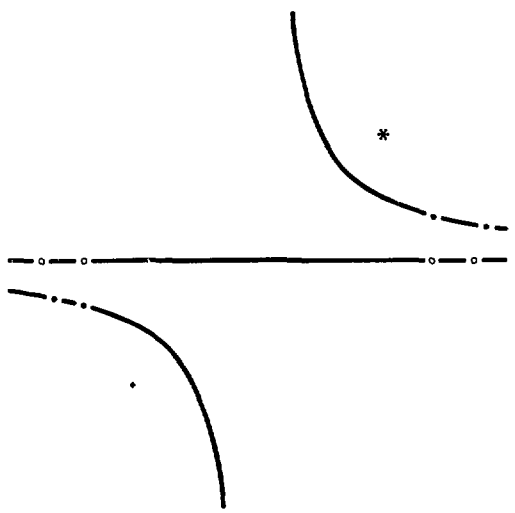
THE

COULOMB

POTENTIAL IN QUANTUM MECHANICS AND RELATED TOPICS



H. van Haeringen

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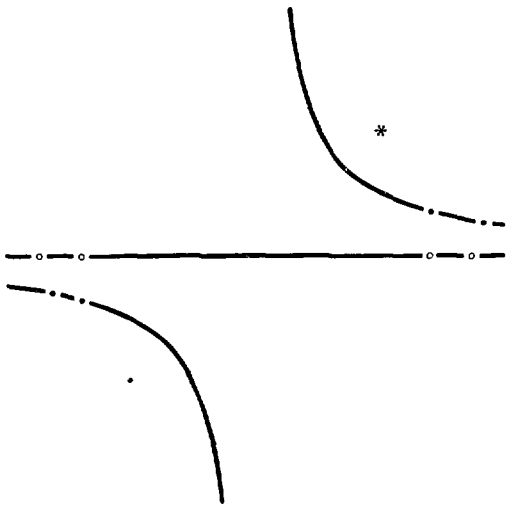

H. van Haeringen

Vrije Universiteit te Amsterdam

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POTENTIAL IN QUANTUM MECHANICS AND RELATED TOPICS

Academisch Proefschrift

ter verkrijging van de graad van
doctor in de wiskunde en natuurwetenschappen
aan de Vrije Universiteit te Amsterdam,
op gezag van
de rector magnificus dr D.M. Schenkeveld,
hoogleraar in de faculteit der letteren,
in het openbaar te verdedigen
op vrijdag 29 september 1978 te 15.30 uur
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De Boelelaan 1105

door

Hendrik van Haeringen

geboren te Dedemsvaart

Krips Repro - Meppel

Promotor: Prof. dr R. van Wageningen
Coreferenten: Dr B.J. Verhaar
Dr L. P. Kok

Stellingen

1

In de niet-relativistische quantummechanische verstrooiingstheorie geldt voor de radiale verstrooiingsgolffunctie $u_\ell(k,r)$ de bekende uitdrukking

$$u_\ell(k,r) = c_\ell(k) \sin(kr - \tfrac{1}{2}\pi\ell + \delta_\ell(k)) + o(1), \quad r \to \infty ,$$

mits de (lokale) potentiaal aan bepaalde voorwaarden voldoet. De in dit verband, met betrekking tot het asymptotische gedrag van de potentiaal, door

W. Franz, Quantentheorie (Springer, Berlin, 1970), p. 168,

genoemde voorwaarde is niet voldoende; anderzijds zijn de voorwaarden genoemd door

G. Baym, Lectures on Quantum Mechanics (Benjamin, New York, 1969), pp. 198, 204,

L.D. Landau and E.M. Lifshitz, Quantum Mechanics, Non-Relativistic Theory (Pergamon Press,London,1958), p.115,

H.M. Nussenzveig, Causality and Dispersion Relations (Academic Press, New York, 1972), pp. 195, 200, 253,

L.I. Schiff, Quantum Mechanics (McGraw-Hill, New York, 1968), Third Edition, p. 118,

en

A.G. Sitenko, Lectures in Scattering Theory (Pergamon Press, Oxford, 1971), p. 54,

weliswaar voldoende maar niet nodig, terwijl verder de voorwaarden genoemd door

A.O. Barut (Ed.), Scattering Theory (Gordon and Breach, New York, 1969), p. 4,

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D.I. Blokhintsev, Quantum Mechanics (Reidel, Dordrecht, 1964), pp. 147, 148,

D. Bohm, Quantum Theory (Prentice-Hall, New York, 1951), pp. 559, 560,

F. Calogero, Variable Phase Approach to Potential Scattering (Academic Press, New York, 1967), p. 3,

F. Constantinescu and E. Magyari, Problems in Quantum Mechanics (Pergamon Press, Oxford, 1971), p. 265,

S. Flügge (Ed.), Encyclopedia of Physics (Springer, Berlin, 1957), Vol. 35, pp. 118, 119,

S. Flügge und H. Marschall, Rechenmethoden der Quantentheorie (Springer, Berlin, 1952, 1965), pp. 118, 119,

N. Fröman and P.O. Fröman, JWKB Approximation (North - Holland, Amsterdam, 1965), pp. 125, 126,

S. Gasiorowicz, Quantum Physics (Wiley, New York, 1974), p. 179,

K. Gottfried, Quantum Mechanics (Benjamin, New York, 1966), Vol. 1, p. 126,

C.C. Grosjean, Formal Theory of Scattering Phenomena (Institut Interuniversitaire des Sciences Nucléaires, Bruxelles, 1960), pp. 11, 105,

A. Messiah, Quantum Mechanics (North - Holland, Amsterdam, 1969), Vol. 1, p. 371,

A. Messiah, Mécanique Quantique (Dunod, Paris, 1959), Tome 1, p. 315,

P.M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill, New York, 1953), Part II, p. 1682,

N.F. Mott and H.S.W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1965), p. 23,

J.L. Powell and B. Crasemann, Quantum Mechanics (Addison - Wesley, Reading, Massachusetts, 1965), p. 248,

L.S. Rodberg and R.M. Thaler, Introduction to the Quantum Theory of Scattering (Academic Press, New York, 1967), p. 63,

P. Roman, Advanced Quantum Theory (Addison - Wesley, Reading, Massachusetts, 1965), p. 161,

D.S. Saxon, Elementary Quantum Mechanics (Holden - Day, San Francisco, 1968), p. 352,

L.I. Schiff, Quantum Mechanics (McGraw - Hill, New York, 1949), First Edition, p. 104,

P. Stehle, Quantum Mechanics (Holden - Day, San Francisco, 1966), p. 193,

J.R. Taylor, Scattering Theory: The Quantum Theory on Non-Relativistic Collisions (Wiley, New York, 1972), p. 260,
N. Tralli and F.R. Pomilla, Atomic Theory (McGraw - Hill, New York, 1969), p. 308,
Ta-You Wu and T. Ohmura, Quantum Theory of Scattering (Prentice - Hall, London, 1962), p. 2,

en

M. Kolsrud, J. Phys. A 11 (1978) 1271 - 1294, p. 1272,

noch nodig noch voldoende zijn; de schijnbare voorwaarde, tenslotte, die in dit verband wordt genoemd door

M.L. Goldberger and K.M. Watson, Collision Theory (Wiley, New York, 1964), pp. 247, 251,

en door

C.J. Joachain, Quantum Collision Theory (North - Holland, Amsterdam, 1975), pp. 67, 68,

heeft geen betekenis.

J.D. Dollard and C.N. Friedman, Ann. Phys. (N.Y.) 111 (1978) 251-266.

2

In het tijdonafhankelijke Schrödingerprobleem met een lokale potentiaal V, waarvoor $r^2V(\vec{r})$ continu is in de oorsprong, is scheiding van variabelen zowel in parabolische coördinaten als in bolcoördinaten, respectievelijk zowel in parabolische coördinaten als in conische coördinaten mogelijk, dan en slechts dan als V, afgezien van een triviale constante, de Coulomb potentiaal is.

P.M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw - Hill, New York, 1953);
L.P. Eisenhart, Phys. Rev. 74 (1948) 87 - 89.

3

De tijdonafhankelijke Schrödingervergelijking met een lokale potentiaal V, waarvoor $r^2V(\vec{r})$ continu is in de oorsprong, is zowel in conische coördinaten als in cilindercoördinaten, respectievelijk zowel in conische coördinaten als in Cartesische coördinaten, respectievelijk zowel in bolcoördinaten als in Cartesische coördinaten, respectievelijk zowel in bolcoördinaten als in bepaalde andere rechthoekige kromlijnige coördinaten separeerbaar, dan en slechts dan als V, afgezien van een triviale constante, de isotrope harmonische oscillator potentiaal is.

P.M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw - Hill, New York, 1953);
L.P. Eisenhart, Phys. Rev. 74 (1948) 87 - 89.

4

De uitspraak „Observabelen corresponderend met niet-verwisselbare operatoren kunnen niet tegelijkertijd scherp gemeten worden" is incorrect.

D. Bohm, Quantum Theory (Prentice - Hall, New York, 1951), p. 206;
F. Constantinescu and E. Magyari, Problems in Quantum Mechanics (Pergamon Press, Oxford, 1971), p. 76;
S. Gasiorowicz, Quantum Physics (Wiley, New York, 1974), p. 119;
E. Merzbacher, Quantum Mechanics (Wiley, New York, 1970), p. 158.

5

De eenvoudige en voor veel mathematisch-fysisch werk nuttige formule

$$\tfrac{1}{2}\,\Gamma(1+\mu)\int_{-1}^{1} P_\ell(x)\,(z-x)^{-\mu-1}\,dx \;=\; (z^2-1)^{-\frac{1}{2}\mu}\,e^{-i\pi\mu}\,Q_\ell^\mu(z)\ ,$$

$(\ell = 0,1,2,\cdots)$, overigens een bijzonder geval van

$$\Gamma(\rho)\,\Gamma(\kappa+\lambda+\sigma-\rho)\int_0^1 t^{\lambda-1}(1-t)^{\sigma-1}\,{}_2F_1(\rho-\kappa,\lambda+\sigma-\rho;\sigma;1-t)\,{}_pF_q([a]_p;[b]_q;zt)\,dt$$

$$=\;\Gamma(\kappa)\,\Gamma(\lambda)\,\Gamma(\sigma)\,{}_{p+2}F_{q+2}([a]_p,\kappa,\lambda;[b]_q,\rho,\kappa+\lambda+\sigma-\rho;z)\ ,$$

ontbreekt ten onrechte in een aantal gangbare mathematisch-fysische handboeken op de voor de hand liggende plaatsen.

B.v.: Bateman Manuscript, edited by A. Erdélyi, Higher Transcendental Functions (McGraw-Hill, New York, 1953), Vols.1 and 2;
Id.,Tables of Integral Transforms (1954), Vols. 1 and 2;
I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series, and Products (Academic Press, New York, 1965).

6

In de mathematisch-fysische literatuur treft men tenminste vier soorten inconsistentie aan met betrekking tot de geassocieerde Legendre functies P_ℓ^m.

D.M.Brink and G.R.Satchler, Angular Momentum(Clarendon,Oxford,1971);
W.Magnus, F.Oberhettinger, and R.P.Soni, Formulas and Theorems for the Special Functions of Mathematical Physics (Springer, New York, 1966);
R.G.Newton, Scattering Theory of Waves and Particles (McGraw-Hill, New York, 1966);
M.E.Rose, Elementary Theory of Angular Momentum (Wiley, New York, 1963);
S.Saxon, Elementary Quantum Mechanics (Holden-Day, San Francisco, 1968);
L.I.Schiff, Quantum Mechanics (McGraw-Hill, New York, 1968);
E.T.Whittaker and G.N.Watson, A Course of Modern Analysis (Cambridge University Press, London, 1950).

7

De omwentelingsconchoïdoïde, die men verkrijgt door die bepaalde conchoïde van Nicomedes, welke gekenmerkt is door het feit dat haar pool tevens keerpunt is, te roteren om haar as van symmetrie, speelt een opmerkelijke rol in de klassieke verstrooiing van geladen deeltjes.

Nicomedes, ca. 240 à 210 v. Chr.;
M. Cantor, Vorlesungen über Geschichte der Mathematik (Teubner, Stuttgart, 1965), Erster Band, S. 350 - 352;
M. Kline, Mathematical Thought from Ancient to Modern Times (Oxford University Press, New York, 1972), pp. 117, 118;
B.L. van der Waerden, Science Awakening (Noordhoff, Leyden, 1975), Vol. 1, Fourth Edition, pp. 82, 235, 236.

8

Het verdient aanbeveling naast twee, in het bijzonder in wiskunde en natuurwetenschappen van belang zijnde, begrippen orde in de betekenis van een antireflexieve asymmetrische transitieve relatie respectievelijk een reflexieve symmetrische niet-transitieve relatie, drie begrippen orde in de betekenis van een reflexieve symmetrische transitieve relatie respectievelijk een reflexieve niet-symmetrische transitieve relatie respectievelijk een antireflexieve asymmetrische transitieve relatie, welke eveneens een belangrijke rol spelen in wiskunde en natuurwetenschappen, te onderscheiden.

Van Dale, Groot Woordenboek der Nederlandse Taal, onder redactie van C. Kruyskamp (Nijhoff, 's-Gravenhage, 1976), Deel II, artikel orde, sub 6 en 13;
G. James and R.C. James, Mathematics Dictionary (Van Nostrand, Princeton, New Jersey, 1960).

9

Het gezegde „De uitzonderingen bevestigen de regel" is een uitzondering op de regel dat een uitspraak op het eerste horen begrijpelijk is, welke uitzondering deze regel niet bevestigt.

Van Dale, Groot Woordenboek der Nederlandse Taal, onder redactie van C. Kruyskamp (Nijhoff, 's-Gravenhage, 1976), Deel II, p. 2015.

10

Het is opmerkelijk dat een bepaald effect van versnelling en zwaartekracht, beschreven in „Autour de la Lune", eveneens optreedt in „Tom Poes en de Nieuwe IJstijd", terwijl het ontbreekt in moderne experimenten.

M.Toonder, Tom Poes en de Nieuwe IJstijd (Nationale Rotterdamse Courant,1947; 7,8 en 10 november), nrs.204-206;
J.Verne, Autour de la Lune (Hetzel, Paris, 1866), Chap. VIII.

11

Het eerste proefschrift dateert van de late prehistorie.

Amsterdam, 29 september 1978 *H. van Haeringen*

Contents

Introduction and Survey

In this thesis we present an analytic study of the Coulomb interaction in nonrelativistic quantum mechanics and some related topics. We investigate in a number of self-contained articles various interesting and important properties of the Coulomb potential. Some of these properties are shared by other potentials which also play a role in quantum mechanics. For such related interactions a comparative study is made of the similarities and differences.

The thesis consists of three parts. In part A we work in the momentum representation whereas in part B the coordinate or position representation will be mainly used. In part C both representations play a role and some connective formulas for special cases are developed.

The great physical importance of the Coulomb interaction follows from the observation that it acts between any pair of charged particles. Since moreover Coulomb's law, describing the force as a function of the relative distance, has the same mathematical form as Newton's law of gravitation, it is obvious that this so-called inverse-distance-squared law of force has received a great deal of attention.

As is well known, the problem of just two particles interacting according to the inverse-distance potential can be solved completely in an analytic way. In this specific situation one can even apply *algebraic* methods, which are more elegant. This is due to an extra symmetry which plays an important role in the *pure* two-particle Coulomb problem, in addition to the ordinary spherical symmetry. By introducing appropriate new variables one finds that the pure Coulomb problem has an intrinsic O_4 symmetry, *i.e.*, that it is invariant under orthogonal rotations in some four-dimensional space. This symmetry results in the existence of the invariant vector of Lenz in classical mechanics, which is defined in connection with the classical conic section orbits. In quantum mechanics the O_4 symmetry generates the additional degeneracy of the energy levels, *e.g.*, in the hydrogen atom. Furthermore, the energy spectrum can be derived in an elegant way by using certain properties of the o_4 algebra.

On the other hand, even the seemingly simple problem of only three particles with such pure inverse-distance potentials between the pairs is of a considerable complexity. In classical mechanics this problem can be successfully attacked in some specific situations by using numerical techniques. However, in nonrelativistic quantum mechanics it constitutes an as yet unsolved problem.

We shall restrict ourselves almost exclusively to a system of at most three spinless particles of which only two are charged. Let us first confine the discussion to just two particles with a Coulomb-like potential. By this we mean that for large distance the potential is approximately the Coulomb one whereas it may be different for short distance. For example one may think of two protons, if the influence of the spins is neglected. In this case the O_4 symmetry is broken. It is convenient then to split off the pure Coulomb part for which the O_4 symmetry can again be used. Moreover, this pure Coulomb part is especially important in connection with certain singularities which will be discussed below.

Such a Coulomb-like potential has a long range, which means that it diminishes rather slowly for increasing distance. This long range has caused a great deal of trouble in quantum mechanical scattering theory. In fact, virtually all difficulties that are encountered in the theory of Coulomb-like potential scattering can be traced back to this long range. Short-range potentials, *e.g.*, with exponentially decreasing asymptotic behavior, are much easier to deal with.

As a matter of fact, the standard quantum mechanical scattering theory which may be found in many textbooks is valid only for short-range potentials. In particular, the scattering amplitude for such a potential is easily obtained from the asymptotic behavior of the scattering wave function in configuration space. However, for a long-range potential this asymptotic behavior of the wave function is more complicated, so that the standard prescription for obtaining the scattering amplitude has to be modified. In the case of a simple two-particle scattering process the necessary modifications are well known. But when a third particle is involved the exact calculations become rather complicated, even if this third particle is subject to short-range forces only.

In the theory of many-particle reactions the transition operator or matrix, usually denoted by T, occupies an important position. The two-particle T operator can be defined as the solution of an operator equation, *viz.* the Lippmann-Schwinger equation. Since in a two-particle reaction the two-particle energy is conserved, one needs in this case only the *on-shell restriction* of the T matrix. This means that the two momentum variables are equal to their values on the energy-shell. This so-called on-shell T matrix is proportional to the scattering amplitude. However, in a reaction involving three particles there is no energy conservation in any of the two-particle subsystems. Indeed, the third particle can, and will in general, carry away energy and momentum. Therefore the complete two-particle T matrix is needed here, without restrictions. In the jargon of quantum mechanical scattering theory it is said that in this case the off-shell part of the two-particle interaction comes into play.

In this thesis we pay attention especially to the off-shell T matrices for Coulomb plus short-range potentials. Such T matrices have branch-point singularities in their half-shell and on-shell points. We study these singularities and we indicate how the physical amplitude has to be obtained from the T matrix for such a Coulomb-like potential. To this end we introduce in the first article, A1, so-called Coulombian asymptotic states. These give an exact mathematical prescription for obtaining the scattering amplitude. We also derive the connection with the 'anomalous' asymptotic behavior of the time-dependent Coulomb scattering states, as obtained by Dollard.

We obtain closed analytic expressions for the partial-wave Coulomb T matrix for $\ell = 0$ (in A2) and for $\ell = 1$ (in A5). Further we introduce in paper A2 the so-called rational separable potentials. Such potentials are nonlocal and have a short range. They are represented by finite-rank operators with form factors which are rational functions of the momenta. For a potential which is the sum of the Coulomb potential and such a rational separable potential the general structure of the off-shell T matrix has been obtained. For some specific cases, in particular for the Coulomb plus Yamaguchi potential, we give simple closed formulas.

In low-energy scattering theory the scattering length and the effective range play

an important role. They provide a convenient way of parametrizing the low-energy scattering data. These two parameters are closely connected with the first two coefficients of the Taylor series expansion in powers of the energy of the effective range function. For a potential which decreases exponentially at large distance this effective range function is an analytic function of the energy in a certain neighborhood of the origin. When the potential decreases more slowly, *e.g.*, like some power of the distance, the definition of the effective range function has to be modified in order to again obtain an analytic function of the energy. We study this modified effective range function in particular for Coulomb plus rational separable potentials and we derive many interesting closed formulas, *e.g.*, for the modified scattering length and effective range, see the papers A3 and A5.

The necessity of the above modification in the definition of the effective range function is closely connected with the long range of the potential. For a Coulomb plus short-range potential this can be understood from the following considerations. First we note that there exists a simple relation between the effective range function and the T matrix. Further it is well known that for any potential the T operator has simple poles at the bound-state energies. The central point is then, that a Coulomb-like potential with an attractive tail gives rise to an infinite number of bound-state energies, which accumulate at the origin in the complex energy plane. This implies that the T matrix corresponding to a Coulomb-like potential has a limit-point of poles in the zero-energy point. This is also true when the tail is *repulsive*. In this case the poles are situated on the unphysical sheet of the complex energy Riemann surface. So we can say that the T operator for any potential with a Coulomb tail has an essential singularity in the origin which is not isolated. In the definition of the effective range function one has to take care of just this singularity at zero energy.

As has just been discussed, any potential with an attractive Coulomb tail gives rise to an infinite number of bound states. We study the bound-state energies in particular for the symmetric shifted Coulomb potential (paper B1), and for the Coulomb plus Yamaguchi potential (paper A4). A well-known peculiarity of any rank-one separable potential, such as the Yamaguchi one, is that it admits of at most one bound state. We prove that also the repulsive Coulomb potential plus any rank-one separable potential gives rise to *at most one* bound state. In the specific Yamaguchi case we derive the strength of the Yamaguchi potential for which this bound state just appears, *i.e.*, for which the bound-state energy is zero (paper A4).

The infinity of the number of bound states is not confined to potentials with a Coulomb tail. It is well known that any potential with an attractive $r^{-\alpha}$ asymptotic behavior, where $\alpha < 2$, has infinitely many bound states. The r^{-2} behavior is here the borderline case. More precisely, when $V(r) = cr^{-2}$ for large r, the number of bound states is finite when $c > -\frac{1}{4}$ and infinite when $c < -\frac{1}{4}$ (in certain units). We prove that for $c = -\frac{1}{4}$ the number of bound states is finite (B2). Furthermore we derive in paper B2 many explicit expressions for the binding energies, and we make interesting comparisons with the case of the symmetric shifted Coulomb potential, studied in the article B1. In particular a curious odd-even staggering phenomenon appears in these two cases, which is discussed in B1 and B2.

In the article A6 we study the exact solution of the integral equations for reactions of three particles of which only two are charged. In these equations the two-particle off-shell Coulomb T matrix plays an important role. One has to deal

here with two different types of problems which are both, of course, generated by the long Coulomb range.

In the first place one has the non-existence of the half-shell and on-shell T matrix, which is related to the different asymptotic behavior of the wave function. This problem can be disposed of by first taking a screened Coulomb potential, *e.g.*, a Yukawa-type potential. The calculations are performed with this screened potential, and afterwards the screening is gradually 'turned off'. In this process a well-known renormalization procedure has to be carried out. An alternative to this 'spatial screening' is presented by the Coulombian asymptotic states discussed before (A1). In this case one lets the energy variable approach the real-positive energy axis from above. Here a different but equivalent renormalization procedure is applied. In analogy to the former case this may be called 'energy-screening'.

The second problem in the solution of the three-particle equations concerns the essential singularity of the Coulomb T matrix at zero energy, discussed before. This singularity is unavoidable when the total three-particle energy is positive or approximately zero, *i.e.*, above or near the break-up threshold. In order to make really exact calculations possible, we derive a number of formulas by means of which this essential singularity is split off in such a way that it is numerically manageable, see paper A6.

There exists a certain 'solution' ψ_s of the three-dimensional Schrödinger equation with the pure Coulomb potential, which has a pleasant asymptotic behavior. Namely, for large distance it is proportional to the Coulomb scattering amplitude times a Coulomb-modified outgoing spherical wave. We often call ψ_s an 'irregular solution'. However, it is in fact a solution of the Schrödinger equation with an inhomogeneous term which contains a Dirac delta function. In the articles B3 and B4 we derive analytic expressions for the partial-wave projections of ψ_s for all $\ell = 0, 1, 2, \ldots$. We prove that these partial-wave projected functions do *not* satisfy the partial-wave Schrödinger equation, but instead an *in*homogeneous type of Schrödinger equation.

Further we consider in paper B4 similar three-dimensional 'irregular solutions' of the Schrödinger equation with different local potentials, notably Coulomb-like and short-range potentials. We investigate whether any such solution might have an asymptotic behavior, similar to that of the irregular solution for the *pure* Coulomb potential. It seems, however, that the pure Coulomb potential constitutes a remarkable exception in this respect.

In part C we pay attention to the connection between quantum mechanical quantities in the coordinate representation and in the momentum representation, respectively. By definition this connection consists of Fourier and Hankel transforms. On the one hand, one is more accustomed to the probability interpretation in the coordinate representation. On the other hand, certain quantities have a simpler form when expressed in the momentum representation. Therefore it is useful to have expressions available in each of the two representations.

It turns out that in the Coulomb case the momentum representation is more suitable for the derivation of analytic expressions for certain quantities. This is explained by recalling the underlying O_4 symmetry that we discussed before. Indeed, a closed form for the three-dimensional off-shell Coulomb T matrix for negative energy can be derived in an elegant way by using the four-dimensional hyperspherical functions, if one works in the momentum representation.

We make some attempts to obtain a closed expression, in terms of hypergeometric functions, of the partial-wave Coulomb T matrix for all $\ell = 0, 1, \ldots$. Such an expression for arbitrary ℓ is rather complicated, as may be guessed from the expressions for $\ell = 0$ and for $\ell = 1$ that we give in A2 and in A5, respectively. Therefore we first consider some closely related, less complicated, functions notably the off-shell Jost functions which have been introduced by Fuda. Indeed, the half-shell T matrix corresponding to a short-range potential is easily obtained from this off-shell Jost function.

In the articles C1 and C2 we derive a large variety of equivalent analytic expressions for the Coulomb off-shell Jost functions for all ℓ, which are useful for various purposes. Moreover we prove that the off-shell Jost functions for a Coulomb plus local short-range central potential have, for all ℓ, exactly the same on-shell singularity as the $\ell = 0$ Coulomb off-shell Jost function, cf. paper C4.

In C3 we study off-shell scattering quantities for local Coulomb-like central potentials. Here a link is made between the coordinate representation and the momentum representation of certain quantities. We derive many interesting expressions, especially for the Jost functions, the off-shell Jost functions, the Jost states, and the off-shell Jost states, for all partial waves. For the pure Coulomb case we obtain explicit analytic expressions for the Jost state and for the off-shell Jost state in the momentum representation, for $\ell = 0$ only.

In the final article, C4, we investigate the $\ell = 0$ off-shell Jost function for Coulomb, Hulthén, and Eckart-type potentials. The Hulthén potential may be considered as a screened Coulomb potential and the Eckart-type potentials as screened r^{-2} potentials. We derive in C4 a number of interesting limiting relations. When the screening is gradually 'turned off', one has to 'renormalize' in order to ensure the existence of the limits of certain scattering quantities. On the other hand, one also has to use a certain renormalization factor when the on-shell quantities are to be obtained from the corresponding off-shell quantities. We derive the appropriate renormalization factors for both these cases.

Synopsis

This dissertation consists of an analytic study of the Coulomb interaction in nonrelativistic quantum mechanics and some related topics. We investigate in a number of self-contained articles various interesting and important properties of the Coulomb potential. Some of these properties are shared by other potentials which also play a role in quantum mechanics. For such related interactions a comparative study is made.

The great physical importance of the Coulomb interaction follows from the observation that it acts between any pair of charged particles. Since moreover Coulomb's law, describing the force as a function of the distance between two particles, has the same mathematical form as Newton's law of gravitation, it is not surprising that this law has received a great deal of attention.

Apart from being important in physics the Coulomb potential is also mathematically of great interest. This is mainly due to the following two characteristic properties. In the first place, the Coulomb Hamiltonian shows in addition to the usual spherical symmetry an extra symmetry, which is closely connected with the invariant vector of Lenz in the classical conic section orbits. The main axis of such a conic section orbit is fixed in space. In the second place, the Coulomb potential and more generally any Coulomb-like potential has a long range. This means that such a potential diminishes rather slowly for increasing distance. The long range generates singularities in certain quantities which play an important role in quantum mechanical scattering theory, notably in the off-shell transition matrix. This so-called T matrix has a branch-point singularity in the half-shell and on-shell points, which requires the application of a certain renormalization procedure. Furthermore, the Coulomb T matrix has an essential singularity in the zero-energy point. This singularity is connected with the infinite number of bound-state poles which accumulate at the origin of the complex energy plane.

In this thesis we pay attention in particular to the off-shell transition matrix for Coulomb plus short-range potentials. Here the short-range potentials are taken to be local as well as nonlocal, separable. We develop analytic expressions involving hypergeometric functions for many quantities. Especially for the case of rational separable potentials we are able to derive relatively simple expressions for the T matrix and for the effective range function.

The principal difficulties in the description of proton-deuteron scattering and break-up reactions, due to the Coulomb interaction, are studied by working out a simple model. These problems concern the two-particle renormalization procedure and the essential singularity at zero energy discussed before.

We study the bound states for the Coulomb plus Yamaguchi potential, for the symmetric shifted Coulomb potential, and for local potentials with an inverse-distance-squared asymptotic behavior.

Further we investigate so-called irregular solutions of the three-dimensional and radial Schrödinger equations. These are closely connected with the Jost solutions. We study for the Coulomb, Hulthén and Eckart potentials the Jost solutions, off-shell Jost solutions, Jost functions, and off-shell Jost functions.

A large variety of simple analytic expressions is obtained for the Coulomb off-shell Jost functions for all values of the angular momentum quantum number. Further we give for some Coulomb Jost states analytic expressions involving hypergeometric functions.

We develop for Coulomb plus short-range potentials a large number of interesting relations between various quantities that play an important role in off-shell scattering theory.

Synopsis

Deze dissertatie bestaat uit een analytische studie van de Coulomb wisselwerking in de niet-relativistische quantummechanica en een aantal hiermee samenhangende onderwerpen. In een aantal onafhankelijke artikelen onderzoeken we diverse belangwekkende en belangrijke eigenschappen van de Coulomb potentiaal. Sommige van deze eigenschappen heeft de Coulomb potentiaal gemeen met andere potentialen die eveneens een rol spelen in de quantummechanica. Voor dergelijke verwante potentialen wordt een vergelijkende studie verricht.

De grote fysische betekenis van de Coulomb wisselwerking volgt uit de constatering dat zij werkt tussen elk paar geladen deeltjes. Bovendien heeft de wet van Coulomb, die de kracht als functie van de afstand tussen twee deeltjes beschrijft, dezelfde wiskundige vorm als de zwaartekrachtwet van Newton. Het is dan ook niet verwonderlijk dat aan deze wet veel aandacht is besteed.

De Coulomb potentiaal is niet alleen belangrijk in de natuurkunde, maar ook wiskundig gezien zeer interessant. Dit is voornamelijk te danken aan de volgende twee karakteristieke eigenschappen. Ten eerste vertoont de Coulomb Hamiltoniaan behalve de gewone bolsymmetrie een extra symmetrie, die in verband staat met de invariante vector van Lenz in de klassieke kegelsnede-banen. De hoofdas van zo'n kegelsnede-baan ligt vast in de ruimte. Ten tweede heeft de Coulomb potentiaal en meer algemeen elke Coulomb plus korte-dracht potentiaal een lange dracht. Dit betekent dat zo'n potentiaal tamelijk langzaam afneemt voor toenemende afstand. De lange dracht veroorzaakt singulariteiten in bepaalde grootheden die een belangrijke rol spelen in de quantummechanische verstrooiingstheorie, met name in de off-shell overgangsmatrix. Deze zogenaamde T matrix heeft een vertakkingspunt-singulariteit in de half-shell en on-shell punten, hetgeen toepassing van een bepaalde renormalisatieprocedure vereist. Verder heeft de Coulomb T matrix in het energienulpunt een essentiële singulariteit, die in direct verband staat met het oneindig groot aantal gebonden toestanden. De hiermee corresponderende polen verdichten zich in de oorsprong van het complexe energievlak.

In dit proefschrift besteden we vooral aandacht aan de off-shell overgangsmatrix voor Coulomb plus korte-dracht potentialen. Hierbij worden zowel lokale als niet-lokale, separeerbare, potentialen beschouwd. We ontwikkelen voor diverse grootheden analytische uitdrukkingen waarin hypergeometrische functies voorkomen. In het bijzonder voor het geval van rationale separeerbare potentialen zijn we in staat relatief eenvoudige uitdrukkingen af te leiden voor de T matrix en voor de effectieve dracht functie.

De voornaamste moeilijkheden in de beschrijving van proton-deuteron verstrooiings- en break-up reacties, veroorzaakt door de Coulomb wisselwerking, worden bestudeerd aan de hand van een eenvoudig model. Het gaat hierbij in feite om de bovengenoemde twee-deeltjes renormalisatieprocedure en de essentiële singulariteit in het energienulpunt.

We bestuderen de gebonden toestanden voor de Coulomb plus Yamaguchi potentiaal, voor de symmetrische verschoven Coulomb potentiaal, en voor lokale potentialen die asymptotisch omgekeerd evenredig zijn met het kwadraat van de afstand.

Verder worden de zogenaamde irreguliere oplossingen van de driedimensionale en radiale Schrödingervergelijkingen onderzocht. Deze staan in nauw verband met de Jost oplossingen. Voor de Coulomb, Hulthén en Eckart potentialen bestuderen we de Jost oplossingen, off-shell Jost oplossingen, Jost functies en off-shell Jost functies.

We leiden een groot aantal eenvoudige analytische uitdrukkingen af voor de Coulomb off-shell Jost functies voor alle waarden van het impulsmomentquantumgetal. Verder geven we voor enkele Coulomb Jost toestanden analytische uitdrukkingen waarin hypergeometrische functies voorkomen.

Voor Coulomb plus korte-dracht potentialen ontwikkelen we een groot aantal interessante relaties tussen diverse grootheden die een belangrijke rol spelen in de off-shell verstrooiingstheorie.

КРАТКОЕ СОДЕРЖАНИЕ

Настоящая диссертация состоит из аналитического исследования кулоновского взаимодействия в нерелятивистской квантовой механике и некоторых связанных с этим тем. В нескольких самостоятельных статьях мы исследуем различные важные и представляющие интерес свойства кулоновского потенциала. Некоторые свойства, характерные для кулоновского потенциала, присущи также другим потенциалам, играющим важную роль в квантовой механике. Для таких родственных взаимодействий производится сравнительное исследование.

Вывод о большом физическом значении кулоновского взаимодействия можно сделать из наблюдения, что такое взаимодействие действительно для любой пары заряженных частиц. Поскольку закон Кулона, описывающий силу как функцию расстояния между двумя частицами, имеет то же самое математическое выражение, что и закон тяготения Ньютона, то совсем неудивительно проявление к этому закону повышенного интереса.

Кулоновский потенциал не только имеет большое значение в физике, но и чрезвычайно интересен с математической точки зрения, главным образом, благодаря двум следующим характерным свойствам. Во-первых, кроме обычной сферической симметрии кулоновские гамильтонианы обнаруживают дополнительную симметрию, которая тесно связана с инвариантным вектором Ленца в классических орбитах конического сечения. Главная ось такой орбиты конического сечения закреплена в пространстве. Во-вторых, кулоновский и вообще любой подобный кулоновскому потенциал отличается дальнодействующим характером. Это значит, что для увеличивающегося расстояния такой потенциал убывает довольно медленно. Дальнодействие вызывает сингулярности в определенных величинах, которые играют существенную роль в квантомеханической теории рассеяния, особенно, в случае матрицы перехода, лежащей вне поверхности энергии. Эта т.н. Т-матрица имеет сингулярность точки ветвления в полуповерхностной и наповерхностной точках, что требует применения определенного метода перенормировки. Кроме того, кулоновская Т-матрица имеет в точке нулевой энергии важную сингулярность,

находящуюся в прямой связи с бесконечным числом связанных состояний, соответствующие полюса которых собираются в исходной точке комплексной плоскости энергии.

Особое внимание в этой диссертации уделяется матрице перехода, лежащей вне поверхности энергии, для кулоновского плюс короткодействующего потенциалов, причем рассматриваются как локальные, так и нелокальные, сепарабельные потенциалы. Мы выводим аналитические выражения, в которых встречаются гипергеометрические функции для многих величин. Особенно в случае сепарабельных потенциалов можно вывести довольно простые выражения для Т-матрицы и для функции эффективной дальности действия.

Основные трудности в описании рассеяния протонов дейтронами и реакций развала, вызванных кулоновским взаимодействием, исследуются путем разработки простой модели. Суть дела фактически заключается в методе перенормировки двух частиц и важной сингулярности при нулевой энергии.

Исследуются связанные состояния для кулоновского плюс ямагушинского потенциалов, для симметричного смещенного кулоновского потенциала и локальных потенциалов с асимптотикой, обратно пропорциональной квадрату расстояния.

Далее мы исследуем т.н. иррегулярные решения трехмерных и радиальных уравнений Шрёдингера. Они вплотную приближаются к решениям Джоста. Для кулоновского, хултенского и экартовского потенциалов мы исследуем решения Джоста, решения Джоста в случае выхода за поверхность энергии, функции Джоста и функции Джоста в случае выхода за поверхность энергии.

Нами получено большое число простых аналитических выражений для кулоновских внеповерхностных функций Джоста для всех значений квантового числа орбитального момента. Для некоторых кулоновских состояний мы даем также аналитические выражения, включающие гипергеометрические функции.

Мы разрабатываем для кулоновского плюс короткодействующего потенциалов большое количество интересных соотношений между различными величинами, которые играют важную роль в теории рассеяния вне поверхности энергии.

梗　概

この学位論文は、非相対論的量子力学におけるクーロン相互作用の解析的研究と、それに関係のあるいくつかの主題とを取扱うものである。私は一連の別の論文において、クーロン・ポテンシャルのいろいろな面白い且つ重要な性質を調べてきた。クーロン・ポテンシャルのある種の性質は、量子力学においてやはり一役を演ずる他のポテンシャルの性質と共通するものである。ここではそのような互に関連のあるポテンシャルについての比較研究を行う。

クーロン相互作用の物理学における重要性は、クーロンの力で任意の一対の荷電粒子間に働くという事実に存する。しかも、力を二つの粒子間の距離の函数として与えるクーロンの法則は、ニュートンの重力法則と同じ数学形式を持っている。だからクーロンの法則が多くの注意を惹いてきたのも決して異とするに足りない。

クーロン・ポテンシャルは物理学において重要なばかりではなく、数学的にみても非常に面白い。その理由は、主として次の二つの特性による。すなわち、第一に、クーロン・ハミルトン演算子は、通常の球対称のほかに、古典円錐曲線軌道の主軸は空間に固定している。第二に、クーロン・ポテンシャル、いやもっと一般的に、クーロン・プラス・近距離ポテンシャルは常に遠達力をもっている。すなわち、このようなポテンシャルは距離が増大すると共にかなり緩かに減少する。この遠達力は、量子力学的散乱理論で重要なある種の量、例えば off-shell 遷移行列、における特異点の原因をなすものである。このいわゆる T 行列は、

half-shell points ならびに on-shell points で分岐点特異点 (branch-point singularity) を持っており、そのため何らかのくりこみの方法を用いることが必要となる。
さらに、クーロン・T行列はエネルギー零点において真性特異点を有しており、これが無限に多い束縛状態のもととなる。これらの状態に対応する極は、複素エネルギー面の原点に密集している。

この学位論文において、私は、特にクーロン・プラス・近距離ポテンシャルに対する off-shell 遷移行列を取扱う。ただし、局所的と非局所的と両方の、分離可能なポテンシャルを考える。そして種々の量に対して、超幾何函数を用いた解析式を展開しよう。特に有理分離可能ポテンシャルの場合には、T行列ならびに有効距離函数に対して比較的簡単な式を導き得ることを示そう。

クーロン相互作用に因る陽子－重陽子の散乱および解体の反応を叙述する場合の主な困難を、一つの単純なモデルによって研究しよう。この問題は、事実上、上述の二粒子間のくりこみ方法とエネルギー零点での真性特異点との問題である。

それから、束縛状態を、クーロン・プラス・山口ポテンシャルの場合、対称的な変位クーロン・ポテンシャルの場合、また漸近的に距離の二乗に逆比例する局所的ポテンシャルの場合について研究する。

さらに三次元のシュレーディンガー方程式の動径部分のいわゆる非正則解のことを調べる。これは Jost の解と密接な関係を持っている。クーロン・ポテンシャル、Hulthén ポテンシャル、および Eckart ポテンシャルに

対して、それぞれ Jost 解、off-shell Jost 解、Jost 函数、ならびに off-shell Jost 函数を検討しよう。

クーロン・off-shell Jost 函数に対して、角運動量量子数のあらゆる値にわたって成立する一連の簡単な解析式を導き出そう。また若干のクーロン・Jost 状態に対して、超幾何函数を用いた解析式を与えよう。

最後に、クーロン・プラス・近距離ポテンシャルに対して、off-shell 散乱理論で重要な諸量間に存在する多数の興味深い関係を導き出そう。

THE

COULOMB

POTENTIAL IN QUANTUM MECHANICS AND RELATED TOPICS

Vrije Universiteit te Amsterdam

THE

COULOMB

POTENTIAL IN QUANTUM MECHANICS AND RELATED TOPICS

Academisch Proefschrift

ter verkrijging van de graad van
doctor in de wiskunde en natuurwetenschappen
aan de Vrije Universiteit te Amsterdam,
op gezag van
de rector magnificus dr D.M. Schenkeveld,
hoogleraar in de faculteit der letteren,
in het openbaar te verdedigen
op vrijdag 29 september 1978 te 15.30 uur
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door

Hendrik van Haeringen

geboren te Dedemsvaart

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Kunt gij de banden der Pleiaden binden,
of de boeien van de Orion slaken?
Doet gij de tekens van de Dierenriem te rechter tijd opgaan,
en bestuurt gij de Beer met zijn jongen?
Kent gij de inzettingen des hemels,
bepaalt gij zijn heerschappij over de aarde?
Kunt gij de bliksemen uitzenden, zodat zij heengaan
en tot u zeggen: Hier zijn wij?

Job 38 : 31-33.35

Ter herinnering aan

mijn Ouders

Contents

Introduction and Survey

In this thesis we present an analytic study of the Coulomb interaction in nonrelativistic quantum mechanics and some related topics. We investigate in a number of self-contained articles various interesting and important properties of the Coulomb potential. Some of these properties are shared by other potentials which also play a role in quantum mechanics. For such related interactions a comparative study is made of the similarities and differences.

The thesis consists of three parts. In part A we work in the momentum representation whereas in part B the coordinate or position representation will be mainly used. In part C both representations play a role and some connective formulas for special cases are developed.

The great physical importance of the Coulomb interaction follows from the observation that it acts between any pair of charged particles. Since moreover Coulomb's law, describing the force as a function of the relative distance, has the same mathematical form as Newton's law of gravitation, it is obvious that this so-called inverse-distance-squared law of force has received a great deal of attention.

As is well known, the problem of just two particles interacting according to the inverse-distance potential can be solved completely in an analytic way. In this specific situation one can even apply *algebraic* methods, which are more elegant. This is due to an extra symmetry which plays an important role in the *pure* two-particle Coulomb problem, in addition to the ordinary spherical symmetry. By introducing appropriate new variables one finds that the pure Coulomb problem has an intrinsic O_4 symmetry, *i.e.*, that it is invariant under orthogonal rotations in some four-dimensional space. This symmetry results in the existence of the invariant vector of Lenz in classical mechanics, which is defined in connection with the classical conic section orbits. In quantum mechanics the O_4 symmetry generates the additional degeneracy of the energy levels, *e.g.*, in the hydrogen atom. Furthermore, the energy spectrum can be derived in an elegant way by using certain properties of the o_4 algebra.

On the other hand, even the seemingly simple problem of only three particles with such pure inverse-distance potentials between the pairs is of a considerable complexity. In classical mechanics this problem can be successfully attacked in some specific situations by using numerical techniques. However, in nonrelativistic quantum mechanics it constitutes an as yet unsolved problem.

We shall restrict ourselves almost exclusively to a system of at most three spinless particles of which only two are charged. Let us first confine the discussion to just two particles with a Coulomb-like potential. By this we mean that for large distance the potential is approximately the Coulomb one whereas it may be different for short distance. For example one may think of two protons, if the influence of the spins is neglected. In this case the O_4 symmetry is broken. It is convenient then to split off the pure Coulomb part for which the O_4 symmetry can again be used. Moreover, this pure Coulomb part is especially important in connection with certain singularities which will be discussed below.

Such a Coulomb-like potential has a long range, which means that it diminishes rather slowly for increasing distance. This long range has caused a great deal of trouble in quantum mechanical scattering theory. In fact, virtually all difficulties that are encountered in the theory of Coulomb-like potential scattering can be traced back to this long range. Short-range potentials, *e.g.*, with exponentially decreasing asymptotic behavior, are much easier to deal with.

As a matter of fact, the standard quantum mechanical scattering theory which may be found in many textbooks is valid only for short-range potentials. In particular, the scattering amplitude for such a potential is easily obtained from the asymptotic behavior of the scattering wave function in configuration space. However, for a long-range potential this asymptotic behavior of the wave function is more complicated, so that the standard prescription for obtaining the scattering amplitude has to be modified. In the case of a simple two-particle scattering process the necessary modifications are well known. But when a third particle is involved the exact calculations become rather complicated, even if this third particle is subject to short-range forces only.

In the theory of many-particle reactions the transition operator or matrix, usually denoted by T, occupies an important position. The two-particle T operator can be defined as the solution of an operator equation, *viz.* the Lippmann-Schwinger equation. Since in a two-particle reaction the two-particle energy is conserved, one needs in this case only the *on-shell restriction* of the T matrix. This means that the two momentum variables are equal to their values on the energy-shell. This so-called on-shell T matrix is proportional to the scattering amplitude. However, in a reaction involving three particles there is no energy conservation in any of the two-particle subsystems. Indeed, the third particle can, and will in general, carry away energy and momentum. Therefore the complete two-particle T matrix is needed here, without restrictions. In the jargon of quantum mechanical scattering theory it is said that in this case the off-shell part of the two-particle interaction comes into play.

In this thesis we pay attention especially to the off-shell T matrices for Coulomb plus short-range potentials. Such T matrices have branch-point singularities in their half-shell and on-shell points. We study these singularities and we indicate how the physical amplitude has to be obtained from the T matrix for such a Coulomb-like potential. To this end we introduce in the first article, A1, so-called Coulombian asymptotic states. These give an exact mathematical prescription for obtaining the scattering amplitude. We also derive the connection with the 'anomalous' asymptotic behavior of the time-dependent Coulomb scattering states, as obtained by Dollard.

We obtain closed analytic expressions for the partial-wave Coulomb T matrix for $\ell = 0$ (in A2) and for $\ell = 1$ (in A5). Further we introduce in paper A2 the so-called rational separable potentials. Such potentials are nonlocal and have a short range. They are represented by finite-rank operators with form factors which are rational functions of the momenta. For a potential which is the sum of the Coulomb potential and such a rational separable potential the general structure of the off-shell T matrix has been obtained. For some specific cases, in particular for the Coulomb plus Yamaguchi potential, we give simple closed formulas.

In low-energy scattering theory the scattering length and the effective range play

an important role. They provide a convenient way of parametrizing the low-energy scattering data. These two parameters are closely connected with the first two coefficients of the Taylor series expansion in powers of the energy of the effective range function. For a potential which decreases exponentially at large distance this effective range function is an analytic function of the energy in a certain neighborhood of the origin. When the potential decreases more slowly, *e.g.*, like some power of the distance, the definition of the effective range function has to be modified in order to again obtain an analytic function of the energy. We study this modified effective range function in particular for Coulomb plus rational separable potentials and we derive many interesting closed formulas, *e.g.*, for the modified scattering length and effective range, see the papers A3 and A5.

The necessity of the above modification in the definition of the effective range function is closely connected with the long range of the potential. For a Coulomb plus short-range potential this can be understood from the following considerations. First we note that there exists a simple relation between the effective range function and the T matrix. Further it is well known that for any potential the T operator has simple poles at the bound-state energies. The central point is then, that a Coulomb-like potential with an attractive tail gives rise to an infinite number of bound-state energies, which accumulate at the origin in the complex energy plane. This implies that the T matrix corresponding to a Coulomb-like potential has a limit-point of poles in the zero-energy point. This is also true when the tail is *repulsive*. In this case the poles are situated on the unphysical sheet of the complex energy Riemann surface. So we can say that the T operator for any potential with a Coulomb tail has an essential singularity in the origin which is not isolated. In the definition of the effective range function one has to take care of just this singularity at zero energy.

As has just been discussed, any potential with an attractive Coulomb tail gives rise to an infinite number of bound states. We study the bound-state energies in particular for the symmetric shifted Coulomb potential (paper B1), and for the Coulomb plus Yamaguchi potential (paper A4). A well-known peculiarity of any rank-one separable potential, such as the Yamaguchi one, is that it admits of at most one bound state. We prove that also the repulsive Coulomb potential plus any rank-one separable potential gives rise to *at most one* bound state. In the specific Yamaguchi case we derive the strength of the Yamaguchi potential for which this bound state just appears, *i.e.*, for which the bound-state energy is zero (paper A4).

The infinity of the number of bound states is not confined to potentials with a Coulomb tail. It is well known that any potential with an attractive $r^{-\alpha}$ asymptotic behavior, where $\alpha < 2$, has infinitely many bound states. The r^{-2} behavior is here the borderline case. More precisely, when $V(r) = cr^{-2}$ for large r, the number of bound states is finite when $c > -\frac{1}{4}$ and infinite when $c < -\frac{1}{4}$ (in certain units). We prove that for $c = -\frac{1}{4}$ the number of bound states is finite (B2). Furthermore we derive in paper B2 many explicit expressions for the binding energies, and we make interesting comparisons with the case of the symmetric shifted Coulomb potential, studied in the article B1. In particular a curious odd-even staggering phenomenon appears in these two cases, which is discussed in B1 and B2.

In the article A6 we study the exact solution of the integral equations for reactions of three particles of which only two are charged. In these equations the two-particle off-shell Coulomb T matrix plays an important role. One has to deal

here with two different types of problems which are both, of course, generated by the long Coulomb range.

In the first place one has the non-existence of the half-shell and on-shell T matrix, which is related to the different asymptotic behavior of the wave function. This problem can be disposed of by first taking a screened Coulomb potential, *e.g.*, a Yukawa-type potential. The calculations are performed with this screened potential, and afterwards the screening is gradually 'turned off'. In this process a well-known renormalization procedure has to be carried out. An alternative to this 'spatial screening' is presented by the Coulombian asymptotic states discussed before (A1). In this case one lets the energy variable approach the real-positive energy axis from above. Here a different but equivalent renormalization procedure is applied. In analogy to the former case this may be called 'energy-screening'.

The second problem in the solution of the three-particle equations concerns the essential singularity of the Coulomb T matrix at zero energy, discussed before This singularity is unavoidable when the total three-particle energy is positive or approximately zero, *i.e.*, above or near the break-up threshold. In order to make really exact calculations possible, we derive a number of formulas by means of which this essential singularity is split off in such a way that it is numerically manageable, see paper A6.

There exists a certain 'solution' ψ_s of the three-dimensional Schrödinger equation with the pure Coulomb potential, which has a pleasant asymptotic behavior. Namely, for large distance it is proportional to the Coulomb scattering amplitude times a Coulomb-modified outgoing spherical wave. We often call ψ_s an 'irregular solution'. However, it is in fact a solution of the Schrödinger equation with an inhomogeneous term which contains a Dirac delta function. In the articles B3 and B4 we derive analytic expressions for the partial-wave projections of ψ_s for all $\ell = 0, 1, 2, \ldots$ We prove that these partial-wave projected functions do *not* satisfy the partial-wave Schrödinger equation, but instead an *in*homogeneous type of Schrödinger equation.

Further we consider in paper B4 similar three-dimensional 'irregular solutions' of the Schrödinger equation with different local potentials, notably Coulomb-like and short-range potentials. We investigate whether any such solution might have an asymptotic behavior, similar to that of the irregular solution for the *pure* Coulomb potential. It seems, however, that the pure Coulomb potential constitutes a remarkable exception in this respect.

In part C we pay attention to the connection between quantum mechanical quantities in the coordinate representation and in the momentum representation, respectively. By definition this connection consists of Fourier and Hankel transforms. On the one hand, one is more accustomed to the probability interpretation in the coordinate representation. On the other hand, certain quantities have a simpler form when expressed in the momentum representation. Therefore it is useful to have expressions available in each of the two representations.

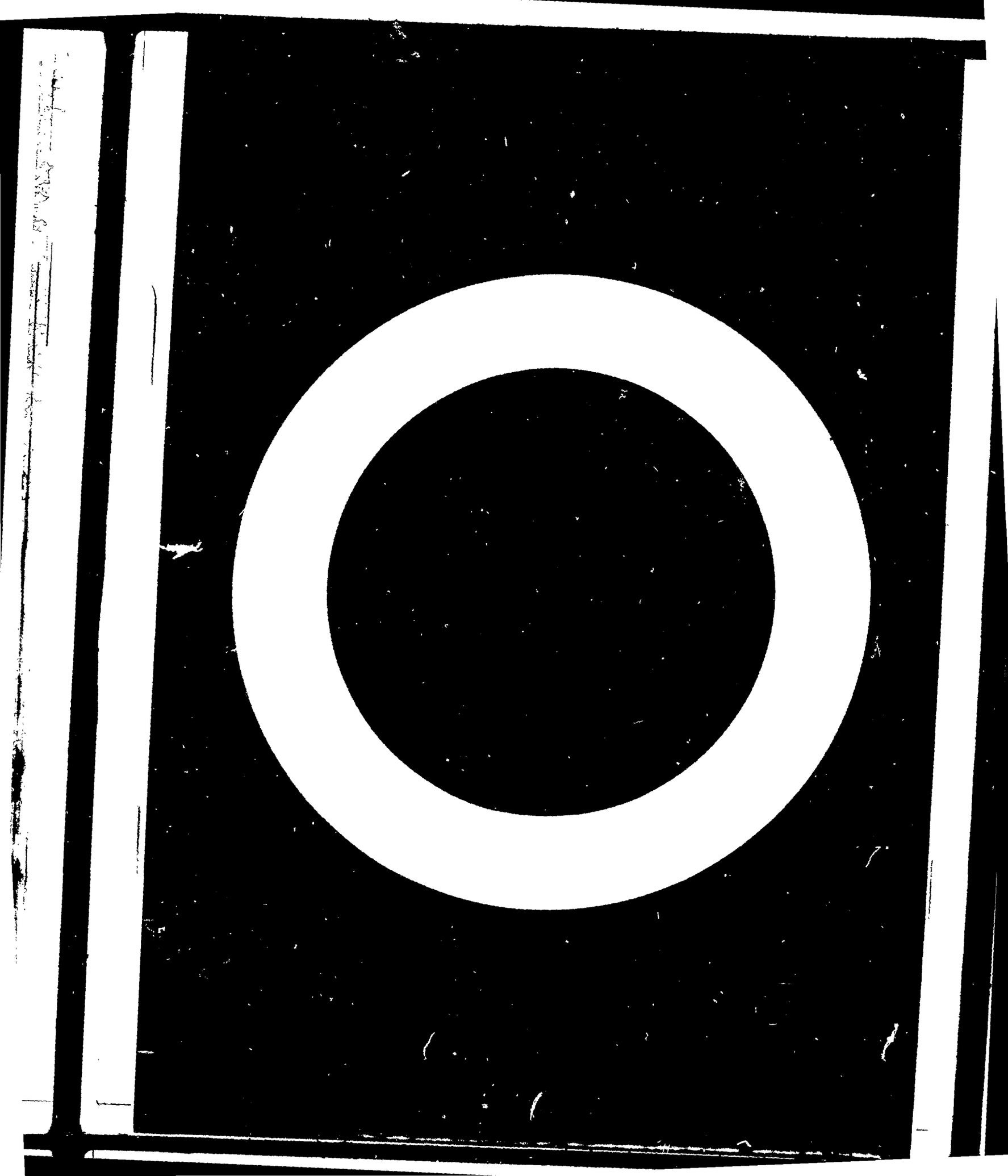
It turns out that in the Coulomb case the momentum representation is more suitable for the derivation of analytic expressions for certain quantities. This is explained by recalling the underlying O_4 symmetry that we discussed before. Indeed, a closed form for the three-dimensional off-shell Coulomb T matrix for negative energy can be derived in an elegant way by using the four-dimensional hyperspherical functions, if one works in the momentum representation.

We make some attempts to obtain a closed expression, in terms of hypergeometric functions, of the partial-wave Coulomb T matrix for all $\ell = 0, 1, \ldots$. Such an expression for arbitrary ℓ is rather complicated, as may be guessed from the expressions for $\ell = 0$ and for $\ell = 1$ that we give in A2 and in A5, respectively. Therefore we first consider some closely related, less complicated, functions notably the off-shell Jost functions which have been introduced by Fuda. Indeed, the half-shell T matrix corresponding to a short-range potential is easily obtained from this off-shell Jost function.

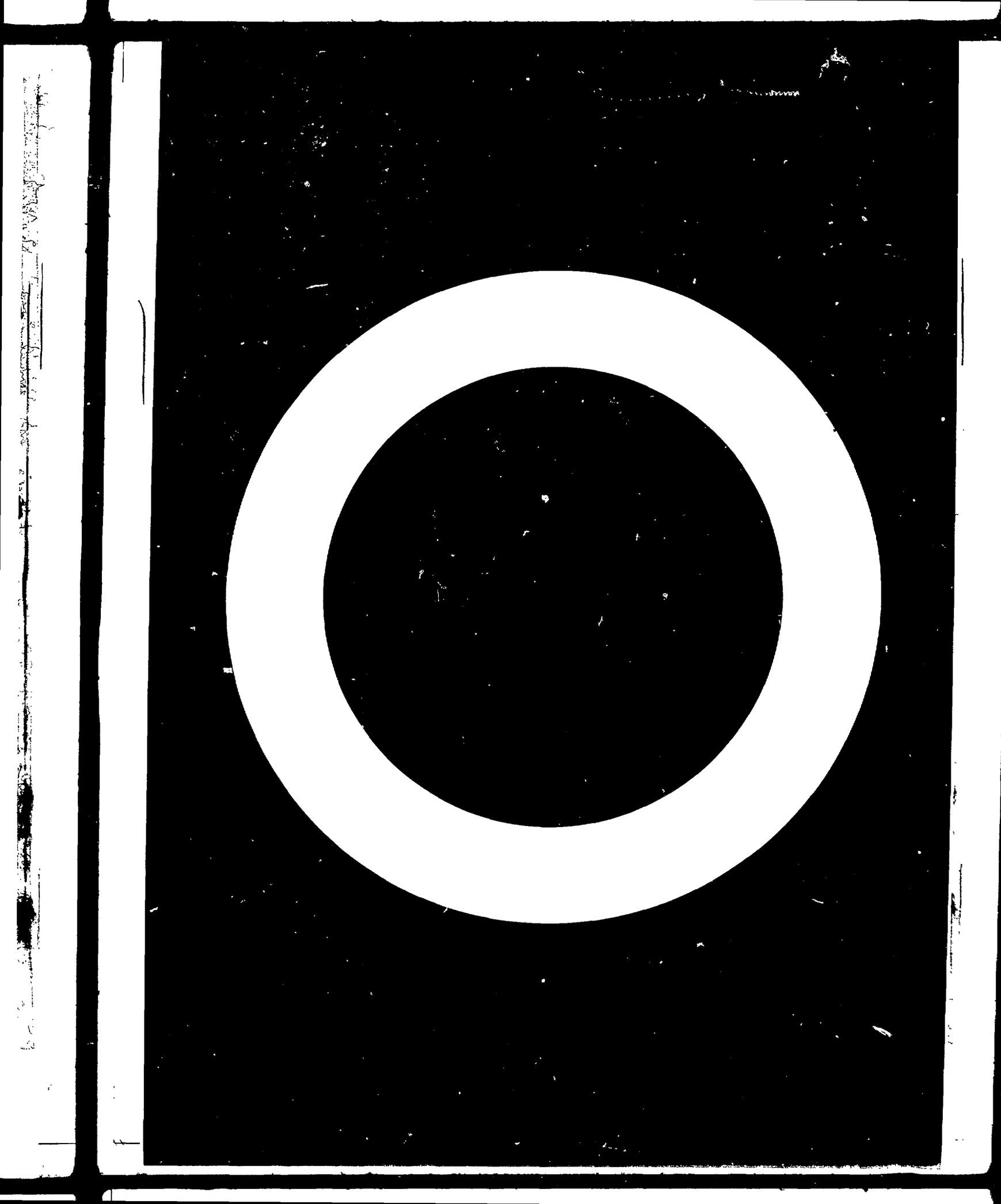
In the articles C1 and C2 we derive a large variety of equivalent analytic expressions for the Coulomb off-shell Jost functions for all ℓ, which are useful for various purposes. Moreover we prove that the off-shell Jost functions for a Coulomb plus local short-range central potential have, for all ℓ, exactly the same on-shell singularity as the $\ell = 0$ Coulomb off-shell Jost function, cf. paper C4.

In C3 we study off-shell scattering quantities for local Coulomb-like central potentials. Here a link is made between the coordinate representation and the momentum representation of certain quantities. We derive many interesting expressions, especially for the Jost functions, the off-shell Jost functions, the Jost states, and the off-shell Jost states, for all partial waves. For the pure Coulomb case we obtain explicit analytic expressions for the Jost state and for the off-shell Jost state in the momentum representation, for $\ell = 0$ only.

In the final article, C4, we investigate the $\ell = 0$ off-shell Jost function for Coulomb, Hulthén, and Eckart-type potentials. The Hulthén potential may be considered as a screened Coulomb potential and the Eckart-type potentials as screened r^{-2} potentials. We derive in C4 a number of interesting limiting relations. When the screening is gradually 'turned off', one has to 'renormalize' in order to ensure the existence of the limits of certain scattering quantities. On the other hand, one also has to use a certain renormalization factor when the on-shell quantities are to be obtained from the corresponding off-shell quantities. We derive the appropriate renormalization factors for both these cases.



Part A



Coulombian asymptotic states

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We define and study Coulombian asymptotic states, denoted by $|\mathbf{k}\,\infty\rangle$, which are useful and important for stationary Coulombian scattering theory. Using these asymptotic states, we are able to derive from the off-shell T matrix the physical on-shell T matrix for Coulomb plus short-range potentials. This function is proportional to the physical scattering amplitude. A generalized Lippmann–Schwinger equation and related equations are derived. Many other applications of the asymptotic states exist. We show the precise connection of $|\mathbf{k}\,\infty\rangle$ with the time-dependent Coulomb scattering theory.

I. INTRODUCTION

The (nonrelativistic two-body) stationary scattering theory for short-range potentials [loosely speaking: $V(r)=O(r^{-\alpha})$, $\alpha>1$, $r\to\infty$] is well founded. If the potential is Coulomb-like, there appear difficulties that *stem from the long range* (in fact, infinite range) of the potential. Two main problems can be discerned: (i) the scattering amplitude is singular in the forward direction, such that it is not an integrable function there; (ii) the scattering states do not approach free states asymptotically (i.e., when $r\to\infty$) and, related to this fact, the T matrix in momentum representation has no half-shell and/or on-shell limit.

To solve problem (i), Herbst[1] and Taylor[2] independently introduced certain distributions (somewhat different from each other) which are suitable to handle the divergencies occurring in the forward direction.

In the present paper we define and study so-called Coulombian asymptotic states, in momentum representation denoted by $\langle\mathbf{p}|\mathbf{k}\,\infty\rangle$, which are suitable to solve problem (ii). They can be thought of as generalized distributions. The phrase "asymptotic state" is an abbreviation of "asymptotically Coulomb-modified improper free state." To be precise, in this paper we consider the *pure* Coulomb potential only. In a forthcoming paper, many applications of $|\mathbf{k}\,\infty\rangle$ will be reported, also to Coulomb plus short-range potential scattering formulas.

We note that the closed formula for $\langle\mathbf{p}|\mathbf{k}\,\infty\rangle$ [see Eqs. (3) and (4)] is not essentially new. Nutt[3] introduced these asymptotic states for the first time, although he defined them inaccurately. To our knowledge, the states have not been used or even mentioned afterwards, up until now. Presumably because an accurate definition and a clear interpretation of these asymptotic states were missing, their importance and usefulness have not been recognized.

In Sec. II we give the exact definition of the asymptotic states and of the class of "test functions" on which they are defined. In Sec. III we derive a generalized Lippmann-Schwinger equation and related equations. We introduce the so-called physical half-shell and on-shell T matrices and we show that the Coulomb scattering amplitude is $-2\pi^2$ times the physical on-shell Coulomb T matrix. In standard scattering theory this relation is well known (the adjective "physical" is then superfluous).

In Sec. IV we investigate the relation between the asymptotic states $\langle\mathbf{p}|\mathbf{k}\,\infty\rangle$ and certain formulas playing a basic role in the time-dependent Coulomb scattering theory. The connection we find there, yields a clear indication for the interpretation of the asymptotic states. Finally, Sec. V contains the summary and discussion.

II. DEFINITION OF THE ASYMPTOTIC STATES $|k\,\infty\rangle$

Already in 1951, Guth and Mullin[4] published an expression for $\langle\mathbf{p}|\mathbf{k}+\rangle_C$, the Coulomb scattering wave function in momentum representation at energy $k^2>0$. We are going to show now that from that expression $\langle\mathbf{p}|\mathbf{k}\,\infty\rangle$ can easily be obtained.

As usual we take $\hbar=2m=1$ (m is the reduced mass) and denote the Coulomb potential by $V_C(r)=2k\gamma/r$. In Sec. IV it will appear preferable to use the k-independent strength parameter $s=-k\gamma$. Throughout this paper we shall be concerned mostly with pure Coulomb formulas. With a few exceptions, the subscript C will be suppressed. We adopt the following normalization:

$$\langle\mathbf{k}'+\ \mathbf{k}+\rangle=\delta(\mathbf{k}'-\mathbf{k}),$$

which differs from the one in Refs. 3 and 4. According to Guth and Mullin[4] one has, with the usual convention $\epsilon\downarrow 0$,

$$\langle\mathbf{p}|V|\mathbf{k}+\rangle = \exp(-\pi\gamma/2)\,\Gamma(1+i\gamma)\,\frac{k\gamma}{\pi^2}\,\frac{|p^2-(k+i\epsilon)^2|^{i\gamma}}{(|\mathbf{p}-\mathbf{k}|^2+\epsilon^2)^{1+i\gamma}}, \tag{1}$$

$$\langle\mathbf{p}|\mathbf{k}+\rangle=\frac{-1}{2k\gamma}\,\frac{d}{d\epsilon}\,\langle\mathbf{p}|V\ \mathbf{k}+\rangle \tag{2}$$

The differentiation with respect to ϵ yields two terms. One of these is

$$\langle\mathbf{p}|\mathbf{k}_\epsilon\rangle\equiv\exp(-\pi\gamma/2)\,\Gamma(2+i\gamma)\,\frac{\epsilon}{\pi^2}\,\frac{|p^2-(k+i\epsilon)^2|^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\gamma}}, \tag{3}$$

where the left-hand side is defined by the right-hand side. We introduce the notation

$$\langle\mathbf{p}|\mathbf{k}\,\infty\rangle\equiv\lim_{\epsilon\downarrow 0}\langle\mathbf{p}|\mathbf{k}_\epsilon\rangle. \tag{4}$$

This is the "plus" state $\langle\mathbf{p}|\mathbf{k}\,\infty+\rangle$. The + sign will mostly be suppressed. The "minus" state is defined by

$$\langle\mathbf{p}|\mathbf{k}_\epsilon-\rangle=\langle\mathbf{p}|\mathbf{k}_\epsilon+\rangle^*, \tag{5}$$

$$\langle\mathbf{p}|\mathbf{k}\,\infty-\rangle=\lim_{\epsilon\downarrow 0}\langle\mathbf{p}|\mathbf{k}_\epsilon-\rangle. \tag{6}$$

Note that this definition is in analogy to the complete physical scattering state $|\mathbf{k}-\rangle$, for which we have

$$\langle \mathbf{p}|\mathbf{k}-\rangle = \langle \mathbf{p}|\mathbf{k}+\rangle^*.$$

We call $|\mathbf{k}_\epsilon \pm\rangle$ and $|\mathbf{k}\,\infty\pm\rangle$ "Coulombian asymptotic states." The limit $\epsilon \downarrow 0$ in Eqs. (1)–(6) should be carefully defined. We give a precise definition of the asymptotic states in the following theorem. The object h_ϵ appearing in the theorem plays the role of the Coulomb T matrix, as will be shown later on.

Theorem. Let $k \equiv |\mathbf{k}| > 0$ and

$$\langle h_\epsilon|\mathbf{p}\rangle \equiv (p-k-i\epsilon)^{i\gamma} f(\mathbf{p}), \tag{7}$$

with $f \in \mathfrak{L}_\infty(\mathbb{R}^3)$ and $f(\mathbf{p})$ continuous at $\mathbf{p}=\mathbf{k}$. Further let $\langle h_\epsilon|\mathbf{k}_\epsilon\rangle$ mean

$$\langle h_\epsilon|\mathbf{k}_\epsilon\rangle \equiv \int_{\mathbb{R}^3} d\mathbf{p}\,\langle h_\epsilon|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle,$$

where $\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle$ has been defined in Eq. (3). Then

$$\lim_{\epsilon\downarrow 0}\langle h_\epsilon|\mathbf{k}_\epsilon\rangle = f(\mathbf{k})[(2k)^{-i\gamma}\exp(-\pi\gamma/2)\,\Gamma(1-i\gamma)]^{-1}. \tag{8}$$

Proof. The proof is essentially a generalization of Simon's "δ-function computation," see Ref. 5: $\lim_{\epsilon\downarrow 0}\epsilon(x^2+\epsilon^2)^{-1} = \pi\delta(x)$. Using Eqs. (3) and (7) and writing $f(\mathbf{p}) = f(\mathbf{p}) - f(\mathbf{k}) + f(\mathbf{k})$, we see that the proof of Eq. (8) is complete once we have proved the following two equations:

$$\text{(i)}\quad \lim_{\epsilon\downarrow 0}\epsilon \int d\mathbf{p}[f(\mathbf{p})-f(\mathbf{k})](p-k-i\epsilon)^{i\gamma} \times \frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\gamma}} = 0. \tag{9}$$

$$\text{(ii)}\quad \lim_{\epsilon\downarrow 0}\frac{\epsilon}{\pi^2}\exp(-\pi\gamma/2)\,\Gamma(2+i\gamma)\int d\mathbf{p}(p-k-i\epsilon)^{i\gamma} \times \frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{2+i\gamma}} = \frac{(2k)^{i\gamma}\exp(\pi\gamma/2)}{\Gamma(1-i\gamma)}. \tag{10}$$

(i) The integral in Eq. (9) exists when $\epsilon > 0$ and it is absolutely dominated by

$$\exp(2\pi|\gamma|)\int d\mathbf{p}\,|f(\mathbf{p})-f(\mathbf{k})|\{|\mathbf{p}-\mathbf{k}|^2+\epsilon^2\}^{-2}.$$

Replace the integration variable $\mathbf{p}$ by $\mathbf{q}=\mathbf{p}-\mathbf{k}$ and define the function $g(\cdot)$ by

$$g(q) \equiv \int d\hat{\mathbf{q}}\,|f(\mathbf{q}+\mathbf{k})-f(\mathbf{k})|. \tag{11}$$

Here $\hat{\mathbf{q}}$ denotes the unit vector in the direction of $\mathbf{q}$, and the domain of integration is the unit sphere. Then $g(\cdot)$ is measurable and essentially bounded, so $g \in \mathfrak{L}_\infty$. Furthermore, $g(0)=0$ and $g(q)$ is continuous at $q=0$. It is now sufficient to prove

$$\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty dq\,\frac{g(q)\,q^2}{(q^2+\epsilon^2)^2} = 0. \tag{12}$$

Take $q \to z = q/\epsilon$, then Eq. (12) becomes

$$\lim_{\epsilon\downarrow 0}\int_0^\infty \frac{dz\,g(\epsilon z)\,z^2}{(z^2+1)^2} = 0.$$

The integrand in this integral converges pointwise to zero and is essentially bounded by $\|g\|_\infty z^2/(z^2+1)^2$, which is integrable, so the integral has zero limit. This proves Eq. (9).

(ii) The integration over the angles in Eq. (10) is easily performed. We have to prove then

$$\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty \frac{dp\,p}{k(p-k-i\epsilon)^{i\gamma}}[p^2-(k+i\epsilon)^2]^{i\gamma}\{[(p-k)^2+\epsilon^2]^{-1-i\gamma} - [(p+k)^2+\epsilon^2]^{-1-i\gamma}\} = \pi\exp(\pi\gamma)(2k)^{i\gamma}|\Gamma(1+i\gamma)|^{-2}. \tag{13}$$

The integral here exists when $\epsilon > 0$. If one excludes any neighborhood of $p=k$, the integral exists also when $\epsilon = 0$. Consequently, the interval of integration $(0,\infty)$ may be replaced by an arbitrary neighborhood of the point $p=k$. This in turn implies that one may in Eq. (13) replace p/k by 1, $(p+k+i\epsilon)^{i\gamma}$ by $(2k)^{i\gamma}$, and neglect the term containing $[(p+k)^2+\epsilon^2]^{-1-i\gamma}$. Finally, one can simplify the integrand by dropping the factor $(p-k-i\epsilon)^{i\gamma}(p-k-i\epsilon)^{-i\gamma}=1$. All this means that it remains to be proved:

$$\lim_{\epsilon\downarrow 0}\int_0^\infty \frac{\epsilon\,dp}{(p-k)^2+\epsilon^2}\frac{(p-k-i\epsilon)^{i\gamma}}{(p-k+i\epsilon)^{i\gamma}} = \pi\exp(\pi\gamma)|\Gamma(1+i\gamma)|^{-2}. \tag{14}$$

The indefinite integral of the integrand in Eq. (14) is easily found, yielding for the left-hand side,

$$\lim_{\epsilon\downarrow 0} -\frac{1}{2\gamma}\frac{(p-k-i\epsilon)^{i\gamma}}{(p-k+i\epsilon)^{i\gamma}}\Big|_{p=0}^{p=\infty} = -\frac{1}{2\gamma}\left(1-\frac{\exp(\pi\gamma)}{\exp(-\pi\gamma)}\right).$$

Utilizing the well-known equality

$$\Gamma(1+i\gamma)\,\Gamma(1-i\gamma) = \pi\gamma/\sinh\pi\gamma,$$

we find that Eq. (14) is valid, so Eq. (19) has been proved. This completes the proof of the theorem.

Reviewing the above theorem and its proof, we find that the domain of integration $\mathbb{R}^3$, implicitly understood in Eq. (8), can be replaced by any neighborhood $\mathcal{N}(\mathbf{k})$ of the point $\mathbf{p}=\mathbf{k}$. In other words: The asymptotic state $\langle \mathbf{p}|\mathbf{k}\,\infty\rangle$ has *support* $\{\mathbf{k}\}$. We deduce from this that the class of "test functions" h_ϵ can be enlarged by relaxing the restrictions. It is sufficient to require only:

$$\begin{aligned} &f(\mathbf{p}) \text{ continuous at } \mathbf{p}=\mathbf{k} \text{ and } f \in \mathfrak{L}_\infty \text{ in some neighborhood } \mathcal{N}(\mathbf{k}),\\ &\langle h_\epsilon|\mathbf{k}_\epsilon\rangle \text{ well defined for all } \epsilon : \epsilon_0 > \epsilon > 0, \text{ some } \epsilon_0 > 0. \end{aligned} \tag{15}$$

Let the symbol $\mathcal{O}_{h_\epsilon}$ mean: in the sense of "generalized distributions" with the above defined "test functions" $\langle h_\epsilon|\mathbf{p}\rangle \equiv (p-k-i\epsilon)^{i\gamma} f(\mathbf{p})$. Then we have, in a formal compact notation, the *extended theorem*:

$$\langle \mathbf{p}|\mathbf{k}\,\infty\rangle = \delta(\mathbf{p}-\mathbf{k})\lim_{\epsilon\downarrow 0}[(p-k-i\epsilon)^{i\gamma}(2k)^{-i\gamma} \times \exp(-\pi\gamma/2)\,\Gamma(1-i\gamma)]^{-1},\ \mathcal{O}_{h_\epsilon}. \tag{16}$$

III. SOME STATIONARY SCATTERING FORMULAS

In Secs. III A–III C we shall derive the following three formulas:

$$|\mathbf{k}+\rangle = |\mathbf{k}\,\infty\rangle + G_0 V|\mathbf{k}+\rangle, \tag{17}$$

$$|\mathbf{k}+\rangle = |\mathbf{k}\,\infty\rangle + G_0 T|\mathbf{k}\,\infty\rangle, \tag{18}$$

$$\langle \mathbf{k}'\infty - |T|\mathbf{k}\,\infty\rangle = \langle \mathbf{k}'\infty - |V|\mathbf{k}+\rangle = \frac{-f^C(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')}{2\pi^2},\quad \hat{\mathbf{k}}' \neq \hat{\mathbf{k}},\quad k' = k \in \mathbb{R}^+. \tag{19}$$

Because of the well-known operator equality $G_0 T = GV$, Eq. (18) implies

$$|\mathbf{k}+\rangle = (\mathbb{1} + GV)|\mathbf{k}\infty\rangle. \tag{20}$$

The operators G, G_0, and T are supposed to have argument $(k+i\epsilon)^2$, $\epsilon \downarrow 0$, and f^C is the Coulomb scattering amplitude,

$$f^C(x) = -\frac{\gamma}{2k}\exp(2i\sigma_0)\left(\frac{1-x}{2}\right)^{-1-i\gamma}. \tag{21}$$

Note that Eqs. (17)—(20) reduce to well-known equations of standard short-range potential scattering theory if one replaces $|\mathbf{k}\infty\rangle$ by the free state $|\mathbf{k}\rangle$. Then Eq. (17) is known as the Lippmann-Schwinger equation and Eq. (19) expresses that the on-shell T matrix is proportional to the amplitude. We call $\langle \mathbf{p}|T|\mathbf{k}\infty\rangle$ the physical half-shell T matrix and $\langle \mathbf{k}'\infty - |T|\mathbf{k}\infty\rangle$ the physical on-shell T matrix $(k'=k)$.

A. Proof of Eq. (17)

In order to derive Eq. (17), we perform the differentiation with respect to ϵ in Eqs. (1) and (2). This gives, at once,

$$\langle \mathbf{p}|\mathbf{k}+\rangle = \lim_{\epsilon\downarrow 0}\langle \mathbf{p}|\mathbf{k}_\epsilon\rangle - \lim_{\epsilon\downarrow 0}\frac{1}{p^2-(k+i\epsilon)^2} \times \exp(-\pi\gamma/2)\,\Gamma(1+i\gamma)\,\frac{k\gamma}{\pi^2}\,\frac{[p^2-(k+i\epsilon)^2]^{i\gamma}}{[|\mathbf{p}-\mathbf{k}|^2+\epsilon^2]^{1+i\gamma}}. \tag{22}$$

The second term on the right-hand side is just $\langle \mathbf{p}|G_0V|\mathbf{k}+\rangle$, as can be seen by inspection. Equation (17) is the formal expression of Eq. (22).

B. Proof of Eq. (18)

Secondly, we have to derive Eq. (18). To this end, we prove that $T|\mathbf{k}\infty\rangle = V|\mathbf{k}+\rangle$, i.e.,

$$\lim_{\epsilon\downarrow 0}\langle \mathbf{p}|T((k+i\epsilon)^2)|\mathbf{k}_\epsilon\rangle = \langle \mathbf{p}|V|\mathbf{k}+\rangle, \quad \hat{\mathbf{p}}\neq\hat{\mathbf{k}}, \tag{23}$$

where the right-hand side is given by Eq. (1) and $\lim_{\epsilon\downarrow 0}$ is understood. Recalling the theorem, it is clear that we need the behavior of the off-shell Coulomb T matrix $\langle \mathbf{p}|T((k+i\epsilon)^2)|\mathbf{p}'\rangle$ at $p'=k$. For this purpose we consider Eqs. (13)—(18) of Ref. 6. The limit $p'\to k$ means in those equations: $x\to -1$, $y\to 0$. Furthermore, $1+I(y)/x \to (-y)^{i\gamma}\Gamma(1+i\gamma)\Gamma(1-i\gamma)$ and $y\to (p^2-k^2)(p'^2-k^2)/(4k^2q^2)$. Assuming $\hat{\mathbf{p}}\neq\hat{\mathbf{p}}'$, we derive from Eqs. (16) and (18) of Ref. 6,

$$\langle \mathbf{p}|T(k^2)|\mathbf{p}'\rangle = k\gamma(\pi q)^{-2}\,\Gamma(1+i\gamma)\,\Gamma(1-i\gamma) \times\left(\frac{(p^2-k^2)(k^2-p'^2)}{4k^2q^2}\right)^{i\gamma} f(p,p';k), \tag{24}$$

where the function f has pleasant properties. Besides on p, p', and k it depends on $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$, but these variables, being unimportant for the discussion, have been suppressed. The variable k is here supposed to be complex, with $\mathrm{Re}k>0$, $\mathrm{Im}k>0$. We let k approach the positive real axis from above. Then f becomes a function of the real positive variables p, p', and k, and this function is continuous at $p=k$ and/or at $p'=k$. Moreover,

$$f(p,k;k) \equiv f(k,p';k) \equiv f(k,k;k) \equiv 1, \tag{25}$$

and this equation is valid for all $\hat{\mathbf{p}}, \hat{\mathbf{p}}'$, provided only that $\hat{\mathbf{p}}\neq\hat{\mathbf{p}}'$. With the above formulas we can derive the physical half-shell limit and, in Sec III C, the physical on-shell limit of the Coulomb T matrix.

Since we wish to apply the theorem to Eq. (24), it is natural to replace k by $k+i\epsilon$ with k real positive. Now let p be fixed with $p\neq k$, and consider the expression between braces in Eq. (24). From the equality

$$[p^2-(k+i\epsilon)^2][(k+i\epsilon)^2-p'^2](k+i\epsilon)^{-2}(k^2+\epsilon^2)^2 = -2ik\epsilon[(k^2+\epsilon^2)^2-p^2p'^2]+(p^2-k^2+\epsilon^2) \times[(k^2+\epsilon^2)^2-p^2p'^2]+p'^2[(p^2-k^2+\epsilon^2)^2+4k^2\epsilon^2], \tag{26}$$

we see that

$$\{[p^2-(k+i\epsilon)^2][(k+i\epsilon)^2-p'^2](k+i\epsilon)^{-2}\}^{i\gamma} \to \exp(-\pi\gamma)\,k^{-2i\gamma}[p^2-(k+i\epsilon)^2]^{i\gamma}[p'^2-(k+i\epsilon)^2]^{i\gamma}, \tag{27}$$

when $p'\to k$, $\epsilon\downarrow 0$. Here γ may be taken real although it depends on $k+i\epsilon$, strictly speaking. We denote now $\mathbf{p}-\mathbf{k}$ by $\mathbf{q}$, which is consistent with the notation $\mathbf{q}=\mathbf{p}-\mathbf{p}'$ of Ref. 6 since $\mathbf{p}'\to\mathbf{k}$. Application of the theorem, in particular Eq. (16), to Eqs. (24) and (27) yields

$$\langle \mathbf{p}|T|\mathbf{k}\infty\rangle = \lim_{\epsilon\downarrow 0} k\gamma\pi^{-2} \times\exp(-\pi\gamma/2)\,\Gamma(1+i\gamma)\,q^{-2-2i\gamma}[p^2-(k+i\epsilon)^2]^{i\gamma}. \tag{28}$$

This expression may be identified with $\langle \mathbf{p}|V|\mathbf{k}+\rangle$ because of $\hat{\mathbf{p}}\neq\hat{\mathbf{k}}$ and the proof of Eq. (18) is complete.

We like to point out that Eq. (27) does not hold, in general. The left-hand side of Eq. (27) has its origin in the expression $(-y)^{i\gamma}$ in Eq. (18) of Ref. 6. Because of the logarithmic cut, running along the negative real axis, $(-y)^{i\gamma}$ cannot be replaced by $\exp(-\pi\gamma)\,y^{i\gamma}$, nor by $\exp(\pi\gamma)\,y^{i\gamma}$. In fact, y *can* become real negative, whereas y *cannot* become real positive, if $q>0$ and $\mathrm{Im}k\neq 0$. This can be seen as follows. Owing to $y=(x+1)/(x-1)$, we have $x=(y+1)/(y-1)$ and the assumption $0\leq y\leq 1$ implies $-\infty\leq x\leq -1$, so $x^2\geq 1$. With the help of Eq. (26), where now either $\epsilon>0$ or $\epsilon<0$, this leads indeed to a contradiction.

In this context it is interesting to note the related fact that $\langle \mathbf{p}'|T(k^2)|\mathbf{p}\rangle$ is a meromorphic function in the complex k plane, cut along the real k axis, and with an arbitrary neighborhood of the origin excluded. See Ref. 6, Eqs. (16)—(18) and also (24), where $T_l(k^2)$ has been expressed in terms of Legendre's second function $\mathfrak{Q}_l$. The branch cut of $\mathfrak{Q}_l$ there is just avoided when $\mathrm{Im}k\neq 0$ and $p'\neq p$, as can be shown with the help of Eq. (26).

C. Proof of Eq. (19)

In order to derive Eq. (19), we can apply the theorem at once to Eq. (28). Taking the epsilons in Eqs. (3) and (28) equal, we get

$$\langle \mathbf{k}'_\epsilon - |T|\mathbf{k}\infty\rangle_{k'=k} \xrightarrow[\epsilon\downarrow 0]{} \frac{-f^C(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')}{2\pi^2}.$$

However, we arrived at this equation in two successive steps. First the physical half-shell limit has been de-

termined and afterwards the physical on-shell limit. The *direct* physical on-shell limit is

$$\lim_{\epsilon \downarrow 0} \langle \mathbf{k}'_\epsilon - | T((k+i\epsilon)^2) | \mathbf{k}_\epsilon \rangle = \frac{-f^C(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')}{2\pi^2}, \quad k' = k \in \mathbb{R}^+. \tag{29}$$

We like to prove this equation in a direct way. Note that the theorem cannot be applied now. However, the following proof of Eq. (29) is very much like the proof of the theorem.

Insert Eqs. (3) and (24) into the expression

$$\lim_{\epsilon \downarrow 0} \int\int d\mathbf{p}\, d\mathbf{p}' \langle \mathbf{k}'_\epsilon - | \mathbf{p}' \rangle \langle \mathbf{p}' | T((k+i\epsilon)^2) | \mathbf{p} \rangle \times \langle \mathbf{p} | \mathbf{k}_\epsilon \rangle, \quad k' = k \in \mathbb{R}^+. \tag{30}$$

The asymptotic states have support $\{\mathbf{k}'\}$ and $\{\mathbf{k}\}$, respectively, so we may replace q^2 by $2k^2(1 - \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')$ and the function f in Eq. (24) by one, according to Eq. (25). The integrations $\int d\hat{\mathbf{p}}$ and $\int d\hat{\mathbf{p}}'$ are now easily evaluated. Consider further

$$i\,\mathrm{Im}[(p-k-i\epsilon)(k+i\epsilon-p')(k+i\epsilon)^{-1}(k^2+\epsilon^2)] = -i\epsilon(k^2+\epsilon^2-pp'),$$

and compare this with Eq. 26). Then it turns out that Eq. (30) can be expressed as

$$\frac{\gamma}{4\pi^2 k} \left(\frac{1 - \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'}{2} \right)^{-1-i\gamma} \Gamma^2(1+i\gamma)\, \Gamma(1-i\gamma) \exp(-\pi\gamma)\, L, \tag{31}$$

with

$$L = \lim_{\epsilon \downarrow 0} \left(\frac{\epsilon}{\pi} \right)^2 \int_0^\infty dp \int_0^\infty dp' \, \frac{(p-k+i\epsilon)^{-i\gamma}}{(p-k)^2+\epsilon^2} \, \frac{(p'-k+i\epsilon)^{-i\gamma}}{(p'-k)^2+\epsilon^2} \times [(p-k-i\epsilon)(k+i\epsilon-p')]^{i\gamma}. \tag{32}$$

Changing variables according to $p - k = \epsilon z$, $p' - k = \epsilon z'$, we get

$$L = \pi^{-2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dz\, dz' \, \frac{(z+i)^{-i\gamma}}{z^2+1} \, \frac{(z'+i)^{-i\gamma}}{z'^2+1} \times [(z-i)(i-z')]^{i\gamma}. \tag{33}$$

The order of integration is unimportant. Now we have ($z, z' \in \mathbb{R}$)

$$\ln(z+i) = \tfrac{1}{2}\ln(z^2+1) + i\,\mathrm{arccot} z$$

and

$$\ln[(z-i)(i-z')] = \tfrac{1}{2}\ln[(z^2+1)(z'^2+1)] + i\arctan z + i\arctan z',$$

where the inverse trigonometric functions are determined by their principal values

$$-\tfrac{1}{2}\pi < \arctan z < \tfrac{1}{2}\pi, \quad 0 < \mathrm{arccot} z < \pi.$$

Using these equations we get

$$L = \pi^{-2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dz\, dz' \, (z^2+1)^{-1}(z'^2+1)^{-1} \times \exp[\gamma(\mathrm{arccot} z - \arctan z + \mathrm{arccot} z' - \arctan z')].$$

This double integral is evaluated by standard means, yielding

$$L = (2\pi\gamma)^{-2}(\exp(-\pi\gamma/2) - \exp(3\pi\gamma/2))^2 = (\pi\gamma)^{-2} \exp(\pi\gamma) \sinh^2 \pi\gamma = \exp(\pi\gamma)\, |\Gamma(1+i\gamma)|^{-4}. \tag{34}$$

Insertion of Eq. (34) into Eq. (31) proves Eq. (29), of which Eq. (19) is the formal expression.

In Sec. IV a different but closely related procedure to obtain the physical on-shell T matrix will be given, see Eq. (51).

Remark. As we said in Sec. I, the asymptotic states defined in the theorem are essentially the asymptotic states introduced by Nutt, see Eq. (15) of Ref. 3. However, Nutt's definition of these states and of the limits $\epsilon \downarrow 0$ is less careful than ours. Also his "minus" state differs from our state $|\mathbf{k}\,\infty -\rangle$. Probably because of these facts, he finds a different result for the Coulomb scattering amplitude. It contains in particular a factor $(2k/\epsilon^2)^{-2i\gamma}$, having no limit when $\epsilon \downarrow 0$.

IV. CONNECTION WITH TIME-DEPENDENT COULOMB SCATTERING

In the time-dependent scattering theory a basic role is played by Møller's wave operators $\Omega_\pm$, defined by

$$\Omega_\pm = s\text{-}\lim_{t \to \mp\infty} \Omega(t), \tag{35}$$

$$\Omega(t) \equiv \exp(iHt) \exp(-iH_0 t), \tag{36}$$

where H is the Hamiltonian $H = H_0 + V$. The strong limits in Eq. (35) exist when V has short range, but they do not exist when V is the Coulomb potential. According to Dollard,[7] the following modification has to be made. Define

$$\Omega^C(t) \equiv \exp(iHt) \exp(-iH_0 t) \exp[-iA(t)], \tag{37}$$

where H is now the Coulomb Hamiltonian, and the "anomalous" operator $A(t)$ is defined by

$$A(t) \equiv -sH_0^{-1/2} \,\mathrm{sgn}(t) \ln(4H_0 |t|), \quad t \neq 0. \tag{38}$$

$\mathrm{sgn}(t)$ denotes the sign of the time t and s is the potential strength, $V(r) = -2s/r$. In Sec. II we chose the notation $V(r) = 2k\gamma/r$, but use of the constant s is here preferable. Because $A(t)$ is a function of H_0, Eq. (37) is equivalent to

$$\Omega^C(t) \equiv \exp(iHt) \exp[(-iH_0 t) - iA(t)].$$

Dollard[7] proved that the strong limits of $\Omega^C(t)$ exist,

$$\Omega^C_\pm = s\text{-}\lim_{t \to \mp\infty} \Omega^C(t), \tag{39}$$

and that $\Omega^C_\pm$ can be correctly interpreted as the Coulomb wave operators.[8] For example, the improper stationary Coulomb scattering states may be written formally as

$$|\mathbf{k}\pm\rangle = \Omega^C_\pm |\mathbf{k}\rangle. \tag{40}$$

It is customary to introduce ϵ'-dependent wave operators $\Omega_{\epsilon'\pm}$ by means of the Bochner integrals (e.g., Prugovečki,[9] pp. 436 and 456),

$$\Omega_{\epsilon'\pm} \equiv \mp\epsilon' \int_0^{\mp\infty} dt \exp(\pm\epsilon' t)\, \Omega(t), \quad \epsilon' > 0. \tag{41}$$

[Here we use ϵ' in order to avoid confusion. Indeed the operators G_0, G, and T turn out to have argument $k^2 + i\epsilon'$. For example, Eqs. (36) and (41) yield formally

$$\Omega_{\epsilon'}|\mathbf{k}\rangle = i\epsilon' G(k^2 + i\epsilon')|\mathbf{k}\rangle. \tag{41'}$$

However, in the preceding sections we preferred to take the argument $(k + i\epsilon)^2$. To first order in ϵ we have $\epsilon' = 2k\epsilon$.] For a short-range potential one has (e.g., Ref. 9, p. 437)

$$\Omega_{\pm} = s\text{-}\lim_{\epsilon' \downarrow 0} \Omega_{\epsilon'\pm}. \tag{42}$$

In the case of the Coulomb potential, Eq. (42) has to be modified also. From the paper by Zorbas[10] (see, p. 122: Lemma) it follows that it should be replaced by

$$\Omega_{\pm}^{C} = s\text{-}\lim_{\epsilon' \downarrow 0} \Omega_{\epsilon'\pm} A_{\epsilon'\pm}^{-1}. \tag{43}$$

Here $\Omega_{\epsilon'\pm}$ are the Møller wave operators for the Coulomb potential, defined by Eqs. (36) and (41), and we have introduced the operators $A_{\epsilon'\pm}^{-1}$ which are defined by[11]

$$A_{\epsilon'\pm} \equiv \mp \epsilon' \int_0^{\mp\infty} dt \exp(\pm \epsilon' t) \exp[iA(t)], \quad \epsilon' > 0. \tag{44}$$

Upon substitution of Eq. (38) for $A(t)$, these integrals become essentially gamma-function integrals. Zorbas obtained the following explicit expressions [Ref. 10, Eq. (13), in different notation and with opposite sign convention, cf. Ref. 8],

$$A_{\epsilon'\pm} = \Gamma(1 \pm isH_0^{-1/2})(4H_0/\epsilon')^{\pm isH_0^{-1/2}}. \tag{45}$$

After this survey of the necessary formulas, we are now in a position to make the final step, and to show explicitly the connection with our asymptotic states. The operators $A_{\epsilon'\pm}$, being functions of H_0, are diagonal in momentum representation. From Eq. (45) we get (recall $\epsilon' \to 2k\epsilon$)

$$\langle \mathbf{p}|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = \delta(\mathbf{p} - \mathbf{k})[(2k/\epsilon)^{-i\gamma}\Gamma(1 - i\gamma)]^{-1} \tag{46}$$

and

$$\langle \mathbf{p}|A_{2k\epsilon-}^{-1}|\mathbf{k}\rangle = \langle \mathbf{p}|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle^*. \tag{47}$$

Here we have turned back to the Sommerfeld parameter $\gamma \equiv -s/k$, and the + subscript has been suppressed. Note that Eq. (47) can also be obtained from the equality $A_{\epsilon'}^{\dagger} = A_{\epsilon'-}$, which is a consequence of the definition of $A_{\epsilon'\pm}$ [Eq. (44)] and of the equalities [cf. Eq. (38)],

$$A^{\dagger}(t) = A(t) = \mathrm{sgn}(t)A(|t|). \tag{48}$$

Now let h_ϵ be a "test function" as defined in Eq. (7),

$$\langle h_\epsilon|\mathbf{p}\rangle \equiv (p - k - i\epsilon)^{i\gamma} f(\mathbf{p}).$$

Then Eq. (46) at once yields

$$\langle h_\epsilon|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = f(\mathbf{k})[(2k)^{-i\gamma}\exp(-\pi\gamma/2)\Gamma(1 - i\gamma)]^{-1}. \tag{49}$$

Comparison of Eq. (49) with Eq. (8) gives

$$\langle h_\epsilon|A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = \lim_{\epsilon \downarrow 0} \langle h_\epsilon|\mathbf{k}_\epsilon\rangle, \tag{50}$$

which we denote formally by [cf. Eq. (16)]

$$|\mathbf{k}\infty\rangle \equiv \lim_{\epsilon \downarrow 0} |\mathbf{k}_\epsilon\rangle = \lim_{\epsilon \downarrow 0} A_{2k\epsilon}^{-1}|\mathbf{k}\rangle, \ \mathcal{O}_{h_\epsilon}. \tag{50'}$$

Furthermore, from Eqs. (46), (47), and (24), (25) we obtain

$$\lim_{\epsilon \downarrow 0} \langle \mathbf{k}'|A_{2k\epsilon-}^{\dagger -1} T((k + i\epsilon)^2) A_{2k\epsilon}^{-1}|\mathbf{k}\rangle = -f^C(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}')/(2\pi^2), \quad k' = k, \tag{51}$$

which should be compared with Eqs. (19) and (29). In the three final equations we have the desired connection of the Coulombian asymptotic states with the time-dependent Coulomb scattering formulas in explicit form.

Eventually two remarks are in order.

(i) The "plus" stationary scattering state $|\mathbf{k}+\rangle$ is connected with the limit $t \to -\infty$; the "minus" state $|\mathbf{k}-\rangle$ with $t \to +\infty$. So if we want to interpret the asymptotic states $|\mathbf{k}\infty\pm\rangle$ in analogy to $|\mathbf{k}\pm\rangle$, it follows from Eq. (47) that we should have

$$\langle \mathbf{p}|\mathbf{k}\infty -\rangle = \langle \mathbf{p}|\mathbf{k}\infty\rangle^*,$$

which agrees with the *definition* of $\langle \mathbf{p}|\mathbf{k}\infty -\rangle$, see Eqs. (4)–(6).

(ii) It is important to realize that $|\mathbf{k}_\epsilon\rangle$ and $A_{2k\epsilon}^{-1}|\mathbf{k}\rangle$ are objects, stemming from quite different starting points. Their equality in the sense $\mathcal{O}_{h_\epsilon}$ [see Eq. (50')] is very satisfactory, for this shows the way how to interpret $|\mathbf{k}_\epsilon\rangle$ in the time-dependent picture.

V. SUMMARY AND DISCUSSION

In Sec. II we defined asymptotic states $|\mathbf{k}\infty\pm\rangle \equiv \lim_{\epsilon\downarrow 0}|\mathbf{k}_\epsilon\pm\rangle$. According to the theorem proved there, these states can be considered as "generalized distributions" defined on a certain class of ϵ-dependent "test functions," see Eq. (16). We showed that the Coulomb T matrix in momentum representation belongs to this class of "test functions." This is an important result since it solves the half-shell and on-shell problems of the Coulomb T matrix. In Sec. III we derived some stationary scattering formulas in which the asymptotic states are applied, see Eqs. (17)–(20). In Sec. IV the connection of our asymptotic states with Dollard's[7] time-dependent formulation and Zorbas's[10] time-independent formulation of Coulomb scattering has been investigated. The main result is here expressed in Eqs. (50) and (51). The approach of this paper differs from the ordinary "screening" approach. With a screened Coulomb potential one gets the ordinary Lippmann-Schwinger equation in place of Eq. (17).

From the time-dependent theory (Sec. IV) it follows that the actual scattering of a particle (occurring at $t \approx 0$, say) should be considered *with respect to its behavior at* $t \to \pm\infty$. The movement of the particle (i.e., the time evolution of the scattering state in Hilbert space) is, at large times, not governed by the usual operator $\exp(-iH_0t)$, but instead by $\exp[-iH_0t - iA(t)]$, see Dollard.[7] The time dependence is translated into the ϵ'- dependence with the help of Eqs. (41) and (44). In this way Zorbas[10] obtained "anomalous" operators which we denote by $A_{\epsilon'\pm}$. In the time-independent picture, the improper free state $|\mathbf{k}\rangle$ has to be replaced by $A_{2k\epsilon}^{-1}|\mathbf{k}\rangle$. One can therefore (small ϵ meaning large times) interpret

$$-2\pi^2\langle \mathbf{k}'|A_{2k\epsilon-}^{\dagger -1} T((k + i\epsilon)^2) A_{2k\epsilon}^{-1}|\mathbf{k}\rangle,$$

with $k' = k$ as the amplitude for the probability, to begin with the distorted free state $A_{2k\epsilon}^{-1}|\mathbf{k}\rangle$ and to find, after the scattering has taken place, the distorted free state denoted by $\langle \mathbf{k}'|A_{2k\epsilon-}^{\dagger -1}$. In the same way we interpret

$$\langle \mathbf{k}'_\epsilon - | T((k+i\epsilon)^2) | \mathbf{k}_\epsilon \rangle,$$

with $k' = k$ as the physical amplitude for an initial distorted free state $|\mathbf{k}_\epsilon\rangle$ and a final distorted free state $\langle \mathbf{k}'_\epsilon - |$. Translating back to the time-dependent picture, we get the correct description of the physical scattering process.

In conclusion we can say that the approaches with our asymptotic states $|\mathbf{k}_\epsilon \pm\rangle$ on the one hand, and with the operators $A^{\pm}_{2\mathbf{k}\epsilon\pm}$ which follow from the paper by Zorbas on the other hand, are equivalent in the sense of Eqs. (50) and (51).

The ideas concerning a "renormalization procedure," as the application of Eq. (16), or something like it, has been called sometimes, have been living in the literature since a long time. A list containing all relevant papers by other authors on this subject would become rather extensive.

The present paper clarifies some obscure points, it shows precisely *how* the asymptotic states can be applied, and, in particular from the connection with the time-dependent theory, it makes clear *why* just the "renormalization procedure" of Eq. (16) should be applied. In general, our asymptotic states restore the analogy of the stationary two-body Coulomb-like potential scattering formulae with the standard scattering formulae. This will be worked out in a subsequent paper, where we shall also have occasion to discuss the approaches by other authors.

From the theorem and Eqs. (16)–(20) it can be seen that $|\mathbf{k}\,\infty\rangle$ is particularly suited to the two-body Coulomb T operator at energy $k^2 > 0$. Furthermore, we can show by means of explicit formulas that exactly the same asymptotic states can be applied to the total T operator when a short-range potential is added to the Coulomb potential. Because the two-body T operator is the basic object in N-body stationary scattering theory, we hope that the approach of this paper can be extended to multiparticle stationary scattering theory involving charged particles.

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A 2

Analytic T matrices for Coulomb plus rational separable potentials

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The $l = 0$ partial wave projected Coulomb off-shell T matrix $T_{c,l=0}$ in momentum representation is obtained in closed form. Problems existing in the literature concerning the half- and on-shell behavior of T_c and $T_{c,l}$ are discussed and clarified by means of explicit formulas. The remaining derivations in this paper are based on $T_{c,l=0}$. We consider the class of N-term separable potentials where the form factors are rational functions of p^2 (in momentum representation). We prove that the $l = 0$ T matrix corresponding to the Coulomb potential plus any such so-called rational separable potential has a very simple form, namely, it can be written in terms of rational functions and the (simple) hypergeometric function with parameters $(1, i\gamma, 1 + i\gamma)$, where γ is the well-known Coulomb parameter. Explicit analytic formulas are derived for a number of simple members of the class, the Yamaguchi potential being one of them. In this particular case the expressions of Zachary and of Bajzer are reproduced who used a method based on the O_4 symmetry

1. INTRODUCTION

The nonrelativistic few-body problem is considerably simplified by the use of nonlocal separable potentials in place of local potentials. This simplification is justified by the observation that short-range local potentials can be approximated by finite-rank separable potentials in a mathematically well-defined sense. In view of the importance of charged particles in few-body systems, the interest in studying potentials consisting of the sum of a short-range finite-rank potential and the Coulomb potential is not surprising.[1-7] Because of the long-range difficulties involved, often a screened Coulomb potential is proposed with a very large screening parameter.[1,8-11] For the pure Coulomb problem, wave functions and Green's functions in coordinate representation are known in closed form.[12-15] Several equivalent[16] momentum representation expressions (in three-dimensional space, $\mathbf{p} \in R^3$) are known for the Green's function and for the off-shell T matrix.[16-22] For the Coulomb plus Yamaguchi[23] potential the off-shell T matrix in momentum representation is known in closed form[5,6] for $l = 0$. This latter is derived using the O_4 group-theoretic approach first discussed at some length by Fock.[24]

As is well known, in conventional (short-range) potential scattering theory the physical scattering amplitude can be obtained by taking the on-shell limit of the off-shell T matrix. This is no longer true when the potential has a long range such as the Coulomb potential; in fact, the on-shell limit is not defined in this case. Because this trouble just comes from the behavior of the potential at large distance, the same fact holds when an arbitrary short-range potential is added to the Coulomb potential. Nevertheless, it is generally expected that one also can extract, in such a situation, all relevant physical information from the off-shell T matrix. Therefore, it seems to be very interesting to have explicit formulas for off-shell T matrices which describe the Coulomb interaction plus a rather general short-range interaction exactly. Once we have gotten the correct relation between the off-shell T matrices and the physical amplitudes, we could obtain information about the short-range interaction by comparing the numerical values resulting from the theory and the experiment respectively. We have been able to establish such a relation, and to give a satisfactory justification for it. This will be reported in detail in a subsequent paper.[25]

In the present paper we obtain the $l = 0$ partial wave projected off-shell Coulomb T matrix in momentum representation $T_{c,l=0}$ analytically, starting from a known expression for the complete T_c in three-dimensional p space (unless stated otherwise we work in momentum representation). Two equivalent explicit formulas for $T_{c,l=0}$ are given at the end of Sec. 3. Concerning the half- and on-shell behavior of T_c and of $T_{c,l}$, some confusion has grown in the literature. As we said above, the difficulties arise exclusively from the long range of the Coulomb potential and remain unaltered when an arbitrary short-range potential is added. These difficulties are discussed in detail in Sec. 4 and clarified with the help of explicit formulas derived in Sec. 3.

In section 5 we give the general formulas to obtain the T matrix corresponding to an arbitrary N-term separable potential plus the Coulomb potential. In Secs. 6 and 7 we derive analytic expressions for a number of off-shell T matrices corresponding to Coulomb plus N-term separable potentials (for $l = 0$ only), starting from one of the explicit expressions for $T_{c,l=0}$ derived in Sec. 3. In particular, for the case of Coulomb plus the (one-term separable) Yamaguchi potential we find complete agreement with the formula of Zachary[5] and of Bajzer.[6] It should be noted, however that we apply only special function theory. Nowhere in this paper do we use the O_4 group-theoretic approach of Zachary and Bajzer.

In Sec. 8 we define the very large class of rational separable potentials. We reveal the general structure of the explicit formulas for the off-shell T matrices corresponding to any such potential plus the Coulomb potential. It appears that the hypergeometric function ${}_2F_1(1, i\gamma; 1 + i\gamma; \cdot)$, where γ is the well-known Coulomb parameter,[12] is the only nonrational function involved. Moreover, the method to obtain any such T matrix in

exact closed form follows immediately from the derivations given in Secs. 6–8.

Finally, in Sec. 9 the results and implications are summarized and discussed.

2. NOTATION

Dirac notation is used throughout. Our normalization is determined by the use of delta functions as basis states in momentum representation,

$$\langle \mathbf{p}|\mathbf{k}\rangle \equiv \delta(\mathbf{p}-\mathbf{k}); \tag{1}$$

in the lth partial wave space

$$\langle p\,l|k\,l\rangle = k^{-2}\delta(p-k). \tag{2}$$

This implies the following basis states in coordinate representation

$$\langle \mathbf{r}|\mathbf{k}\rangle \equiv (2\pi)^{-3/2}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{3}$$

$$\langle r\,l|k\,l\rangle \equiv (2/\pi)^{1/2}i^l j_l(kr). \tag{4}$$

Here the variable k stands for the square root of the energy,

$$E \equiv k^2. \tag{5}$$

Functions of k will be defined in the upper-half of the complex k-plane, i.e.,

$$\mathrm{Im}\,k > 0. \tag{6}$$

Generalized functions (distributions) like (1) and (2) may be defined as limits of functions of k where the appropriate limit

$$\mathrm{Im}\,k \to 0 \tag{7}$$

is taken, cf., e.g., Ref. 12. The partial wave projection of a rotationally invariant operator A is defined by

$$\langle x'|A_l|x\rangle \equiv \int d\hat{\mathbf{x}}\,P_l(\hat{\mathbf{x}}'\cdot\hat{\mathbf{x}})\,\langle \mathbf{x}'|A|\mathbf{x}\rangle, \tag{8}$$

where x stands for r or p. This implies

$$\langle \mathbf{x}'|A|\mathbf{x}\rangle = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\hat{\mathbf{x}}'\cdot\hat{\mathbf{x}})\langle x'|A_l|x\rangle. \tag{9}$$

In Eq. (9) the infinite sum converges generally not pointwise, but only in the sense of distributions[12,26,27]; compare Sec. 4.

3. THE PARTIAL WAVE PROJECTED COULOMB T OPERATOR $T_{c,l}$

In this section an integral representation for $T_{c,l}$ is derived from one of the known expressions for the complete T_c. At the end of the section $T_{c,l=0}$ is explicitly obtained; the derivations of Secs. 6–8 are based on this expression for $T_{c,l=0}$.

Our starting point is the complete Coulomb T matrix T_c. There are several equivalent[16] expressions known for this function.[16–21] In particular, Schwinger's[19] derivation, based on the O_4 symmetry exhibited by the Coulomb potential, is elegant. Chen and Chen[16] give a fairly complete survey of the work done on two-body Coulomb amplitudes. In place of T_c the resolvent G_c is given by many authors, but in momentum representation the explicit expressions for G_c and T_c are related in a trivial way because one has

$$G_c(E) = G_0(E) + G_0(E)T_c(E)G_0(E). \tag{10}$$

Below we mention some useful expressions for T_c. We define the Coulomb potential

$$V_c(r) \equiv 2k\eta/r. \tag{11}$$

Here the notation of Messiah[12] is followed. Units are such that $\hbar = 2m = 1$ where m is the reduced mass. It is important to note that the parameter η is energy-dependent, for (recall $E = k^2$, $\mathrm{Im}\,k > 0$)

$$k\eta = \text{real const.} \tag{12}$$

Defining

$$\mathbf{q} \equiv \mathbf{p}'-\mathbf{p}, \quad q \equiv |\mathbf{q}|,$$

we get from (11)

$$\mathbf{p}'|V_c|\mathbf{p} = -\frac{k\eta}{\pi^2 q^2}. \tag{13}$$

Define further

$$x \equiv 1-(p^2+k^2)(p'^2-k^2)^{-1}k^{-2}q^2,$$

$$\nu \equiv (x+1)^{1/2}(x-1)^{1/2},$$

then T_c can be expressed as

$$\mathbf{p}'|T_c(k^2)|\mathbf{p} = -\frac{k\eta}{\pi^2 q^2}\cdot\frac{4ik^3\eta^2}{\pi^2(p^2-k^2)(p'^2-k^2)} \times\int_0^1 dt\,t^{i\eta}(1-t\nu)^{-1}(1-t/\nu)^{-1}. \tag{14}$$

The first term of the rhs is just the potential term; see Eq. (13). Using the integral representation[28]

$${}_2F_1(1,i\eta;1+i\eta;\nu) = i\eta\int_0^1 dt\,t^{i\eta-1}(1-t\nu)^{-1} \tag{15}$$

of this h.f. (hypergeometric function) we get from (14)

$$\langle \mathbf{p}'|T_c(k^2)|\mathbf{p}\rangle = \frac{k\eta}{\pi^2 q^2}\left(1+\frac{I(\nu)}{\nu}\right), \tag{16}$$

with

$$I(\nu) = {}_2F_1(1,i\eta,1+i\eta;\nu) - {}_2F_1(1,i\eta,1+i\eta,1/\nu). \tag{17}$$

It is clear that $I(\nu)/\nu$ is invariant for the transformation $\nu \to -\nu$. Thus the sign of the real part of ν may be chosen freely. Choose then

$$\mathrm{Re}\,\nu < 0,$$

this implies

$$|\nu| < 1.$$

Using well-known properties of the h.f.[28] [cf., Eq. (32)] and writing it in its infinite series representation, we get the result

$$I(\nu) = 1-(-\nu)^{i\eta}\Gamma(1+i\eta)\Gamma(1-i\eta) + 2\eta^2\sum_{n=1}^{\infty}\frac{\nu^n}{n^2+\eta^2}. \tag{18}$$

We can rewrite Eq. (14) in a different form,

$$\langle \mathbf{p}'|T_c(k^2)|\mathbf{p}\rangle = \frac{k\eta}{\pi^2 q^2} + \frac{4k\eta^2}{i\pi^2 q^2}\int_0^1\frac{dt\,t^{i\eta}}{4t-(1-t)^2(\nu^2-1)}. \tag{19}$$

This expression is more convenient for the derivation of

$T_{c,l}$. According to (8), multiplying Eq. (19) by the Legendre polynomial $P_l(\hat{\mathbf{p}}'\cdot\hat{\mathbf{p}})$ and integrating over the angles yields $T_{c,l}$. Now we have the well-known relation between P_l and the Legendre function of the second kind Q_l:

$$Q_l(z)=\frac{1}{2}\int_{-1}^{1} d\alpha\, P_l(\alpha)(z-\alpha)^{-1}. \tag{20}$$

Equation (20) immediately yields the partial wave projected potential matrix elements from Eq. (13):

$$\langle p'|V_{c,l}|p\rangle=\frac{2k\gamma}{\pi pp'}Q_l\left(\frac{p^2+p'^2}{2pp'}\right). \tag{21}$$

Applying Eqs. (8) and (20) to Eq. (19) gives, after interchanging the order of integration (this is permitted, compare Sec. 4B),

$$\langle p'|T_{c,l}(k^2)|p\rangle=\frac{2k\gamma}{\pi pp'}\left(Q_l\left(\frac{p^2+p'^2}{2pp'}\right)-i\gamma\int_0^1 dl\, l^{i\gamma-1}Q_l(z)\right), \tag{22}$$

with

$$z=\frac{1}{2pp'}\left(p^2+p'^2-\frac{(1-l)^2}{l}\cdot\frac{(p^2-k^2)(p'^2-k^2)}{4k^2}\right). \tag{23}$$

Difficulties may occur in the integrals of the form $\int dl\, l^{i\gamma}\cdots$ in the neighborhood of $l=0$. These are discussed in Sec. 4B. In effect we may assume that the exponent $i\gamma$ contains a small positive real part. We simplify Eq. (22) by means of integration by parts. The integrated term just cancels the first term in the rhs of Eq. (22); thus we get

$$\langle p'|T_{c,l}(k^2)|p\rangle=\frac{2k\gamma}{\pi pp'}\int_0^1 dl\, l^{i\gamma}\frac{d}{dl}Q_l(z). \tag{24}$$

Whether this formula is useful for a derivation of $T_{c,l}$ in closed form remains to be seen. In this paper we use only $T_{c,l=0}$ for further derivations. This function follows rather easily from Eq. (24). Because of the simple relation

$$\frac{d}{dz}Q_0(z)=(1-z^2)^{-1}, \tag{25}$$

the integral in Eq. (24) can (in case $l=0$) be written in terms of h.f.'s. Rearranging and collecting terms yields the final result

$$\langle p'|T_{c,l=0}(k^2)|p\rangle=\frac{ik}{\pi pp'}D, \tag{26}$$

$$D\equiv {}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ a'a)-{}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ a/a') \tag{27}$$
$$+{}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ 1/(a'a))-{}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ a'/a),$$

with

$$a\equiv(p-k)/(p+k), \tag{28}$$

$$a'\equiv(p'-k)/(p'+k). \tag{29}$$

A different expression for D is convenient if one wishes to study its half-shell behavior, i.e., $p'\to k$ thus $a'\to 0$. This expression reads

$$D\equiv\Gamma(1+i\gamma)\Gamma(1-i\gamma)\left[(-a'a)^{i\gamma}-(-a'/a)^{i\gamma}\right]$$
$$+{}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ a'a)-{}_2F_1(1,\ -i\gamma;\ 1-i\gamma;\ a'a)$$
$$-{}_2F_1(1,i\gamma;1+i\gamma;a'/a)+{}_2F_1(1,-i\gamma;1-i\gamma;a'/a). \tag{30}$$

Equation (30) can be obtained from Eq. (27) as follows. Utilizing the relation[29,30]

$${}_2F_1(\lambda,\mu;\nu;z)=\frac{\Gamma(\nu)\Gamma(\mu-\lambda)}{\Gamma(\mu)\Gamma(\nu-\lambda)}(-z)^{-\lambda}$$
$$\times\ {}_2F_1(\lambda,1-\nu+\lambda,1-\mu+\lambda;1/z)$$
$$+\frac{\Gamma(\nu)\Gamma(\lambda-\mu)}{\Gamma(\lambda)\Gamma(\nu-\mu)}(-z)^{-\mu}$$
$$\times\ {}_2F_1(\mu,1-\nu+\mu,1-\lambda+\mu;1/z), \tag{31}$$

we derive

$${}_2F_1(1,i\gamma,1+i\gamma,z)+{}_2F_1(1,-i\gamma;1-i\gamma;1/z)$$
$$=1+\Gamma(1+i\gamma)\Gamma(1-i\gamma)(-z)^{-i\gamma}. \tag{32}$$

It is well known that ${}_2F_1$ has a branch point at infinity.[29] In Eq. (27) it is then clear that two of the four h.f.'s have to be transformed, this is done with the help of Eq. (32), and Eq. (30) is obtained at once. In Eq. (30), the singular behavior of D in the neighborhood of $a'=0$ is written out in its most transparent form.

Finally, it should be noted that the off-shell $l=0$ T matrix for the Hulthén potential is known in closed form.[31] Because the Hulthén potential can be seen as a screened Coulomb potential, one could in principle obtain $T_{c,l=0}$ from the analytic formula of Bahethi and Fuda, by letting the screening parameter go to infinity. This formula contains hypergeometric functions ${}_4F_3$ and ${}_3F_2$, however, so it seems that our (more direct) approach is easier.

4. HALF- AND ON-SHELL BEHAVIOR OF THE COULOMB T MATRICES

In this section we discuss the half-shell behavior $p'\to k$ and the on-shell behavior $p'\to k$, $p\to k$ of the complete T_c and of all partial wave projected $T_{c,l}$, i.e., we consider

$$\langle\mathbf{p}'|T_c(k^2)|\mathbf{p}\rangle$$

and

$$\langle p'|T_{c,l}(k^2)|p\rangle,\quad l=0,\ 1,\cdots,$$

for $p'\to k$ and for $p'\to k$, $p\to k$. Obviously, k has to be (almost) real, for p' and p are real by definition. Therefore, we take, in this section only, k exactly real (and positive) and we replace k by $k+i\epsilon$ with $\epsilon>0$ [recall Eq. (6)], whenever it is important to distinguish between k and $k+i\epsilon$.

A. The functions T_c and $T_{c,l}$

We first concentrate on Eq. (19) where the complete T_c is given. The integral in the rhs exists on the condition that

$$\mathrm{Re}\, i\gamma > -1. \tag{33}$$

This restriction can be removed by replacing the integral along the real axis with a contour integral[19,20]

$$\int_0^1 dt\, t^{i\gamma}(\cdots) \;\Rightarrow\; \frac{1}{e^{-2\pi\gamma}-1}\int_C dt\, t^{i\gamma}(\cdots). \tag{34}$$

The contour C begins at $t=1+i\delta$ where the phase of t is zero, moves to the origin, circles it once and continues to $t=1-i\delta$ with $\delta \downarrow 0$. Equation (19) and (34) together give the most general expression for T_c.[32] Now we take p' equal to k in Eq. (19). Then x^2 becomes equal to one, and we see that the resulting integral in the rhs of Eq. (19)

$$\int_0^1 dt\, t^{i\gamma-1} \tag{35}$$

is divergent, because $i\gamma$ is imaginary. In this case (34) is of no help. The half-shell limit of T_c simply is not defined. In Eqs. (16), (17) this fact becomes manifest; $p' \to k$ implies $y \to 0$ (or $y \to \infty$) and it is well known that the h.f. has a branch point at infinity. In Eq. (18) the singularity is made explicit:

$$\lim_{y\to 0} y^{i\gamma} \tag{36}$$

is not defined. $T_{c,l}$ contains the same singularity. Taking $p'=k$ in Eqs. (22), (23) we get a divergent integral like (35). In the case $l=0$ we also have the more explicit formula Eq. (30); the limit $p' \to k$ here again becomes a limit like (36).

Everything we have said about $p' \to k$ applies a fortiori to the on-shell limit $p' \to k$, $p \to k$.

Finally, we remark that for $p' \to p \neq k$ there appear singularities, too. From Eq. (21) it follows that $V_{c,l}$ has a logarithmic singularity, and in Eqs. (26), (27) it can be seen that the same holds for $T_{c,l=0}$, because this h.f. has a logarithmic singularity for the argument becoming equal to one.[28–30] Concerning these singularities we found a discrepancy in the literature (see Ref. 17 of Ref. 33 and compare Ref. 34). This discrepancy seems to have been caused mainly by the mistake of Nutt.[22] See the discussion following (47). These singularities are less interesting so we will not discuss them further in this paper.

B. The distributions T_c and $T_{c,l}$

In Sec. 4A we considered T_c and $T_{c,l}$ as ordinary functions. Now we want to discuss a different approach: We consider T_c and $T_{c,l}$ as distributions (also called generalized functions). Distributions are often tacitly applied by physicists. Such applications are not restricted to the well-known Dirac delta function/distribution. For example, the Coulomb potential in momentum representation can only be obtained with the help of distributions. Straightforward derivation of Eq. (13) from Eq. (11) goes wrong because the Fourier transform of $V_c(r)$ yields a divergent integral. As is (implicitly or explicitly) done in all textbooks, one multiplies by $e^{-\epsilon r}$ and takes the limit $\epsilon \downarrow 0$ after the integration has been carried out; this procedure easily yields Eq. (13) for $\langle \mathbf{p}' | V_c | \mathbf{p} \rangle$.

Because there are several types of distributions (see Refs. 26, 27 and references quoted there), we ought to specify the particular one we are going to apply. The distribution appropriate to our purpose is in fact the same as studied by Herbst.[35] According to Herbst the pure Coulomb S matrix, usually written

$$\langle \mathbf{k} | S_c | \mathbf{k}' \rangle = \frac{\gamma}{2\pi i k}\, e^{2i\sigma_0(k)}\delta(k'^2-k^2)\left(\frac{1-\hat{\mathbf{k}}'\cdot\hat{\mathbf{k}}}{2}\right)^{-1-i\gamma}, \tag{37}$$

is undefined as it stands because it is not an integrable function. Furthermore, any extension is unique only up to a distribution with support at $\hat{\mathbf{k}}'=\hat{\mathbf{k}}$. Herbst proves that there is at most one unitary extension (in the sense of distributions) of (37) to all $\mathbf{k}'$ and $\mathbf{k}$. This extension is just given by the substitution

$$(1-\hat{\mathbf{k}}'\cdot\hat{\mathbf{k}})^{-1-i\gamma} \;\to\; \lim_{\eta\downarrow 0}(1-\hat{\mathbf{k}}'\cdot\hat{\mathbf{k}})^{\eta-1-i\gamma}. \tag{38}$$

This means that S_c is a distribution, defined by

$$\langle \mathbf{k} | S_c | f \rangle = \lim_{\eta\downarrow 0}\frac{\gamma}{2\pi i k}\, e^{2i\sigma_0(k)}\int_{R^3} d\mathbf{k}'\,\delta(k'^2-k^2) \tag{39}$$

$$\times\left(\frac{1-\hat{\mathbf{k}}'\cdot\hat{\mathbf{k}}}{2}\right)^{\eta-1-i\gamma}\langle \mathbf{k}' | f \rangle,$$

where $\langle \mathbf{k}' | f \rangle$ is a continuously differentiable and square integrable function. The so-called test functions f belonging to this type of distribution are dense in $L^2(R^3)$.

Analogous to Herbst we define the substitution

$$(\cdots)^{i\gamma} \longrightarrow \lim_{\eta\downarrow 0}(\cdots)^{\eta+i\gamma}. \tag{40}$$

We apply (40) in every situation where $i\gamma$ appears in the exponent. It is important to note that this has nothing to do with the fact that $i\gamma$ itself contains a small real part when k contains a small imaginary part according to (12). Remark that there should be, in this respect, no distinction between a repulsive force and an attractive force. Indeed, there *is* no distinction because (40) is not essentially modified when γ is replaced by $-\gamma$. The limits $\epsilon \downarrow 0$ (ϵ occurring in $k+i\epsilon$) and $\eta \downarrow 0$ are taken independently, *the latter after the former*. There is an important difference between (38) and (40) as we use it for T_c and $T_{c,l}$. In (38) the singularity is worse than a pole while the singularities in T_c and $T_{c,l}$ are much weaker than poles; in effect they are quite harmless. Therefore, the corresponding test functions are certainly dense in the Hilbert space of square integrable functions.

Applying (40) to Eqs. (16), (18) [or to Eq. (19)] we see that the half- and on-shell T_c are exactly zero. From Eq. (30) it is seen that the same fact holds for $T_{c,l=0}$. This is so because

$$\lim_{\eta\downarrow 0}\lim_{p\to k}\lim_{\epsilon\downarrow 0}\left(\frac{p-k-i\epsilon}{p+k+i\epsilon}\right)^{\eta+i\gamma}=0. \tag{41}$$

Obviously, the second and the third limit may be interchanged. Finally, in Eq. (23) z becomes equal to $(p^2+p'^2)/(2pp')$ when $p' \to k$ or when $p' \to k$, $p \to k$, and in Eq. (22) the Legendre function Q_l then becomes a constant with respect to the integration variable t, the integral becomes elementary, and the half- and on-shell $T_{c,l}$ are exactly zero for all l.

In all other (nonsingular) points convention (40) makes

no difference whatsoever. In conclusion we may say that T_c and $T_{c,l}$ are only altered in the on- and half-shell points, where they were not defined before, and in these points they become exactly zero.

Convention (40) is of considerable value because it simplifies the evaluation of our integrals, while we still know what we are doing. Interchanging the order of integrations, as for example has been done to derive Eq. (22), is now justified with the help of (40). Because all occurring integrals are absolutely convergent, the theorems of Fubini and Tonelli may be applied[36] and thus the correct evaluation is easily performed.

C. The operators T_c and $T_{c,l}$

In this section we consider T_c and $T_{c,l}$ as operators (defined in the corresponding Hilbert spaces of square integrable functions). They may be defined in terms of the resolvents

$$G_0(E) \equiv (E-H_0)^{-1}, \tag{42}$$

$$G_c(E) \equiv (E-H_0-V_c)^{-1}, \tag{43}$$

where H_0 is the kinetic energy operator. These definitions are

$$G_c = G_0 + G_0 T_c G_0, \quad G_{c,l} = G_{0,l} + G_{0,l} T_{c,l} G_{0,l}, \tag{44}$$

where the energy-dependence has been suppressed. Alternatively, they can be defined by the Lippmann–Schwinger (L–S) equations

$$T_c(E) = V_c + V_c G_0(E) T_c(E), \tag{45a}$$

$$T_{c,l}(E) = V_{c,l} + V_{c,l} G_{0,l}(E) T_{c,l}(E). \tag{45b}$$

It is essential that E is not in the spectrum of the Hamilton operators H_0 and $H_0 + V_c$, for in that case that resolvents are not defined. For E not real positive, the kernels of the L–S equations are of Hilbert–Schmidt class if the potential satisfies certain conditions.[13] This guarantees that the L–S equations have unique solutions for these potentials. Even for the Coulomb potential, the kernel $V_{c,l} G_{0,l}(E)$ is of Hilbert–Schmidt class (provided E is not positive), and therefore the solution $T_{c,l}(E)$ of equation (45b) is unique.

Writing the operators in momentum representation gives the matrix elements $\langle \mathbf{p}' | T_c(E) | \mathbf{p} \rangle$ and $\langle p' | T_{c,l}(E) | p \rangle$. They can be considered as functions of the momenta and of the energy. If the potential has short range (in a certain well defined sense), it is known that these functions are meromorphic in the complex E-plane, cut along the positive real axis. Besides bound-state poles (cf. Ref. 32) other poles can occur. The cut $0 < E < \infty$ is called the unitarity cut. The limits at the upper and lower rim of the unitarity cut exist if the potential has short range. As we have seen, the limits $k \to p$ and $k \to p'$ [cf., Eq. (5)] of the Coulomb T matrices do not exist. These additional singularities, characteristic for the Coulomb potential (and probably for other long-range potentials), are of the type $(p-k)^{i\nu}$, $(p'-k)^{i\nu}$. These singularities are clearly integrable. So if we consider $T_c|f\rangle$, where $|f\rangle$ is a Hilbert space vector,

$$\langle \mathbf{p}' | T_c(k^2) | f \rangle = \int_{R^3} d\mathbf{p}\, \langle \mathbf{p}' | T_c(k^2) | \mathbf{p} \rangle \langle \mathbf{p} | f \rangle, \tag{46}$$

we get no trouble at all in this integral because $\langle \mathbf{p}|f\rangle$, being square integrable, is locally integrable.[36] The value of $\langle \mathbf{p}' | T_c(k^2) | \mathbf{p} \rangle$ at $p = k$ is here unimportant.

Strictly speaking, the half- and on-shell points make sense only for the matrix elements, not for the operators. So we may say equally well that the half- and on-shell values of T_c and of $T_{c,l}$, considered as operators, are irrelevant.

D. Summary and discussion

We can summarize the discussion of Secs. 4A–4C as follows. When T_c and $T_{c,l}$ are considered as

$$\left\{\begin{matrix}\text{functions}\\ \text{distributions}\\ \text{operators}\end{matrix}\right\} \text{their half- and on-shell values are} \left\{\begin{matrix}\text{not defined}\\ \text{exactly zero}\\ \text{irrelevant}\end{matrix}\right\}. \tag{47}$$

In this connection it is useful to remark that in the literature considerable confusion has arisen about the half- and on-shell Coulomb T matrices. West[37] finds exactly zero for the on-shell T_c. He adds a physical interpretation: $\langle \mathbf{p}' | T_c | \mathbf{p} \rangle$ may be interpreted as the probability to scatter a free state denoted by $|\mathbf{p}\rangle$ into the free state $\langle \mathbf{p}'|$. This probability should indeed be zero because in practice one never has a free state when the pure Coulomb force acts. This is due to its long range. Nutt[22] obtained zero, too, but his derivation is wrong as was shown, e.g., by Nuttall and Stagat.[38] Shastry and Rajagopal,[33] following Nutt, also found zero for the on-shell partial wave projected $T_{c,l}$. Most authors obtain the branch-point singularities (of T_c only; to our knowledge $T_{c,l}$ is not known in explicit form). The result (47) applies as well when an arbitrary short-range *separable* potential is added to the Coulomb potential. The proof of this statement follows easily from Eqs. (48)–(58) given in the next section. We conjecture that (47) will hold also for the Coulomb potential plus an arbitrary (suitably defined) short-range potential. This can be expected because in the Fourier transform a neighborhood of the point $p = k$ is related to a neighborhood of the point $r = \infty$ (in coordinate representation). Furthermore, only the tail of the potential is important for the behavior of all relevant functions at large distances. Explicit examples of such T matrices corresponding to Coulomb-like potentials are given in the following sections.

We may understand (47) as the formal solution of the T matrix problems. However, concerning the *physical* interpretation more has to be said. This will be done in a forthcoming paper.[25] Compare also the work of Taylor[39,40] and of Marquez.[41]

5. THE TOTAL T OPERATOR

Let the potential V be the sum of two potentials V_c and V_s which are not specified for the time being,

$$V = V_c + V_s. \tag{48}$$

In the Gell-Mann—Goldberger two-potential formalism[42] it follows that the corresponding total T operator can be written[6,7]

$$T = T_c + T_{cs}, \tag{49}$$

where T_c is the T operator corresponding to V_c [cf., Eqs. (44), (45)] and T_{cs} is given by

$$T_{cs}(E) = [1 + T_c(E)G_0(E)]\, t_{cs}(E)[1 + G_0(E)T_c(E)], \tag{50}$$

where the operator $t_{cs}(E)$ satisfies the equation

$$t_{cs}(E) = V_s + V_s G_c(E) t_{cs}(E). \tag{51}$$

The resolvents G_0 and G_c have been introduced already in Eqs. (42), (43). The orbital angular momentum projections of the operators occurring in Eqs. (48)–(51) satisfy these same equations.

Now we specify the operators V_c and V_s. Let V_c be the Coulomb potential [given by Eq. (11) or (13)] and let V_s be an operator of finite rank N (also called an N-term separable potential), which works only in a subspace corresponding to one particular value of the orbital angular momentum l,

$$V_s = -\sum_{i=1}^{N} |g_i\rangle \lambda_i \langle g_i|. \tag{52}$$

In Eq. (52) the projection operator projecting onto the lth partial wave space and the corresponding subscripts l are suppressed. The same is done in the rest of this section. The λ_i are real numbers in order that V_s be Hermitian. Time reversal invariance requires that $\langle p|g_i\rangle$ and $\langle r|g_i\rangle$ are real functions of p and r, respectively. It is well known that the T operator T_s corresponding to the separable potential V_s is separable itself and may be written

$$T_s(E) = -\sum_{i,j=1}^{N} |g_i\rangle \tau_{ij}(E) \langle g_j|. \tag{53}$$

Here the $N \times N$ matrix τ is defined via its inverse:

$$(\tau^{-1}(E))_{ij} \equiv (\Lambda^{-1})_{ij} + \langle g_i | G_0(E) | g_j \rangle, \tag{54}$$

where Λ is a diagonal matrix with elements $\lambda_i \delta_{ij}$. Now $T_s(E)$ is the unique solution of the equation

$$T_s(E) = V_s + V_s G_0(E) T_s(E). \tag{55}$$

Also Eq. (51) has a unique solution. The uniqueness follows almost trivially from the fact that V_s is of finite rank. Because of the resemblance of Eq. (51) to Eq. (55), we can write down the solution of Eq. (51) at once: All we have to do is replace G_0 by G_c in Eqs. (53), (54). Thus in terms of the Coulomb-modified (energy-dependent) form factors $|g_i^c(E)\rangle$ defined by

$$|g_i^c(E)\rangle \equiv (1 + T_c(E)G_0(E))\, |g_i\rangle, \tag{56}$$

we obtain our final result for T_{cs} [cf., Eq. (50)],

$$T_{cs}(E) = -\sum_{i,j=1}^{N} |g_i^c(E)\rangle\, \tau_{ij}^c(E) \langle g_j^c(E^*)|, \tag{57}$$

with

$$(\tau^c(E))_{ij}^{-1} \equiv (\Lambda^{-1})_{ij} + \langle g_i | G_c(E) | g_j \rangle. \tag{58}$$

Equation (44) and definition (56) imply the useful identity

$$G_0(E)\, |g_i^c(E)\rangle \equiv G_c(E)\, |g_i\rangle. \tag{59}$$

It is clear from Eqs. (49), (56)—(58) that the total T matrix has been obtained in closed form, once we have derived explicit expressions for $\langle p|g_i^c\rangle$ and for $\langle g_i|G_c|g_j\rangle$. This is what we are going to do in the next sections, for some simple form factors $|g_i\rangle$ in $l=0$ partial wave space.

6. THE COULOMB MODIFIED FORM FACTORS $\langle p|g^c\rangle$

From now on we consider only the case $l=0$ and we suppress the subscript l throughout. The form factors $\langle p|g\rangle$ are supposed to be rational functions of p^2. The simplest rational function that is physically acceptable as form factor is the Yamaguchi[23] one

$$\langle p|g_\beta\rangle = \sqrt{2/\pi}\ \frac{1}{p^2+\beta^2}. \tag{60}$$

Differentiation with respect to the parameter β yields (apart from a trivial factor)

$$\langle p|g_{\beta\beta}\rangle = \sqrt{2/\pi}\ \frac{1}{(p^2+\beta^2)^2}. \tag{61}$$

In coordinate representation one has

$$\langle r|g_\beta\rangle = e^{-\beta r}/r, \tag{62}$$

$$\langle r|g_{\beta\beta}\rangle = e^{-\beta r}/(2\beta). \tag{63}$$

We obtain the Coulomb-modified form factor

$$\langle p|g_\beta^c(k^2)\rangle = \langle p|(1+T_c(k^2)G_0(k^2))|g_\beta\rangle \tag{64}$$

in closed form with the help of Eqs. (26), (27), and (15). The result is a double integral of the type

$$\int_0^\infty dp' \int_0^\infty dt \cdot \cdot \frac{1}{p'} \times \left(\frac{1}{1-ta'a} - \frac{1}{1-ta'/a} + \frac{1}{1-t/(a'a)} - \frac{1}{1-ta/a'}\right), \tag{65}$$

where as before $a = (p-k)/(p+k)$, $a' = (p'-k)/(p'+k)$, [Eqs. (28), (29)]. The four terms of the integrand in Eq. (65) are taken two by two; the integrand then appears to be a function of $(p')^2$. Interchanging the order of the integrations (this is permitted according to Sec. 4B), one easily performs the integration $\int dp'$. The remaining integral $\int dt$ is again an h.f.. The actual derivation is given at the end of this section. In advance we give here the final result

$$\langle p|g_\beta^c(k^2)\rangle = \frac{\sqrt{2/\pi}}{\beta^2+p^2} - \frac{\sqrt{2/\pi}}{\beta^2+k^2}\ \frac{k}{p}\,[F_{i\gamma}(Ba) - F_{i\gamma}(B/a)], \tag{66}$$

where

$$B \equiv (\beta + ik)/(\beta - ik). \tag{67}$$

In addition, we introduced here the notation

$$F_{i\gamma}(z) \equiv {}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ z) \tag{68}$$

which we shall use from now on in this paper. Equation (66) can be converted into [e.g. with the help of Eq. (85)]

$$\langle p|g^c_\beta(k^2)\rangle = \frac{1}{2p(\beta-ik)}\frac{\sqrt{2/\pi}}{1+i\gamma} \times\left(\frac{p-k}{\beta-ip}\,{}_2F_1(1,\ i\gamma;\ 2+i\gamma;\ B\alpha) + \frac{p+k}{\beta+ip}\,{}_2F_1(1,\ i\gamma;\ 2+i\gamma;\ B/\alpha)\right). \tag{69}$$

In Eq. (69) a result of Zachary[5] and of Bajzer[6] is reproduced. [Note the misprint in Eq. (49) of Ref. 6; the argument $(B\alpha)^{-1}$ of the h.f. mentioned there should be B/α (in our notation)] The h.f.'s occurring in Eq. (69) differ from the h.f. in (68) with regard to their third parameter. More generally, we meet in this game several different h.f.'s which all have one common property, i.e., they are of the type

$${}_2F_1(\lambda,\ \mu-1+i\gamma;\ \nu+\mu-1+i\gamma;\ z),\quad \lambda,\ \mu,\ \nu=1,\ 2,\ \cdots. \tag{70}$$

All these functions can be expressed in any one representative of the class (70) plus rational functions of z. This can be proven with the help of their integral representations.[28] We chose already ${}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ z)$ as a simple and convenient representative [see (68)]. This has the additional advantage that it facilitates the comparison of different expressions for the same object, such as in Eqs. (66) and (69). Therefore, $F_{i\gamma}$ will be our standard hypergeometric function throughout this paper.

The derivative of the standard h.f. $F_{i\gamma}$ can also be written in terms of $F_{i\gamma}$ and rational functions. The following equality is easily established:

$$\frac{d}{dz}F_{i\gamma}(z) = \frac{i\gamma}{z}\left(\frac{1}{1-z} - F_{i\gamma}(z)\right). \tag{71}$$

Utilizing (71) we obtain from (66) by differentiation with respect to β [cf. (61)]

$$\langle p|g^c_{\beta\beta}(k^2)\rangle = \sqrt{2/\pi}\left(\frac{1}{(\beta^2+p^2)^2} + \frac{k\gamma/\beta}{(\beta^2+p^2)(\beta^2+k^2)} - \frac{1+k\gamma/\beta}{(\beta^2+k^2)^2}\,\frac{k}{p}\,[F_{i\gamma}(B\alpha) - F_{i\gamma}(B/\alpha)]\right). \tag{72}$$

The rest of this section is devoted to the derivation of Eq. (66). The reader who is not interested in the details of the proof can immediately go on to Sec. 7. We calculate the integral in the rhs of the following equation:

$$\langle p|T_c(k^2)G_0(k^2)|g_\beta\rangle = -\sqrt{2/\pi}\int_0^\infty dp' p'^2\,\frac{\langle p|T_c(k^2)|p'\rangle}{(p'^2+\beta^2)(p'^2-k^2)}. \tag{73}$$

Substitute for $\langle p|T_c|p'\rangle$ Eqs. (26), (27), utilize the integral representation of the h.f. Eq. (15), and interchange the order of the two integrations, then one obtains

$$\langle p|T_c(k^2)G_0(k^2)|g_\beta\rangle = \sqrt{2/\pi}\,\frac{k\gamma}{\pi p}\int_0^1 dt\, t^{i\gamma-1} \times\int_0^\infty \frac{dp' p'}{(p'^2+\beta^2)(p'^2-k^2)} \times\left(\frac{1}{1-t\alpha(p'-k)/(p'+k)}\ \ \frac{1}{1-t\alpha(p'+k)/(p'-k)}\right) + (\text{idem, with } p\to -p \text{ thus } \alpha\to 1/\alpha). \tag{74}$$

The integral $\int dp'$ in Eq. (74) can be simplified utilizing the variable x defined by

$$x \equiv k(1+t\alpha)/(1-t\alpha), \tag{75}$$

where $\mathrm{Im}\,x > 0$ holds because $\mathrm{Im}\,k > 0$ This integral then appears to be an elementary one; we get

$$\int_0^\infty dp'\cdots \text{ in (74)} = \frac{-4kt\alpha}{(1-t\alpha)^2}\int_0^\infty \frac{dp'p'^2}{(p'^2+\beta^2)(p'^2-k^2)(p'^2-x^2)} = \frac{-4kt\alpha}{(1-t\alpha)^2}\,\frac{i\pi/2}{(\beta-ik)(\beta-ix)(k+x)}. \tag{76}$$

From (75) we have

$$\beta - ix = (\beta-ik)(1-tB\alpha)/(1-t\alpha),\qquad k+x = 2k/(1-t\alpha), \tag{77}$$

so that the factors $(1-t\alpha)$ occurring in the integral $\int dl\cdots$ drop out, and this integral appears to be again an h.f. ${}_2F_1$ according to

$$\int_0^1 dl\,\frac{l^{i\gamma}}{1-tB\alpha} = \frac{1}{1+i\gamma}\,{}_2F_1(1,\ 1+i\gamma;\ 2+i\gamma;\ B\alpha). \tag{78}$$

This h.f. is reduced to the standard $F_{i\gamma}$ by means of

$$F_{i\gamma}(z) \equiv {}_2F_1(1, i\gamma;\ 1+i\gamma;\ z) = 1 + \frac{i\gamma z}{1+i\gamma} \times {}_2F_1(1,\ 1+i\gamma;\ 2+i\gamma,\ z). \tag{79}$$

Performing all this in Eq. (74), we get the final result

$$\langle p|T_c(k^2)G_0(k^2)|g_\beta\rangle = \frac{-k\sqrt{2/\pi}}{p(\beta-ik)^2}\cdot\frac{i\gamma}{1+i\gamma} \tag{80}$$

$$\times[\alpha\ {}_2F_1(1,1+i\gamma;2+i\gamma;\ B\alpha) - 1/\alpha\ {}_2F_1(1,1+i\gamma;2+i\gamma;\ B/\alpha)]$$

$$= -\frac{\sqrt{2/\pi}}{\beta^2+k^2}\,\frac{k}{p}\,[F_{i\gamma}(B\alpha) - F_{i\gamma}(B/\alpha)]. \tag{81}$$

Equation (81) proves Eq. (66).

7. THE IN-PRODUCTS $\langle g|G_c|g\rangle$

In this section we obtain analytic expressions for the in-products $\langle g_i|G_c|g_j\rangle$ occurring in the T_{cs}-formula, cf. Eqs. (57), (58). The operators V_s and T_{cs} are fixed once we have fixed the N form factors $|g_i\rangle$, $i=1,\ \ldots,\ N$ (plus λ_i and the energy, of course). We suppose that these form factors are of the type (60) and/or (61); their parameters β are possibly different. Because "cross products" $\langle g_i|G_c|g_j\rangle$ with $i\neq j$ occur, we have to calculate three different expressions, namely, $\langle g_\alpha|G_c|g_\beta\rangle$, $\langle g_{\alpha\alpha}|G_c|g_\beta\rangle$, and $\langle g_{\alpha\alpha}|G_c|g_{\beta\beta}\rangle$ where α and β are independent parameters. From these three, all possible combinations can be made. Obviously this is sufficient to obtain T_{cs} in closed form [in combination with Eqs. (66) and (72)].

The derivation of $\langle g_\alpha|G_c|g_\beta\rangle$ is given at the end of this section. It has to be noted that one could start with Eq. (66), because from Eq. (59) one has the identity

$$\langle g_i|G_c(k^2)|g_j\rangle \equiv \langle g_i|G_0(k^2)|g^c_j(k^2)\rangle, \tag{82}$$

We obtain

$$\langle g_\alpha | G_c(k^2) | g_\beta \rangle = \frac{-{}_2F_1(1, i\gamma; 2+i\gamma; AB)}{(1+i\gamma)(\alpha+\beta)(\alpha-ik)(\beta-ik)}, \tag{83}$$

with

$$A \equiv (\alpha+ik)/(\alpha-ik), \quad B \equiv (\beta+ik)/(\beta-ik). \tag{84}$$

Taking $\alpha=\beta$ in Eq. (83) we reproduce the result of Zachary.[5] Utilizing the relation

$$\frac{1}{1+i\gamma}\,{}_2F_1(1,\ i\gamma;\ 2+i\gamma;\ z) = 1/z + (1-1/z)F_{i\gamma}(z), \tag{85}$$

Eq. (83) can be converted into an equation where $F_{i\gamma}$ is the only nonelementary function,

$$\langle g_\alpha | G_c(k^2) | g_\beta \rangle = \frac{-1}{(\alpha+\beta)(\alpha+ik)(\beta+ik)} - \frac{2ik}{(\alpha^2+k^2)(\beta^2+k^2)} F_{i\gamma}(AB). \tag{86}$$

Differentiation of Eq. (86) with respect to α, β and utilizing Eq. (71) yields the final results

$$\langle g_{\alpha\alpha} | G_c(k^2) | g_\beta \rangle = \frac{1}{2\alpha(\alpha+\beta)^2(\alpha^2+k^2)} - \frac{\alpha+k\gamma}{\alpha(\alpha+\beta)(\alpha+ik)(\beta+ik)(\alpha^2+k^2)} - \frac{2ik(\alpha+k\gamma)}{\alpha(\alpha^2+k^2)^2(\beta^2+k^2)} F_{i\gamma}(AB) \tag{87}$$

and

$$\langle g_{\alpha\alpha} | G_c(k^2) | g_{\beta\beta} \rangle = \frac{\alpha^2+\alpha\beta+\beta^2+k^2+k\gamma(\alpha+\beta)}{2\alpha\beta(\alpha+\beta)^3(\alpha^2+k^2)(\beta^2+k^2)} - \frac{(\alpha+k\gamma)(\beta+k\gamma)}{\alpha\beta(\alpha+\beta)(\alpha+ik)(\beta+ik)(\alpha^2+k^2)(\beta^2+k^2)} - \frac{2ik(\alpha+k\gamma)(\beta+k\gamma)}{\alpha\beta(\alpha^2+k^2)^2(\beta^2+k^2)^2} F_{i\gamma}(AB), \tag{88}$$

Now we give the proof of Eq. (83), or alternatively of Eq. (86). According to Eq. (81), we may write

$$\langle g_\alpha | G_0(k^2) T_c(k^2) G_0(k^2) | g_\beta \rangle = \int_0^\infty dp\, \frac{p^2}{(p^2+\alpha^2)(p^2-k^2)} \times \frac{2k}{\pi p}\, \frac{i\gamma}{\beta^2+k^2} \int_0^1 dl\, l^{i\gamma-1} \left(\frac{1}{1-lBa} - \frac{1}{1-lB/a} \right). \tag{89}$$

Define the variable y,

$$y \equiv k\, \frac{1+lB}{1-lB}, \tag{90}$$

interchange the order of the two integrations (cf. Sec. 4B) and recall from Eq. (28) that

$$a - 1/a = -4pk/(p^2-k^2), \tag{91}$$

$$a + 1/a = 2(p^2+k^2)/(p^2-k^2), \tag{92}$$

then one arrives at the following formula which shows a strong resemblance to Eq. (76):

$$\langle g_\alpha | G_0(k^2) T_c(k^2) G_0(k^2) | g_\beta \rangle = \frac{-8k^2B}{\pi(\beta^2+k^2)} \times i\gamma \int_0^1 \frac{dl\, l^{i\gamma}}{(1-lB)^2} \int_0^\infty \frac{dp\, p^2}{(p^2+\alpha^2)(p^2-k^2)(p^2-\gamma^2)}. \tag{93}$$

So this derivation runs along the same lines as the derivation of Eq. (66) in Sec. 6. The integration $\int dp$ gives in analogy to Eq. (76) a factor $(\alpha - iy)$ that can be written

$$\alpha - iy = (\alpha - ik)(1-lAB)/(1-lB) \tag{94}$$

The factors $(1-lB)$ cancel and one obtains

$$\langle g_\alpha | G_0(k^2) T_c(k^2) G_0(k^2) | g_\beta \rangle = \frac{2k\gamma}{(\alpha-ik)^2(\beta-ik)^2} \int_0^1 dl\, \frac{l^{i\gamma}}{1-lAB}. \tag{95}$$

With the help of Eqs. (78), (79), and (82), Eqs. (83) and (86) follow easily from Eq. (95).

8. T MATRIX FOR COULOMB PLUS ARBITRARY $l=0$ RATIONAL SEPARABLE POTENTIAL

We call a potential of the form

$$V_c = \sum_{i=1}^{N} |g_i\rangle \lambda_i \langle g_i|,$$

where the form factors $|g_i\rangle$ in momentum representation, $\langle p | g_i \rangle$,

1. are real rational functions of p^2,
2. are zero at infinity, (96)
3. and have no poles on the positive axis $0 \le p^2 < \infty$,

a *rational separable potential*. Any such form factor can be written (for some $\nu = 1, 2, \cdots$)

$$\langle p | g_{\{\beta\}} \rangle \equiv \frac{P(p^2)}{(p^2+\beta_1^2)(p^2+\beta_2^2)\cdots(p^2+\beta_\nu^2)}, \tag{97}$$

where P is some (real) polynomial of degree smaller than ν. Its realness follows from the fact that the form factor is real. The denominator of the rhs of definition (97) is real, too, but the β's may be complex. They can and will always be chosen such that they satisfy

$$\mathrm{Re}\,\beta_n > 0, \quad n = 1, \ldots, \nu. \tag{98}$$

These parameters β_n need not all be different. The notation in definition (97) is such that the symbol $\{\beta\}$ stands for $(\beta_1, \ldots, \beta_\nu)$. In (61) we had the particular case $\nu=2$, we took $\beta_1=\beta_2=\beta$ and the polynomial P was taken constant there. Our potential is built up from N form factors $|g_i\rangle$, $i=1, \ldots, N$. Each form factor has the form (97), but possibly with a different set of β's, e.g.,

$$\beta_{i,1},\ \beta_{i,2}, \cdots, \beta_{i,\nu_i} \quad \text{for each } i = 1, \ldots, N.$$

This more complete notation is cumbersome and would not clarify our formulas so we will not use it. We suppress the index i when the deal with the general form factors $|g\rangle$.

Recalling the discussion following (65), it becomes clear that we need in effect integrals of the type

$$\int_0^\infty dp\, P(p^2) \prod_{n=1}^{s} (p^2+\beta_n^2)^{-1}. \tag{99}$$

Quite a lot of such integrals are known in closed form.[43,44] Moreover, the general structure can easily be found. In this way one can derive the desired formulas for the $\langle p | g^c \rangle$'s and for the $\langle g | G_c | g \rangle$'s. This will be done at

the end of this section. We give the final results here in advance:

$$\langle p|g^{\gamma}_{\{\beta\}}(k^2)\rangle = R_0(p^2) + \sum_{n=1}^{\nu} R_n(p^2)\,\frac{1}{p}[F_{i\gamma}(B_n a) - F_{i\gamma}(B_n/a)] \tag{100}$$

and

$$\langle g_{\{\alpha\}}|G_c(k^2)|g_{\{\beta\}}\rangle = R_{00} + \sum_{m=1}^{\mu}\sum_{n=1}^{\nu} R_{mn}F_{i\gamma}(A_m B_n), \tag{101}$$

where as before $a=(p-k)/(p+k)$, and in analogy to Eq. (84) [cf. Eq. (120)]

$$A_m \equiv (\alpha_m + ik)/(\alpha_m - ik), \quad m=1, 2, \ldots, \mu, \tag{102}$$

$$B_n \equiv (\beta_n + ik)/(\beta_n - ik), \quad n=1, 2, \ldots, \nu. \tag{103}$$

R_0 and R_n are rational functions of k, γ, $\beta_1, \ldots, \beta_\nu$, p^2. R_{00} and R_{mn} are rational functions of k, γ, $\beta_1, \ldots, \beta_\nu$, $\alpha_1, \ldots, \alpha_\mu$.

The T matrix corresponding to a rational separable potential plus the Coulomb potential is given by Eqs. (49), (57), (58) and (100), (101). The important point is that, apart from rational functions, only the h.f. $F_{i\gamma}$ shows up in the final expressions for T. The arguments occurring in $F_{i\gamma}$ can easily be found. They are exclusively defined by the *poles* of all form factors involved (and by k and p of course), as can be seen from the Eqs. (26), (27), (97), (100)–(103), and (120).

The remaining part of this section is entirely devoted to the derivation of Eqs. (100) and (101). The proof of these equations is in fact a generalization of the proofs given in Secs. 6 and 7, respectively.

We start with the integral

$$^{(s)}I \equiv \int_0^\infty dp\, p^2 \prod_{n=1}^{s} (p^2+\beta_n^2)^{-1}, \quad s=2, 3, 4, \cdots, \tag{104}$$

where

$$\mathrm{Re}\,\beta_n > 0 \quad \text{for } n=1, 2, \ldots, s. \tag{105}$$

The following result holds[44]

$$^{(s)}I = \frac{\pi}{2} P_s(\beta_1, \ldots, \beta_s) \prod_{m<n=1}^{s} (\beta_n+\beta_m)^{-1}. \tag{106}$$

Here P_s is a symmetric homogeneous polynomial in the variables $(\beta_1 \ldots, \beta_s)$. *Its degree is* $\frac{1}{2}(s-2)(s-3)$, *but the* highest power of any one of the β's is $s-3$ if $s>2$, and for $s=2$ this power is zero. Explicitly we have for the first three polynomials

$$P_2 = P_3 = 1, \tag{107}$$

$$P_4 = \beta_1+\beta_2+\beta_3+\beta_4. \tag{108}$$

With the generalized Yamaguchi form factor

$$\langle p|g_{\{\beta\}}\rangle = \prod_{n=1}^{\nu} (p^2+\beta_n^2)^{-1}, \tag{109}$$

which is a special case of (97), we get in the same way as in Sec. 6

$$\langle p|T_c(k^2)G_0(k^2)|g_{\{\beta\}}\rangle = -\frac{4k^2\gamma}{\pi p}\int_0^1 \frac{dt\, t^{i\nu}a}{(1-ta)^2}$$

$$\times \int_0^\infty \frac{dp' p'^2}{(p'^2-k^2)(p'^2-x^2)(p'^2+\beta_1^2)\cdots(p'^2+\beta_\nu^2)}$$

$$+ (\text{idem, with } p\to -p \text{ thus } a\to 1/a). \tag{110}$$

As before the variable x is given by $x/k=(1+ta)/(1-ta)$, where $\mathrm{Im}\,x>0$ holds because of $\mathrm{Im}\,k>0$. Application of Eq. (106) gives for the integral $\int dp'$ in the rhs of Eq. (110) the expression

$$\frac{i\pi}{4k}$$

$$\times \frac{(1-ta)P_{\nu+2}(-ix, -ik, \beta_1, \ldots, \beta_\nu)}{(\beta_1-ix)\cdots(\beta_\nu-ix)(\beta_1-ik)\cdots(\beta_\nu-ik)(\beta_1+\beta_2)\cdots(\beta_{\nu-1}+\beta_\nu)} \tag{111}$$

where the polynomial $P_{\nu+2}$ contains at most terms with $x^{\nu-1}$. It contains no terms with higher powers of x. In analogy to Eq. (77) we have

$$\beta_n - ix = (\beta_n - ik)(1-taB_n)/(1-ta). \tag{112}$$

Multiply numerator and denominator of expression (111) by the factor $(1-ta)^\nu$. The polynomial $P_{\nu+2}$ then becomes a polynomial in the variables $(ta, k, \beta_1, \ldots, \beta_\nu)$, and the numerator contains further a factor $(1-ta)^2$. The denominator becomes a product of the factors $(1-taB_n)$ and of the factors $(\beta_n-ik)^2(\beta_n+\beta_m)$ with $m<n=1, 2, \ldots, \nu$.

In the rhs of Eq. (110) we see a factor $(1-ta)^2$ in the denominator, so this factor cancels. Equation (110) then simplifies considerably; we get

$$\langle p|T_c(k^2)G_0(k^2)|g_{\{\beta\}}\rangle$$

$$= \frac{1}{(\beta_1-ik)^2\cdots(\beta_\nu-ik)^2(\beta_1+\beta_2)\cdots(\beta_{\nu-1}+\beta_\nu)}$$

$$\times \frac{k\gamma}{ip}\int_0^1 dt\, \frac{a t^{i\nu} P''_{\nu+2}(ta, k, \beta_1, \ldots, \beta_\nu)}{(1-taB_1)\cdots(1-taB_\nu)}$$

$$+ (\text{idem, with } p\to -p \text{ thus } a\to 1/a). \tag{113}$$

For $\nu=1$ the polynomial $P''_{\nu+2}$ is just 1, and Eq. (113) reduces to Eq. (80), apart from a factor $\sqrt{2/\pi}$.

The denominator of the integrand in Eq. (113) can be written in partial fractions. Then we get a sum of ν terms as follows:

$$\prod_{n=1}^{\nu}(1-taB_n)^{-1} = \sum_{n=1}^{\nu} P'_n/(1-taB_n), \tag{114}$$

where the P'_n are certain polynomials of $(ta, B_1, \ldots, B_\nu)$. Now we know[28]

$$\int_0^1 dt\, t^{i\gamma-1}\,\frac{t^\lambda}{1-tz} = \frac{1}{\lambda+i\gamma}\,{}_2F_1(1, \lambda+i\gamma; \lambda+1+i\gamma; z),$$

$$\lambda = 0, 1, \cdots. \tag{115}$$

Furthermore, iteration of Eq. (79) yields

$$F_{i\gamma}(z) = 1 + \frac{i\gamma z}{1+i\gamma} + \cdots + \frac{i\gamma z^{\lambda-1}}{\lambda-1+i\gamma} + \frac{i\gamma z^\lambda}{\lambda+i\gamma}F_{\lambda+i\gamma}(z); \tag{116}$$

recall from Eq. (68) the notation

$$F_{\lambda+i\gamma}(z) \equiv {}_2F_1(1, \lambda+i\gamma; \lambda+1+i\gamma; z). \tag{68'}$$

This implies that the integral

$$\int_0^1 dl\, l^{i\gamma-1}(la)^\lambda/(1-laB_n) \tag{117}$$

can be written in terms of $F_{i\gamma}(aB_n)$ plus rational functions, for $\lambda = 0, 1, \cdots$. The same holds then if the factor $(la)^\lambda$ in the integrand of (117) is replaced by an arbitrary polynomial of la, like we have from Eqs. (113), (114). Applying all this to Eq. (113) we get the result

$$\langle p|\, T_c(k^2)G_0(k^2)\,|g_{\{\beta\}}\rangle = r_0 + \sum_{n=1}^{\nu} r_n \frac{1}{p} \times [F_{i\gamma}(B_n a) - F_{i\gamma}(B_n/a)], \tag{118}$$

where r_0 and the r_n are rational functions of $(p^2, k, \gamma, \beta_1, \ldots, \beta_\nu)$. They are functions of p^2 (and not only of p) because $\langle p|\, T_c G_0|g\rangle$ is *even* in p.

Now that we have evaluated this expression where the form factor is given by Eq. (109), it is only one step further to prove Eq. (118) for a form factor that is an arbitrary rational function of p^2 [see definition (97)]. Write any term $p^{2\lambda}$ occurring in the polynomial in (97) as

$$p^{2\lambda} = p^{2\lambda-2}(p^2 + \beta_1^2 - \beta_1^2). \tag{119}$$

The term containing the factor $(p^2 + \beta_1^2)$ is then reduced by dividing that factor out. Iteration of this procedure reduces the exponent to zero, so any rational form factor can be reduced to a sum of form factors of the type given in Eq. (109). Therefore, Eq. (118) holds for an arbitrary rational form factor, and Eq. (100) has been proven.

The proof of Eq. (101) which we shall give now is not essentially different in structure from the one just given for Eq. (100). With the form factor

$$\langle p|\, g_{\{\alpha\}}\rangle = \prod_{m=1}^{\mu} (p^2 + \alpha_m^2)^{-1}, \tag{120}$$

we have [cf. Eqs. (118) and (15)]

$$\langle g_{\{\alpha\}}|\, G_0(k^2)T_c(k^2)G_0(k^2)\,|g_{\{\beta\}}\rangle = r_{00} - \sum_{n=1}^{\nu} \int_0^\infty dl \int_0^\infty dp \times \frac{p^2 r_n(p^2)}{(p^2-k^2)(p^2+\alpha_1^2)\cdots(p^2+\alpha_\mu^2)} \frac{i\gamma l^{i\gamma-1}}{p} \times \left(\frac{1}{1-lB_n a} - \frac{1}{1-lB_n/a}\right) \tag{121}$$

Here r_{00} is a rational function of $(k, \gamma, \alpha_m, \beta_n)$ with $m = 1, \ldots, \mu$; $n = 1, \ldots, \nu$. As in (90) define

$$y_n \equiv k(1 + lB_n)/(1 - lB_n), \tag{122}$$

in terms of which Eq. (121) reads

$$\langle g_{\{\alpha\}}|\, G_0(k^2)T_c(k^2)G_0(k^2)\,|g_{\{\beta\}}\rangle = r_{00} + 4ik\gamma \sum_{n=1}^{\nu} \int_0^1 dl\, l^{i\gamma-1} \frac{lB_n}{(1-lB_n)^2} \times \int_0^\infty \frac{dp\, p^2 r_n(p^2)}{(p^2-k^2)(p^2-y_n^2)(p^2+\alpha_1^2)\cdots(p^2+\alpha_\mu^2)}. \tag{123}$$

Utilizing

$$\alpha_m - iy_n = (\alpha_m - ik)(1 - lA_mB_n)/(1 - lB_n), \tag{124}$$

and recalling the discussion following Eq. (110), one finds that all factors $(1-lB_n)$ cancel. The denominator of the integrand in the integral $\int dl$ then contains only factors $(1-lA_mB_n)$ and other factors that are constant with respect to the variable of integration l. The product of these factors can be written as a sum by means of partial fractions just as in Eq. (114),

$$\prod_{m=1}^{\mu} \frac{1}{1-lA_mB_n} = \sum_{m=1}^{\mu} \frac{P'_m}{1-lA_mB_n}, \tag{125}$$

where the P'_m are polynomials in $(lB_n, A_1, \ldots, A_\mu)$. Thus we get again integrals of the type (117). All these integrals are then transformed into rational functions of $(k, \gamma, \alpha_1, \ldots, \alpha_\mu, \beta_1, \ldots, \beta_\nu)$ and the h.f.'s $F_{i\gamma}(A_mB_n)$. Then the same result is valid if one takes arbitrary rational form factors $g_{\{\alpha\}}$ instead of the form factors of Eq. (120). Finally, for G_c the same holds as for $G_0T_cG_0$ according to Eq. (10). This completes the proof of Eq. (101).

9. SUMMARY AND DISCUSSION

We discussed and resolved the half- and on-shell problems which occur in the T matrices (in complete three-dimensional space and in the partial wave spaces $l = 0, 1, \cdots$, respectively) of any Coulomb-like potential $V = V_c + V_s$ where V_s is an arbitrary short-range separable potential (Sec. 4). In Secs. 5–7 we obtained exact explicit formulas for off-shell T matrices corresponding to several Coulomb-plus-rational-separable potentials (for $l = 0$ only). To this end, we first derived in Sec. 3 the pure Coulomb $T_{c,l=0}$ from a known expression for the complete T_c in three-dimensional space. Equations (26), (27), and (30) give two equivalent explicit formulas for $T_{c,l=0}$. Finally, in Sec. 8 we derived a general formula for the off-shell T matrix corresponding to any member of the very large class of potentials consisting of the Coulomb potential plus an arbitrary rational separable potential, as defined in (96). Apart from rational functions, the final expressions [Eqs. (100) and (101)] contain only the h.f. ${}_2F_1(1, i\gamma; 1 + i\gamma; \cdot)$ where γ is the well-known Coulomb parameter.[12]

As for the physical relevance of the obtained formulas, we like to discuss some important points.

In scattering experiments with charged particles one often deals with the combination of the Coulomb interaction plus some short-range interaction. For example, nonrelativistic models for proton–proton scattering have a short-range potential built in to account for the strong interaction, the Coulomb potential taking care of the charges. The strong interaction here is almost completely unknown at very short distance (< 1 fm), so one looks for a phenomenological fit. The model potential may then be (partly) local or nonlocal (e.g. separable); often one takes the sum of a local potential (for the longer distances) and a nonlocal separable potential (for the short distances). Moreover, as we said already in the introduction, any local short-range potential can be approximated by an N-term separable potential in a mathematically well-defined sense. This explains and justifies our interest in a general kind of separable potential.

Due to the long range of the Coulomb potential, diffi-

culties occur in the theoretical description of the scattering. As we said before, the physical scattering amplitude is (in conventional short-range potential scattering theory) just the on-shell T matrix, apart from a simple factor. This cannot be the case in long-range potential scattering theory, because the on-shell limit is not defined then, as is known (compare Sec. 4). We repeat that this trouble is unaffected by any short-range potential; it is only the Coulomb potential that generates the problems.

As a way out of these problems it has been proposed to screen the Coulomb potential; eventually this screening is then removed by letting the screening radius go to infinity.[1,8-11,45] Since some time this approach can be interpreted in a rather satisfactory way[40,46] at least for two-particle scattering. In practice, of course, one always has screening at some very large distance. But even then it could be questionable whether one is allowed to apply conventional short-range scattering theory; the range of the potential is (very) large, though not infinite. This is a delicate question. Moreover, the screening approach is hampered by the fact that the scattering formulas (T matrices and the like) are not known analytically in general, and they are much more difficult to obtain. Screening can also be applied as long as it appears useful in singular expressions (cf. Refs. 7, 47, 48). This is implicitly done in the application of the on-shell Gell-Mann–Goldberger[12] two-potential formula to Coulomb-like potentials (cf. Ref. 6). The long-range troubles have often caused inaccuracies and inconsistencies in the past. In Sec. 4 we mentioned a few examples of such inconsistencies we found in the literature. Here we give some more. The Coulomb scattering state is often written (e.g. Refs. 17, 7)

$$|\mathbf{k}\pm\rangle_c = (1 + G_c(k^2 \pm i\epsilon)V_c)|\mathbf{k}\rangle, \tag{126}$$

where G_c is the Coulomb Green's function. Although the formula analogous to (126) for a short-range potential is correct, (126) is at least inaccurate because the limit of $G_c(k^2 \pm i\epsilon)$ for $\epsilon \to 0$ is not clearly defined. Related to this we have the equation (see, e.g., Refs. 1, 21, 49)

$$\langle \mathbf{p}'|T_c|\mathbf{p}\rangle = \langle \mathbf{p}'|V_c|\mathbf{p}+\rangle_c. \tag{127}$$

This equation is known to be correct when V has short range, but it is inaccurate, to say the least, when V is the Coulomb potential because the half-shell limit of T_c which is implicitly understood in Eq. (127) is not defined. In fact, we claim that the T_c given by Eq. (127) is *not* the conventional T_c defined by the (off-shell-) Eq. (10),

$$G_c(E) = G_0(E) + G_0(E)T_c(E)G_0(E).$$

To summarize one has:

(i) Exact analytic formulas without application of screening, but in such a situation no satisfactory physical interpretation is known.

(ii) A rather satisfactory interpretation when screening is applied, but in general no analytic formulas are known then. There might be problems also in this case because the range is (very) large though not infinite.

This whole problem can be attacked in a rigorous manner to obtain a correct physical interpretation without the application of screening. All formulations then have to be set in an appropriate distribution-theoretic framework. Our approach is in a certain sense akin to the work of Herbst,[35] Taylor,[40] and Prugovečki and Zorbas.[50] We shall discuss this problem in a subsequent paper.[25] In this connection we note that Sec. 4 of the present paper solves only the *formal* difficulties as we found them in the literature. This is just a first step in the process to obtain the complete solution.

With the approach just mentioned we can in principle derive the desired physical quantities from the T matrix formulas obtained in the present paper, for example, amplitudes and effective range parameters. In advance we report here already that we found a means of obtaining the scattering length a_{cs} and the effective range r_{cs} in closed form for *all* our potentials. For the simplest one of our potentials, namely, Coulomb plus Yamaguchi, these two parameters have been obtained (i) by Harrington[1] in first order perturbation, (ii) by Ali and Rahman and Husain[51] purely numerically. It appears that the first order approximation of our result agrees exactly with the formulas derived by Harrington. The numerical results of Ref. 51 also agree with our closed formulas. More details about this subject will be reported.[25]

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SCATTERING LENGTH AND EFFECTIVE RANGE IN CLOSED FORM FOR THE COULOMB PLUS YAMAGUCHI POTENTIAL

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Abstract: From the known expression for the off-shell T-matrix corresponding to the potential consisting of the sum of the Coulomb potential and the Yamaguchi potential, the physical scattering amplitude can be derived in a satisfactory way. We derive simple exact closed formulae for the scattering length a_{cs} and the effective range r_{cs} from this amplitude. These are compared with approximate formulae derived by Harrington. Also a few numerical calculations are reported and compared with results obtained by Harrington and by Ali *et al.*

1. Introduction and notation

The theoretical description of few-body scattering is considerably simplified by the use of separable potentials for the two-particle interactions. As is well known, the two-body Lippmann-Schwinger equation can be solved by purely algebraic means for such a potential. This yields the two-body transition operator T. In contradistinction to the situation in the two-body problem, the *complete* two-body T-operator is needed for the solution of the N-body problem if $N > 2$. This means that the T-matrix elements in momentum representation are required also off the energy shell, in addition to the on-shell T-matrix elements.

Because the non-relativistic potential model has no clear meaning for high energies, the domain of application of the model is restricted to low energies. Often the effective-range parameters are used to parametrize the scattering at low energies, and to facilitate the comparison of experimental with theoretical values. The effective-range parameters for pp (proton-proton), nn (neutron-neutron) and pn (proton-neutron) scattering have been objects of special interest for a long time.

Experimentally, charged particles are preferred to neutral particles because they are easier to handle. Theoretically, the Coulomb potential causes special problems in scattering theory because of its long range. In two-particle reactions these problems can be overcome. To derive the scattering amplitude for the Coulomb potential plus a short-range potential, one may apply the on-shell Gell-Mann–Goldberger two-potential formula. This has been proven recently by Zorbas [1]). The formula has been used over a long period. Harrington [2]) applied it in his study on the Coulomb plus Yamaguchi potential.

The off-shell T-matrix for the Coulomb plus Yamaguchi potential was first derived by Zachary [3]) and then by Bajzer [4]) making use of the O_4 symmetry of the Coulomb

Hamiltonian. A different derivation, without using this O_4 symmetry, has been given by Van Haeringen and Van Wageningen [5]). We recently derived the physical amplitude from this off-shell T-matrix †. From this physical amplitude, the Coulomb-modified scattering length a_{cs} and effective range r_{cs} for the Yamaguchi potential can be derived. Harrington [2]) has obtained formulae for a_{cs} and r_{cs} in the first-order approximation. Ali *et al.* [8]) obtained values for a_{cs} and r_{cs} purely numerically by solving equations in co-ordinate representation.

In the present paper we obtain simple exact closed formulae for a_{cs} and r_{cs}. The first-order approximations of these formulae agree exactly with the Harrington [2]) expressions. The numerical values which follow from our formulae are in satisfactory agreement with the results of Harrington [2]) and of Ali *et al.* [8]).

In a previous paper [5]) we derived the general structure of exact analytic formulae for the off-shell T-matrices corresponding to the Coulomb potential plus so-called rational separable potentials. Applying the necessary adaptation on the energy shell, the amplitudes can be obtained for all these potentials. The final expressions contain only one non-elementary function, namely the hypergeometric function with parameters $(1, i\gamma; 1+i\gamma)$, where γ is the well known Sommerfeld parameter [9]). To obtain the effective range parameters, only one difficulty has to be overcome. The problem is to expand the hypergeometric function in a power series in the energy parameter. We solve this problem in the present paper. Using this result, one can therefore derive the effective-range parameters in closed form for the Coulomb potential plus an arbitrary rational separable potential in a relatively simple manner.

In sect. 2 we give the general formalism that is needed in sect. 3 to derive the expansion coefficients of the effective-range expansion. In sect. 3 we also report the numerical results and study the sensitivity of a_{cs} and r_{cs} with respect to variation of the parameters of the Yamaguchi potential. In sect. 4 we summarize and discuss the results.

We use the delta-function normalization, $\langle \boldsymbol{p}|\boldsymbol{k}\rangle = \delta(\boldsymbol{p}-\boldsymbol{k})$. The variable k stands for the square root of the energy, $E \equiv k^2$, with $\mathrm{Im}\, k > 0$. The (real positive) physical energy is obtained by taking the appropriate limit, $\mathrm{Im}\, k \downarrow 0$, $\mathrm{Re}\, k > 0$.

Unless stated otherwise, we work in momentum representation.

2. General formalism

This section contains the necessary formalism. After the definition of the Coulomb potential we give a short enumeration of the relevant formulae, conventionally used for scattering by Coulomb plus arbitrary short-range potentials. The main part of the section is devoted to general scattering theory. In the final part we give explicit formulae for the Coulomb plus Yamaguchi potential.

† We developed a physically justifiable adaptation [6]) which can be applied to the off-shell T-matrix to give the on-shell amplitude. In the particular case of "two-potential scattering", application of this adaptation immediately yields the on-shell two-potential formula [1, 7]).

The Coulomb potential is given by

$$V_c(r) = \frac{2k\gamma}{r} \equiv \frac{-2s}{r}, \tag{1}$$

where γ is the well known Sommerfeld parameter [9]). Because

$$k\gamma \equiv -s = \text{real constant}, \tag{2}$$

it follows that γ is energy-dependent. For $s > 0$ we have attraction, for $s < 0$ repulsion. Choosing units such that $\hbar = 2m = 1$ where m is the reduced mass, we get

$$|s|^{-1} = \text{the Bohr radius}. \tag{3}$$

The scattering amplitude for the sum of the Coulomb potential V_c and a short-range potential V_s of any type (either local or non-local) may be written as

$$f(\theta) = f_c(\theta) + f_{cs}(\theta), \tag{4}$$

where $f_c(\theta)$ is the well known Coulomb amplitude. The conventional partial wave expansion of $f_{cs}(\theta)$ is given by

$$f_{cs}(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{2i\sigma_l}e^{i\delta_l^c}\sin\delta_l^c P_l(\cos\theta), \tag{5}$$

where the σ_l are the well known Coulomb phases and the δ_l^c are called the Coulomb-modified nuclear phase shifts. These are *not* the phases for V_s separately. Of course f_c, f_{cs}, σ_l and δ_l^c are k-dependent. We shall be concerned in the following mainly with s-waves. The subscript $l = 0$ will be suppressed.

For the short-range potential V_s one can expand the function $k\cot\delta_s$ in a power series in k^2 as follows

$$k\cot\delta_s = -\frac{1}{a_s} + \tfrac{1}{2}r_s k^2 - \ldots. \tag{6}$$

Here δ_s is the phase shift, a_s is the scattering length and r_s the effective range for V_s. A modification of this formula is needed when the Coulomb potential is included. The following expansion is then known to hold [see Hamilton *et al.* [10]) and references quoted therein],

$$\frac{2\pi\gamma}{e^{2\pi\gamma}-1}k\cot\delta^c + 2k\gamma h(\gamma) = -\frac{1}{a_{cs}} + \tfrac{1}{2}r_{cs}k^2 - \ldots. \tag{7}$$

The function $h(\gamma)$ in this formula is defined by

$$h(\gamma) \equiv -C - \ln\gamma + \gamma^2\sum_{n=1}^{\infty}\frac{1}{n(n^2+\gamma^2)}, \tag{8}$$

where $C = 0.5772\ldots$ is Euler's constant. Up to order γ^{-4} we have

$$h(\gamma) = \frac{1}{12\gamma^2} + \frac{1}{120\gamma^4} + O(\gamma^{-6}), \qquad \gamma \to \infty. \tag{9}$$

We shall see explicitly [eqs. (35)–(37) below and the discussion given there] that $h(\gamma)$ is essential for the validity of the effective-range formula, eq. (7).

The main result of the present paper is a simple exact closed formula for a_{cs} and for r_{cs}, when the total potential consists of the sum of the Coulomb and the Yamaguchi potential.

It is well known that the scattering amplitude $f(\theta)$ for a short-range potential may be obtained by taking the on-shell limit of the off-shell T-matrix. The latter is defined by the operator equation

$$T(E) = V + VG_0(E)T(E), \tag{10}$$

where $G_0(E)$ is the resolvent $(E-H_0)^{-1}$ of the kinetic-energy operator H_0. Now let V be the sum of the Coulomb potential V_c and the Yamaguchi potential V_s [in the notation of ref. [5])],

$$V = V_c + V_s, \tag{11}$$

$$V_s = -\lambda|g\rangle\langle g|, \tag{12}$$

where the form factor g in momentum representation is given by

$$\langle p|g\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{p^2+\beta^2}. \tag{13}$$

As V_s is a one-term separable potential working in $l = 0$ partial wave space only, we then have

$$T = T_c + T_{cs}, \tag{14}$$

where T_c is the well known pure Coulomb T-operator [11]) and T_{cs} is given in closed form by [5])

$$\langle p'|T_{cs}(k^2)|p\rangle = -\langle p'|g^c(k^2)\rangle\tau_c(k^2)\langle g^c(k^{2*})|p\rangle, \tag{15}$$

with

$$\tau_c^{-1}(k^2) = \lambda^{-1} + \langle g|G_c(k^2)|g\rangle, \tag{16}$$

$$\langle g|G_c(k^2)|g\rangle = \frac{-1}{2\beta(\beta+ik)^2} - \frac{2ik}{(\beta^2+k^2)^2}F_{i\gamma}(B^2). \tag{17}$$

In these expressions G_c is the pure Coulomb resolvent, and

$$B \equiv (\beta+ik)/(\beta-ik).$$

The Coulomb-modified form factor g^c is given by

$$\langle p|g^c(k^2)\rangle = \frac{\sqrt{2/\pi}}{\beta^2+p^2} - \frac{\sqrt{2/\pi}}{\beta^2+k^2}\frac{k}{p}[F_{i\gamma}(Ba) - F_{i\gamma}(B/a)], \tag{18}$$

where

$$a \equiv (p-k)/(p+k).$$

The function

$$F_{i\gamma}(z) \equiv {}_2F_1(1,\ i\gamma;\ 1+i\gamma;\ z) \tag{19}$$

is simply connected with the incomplete beta function [12]). It turns out that this function $F_{i\gamma}$ is convenient for practical applications.

From T_c and T_{cs} we can derive the physical on-shell T-matrices which we denote by t_c and t_{cs}. Their relations with the phase shifts are

$$t_c(k) = \frac{i}{\pi k} e^{2i\sigma}, \tag{20}$$

$$t_{cs}(k) = \frac{i}{\pi k} e^{2i\sigma}(e^{2i\delta^c}-1) = -\frac{2}{\pi k} e^{2i\sigma} e^{i\delta^c} \sin \delta^c. \tag{21}$$

Note that the term -1 in eq. (20) is missing. This is one of the remarkable features of the Coulomb potential. From eq. (21) we get at once

$$k \cot \delta^c = -\frac{2}{\pi} \mathrm{Re}(e^{2i\sigma}/t_{cs}). \tag{22}$$

We can express t_{cs} in terms of eqs. (15)–(18). Eq. (22) is then written as

$$\frac{2\pi\gamma}{e^{2\pi\gamma}-1} k \cot \delta^c = B^{2i\gamma}(\beta^2+k^2)^2 \mathrm{Re}\, \tau_c^{-1}. \tag{23}$$

Note that $B^{2i\gamma}$ is real because

$$|B| = 1 \Rightarrow B = e^{i\phi}, \qquad \phi \text{ real}.$$

Eqs. (16) and (17) imply

$$(\beta^2+k^2)^2 \mathrm{Re}\, \tau_c^{-1} = \frac{(\beta^2+k^2)^2}{\lambda} + \frac{k^2-\beta^2}{2\beta} + 2k \mathrm{Im}\, F_{i\gamma}(B^2). \tag{24}$$

Combining eqs. (7), (23) and (24), we see that we have to expand $2k$ Im $F_{i\gamma}(B^2)$ in a power series in k^2. This will be done in the next section.

3. The exact closed formulae for the effective-range parameters and numerical results

The expansion of the function

$$k \mathrm{Im}\, {}_2F_1(1, i\gamma; 1+i\gamma; [(\beta+ik)/(\beta-ik)]^2),$$

in a power series in k^2 [or in a power series in γ^{-2}, which is equivalent to this according to eq. (2)] is tricky because k occurs in the argument of the hypergeometric function as well as in its parameters. Because the argument is 1 for $k = 0$, we can profitably use an expansion of $F_{i\gamma}(z)$ in powers of $(1-z)$. Such an expansion is known [ref. [12]), p. 49] and reads in this case

$${}_2F_1(1, i\gamma; 1+i\gamma; z) = i\gamma \sum_{n=0}^{\infty} \frac{(i\gamma)_n}{n!} (1-z)^n [\psi(n+1) - \psi(n+i\gamma) - \ln(1-z)], \tag{25}$$

where ψ is the logarithmic derivative of the gamma function and $(i\gamma)_n$ is Pochhammer's

symbol. As is well known, $F_{i\gamma}(z)$ has a branch point at $z = 1$ [ref. [12])]. The function $\ln(1-z)$ shows this branch point in the r.h.s. of eq. (25). It is important to notice, however, that the limit $k \to 0$ does not necessarily take us to a branch point of the function ${}_2F_1(1, i\gamma; 1+i\gamma; [(\beta+ik)/(\beta-ik)]^2)$, because two of the three parameters go to $\pm i\,\infty$ at the same time when the argument goes to 1. It indeed appears that a power series expansion

$$\mathrm{Re}\left[\frac{1}{i\gamma} F_{i\gamma}(B^2)\right] = c_0 + \frac{c_2}{(i\gamma)^2} + \ldots, \tag{26}$$

is possible. We calculate c_0 and c_2 by expanding all expressions occurring in the r.h.s. of eq. (25) in powers of $1/i\gamma$ and collecting corresponding terms. To this end, the following equalities are utilized [12]),

$$\psi(n+1) = -C + \sum_{m=1}^{n} \frac{1}{m}, \tag{27}$$

$$\sum_{n=0}^{\infty} \frac{z^n}{n!}(C+\psi(n+1)) = -\mathrm{e}^z \sum_{n=1}^{\infty} \frac{(-z)^n}{nn!}, \tag{28}$$

$$-\Gamma(0, z) = C + \ln z + \sum_{n=1}^{\infty} \frac{(-z)^n}{nn!}, \qquad |\arg z| < \pi, \tag{29}$$

$$\psi(z) \sim \ln z - \frac{1}{2z} - \sum_{n=1}^{\infty} \frac{B_{2n}}{2nz^{2n}}, \qquad |\arg z| < \pi. \tag{30}$$

In these formulae, $\Gamma(0, z)$ is the incomplete gamma function, B_{2n} are the Bernoulli numbers and C is Euler's constant.

After a straightforward derivation we obtain the following results,

$$c_0 = \mathrm{e}^{4v}\Gamma(0, 4v), \tag{31}$$

$$c_2 = \tfrac{1}{12}(1+4v-4v^2+16v^3c_0), \tag{32}$$

where the parameter v is defined by

$$v \equiv \frac{k\gamma}{\beta} \equiv -\frac{s}{\beta}. \tag{33}$$

Application of these expressions for c_0 and c_2 to eqs. (7), (23), (24) and (26) yields the desired closed formulae for the effective range parameters,

$$-\frac{1}{a_{cs}} = \mathrm{e}^{-4v}\left(\frac{\beta^4}{\lambda} - \tfrac{1}{2}\beta\right) + 2\beta v\Gamma(0, 4v), \tag{34}$$

$$\tfrac{1}{2}r_{cs} = \frac{1-\mathrm{e}^{-4v}}{6\beta v} + \mathrm{e}^{-4v}\left(-\frac{1}{6\beta} + \frac{2\beta^2}{\lambda} + \frac{4\beta^2}{3\lambda}v\right). \tag{35}$$

The contribution of the function $h(\gamma)$ in eq. (7) to these expressions consists merely

in the first term of the r.h.s. of eq. (35), namely $1/6\beta\nu$. There is no contribution to a_{cs} because $h(\gamma) = 0(k^2)$ for $k \to 0$.

We can see explicitly in eq. (35) that the function $h(\gamma)$ in the effective-range formula is essential. If the term $1/6\beta\nu$ is left out, r_{cs} would become infinite for $\nu \to 0$, i.e. for $s \to 0$ where as before s is the Coulomb strength parameter.

At first sight it seems rather embarrassing that $h(\gamma)$ plays an essential role when we turn off the Coulomb potential. For $s \to 0$, the Coulomb effective-range formula eq. (7) goes over into the ordinary effective-range formula eq. (6) and the term $2k\gamma h(\gamma)$ vanishes. How can this term then be essential, in particular for $s \to 0$?

This difficulty arises from the fact that we are concerned here with two different limits. We can find the solution by considering the behaviour of the term $2k\gamma h(\gamma)$ in these two limits, cf. eqs. (7)–(9),

$$2k\gamma h(\gamma) = 2s \ln|s| + O(s), \qquad \text{for } s \to 0,\ k \text{ constant}, \tag{36}$$

$$2k\gamma h(\gamma) = -\frac{k^2}{6s} + O(k^4), \qquad \text{for } k \to 0,\ s \text{ constant}. \tag{37}$$

So we see that the coefficient of k^2 becomes indeed infinite for $s \to 0$ although the whole term then tends to zero! In fact, this coefficient $-1/6s$ is just the term $1/6\beta\nu$ discussed before, cf. eqs. (33), (35).

We may rewrite a_{cs} and r_{cs} in terms of the well known Yamaguchi effective-range parameters a_s and r_s, given by

$$-\frac{1}{a_s} = \frac{\beta^4}{\lambda} - \tfrac{1}{2}\beta, \tag{38}$$

$$\tfrac{1}{2}r_s = \frac{2\beta^2}{\lambda} + \frac{1}{2\beta}. \tag{39}$$

Eqs. (34) and (35) then become

$$-\frac{1}{a_{cs}} = -\frac{e^{-4\nu}}{a_s} + 2\beta\nu\Gamma(0, 4\nu), \tag{40}$$

$$\tfrac{1}{2}r_s = e^{-4\nu}\left[\tfrac{1}{2}r_s + \frac{4\beta^2}{3\lambda}\nu + \frac{e^{4\nu}-1-4\nu}{6\beta\nu}\right]. \tag{41}$$

To first order in ν we get

$$-\frac{1}{a_{cs}} = -\frac{1}{a_s}(1-4\nu) - 2\beta\nu(C + \ln 4\nu) + O(\nu^2), \tag{42}$$

$$\tfrac{1}{2}r_{cs} = \tfrac{1}{2}r_s - \frac{2\nu}{3}\left(\frac{1}{\beta} + \frac{10\beta^2}{\lambda}\right) + O(\nu^2) \tag{43}$$

$$= \tfrac{1}{2}r_s(1-4\nu) + \frac{2\nu}{\beta}\left(1 - \frac{2}{3\beta a_s}\right) + O(\nu^2). \tag{44}$$

It is easy to see that (a_{cs}, r_{cs}) become equal to (a_s, r_s) in the limit $s \to 0$, as one would expect.

Now that we have derived the exact formulae for a_{cs} and r_{cs} [eqs. (34), (35)] we can compare our formulae with published results. Firstly, Harrington [2]) derived analytic formulae valid to first order in v, and he applied these to the nucleon-nucleon system. His formulae are just our eqs. (42) and (44) so in this respect there is complete agreement. Secondly, Ali *et al.* [8]) calculated a_{cs} and r_{cs}. Their method involved the numerical evaluation of a double integral involving Coulomb wave functions.

We therefore did some calculations with the same parameter sets used by Harrington and by Ali. These authors chose the Yamaguchi parameters λ and β such that a_{cs} and r_{cs} are near the experimental proton-proton effective-range parameter values.

The numerical results are listed in table 1. We took $(2k\gamma)^{-1} \equiv (2\beta\nu)^{-1} = 28.80$ fm. This is the proton Bohr radius. Of course, the Bohr radius for the pp system is twice this value, cf. eq. (3).

TABLE 1

Effective-range parameters for Yamaguchi (a_s, r_s) and for Coulomb plus Yamaguchi (a_{cs}, r_{cs})

	β (fm^{-1})	λ (fm^{-3})	a_s (fm)	r_s (fm)	a_{cs} (fm)	r_{cs} (fm)
	1.100	2.405	−17.015	2.922	−7.507	2.799
	1.095	2.400	−19.408	2.912	−7.921	2.790
	1.100	2.400	−16.655	2.926	−7.440	2.803
First order	1.100	2.400	−16.655	2.926	−7.568	2.801
Harrington (first order)	1.10	2.40	−18.0	2.93	−7.81	2.80
	1.075	2.250	−17.844	2.985	−7.703	2.857
	1.074	2.240	−17.551	2.991	−7.653	2.863
	1.074	2.260	−19.335	2.973	−7.953	2.846
	1.074	2.250	−18.404	2.982	−7.801	2.854
Ali *et al.*	1.074	2.25			−7.717	2.84

$(2k\gamma)^{-1} = 28.80$ fm.

It should be noted that we can compute a_{cs} very accurately by using the expansion eq. (29) for the incomplete gamma function in the exact expressions for a_{cs}, eqs. (34) and (40). Because of the smallness of the parameter $\nu(\nu \approx 0.016$ for $\beta \approx 1)$, the power series converges very rapidly.

Upon variation of the Coulomb strength $\beta\nu \equiv -s$ it turned out that the effective-range parameters are not sensitive with respect to s. We also varied the Yamaguchi parameters λ and β. As can be seen from table 1, we find that a_s and a_{cs} both are rather sensitive to small variations in λ and β. It appears that r_s and r_{cs} are much less sensitive.

First-order calculations [using eqs. (42)–(44)] are shown in the fourth row of table 1. These can be compared with Harrington's first-order results, given in the fifth row. Comparing the fourth row with the third one, we see that the first-order values do not differ much from the exact values. The values of a_s and r_s in rows 3 and 4 are, of course, exactly the same. In rows 6–10 our results are compared with those of Ali *et al.*

In view of the sensitivity of the scattering lengths a_s and a_{cs} with respect to λ and β, we may say that our numerical values are in satisfactory agreement with the values of Harrington and of Ali *et al.* †.

4. Summary and discussion

We derived simple exact closed formulae for the effective-range parameters a_{cs} and r_{cs} for the Coulomb plus Yamaguchi potential, [eqs. (34), (35)]. In terms of the pure Yamaguchi effective-range parameters a_s and r_s the expressions for a_{cs} and r_{cs} are [eqs. (40), (41)],

$$-\frac{1}{a_{cs}} = -\frac{e^{-4\nu}}{a_s} + 2\beta\nu\Gamma(0, 4\nu),$$

$$\tfrac{1}{2}r_{cs} = e^{-4\nu}\left[\tfrac{1}{2}r_s + \frac{4\beta^2}{3\lambda}\nu + \frac{e^{4\nu}-1-4\nu}{6\beta\nu}\right].$$

The first-order approximations of these expressions, [eqs. (42)–(44)], are in complete agreement with the first-order formulae obtained by Harrington [2]). We gave numerical results and compared these with the results of Harrington [2]) and of Ali *et al.* [8]). We showed that the scattering lengths a_s and a_{cs} are rather sensitive to small variations in the Yamaguchi parameters λ and β. If we take this sensitivity into account, we may say that the agreement with the results of Harrington and Ali is satisfactory.

As Harrington reported already, the values for a_s and r_s are in reasonable agreement with previous calculations based upon charge symmetry, and with experimental values for the neutron-neutron parameters, if λ and β are chosen such that a_{cs} and r_{cs} agree approximately with the experimental proton-proton parameters.

In a previous paper [5]) we revealed the general structure of exact analytic expressions for the off-shell T-matrices corresponding to the Coulomb potential plus so-called rational separable potentials. It turns out that the final formulae for the physical scattering amplitudes contain the hypergeometric function $F_{i\gamma}$ [defined in eq. (19)] as the only non-elementary function. We can therefore extend the results of the present paper to this very large class of rational separable potentials, using the same method and in particular the expansion of $F_{i\gamma}$ given in eqs. (26), (31) and (32).

† After completion of the manuscript we noticed that Thomas and Afnan [13]) have calculated a_{cs} using the numerical procedure of Vincent and Phatak [14]). With Harrington's values for β, λ they find $a_{cs} = -7.43$ fm, in good agreement with our value -7.440 fm.

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A 4

The number of bound states of the Coulomb plus Yamaguchi potential

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It is shown that certain assertions on the number of bound states of a Coulomb plus Yamaguchi potential which Zachary [J. Math. Phys. **12**, 1379 (1971); **14**, 2018 (1973)] claims to have proved are incorrect. We prove that there are always infinitely many bound states if the Coulomb part of the potential is attractive and that, in case the Coulomb part of the potential is repulsive, there is one bound state only if the Yamaguchi potential is sufficiently attractive.

In this paper we correct some assertions which Zachary[1] claims to have proved concerning the number of bound states (in the $l=0$ partial wave projected space) for the Coulomb plus Yamaguchi potential.

We prove that the number of s wave bound states is always infinite if the Coulomb part of the potential is attractive, for a repulsive as well as for an attractive Yamaguchi potential. Zachary found (by means of numerical calculations) that the number of bound states would be 0 or 1 in this case.

In case the Coulomb part of the potential is repulsive, we prove that there is one and only one bound state if the Yamaguchi potential is sufficiently attractive, and that there is no bound state otherwise. Zachary found in this case that the number of bound states could be 0, 1, or 2. See Ref. 1, pp. 1384 and 1385.

We start with the observation that all the bound states are given by the poles of the T operator. In the notation of Ref. 2, we have $V=V_c+V_s$. Here V_s is the rank-one separable Yamaguchi potential with strength λ and range parameter β. V_s is attractive or repulsive when $\lambda>0$ or $\lambda<0$, respectively. Further, V_c is the pure Coulomb potential with strength s, V_c being attractive when $s>0$ and repulsive when $s<0$. Furthermore we shall use the variable κ which is connected to the energy by $E=-\kappa^2$, $\kappa>0$. Then

$$T=T_c+T_{cs}, \tag{1}$$

$$T_{cs}=-\frac{|g^c\rangle\langle g^c|}{\lambda^{-1}+\langle g|G_c|g\rangle}, \tag{2}$$

where g^c is the Coulomb-modified form factor. When V_c is repulsive, neither T_c nor g^c has poles. Below we shall show[3] that, when V_c is attractive, the pure Coulomb poles in T_c are cancelled by corresponding poles in T_{cs}. Then it follows that the poles of T are obtained by solving the equation

$$\lambda^{-1}+\langle g|G_c|g\rangle=0. \tag{3}$$

In the case g is the Yamaguchi form factor, the second term is known in closed form [cf. Eq. (83) of Ref. 2] and we have

$$\lambda^{-1}=\frac{1}{2\beta(\beta+\kappa)^2}\,\frac{1}{1-s/\kappa}\,{}_2F_1\left(1,-s/\kappa;2-s/\kappa;[(\beta-\kappa)/(\beta+\kappa)]^2\right). \tag{4}$$

This is essentially Eq. (31) of Zachary.

We now first consider the case that V_c is attractive, i.e., $s>0$. In that case T_c has the pure Coulomb bound-state poles at $\kappa=s/n$, $n=1, 2, \cdots$. The origin $\kappa=0$ is the limit point of these poles. However, we do not expect bound states of V_c+V_s at *these* energies. In fact, T_{cs} has poles at exactly the same points $\kappa=s/n$ and its residues cancel the residues of T_c. It follows that T_c+T_{cs} has for these values of κ "removable poles" (in the terminology of Ref. 4). This can be shown in the following way. In the neighborhood of the point $\kappa=s/n$, where we fix n for the moment, we have

$$T_c\approx\frac{G_0^{-1}|\kappa_n\rangle\langle\kappa_n|G_0^{-1}}{-\kappa^2+s^2/n^2}\quad(\kappa\approx s/n), \tag{5}$$

where $|\kappa_n\rangle$ is the pure Coulomb bound state vector. Using then

$$G_c=G_0+G_0T_cG_0\approx G_0T_cG_0,$$

$$|g^c\rangle=(1+T_cG_0)|g\rangle\approx T_cG_0|g\rangle,$$

where both approximations hold near the pure Coulomb bound state poles, we get from Eqs. (1) and (2),

$$T\approx T_c-\frac{T_cG_0|g\rangle\langle g|G_0T_c}{\langle g|G_0T_cG_0|g\rangle}. \tag{6}$$

Insertion of Eq. (5) into Eq. (6) shows that the residues of T_c and T_{cs} cancel,[3] i.e.,

$$\lim_{\kappa\to s/n}(-\kappa^2+s^2/n^2)T=0. \tag{7}$$

It is also clarifying to consider the following interesting equality, which holds without approximation,

$$\langle g|G|g\rangle^{-1}=\lambda+\langle g|G_c|g\rangle^{-1}. \tag{8}$$

Clearly, the poles of $\langle g|G_c|g\rangle$ are no poles of $\langle g|G|g\rangle$ (and vice versa) as long as $\lambda\neq0$. Furthermore, the *resolvent G and the T operator have the same poles*, which follows easily from

$$G=G_0+G_0TG_0.$$

We now turn to the solution of Eq. (4). All the variables in Eq. (4) are real and it follows that the whole expression is real. Due to $s>0$ we have $-s/\kappa<0$. Now it is known that ${}_2F_1(a,b;c;z)/\Gamma(c)$ is an entire analytic function of a, b, and c if z is fixed and $|z|<1$. It follows that the expression on the right-hand side of Eq. (4) has simple poles at $s/\kappa=n=1, 2, \cdots$. (These are just the pure Coulomb bound state poles.) At such a pole it

behaves as[3]

$$(n - s/\kappa)^{-1}\, 2s(\beta - s/n)^{2n-2}(\beta + s/n)^{-2n-2},$$

from which it follows that the residues have the same sign for all n. Therefore, if we vary κ from $s/(n+1)$ to s/n (i.e., between any pair of consecutive poles), that expression varies continuously from $+\infty$ to $-\infty$ and adopts every real number at least once. (Below we shall find that it adopts every real number *just* once.) This holds for every $n = 1, 2, \cdots$, so Eq. (4) has infinitely many solutions for every real value of λ, i.e., there is a bound state corresponding to $\kappa = s/n$ $(n = 1, 2, \cdots)$ for an arbitrarily strongly repulsive or attractive amaguchi potential. The origin $\kappa = 0$ (zero energy) is the only accumulation point of the bound state energies.

A second way to prove this, which at the same time gives more detailed information about the position of the bound state energies with respect to the pure Coulomb bound states, is to insert the completeness relation

$$\mathbb{1} = \sum_{n=1}^{\infty} |\kappa_n\rangle\langle\kappa_n| + \int_0^{\infty} dk\, k^2 |k+\rangle\langle k+| \tag{9}$$

into Eq. (3). Here again $|\kappa_n\rangle$ are the bound state vectors and $|k+\rangle$ are the scattering states of the attractive pure Coulomb potential. Using then $G_c = -(\kappa^2 + H_c)^{-1}$ where $H_c = H_0 + V_c$, we get

$$\lambda^{-1} = \sum_{n=1}^{\infty} \frac{\langle g|\kappa_n\rangle\langle\kappa_n|g\rangle}{\kappa^2 - s^2/n^2} + \int_0^{\infty} \frac{dk\, k^2}{\kappa^2 + k^2} \langle g|k+\rangle\langle k+|g\rangle. \tag{10}$$

The integrand and each term of the infinite sum is a monotonically decreasing function of κ on each of the intervals $s/(n+1) < \kappa < s/n$, $n = 0, 1, \cdots$; This can be seen either by inspection or by means of differentiation with respect to κ^2. It follows that the right-hand side of Eq. (10) is a monotonically decreasing function of κ on the above intervals. So if κ increases between any pair of adjacent poles[3] [from $s/(n+1)$ to s/n, say], the expression on the right-hand side of Eq. (10) *decreases continuously and monotonically* from $+\infty$ to $-\infty$. Therefore, Eq. (10) has for every real value of λ one and only one solution in the interval $s/(n+1) < \kappa < s/n$, for $n = 1, 2, \cdots$. Furthermore, in the $n = 0$ interval $s < \kappa < \infty$ there is one and only one solution for every real *positive* value of λ, since the right-hand side of Eq. (10) varies then continuously and monotonically from $+\infty$ to 0.

This means that in the case of an attractive Yamaguchi part there is just one bound state below the pure Coulomb ground state, with binding energy $E_B < -s^2$. This is the ground state of $V_c + V_s$. By increasing the Yamaguchi strength, $\lambda \to \infty$, we get an infinite binding energy as expected, $E_B \to -\infty$. Also all other bound states of $V_c + V_s$, namely those with $n = 2, 3, \cdots$, are shifted downwards with respect to the corresponding pure Coulomb bound states. But in this case the bound states always remain above the next lower pure Coulomb bound states. On the other hand, if the Yamaguchi part is repulsive, all bound states are shifted upwards with respect to the pure Coulomb bound states, but every state remains below the next higher pure Coulomb state, no matter how strongly repulsive V_s is. This is a remarkable and quite unexpected phenomenon.

Now we consider the case that V_c is repulsive. In this case the pure Coulomb scatterin ; states $|k+\rangle$ form a complete set in the $l = 0$ space. The completeness relation now takes the form

$$1 = \int_0^{\infty} dk\, k^2 |k+\rangle\langle k+|. \tag{11}$$

Again, we insert Eq. (11) into Eq. (3) and use the fact that $G_c = -(\kappa^2 + H_c)^{-1}$ with $H_c|k+\rangle = k^2|k+\rangle$. Then Eq. (3) becomes

$$\lambda^{-1} - \int_0^{\infty} \frac{dk\, k^2}{\kappa^2 + k^2} \langle g|k+\rangle\langle k+|g\rangle = 0. \tag{12}$$

The integrand is clearly real positive and it is a continuous and monotonically decreasing function of κ for $0 < \kappa < \infty$. The same holds for the integral. It is maximal for $\kappa = 0$. We denote the corresponding strength by λ_0,

$$\lambda_0^{-1} = \int_0^{\infty} dk \langle g|k+\rangle\langle k+|g\rangle. \tag{13}$$

It follows by inspection that Eq. (12) has one and only one solution if the Yamaguchi potential is sufficiently attractive, i.e., if $\lambda \geq \lambda_0$. When $\lambda < \lambda_0$ there is no solution and therefore no bound state. An explicit expression for λ_0 follows from

$$\beta^3/\lambda_0 = \tfrac{1}{2} - 2\nu \exp(4\nu)\,\Gamma(0, 4\nu), \tag{14}$$

in the notation of Ref. 5 $(\nu = -s/\beta > 0)$. For this value of λ_0, the Coulomb-modified scattering length is infinite, $a_{cs}^{-1} = 0$, see Eq. (34) of Ref. 5. We notice that

$$0 < x \exp(x)\Gamma(0, x) = x \exp(x) \int_x^{\infty} dt\, t^{-1} \exp(-t) < 1, \quad x > 0,$$

so that the right-hand side of Eq. (14) is always positive and therefore $\lambda_0^{-1} > 0$, cf. Eq. (13). It also follows from Eq. (14) that $\beta^3/\lambda_0 < \frac{1}{2}$. This is satisfactory since it is known that for the *pure* Yamaguchi potential the bound state appears just at zero energy if the strength λ is equal to $2\beta^3$. Addition of the repulsive Coulomb potential must have the effect that $\lambda_0 > 2\beta^3$.

Finally we note that Eq. (12) implies that the expression on the right-hand side of Eq. (4) is a continuous and monotonically decreasing function of κ for $0 < \kappa < \infty$ if $s < 0$. This can be proved directly, but with considerably more effort, as follows. Starting from a well-known integral representation for the hypergeometric function, we can recast Eq. (4) into the form

$$\lambda^{-1} = 2\kappa \int_0^1 dt\, t^{-s/\kappa} N^{-2}, \tag{15}$$

with

$$N = (\beta + \kappa)^2 - t(\beta - \kappa)^2 \geq 0.$$

Here we have also utilized

$${}_2F_1(1, i\gamma; 2 + i\gamma; z) = (1 - z)\, {}_2F_1(2, 1 + i\gamma; 2 + i\gamma; z).$$

We differentiate the right-hand side of Eq. (15) with respect to κ and obtain, after a few partial integrations,

$$2\int_0^1 dt\, t^{-s/\kappa} N^{-3} \{2(\beta^2 - \kappa^2)(1 - t) + \ln t[(\beta + \kappa)^2 + t(\beta - \kappa)^2]\}. \tag{16}$$

One easily verifies that

$$\ln t = \sum_{n=1}^{\infty} \frac{2}{2n-1} \left(\frac{t-1}{t+1}\right)^{2n-1} < 2\frac{t-1}{t+1}, \quad 0 < t < 1.$$

Substitution of this inequality shows that the integrand is dominated by

$$t^{-s/\kappa}N^{-3}\,4\kappa(t-1)[\kappa+\beta(1-t)/(1+t)],$$

which is clearly negative for $0<t<1$, so that the integral of Eq. (16) is also negative. This proves the monotonicity.

We note that almost all the assertions of this paper remain valid when the Yamaguchi potential is replaced by an arbitrary rank-one separable potential. It is not difficult to verify this. There is one important exception, however. When we discussed the solutions of Eq. (4), we assumed the energy to be negative. It can be shown, with the help of Eqs. (10) and (12), that Eq. (4) has indeed no solution for positive energy if g is the Yamaguchi form factor. That is, there is no bound state in the continuum. However, by a special choice of the form factor it is possible to construct a bound state at positive energy. Such a pathological situation will not be discussed here.

The results of this paper agree with our intuitive idea, namely that the range of V_c+V_s, being still infinite, causes an infinite number of bound states in case V_c is attractive. On the other hand, it is known that an attractive rank-one separable potential has at most one bound state at negative energy. Addition of a repulsive Coulomb potential should not change the situation.

The mistake of Zachary shows that the hypergeometric functions occurring here are complicated objects. The source of the difficulties is that the energy variable is contained in the parameters of ${}_2F_1$ as well as in its argument. In particular in the zero energy region one should be careful. Numerical calculations might fail here because the well known ordinary power series of ${}_2F_1$ converges very slowly. A method for practical calculations, in particular useful in this region, has been developed in Ref. 4.

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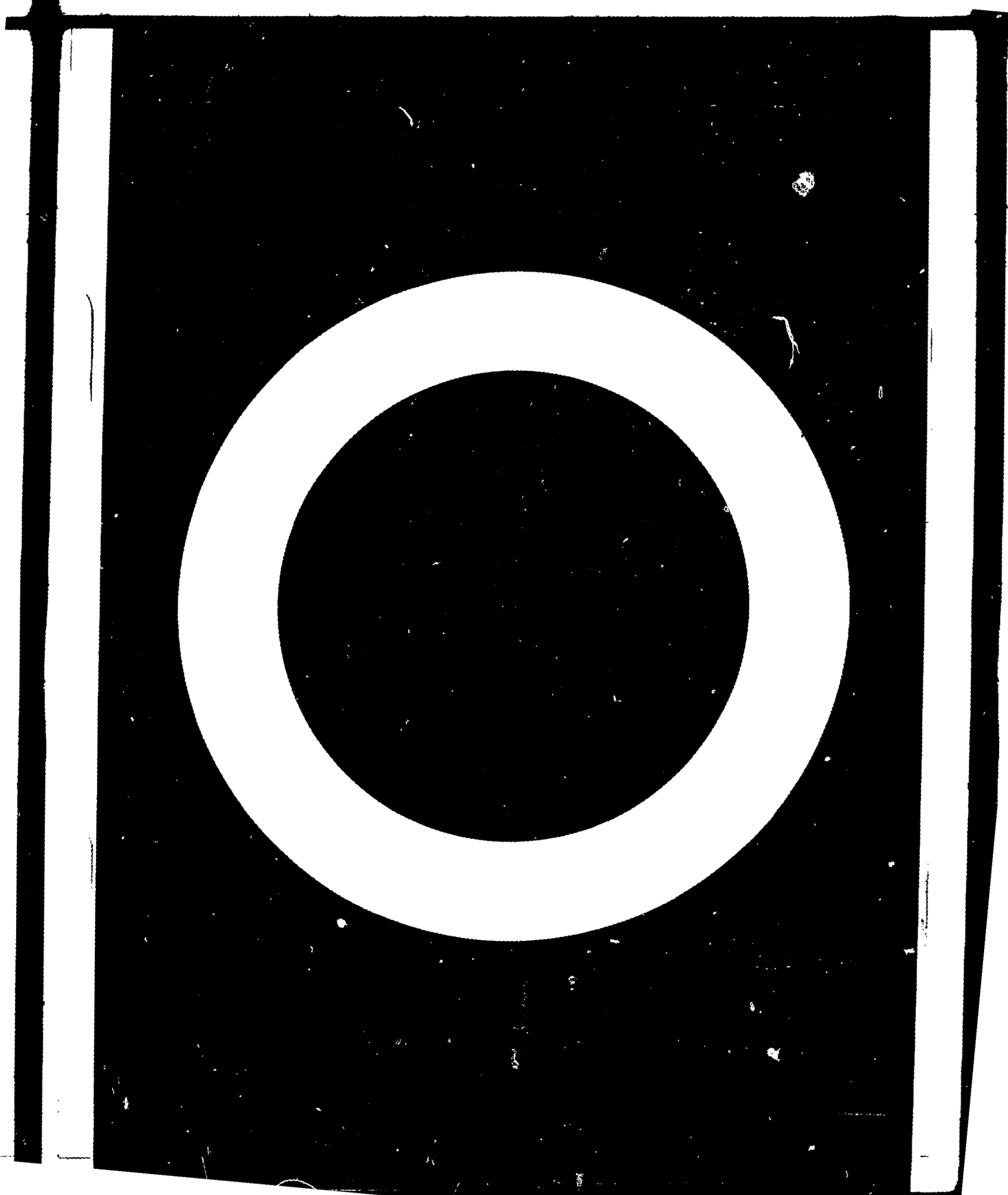

A 5

T matrix and effective range function for Coulomb plus rational separable potentials especially for $l=1$

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The off-shell $l=1$ T matrix in the momentum representation for the pure Coulomb potential and for the Coulomb plus a rational separable potential of the Yamaguchi type is obtained in closed form. The amplitude, the effective range function, and the effective range parameters are derived from the T matrix and are given in closed form. For a large number of rational separable potentials we prove that the effective range function is real analytic at zero energy. We give, however, an example of a potential for which this effective range function has a *pole* at the origin. From these effective range functions a certain function W is extracted which does not depend either on l or on the particular potential. This function W is studied in detail. We indicate how the results of this paper can be generalized to arbitrary values of l and to all Coulomb plus rational separable potentials.

1. INTRODUCTION

In Sec. 2 we present a number of results for scattering by a potential which is the sum of the Coulomb potential and a rational separable potential[1] in the $l=1$ partial wave space. Analogous results for $l=0$ have been published in Refs. 1 and 2.

We give a closed formula for the pure Coulomb T matrix for $l=1$ in Eq. (2.1). Further we consider a rank-one separable potential with form factor of the type $p^l/(p^2+\beta_1^2)^{l+1}$. For $l=1$ we obtain the T matrix for the Coulomb potential plus a potential of the above type. By applying the asymptotic states defined and studied by the author to this T matrix we obtain the $l=1$ partial wave projected physical scattering amplitude. The effective range parameters a_1 and r_1 are derived from the amplitude in the well-known way and given in closed form, see Eqs. (2.9) and (2.10).

The larger part of this paper, Secs. 3–6, is mainly concerned with the so-called effective range function K and related functions. The function K, being analytic at zero energy ($k^2=0$), can be expanded in a Taylor series,

$$K_l(k^2) = -a_l^{-1} + \tfrac{1}{2} r_l k^2 - \cdots,$$

where a_l, r_l, $\cdots$ are real. An analytic function with real expansion coefficients is called real analytic.

In Ref. 2 we *assumed* that K_0 is real analytic, and we derived closed expressions for a_0 and r_0. In the present paper we *prove* the real analyticity of K_l for a large number of rational separable potentials [see Eq. (3.11)]. To our knowledge, no such proof has been given before when the additional potential is nonlocal. Only for Coulomb plus *local* short-range potentials the analytic properties of the effective range function K_l have been studied and the real analyticity of K_l has been proved, see Hamilton *et al.*[3] and Cornille and Martin.[4]

In the following we shall use several variables. In the first place we have the strength s of the Coulomb potential. It is real and in this paper it is kept fixed; however, both $s>0$ and $s<0$ will be considered. Secondly we have the strengths λ_i of the separable potential which play only a role of minor importance. Further we have α and β which are parameters related to the range of the rational separable potential. Finally we have the wavenumber k which is equal to the square root of the energy. It is often convenient to use instead of k, α, β the variables γ, μ, ν defined by

$$\mu\alpha \equiv \nu\beta \equiv k\gamma \equiv -s.$$

We shall consider functions of k and also functions of k^2. It is important to note that the so-called physical complex k^2-plane corresponds to the upper half of the complex k-plane, i.e., $\mathrm{Im}k \geq 0$. Consequently, the physical complex γ-half-plane depends on the sign of the Coulomb strength s. It is determined by $s\,\mathrm{Im}\gamma \geq 0$. The Coulomb bound states occur only if $s<0$ and are given by $\gamma = in$, $n=1,2,\cdots$.

In Sec. 3 we extract from the effective range functions K_l (corresponding to different potentials) a certain function $W(\gamma;\mu,\nu)$ which depends neither on l nor on the particular potential. If W is real analytic so is K_l, with the exception of possible poles, for a large number of potentials defined in Sec. 3. We claim that this even holds for all rational separable potentials. We shall prove that $W(\gamma;\mu,\nu)$ is indeed real analytic at $\gamma^{-2}=0$ for real μ and ν.

Related to W is the hypergeometric function $F_{i\gamma}(AB) \equiv {}_2F_1(1, i\gamma; 1+i\gamma; AB)$ [with $A \equiv (\alpha+ik)/(\alpha-ik)$, $B \equiv (\beta+ik)/(\beta-ik)$] that we encountered before.[1] In Sec. 4 we shall study $F_{i\gamma}(AB)$ for real positive k, α and β, i.e., for real γ, μ and ν. In Sec. 5 we investigate $W(\gamma;\mu,\nu)$ for real μ, ν and complex γ. We introduce there the function $W(\gamma;\xi)$ which is related to but simpler than $W(\gamma;\mu,\nu)$. This function $W(\gamma;\xi)$ is useful for the exact numerical computation of $W(\gamma;\mu,\nu)$ and therefore of the effective range functions, see Eq. (5.11).

Eventually in Sec. 6 all variables are taken complex and the proof of the real analyticity of $W(\gamma;\mu,\nu)$ at $k=0$ (for real μ and ν) is given. To achieve this, related functions $V(\gamma;\mu,\nu)$ and $V(\gamma;\xi)$ will be introduced which are analytic in all their variables. Section 7 summarizes the results.

2. *T* MATRIX, AMPLITUDE AND EFFECTIVE RANGE PARAMETERS

In this section we present the Coulomb T matrix, the T matrix for the Coulomb plus Yamaguchi-type poten-

tial and the corresponding amplitude and effective range parameters in explicit form, all for $l=1$. The analogous $l=0$ quantities have been presented in Refs. 1 and 2. We use here the same notation.

The $l=1$ pure Coulomb T matrix is obtained from Eq. (24) of Ref. 1, in the same way as $T_{c,\,l=0}$ has been derived. The result is as follows:

$$\begin{aligned}\langle p'|\,T_{c,\,l=1}(k^2)\,|p\rangle &= \frac{ik}{\pi pp'}\,\frac{1}{1+\gamma^2}\Big[2i\gamma(1-i\gamma)+i\gamma\,\frac{p^2-k^2}{2pk}\,\frac{p'^2-k^2}{2p'k}\,\ln\Big(\frac{p'+p}{p'-p}\Big)^2\\ &+\Big(i\gamma-\frac{p^2+k^2}{2pk}\Big)\Big(i\gamma-\frac{p'^2+k^2}{2p'k}\Big)\,F_{i\gamma}(aa')\\ &+\Big(i\gamma+\frac{p^2+k^2}{2pk}\Big)\Big(i\gamma+\frac{p'^2+k^2}{2p'k}\Big)\,F_{i\gamma}\Big(\frac{1}{aa'}\Big)\\ &+\Big(i\gamma-\frac{p^2+k^2}{2pk}\Big)\Big(i\gamma+\frac{p'^2+k^2}{2p'k}\Big)\,F_{i\gamma}\Big(\frac{a}{a'}\Big)\\ &+\Big(i\gamma+\frac{p^2+k^2}{2pk}\Big)\Big(i\gamma-\frac{p'^2+k^2}{2p'k}\Big)F_{i\gamma}\Big(\frac{a'}{a}\Big)\Big]. \qquad (2.1)\end{aligned}$$

Here $F_{i\gamma}(\cdot)$ is the hypergeometric function ${}_2F_1(1, i\gamma; 1+i\gamma; \cdot)$ and $a=(p-k)/(p+k)$, $a'=(p'-k)/(p'+k)$.

In Ref. 1 we have introduced what we call the rational separable potentials in the $l=0$ space. The definition of a rational separable potential can be extended to all l in an obvious way. Here we consider only the form factor

$$\langle p|\,g_{\beta,\,l}\rangle=(2/\pi)^{1/2}\,p^l(\beta^2+p^2)^{-l-1}. \qquad (2.2)$$

This form factor is often proposed to describe nucleon–nucleus and nucleon–nucleon scattering (e.g., Cattapan[5] and Črepinšek[6]). We would like to have closed formulas for the T matrices corresponding to potentials $V=V_c+V_s$, where V_c is the Coulomb potential and V_s a separable potential of finite rank with form factors of the type of Eq. (2.2). According to Sec. 5 of Ref. 1 it is for this purpose sufficient to derive closed formulas for the following two objects:

$$\langle p|\,g^c_{\beta,\,l}(k^2)\rangle\equiv\langle p|\,[1+T_{c,\,l}(k^2)\,G_{0,\,l}(k^2)]\,|\,g_{\beta,\,l}\rangle$$

and

$$\langle g_{\alpha,\,l}|\,G_{c,\,l}(k^2)\,|\,g_{\beta,\,l}\rangle\equiv\langle g_{\alpha,\,l}|\,G_{0,\,l}(k^2)\,|\,g^c_{\beta,\,l}(k^2)\rangle.$$

With the help of Eq. (2.1) this plan of action has been carried out for $l=1$. By applying the straightforward method of Secs. 6 and 7 of Ref. 1 we find, with $A=(\alpha+ik)/(\alpha-ik)$ and $B=(\beta+ik)/(\beta-ik)$,

$$\begin{aligned}\langle p|\,g^c_{\beta,\,l=1}(k^2)\rangle &= \frac{(2/\pi)^{1/2}p}{(\beta^2+p^2)^2}-\frac{(2/\pi)^{1/2}i\gamma k^2}{p(\beta^2+k^2)^2}+\frac{(2/\pi)^{1/2}\beta k\gamma(p^2-k^2)}{p(\beta^2+p^2)(\beta^2+k^2)^2}\\ &+\frac{(2/\pi)^{1/2}k^2}{p(\beta^2+k^2)^2}\Big[\Big(i\gamma-\frac{p^2+k^2}{2pk}\Big)\,F_{i\gamma}(B a)\\ &+\Big(i\gamma+\frac{p^2+k^2}{2pk}\Big)\,F_{i\gamma}\Big(\frac{B}{a}\Big)\Big], \qquad (2.3)\end{aligned}$$

and

$$\begin{aligned}\langle g_{\alpha,\,l=1}|\,G_{c,\,l=1}\,|\,g_{\beta,\,l=1}\rangle &= \frac{2ik^3}{(\alpha^2+k^2)^2(\beta^2+k^2)^2}\,[1-(1+\gamma^2)\,F_{i\gamma}(AB)]\\ &+\frac{ik}{2(\alpha+\beta)^2(\alpha-ik)^2(\beta-ik)^2}-\frac{1}{2(\alpha+\beta)^3(\alpha-ik)(\beta-ik)}\\ &+\frac{k\gamma}{2(\alpha+\beta)^2(\alpha^2+k^2)(\beta^2+k^2)}\\ &-\frac{(k\gamma)^2}{(\alpha+\beta)(\alpha+ik)(\beta+ik)(\alpha^2+k^2)(\beta^2+k^2)}. \qquad (2.4)\end{aligned}$$

In order to obtain the scattering amplitude from the off-shell T matrix, one should take the physical on-shell T matrix, i.e., sandwich the T matrix with the appropriate asymptotic states as has been discussed by the author.[7]

Let V_s from now on be restricted to a rank-one potential defined in the partial wave space characterized by l,

$$V_{s,\,l}=-\lambda_l\,|\,g_{\beta,\,l}\rangle\langle g_{\beta,\,l}\,|, \qquad (2.5)$$

where the form factor is given by Eq. (2.2). Suppressing now the subscript β, we get for the physical on-shell Coulomb-modified T matrix,

$$\begin{aligned}t_{cs,\,l}(k)&\equiv\langle k^\infty-|\,T_{cs,\,l}(k^2)\,|\,k^\infty\rangle\\ &=-\tau^c_l\langle k^\infty-|\,g^c_l\rangle\langle g^c_l|\,k^\infty\rangle, \qquad (2.6)\end{aligned}$$

with

$$\tau_l^{c\,-1}=\lambda_l^{-1}+\langle g_l|\,G_c\,|\,g_l\rangle,$$

and the amplitude is proportional to $t_{c,\,l}+t_{cs,\,l}$.

At this point we are able to give a closed formula for the amplitude for $l=1$. Indeed, from Ref. 7 we derive

$$\langle g^c_l|\,k^\infty\rangle=\langle g_l|\,kl+\rangle_c, \qquad (2.7)$$

where the right-hand side is known,

$$\langle g_l|\,kl+\rangle_c=(2/\pi)^{1/2}[i^{i\gamma}(l+i\gamma)!/l!\,]\,k^l(\beta^2+k^2)^{-l-1}\,B^{-i\gamma}. \qquad (2.8)$$

We checked this expression explicitly for $l=1$, using Eq. (2.3) (cf. Ref. 8). Furthermore, a closed form for $\tau^c_{l=1}$ is obtained from Eq. (2.4).

In particular we are now able to express the Coulomb-modified low energy scattering parameters for $l=1$ in terms of known functions. For a repulsive Coulomb potential ($\nu=k\gamma/\beta>0$) the results are

$$\begin{aligned}-a^{-1}_{cs,\,l=1}&=2\beta^3\nu^3\Gamma(0,4\nu)\\ &+\tfrac{1}{16}\,\beta^3\exp(-4\nu)(16\beta^5/\lambda-1+2\nu-8\nu^2), \qquad (2.9)\\ \tfrac{1}{2}r_{cs,\,l=1}&=2\beta\nu\Gamma(0,4\nu)\\ &+\tfrac{1}{6}\,\beta\nu+\exp(-4\nu)[-\tfrac{9}{16}\,\beta+(4+\tfrac{4}{3}\nu)\,\beta^6/\lambda]. \qquad (2.10)\end{aligned}$$

For an attractive Coulomb potential ($\nu<0$) the incomplete gamma function must be replaced by its real part in both equations. The explicit derivation of these formulas will be given in Sec. 4.

For vanishing Coulomb strength: $k\gamma\to 0$, i.e., $\nu\to 0$, Eqs. (2.9) and (2.10) become

$$-a^{-1}_{s,\,l=1}=\beta^8/\lambda-\beta^3/16,$$

$$\tfrac{1}{2}r_{s,\,l=1}=4\beta^6/\lambda-9\beta/16.$$

These expressions just give the effective range parameters for the rank-one potential of Eq. (2.5).

3. THE EFFECTIVE RANGE FUNCTION

It is well known that in the theory of scattering by a short-range potential the so-called effective range function

$$K_l(k^2) = k^{2l+1}\cot\delta_l(k) \tag{3.1}$$

plays an important role. It has been proved that (under certain conditions on the potential) this function is real analytic at the origin. Its first two expansion coefficients are related to the scattering length a_l and the effective range r_l according to[9]

$$K_l(k^2) = -a_l^{-1} + \tfrac{1}{2} r_l k^2 - \cdots. \tag{3.2}$$

If the potential is equal to $V = V_c + V_s$, where V_c is the repulsive Coulomb potential, the effective range function is modified, and may be taken as

$$K_{cs,l}(k^2) = k^{2l+1}\binom{l+i\gamma}{l}\binom{l-i\gamma}{l} \times\left[2\gamma\, h(\gamma) + \frac{2\pi\gamma}{\exp(2\pi\gamma)-1}\left(\cot\delta_l^c - i\right)\right], \tag{3.3}$$

where the function $h(\gamma)$ is defined by[10]

$$h(\gamma) \equiv -2\int_0^\infty \frac{t\,dt}{(t^2+\gamma^2)[\exp(2\pi t)-1]}, \quad \mathrm{Re}\,i\gamma \geq 0. \tag{3.4}$$

If the Coulomb potential is attractive the function $h(\gamma)$ should be replaced by

$$h(\gamma) + i\pi\coth\pi\gamma.$$

Now we know from the work of Cornille and Martin[4] and that of Hamilton *et al.*[3] that for certain classes of *local* potentials the function $K_{cs,l}(k^2)$ is again a real analytic function of k^2 at $k^2 = 0$ with a branch cut on (part of) the negative real axis and possibly with isolated poles in the cut complex k^2 plane. The first two expansion coefficients are related to the Coulomb-modified scattering length $a_{cs,l}$ and effective range $r_{cs,l}$,

$$K_{cs,l}(k^2) = -a_{cs,l}^{-1} + \tfrac{1}{2} r_{cs,l} k^2 - \cdots. \tag{3.5}$$

In this section we shall discuss the effective range function for the case that V_s is a *separable* interaction of finite rank with *rational* form factors. For simplicity we shall restrict ourselves mainly to the simple potential of Eqs. (2.2) and (2.5), and we shall discuss only a few examples of more general rational separable potentials.

The main purpose of the rest of this paper will be to prove for those rational separable potentials the real analyticity of $K_{cs,l}(k^2)$ at $k=0$ for real α and β, to derive a method for exact practical calculations of $K_{cs,l}$, and to investigate it in general.

First we note that the function [cf. also Eq. (27) of Ref. 4]

$$H(\gamma) \equiv \psi(i\gamma) + (2i\gamma)^{-1} - \ln[-i\gamma\,\mathrm{sgn}(s)], \tag{3.6}$$

where ψ is the digamma function, is more useful than $h(\gamma)$. Indeed, by using[11]

$$\psi(i\gamma) = \psi(-i\gamma) - (i\gamma)^{-1} + i\pi\coth\pi\gamma, \tag{3.7}$$

we find that substitution of $h(\gamma)$ by $H(\gamma)$ in Eq. (3.3) yields the general formula for $K_{cs,l}$ which is valid for a repulsive ($s < 0$) as well as for an attractive ($s > 0$) Coulomb potential. (Recall $k\gamma \equiv -s$, so that on the physical domain $\mathrm{Im}\,k \geq 0$ we have $\mathrm{Re}\,i\gamma > 0$ if $s < 0$ and $\mathrm{Re}\,i\gamma < 0$ if $s > 0$). Furthermore, by taking the limit $s \to 0$ in Eq. (3.3) [with $H(\gamma)$ instead of $h(\gamma)$] we obtain Eq. (3.1), independently of the sign of s. This follows from the fact that

$$\lim_{s\to 0} 2\gamma H(\gamma) = i.$$

Some useful equalities in connection with Eq. (3.3) are

$$2\pi\gamma[\exp(2\pi\gamma)-1]^{-1} = \exp(-\pi\gamma)\,\Gamma(1+i\gamma)\,\Gamma(1-i\gamma),$$

and

$$\binom{l+i\gamma}{l}\binom{l-i\gamma}{l} = \prod_{m=1}^{l}(1+\gamma^2/m^2).$$

Now we have to express $\cot\delta_l^c$ occurring in Eq. (3.3) in terms of known functions. The relation of the phase shifts σ_l and δ_l^c with the physical on-shell t matrices is as follows:

$$\begin{aligned} t_{c,l}(k) &= [i^{l}/(\pi k)]\exp(2i\sigma_l), \\ t_{cs,l}(k) &= t_{c,l}(k)[\exp(2i\delta_l^c)-1]. \end{aligned} \tag{3.8}$$

It is now easy to derive

$$\cot\delta_l^c - i = -2\exp(2i\sigma_l)/(\pi k t_{cs,l}),$$

and, with the help of Eq. (2.6) for $t_{cs,l}$, $K_{cs,l}$ is obtained in closed form. For the simple Yamaguchi-type potential of Eqs. (2.2) and (2.5) this yields

$$K_l(k^2) = 2\gamma H(\gamma)\,k^{2l+1}\binom{l+i\gamma}{l}\binom{l-i\gamma}{l} + (\beta^2+k^2)^{2l+2}B^{2l}\{\lambda_l^{-1} + \langle g_l|\,G_{c,l}(k^2)\,|g_l\rangle\}, \tag{3.9}$$

where the subscripts cs and s have been suppressed. An explicit expression for $\langle g_l|G_{c,l}|g_l\rangle$ is known[1] in the case $l=0$, and for $l=1$ we found the expression (2.4).

For a general rational separable potential the function K_l is much more complicated than the one of Eq. (3.9). We claim, however, that, for *any* rational separable potential, K_l can be expressed[12] in terms of simple real analytic functions and a certain function W which we define by

$$W(\gamma;\mu,\nu) \equiv (i\gamma)^{-1}A^{i\gamma}B^{i\gamma}[F_{i\gamma}(AB) - \tfrac{1}{2}] + H(\gamma). \tag{3.10}$$

This function depends on $\mu = k\gamma/\alpha$ and $\nu = k\gamma/\beta$ through A and B respectively. A warning is appropriate here, that $A^{i\gamma}B^{i\gamma}$ is not everywhere equal to $(AB)^{i\gamma}$. This will be discussed in Secs. 4 and 5. Note that W is independent of l and of the particular potential employed. We have worked out three examples for different types of potentials, in order to make the above conjecture plausible. These three cases describe the principal generalizations of the Yamaguchi potential that one can imagine.

(i) The rank-one potential of Eqs. (2.2) and (2.5) for all l, that is, Eq. (3.9). In this case we find

$$K_l = R_l^{(1)} + R_l^{(2)}\,W(\gamma;\nu,\nu), \tag{3.11}$$

with

$$R_l^{(2)} = 2\gamma k^{2l+1} \binom{l+i\gamma}{l} \binom{l-i\gamma}{l},$$

and $R_l^{(1)}$ is regular at zero energy.

(ii) A rank-one potential with form factor

$$g(p) = (p^2+\alpha^2)^{-1} + b(p^2+\beta^2)^{-1},$$

for $l=0$ only (b is a real parameter). This yields the expression

$$K_l = R^{(0)} + R^{(\mu)} W(\gamma;\mu,\mu) + R^{(\nu)} W(\gamma;\nu,\nu) + R^{(\mu\nu)} W(\gamma;\mu,\nu) \tag{3.12}$$

(iii) A rank-two potential with form factors of the type of Eq. (2.2), for $l=0$ only. Then we get

$$K_0 = 2k\gamma \times \frac{[R_\alpha + W(\gamma;\mu,\mu)][R_\beta + W(\gamma;\nu,\nu)] - [R_{\alpha\beta} + W(\gamma;\mu,\nu)]^2}{R_\alpha + R_\beta - 2R_{\alpha\beta} + W(\gamma;\mu,\mu) + W(\gamma;\nu,\nu) - 2W(\gamma;\mu,\nu)}. \tag{3.13}$$

The R's denote simple real analytic functions. Their dependence on k (or γ) is contained in the quantities $A^{i\gamma}$, $B^{i\gamma}$, and rational functions of k^2 with real coefficients. We shall derive in Sec. 4 the equality [recall $A = (1+i\mu^{-1}\gamma)/(1-i\mu^{-1}\gamma)$]

$$A^{i\gamma} = \exp[-2\gamma \arctan(\mu/\gamma)] = \exp[(2s/k)\arctan(k/\alpha)],$$

from which it easily follows that $A^{i\gamma}$ and similarly $B^{i\gamma}$ is real analytic at $k=0$ for real α and β respectively.

Our main task will be to prove that $W(\gamma;\mu,\nu)$ is a real analytic function of γ^{-2} at $\gamma^{-2}=0$. Once this proof has been given, it is relatively easy to investigate the effective range function itself. We shall find that the only singularities of W are the branch cuts $-\infty < k^2 < -\alpha^2$ and $-\infty < k^2 < -\beta^2$. The only additional singularities of K_l can be (isolated) poles of finite order, i.e., K_l is a meromorphic function in the cut k^2 plane. The position of these poles depends on the particular potential and cannot be predicted in general. We have been able to show that K_l of Eq. (3.11) is real analytic at $k=0$. However, in general even a pole at $k=0$ can occur although this is exceptional. It may be interesting to consider an example in some detail.

We take the rank-one potential of Eq. (2.5) for $l=0$, with form factor

$$g(p^2) = \left(\frac{2}{\pi}\right)^{1/2} \left(p^2 - \frac{\beta^2 s}{\beta - s}\right) (p^2+\beta^2)^{-2}. \tag{3.14}$$

With this form factor g we obtain from Eq. (2.8)

$$\langle g | k+\rangle_c = (2/\pi)^{1/2} i^{i\gamma} \Gamma(1+i\gamma) k^2 (\beta^2+k^2)^{-2} B^{-i\gamma}. \tag{3.15}$$

Utilizing Eqs. (86)—(88) of Ref. 1 we derive $\langle g | G_c | g\rangle$, and for the effective range function we get then

$$K_0 = 2k\gamma W(\gamma;\nu,\nu) + k^{-4}R, \tag{3.16}$$

where R is a certain real analytic function of k^2 which is regular and different from zero at $k=0$. Consequently, K_0 has a pole of fourth order at the origin.

We like to discuss a few properties of the Coulomb-modified phase shift δ_l^c. At a bound state of $V_c + V_s$ we have in general

$$\cot\delta_l^c = i, \quad \delta_l^c = -i\infty. \tag{3.17}$$

This corresponds with the situation for a pure short-range potential, where we have

$$t_{s,l}(k) = [1 - \exp(2i\delta_{s,l})]/(i\pi k). \tag{3.18}$$

In general $t_{s,l}(k)$ has a pole at the bound state, so that

$$\cot\delta_{s,l} = i, \quad \delta_{s,l} = -i\infty. \tag{3.19}$$

Since $t_{s,l}(k)$ is always real for negative energy, it also follows from Eq. (3.18) that $\delta_{s,l}(k)$ is (purely) imaginary when k is imaginary. In contrast, this does *not* hold for $\delta_l^c(k)$; from Eq. (3.3) we see that the expression

$$(\cot\delta_l^c - i)/[\exp(2\pi\gamma) - 1] \tag{3.20}$$

must be real for negative energy because $h(\gamma)$ is then real.

Finally we note that the central function on the right-hand side of Eq. (3.10) is $F_{i\gamma}(AB)$. We have met this function before.[1,2] Its behavior at $k=0$ is particularly interesting but complicated. Now it seems that just this function appears in the off-shell T matrix formula for the Coulomb plus any rational separable potential. For the case $l=0$ this has been proved by van Haeringen and van Wageningen.[1] See also the recent paper by Bajzer.[13] Equations (2.3) and (2.4) of the present paper suggest that the same holds for $l=1$ and we have reasons to believe that it is true for all l. Moreover, it is very likely that also the *pure* Coulomb transition matrices $T_{c,l}$ contain functions $F_{i\gamma}$ with a similar structure, see, e.g., Eq. (2.1). For these reasons we devote the following section to an investigation of $F_{i\gamma}(AB)$.

4. THE FUNCTION $F_{i\gamma}(AB)$

As a first step in our proof we shall consider in this section the function $F_{i\gamma}(AB)$ for real positive k, α, and β, so γ is real. The series representation

$$F_{i\gamma}(z) = i\gamma \sum_{n=0}^{\infty} z^n/(n+i\gamma) \tag{4.1}$$

reminds us of the logarithmic function series

$$-\ln(1-z) = \sum_{n=1}^{\infty} z^n/n.$$

Indeed we have (Ref. 11, pp. 13 and 49)

$$\lim_{\gamma\to 0} (1 - F_{i\gamma}(z))/(i\gamma) = \ln(1-z)$$

and

$$\lim_{z\to 1}[\ln(1-z) + (1/i\gamma)F_{i\gamma}(z)] = -C - \psi(i\gamma) = \sum_{n=0}^{\infty}\left(\frac{1}{n+i\gamma} - \frac{1}{n+1}\right). \tag{4.2}$$

Here ψ is the digamma function as before, $\psi(z) = \Gamma'(z)/\Gamma(z)$ and $C = 0.5772\ldots$ is the constant of Euler or Mascheroni. We have substituted $-C$ for $\psi(1)$.

The infinite series in Eq. (4.1) is convergent if $|z| \le 1$, $z \neq 1$. When $|z| > 1$, but z not real positive, one can find an expression for $F_{i\gamma}(z)$ by applying the very useful formula [see Eq. (32) of Ref. 1]

$$F_{i\gamma}(z) + F_{-i\gamma}(1/z) = 1 + \Gamma(1+i\gamma)\Gamma(1-i\gamma)(-z)^{-i\gamma}, \tag{4.3}$$

since the series (4.1) for $F_{-i\gamma}(1/z)$ converges in that case.

Now we have $A=(\alpha+ik)/(\alpha-ik)$, $B=(\beta+ik)/(\beta-ik)$ with $\alpha,\beta,k>0$, so $A^*=A^{-1}$, $B^*=B^{-1}$ and Eq. (4.3) gives

$$2\,\mathrm{Re}F_{i\gamma}(AB)=F_{i\gamma}(AB)+F_{-i\gamma}(A^{-1}B^{-1})$$
$$=1+|\Gamma(1+i\gamma)|^2(-AB)^{-i\gamma}. \tag{4.4}$$

However, $\mathrm{Im}F_{i\gamma}(AB)$ is somewhat more complicated. In Ref. 2 we have obtained the coefficients c_0 and c_2 (in the restricted case $A=B$) of the asymptotic expansion

$$\gamma^{-1}\mathrm{Im}F_{i\gamma}(AB)=\mathrm{Re}(i\gamma)^{-1}F_{i\gamma}(AB)$$
$$=c_0+c_2(i\gamma)^{-2}+O(\gamma^{-4}),\quad \gamma^2\to\infty.$$

Since then we have found that the coefficients d_{2n} of the asymptotic expansion

$$A^{i\gamma}B^{i\gamma}\,\mathrm{Re}(i\gamma)^{-1}F_{i\gamma}(AB)$$
$$=d_0+d_2(i\gamma)^{-2}+d_4(i\gamma)^{-4}+O(\gamma^{-6}),\quad \gamma^2\to\infty, \tag{4.5}$$

have simpler closed expressions than c_{2n}. We shall derive d_0, d_2, and d_4 in explicit form. Let us first investigate the factor $A^{i\gamma}B^{i\gamma}$. We use for convenience the parameters μ and ν, defined before by

$$\mu\alpha\equiv\nu\beta\equiv k\gamma\equiv -s. \tag{4.6}$$

If arctan denotes the principal value determined by

$$-\tfrac{1}{2}\pi<\arctan x<\tfrac{1}{2}\pi,\quad -\infty<x<\infty,$$

then the following equalities hold for $k>0$:

$$(1/2i)\ln(-AB)=\arctan[(k^2-\alpha\beta)/k(\alpha+\beta)]$$
$$=\arctan[(\mu\nu-\gamma^2)/\gamma(\mu+\nu)]$$
$$=-\tfrac{1}{2}\pi+\arctan(k/\alpha)+\arctan(k/\beta)$$
$$=\tfrac{1}{2}\pi-\arctan(\gamma/\mu)-\arctan(\gamma/\nu), \tag{4.7}$$

$$(1/2i)\ln(AB)=\arctan[k(\alpha+\beta)/(\alpha\beta-k^2)]$$
$$=\arctan[\gamma(\mu+\nu)/(\gamma^2-\mu\nu)]$$
$$=-\pi+\arctan(k/\alpha)+\arctan(k/\beta)\quad \text{if } k^2>\alpha\beta$$
$$=\arctan(k/\alpha)+\arctan(k/\beta)\quad \text{if } k^2<\alpha\beta. \tag{4.8}$$

Therefore

$$(-AB)^{i\gamma}=\exp(\pi\gamma)A^{i\gamma}B^{i\gamma}, \tag{4.9}$$

$$(AB)^{i\gamma}=\exp(2\pi\gamma)A^{i\gamma}B^{i\gamma}\quad \text{if } k^2>\alpha\beta,\ \text{i.e., if } \gamma^2<\mu\nu,$$
$$=A^{i\gamma}B^{i\gamma}\quad \text{if } k^2<\alpha\beta,\ \text{i.e., if } \gamma^2>\mu\nu, \tag{4.10}$$

which shows that indeed $A^{i\gamma}B^{i\gamma}$ is not everywhere equal to $(AB)^{i\gamma}$, cf. Sec. 3. We shall work in the region defined by $0<k<\min(\alpha,\beta)$, which means that we can write $(AB)^{i\gamma}$ for $A^{i\gamma}B^{i\gamma}$, and we can expand $\arctan(k/\alpha)$ and $\arctan(k/\beta)$ at $k=0$ in the well-known way. From

$$A^{i\gamma}=\exp[-2\gamma\arctan(\mu/\gamma)]=\exp[(2s/k)\arctan(k/\alpha)] \tag{4.11}$$

we see that $A^{i\gamma}$ is real analytic at $k=0$, and so is $(AB)^{i\gamma}$. This means in particular that $A^{i\gamma}$ and $(AB)^{i\gamma}$ are real for real k, α, and β.

After these introductory formulas we are now in the position to derive the coefficients d_{2n} of Eq. (4.5). The integral representation

$$F_{i\gamma}(AB)=i\gamma\int_0^1 t^{i\gamma-1}(1-ABt)^{-1}\,dt,$$

which holds for $\mathrm{Re}\,i\gamma>0$, can be recast into the form

$$(AB)^{i\gamma}[F_{i\gamma}(AB)-1]=i\gamma\int_0^{AB}t^{i\gamma}(1-t)^{-1}\,dt. \tag{4.12}$$

This equation is valid for $0<k<\alpha$, $0<k<\beta$. We differentiate both sides of this equation with respect to μ. By splitting the derivatives into real and imaginary parts we find, using Eq. (4.5),

$$\frac{(AB)^{i\gamma}}{\mu+\nu}\,\frac{\mu\nu-\gamma^2}{\mu^2+\gamma^2}=d_0'+d_2'(i\gamma)^{-2}+d_4'(i\gamma)^{-4}+O(\gamma^{-6}), \tag{4.13}$$

with $d_{2n}'\equiv d_{2n}'(\mu,\nu)\equiv(d/d\mu)d_{2n}(\mu,\nu)$. By taking the limit for $\gamma^{-2}\to 0$ of both sides of Eq. (4.13) we obtain

$$d_0'=-\exp(-2\mu-2\nu)\quad(\mu+\nu). \tag{4.14}$$

By inserting this expression into Eq. (4.13) and multiplying with $\exp(2\mu+2\nu)$ we get

$$\exp(2\mu+2\nu)\sum_{n=1}^{\infty}d_{2n}'(i\gamma)^{-2n}$$
$$=\frac{1}{\mu+\nu}\,[1-(AB)^{i\gamma}\exp(2\mu+2\nu)]$$
$$+\frac{\mu}{\mu^2+\gamma^2}\,(AB)^{i\gamma}\exp(2\mu+2\nu). \tag{4.15}$$

(The series $\sum d_{2n}'(i\gamma)^{-2n}$ converges, although $\sum d_{2n}(i\gamma)^{-2n}$ diverges.)

Now Eq. (4.8) yields

$$(AB)^{i\gamma}\exp(2\mu+2\nu)$$
$$=\exp\left[2\mu+2\nu-2\gamma\arctan\frac{(\mu+\nu)/\gamma}{1-\mu\nu/\gamma^2}\right]$$
$$=\exp\left[(2\mu+2\nu)\left(\frac{-\mu\nu/\gamma^2}{1-\mu\nu/\gamma^2}+\frac{1}{3}\,\frac{(\mu+\nu)^2/\gamma^2}{(1-\mu\nu/\gamma^2)^3}\right.\right.$$
$$\left.\left.-\frac{1}{5}\,\frac{(\mu+\nu)^4/\gamma^4}{(1-\mu\nu/\gamma^2)^5}+\cdots\right)\right].$$

Consequently, we have the interesting relation

$$(AB)^{i\gamma}\exp(2\mu+2\nu)=1-(2\mu+2\nu)\sum_{n=1}^{\infty}b_{2n}(i\gamma)^{-2n}, \tag{4.16}$$

where $b_{2n}\equiv b_{2n}(\mu,\nu)$ are certain symmetric *polynomials* in μ and ν, of degree $3n-1$. Therefore, the factor $1/(\mu+\nu)$ in Eq. (4.15) cancels. Upon substitution of Eq. (4.16) into Eq. (4.15) we find

$$\exp(2\mu+2\nu)\,d_{2n}'=2b_{2n}-\mu^{2n-1}+(2\mu+2\nu)\sum_{m=2}^{n}b_{2m-2}\,\mu^{2n-2m+1}.$$

So d_{2n}' is equal to $\exp(-2\mu-2\nu)$ times some polynomial in μ and ν of degree $3n-1$. For $n=1$ and $n=2$ we have obtained

$$d_2'=\tfrac{1}{3}\exp(-2\mu-2\nu)[2\mu^2+2\nu^2-\mu(2\nu+3)],$$
$$d_4'=-\tfrac{1}{45}\exp(-2\mu-2\nu)[10\mu^5-2\mu^4(5\nu+24)$$
$$+\mu^3(10\nu^2+18\nu+45)+2\mu^2\nu^2(5\nu-9)$$
$$-2\mu\nu^3(5\nu+6)+2\nu^4(5\nu-9)]. \tag{4.17}$$

Integration of d_{2n}' with respect to μ yields d_{2n} up to some

function of ν. Because $d_{2n}(\mu,\nu)$ must be symmetric in μ and ν, it follows from the special form of d'_{2n} that this function can only be a constant. This integration constant will be determined below.

It is easy to see that the integration of an expression of the form $\exp(z)\,\mathrm{Pol}(z)$ yields $\exp(z)$ times a polynomial of the same degree. Therefore, d_{2n} is (just as d'_{2n}) equal to $\exp(-2\mu-2\nu)$ times a polynomial of degree $3n-1$ (for $n>0$). This polynomial is now, to course, symmetric in μ and ν. An economical way to obtain d_{2n} from d'_{2n} is to make use of the equalities

$$\frac{d}{dz}\,\Gamma(n+1,\lambda z) = -\lambda(\lambda z)^n \exp(-\lambda z)$$

and

$$\Gamma(n+1,\ z) = n!\, e_n(z)\exp(-z) \tag{4.18}$$

Here the polynomial e_n is defined by (Ref. 11, p. 338)

$$e_n(z) \equiv \sum_{m=0}^{n} z^m/m! \tag{4.19}$$

and $\Gamma(n+1,z)$ is the incomplete gamma function.

We have obtained the following explicit expressions:

$$\begin{aligned}
d_0 &= \mathrm{Re}\,\Gamma(0, 2\mu+2\nu),\\
d_2 &= \tfrac{1}{12}\exp(-2\mu-2\nu)\{1+(2\mu+2\nu)\\
&\quad +(1/2!)(2\mu+2\nu)^2 - 6(\mu^2+\nu^2)\}\\
&= \tfrac{1}{12}\exp(-2\mu-2\nu)\{e_2(2\mu+2\nu) - 6(\mu^2+\nu^2)\},\\
d_4 &= -\tfrac{1}{120}\exp(-2\mu-2\nu)\{1+(2\mu+2\nu)+(1/2!)(2\mu+2\nu)^2\\
&\quad +(1/3!)(2\mu+2\nu)^3+(1/4!)(2\mu+2\nu)^4+30(\mu^4+\nu^4)\\
&\quad -\tfrac{40}{3}(\mu^5-\mu^4\nu+\mu^3\nu^2+\mu^2\nu^3-\mu\nu^4+\nu^5)\}\\
&= \tfrac{1}{4}\exp(-2\mu-2\nu)\{B_3 e_3(2\mu+2\nu) - \mu^4-\nu^4\\
&\quad +\tfrac{1}{9}(\mu^5-\mu^4\nu+\mu^3\nu^2+\mu^2\nu^3-\mu\nu^4+\nu^5)\}.
\end{aligned} \tag{4.20}$$

The expression for d_0 is in agreement with the expression for c_0 given in Eq. (31) of Ref. 2. [Notice that $\Gamma(0,z)$ is real for real positive z. Along the negative real axis it has a branch cut, but the real part of $\Gamma(0,z)$ is continuous across this cut so that $\mathrm{Re}\,\Gamma(0,z)$ is well defined for $z<0$, cf. Eq. (6.3)]. It is interesting to compare Eq. (4.20) with the general formula for d_{2n} in Eq. (5.20) below. In Eq. (4.20) the correct integration constants have already been inserted in the expressions for d_2 and d_4. Now we are going to determine these constants. This will be done by considering Eq. (4.5) for $\mu,\nu\to 0$ and $\alpha,\beta\to\infty$, such that $\mu\alpha=\nu\beta=k\gamma=-s$ remains constant. Utilizing

$$\lim_{\alpha\to\infty} A^{i\gamma} = \lim_{\beta\to\infty} B^{i\gamma} = 1$$

we get from Eq. (4.5)

$$\begin{aligned}
&\lim_{\substack{\mu,\nu\to 0\\ \alpha,\beta\to\infty}} \mathrm{Re}(1/(i\gamma)\,F_{i\gamma}(AB) - d_0)\\
&\quad = \lim_{\mu,\nu\to 0}(d_2(i\gamma)^{-2} + d_4(i\gamma)^{-4} + \cdots).
\end{aligned} \tag{4.21}$$

From Eq. (25) of Ref. 2 [see Eq. (4.28) below] it follows that

$$\begin{aligned}
1/(i\gamma)\,F_{i\gamma}(AB) &= \psi(1) - \psi(i\gamma) - \ln(1-AB)\\
&\quad + O(1-AB),\quad AB\to 1.
\end{aligned}$$

Using Eqs. (29) and (30) of Ref. 2, we get [recall that $\psi(1)=-C$]

$$\begin{aligned}
&\lim_{\mu,\nu\to 0} \mathrm{Re}(1/(i\gamma)\,F_{i\gamma}(AB) - d_0) = \mathrm{Re}[\ln\gamma - \psi(i\gamma)]\\
&\quad \sim \sum_{n=1}^{\infty} (i\gamma)^{-2n} B_{2n}/(2n),
\end{aligned} \tag{4.22}$$

where B_{2n} are the Bernoulli numbers. The symbol $\sim$ denotes an asymptotic expansion. Note that the infinite series in Eq. (4.22) is divergent for all finite γ. Comparison of Eq. (4.22) with Eq. (4.21) yields

$$\lim_{\mu,\nu\to 0} d_{2n}(\mu,\nu) = B_{2n}/(2n),\quad n=1,2,\cdots,$$

and this determines the above mentioned constant of the μ integration, if the symmetry with respect to μ and ν is taken into account.

We summarize the results obtained so far. The coefficients $d_{2n} = d_{2n}(\mu,\nu)$ of the asymptotic expansion

$$(AB)^{i\gamma}\,\mathrm{Re}\left(\frac{1}{i\gamma}\,F_{i\gamma}(AB)\right) \sim \sum_{n=0}^{\infty} d_{2n}(i\gamma)^{-2n} \tag{4.23}$$

are symmetric functions of μ and ν. For $n>0$ we have

$$d_{2n}(\mu,\nu) = \exp(-2\mu-2\nu)\,P_{3n-1}(\mu,\nu), \tag{4.24}$$

where P is a certain polynomial of degree $3n-1$ and symmetric in μ and ν. Its value for $\mu=\nu=0$ can be expressed in terms of the Bernoulli numbers B_{2n},

$$d_{2n}(0,0) = P_{3n-1}(0,0) = B_{2n}/(2n),\quad n=1,2,\cdots. \tag{4.25}$$

Equation (4.20) gives d_0, d_2, and d_4 in closed form. The expressions for c_0 and c_2, which follow from $d_0(\nu,\nu)$ and $d_2(\nu,\nu)$, agree with Eqs. (31) and (32) of Ref. 2. The effective range parameters for $l=1$ given in Eqs. (2.9) and (2.10) can easily be obtained with the help of the expressions for d_0 and d_2.

We conclude this section with a few formulas that are useful for the high-energy limit: $k\to\infty$. It turns out that $\mathrm{Re}F_{i\gamma}(AB)$ can be expanded in a power series at $\gamma=0$. Let $|\gamma|\ll 1$, $|\gamma|\ll|\mu|$, and $|\gamma|\ll|\nu|$. Apply Eqs. (4.4) and (4.7) and recall that γ, μ, and ν have equal signs since k, α, and β are real positive by definition. With the help of the well-known equality

$$\begin{aligned}
&\exp(\pi\gamma)\,\Gamma(1+i\gamma)\,\Gamma(1-i\gamma)\\
&\quad = 1+\pi\gamma+\sum_{n=1}^{\infty}(2\pi\gamma)^{2n}B_{2n}/(2n)!,\quad |\gamma|\ll 1\\
&\quad = \sum_{n=0}^{\infty}(-2\pi\gamma)^n B_n/n!,\quad |\gamma|\ll 1,
\end{aligned} \tag{4.26}$$

the following interesting equality is readily established:

$$\begin{aligned}
&2\,\mathrm{Re}F_{i\gamma}(AB)\\
&\quad = 1+\exp\left[-2\gamma\arctan\frac{\gamma(\mu+\nu)}{\mu\nu-\gamma^2}\right]\sum_{n=0}^{\infty}(-2\pi\gamma)^n\frac{B_n}{n!},\quad |\gamma|\ll 1.
\end{aligned} \tag{4.27}$$

The exponential function here is recast into [cf. Eq. (4.7)]

$$\exp\{-2\gamma[\arctan(\gamma/\mu)+\arctan(\gamma/\nu)]\},$$

and this function can easily be expanded in powers of γ^2. Alternatively one can start from Eq. (25) of Ref. 2 which can be rewritten as

$$F_{i\gamma}(z) = i\gamma \sum_{n=0}^{\infty} \binom{n+i\gamma-1}{n} (1-z)^n \times [\psi(n+1) - \psi(n+i\gamma) - \ln(1-z)], \quad |1-z|<1, \quad |\arg(1-z)|<\pi. \tag{4.28}$$

Further one has to use the Laurent expansion of the digamma function $\psi(z)$ at $z=0$ (Ref. 11, p. 13, corrected for the misprint),

$$\psi(z) = -\frac{1}{z} - C - \sum_{n=1}^{\infty} \zeta(n+1)(-z)^n, \quad 0<|z|<1, \tag{4.29}$$

where ζ is Riemann's zeta function. After a few manipulations one arrives at the expansion

$$F_{i\gamma}(AB) = 1 + \tfrac{1}{2}\pi\gamma + \gamma^2\left(\frac{\pi^2}{6} - \frac{1}{\mu} - \frac{1}{\nu}\right) - i\gamma \ln\left(\frac{2\gamma}{\mu} + \frac{2\gamma}{\nu}\right) + O(\gamma^3 \ln|\gamma|), \quad \gamma \to 0. \tag{4.30}$$

The real part of this expression agrees with the second-order approximation obtained from Eq. (4.27).

5. THE FUNCTIONS $W(\gamma;\mu,\nu)$ AND $W(\gamma;\xi)$

In this section we are going to investigate the function $W(\gamma;\mu,\nu)$ introduced in Eq. (3.10). We shall *assume* in this section that $W(\gamma;\mu,\nu)$ is real analytic at γ^{-2} for real μ and ν. The proof will be given in Sec. 6A. The three independent variables γ, μ, and ν are related to k, α, and β respectively through Eq. (4.6), where the strength s is supposed to be fixed.

It turns out that it is useful to investigate in addition a closely related but somewhat simpler function, which we denote by $W(\gamma;\xi)$. This function is also real analytic at $\gamma^{-2}=0$ (which will be proved in Sec. 6B). We shall obtain all its expansion coefficients in closed form. In this whole section we still take μ, ν, and ξ real, and only (k and) γ complex.

A. The function $W(\gamma;\mu,\nu)$

The defining expression for $W(\gamma;\mu,\nu)$ is obtained from Eqs. (3.6) and (3.10),

$$W(\gamma;\mu,\nu) = (i\gamma)^{-1} A^{i\gamma} B^{i\gamma} [F_{i\gamma}(AB) - \tfrac{1}{2}] + \psi(i\gamma) + (2i\gamma)^{-1} - \ln[-i\gamma\,\mathrm{sgn}(s)], \tag{5.1}$$

where the last three terms are equal to $H(\gamma)$. Since we have assumed that W is real analytic at $\gamma^{-2}=0$, we may write

$$W(\gamma;\mu,\nu) = \sum_{n=0}^{\infty} w_{2n}(\mu,\nu)(i\gamma)^{-2n}, \tag{5.2}$$

where the coefficients $w_{2n}(\mu,\nu)$ are real symmetric functions of μ and ν.

We are interested in the radius of convergence of the expansion (5.2) and in closed expressions for $w_{2n}(\mu,\nu)$. When we take γ real for the moment, we can write

$$W(\gamma;\mu,\nu) = \mathrm{Re}[H(\gamma)] + \mathrm{Re}\{(i\gamma)^{-1} A^{i\gamma} B^{i\gamma} [F_{i\gamma}(AB) - \tfrac{1}{2}]\},$$

because $W(\gamma;\mu,\nu)$ is a real-valued function for real γ, μ, and ν. From Eq. (30) of Ref. 2 and Eq. (3.6) we have the asymptotic expansion

$$\mathrm{Re}H(\gamma) \sim -\sum_{n=1}^{\infty} (i\gamma)^{-2n} B_{2n}/(2n). \tag{5.3a}$$

Notice that the infinite series diverges for all finite γ. Further Eq. (4.23) yields

$$\mathrm{Re}\{(i\gamma)^{-1} A^{i\gamma} B^{i\gamma} [F_{i\gamma}(AB) - \tfrac{1}{2}]\} \sim \sum_{n=0}^{\infty} d_{2n}(i\gamma)^{-2n}. \tag{5.3b}$$

Addition of Eqs. (5.3a) and (5.3b) gives $W(\gamma;\mu,\nu)$. Because the asymptotic series expansions are unique, it follows that

$$w_0 = d_0 = \mathrm{Re}\Gamma(0, 2\mu+2\nu),$$
$$w_{2n} = d_{2n} - B_{2n}/(2n), \quad n = 1, 2, \cdots. \tag{5.4}$$

It is interesting that the summation of the two divergent asymptotic series in Eqs. (5.3a) and (5.3b) yields a convergent series, that is, the power series (5.2).

In order to investigate the radius of convergence of the latter, we shall study the singularities of the functions occurring on the right-hand side of Eq. (5.1). We discern four sources of singularities namely those originating from

(i) $A^{i\gamma}B^{i\gamma}$,

(ii) the hypergeometric function $F_{i\gamma}(AB)$,

(iii) the logarithmic function,

(iv) the digamma function $\psi(i\gamma)$.

(i) In the first place, $A^{i\gamma} \equiv \exp(i\gamma \ln A)$ has a branch cut for real negative A and similarly $B^{i\gamma}$ for real negative B. The location of these branch cuts in the complex k plane is easily found. For real positive α and complex k we have

$$A = \frac{\alpha+ik}{\alpha-ik} = \frac{\alpha^2 - |k|^2 + 2i\alpha\,\mathrm{Re}k}{(\alpha+\mathrm{Im}k)^2 + (\mathrm{Re}k)^2}.$$

Since the denominator is clearly always positive (or zero), it follows that A is real and negative if and only if $\mathrm{Re}k=0$ and $|k|>\alpha$. The branch cut, therefore, consists of the two intervals $(-i\infty, -i\alpha)$ and $(i\alpha, i\infty)$ along the imaginary k axis. The product $A^{i\gamma}B^{i\gamma}$ has in the k plane the following four branch cuts:

$$(i\alpha, i\infty), \quad (-i\infty), \quad -i\alpha), \quad (i\beta, i\infty), \quad (-i\infty, -i\beta). \tag{5.5}$$

We have used $(-AB)^{i\gamma}$ in Eqs. (4.4) and (4.9). It is useful to know the branch cuts of this quantity. They are determined by $\mathrm{Im}AB=0$, $\mathrm{Re}AB<0$. Now

$$\mathrm{Im}AB = D^{-1}(\alpha+\beta)(\alpha\beta - |k|^2)\mathrm{Re}k,$$

where D is real nonnegative. Therefore, AB is real if and only if either $|k|^2=\alpha\beta$ or $\mathrm{Re}k=0$. Assuming $\alpha>\beta$ for definiteness, one can easily verify:

$$AB>1 \iff k\in(-i\infty, -i\beta)\cup(-i\alpha, 0), \tag{5.6a}$$

$$AB<0 \iff k\in(-i\infty, -i\beta)\cup(-i\alpha, i\alpha)\cup(i\beta, i\infty), \tag{5.6b}$$

$$AB<0 \iff k\in(-i\beta, -i\alpha)\cup(i\alpha, i\beta) \text{ or } |k|^2=\alpha\beta. \tag{5.6c}$$

Therefore $(-AB)^{i\gamma}$ has the three branch cuts of Eq. (5.6b). Furthermore, we have in the k plane, cut along the imaginary axis,

$$(-AB)^{i\gamma} = \exp(\pm\pi\gamma) A^{i\gamma} B^{i\gamma}, \quad \mathrm{Re}k \gtrless 0. \tag{5.7a}$$

Note that the origin is an exceptional point here since $k=0$ is an isolated essential singularity of $\exp(\pm\pi\gamma)$.

Although $(AB)^{i\gamma}$ plays no role in the physical quantities, it is interesting to compare also this function with $A^{i\gamma}B^{i\gamma}$. The branch cut of $(AB)^{i\gamma}$ is given by Eq. (5.6c). It has a rather peculiar shape. There are four branch points namely $\pm i\alpha$, $\pm i\beta$ and the cut connecting them is only one curve, composed of a circle and two finite intervals. Inside the circle $|k|^2=\alpha\beta$ we have

$$(AB)^{i\gamma}=A^{i\gamma}B^{i\gamma}, \quad |k|^2<\alpha\beta, \tag{5.7b}$$

and, outside the circle,

$$(AB)^{i\gamma}=\exp(\pm 2\pi\gamma)A^{i\gamma}B^{i\gamma}, \quad \mathrm{Re}k\geq 0, \quad |k|^2>\alpha\beta. \tag{5.7c}$$

(ii) Secondly, $F_{i\gamma}(AB)$ has a branch cut for real AB with $1<AB<\infty$. According to Eq. (5.6a) AB is real and larger than one if and only if k lies in either the interval $(-i\infty, -i\beta)$ or the interval $(-i\alpha, 0)$. The discontinuity across the cut $(-i\alpha, 0)$ of the expression

$$(i\gamma)^{-1}A^{i\gamma}B^{i\gamma}F_{i\gamma}(AB)$$

in Eq. (5.1) is equal to $2\pi i$; see Eq. (6.19) below. It is remarkable that this discontinuity is independent of α and β, despite the fact that the expression itself does depend on α and β.

Further $F_{i\gamma}(z)/\Gamma(1+i\gamma)$ is an entire function of $i\gamma$ for fixed z. This implies that $F_{i\gamma}(z)$ has simple poles at $i\gamma=-n$ for $n=1,2,\cdots$.

(iii) In the third place $\ln[-i\gamma\,\mathrm{sgn}(s)]$ yields a branch cut for $0<ik<\infty$, that is, for k on the negative imaginary axis. The discontinuity across the cut is $-2\pi i$. If we combine this with the branch cut $0<ik<\alpha$ from (ii), we see that the discontinuities cancel. Therefore, we call $(-i\alpha, 0)$ a "removable branch cut" of $W(\gamma;\mu,\nu)$. Below we shall find other removable singularities.

The above considerations lead us to the conjecture that the infinite series in Eq. (5.2) converges provided that

$$|k|<\min(\alpha,\beta), \quad \text{i.e.,} \quad |\gamma|^2>\max(\mu^2,\nu^2). \tag{5.8}$$

(iv) In the fourth place the digamma function $\psi(i\gamma)$ is a meromorphic function having simple poles at $i\gamma=-n$, $n=0,1,2,\cdots$. The pole at $i\gamma=0$ is always located outside the domain defined by Eq. (5.8). Now $F_{i\gamma}(AB)$ has simple poles at $i\gamma=-n$ for $n=1,2,\cdots$ [see (ii)]. It will be shown below that the residues of $\psi(i\gamma)$ at these poles cancel the residues of $1/(i\gamma)A^{i\gamma}B^{i\gamma}F_{i\gamma}(AB)$, despite the fact that this latter expression depends also on α and β. Consequently, $W(\gamma;\mu,\nu)$ can be made regular at these "Coulomb bound-state poles." We may call them "removable poles." The limit for $n\to\infty$ is particularly interesting. This point $i\gamma=-\infty$ is the origin $k=0$, and we will find that this singularity is removable as well.

We conclude this section now with a short derivation of the value of $W(\gamma;\mu,\nu)$ at $i\gamma=-n$, and for comparison at $i\gamma=n$, for $n=1,2,\cdots$. In the limit $n\to\infty$ we shall obtain in both cases the value w_0 which is just what we expect from Eq. (5.2).

Utilizing

$$\lim_{x\to -n}[\psi(x)+1/(x+n)]=\psi(n+1)$$

and l'Hôspital's theorem, we find

$$\lim_{i\gamma\to -n}\left[\psi(i\gamma)+\frac{z^{i\gamma}}{i\gamma}F_{i\gamma}(z)\right]$$
$$=\psi(n+1)+\ln z+\sum_{\substack{m=0\\ m\neq n}}^{\infty}\frac{z^{m-n}}{m-n}$$
$$=-C-\ln\frac{1-z}{z}+\sum_{m=1}^{n}\frac{1-z^m}{m}.$$

Let $0<s<\alpha,\beta$ and so $-1<\mu,\nu<0$. (Note that the poles occur only in case of attraction, i.e., if s is positive). Then we obtain from Eq. (5.1) with the help of the above formulas,

$$\lim_{i\gamma\to -n}W(\gamma;\mu,\nu)=-C-\ln(-2\mu-2\nu)$$
$$+\ln\left[\left(\frac{n+\mu}{n}\right)\left(\frac{n+\nu}{n}\right)\right]-\sum_{m=1}^{n}{}'\frac{1}{m}\left[\left(\frac{n-\mu}{n+\mu}\,\frac{n-\nu}{n+\nu}\right)^m-1\right]. \tag{5.9a}$$

The prime in $\sum'$ means that the last term ($m=n$) should be divided by 2. The limit for $n\to\infty$ of the right-hand side of Eq. (5.9a) must be equal to $W(\gamma;\mu,\nu)$ at $k=0$, that is, $w_0(\mu,\nu)$ for which we have the closed form (5.4). That this limit has indeed the correct value can be checked as follows. The formula

$$\lim_{n\to\infty}\sum_{m=1}^{n}\frac{1}{m}\left[\left(1+\frac{x}{n}\right)^m-1\right]=\sum_{l=1}^{\infty}\frac{x^l}{l\cdot l!}$$

can be proved by using the binomial theorem for $(1+x/n)^m$, interchanging the two finite summations and applying the equality

$$\sum_{m=j}^{n}\frac{(m-1)!}{(m-j)!}=\frac{n!}{j(n-j)!}.$$

By applying the above formula to Eq. (5.9a) we obtain

$$\lim_{n\to\infty}\lim_{i\gamma\to -n}W(\gamma;\mu,\nu)=-C-\ln(-2\mu-2\nu)$$
$$-\sum_{l=1}^{\infty}\frac{(-2\mu-2\nu)^l}{l\cdot l!}.$$

This expression is indeed equal to $w_0=d_0$ $=\mathrm{Re}\Gamma(0,2\mu+2\nu)$ according to Eq. (29) of Ref. 2.

One should keep in mind that for $s<0$ there are no poles in the physical region, neither in $\psi(i\gamma)$ nor in $F_{i\gamma}(AB)$. So $W(\gamma;\mu,\nu)$ is regular at $i\gamma=n$, for $n=1,2,\cdots$. Nevertheless, it is interesting to calculate the value of W at $i\gamma=n$. We find

$$W(-in;\mu,\nu)=(1-z^n)/(2n)-\ln n+\psi(n)+\sum_{m=n}^{\infty}z^m/m, \tag{5.9b}$$

with

$$z=\frac{n-\mu}{n+\mu}\,\frac{n-\nu}{n+\nu}.$$

In order to derive the limit of $W(-in;\mu,\nu)$ for $n\to\infty$ we proceed as follows. First, observe that

$$n^{-1}\sum_{m=n}^{\infty}(1-x/n)^{m-1}=x^{-1}(1-x/n)^{n-1},$$

where the convergence is uniform for $0<\epsilon\leq x\leq n$. Integration with respect to x yields

$$\sum_{m=n}^{\infty}m^{-1}(1-x/n)^m=\int_x^n t^{-1}(1-t/n)^{n-1}\,dt, \quad 0<x\leq n.$$

We now apply the inequalities

$$0 < \exp(-t) - (1 - t/y)^y \leq 1/(ey), \quad 0 < t \leq y,$$

to the above integral and obtain (which follows also from Tannery's theorem)

$$\lim_{n\to\infty} \int_x^n t^{-1}(1 - t/n)^{n-1}\,dt = \int_x^\infty t^{-1}\exp(-t)\,dt, \quad x > 0.$$

This latter integral equals $\Gamma(0, x)$ [cf. Eq. (5.15a)], so that

$$\lim_{n\to\infty} \sum_{m=n}^{\infty} m^{-1}(1 - x/n)^m = \Gamma(0, x), \quad x > 0.$$

Finally we utilize the well-known fact

$$\lim_{n\to\infty}[\psi(n) - \ln n] = \lim_{n\to\infty}\left(-C - \ln n + \sum_{m=1}^{n-1} m^{-1}\right) = 0.$$

In this way we obtain

$$\lim_{n\to\infty} W(-in; \mu, \nu) = \Gamma(0, 2\mu + 2\nu) = w_0(\mu, \nu),$$

where now $\mu > 0$ and $\nu > 0$ since $s < 0$.

One should be careful in applying here the equality $W(\gamma; \mu, \nu) = W(-\gamma; \mu, \nu)$, since W depends also on the sign of s, and therefore on the sign of μ and ν. In Eq. (5.9a) μ and ν are negative, in Eq. (5.9b) μ and ν are positive. It can be shown that the expression of Eq. (5.9a) becomes equal to the expression of Eq. (5.9b) if one replaces $\ln(-2\mu - 2\nu)$ by $\ln(2\mu + 2\nu)$.

B. The function $W(\gamma; \xi)$

We define $W(\gamma;\xi)$ for real ξ by

$$W(\gamma;\xi) \equiv (i\gamma)^{-1}\exp(-\xi)\{F_{i\gamma}[\exp(i\xi/\gamma)] - \tfrac{1}{2}\} + H(\gamma). \tag{5.10}$$

The function $W(\gamma;\mu,\nu)$ is obtained from $W(\gamma;\xi)$ if one takes

$$\xi = 2\gamma[\arctan(\mu/\gamma) + \arctan(\nu/\gamma)].$$

One easily verifies that with this expression for ξ one has $\exp(i\xi/\gamma) = AB$ and $\exp(-\xi) = A^{i\gamma}B^{i\gamma}$, cf. Eq. (4.11). The following important equality holds, therefore:

$$W(\gamma;\mu,\nu) = W(\gamma;2\gamma[\arctan(\mu/\gamma) + \arctan(\nu/\gamma)]). \tag{5.11}$$

Now in order to calculate $W(\gamma;\mu,\nu)$ for some value of γ, μ, and ν, one first has to calculate ξ from the above expression, and this value of ξ has to be used then in $W(\gamma;\xi)$. In Eq. (5.14) we give closed expressions for the coefficients of the power series of $W(\gamma;\xi)$ at $\gamma^{-2} = 0$. Therefore, $W(\gamma;\xi)$ is useful for the exact numerical computation of $W(\gamma;\mu,\nu)$. For real μ, ν, and γ one has clearly $|\xi| < 2\pi|\gamma|$. We shall find that $W(\gamma;\xi)$ is analytic in γ on this same domain, see Eqs. (6.32) and (6.34). For values of ξ, μ, and ν which are small compared with γ the functions $W(\gamma;\xi)$ and $W(\gamma;\mu,\nu)$ are comparable according to

$$\xi \to 2\mu + 2\nu: \quad W(\gamma;\xi) \approx W(\gamma;\mu,\nu). \tag{5.12}$$

Notice in particular that ξ, μ, and ν have equal signs here.

By repeating the procedure that we described for $W(\gamma;\mu,\nu)$ we obtain an asymptotic expansion and a Taylor series for the ξ functions which are the analogs of Eqs. (4.23) and (5.2) respectively. The coefficients are denoted by $d_{2n}(\xi)$ and $w_{2n}(\xi)$. At the "Coulomb-bound-state poles" $i\gamma = -n$ we have the analog of Eq. (5.9a),

$$\lim_{i\gamma\to -n} W(\gamma;\xi) = -C - \ln n - \ln[1 - \exp(\xi/n)] + \xi/n - \sum_{m=1}^{n}{}' m^{-1}[\exp(-\xi m/n) - 1],$$

where $\xi < 0$ since $s > 0$ (compare $\mu, \nu < 0$). At zero energy we get

$$\lim_{n\to\infty}\lim_{i\gamma\to -n} W(\gamma;\xi) = -C - \ln(-\xi) - \sum_{l=1}^{\infty}\frac{(-\xi)^l}{l\cdot l!} = \mathrm{Re}\,\Gamma(0,\xi) = w_0(\xi).$$

We have obtained the following simple closed formulas for $d_{2n}(\xi)$:

$$d_{2n}(\xi) = [B_{2n}/(2n)!\,]\,\Gamma(2n, \xi), \tag{5.13a}$$

$$= [B_{2n}/(2n)!\,]\exp(-\xi)\,\xi^{2n-1}\,{}_2F_0(1, 1 - 2n; -1/\xi), \tag{5.13b}$$

$$= [B_{2n}/(2n)]\exp(-\xi)\,e_{2n-1}(\xi), \qquad n > 0, \tag{5.13c}$$

$$= -[B_{2n}/(2n)]\exp(-\xi)\,L_{2n-1}^{(-2n)}(\xi), \quad n > 0. \tag{5.13d}$$

Here ${}_2F_0$ is a generalized hypergeometric function, e_{2n-1} is the exponential polynomial of Eq. (4.19), and L is the generalized Laguerre polynomial. Equations (5.13) are valid for all real ξ if $n > 0$, and for positive ξ if $n = 0$. When ξ is negative, d_0 is equal to the real part of the right-hand side of Eqs. (5.13a) or (5.13b). For the coefficients $w_{2n}(\xi)$ of the expansion

$$W(\gamma;\xi) = \sum_{n=0}^{\infty} w_{2n}(\xi)(i\gamma)^{-2n}, \quad |\xi| < 2\pi|\gamma|,$$

we have obtained:

$$w_0(\xi) = d_0(\xi) = \mathrm{Re}\,\Gamma(0, \xi), \tag{5.14a}$$

$$w_{2n}(\xi) = -[B_{2n}/(2n)!\,]\,\gamma(2n, \xi), \quad n > 0, \tag{5.14b}$$

$$= -[B_{2n}/(2n)!\,][\xi^{2n}/(2n)]\exp(-\xi)\,{}_1F_1(1; 2n + 1; \xi) \qquad n > 0, \tag{5.14c}$$

$$= -[B_{2n}/(2n)!\,][\xi^{2n}/(2n)]\,{}_1F_1(2n; 2n + 1; -\xi), \qquad n > 0. \tag{5.14d}$$

These Eqs. (5.13) and (5.14) have been derived with the help of Eqs. (6.31) and (6.36). The incomplete gamma functions are defined by

$$\Gamma(2n, \xi) = \int_\xi^\infty \exp(-t)\,t^{2n-1}\,dt, \tag{5.15a}$$

$$\gamma(2n, \xi) = \int_0^\xi \exp(-t)\,t^{2n-1}\,dt. \tag{5.15b}$$

One should not confuse $\gamma(2n, \xi)$ and the variable γ. From Eqs. (5.13a) and (5.14b) it follows that

$$w_{2n}(\xi) = d_{2n}(\xi) - B_{2n}/(2n), \quad n > 0, \tag{5.16}$$

which should be compared with Eq. (5.4). The polynomial in Eq. (5.13c) is just a cutoff Taylor series expansion of $\exp(\xi)$. This polynomial is multiplied by $\exp(-\xi)$ and therefore we have

$$d_{2n}(\xi) = B_{2n}/(2n) + O(\xi^{2n}), \quad \xi \to 0, \tag{5.17}$$

and so

$$w_{2n}(\xi) = O(\xi^{2n}), \quad \xi \to 0, \tag{5.18}$$

which follows also from Eqs. (5.14c) and (5.14d). Now if we replace ξ by $2\mu + 2\nu$ according to Eq. (5.12), we get analogous formulas for $d_{2n}(\mu, \nu)$ and $w_{2n}(\mu, \nu)$,

$$d_{2n}(\mu, \nu) = B_{2n}/(2n) + O_{2n}(\mu, \nu), \quad \mu, \nu \to 0,$$
$$w_{2n}(\mu, \nu) = O_{2n}(\mu, \nu), \quad \mu, \nu \to 0,$$

where $O_{2n}(\mu, \nu)$ contains terms of degree $\geq 2n$ in μ and ν together. The proof of this remarkable fact will be given in Sec. 6. There we will obtain the more precise expression [cf. Eq. (6.29)]

$$w_{2n}(\mu, \nu) = -\frac{1}{2n}\left(\mu^{2n} + \nu^{2n}\right) + O_{2n+1}(\mu, \nu), \quad \mu, \nu \to 0, \tag{5.19}$$

valid for $n > 0$. By combining this result with the already known properties of d_{2n} we arrive at the following interesting expression:

$$d_{2n}(\mu, \nu) = (2n)^{-1} \exp(-2\mu - 2\nu) \times [B_{2n} e_{2n}(2\mu + 2\nu) - (\mu^{2n} + \nu^{2n}) + f_{2n}(\mu, \nu)] \tag{5.20}$$

for $n > 0$. Here $f_{2n}(\mu, \nu)$ is a certain symmetric polynomial in μ and ν with the property that the degree of its terms is at least $2n + 1$ and at most $3n - 1$. Obviously $f_2 = 0$ and f_4 has only terms of degree 5. In the particular cases $n = 1$ and $n = 2$ we have checked Eqs. (5.19) and (5.20) explicitly. The expressions for d_2 and d_4 have been given in Eq. (4.20).

We conclude this section with two remarks.

(i) Equation (5.14d) can also be derived directly from Eq. (5.10) by using the last formula on p. 33 of Ref. 11. We note that this formula must be corrected as follows: Replace $\Gamma(m+2)$ by $(m+1)\Gamma(m+2)$. The function $F_{i\gamma}(z)$ is simply connected to Lerch's function Φ,

$$F_{i\gamma}(z) = i\gamma\, \Phi(z, 1, i\gamma). \tag{5.21}$$

We have then

$$(i\gamma)^{-1} z^{i\gamma} F_{i\gamma}(z) = -C - \psi(i\gamma) - \ln(\ln z^{-1}) - \sum_{n=1}^{\infty} \frac{(\ln z)^n}{n \cdot n!} B_n(i\gamma), \quad |\ln z| < 2\pi, \tag{5.22}$$

where $B_n(i\gamma)$ are the Bernoulli polynomials. We insert Eq. (5.22) with $z = \exp(i\xi/\gamma)$ into Eq. (5.10). Comparison with

$$W(\gamma; \xi) = \sum_{n=0}^{\infty} (i\gamma)^{-2n} w_{2n}(\xi) \tag{5.23}$$

yields after some manipulations agreement with the expression (5.14d) for $w_{2n}(\xi)$.

(ii) The integral in Eq. (3.4) for $h(\gamma)$ is reminiscent of the Mellin–Barnes integral representation[11] of $F_{i\gamma}$,

$$F_{i\gamma}(z) = i\gamma \int_{-\infty}^{\infty} \frac{dt}{t + \gamma} \frac{(-z)^{it}}{2 \sinh \pi t}, \quad |\arg(-z)| < \pi. \tag{5.24}$$

The path of integration is chosen such that the points $t = 0, -i, -2i, \cdots$, are under the contour and the point $t = -\gamma$ is above the contour. Therefore γ cannot be equal to $0, i, 2i, \cdots$. It might be that this integral is a good starting point to prove the real analyticity of $W(\gamma; \mu, \nu)$. However, we have not been able to take advantage of the similarity.

6. PROOF OF THE ANALYTICITY OF V AND W

In Sec. 6 A we shall prove that $W(\gamma; \mu, \nu)$ is a real analytic function of γ^{-2} at $\gamma^{-2} = 0$ when μ and ν are real For this purpose it is convenient to introduce a closely related function $V(\gamma; \mu, \nu)$ which is analytic in the three complex variables γ, μ and ν, on the domain defined by $|\mu/\gamma| < 1$, $|\nu/\gamma| < 1$.

In Sec. 6 B we shall introduce the function $V(\gamma; \xi)$, which is similarly related to $W(\gamma; \xi)$, and prove that it is analytic in γ and in ξ on the domain defined by $|\xi/\gamma| < 2\pi$. We will obtain simple closed expressions for the expansion coefficients $v_{2n}(\xi)$ (expansion in powers of γ^{-2}), and for $\bar{v}_n(\gamma)$ (expansion in powers of ξ).

A. The functions $V(\gamma; \mu, \nu)$ and $W(\gamma; \mu, \nu)$

The function $W(\gamma; \mu, \nu)$ has been defined in Eq. (5.1) for real μ and ν. Let us first take $\nu = 0$. Then we have

$$W(\gamma; \mu, 0) = (i\gamma)^{-1} A^{i\gamma} [F_{i\gamma}(A) - \tfrac{1}{2}] + H(\gamma), \tag{6.1}$$

with $A = (1 + i\mu/\gamma)/(1 - i\mu/\gamma)$ and [Eq. (3.6)]

$$H(\gamma) = \psi(i\gamma) + 1/(2i\gamma) - \ln[-i\gamma \operatorname{sgn}(s)].$$

Assuming first μ real, we define

$$V(\gamma; \mu, 0) \equiv W(\gamma; \mu, 0) + C + \ln[-2\mu \operatorname{sgn}(s)]. \tag{6.2}$$

The Euler constant C has been added for convenience only, but the term $\ln[-2\mu \operatorname{sgn}(s)]$ has the effect to cancel the singularity of $w_0(\mu, 0) = \operatorname{Re}\Gamma(0, 2\mu)$, see Eq. (5.4). In fact we have

$$\Gamma(0, z) + \ln z + C = -\sum_{n=1}^{\infty} \frac{(-z)^n}{n \cdot n!}. \tag{6.3}$$

This is an entire function for which we have the following useful integral representations:

$$\Gamma(0, z) + \ln z + C = \int_0^z \frac{dt}{t} [1 - \exp(-t)] = \int_0^1 \frac{dt}{t} [1 - \exp(-zt)]. \tag{6.4}$$

The combination of Eqs. (6.1), (6.2), and (3.6) yields

$$V(\gamma; \mu, 0) = (1/i\gamma) A^{i\gamma} [F_{i\gamma}(A) - \tfrac{1}{2}] + \psi(i\gamma) + 1/(2i\gamma) + C + \ln(2\mu/i\gamma). \tag{6.5}$$

Notice that sgn(s) has disappeared. Below we shall find that the right-hand side of Eq. (6.5) can be analytically continued into the complex μ plane on the domain defined by

$$|\mu/\gamma| < 1. \tag{6.6}$$

We shall derive now a simple integral representation for $V(\gamma; \mu, 0)$ from which the analytical properties can easily be obtained.

We differentiate Eq. (6.5) with respect to μ. Utilizing the following integral representation [cf. Eq. (4.12)],

$$\frac{1}{(i\gamma)} z^{i\gamma} F_{i\gamma}(z) = \int_0^z \frac{t^{i\gamma - 1}}{1 - t}\, dt, \quad \operatorname{Re} i\gamma > 0, \tag{6.7}$$

we obtain

$$\frac{d}{d\mu}\ V(\gamma;\mu,0)=\frac{1}{\mu}\left(1-\frac{A^{i\gamma}}{1+\mu^2/\gamma^2}\right). \tag{6.8}$$

Further we know that $w_0(\mu,0)=\mathrm{Re}\Gamma(0,2\mu)$ and so

$$\lim_{\mu\to 0} V(\gamma;\mu,0)=0, \tag{6.9}$$

where we utilized Eq. (6.3). From Eqs. (6.8) and (6.9) we obtain the desired integral representation

$$V(\gamma;\mu,0)=\int_0^{\mu}\frac{dl}{l}\left[1-\frac{1}{1+l^2/\gamma^2}\left(\frac{1+il/\gamma}{1-il/\gamma}\right)^{i\gamma}\right], \tag{6.10}$$

which can be recast into the form

$$V(\gamma;\mu,0)=\int_0^{\mu}\frac{dl}{l}\left[1-\frac{1}{1+l^2/\gamma^2}\exp[-2\gamma\arctan(l/\gamma)]\right] \tag{6.11}$$

or

$$V(\gamma;\mu,0)=\int_0^{1}\frac{dl}{l}\left[1-\frac{1}{1+\mu^2l^2/\gamma^2}\left(\frac{1+i\mu l/\gamma}{1-i\mu l/\gamma}\right)^{i\gamma}\right]. \tag{6.12}$$

The integrand of the integral in Eq. (6.12) is analytic provided that

$$0<|l|<|\gamma/\mu|,$$

and it can be analytically continued to $l=0$. It follows that $V(\gamma;\mu,0)$ is an analytic function of γ and μ on the domain defined by Eq. (6.6), that is, $|\mu|<|\gamma|$. By making the substitution $\gamma\to-\gamma$ in either of the Eqs. (6.10)–(6.12) we see that $V(\gamma;\mu,0)$ is actually a function of γ^2 rather than of γ.

We have obtained in Eqs. (6.5) and (6.12) two important expressions for the function $V(\gamma;\mu,0)$. Since the expressions (6.5) on the one hand and (6.10)–(6.12) on the other hand look quite different, they deserve a detailed investigation. In particular we shall compare their singularities. In Eq. (6.5) we see simple poles at $i\gamma=-n$, for $n=1,2,\cdots$. They are removable and have been discussed before. Further we see a removable singularity at $\mu=0$, that is, at $A=1$. In virtue of Eq. (4.2) the function $V(\gamma;\mu,0)$ can be made continuous at $\mu=0$ with $V(\gamma;0,0)=0$.

More interesting are the nonremovable singularities which we are going to discuss now. For this purpose it is convenient to introduce the new function U by $U(\gamma;\rho)\equiv V(\gamma;\mu,0)$ with the new variable $\rho\equiv i\mu/\gamma$. We get from Eq. (6.5)

$$U(\gamma;\rho)=(i\gamma)^{-1}\left(\frac{1+\rho}{1-\rho}\right)^{i\gamma}\left[F_{i\gamma}\left(\frac{1+\rho}{1-\rho}\right)-\frac{1}{2}\right]+\ln(-2\rho)+\psi(i\gamma)+(2i\gamma)^{-1}+C, \tag{6.13}$$

and from Eq. (6.12)

$$U(\gamma;\rho)=\int_0^{\rho}\frac{dl}{l}\left[1-\frac{1}{1-l^2}\left(\frac{1+l}{1-l}\right)^{i\gamma}\right]. \tag{6.14}$$

Now that we have obtained these two expressions after several manipulations, we note that a second proof of their equality is obtained by using Eq. (6.7) and the following integral representation of the digamma function[11]

$$\psi(z)=-\frac{1}{2z}-\ln 2-C+\int_0^{1}\frac{dl}{l}\left[1-\frac{1}{1-l^2}\left(\frac{1-l}{1+l}\right)^{z}\right],\quad \mathrm{Re}\,z>0. \tag{6.15}$$

From the definition of $U(\gamma;\rho)$ and the equality $V(\gamma;\mu,\nu)=V(-\gamma;\mu,\nu)$ it follows that

$$U(\gamma;\rho)=U(-\gamma;-\rho). \tag{6.16}$$

One can derive this equality easily from Eq. (6.14). It follows also from Eq. (6.13), by using Eq. (4.3) and observing that

$$U(\gamma;\rho)-U(-\gamma;-\rho)=\psi(i\gamma)-\psi(-i\gamma)+(i\gamma)^{-1}+\ln(-\rho)-\ln(\rho)+(i\gamma)^{-1}\Gamma(1+i\gamma)\Gamma(1-i\gamma)\left(\frac{1-\rho}{1+\rho}\right)^{-i\gamma}\left(\frac{\rho-1}{\rho+1}\right)^{i\gamma} \tag{6.17}$$

vanishes identically for all nonreal ρ. This can be derived with the help of Eq. (3.7),

$$\psi(i\gamma)-\psi(-i\gamma)+(i\gamma)^{-1}=i\pi\coth\pi\gamma.$$

By means of analytical continuation we then find that the expression of Eq. (6.17) is identically zero and this again proves Eq. (6.16).

Considered as functions of ρ, the expressions in Eqs. (6.13) and (6.14) show several branch cuts. Taken together, they must yield the same branch cut with the same discontinuity for both expressions separately. We are going to show that this is indeed true. For the purpose of this paper the discontinuity of a function f across a branch cut in a point z on the cut can be defined by

$$\mathrm{Disc.}\ f(z)\equiv\lim_{\epsilon\to 0}[f(z(1+i\epsilon))-f(z(1-i\epsilon))]. \tag{6.18}$$

For example,

$$\mathrm{Disc.}\ \ln(-z)=-2\pi i,\quad z>0,$$

and, with the help of Eq. (4.3) [cf. also Eq. (5.22)],

$$\mathrm{Disc.}\ (i\gamma)^{-1}z^{i\gamma}F_{i\gamma}(z)=2\pi i,\quad z>1. \tag{6.19}$$

For the discontinuity across the cut $-\infty<\rho<-1$ arising from the integrand in Eq. (6.14), we obtain

$$D_\gamma\equiv D(\gamma;\rho)=2(i\gamma)^{-1}\sinh(\pi\gamma)\times\left(\frac{\rho-1}{\rho+1}\right)^{i\gamma}\left[F_{i\gamma}\left(\frac{1-\rho}{1+\rho}\right)-\frac{1}{2}\right]. \tag{6.20}$$

We need this function only for $-\infty<\rho<-1$ and for $1<\rho<\infty$, where it is regular. Equation (6.16) implies at once that the discontinuity across the cut $1<\rho<\infty$ arising from the integrand in Eq. (6.14) is equal to $D_{-\gamma}=D(-\gamma;\rho)$. One can verify with the help of Eq. (4.3) that

$$D(\gamma;\rho)+D(-\gamma;-\rho)=-2\pi i.$$

The derivation of all the discontinuities will not be given here. We summarize the results in the following scheme.

Branch cut	Discontinuity	Arising from
$-\infty<\rho<-1$	D_γ	Eq. (6.14)
$1<\rho<\infty$	$D_{-\gamma}$	Eq. (6.14)
$-\infty<\rho<-1$	D_γ	$((1+\rho)/(1-\rho))^{i\gamma}$
$1<\rho<\infty$	$D_{-\gamma}+2\pi i$	$((1+\rho)/(1-\rho))^{i\gamma}$
$0<\rho<1$	$2\pi i$	$F_{i\gamma}((1+\rho)/(1-\rho))$
$0<\rho<\infty$	$-2\pi i$	$\ln(-2\rho)$

The first two lines concern Eq. (6.14): the last four lines concern the respective expressions of Eq. (6.13). On the third line we see the same branch cut as on the first line. Furthermore, combination of the last three lines just gives the branch cut of the second line. So we see that Eqs. (6.13) and (6.14) have indeed the same branch cut structure.

So far we have studied $W(\gamma;\mu,0)$. However, our goal is the function $W(\gamma;\mu,\nu)$. The final step now is the observation that $W(\gamma;\mu,0)$ is transformed into $W(\gamma;\mu,\nu)$ by means of the substitution

$$\mu \to (\mu+\nu)/(1-\mu\nu/\gamma^2),$$

under the restriction

$$|\mu/\gamma|<1, \quad |\nu/\gamma|<1. \tag{6.21}$$

It is easy to find that this substitution yields

$$A \to AB, \quad A^{i\gamma} \to A^{i\gamma}B^{i\gamma},$$

where $B=(1+i\nu/\gamma)/(1-i\nu/\gamma)$, see Eqs. (4.8) and (5.7). So we have

$$W(\gamma;\mu,\nu)=W\left(\gamma;\frac{\mu+\nu}{1-\mu\nu/\gamma^2},\ 0\right). \tag{6.22}$$

By defining

$$V(\gamma;\mu,\nu)\equiv V\left(\gamma;\frac{\mu+\nu}{1-\mu\nu/\gamma^2},\ 0\right), \tag{6.23}$$

we get the following expressions

$$V(\gamma;\mu,\nu)=W(\gamma;\mu,\nu)+C+\ln\frac{(-2\mu-2\nu)\,\mathrm{sgn}(s)}{1-\mu\nu/\gamma^2} \tag{6.24}$$

$$=\frac{1}{i\gamma}A^{i\gamma}B^{i\gamma}\left[\mathcal{F}_{i\gamma}(AB)-\tfrac{1}{2}\right]+\psi(i\gamma)+\frac{1}{2i\gamma}+C$$
$$+\ln\left(\frac{2\mu+2\nu}{i\gamma}\,\frac{1}{1-\mu\nu/\gamma^2}\right) \tag{6.25}$$

$$=\int_0^{(\mu+\nu)/(1-\mu\nu/\gamma^2)}\frac{dt}{t}\left[1-\frac{1}{1+t^2/\gamma^2}\left(\frac{1+it/\gamma}{1-it/\gamma}\right)^{i\gamma}\right]. \tag{6.26}$$

By means of changing the variable of integration according to

$$t\to\tau, \quad t=\frac{\tau(\mu+\nu)}{1-\mu\nu\tau^2/\gamma^2},$$

and, denoting τ again by t, we obtain from Eq. (6.26)

$$V(\gamma;\mu,\nu)=\int_0^1\frac{dt}{t}\,\frac{1+\mu\nu t^2/\gamma^2}{1-\mu\nu t^2/\gamma^2}$$
$$\times\left[1-\frac{(1-\mu\nu t^2/\gamma^2)^2}{(1+\mu^2t^2/\gamma^2)(1+\nu^2t^2/\gamma^2)}\right.$$
$$\left.\times\left(\frac{1+i\mu t/\gamma}{1-i\mu t/\gamma}\right)^{i\gamma}\left(\frac{1+i\nu t/\gamma}{1-i\nu t/\gamma}\right)^{i\gamma}\right]. \tag{6.27}$$

The integrand of the integral in Eq. (6.27) is analytic in t, γ, μ, and ν on the domain defined by

$$0<|t|<\min(|\gamma/\mu|,\ |\gamma/\nu|),$$

and it can be analytically continued to $t=0$, so $V(\gamma;\mu,\nu)$ is analytic in γ, μ, and ν on the domain defined by Eq. (6.21),

$$|\mu/\gamma|<1, \quad |\nu/\gamma|<1.$$

Since the integrand in Eq. (6.2^7) is real if t, γ, μ, and ν are real, $V(\gamma;\mu,\nu)$ is a real-valued function for real γ, μ, and ν. Consequently, $V(\gamma;\mu,\nu)$ is *real* analytic in any one of the three variables if the other two are real. We point out that the desired analytical properties of $W(\gamma;\mu,\nu)$ follow from Eq. (6.24).

Now we shall give the proof of Eq. (5.19). For this purpose we introduce the variable $\sigma\equiv i\nu/\gamma$ in addition to $\rho=i\mu/\gamma$ used before [Eq. (6.13)]. We consider the limit of $V(\gamma;\mu,\nu)$ for $\gamma,\mu,\nu\to 0$ such that ρ and σ remain constant. In view of Eq. (6.21) we have to require $|\rho|<1$, $|\sigma|<1$. From Eq. (6.26) it easily follows that

$$\lim_{\substack{\gamma,\mu,\nu\to 0\\ |\rho|<1,\ |\sigma|<1}} V(\gamma;\mu,\nu)=\int_0^{-i(\rho+\sigma)/(1+\rho\sigma)}\frac{dt}{t}\left[1-\frac{1}{1+t^2}\right]$$
$$=\tfrac{1}{2}\ln\frac{(1-\rho^2)(1-\sigma^2)}{(1+\rho\sigma)^2}. \tag{6.28}$$

The power series expansion of this expression yields

$$\lim_{\substack{\gamma,\mu,\nu\to 0\\ |\rho|<1,\ |\sigma|<1}} w_{2n}(\mu,\nu)(i\gamma)^{-2n}=-\frac{1}{2n}\left[\rho^{2n}+\sigma^{2n}-2(-\rho\sigma)^n\right].$$

Considering now W and w_{2n}, we observe that the term $-\ln(1-\mu\nu/\gamma^2)$ occurring in Eq. (6.24) has the effect of cancelling the term $-\frac{1}{2}\ln(1+\rho\sigma)^2$ in Eq. (6.28). Therefore, we have

$$\lim_{\substack{\gamma,\mu,\nu\to 0\\ |\rho|<1,\ |\sigma|<1}} w_{2n}(\mu,\nu)(i\gamma)^{-2n}=-\frac{1}{2n}\left(\rho^{2n}+\sigma^{2n}\right), \quad n\neq 0, \tag{6.29}$$

and this proves Eq. (5.19).

Finally we report that we have utilized Eq. (6.22) to derive (for $n=0,1,2$) $w_{2n}(\mu,\nu)$ from $w_{2n}(\mu,0)$ which is much easier to obtain. This alternative method yields a check on the derivation of $d_{2n}(\mu,\nu)$ performed in Sec. 4, see Eqs. (4.17) and (4.25). Since $w_0(\mu,0)=d_0(\mu,0)=\Gamma(0,2\mu)$ for $\mu\neq 0$, we have to expand

$$\Gamma\left(0,\frac{2\mu+2\nu}{1-\mu\nu/\gamma^2}\right)$$

in powers of γ^{-2}. The expansion is carried out with the help of the addition theorem for the incomplete gamma functions (Ref. 11, p. 341):

$$\Gamma(a,x)-\Gamma(a,x+y)=\gamma(a,x+y)-\gamma(a,x)$$
$$=\exp(-x)\,x^{a-1}\sum_{n=0}^{\infty}(-x)^{-n}(1-a)_n$$
$$\times[1-\exp(-y)\,e_n(y)], \quad |y|<|x|,$$

which implies in particular

$$\Gamma(0,x+y)=\Gamma(0,x)$$
$$+\exp(-x)\left[-\frac{y}{x}+\frac{y^2}{x^2}\,\frac{1+x}{2}\right]+O(y^3), \quad y\to 0.$$

B. The functions $V(\gamma;\xi)$ and $W(\gamma;\xi)$

The function $W(\gamma;\xi)$ has been defined in Eq. (5.10) for real ξ,

$$W(\gamma;\xi)=(i\gamma)^{-1}\exp(-\xi)\left[F_{i\gamma}(\exp(i\xi/\gamma))-\tfrac{1}{2}\right]+H(\gamma).$$

Repeating the procedure of Sec. 6A, we get

$$V(\gamma;\xi)=W(\gamma;\xi)+C+\ln[-\xi\,\mathrm{sgn}(s)], \tag{6.30a}$$

and

$$V(\gamma;\xi) = (1/i\gamma)\exp(-\xi)[F_{i\gamma}(\exp(i\xi/\gamma)) - \tfrac{1}{2}] + \psi(i\gamma) + 1/(2i\gamma) + C + \ln(\xi/i\gamma). \quad (6.30b)$$

The latter expression can be analytically continued into the complex ξ plane. We obtain

$$\frac{d}{d\xi}\, V(\gamma;\xi) = \frac{1}{\xi} - \frac{1}{2\gamma}\, \exp(-\xi)\cot\frac{\xi}{2\gamma},$$

and

$$\lim_{\xi\to 0} V(\gamma;\xi) = 0,$$

so

$$V(\gamma;\xi) = \int_0^1 \frac{dl}{l}\left[1 - \exp(-\xi l)\,\frac{\xi l}{2\gamma}\,\cot\frac{\xi l}{2\gamma}\right]. \quad (6.31)$$

This integral representation implies that $V(\gamma;\xi)$ is analytic in γ and in ξ on the domain defined by

$$|\xi/\gamma| < 2\pi. \quad (6.32)$$

Let us briefly consider the singularities outside the domain (6.32). From Eq. (6.30b) we see that $\ln[\xi/(i\gamma)]$ yields a branch cut $0 < i\xi/\gamma < \infty$, and $F_{i\gamma}$ yields a branch cut $1 < \exp(i\xi/\gamma) < \infty$. It turns out that the first branch cut can be removed and that the actual branch cuts are given by

$$0 < i\xi/\gamma + 2\pi i n < \infty, \quad n = \pm 1, \pm 2, \cdots. \quad (6.33)$$

So we have in the plane of the complex variable ξ/γ a set of branch cuts consisting of vertical lines parallel to the imaginary axis, starting from the points $2\pi n$ $(n = \pm 1, \pm 2, \cdots)$ on the real axis and going downwards. Only the negative imaginary axis itself $(n = 0)$ is a removable branch cut.

The series expansion in powers of $(i\gamma)^{-2}$ converges if Eq. (6.32) is satisfied,

$$V(\gamma;\xi) = \sum_{n=0}^{\infty} v_{2n}(\xi)(i\gamma)^{-2n}, \quad |\xi| < 2\pi|\gamma|. \quad (6.34)$$

The coefficients v_{2n} are closely related to the coefficients w_{2n} of W [see Eq. (5.14)],

$$v_0(\xi) = \Gamma(0,\xi) + \ln\xi + C = -\sum_{n=1}^{\infty} \frac{(-\xi)^n}{n\cdot n!},$$

$$v_{2n}(\xi) = w_{2n}(\xi), \quad n > 0. \quad (6.35)$$

The closed expressions for $v_{2n}(\xi)$ follow easily from Eq. (6.31) if one utilizes the expansion

$$z\cot z = \sum_{n=0}^{\infty} (-)^n (2z)^{2n} B_{2n}/(2n)!, \quad |z| < \pi. \quad (6.36)$$

The coefficients of the expansion in powers of ξ can also be obtained in closed form. We write

$$V(\gamma;\xi) = -\sum_{n=1}^{\infty} \bar{v}_n(\gamma)(-\xi)^n/n!, \quad |\xi| < 2\pi|\gamma|. \quad (6.37)$$

Starting from Eq. (6.31) and applying the generating function of the Bernoulli polynomials $B_n(\cdot)$, we find after some manipulations [cf. Eq. (5.22)]

$$\bar{v}_n(\gamma) = 1/(2i\gamma) + (1/n)(i\gamma)^{-n} B_n(i\gamma). \quad (6.38)$$

We know that $V(\gamma;\xi)$ and $\bar{v}_n(\gamma)$ are functions of γ^2 rather than of γ, and we show this explicitly by recasting Eqs. (6.37) and (6.38) into the form

$$V(\gamma;\xi) = -\sum_{n=1}^{\infty} \frac{(-\xi)^n}{n\cdot n!} \sum_{m=0}^{[n/2]} \binom{n}{2m} (i\gamma)^{-2m} B_{2m}. \quad (6.39)$$

Here $[n/2]$ means the integral part of $n/2$ and we have used the relation

$$B_n(x) = \sum_{m=0}^{n} \binom{n}{m} x^{n-m} B_m \quad (6.40)$$

and the fact that $B_m = 0$ for $m = 3, 5, 7, \cdots$.

7. SUMMARY AND DISCUSSION

We have given in Sec. 2 closed expressions for $T_{c,\,l=1}(p,p';k^2)$, for $T_{cs,\,l=1}(p,p';k^2)$ and for a_1 and r_1, corresponding to $V_c + V_s$ with V_c the $l=1$ Yamaguchi-type potential. In Eq. (3.6) we introduced the function

$$H(\gamma) = \psi(i\gamma) + (2i\gamma)^{-1} - \ln[-i\gamma\,\mathrm{sgn}(s)],$$

which replaces the often used function $h(\gamma)$ in the definition of the effective range function if the Coulomb potential V_c is attractive. When V_c is repulsive, $H(\gamma)$ is identical to $h(\gamma)$. The effective range functions corresponding to $V_c + V_{rs}$ for several rational separable potentials V_{rs} have been discussed in Sec. 3, and the function $W(\gamma;\mu,\nu)$, which plays the central role here, has been introduced.

In Sec. 4 we investigated $F_{i\gamma}(AB)$. This section concludes with some formulas useful for the high-energy limit, $k\to\infty$. In Sec. 5 we studied $W(\gamma;\mu,\nu)$ of Eq. (3.10) and an auxiliary function $W(\gamma;\xi)$; see Eq. (5.10). This function is very useful for numerical computations, due to the relationship

$$W(\gamma;\mu,\nu) = W(\gamma;2\gamma[\arctan(\mu/\gamma) + \arctan(\nu/\gamma)]) \quad (5.11)$$

and the fact that we found simple closed expressions for the expansion coefficients $w_{2n}(\xi)$ of $W(\gamma;\xi)$. The equality

$$w_{2n} = d_{2n} - B_{2n}/(2n)$$

holds for $w_{2n}(\xi)$ and $d_{2n}(\xi)$ as well as for $w_{2n}(\mu,\nu)$ and $d_{2n}(\mu,\nu)$. We have obtained

$$d_{2n}(\xi) = (2n)^{-1}\exp(-\xi)\,B_{2n}\,e_{2n-1}(\xi) \quad (5.13c)$$

and

$$d_{2n}(\mu,\nu) = (2n)^{-1}\exp(-2\mu-2\nu) \times[B_{2n}e_{2n}(2\mu+2\nu) - (\mu^{2n}+\nu^{2n}) + f_{2n}(\mu,\nu)]. \quad (5.20)$$

In Eq. (4.20) d_0, d_2, and d_4 have been given explicitly.

In Sec. 6 we have proved that $W(\gamma;\mu,\nu)$ is a real analytic function of γ^2 for real μ and ν. The only singularities in the complex γ plane are the branch cuts

$$(-i\mu, i\mu), \quad (-i\nu, i\nu).$$

They correspond in the complex k plane to the branch cuts

$$(i\alpha, i\infty), \quad (-i\infty, -i\alpha), \quad (i\beta, i\infty), \quad (-i\infty, -i\beta).$$

The power series

$$\sum_{n=0}^{\infty} (i\gamma)^{-2n} w_{2n}(\xi),$$

where ξ has the value

$$\xi = 2\gamma \arctan(\mu/\gamma) + 2\gamma \arctan(\nu/\gamma),$$

is equal to $W(\gamma;\mu,\nu)$. It converges if

$$|\xi| < 2\pi|\gamma|. \tag{6.32}$$

The map of this region into the complex k plane gives a region of convergence which is much larger than the disk $|k| < \min(\alpha,\beta)$. [However, this disk is not wholly contained in (6.32)]. In particular the whole real k axis belongs to the region of convergence determined by Eq. (6.32).

The effective range function K_l of the examples of the potentials in Sec. 3 is a real analytic function of k^2 with the branch cut $-\infty < k^2 < \max(-\alpha^2, -\beta^2)$ and possibly with isolated poles of finite order. The position of these poles depends on the particular potential and is in general difficult to predict. In Eq. (3.11) K_l is regular at $k=0$. We have also given an example of a potential for which K_0 has a *pole* at $k=0$ [Eqs. (3.14)–(3.16)]. For a general rational separable potential with real positive β_i [Ref. 1, Eq. (97)] we conjecture that, except for the branch cut $-\infty < k^2 < \max(-\beta_1^2, \ldots, -\beta_n^2)$, the effective range function K_l is a "real-meromorphic" function of k^2 (i.e., real analytic except for a finite number of poles of finite order).

The singularities of the effective range function have thus been determined in principle. Its numerical calculation is facilitated, which is in particular due to Eq. (5.11)ff. The use of these equations is not restricted to the effective range function. They can also be applied to other quantities playing a role in the scattering by $V_c + V_{rs}$.

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A 6

ON THE EXACT SOLUTION OF THE SCATTERING AND BREAK-UP EQUATIONS FOR THREE-PARTICLE SYSTEMS WITH COULOMB INTERACTION

We investigate the problems connected with the incorporation of the Coulomb interaction in the equations which describe reactions involving charged particles. In particular a simple model for the proton-deuteron scattering and break-up reactions in the formalism of Alt, Sandhas and Ziegelmann is considered. Here various Coulomb quantities play a role which all have a so-called essential singularity in the zero-energy point. This singularity has to be taken care of when the total three-particle energy is near or above the break-up threshold. We have developed formulas, both for the case of a repulsive and an attractive Coulomb potential, by means of which the essential singularity is split off in a satisfactory way. This allows one to make really exact calculations for simple models. We have indicated a reason why a comparison of such exact calculations with known approximations is indeed desirable.

1. INTRODUCTION

A long-standing problem in nuclear physics, especially in the proton-deuteron system, concerns the incorporation of the Coulomb interaction between the protons in the description of nuclear reactions involving charged particles. In particular only crude ad hoc approximations for the Coulomb interaction have been used in proton-deuteron break-up calculations, e.g., by Van Oers and Brockmann [1], Bruinsma et al.[2] and Stuivenberg and Bruinsma [3].

As is well known, three-particle reactions are conveniently described by using the integral equations of Faddeev [4] or equivalent equations. However, the validity of these equations is restricted to interactions of short range so that the long-range Coulomb potential has to be excluded. Similar problems which play a role in the scattering of only two charged particles can be solved by applying a renormalization technique which is based on screening of the long-range potential, see Gorshkov [5]. The two-particle Coulomb difficulties and peculiarities have been studied extensively and are well understood.

By using Gorshkov's renormalization technique, Veselova[6] has developed a system of regular integral equations for reactions of three particles of which only two are charged. She restricted the total three-particle energy to negative values thereby excluding break-up reactions. Kharchenko and Storozhenko [7] have derived integral equations for the proton-deuteron system with separable nuclear interactions by using

the Gorshkov-Veselova method. Recently Alt, Sandhas and Ziegelmann [8] (see also Ref.9) have extended the AGS three-particle formalism [10] to include Coulomb interaction between two of the particles. They have given a comprehensive description of Coulomb-modified integral equations which allow exact calculations, for the case of general short-range interactions. Gorshkov's screening approach is used here, too. It is important to note that the three-particle energy may be positive as well as negative so that in particular break-up reactions may be described [8].

The basic idea in the approaches of Veselova and of Alt et al. described above, is to exploit to great similarity with the problem of just two charged particles. For the case of three charged particles such a similarity is not obvious. In this case additional singularities appear in the amplitudes (e.g., Veselova [11]). However, when only two charged fragments are present in the initial and final configurations, the approach of Alt et al. can again be used, see Alt [12]. Break-up equations for three charged particles are expected to be more complicated, since in this case the long-range Coulomb interaction between the three particle-pairs gives rise to more complicated asymptotic states (e.g.[11,13,14]).

In calculations with three-particle equations one usually works in the momentum representation. Merkuriev et al. [15] have studied such equations in the coordinate representation. The asymptotic form of the wave functions for three charged particles has been obtained by Merkuriev [13], below as well as above the break-up threshold. It may be expected that exact calculations can be obtained along these lines.

The problems in two-particle Coulomb scattering can be understood by considering the Lippmann-Schwinger equation for the off-shell T matrix in the momentum representation,

$$\langle \vec{q} \,|T_C(E)\,| \vec{q}' \rangle = \langle \vec{q} \,|V_C\,| \vec{q}' \rangle + \int d\vec{q}'' \langle \vec{q} \,|\, V_C \,|\, \vec{q}'' \rangle (E - q''^2)^{-1} \langle \vec{q}'' |T_C(E)| \vec{q}' \rangle . \qquad (1.1)$$

The Coulomb potential term in the kernel of this integral equation has a singularity at $\vec{q}'' = \vec{q}$, of the type $|\vec{q}'' - \vec{q}|^{-2}$. When the energy E equals q^2, this singularity coincides with the one of the Green function. This observation "explains" the singularity of T_C half-off the energy-shell, i.e. for $E = q^2$.

We now turn to the three-particle system. We consider in particular a very simple model in which the short-range nuclear forces are described by rank-one separable operators, and in which there is in addition repulsive Coulomb interaction between two of the particles. Alt et al. [8] have derived effective two-particle integral equations for the amplitudes $\mathbf{T}_{\beta\alpha}$ which are similar to Eq.(1.1) (cf. Eq.(2.20)),

$$\langle \vec{q}_\beta \,|\, \mathbf{T}_{\beta\alpha}(z) \,|\, \vec{q}_\alpha' \rangle = \langle \vec{q}_\beta \,|\, \mathbf{V}_{\beta\alpha}(z) \,|\, \vec{q}_\alpha' \rangle$$

$$+ \sum_\gamma \int d\vec{q}_\gamma'' \langle \vec{q}_\beta \,|\, \mathbf{V}_{\beta\gamma}(z) \,|\, \vec{q}_\gamma'' \rangle (z - \hat{E}_\gamma - \tfrac{3}{4}(q_\gamma'')^2)^{-1} \langle \vec{q}_\gamma'' \,|\, \mathbf{T}_{\gamma\alpha}(z) \,|\, \vec{q}_\alpha' \rangle . \qquad (1.2)$$

Here we have taken the masses equal to 1 for convenience. The formalism of Ref.8 is more general in that it is valid for rank N separable and local potentials as well, but the Coulomb interaction is taken care of in essentially the same way.

It is interesting to discuss the similarity of Eqs.(1.1)

and (1.2). The effective potentials $\mathbf{V}$ occurring in (1.2) are energy-dependent. As is shown in Ref.8, $\mathbf{V}_{\alpha\alpha}$ has on the energy-shell the same singularity as the pure two-particle Coulomb potential. Since, therefore, the singularity structure of Eq. (1.2) is similar to that of Eq.(1.1), the renormalization procedure of Gorshkov [5] is also applicable in this case.

There are, however, some additional problems. These concern the exact calculations of the effective two-particle potential $\mathbf{V}_{\beta\alpha}(z)$ itself. This quantity equals an integral involving the three-dimensional two-particle Coulomb T matrix, T_C. Moreover one needs Coulomb-modified form factors and their overlap integrals with the form factors of the rank-one separable potentials. In these quantities the partial-wave projection of T_C occurs. Now T_C is a complicated object. Although a number of integral- and series representations are known for $< \vec{q} \mid T_C(E) \mid \vec{q}' >$, these are not suitable for the zero-energy region.

This is related to the fact that $E = 0$ is a highly singular point of $T_C(E)$. As is well known, the bound-state energies for a potential appear as poles in the transition operator. Since the attractive Coulomb potential has an infinity of bound states, it follows that $T_C(E)$ has an accumulation point of poles in $E = 0$. This is also the case for a *repulsive* Coulomb interaction, even though the poles themselves occur for non-physical energies, see figs.1 and 2 at the end of Section 4B. As we will show in Section 3, the two-particle Coulomb T matrix at *zero* energy is always involved in the equations for reactions with *positive* (or zero) three-particle energy. It is therefore of interest to have a method which makes an exact calculation

of $T_C(E)$ possible, in particular in the vicinity of $E = 0$.

A natural approximation consists of replacing T_C by its first Born term, V_C, and similarly $T_{C,\ell}$ by $V_{C,\ell}$. In this case the calculations are considerably simplified. However, it is not clear how a reliable estimate of the accuracy of these approximations could be made.

In this connection it is worthwhile to consider the effect of these approximations on the renormalization factors. As we will show in Section 3, these factors remain unaltered when the three-dimensional Coulomb transition matrix T_C is replaced by V_C, since V_C alone generates the kernel-singularity which determines the renormalization factors. It is important to note, however, that an approximation of the overlap-integrals of the Coulomb-modified form factors with the form factors of the separable potentials *does* affect the renormalization factors since these quantities occur in the "residue" of the singularity of the kernel.

It follows from the above discussion that the off-shell two-particle Coulomb T matrix T_C is of considerable importance for exact calculations of three-body reactions involving charged particles. Moreover it may be expected that in all many-charged-particles-reaction-equations this quantity will play a basic and fundamental role. Therefore a study of T_C is of great interest.

The main purpose of this paper is to provide formulas for T_C and related quantities in particular in the vicinity of zero energy, which make an exact numerical calculation of the effective two-particle potentials possible. By using these formulas, really exact calculations can be performed for simple models. In this way reliable estimates can be made of various approximations.

In Section 2 we briefly discuss the formalism of Alt, Sandhas and Ziegelmann. In Section 3 we consider the zero-energy singularity playing a role in the effective two-particle potentials and in Section 4 we indicate the way in which this singularity should be treated. At the end of Section 4 we discuss a reason why the approximation in which T_C is replaced by V_C should be studied judiciously. Finally in Section 5 the results are summarized and discussed.

In Sections 2 and 3 we shall use mainly the notation of Ref.8. However, for the study of the Coulomb singularities in Section 4 we will use the notation of Refs.16 and 17 which is more suitable here.

2. A BRIEF DERIVATION OF THE EQUATIONS

In this section the derivation of the integral equations is briefly reviewed. We shall mainly use the notation of Ref.8. In particular, z is the total three-particle energy, $\vec{p}_\alpha$ is the relative momentum of particles β and γ, and $\vec{q}_\alpha$ the relative momentum of particle α and the system of particles (β,γ). For convenience we assume the masses m to be equal, and we take units such that $\hbar = m = 1$. Two-body quantities are characterized by a hat, e.g., $\hat{E}_\alpha$ is the bound-state energy of the (β,γ) pair. Then

$$z = \hat{E}_\alpha + \tfrac{3}{4} q_\alpha^2, \tag{2.1a}$$

$$z = p^2 + \tfrac{1}{4} q^2 , \tag{2.1b}$$

give the on-shell relations for scattering and break-up, respectively. Following Ref.8, Section 3, we take rank-one operators for the nuclear pair-interactions and we suppose that there is just one bound state in each channel.

The AGS equations [10] for the amplitudes $U_{\beta\alpha}(z)$ are

$$U_{\beta\alpha} = \bar{\delta}_{\beta\alpha}\, G_0^{-1} + \sum_\gamma \bar{\delta}_{\beta\gamma}\, T_\gamma\, G_0\, U_{\gamma\alpha}, \tag{2.2}$$

where $\bar{\delta}_{\beta\alpha} = 1 - \delta_{\beta\alpha}$ and the energy variable z has been suppressed. When the transition operator T_γ is written as the sum of a rank-one operator and a rest part T_γ',

$$T_\gamma = |\, \gamma > \tau_\gamma < \gamma\, | + T_\gamma', \tag{2.3}$$

one obtains, by inserting (2.3) in (2.2), the following equations for $U_{\beta\alpha}$,

$$U_{\beta\alpha} = U'_{\beta\alpha} + \sum_\gamma U'_{\beta\gamma}\, G_0\, |\, \gamma > \tau_\gamma < \gamma\, |\, G_0\, U_{\gamma\alpha}. \tag{2.4}$$

Here the $U'_{\beta\alpha}$ are the solutions of the equations

$$U'_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_0^{-1} + \sum_\gamma \bar{\delta}_{\beta\gamma} T'_\gamma G_0 U'_{\gamma\alpha}. \tag{2.5}$$

Now suppose that particle 3 is the neutral one, i.e., $T'_\gamma = \delta_{\gamma 3} T_C$. In this case Eq.(2.5) reduces to

$$U'_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_0^{-1} + \bar{\delta}_{\beta 3} T_C G_0 U'_{3\alpha},$$

which can be solved immediately,

$$U'_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_0^{-1} + \bar{c}_{\beta 3} \bar{\delta}_{3\alpha} T_C. \tag{2.6}$$

Therefore the first quasi-Born approximation is exact in this case.

One usually introduces transition operators $X_{\beta\alpha}$ and effective potentials $Z_{\beta\alpha}$ in an effective two-particle space by putting

$$X_{\beta\alpha} \equiv < \beta \mid G_0 U_{\beta\alpha} G_0 \mid \alpha >, \tag{2.7a}$$

$$Z_{\beta\alpha} \equiv < \beta \mid G_0 U'_{\beta\alpha} G_0 \mid \alpha >. \tag{2.7b}$$

In order to get the *amplitudes*, one has to sandwich these operators between plane wave states $\mid \vec{q} >$. From Eq.(2.4) one obtains

$$X_{\beta\alpha} = Z_{\beta\alpha} + \sum_\gamma Z_{\beta\gamma} \tau_\gamma X_{\gamma\alpha}. \tag{2.8}$$

We now concentrate on the effective potentials $Z_{\beta\alpha}$. When the strong interactions are described by rank-one operators with form factors $\mid g_\alpha >$, the form factors occurring in (2.3) are given by

$$\mid \gamma > = (1 + T'_\gamma G_0) \mid g_\gamma >.$$

Since only particles 1 and 2 are charged, we see that only $\mid 3 >$ is a Coulomb-modified form factor: From $T'_\gamma = \delta_{\gamma 3} T_C$ we have

$$\mid \gamma > = (1 + \delta_{\gamma 3} T_C G_0) \mid g_\gamma >. \tag{2.9}$$

We insert (2.9) in (2.7b) and obtain, by using (2.6), the following

simple exact expression for the effective potentials,

$$Z_{\beta\alpha} = \langle g_\beta \mid G_C - \delta_{\beta\alpha}\, G_0 \mid g_\alpha \rangle, \quad (\beta,\alpha) \neq (3,3),$$

$$Z_{33} = 0. \tag{2.10}$$

This is essentially Eq.(3.23) of Ref.8.

It is convenient to recast Eq.(2.8) into an effective two-particle equation which resembles the ordinary Lippmann-Schwinger (LS) equation. In Ref.8 this is performed by rewriting τ_γ and by introducing new amplitudes $\mathbf{T}_{\beta\alpha}(z)$ and effective potentials $\mathbf{V}_{\beta\alpha}(z)$. Let us first consider τ_γ. According to the above assumptions we have

$$V_\gamma = \mid g_\gamma \rangle \lambda_\gamma \langle g_\gamma \mid + \delta_{\gamma 3}\, V_C, \tag{2.11}$$

and so (cf. Eq.(2.3))

$$\hat{\tau}_3^{-1}(z_3) = \lambda_3^{-1} - \langle g_3 \mid \hat{G}_C(z_3) \mid g_3 \rangle. \tag{2.12}$$

A similar expression, with $\hat{G}_C$ replaced by $\hat{G}_0$, holds for $\hat{\tau}_1$ and $\hat{\tau}_2$. At the two-body bound-state energy, $\hat{E}_\alpha$, the T operator has a pole and so one has $\hat{\tau}_\alpha^{-1}(\hat{E}_\alpha) = 0$. By using the identity

$$\hat{G}(\hat{E}) - \hat{G}(z) = (z - \hat{E})\, \hat{G}(\hat{E})\, \hat{G}(z), \tag{2.13}$$

we obtain

$$\hat{\tau}_\alpha(z_\alpha) = \hat{s}_\alpha(z_\alpha) / (z_\alpha - \hat{E}_\alpha),$$

where

$$\hat{s}_\alpha(z_\alpha) \equiv \langle g_\alpha \mid \hat{G}_0(\hat{E}_\alpha)\, \hat{G}_0(z_\alpha) \mid g_\alpha \rangle^{-1}, \quad \alpha = 1,2, \tag{2.14}$$

$$\hat{s}_3(z_3) \equiv \langle g_3 \mid \hat{G}_C(\hat{E}_3)\, \hat{G}_C(z_3) \mid g_3 \rangle^{-1}. \tag{2.15}$$

The bound-state wave functions may be taken normalized to one, so

$$\hat{s}_\alpha(\hat{E}_\alpha) = 1, \quad \alpha = 1,2,3. \tag{2.16}$$

The operator $T_\gamma(z)$ in three-particle space is connected to the two-particle transition operator by

$$\langle \vec{q}_\gamma', \vec{p}_\gamma' | T_\gamma(z) | \vec{p}_\gamma, \vec{q}_\gamma \rangle = \delta(\vec{q}_\gamma' - \vec{q}_\gamma) \langle \vec{p}_\gamma' | \hat{T}_\gamma(z - \tfrac{3}{4} q_\gamma^2) | \vec{p}_\gamma \rangle.$$

One also has

$$\langle \vec{q}_\gamma' | \tau_\gamma(z) | \vec{q}_\gamma \rangle = \delta(\vec{q}_\gamma' - \vec{q}_\gamma) \hat{\tau}_\gamma(z - \tfrac{3}{4} q_\gamma^2).$$

Now we recall Eq.(2.8) which is rewritten more completely as

$$\langle \vec{q}_\beta' | X_{\beta\alpha}(z) | \vec{q}_\alpha \rangle = \langle \vec{q}_\beta' | Z_{\beta\alpha}(z) | \vec{q}_\alpha \rangle + \sum_\gamma \int d\vec{q}_\gamma'' \langle \vec{q}_\beta | Z_{\beta\gamma}(z) | \vec{q}_\gamma'' \rangle \hat{\tau}_\gamma(z - \tfrac{3}{4}(q_\gamma'')^2) \langle \vec{q}_\gamma'' | X_{\gamma\alpha}(z) | \vec{q}_\alpha \rangle. \tag{2.17}$$

In Ref.8 new amplitudes and effective potentials are introduced by

$$\langle \vec{q}_\beta' | \mathbf{T}_{\beta\alpha}(z) | \vec{q}_\alpha \rangle \equiv \hat{s}_\beta^{\frac{1}{2}}(z - \tfrac{3}{4} q_\beta'^2) \langle \vec{q}_\beta' | X_{\beta\alpha}(z) | \vec{q}_\alpha \rangle \hat{s}_\alpha^{\frac{1}{2}}(z - \tfrac{3}{4} q_\alpha^2), \tag{2.18}$$

$$\langle \vec{q}_\beta' | \mathbf{V}_{\beta\alpha}(z) | \vec{q}_\alpha \rangle \equiv \hat{s}_\beta^{\frac{1}{2}}(z - \tfrac{3}{4} q_\beta'^2) \langle \vec{q}_\beta' | Z_{\beta\alpha}(z) | \vec{q}_\alpha \rangle \hat{s}_\alpha^{\frac{1}{2}}(z - \tfrac{3}{4} q_\alpha^2). \tag{2.19}$$

Note that, because of $\hat{s}_\alpha(\hat{E}_\alpha) = 1$ (Eq.(2.16)), $\mathbf{T}_{\beta\alpha}$ coincides with $X_{\beta\alpha}$ on the energy-shell (see Eq.(2.1)). With the help of the above equations one obtains for the new operators $\mathbf{T}_{\beta\alpha}$ the following effective two-particle equations,

$$\mathbf{T}_{\beta\alpha}(z) = \mathbf{V}_{\beta\alpha}(z) + \sum_\gamma \mathbf{V}_{\beta\gamma}(z) \mathbf{G}_{0;\gamma}(z) \mathbf{T}_{\gamma\alpha}(z), \tag{2.20}$$

where

$$\langle \vec{q}_\alpha' | \mathbf{G}_{0;\alpha}(z) | \vec{q}_\alpha \rangle = \delta(\vec{q}_\alpha' - \vec{q}_\alpha) (z - \hat{E}_\alpha - \tfrac{3}{4} q_\alpha^2)^{-1}. \tag{2.21}$$

Obviously (2.20) has the form of a set of LS equations with energy-

dependent effective potentials $\mathbf{V}_{\beta\alpha}(z)$.

The three-particle *break-up* operators $\mathbf{T}_{0\alpha}$ can be calculated by quadrature [10] from the elastic and rearrangement operators $\mathbf{T}_{\beta\alpha}$,

$$\mathbf{T}_{0\alpha}(z) = \mathbf{V}_{0\alpha}(z) + \sum_{\gamma} \mathbf{V}_{0\gamma}(z)\ \mathbf{G}_{0;\gamma}(z)\ \mathbf{T}_{\gamma\alpha}(z). \qquad (2.22)$$

For the break-up effective potentials $\mathbf{V}_{0\alpha}$ occurring here an expression involving again the two-particle Coulomb T matrix can be given, see Eq.(3.56) of Ref.8. We may restrict ourselves for the moment to the $\mathbf{T}_{\beta\alpha}$, which have to be calculated from (2.20), that is, from the corresponding integral equations (1.2). The singularities of $\mathbf{T}_{\beta\alpha}$ can be deduced from the singularities of the kernels of the integral equations (1.2). Therefore we shall investigate the effective potentials $\mathbf{V}_{\beta\alpha}$ in the next section.

3. ON THE EXACT CALCULATION OF THE EFFECTIVE POTENTIALS

In this section we shall discuss the complicated Coulomb singularities that play a role in the exact calculation of the effective potentials $\mathbf{V}_{\beta\alpha}$. We will also briefly consider the singularity structure of the effective two-particle equations (1.2) and show the similarity with the two-particle Coulomb LS equation (1.1).

According to Eqs.(2.10) and (2.19) the Coulomb interaction occurs in the quantities $< g_\beta \mid G_C \mid g_\alpha >$ or $Z_{\beta\alpha}$, and in $\hat{s}_3(z - \frac{3}{4}q_3^2)$, which is given by Eq.(2.15). By using Eq.(2.13) we see that in order to obtain $\hat{s}_3$, only $< g_3 \mid \hat{G}_C \mid g_3 >$ has to be calculated, for different energies.

Since $G_C = G_3'$, the quantities $< g_\beta \mid G_C \mid g_\alpha >$ appear in three different types (cf. fig.1 of Ref.8). Examples of the first type are $< g_3 \mid G_C \mid g_1 >$ and $< g_3 \mid G_C \mid g_2 >$. These quantities are essentially given by Coulomb-modified form factors, $g^C(z - \frac{3}{4}q^2)$ (cf. Eq.(A.2) of Ref.8). Type two is exemplified by $< g_2 \mid G_C \mid g_1 >$, and type three by $< g_1 \mid G_3 \mid g_1 >$ and $< g_2 \mid G_3 \mid g_2 >$. These quantities can be expressed by three-dimensional integrals involving the two-particle Coulomb Green function or T matrix.

Let us first write out $Z_{\alpha\alpha}$ $(\alpha = 1,2)$ explicitly (cf. Eq.(2.10)),

$$< \vec{q}_\alpha' \mid Z_{\alpha\alpha}(z) \mid \vec{q}_\alpha > =$$

$$\int d\vec{p}\, \frac{g_\alpha(\frac{1}{2}\vec{q}_\alpha' + \vec{p})\ \hat{T}_C(\vec{q}_\alpha' + \frac{1}{2}\vec{p}, \vec{q}_\alpha + \frac{1}{2}\vec{p}; z - \frac{3}{4}p^2)\ g_\alpha(\frac{1}{2}\vec{q}_\alpha + \vec{p})}{(z - p^2 - q_\alpha'^2 - \vec{q}_\alpha' \cdot \vec{p})(z - p^2 - q_\alpha^2 - \vec{q}_\alpha \cdot \vec{p})}. \qquad (3.1)$$

This expression corresponds to diagram d, fig.1 of Ref.8. The form factors are in fact only functions of the magnitude of their argument. By inserting

$$\hat{T}_C = \hat{V}_C + (\hat{T}_C - \hat{V}_C) \qquad (3.2)$$

in (3.1) one obtains two terms. The first one can be written as

$$\hat{V}_C(\vec{q}_\alpha', \vec{q}_\alpha)\ F_\alpha(\vec{q}_\alpha', \vec{q}_\alpha;\ z), \tag{3.3}$$

with

$$F_\alpha(\vec{q}_\alpha', \vec{q}_\alpha;\ z) = \int d\vec{k}\, \frac{g_\alpha(\vec{k})\ g_\alpha(\vec{k} + \tfrac{1}{2}(\vec{q}_\alpha' - \vec{q}_\alpha))}{(k^2 + \tfrac{3}{4} q_\alpha'^2 - z)\,(\,|\,\vec{k} + \tfrac{1}{2}(\vec{q}_\alpha' - \vec{q}_\alpha)\,|^2 + \tfrac{3}{4} q_\alpha^2 - z)}, \tag{3.4}$$

where the new variable of integration $\vec{k} = -\vec{p} - \tfrac{1}{2}\vec{q}_\alpha'$ has been used.

The expression (3.3) is singular for $\vec{q}_\alpha' = \vec{q}_\alpha$. When in addition q_α and q_α' are on the energy-shell (see Eq.(2.1)), it has exactly the same singularity as the pure Coulomb potential $\hat{V}_C$. This follows by noting that F_α in this case reduces to the normalization integral of the bound-state wave function, which is taken to be one according to Eq.(2.16). The singularity of $\mathbf{G}_{0;\alpha}$ in Eq.(1.2) coincides with the one of the effective potential $\mathbf{V}_{\alpha\alpha}$, in the on-shell case. The second term of (3.2), $\hat{T}_C - \hat{V}_C$, has for $\vec{q}_\alpha' \simeq \vec{q}_\alpha$ a behavior like $c\,|\,\vec{q}_\alpha' - \vec{q}_\alpha\,|^{-1}$ (see Eq.(4.40)), so it is integrable there.

For Z_{21} an expression similar to (3.1) holds, where now, however, the matrix element with $\hat{T}_C$ on the right-hand side is replaced by

$$\hat{T}_C(-\vec{q}_\beta' - \tfrac{1}{2}\vec{p},\ \vec{q}_\alpha + \tfrac{1}{2}\vec{p};\ z - \tfrac{3}{4} p^2).$$

Obviously the first Born term $\hat{V}_C$ gives in this case an integral of the type $\int d\vec{p}\,|\,\vec{p} + \vec{q}_\alpha + \vec{q}_\beta'\,|^{-2} \ldots$ in (3.1), which shows that Z_{21} has no "dangerous" singularity.

Finally, also the operators Z_{31} and Z_{32}, which can be expressed in terms of the Coulomb-modified form factors, contain no dangerous singularity.

The effective potentials are also needed *off* the energy shell. It can be shown [8] that there are no other "dangerous" singularities,

not only for negative total energy z, but also for positive z. There are of course no difficulties when $\vec{q}_\alpha' \neq \vec{q}_\alpha$. So let us consider only F_α with $\vec{q}_\alpha' = \vec{q}_\alpha$ and $z = E + i\eta$, $\eta \downarrow 0$, where $E > \frac{3}{4} q_\alpha^2$,

$$F_\alpha(\vec{q}_\alpha, \vec{q}_\alpha; E + i\eta) = \int d\vec{k} \, [g(\vec{k}) / (k^2 + \tfrac{3}{4} q_\alpha^2 - E - i\eta)]^2 .$$

The integrand here has a pole of the second order, so it is integrable.

The conclusion is that only $Z_{\alpha\alpha}$ ($\alpha = 1,2$) contains the singularity from which the renormalization factors have to be deduced. So the effective two-particle integral equations have the same singularity structure as the ordinary LS equation with the Coulomb potential, and therefore the well-known two-particle Coulomb renormalization procedure can be applied. For more details we refer to the paper of Alt et al. [8].

Now that the formalism has been briefly sketched, we come to the *exact* calculation of the effective potentials. We see from Eq.(3.1) in particular, that for any reaction where the total three-particle energy is above the break-up threshold, $z = 0$, one has to calculate the two-particle Coulomb T matrix for negative *and* positive energies. Especially the zero-energy region is difficult since $z = 0$ is a so-called essential singular point of $\hat{T}_C(z)$. Because of the infinity of bound states for an attractive Coulomb interaction, $\hat{T}_C(z)$ has an accumulation point of poles at $z = 0$. In the case of a repulsive $\hat{V}_C$ these poles are situated on the second Riemann-sheet of the complex energy plane. Therefore the origin is limit point of poles also in the repulsive case. In order to perform the integration in (3.1) one needs a representation of $\hat{T}_C$ which is different from the known series- and integral representations. We shall deduce such a representation in the next section. There we shall

also discuss the Coulomb-modified form factors and the factors $\hat{s}_\alpha$, where the same $\hat{T}_C$-zero-energy problems play a role.

Finally a remark on some approximations is appropriate here. When in Eq.(3.1) $\hat{T}_C$ is replaced by $\hat{V}_C$, the calculations are very much simplified. In this case the renormalization factors remain unaltered, as will be clear from Eq.(3.3) and the discussion following. However, when an approximation for $\hat{s}_\alpha$ is used, the renormalization factors have to be adapted. The reason is that the factors $\hat{s}_\alpha^{\frac{1}{2}}$ appear in the "residue" of the singularity of the kernel. Although on the energy-shell $\hat{s}_\alpha$ may be *defined* to be 1 (Eq.(2.16)), its exact calculation is *not* easy, even in the simple case when the form factors g_α are Yamaguchi ones. We shall investigate $\hat{s}_\alpha$ in particular for these form factors.

4. REDUCTION OF THE ZERO-ENERGY ESSENTIAL SINGULARITY OF VARIOUS COULOMB QUANTITIES

In this section we shall study the zero-energy singularity of the Coulomb quantities occurring in the effective potentials which have been discussed in Sections 2 and 3. We shall deduce asymptotic series expansions for these quantities that are usable especially when the energy is close to zero.

The notation here differs from the one used in Sections 2 and 3. We will mainly use the notation of Refs.16 and 17, which is more appropriate for two-particle off-shell quantities. The mass of each particle equals one as before, but the energy E is denoted by k^2 with $\mathrm{Im}\, k > 0$. The energy-dependence will often be suppressed. It is important to note that the subscripts α and β to the form factors g have a different meaning here. In Sections 2 and 3, α denotes the channels, whereas in Ref.16 α is connected with the range of the nuclear interaction. In particular, for the Yamaguchi potential g_α is given by

$$g_\alpha(p) = (2/\pi)^{\frac{1}{2}} (p^2 + \alpha^2)^{-1}, \quad \alpha > 0.$$

The subscripts α, β and γ used in Sections 2 and 3 to denote the particles are irrelevant here and will be suppressed. For the sake of comparison with Refs. 16 and 17 we shall use the momentum variables p, p', $\vec{p}$ and $\vec{p}'$. Furthermore we will denote $|\vec{p} - \vec{p}'|$ by q, which should not be confused with the variable q used before. In actual three-particle calculations one should of course replace the momenta and energies used here, by the appropriate expressions occurring in Sections 2 and 3.

This section contains three subsections. In Section 4A some

preliminaries will be given. In 4B we investigate the hypergeometric function (h.f.) $F_{i\gamma}(AB)$ with complex α and β. This function is the basic object in the expressions for

(i) the Coulomb-modified form factors,

(ii) their overlap integrals with the form factors of the separable potentials, and

(iii) the partial-wave Coulomb T matrix.

Finally in Section 4C we present our study of the three-dimensional Coulomb T matrix.

4A. *Preliminaries*

It turns out that in all expressions we need, a central role is played by a certain hypergeometric function [18] which we have previously denoted by $F_{i\gamma}$, namely

$$F_{i\gamma}(z) \equiv {}_2F_1(1, i\gamma;\ 1 + i\gamma;\ z). \tag{4.1}$$

Let us start by considering the case $\ell = 0$. In the first place the $\ell = 0$ partial wave Coulomb T matrix is given by [16]

$$\langle p' \mid \hat{T}_{C,\ell=0} \mid p \rangle = \frac{ik}{\pi pp'} \left[F_{i\gamma}(aa') + F_{i\gamma}\left(\frac{1}{aa'}\right) - F_{i\gamma}\left(\frac{a}{a'}\right) - F_{i\gamma}\left(\frac{a'}{a}\right) \right], \tag{4.2}$$

where

$$a \equiv (p - k) / (p + k), \quad a' \equiv (p' - k) / (p' + k).$$

This quantity $\langle p' \mid \hat{T}_{C,\ell=0} \mid p \rangle$ is needed in particular when calculations with nonrational form factors are made.

Secondly, for the calculation of the quantities $\hat{s}$ discussed in Section 2 we need an expression for $\langle g \mid \hat{G}_{C,\ell=0} \mid g \rangle$. Suppose that the form factor g is a linear combination of two Yamaguchi form factors,

$$g(p) = c_\alpha\, g_\alpha(p) + c_\beta\, g_\beta(p).$$

Then we may restrict the considerations to $< g_\alpha \mid \hat{G}_{C,\ell=0} \mid g_\beta >$. Indeed, by taking $\alpha \neq \beta$, $\alpha \to \beta$, and $\beta \to \alpha$ respectively, one obtains $< g \mid \hat{G}_{C,\ell=0} \mid g >$. A number of closed expressions for $< g_\alpha \mid \hat{G}_{C,\ell=0} \mid g_\beta >$ are available, e.g. [16]

$$< g_\alpha \mid \hat{G}_{C,\ell=0}(k^2) \mid g_\beta > = \frac{-1}{(\alpha+\beta)(\alpha+ik)(\beta+ik)} - \frac{2ik}{(\alpha^2+k^2)(\beta^2+k^2)} F_{i\gamma}(AB), \quad (4.3)$$

in which A and B, occurring in the argument of the h.f. $F_{i\gamma}$, are defined by

$$A \equiv \frac{\alpha + ik}{\alpha - ik}, \qquad B \equiv \frac{\beta + ik}{\beta - ik}.$$

The Coulomb-modified form factor g_β^C corresponding to g_β is given by [16,19]

$$< p \mid g_\beta^C(k^2) > \equiv < p \mid (1 + \hat{T}_{C,\ell=0}\ \hat{G}_{0,\ell=0}) \mid g_\beta >$$

$$= \frac{(2/\pi)^{\frac{1}{2}}}{p^2 + \beta^2} - \frac{(2/\pi)^{\frac{1}{2}} k/p}{k^2 + \beta^2} \left| F_{i\gamma}(Ba) - F_{i\gamma}(B/a) \right|. \quad (4.4)$$

Instead of a superposition of Yamaguchi form factors one can use more general rational form factors. Further the above discussion on the $\ell = 0$ case can be extended to higher values of ℓ. This leads to more complicated expressions which are, however, still composed of simple functions and the h.f. $F_{i\gamma}$. In particular, when the form factor g_ℓ is normalizable and $p^{-\ell} g_\ell(p)$ is a rational function of p^2, $< p \mid g_\ell^C >$ and $< g_\ell \mid \hat{G}_{C,\ell} \mid g_\ell >$ can most likely be expressed in terms of simple functions and the h.f. $F_{i\gamma}$ with *exactly* the same arguments as in (4.3) and (4.4). Furthermore, $< p' \mid \hat{T}_{C,\ell} \mid p >$ can be written in terms of simple functions and $F_{i\gamma}$ with *exactly* the same arguments as occur in Eq.(4.2). Such expressions have, however, only been published for $\ell = 1$, see Eqs.(2.1) - (2.4) of Ref.17, where we also have given a more detailed discussion.

In the third place we encounter the complete three-dimensional two-particle Coulomb T matrix in the momentum representation. An expression for this quantity has been known for a long time [20,21]. It is convenient here to subtract the potential term, $\hat{V}_C$. In the notation of Ref.16 we have

$$\langle \vec{p}' | \hat{V}_C | \vec{p} \rangle = k\gamma \pi^{-2} q^{-2} = -s \pi^{-2} q^{-2},$$

$$\langle \vec{p}' | \hat{T}_C - \hat{V}_C | \vec{p} \rangle = k\gamma \pi^{-2} q^{-2} x^{-1} \left[F_{i\gamma}(y) - F_{i\gamma}(1/y) \right]. \qquad (4.5)$$

Here $q \equiv |\vec{p}' - \vec{p}|$ and

$$x^2 \equiv 1 + (p^2 - k^2)(p'^2 - k^2) k^{-2} q^{-2},$$

$$y \equiv (x+1) / (x-1). \qquad (4.6)$$

In Eqs.(4.2) - (4.5) the h.f. $F_{i\gamma}(z)$ occurs with various expressions for z: AB, Ba, B/a, aa', $(aa')^{-1}$, a/a', a'/a, y and 1/y. All these expressions have one common property: For zero energy, i.e. $k = 0$, they are all equal to 1, when α, β, p, p' and q are different from zero. It is well known that $F_{i\gamma}(z)$ has a singularity at $z = 1$, of a logarithmic type, cf. Eq.(4.2) of Ref.17. Furthermore it should be noted that $|\gamma| \to \infty$ when $k \to 0$ since $k\gamma = -s =$ constant. It follows in particular that the above functions $F_{i\gamma}(z)$, considered as functions of k, are *no* h.f.'s since not only their argument but also two parameters are functions of k.

As a matter of fact, the $F_{i\gamma}$'s that appear in Eqs.(4.2) - (4.4) can all be represented by $F_{i\gamma}(AB)$ if we allow α and β to be complex numbers. Only $F_{i\gamma}(y)$ and $F_{i\gamma}(1/y)$ (Eq.(4.5)) are somewhat different, since y is a more complicated function of k. Therefore we are now going to discuss $F_{i\gamma}(AB)$. In section 4C we will consider $F_{i\gamma}(y)$ and the three-dimensional Coulomb T matrix $\hat{T}_C$.

4B. $F_{i\gamma}(AB)$ *with complex* α *and* β

In order to study $F_{i\gamma}(AB)$ with complex $A = (\alpha + ik)/(\alpha - ik)$, $B = (\beta + ik)/(\beta - ik)$, we use some results obtained previously [17]. There, in Eq.(6.30), we defined a function V by

$$V(\gamma;\xi) \equiv (i\gamma)^{-1} e^{-\xi} \left[F_{i\gamma}(e^{i\xi/\gamma}) - \tfrac{1}{2} \right] + \psi(i\gamma) + (2i\gamma)^{-1} + C - \ln(i\gamma/\xi), \tag{4.7}$$

where C is Euler's constant and ψ is the digamma function, $\psi(z) = \Gamma'(z) / \Gamma(z)$. The variable ξ will be chosen appropriately below.

One of the basic results of Ref.17 consists of the proof that $V(\gamma;\xi)$ is analytic in γ and in ξ on the domain defined by

$$| \xi/\gamma | < 2\pi, \tag{4.8}$$

where the expansion

$$V(\gamma;\xi) = \sum_{n=0}^{\infty} v_{2n}(\xi)(i\gamma)^{-2n}, \quad | \xi | < 2\pi | \gamma | \tag{4.9}$$

holds (Eq.(6.34) of Ref.17). The first expansion coefficient v_0 is given by

$$v_0(\xi) = \Gamma(0,\xi) + \ln \xi + C = -\sum_{n=1}^{\infty} (-\xi)^n/(n\,n!), \tag{4.10}$$

where $\Gamma(0,\xi)$ is the incomplete gamma function [18]. For $v_{2n}(\xi)$, $n > 0$, we have obtained a number of equivalent expressions, see Eqs.(5.13), (5.14), (5.16) and (6.35) of Ref.17. For the moment the following closed expression will suffice,

$$v_{2n}(\xi) = -\frac{B_{2n}}{(2n)!} \frac{\xi^{2n}}{2n} e^{-\xi} {}_1F_1(1; 2n+1; \xi), \quad n > 0. \tag{4.11}$$

Here B_{2n} are Bernoulli's numbers and ${}_1F_1$ is the confluent hypergeometric function [18].

In order to apply these results we first recast Eq.(4.7) in the form

$$F_{i\gamma}(e^{i\xi/\gamma}) = \tfrac{1}{2} + i\gamma\, e^{\xi} V(\gamma;\xi) - i\gamma\, e^{\xi}\left[\psi(i\gamma) + (2i\gamma)^{-1} + C - \ell n\,(i\gamma/\xi)\right]. \qquad (4.12)$$

The important step is then, to construct an expression for ξ such that the various arguments of $F_{i\gamma}$, such as AB, Ba, aa', are reproduced.

In order to achieve this for the argument AB, we choose

$$\xi = 2\gamma \arctan\,(k/\alpha) + 2\gamma \arctan\,(k/\beta). \qquad (4.13)$$

Note that this ξ is a rather simple function of k^2. Furthermore, ξ is real for real or imaginary k when α and β are real. By using

$$i \arctan z = \operatorname{Artanh} iz = \tfrac{1}{2}\,\ell n\,\frac{1+iz}{1-iz}\,, \qquad (4.14)$$

and Eq.(4.13) we obtain

$$e^{i\xi/\gamma} = \frac{\alpha+ik}{\alpha-ik}\,\frac{\beta+ik}{\beta-ik} = AB \qquad (4.15)$$

and

$$e^{\xi} = (\exp(i\xi/\gamma))^{-i\gamma} = (AB)^{-i\gamma}.$$

Clearly, substitution of (4.13) in (4.12) yields the desired expression for $F_{i\gamma}(AB)$ which is indeed usable near zero energy, $k \approx 0$. The zero energy limit of ξ is easily obtained from Eq.(4.13),

$$\lim_{k\to 0} \xi \equiv \xi_0 = -2s(\alpha^{-1} + \beta^{-1}),$$

where we have made use of the equality $k\gamma = -s$. In terms of the alternative variables $\mu = -s/\alpha$ and $\nu = -s/\beta$ which are used in Ref.17, we have

$$\xi_0 = 2\mu + 2\nu.$$

Let us discuss $F_{i\gamma}(e^{i\xi/\gamma})$ in particular for small k. On the

right-hand side of Eq.(4.12) we see three nontrivial functions, namely $V(\gamma;\xi)$, $\psi(i\gamma)$ and $\ell n(i\gamma/\xi)$. We shall first consider V, for which the expansion (4.9) has been given. The coefficients $v_{2n}(\xi$, are rather simple functions of ξ. In particular, the well-known power series for the h.f ${}_1F_1$,

$$ {}_1F_1(1;\, 2n+1;\, \xi) = (2n)! \sum_{m=0}^{\infty} \xi^m/(2n+m)! $$

converges for all ξ.

It is worthwhile to investigate the domain of the convergence of the expansion in (4.9), i.e., $|\xi| < 2\pi|\gamma|$. We would like to have an inequality which gives the domain of convergence in the complex k-plane. By inserting the expression (4.13) for ξ we obtain

$$ |\arctan(k/\alpha) + \arctan(k/\beta)| < \pi . \qquad (4.16) $$

This condition is fulfilled for all real k, $\alpha \neq 0$ and $\beta \neq 0$. For negative energy k is purely imaginary. More generally, when α and β are complex, we deduce from Eq.(4.16) with the help of Eq.(4.14) that a sufficient condition is given by

$$ |k/\alpha| \text{ and } |k/\beta| < \frac{e^{\pi}-1}{e^{\pi}+1} = \tanh(\pi/2) \approx 0.917. \qquad (4.17) $$

This condition can be satisfied rather easily. Moreover, when $|k/\alpha|$ and $|k/\beta|$ are much smaller than 1, a few terms of the series in Eq.(4.9) will presumably give a good approximation.

Now we are going to discuss $\psi(i\gamma)$ and $\ell n(i\gamma/\xi)$ occurring on the right-hand side of Eq.(4.12). We shall first consider the repulsive case, $s < 0$. The digamma function $\psi(i\gamma)$ is meromorphic. It has simple poles at $i\gamma = -n$, $n = 0,1,2, \ldots$. In the complex k-plane these poles are situated on the negative-imaginary k-axis in the points $k = is/n$, and they accumulate at the origin, see fig.1. Since

the physical region is the *upper* half of the complex k-plane, these poles are nonphysical, which is indeed obvious for a repulsive potential. In this case we can apply the following asymptotic expansion,

$$\psi(z) = \ln z - (2z)^{-1} - \sum_{n=1}^{m} z^{-2n} B_{2n}/(2n) + O(z^{-2m-2}), \quad |z| \to \infty, \quad |\arg z| < \pi. \quad (4.18)$$

Note that, for physical k: $\mathrm{Im}\, k > 0$, $i\gamma$ cannot become real negative when $s < 0$. By considering the term $\ln z$ on the right-hand side of Eq.(4.18) we see that the logarithmic singularity of $F_{i\gamma}(AB)$ (cf. Eq.(4.12)) is only apparent in this case. Since $\psi(i\gamma) - \ln(i\gamma)$ goes to zero for $k \to 0$, i.e. $|\gamma| \to \infty$, we have, with the help of Eq.(4.10),

$$\lim_{k\to 0} (i\gamma)^{-1} F_{i\gamma}(AB) = e^{\xi_0} \Gamma(0, \xi_0), \qquad s < 0, \ \alpha > 0, \ \beta > 0,$$

where $\xi_0 = 2\mu + 2\nu$ as before.

The importance of Eq.(4.12) is that the essential singularity in the point $k = 0$ is contained in the digamma function, for which the asymptotic series (4.18) is known. Indeed, when we have to use $F_{i\gamma}(AB)$ in the calculations for the three-particle equations, the above essential singularity will cause no difficulties any more. Recall from Eqs.(1.2), (2.14), (2.18), (2.19), and (3.1) that for these calculations integrations have to be performed in the complex energy-plane along the line $E + i\eta$, where $\eta \downarrow 0$ and $-\infty < E < z$ with $z > 0$. We have sketched this path of integration in the complex k-plane in fig.1. It clearly shows that this path just touches the *upper* side of the essential singularity in $k = 0$, where this singularity is not "dangerous".

In the second place we now consider the case of an attractive Coulomb potential, $s > 0$. As is well known the Coulomb T matrix has simple poles at the bound-state energies, which are given by $-s^2/n^2$,

$n = 1,2,3, \ldots$. In this case the poles are physical. Indeed, they lie on the *positive*-imaginary k-axis, in $k = is/n$, see fig.2. These are just the poles $i\gamma = -n$, $n = 1,2,3, \ldots$, of the digamma function $\psi(i\gamma)$ discussed above. So we see that again the essential singularity in $k = 0$, due to the accumulation of the Coulomb bound-state poles, is contained in $\psi(i\gamma)$.

Just as before one has to perform an integration in the complex k-plane. The path of integration has been sketched in fig.2. Since in the attractive case one really has to integrate closely along all the poles, a part of the integration has to be done by analytical means. For this purpose the following expression may be helpful

$$\psi(i\gamma) = -C + \sum_{n=0}^{\infty} \left(\frac{1}{n+1} - \frac{1}{n+i\gamma} \right),$$

in which the poles of ψ are clearly shown. It is not difficult to work out a simple example in which an integration of $\psi(i\gamma)$ is carried out along the path shown in fig.2. For more details we refer to Ref.17.

In conclusion we can say that by the manipulations discussed above we have split off the essential singularity of the Coulomb quantities at zero energy in a satisfactory way. With the help of Eqs.(4.9) - (4.12) it is possible to make the necessary calculations in an exact way.

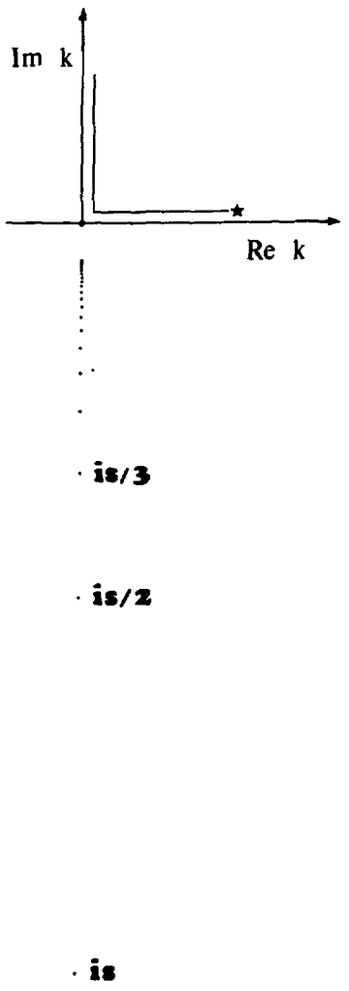

Fig. 1

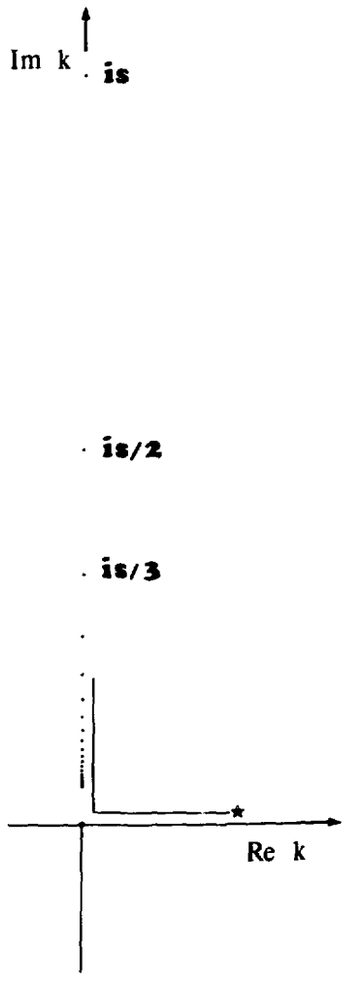

Fig. 2

Figs.1 and 2. The bound-state poles at $k = is/n$, $n = 1,2,3, \ldots$, for a repulsive Coulomb potential ($s < 0$: fig.1) and for an attractive Coulomb potential ($s > 0$: fig.2). The path of the integrations playing a role in the three-particle equations is indicated by a little star in both figures.

4C. $F_{i\gamma}(y)$ and the three-dimensional Coulomb T matrix in the vicinity of zero energy

In this subsection we shall analyse the three-dimensional Coulomb T matrix by using the function $F_{i\gamma}(e^{i\xi/\gamma})$ of Eq.(4.12). In this case a different and more complicated expression for ξ has to be found. Apart from a differing ξ the situation is just as has been sketched in figs.1 and 2. Again one has to integrate along the essential singularity at zero energy, cf. Eq.(3.1).

Let us first give a few known formulas [20,21]. These may be used only for energies different from zero. In the notation of Ref.16 we have (cf. Eqs.(4.5) and (4.6))

$$\langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = 4k\gamma^2(i\pi^2q^2)^{-1}\int_0^1 t^{i\gamma}[4t-(1-t)^2(x^2-1)]^{-1}\,dt$$

$$= k\gamma(\pi^2q^2x)^{-1}[F_{i\gamma}(y) - F_{i\gamma}(1/y)]. \qquad (4.19)$$

By choosing Re $\mathbf{x} < 0$, which implies $|y| < 1$, one obtains

$$F_{i\gamma}(y) - F_{i\gamma}(1/y) = 1-(-y)^{i\gamma}\,\Gamma(1+i\gamma)\,\Gamma(1-i\gamma) + 2\gamma^2\sum_{n=1}^{\infty} y^n(n^2+\gamma^2)^{-1}. \qquad (4.20)$$

Other expressions are known which are essentially equivalent to those given here.

Our aim will be to reduce $F_{i\gamma}(y)$ and $F_{i\gamma}(1/y)$ such that we get practical expressions which are usable in the vicinity of zero energy. Just as in Section 4B we use Eqs.(4.9) and (4.12) as a starting point. In this case an expression for ξ is needed such that $e^{i\xi/\gamma}$ equals y, and 1/y, respectively. We first introduce two new variables,

$$\zeta \equiv [1 - 2k^2\vec{p}\cdot\vec{p}'(pp')^{-2} + k^4(pp')^{-2}]^{-\frac{1}{2}},$$

and

$$\rho \equiv i k\gamma q \zeta/(pp').$$

We assume that p,p' and q are positive. Then ζ is positive and finite when $|k^2| < pp'$, and further

$$\zeta_0 \equiv \lim_{k\to 0} \zeta = 1.$$

By taking Re x <0 as before, we have for Re k > 0,

$$x = -pp'/(k q \zeta), \tag{4.21}$$

and according to Eq.(4.6),

$$y = \frac{pp' - k q \zeta}{pp' + k q \zeta}.$$

Now we are in a position to give the desired expression for ξ,

$$\xi = 2\gamma \arctan(\rho/\gamma). \tag{4.22a}$$

With the help of Eq.(4.14) this can be rewritten as

$$\xi = -i\gamma \ell n \frac{pp' - k q \zeta}{pp' + k q \zeta} = -i\gamma \ell n\, y. \tag{4.22b}$$

It can be seen by inspection that

$$e^{i\xi/\gamma} = y, \qquad e^{-\xi} = y^{i\gamma}.$$

Furthermore, $F_{i\gamma}(1/y)$ is obtained from $F_{i\gamma}(y)$ by taking $F_{i\gamma}(e^{-i\xi/\gamma})$, i.e., we only have to replace ξ by $-\xi$.

We note that ξ and ρ are purely imaginary, for positive energy as well as for negative energy. Their signs are determined by the sign of the Coulomb potential,

$$i\xi s > 0, \tag{4.23a}$$

$$i\rho s > 0. \tag{4.23b}$$

For zero energy one has

$$\xi_0 \equiv \lim_{k\to 0} \xi = -2\,i\,s\,q/(pp'), \tag{4.24a}$$

$$\rho_0 \equiv \lim_{k\to 0} \rho = \tfrac{1}{2}\xi_0 = -i\,s\,q/(pp'). \tag{4.24b}$$

In order to proceed with $\hat{T}_C$ we use Eqs.(4.5), (4.12) and (4.22), and obtain

$$\langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = k\gamma(\pi q)^{-2}\ \rho\ \Xi(\gamma,\xi), \tag{4.25a}$$

in which we have introduced the new function

$$\begin{aligned}\Xi(\gamma,\xi) &\equiv (i\gamma)^{-1}\,[\,F_{i\gamma}(e^{-i\xi/\gamma}) - F_{i\gamma}(e^{i\xi/\gamma})\,] \\ &= e^{\xi}\,[\,-V(\gamma;\xi) + \psi(i\gamma) + (2i\gamma)^{-1} + C - \ell n(i\gamma/\xi)\,] \\ &\quad -e^{-\xi}[\,-V(\gamma;-\xi) + \psi(i\gamma) + (2i\gamma)^{-1} + C - \ell n(-i\gamma/\xi)\,].\end{aligned} \tag{4.25b}$$

It is convenient to recast Eq.(4.25b) into a more suitable form. To achieve this we make a number of changes.

First we introduce the function $H(\gamma)$ that has been defined in Eq.(3.6) of Ref.17,

$$H(\gamma) \equiv \psi(i\gamma) + (2i\gamma)^{-1} - \ell n(-i\gamma\,\mathrm{sgn}\,(s)). \tag{4.26}$$

In the case of repulsion $i\gamma$ cannot become real negative when $\mathrm{Im}\,k > 0$. In this case the following asymptotic expansion

$$H(\gamma) = \sum_{n=1}^{m} \gamma^{-2n}\,|\,B_{2n}\,|\,/(2n) + O(\gamma^{-2m-2}),\quad |\,\gamma\,| \to \infty,\ k \to 0, \tag{4.27}$$

may be used. This expression follows from Eqs.(4.18) and (4.26) by inserting the equality $B_{2n} = (-)^{n+1}\,|\,B_{2n}\,|$.

Furthermore we split off from V its first term v_0 (see Eq. (4.9)) and use the explicit expression for v_0 given by Eq.(4.10).

In the third place we split the logarithmic terms on the right-hand side of Eq.(4.25b). By using Eq.(4.23a) and the fact

that for positive energy, k has a small positive-imaginary part, we obtain for the case of repulsion,

$$\ell n(i\gamma/\xi) = \ell n(i\gamma) - \ell n\,\xi, \qquad s < 0,$$

$$\ell n(-i\gamma/\xi) = \ell n(i\gamma) - \ell n(-\xi), \quad s < 0. \tag{4.28}$$

The terms $\ell n(\pm\xi)$ are combined with $v_0(\pm\xi)$, and $\ell n(i\gamma)$ is used to construct $H(\gamma)$. In this way we obtain from Eq.(4.25b),

$$\Xi(\gamma,\xi) = H(\gamma)\ (e^{\xi} - e^{-\xi}) + e^{-\xi}\ \Gamma(0,-\xi) - e^{\xi}\,\Gamma(0,\xi)$$

$$+ e^{-\xi}\ [V(\gamma;-\xi) - v_0(-\xi)] - e^{\xi}[V(\gamma;\xi) - v_0(\xi)], \qquad s < 0.$$

Substitution of Eqs.(4.9), (4.11) and [18]

$$e^{\xi}\ \Gamma(0,\xi) = U(1,1,\xi)$$

yields

$$\Xi(\gamma,\xi) = 2\,H(\gamma)\sinh\xi + U(1,1,-\xi) - U(1,1,\xi)$$

$$+ \sum_{n=1}^{\infty}\left(\frac{i\xi}{\gamma}\right)^{2n}\frac{B_{2n}}{2n(2n)!}\,[{}_1F_1(1;2n+1;\xi) - {}_1F_1(1;2n+1;-\xi)],$$

$$|\,\xi\,| < 2\pi\,|\,\gamma\,|, \qquad s < 0. \tag{4.29}$$

The two confluent h.f.'s ${}_1F_1$ can be combined in one generalized hypergeometric function ${}_1F_2$ which has a rapidly converging power series,

$${}_1F_1(1;2n+1;\xi) - {}_1F_1(1;2n+1;-\xi) = 2\xi(2n)!\sum_{m=0}^{\infty}\xi^{2m}/(2n+2m+1)!$$

$$= \xi(n+\tfrac{1}{2})^{-1}\ {}_1F_2(1;n+1,n+3/2;\xi^2/4).$$

Therefore we finally have

$$\Xi(\gamma,\xi) = 2\,H(\gamma)\sinh\xi + U(1,1,-\xi) - U(1,1,\xi)$$

$$+ \xi\sum_{n=1}^{\infty}\left(\frac{i\xi}{\gamma}\right)^{2n}\frac{B_{2n}}{n(2n+1)!}\ {}_1F_2(1;n+1,n+3/2;\xi^2/4),$$

$$|\,\xi\,| < 2\pi\,|\,\gamma\,|, \quad s < 0. \tag{4.30}$$

In the case of an *attractive* Coulomb potential the expression for Ξ given in Eq.(4.25b) may be refashioned in a similar way. There is only one notable difference. This concerns the splitting of the logarithmic term $\ell n(\pm i\gamma/\xi)$. Because of the branch cut of the logarithmic function we now obtain with the help of Eq.(4.23a),

$$\ell n(i\gamma/\xi) = \ell n(-i\gamma) - \ell n(-\xi) = \ell n(-i\gamma) - \ell n(\xi) - i\pi, \qquad s > 0,$$

$$\ell n(-i\gamma/\xi) = \ell n(-i\gamma) - \ell n\ \xi \quad = \ell n(-i\gamma) - \ell n(-\xi) + i\pi, \qquad s > 0. \quad (4.31)$$

This may be compared with Eq.(4.28). So we have the same expression as before (Eq.(4.30)), but in addition we get a term $2i\pi\cosh\xi$. Therefore in the case of attraction we have the following expression,

$$\Xi(\gamma,\xi) = 2H(\gamma)\sinh\xi + 2i\pi\cosh\xi + U(1,1,-\xi) - U(1,1,\xi)$$
$$+ \xi \sum_{n=1}^{\infty} \left(\frac{i\xi}{\gamma}\right)^{2n} \frac{B_{2n}}{n(2n+1)!}\, {}_1F_2(1; n+1, n+3/2; \xi^2/4),$$
$$|\xi| < 2\pi\,|\gamma|, \qquad s > 0. \qquad (4.32)$$

Let us examine the domain of convergence of Eqs.(4.30) and (4.32), $|\xi| < 2\pi|\gamma|$. By substituting Eq.(4.22a) we get

$$|\arctan(\rho/\gamma)| < \pi,$$

or

$$|\arctan(ikq\zeta/(pp'))| < \pi.$$

This condition is fulfilled for all negative energies. In the case of positive energy ($k > 0$) it is more useful to insert Eq. (4.22b) which yields

$$\left|\ell n \frac{pp' - kq\zeta}{pp' + kq\zeta}\right| < 2\pi.$$

This inequality can be reduced to

$$(p^2 - k^2)(p'^2 - k^2) > k^2q^2(\sinh\pi)^{-2} \simeq 0.0075\, k^2q^2. \qquad (4.33)$$

So we see that the infinite series on the right-hand sides of Eqs. (4.30) and (4.32) are convergent up to energies close to the half-shell values $k^2 = p^2$ and $k^2 = p'^2$. It is not surprising that these points are excluded. As is well known, $\hat{T}_C$ is singular in the half-shell points. These singularities are of the type $(p^2 - k^2)^{i\gamma}$, so they are integrable.

The zero-energy limit of $\hat{T}_C$ can easily be read off from Eqs. (4.25) and (4.30) for the repulsive case,

$$\lim_{k\to 0} \langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = \tfrac{1}{2} s \pi^{-2} q^{-2} \xi_0 [U(1,1,\xi_0) - U(1,1,-\xi_0)], \quad (4.34)$$

where ξ_0 is given by Eq.(4.24a). For the sake of comparison with results of other authors [21,22] we shall rewrite Eq.(4.34) in terms of the sine- and cosine integrals,

$$si(z) = -\int_z^\infty t^{-1} \sin t \, dt,$$

$$Ci(z) = -\int_z^\infty t^{-1} \cos t \, dt.$$

By inserting [18]

$$\Gamma(0,iz) = -Ci(z) + i\, si(z),$$

$$\Gamma(0,-iz) = -Ci(z) - i\, si(z)$$

in Eq.(4.34) we obtain

$$\lim_{k\to 0} \langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = s(\pi q)^{-2}$$

$$\times (\xi_0/i) [\sin(\xi_0/i)\, Ci(\xi_0/i) - \cos(\xi_0/i)\, si(\xi_0/i)], \quad s < 0 \quad (4.35a)$$

$$= s(\pi q)^{-2} (\xi_0/i) \int_0^\infty (1+t)^{-1} \sin(t\,\xi_0/i)\, dt, \qquad s < 0. \quad (4.35b)$$

Here $\xi_0/i = -2\,s\,q/(pp')$ is positive since the Coulomb potential

is repulsive ($s < 0$), by assumption.

In the case of attraction the zero-energy limit makes no sense because of the bound-state poles. We can, however, consider the limit for vanishing potential strength, $s \to 0$, both for repulsion and attraction. This gives a partial check on Eqs.(4.30) and (4.32). We note that $\xi \to 0$ and $\gamma \to 0$ when $s \to 0$. Since

$$\psi(z) \sim -z^{-1}, \quad z \to 0,$$

we have

$$\lim_{\gamma \to 0} 2i\gamma\, H(\gamma) = -1.$$

By using further

$$U(1,1,\xi) = e^{\xi}\, \Gamma(0,\xi) \simeq -\ell n\, \xi, \quad \xi \to 0,$$

we obtain from Eq.(4.30),

$$\lim_{s \to 0} s^{-2} \langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = \frac{i\zeta}{\pi^2 q\, pp'} \lim_{\xi \to 0} (\ell n\, y + \ell n\, \xi - \ell n(-\xi)).$$

From Eq.(4.32) a similar expression can be found, but here in addition the term $2i\pi \cosh \xi$ appears between the brackets. By using $i\,\xi\, s > 0$ we obtain for *both* cases $s < 0$ and $s > 0$, the simple expression,

$$\lim_{s \to 0} s^{-2} \langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = \frac{i\zeta}{\pi^2 q\, pp'} (i\pi + \ell n\, y)\,. \tag{4.36}$$

On the other hand, with the help of

$$\lim_{\gamma \to 0} (i\gamma)^{-1} (1 - F_{i\gamma}(y)) = \ell n(1 - y), \tag{4.37}$$

and

$$\ell n(y - 1) = -i\pi + \ell n(1 - y),$$

one obtains from Eq.(4.5), both for $s < 0$ and $s > 0$,

$$\lim_{s \to 0} s^{-2} \langle \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} \rangle = \frac{-i(i\pi + \ell n\, y)}{\pi^2 q^2\, kx}. \tag{4.38}$$

Since $x = -pp'/(k\,q\,\zeta)$ (Eq.(4.21)), this agrees with Eq.(4.36).

Finally we note that the limiting behavior of $\hat{T}_C - \hat{V}_C$ for $q \to 0$ can be obtained in a similar way. This limit $q \to 0$ has been briefly discussed in Section 3. For $\vec{p}' \to \vec{p}$ we have

$$\zeta \to p^2/(p^2 - k^2),$$

$$\rho \to i k\gamma\, q/(p^2 - k^2) \to 0,$$

$$\xi \to 2\rho \to 0.$$

We insert these expressions in (4.30) and (4.32), respectively, and proceed in the same way as before. This yields

$$\lim_{q\to 0} q < \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} > \; = -s^2\, \pi^{-1} (p^2 - k^2)^{-1}, \tag{4.39}$$

which is again valid for $s < 0$ and for $s > 0$. Note that $k^2 < p^2$ is assumed here. In the notation of Sections 2 and 3, Eq.(4.39) reads

$$\lim_{\vec{q}_\alpha' \to \vec{q}_\alpha} \; | \vec{q}_\alpha' - \vec{q}_\alpha | < \vec{q}_\alpha' \mid \hat{T}_C(E) - \hat{V}_C \mid \vec{q}_\alpha > \; = -s^2\, \pi^{-1} (q_\alpha^2 - E)^{-1}. \tag{4.40}$$

Now that we have obtained a number of formulas for various cases, we are in a position to consider the approximation in which $\hat{T}_C$ is replaced by $\hat{V}_C$ (cf.Section 1) in more detail. To this end we introduce the dimensionless quantity

$$\tau \equiv < \vec{p}' \mid \hat{T}_C - \hat{V}_C \mid \vec{p} > / < \vec{p}' \mid \hat{V}_C \mid \vec{p} >. \tag{4.41}$$

The above approximation would certainly be justified if one could show that τ is close to zero for all values of $\vec{p}$, $\vec{p}'$ and k. However, we will prove that (in the repulsive case) for small k and small p' (or p) τ approaches -1, for all

positive p (or p', respectively). This means that a careful comparison of an exact calculation with the result of this approximation is highly desirable.

We shall deduce $\lim_{p'\to 0}\lim_{k\to 0}\tau$ and $\lim_{k\to 0}\lim_{p'\to 0}\tau$, respectively, both for the case of a repulsive Coulomb potential. So let us start with the limit for $k \to 0$. From Eq.(4.34) we have

$$\lim_{k\to 0}\tau = \tfrac{1}{2}\xi_0[U(1,1,-\xi_0) - U(1,1,\xi_0)].$$

Now we let p' go to zero. Then $\xi_0 \sim -2is/p'$, so $-i\xi_0 \to +\infty$, cf. Eq.(4.24). By using further

$$U(1,1,z) \sim z^{-1} - z^{-2}, \quad |z| \to \infty, \tag{4.42}$$

we obtain

$$\lim_{p'\to 0}\lim_{k\to 0}\tau = -1. \tag{4.43}$$

Now we shall reverse the order in which these two limits are taken. By letting first p' go to zero we have

$$x \to -k/p,$$

and

$$y \to -a,$$

where $a = (p-k)/(p+k)$ as before (Eq.(4.2)). Therefore

$$\lim_{p'\to 0}\tau = \frac{a+1}{a-1}[F_{i\gamma}(-a) - F_{i\gamma}(-1/a)]. \tag{4.44}$$

We have to find the limit of this expression for $k \to 0$. It is tempting to use the series expansion of Eq.(4.20), but it turns out that this expression is not easily applicable. By using the integral representation of Eq.(4.19) we have found that the interchange of the limits in Eq.(4.43) does not alter the result, i.e.,

$$\lim_{k\to 0}\lim_{p'\to 0}\tau = -1. \tag{4.45}$$

We wish to confirm this result by using again Eq.(4.12). In the derivation following below we shall give an interesting asymptotic series for the function Ξ which may have other applications (Eq.(4.49)).

We note that the arguments of $F_{i\gamma}$ now approach -1 instead of +1 as they did in all cases considered so far. In order to use Eq.(4.12) we have to take a *different expression for* ξ, since the condition for convergence, Eq.(4.33), is not fulfilled in the present case. We take the following expression for ξ,

$$\xi = \pi\gamma + i\gamma \ln a, \tag{4.46}$$

which implies $e^{-i\xi/\gamma} = -a$. In view of Eqs.(4.25) and (4.44) we have

$$\lim_{p^t \to 0} \tau = -i\gamma\, p\, k^{-1}\, \Xi(\gamma,\xi). \tag{4.47}$$

By inserting (4.46) in (4.28) we get an equality, and therefore the expression for Ξ on the right-hand side of Eq.(4.29) is valid in this case.

We want to obtain the limit of the right-hand side of Eq.(4.47) for $k \to 0$. Since $|\xi| \to \infty$ when k goes to zero, we first have to recast the expressions for Ξ given by Eqs.(4.29) and (4.30) in a more suitable form. To this end we insert the asymptotic series for $H(\gamma)$ (Eq.(4.27)) in (4.29), and use Eqs.(5.13c), (5.14c) and (5.16) of Ref.17. In this way we obtain

$$\Xi(\gamma,\xi) = U(1,1,-\xi) - U(1,1,\xi)$$

$$+ \sum_{n=1}^{m-1} (i\gamma)^{-2n} (e_{2n-1}(-\xi) - e_{2n-1}(\xi))\, B_{2n}/(2n) + O(\gamma^{-2m}), |\gamma| \to \infty \quad (s<0). \tag{4.48}$$

Here e_{2n-1} is the exponential polynomial,

$$e_n(z) = \sum_{\mu=0}^{n} z^\mu/\mu! \ .$$

So Eq.(4.48) may be recast in the form

$$\Xi(\gamma,\xi) = U(1,1,-\xi) - U(1,1,\xi)$$

$$- \sum_{n=1}^{m-1} (i\gamma)^{-2n} n^{-1} B_{2n} \sum_{\nu=0}^{n-1} \xi^{2\nu+1}/(2\nu+1)! + O(\gamma^{-2m}), \ |\gamma| \to \infty \ (s<0). \quad (4.49)$$

This asymptotic series for Ξ can be used in particular in the present case where we let k go to zero. With the help of Eq. (4.42) we obtain from Eq.(4.49),

$$\Xi(\gamma,\xi) \underset{k\to 0}{\sim} (-2/\xi) \left[1 + \sum_{n=1}^{\infty} (i\xi/\gamma)^{2n} B_{2n}/(2n)! \right].$$

Further we use the equality [18]

$$\sum_{n=1}^{\infty} z^{2n} B_{2n}/(2n)! = -1 + \tfrac{1}{2}z + z/(e^z - 1), \quad |z| < 2\pi. \quad (4.50)$$

In this way we get

$$\Xi(\gamma,\xi) \underset{k\to 0}{\sim} (i\gamma)^{-1} + 2(i\gamma)^{-1}/(e^{i\xi/\gamma} - 1) = (i\gamma)^{-1}(1-a)/(1+a).$$

Substitution of this expression in Eq.(4.47) yields the desired proof of Eq.(4.45).

This result implies that for a repulsive Coulomb potential $\langle \vec{p}' \mid \hat{T}_C \mid \vec{p} \rangle$ is approximately zero when k and p' are close to zero, for all $\vec{p}$ $(p \neq 0)$.

5. SUMMARY AND DISCUSSION

In this paper we have studied certain problems connected with the incorporation of the Coulomb interaction in the equations for systems involving charged particles. In Section 2 we have considered a particularly simple model of one neutral and two charged particles, without spins, in the formalism of Ref.8. The exact calculation of the effective potentials occurring in the three-particle equations has been discussed in Section 3.

Section 4 constitutes the main part of this paper. Here we have developed formulas which are usable for the exact calculations of the effective potentials. In such calculations, and in the three-particle integral equations, one has to perform integrations of various Coulomb quantities closely along the zero energy point, when the total three-particle energy is positive or approximately zero, i.e., above or near the break-up threshold. This point is a so-called essential singularity, which is generated by the infinite number of Coulomb bound-state poles accumulating at zero energy. The situation has been sketched in fig.1 and in fig.2, for a repulsive and for an attractive Coulomb potential, respectively.

We have split off this essential singularity at zero energy in a satisfactory way. In Eqs.(4.9) - (4.12) the basic formulas have been given in which the various Coulomb quantities can be expressed. The central function here is the h.f. $F_{i\gamma}(e^{i\xi/\gamma})$, where ξ has to be chosen appropriately for various cases. In Section 4C we have investigated in particular the three-dimensional Coulomb T matrix. For this case the more important formulas are given by Eqs.(4.25), (4.30) and (4.32), where ξ is chosen according to Eq.(4.22). In Eq. (4.49) an interesting asymptotic series has been given which is

especially useful when a different expression for ξ is taken.

At the end of Section 4 we have considered in particular the approximation in which the three-dimensional Coulomb T matrix is replaced by the Coulomb potential, for the repulsive case only. We have shown that for certain values of $\vec{p},\vec{p}'$ and k this approximation is not satisfactory, cf. Eqs.(4.41) ff. Therefore a careful comparison of exact calculations with the results of the approximate calculations in the three-particle equations is highly desirable.

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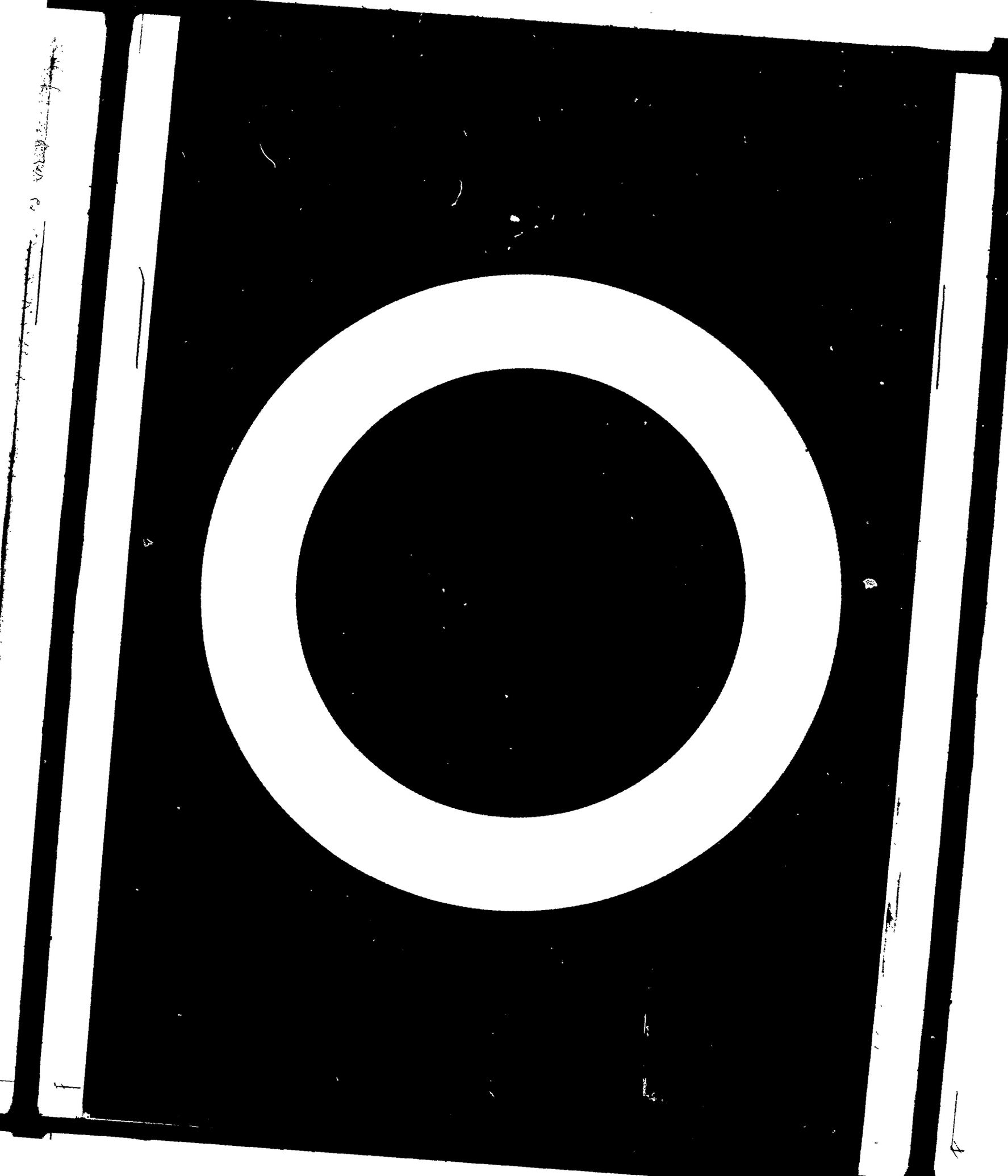
Part B



B 1

THE BOUND STATES FOR THE SYMMETRIC SHIFTED COULOMB POTENTIAL

We investigate the bound states for the symmetric one-dimensional shifted Coulomb potential, $V(x) = -2s(|x| + d)^{-1}$. Explicit approximate expressions for the infinite number of bound-state energies are obtained. For small s the ground-state energy is $O(s^2 \ell n^2 sd)$, whereas the energies of the excited states are $O(s^2)$. We prove that the square roots of the binding energies form approximately a harmonic progression, both for the even solutions and for the odd solutions. This is also true for the sequence of <u>all</u> solutions when sd is not small. However, when $sd \ll 1$ this sequence shows an interesting odd-even staggering phenomenon.

1. INTRODUCTION

In this paper we shall deduce explicit approximate expressions for the binding energies for the symmetric one-dimensional shifted Coulomb potential,

$$V(x) = -2s(|x|+d)^{-1}, \quad s>0, \quad -\infty<x<\infty, \tag{1.1}$$

where d is some positive parameter. For $x>0$ the odd bound-state wave functions for this symmetric potential are, if we write r for x, proportional to the $\ell=0$ radial bound-state wave functions for the three-dimensional shifted Coulomb potential,

$$V(r) = -2s(r+d)^{-1}. \tag{1.2}$$

We take units such that $\hbar = 2m = 1$. Moreover, for the treatment of the Coulomb potential it is convenient to use Sommerfeld's parameter $\gamma = -s/k$, where k is the square root of the energy E.

In this investigation an important role will be played by the Jost solution [1,2]. The pure Coulomb Jost solution for $\ell=0$ is given by

$$f_C(k,r) = e^{ikr+\pi\gamma/2}\, U(i\gamma,\, 0,\, -2ikr), \tag{1.3}$$

where U is an irregular solution of the confluent hypergeometric differential equation [3]. The asymptotic behavior of f_C is given by

$$\lim_{r\to\infty} f_C(k,r)\, \exp(-ikr + i\gamma\, \ell n(2kr)) = 1. \tag{1.4}$$

It easily follows that the function

$$f(k,r) \equiv e^{-ikd}\, f_C(k,r+d) = e^{ikr+\pi\gamma/2}\, U(i\gamma,0,-2ik(r+d)) \tag{1.5}$$

is a solution of the Schrödinger equation with the shifted potential (1.2). Since its asymptotic behavior is the same as that of $f_C(k,r)$, we may call $f(k,r)$ the Jost solution for the shifted Coulomb potential (1·2).

We consider negative energies, so we put $k = i\kappa$ with $\kappa > 0$, the corresponding energies being $E = -\kappa^2$. Then the bound-state wave functions we are looking for follow from $f(i\kappa,r)$ by imposing the appropriate boundary conditions at $r = 0$. The odd wave functions satisfy

$$\lim_{r\to 0} f(i\kappa,r) = 0, \tag{1.6}$$

whereas for the even wave functions we have

$$\lim_{r\to 0} (d/dr)\, f(i\kappa,r) = 0. \tag{1.7}$$

From Eq.(1.6) we shall deduce a discrete set $\kappa = \kappa_n^{(-)}$, $n = 1,2, \ldots$, for which the equation holds. The $\kappa_n^{(-)}$ will be called the odd solutions. For $d = 0$ we get the well-known pure Coulomb solutions $\kappa_n = s/n$. The values $\kappa = \kappa_n^{(+)}$, $n = 0,1,2, \ldots$, for which Eq.(1.7) holds will be called the even solutions. The even ground-state solution, $\kappa_0^{(+)}$, plays a special role.

The way in which we are going to derive approximate expressions for $\kappa_n^{(-)}$ and $\kappa_n^{(+)}$ depends critically on the magnitude of sd. Therefore in Section 2 we restrict ourselves to the case $sd \ll 1$. Mehta and Patil [4] have given an expression for $\kappa_n^{(-)}$ in the case of small sd. Our expression (Eq.(2.8)) is in agreement with theirs [4, Eq.(27)]. We can understand why the product sd plays an important role by transforming the Schrödinger equation according to $u(r) = v(y)$, $y = r(2s/d)^{\frac{1}{2}}$,

which yields

$$v'' + (1 + y(2sd)^{-\frac{1}{2}})^{-1} v = v\kappa^2 d/(2s). \tag{1.8}$$

This equation has again the form of a Schrödinger equation, with a potential which depends only on sd. Note also that the first-order perturbation with respect to the pure Coulomb potential (d = 0) depends on sd,

$$V(r) = \frac{-2s}{r+d} = \frac{-2s}{r} + \frac{2sd}{r^2} - \frac{2sd^2}{r^2(r+d)} . \tag{1.9}$$

In Section 3 we consider the case when sd is not small, of the order 1 or bigger. Here we discuss some simple explicit expressions for the lowest odd and even states. We prove that

$$\lim_{sd\to\infty} \kappa(2s/d)^{-\frac{1}{2}} = 1 \tag{1.10}$$

for all binding energies. Note that Eq.(1.8) implies $\kappa^2 \leq 2s/d$.

We point out that for intermediate values of sd < 1, approximate values for the binding energies can be obtained by means of interpolation. In Section 4 some interesting special points will be considered. In particular we discuss an interesting phenomenon which occurs in the complete sequence $\{\kappa_n^{(-)}, \kappa_n^{(+)}\}$. It turns out that this sequence shows a very curious odd-even staggering for small values of sd. Section 5 contains a short summary.

2. THE CASE sd << 1.

In this section we shall derive approximate expressions for the odd solutions $\kappa_n^{(-)}$ and for the even solutions $\kappa_n^{(+)}$, assuming throughout that $sd << 1$.

The odd solutions follow from Eqs.(1.5) and (1.6), i.e. we have to find those values of $\kappa > 0$ for which the equation

$$U(-s/\kappa,\ 0,\ 2\kappa d) = 0 \tag{2.1}$$

holds. First we shall prove that this equation has no solution $\kappa > s$. To this end we use the integral representation

$$\Gamma(a+1)\,U(a,0,z) = \int_0^\infty (a+1+z(1+t))\,t^a(1+t)^{-a-2}\,e^{-zt}dt,\quad \mathrm{Re}\,z>0,\mathrm{Re}\,a>-1. \tag{2.2}$$

Since for $a = -s/\kappa > -1$ the integrand is positive for all t, it follows that Eq.(2.1) has no solution in this case (cf. also Eq.(1.8)). So we may restrict ourselves to $\kappa \le s$, i.e. $\kappa d \le sd$, so $\kappa d << 1$ since $sd << 1$.

In order to solve Eq.(2.1), we use

$$U(a,c,z) = z^{1-c}\,U(a+1-c,\ 2-c,\ z), \tag{2.3}$$

and Eq.(13) of [5, Vol.1, p.261], and obtain

$$\Gamma(a)\,U(a,0,z) = a^{-1} + z\,\ell n\,z\ {}_1F_1(a+1;\ 2;\ z)$$
$$+ \sum_{n=0}^{\infty} (\psi(a+n+1) - \psi(n+1) - \psi(n+2))\ \ z^{n+1}\ (a+1)_n/(n!(n+1)!). \tag{2.4a}$$

Here ψ is the logarithmic derivative of the gamma function, $\psi(z) = \Gamma'(z)/\Gamma(z)$. For small z we have

$$\Gamma(a)\,U(a,0,z) \simeq a^{-1} + z\,\ell n\,z + z\,\psi(a+1), \qquad z \to 0. \tag{2.4b}$$

We use the fact that the product of a and z, which is here -2sd, is close to zero. By combining Eqs. (2.1), (2.4a) and (2.4b) we see that we have to solve the equation

$$(2sd)^{-1} \simeq \ell n(2\kappa d) + \psi(1 - s/\kappa). \tag{2.5}$$

This equation can only have a solution when $1 - s/\kappa$ is near one of the poles of ψ. By using

$$\psi(z) \simeq -\frac{1}{z+n} + \psi(n+1), \text{ if } z \simeq -n, \quad n = 0,1,2, \ldots , \tag{2.6}$$

and

$$\psi(n+1) \simeq \ell n\, n , \quad n \to \infty,$$

we obtain from Eq.(2.5),

$$(2sd)^{-1} \simeq \ell n(2n\kappa d) - (n - s/\kappa)^{-1}.$$

Therefore the approximate odd solutions $\kappa_n^{(-)}$ follow from

$$s/\kappa_n^{(-)} \simeq n + 2sd(1 + 2sd\ \ell n(2sd)), \tag{2.7}$$

and are explicitly given by

$$\kappa_n^{(-)} \simeq sn^{-1} - 2s^2 d\, n^{-2}(1 + 2sd\ \ell n(2sd)). \tag{2.8}$$

This expression is in agreement with Eq. (27) of Mehta and Patil [4]. We note that the logarithmic term in Eqs.(2.7) and (2.8) may be neglected since $\lim_{z\to 0} z\, \ell n\, z = 0$, so we have

$$s/\kappa_n^{(-)} \simeq n + 2sd, \qquad n = 1,2, \ldots , \tag{2.9}$$

and

$$\kappa_n^{(-)} \simeq s/n - 2s^2 d/n^2, \quad n = 1,2, \ldots . \tag{2.10}$$

It is interesting to note that the bound-state energies which we have deduced here, can also be obtained by applying

first-order perturbation theory. On the one hand, we have from Eq.(2.10)

$$E_n = -\kappa_n^2 \simeq -s^2/n^2 + 4s^3 d/n^3. \qquad (2.11)$$

On the other hand, we can consider $2sd/r^2$ as a perturbation of the pure Coulomb potential, according to Eq.(1.9). The first-order perturbation of the energy is then

$$\Delta E_n = 2sd \langle r^{-2} \rangle_n = 2sd \cdot 2s^2/n^3,$$

and the total energy, $E_n = -s^2/n^2 + \Delta E_n$, is in agreement with Eq.(2.11).

Now we turn to the even solutions $\kappa_n^{(+)}$, which have to be deduced from Eq.(1.7). Let us first rewrite this equation. By using Eq.(1.5) and well-known properties of the function U we obtain

$$\frac{d}{dr} f(k,r) = -ik\, e^{ikr+\pi\gamma/2} \left[U(i\gamma,0,-2ik(r+d)) - 2U(i\gamma,1,-2ik(r+d))\right]. \qquad (2.12)$$

Therefore we have to find the solutions $\kappa = \kappa_n^{(+)}$ of the equation

$$U(-s/\kappa,0,2\kappa d) = 2\,U(-s/\kappa,1,2\kappa d). \qquad (2.13)$$

First we shall show that this equation has no solution when κd is not small. To this end, we suppose that $\kappa d \gg sd$ (recall that $sd \ll 1$), so $\kappa \gg s$. We now use the integral representation

$$\Gamma(a+1)\, U(a,1,z) = \int_0^\infty (a+z(1+t))\, t^a (1+t)^{-a-1} e^{-zt}\, dt, \quad \mathrm{Re}\, z > 0, \mathrm{Re}\, a > -1, \qquad (2.14)$$

together with Eq.(2.2). It follows that we must have $1 \sim 2a \ln z \to 0$ when $a \to 0$ for the solution of Eq.(2.13), i.e., $z \equiv 2\kappa d$ must be small since $a \equiv -s/\kappa \simeq 0$. Therefore we may restrict ourselves to the case that κd is small (cf. also Eq.(1.8)).

In order to solve Eq.(2.13), we use Eq.(2.4) and the expansion [5, Vol.1, p.261]

$$\Gamma(a)\, U(a,1,z) = -\ell n\, z\, {}_1F_1(a;1;z) - \sum_{n=0}^{\infty} (\psi(a+n) - 2\psi(1+n))\, (a)_n\, z^n/(n!)^2, \tag{2.15a}$$

which becomes for small z,

$$\Gamma(a)\, U(a,1,z) \simeq -\ell n\, z - \psi(a). \tag{2.15b}$$

By applying Eqs.(2.4) and (2.15) to Eq.(2.13), and using

$$\psi(a) = \psi(1+a) - a^{-1}, \tag{2.16}$$

and the fact that κd is small, we find that our equation to be solved turns out to be

$$\kappa/(2s) + \ell n(2\kappa d) + \psi(1 - s/\kappa) \simeq 0. \tag{2.17}$$

It is useful to distinguish two cases, either s/κ is small (e.g. $s/\kappa < \frac{1}{2}$), or not.

(i) In the first case, when s/κ is small, we may neglect $\psi(1 - s/\kappa)$ and Eq.(2.17) may be rewritten as

$$\kappa d \simeq -2sd\ \ell n(2\kappa d). \tag{2.18a}$$

Put for convenience $2\kappa d \equiv z$ and $4sd \equiv \lambda$. Now let $z_0 = z_0(\lambda)$ be the solution of the equation

$$z = -\lambda\, \ell n\, z. \tag{2.18b}$$

For $0 < \lambda < e^{-1}$, this solution z_0 is easily calculated numerically by means of iteration. Graphically we can prove that

$$f(\lambda) \equiv \frac{\lambda\, |\, \ell n\, \lambda\, | - z_0(\lambda)}{\lambda\, \ell n |\, \ell n\, \lambda\, |} \tag{2.18c}$$

is a decreasing function of λ, even for $0 < \lambda < 1$. We have $f(0) = 1$, $f(e^{-1}) = \frac{1}{2}$, and $f(1) = 0$. It follows that the approximate solution of Eq.(2.18a) is

$$\kappa_0^{(+)} \simeq -2s \ln(4sd). \tag{2.19}$$

This is the ground-state solution, which is for this reason denoted by $\kappa_0^{(+)}$. We note that indeed $s/\kappa_0^{(+)}$ is small because $sd << 1$, so that our above condition is satisfied, and therefore this $\kappa_0^{(+)}$ is indeed the correct solution.

If we now take d fixed, and let s go to zero, we have

$$\lim_{s\to 0} \kappa_0^{(+)} / (s \ln sd) = -2. \tag{2.20}$$

On the other hand we can fix s and let d go to zero. In this case we have

$$\lim_{d\to 0} \kappa_0^{(+)} / (\ln sd) = -2s,$$

and therefore,

$$\lim_{d\to 0} \kappa_0^{(+)} = +\infty \tag{2.21}$$

So the binding energy of the ground state for the one-dimensional shifted Coulomb potential becomes infinite for $d \to 0$. This is in agreement with the well-known fact that the Hamiltonian with a pure Coulomb potential is not bounded below in the one-dimensional case.

(ii) In the second case, when s/κ is not small, we may neglect the term $\kappa/(2s)$ in Eq.(2.17). Since $-\ln(2\kappa d)$ is large, it follows that $1 - s/\kappa$ must be near one of the poles of the ψ function. We use Eq.(2.6) as before and furthermore we have

$$\ln(2\kappa d) + \psi(n) \simeq \ln(2n\kappa d) \simeq \ln(2sd),$$

since $n\kappa$ approximately equals s. In this way we obtain from Eq.(2.17),

$$(n - s/\kappa)^{-1} \simeq \ell n(2sd),$$

and therefore,

$$s/\kappa_n^{(+)} \simeq n - (\ell n(2sd))^{-1}, \qquad n = 1,2, \ldots, \tag{2.22}$$

or

$$\kappa_n^{(+)} \simeq \frac{s}{n} + \frac{s}{n^2 \ell n(2sd)}, \qquad n = 1,2, \ldots . \tag{2.23}$$

It is instructive to compare the expressions for the even solutions with those for the odd solutions, see fig.1. From Eqs. (2.10) and (2.23) one easily verifies that

$$\kappa_0^{(+)} >> \kappa_1^{(-)} > \kappa_1^{(+)} > \kappa_2^{(-)} > \kappa_2^{(+)} \ldots . \tag{2.24}$$

The solutions $\kappa_n^{(\pm)}$ are somewhat smaller than the corresponding pure Coulomb solutions $\kappa_n = s/n$,

$$\kappa_n^{(+)} < \kappa_n^{(-)} < s/n, \qquad n = 1,2, \ldots . \tag{2.25}$$

This is clear since our potential is everywhere less attractive than the pure Coulomb potential. The phenomenon that both $\kappa_n^{(+)}$ and $\kappa_n^{(-)}$ are close to s/n for all n = 1,2, ... may be called "odd-even staggering", see fig.1.

Finally we note that our Eqs.(2.10), (2.20) and (2.23) show that the conjecture of Blankenbecler et al. [6, p.70], at least for this potential which satisfies $V(r) = O(r^{-1})$, $r \to \infty$, is correct. Indeed, for the ground-state energy we have

$$E_0 = O(s^2 \ell n^2 sd), \qquad s \to 0, \tag{2.26}$$

and for the excited states,

$$E_n = O(s^2), \qquad s \to 0. \tag{2.27}$$

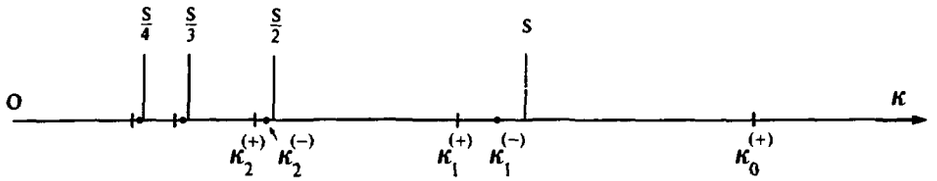


Fig.1. The odd solutions $\kappa_n^{(-)}$ (dots) and the even solutions $\kappa_n^{(+)}$ (small vertical lines) for the shifted Coulomb potential in the case $sd \ll 1$, as compared with the pure Coulomb solutions $\kappa_n = s/n$.

3. THE CASE WHEN sd IS NOT SMALL

When sd is not small, the series expansions of the functions U (Eqs.(2.4) and (2.15)) are not very useful. In this case a different approach is more appropriate. We fix s/κ at some integer value,

$$s/\kappa = n, \qquad n = 1,2, \ldots , \tag{3.1}$$

and we look for those values of d for which the bound states occur. Once these have been found, we shall deduce an approximate expression for $\kappa_n^{(\pm)}$ by means of interpolation. We shall restrict ourselves to the case that $sd \geq \frac{1}{2}$ or bigger.

We use the equality

$$U(-n,\nu+1,x) = (-)^n n!\, L_n^{(\nu)}(x) = (-)^n(\nu+1)_n\, {}_1F_1(-n;\nu+1;x), \tag{3.2}$$

where $L_n^{(\nu)}$ is the Laguerre polynomial ($L_n^{(0)} \equiv L_n$). For the odd solutions the required values of d are then obtained from (cf. Eq.(2.1))

$$L_n^{(-1)}(2sd/n) = 0, \tag{3.3}$$

and the even solutions from (cf. Eq.(2.13))

$$L_n^{(-1)}(2sd/n) = 2\, L_n(2sd/n). \tag{3.4}$$

By using the equality

$$n\, L_n^{(-1)}(x) = -x\, L_{n-1}^{(1)}(x),$$

the equation for the odd solutions is rewritten as

$$L_{n-1}^{(1)}(2sd/n) = 0, \tag{3.5}$$

and the equation for the even solutions as

$$L_n(2sd/n) = -sd\, n^{-2}\, L_{n-1}^{(1)}(2sd/n), \tag{3.6}$$

or

$$L_n(2sd/n) + L_{n-1}(2sd/n) = 0. \tag{3.7}$$

Let us first restrict ourselves to large n ($n \gg sd$). In this case the zeros of the Laguerre polynomials are closely related to the zeros of the Bessel function J_ν, see Szegö [7, pp. 127 - 129]:

Let $x_{nm}(\nu)$, $m = 1,2, \ldots, n$, be the zeros of $L_n^{(\nu)}(x)$ in increasing order ($\nu > -1$), and let $j_{\nu,m}$, $m = 1,2, \ldots$, be the positive zeros of $J_\nu(z)$ in increasing order. Then we have

$$x_{nm}(\nu) > (\tfrac{1}{2} j_{\nu,m})^2 / (n + (\nu+1)/2), \quad m = 1,2, \ldots, n, \tag{3.8}$$

and

$$\lim_{n\to\infty} n\, x_{nm}(\nu) = (\tfrac{1}{2} j_{\nu,m})^2, \quad m = 1,2, \ldots. \tag{3.9}$$

We deduce from Eqs.(3.5) and (3.9) that the approximate odd solutions are, for large n, given by

$$2\kappa dn = 2sd \simeq (\tfrac{1}{2} j_{1,m})^2, \quad m = 1,2, \ldots. \tag{3.10}$$

In order to find the even solutions, we consider Eq.(3.6) and use the asymptotic behavior of the Laguerre polynomials, see Szegö [7, p.198]. We conclude that, for sufficiently large n, Eq.(3.6) may be replaced by

$$L_n(2sd/n) \simeq 0. \tag{3.11}$$

By combining this with Eq.(3.9), we find that the approximate even solutions are given by

$$2\kappa dn = 2sd \simeq (\tfrac{1}{2} j_{0,m})^2, \quad m = 1,2, \ldots. \tag{3.12}$$

Finally we obtain the approximate solutions for general

values of sd ($> \frac{1}{2}$) by means of interpolation. From Eq.(3.10) we deduce the odd solutions,

$$s/\kappa_n^{(-)} \simeq n + m + \frac{(8sd)^{\frac{1}{2}} - j_{1,m}}{j_{1,m+1} - j_{1,m}}, \tag{3.13}$$

where the integer m is defined by the inequality

$$j_{1,m} \leq (8sd)^{\frac{1}{2}} < j_{1,m+1}. \tag{3.14}$$

In case $(8sd)^{\frac{1}{2}}$ is smaller (but not much) than $j_{1,1} = 3.83\ ..$, we have

$$s/\kappa_n^{(-)} \simeq n + (8sd)^{\frac{1}{2}}/j_{1,1}. \tag{3.15}$$

Similarly, for the even solutions we deduce from Eq. (3.12),

$$s/\kappa_n^{(+)} \simeq n + m + \frac{(8sd)^{\frac{1}{2}} - j_{0,m}}{j_{0,m+1} - j_{0,m}}, \tag{3.16}$$

where m is defined by

$$j_{0,m} \leq (8sd)^{\frac{1}{2}} < j_{0,m+1}. \tag{3.17}$$

When $(8sd)^{\frac{1}{2}}$ is smaller (but not much) than $j_{0,1} = 2.40\ ..$, we have

$$s/\kappa_n^{(+)} \simeq n + (8sd)^{\frac{1}{2}}/j_{0,1}. \tag{3.18}$$

It is interesting to compare Eqs.(3.15) and (3.18) with the corresponding expressions, valid for small sd, i.e. Eqs. (2.9) and (2.22):

$$s/\kappa_n^{(-)} \simeq n + 2sd, \quad n = 1,2, \ldots, \quad sd \ll 1,$$

and

$$s/\kappa_n^{(+)} \simeq n + (-\ell n\, 2sd)^{-1}, \quad n = 1,2, \ldots, \quad sd \ll 1.$$

When m is large, we may use the asymptotic expressions for the zeros of the Bessel functions J_1 and J_0,

$$j_{1,m} \simeq \pi(m + \tfrac{1}{4}), \tag{3.19}$$

$$j_{0,m} \simeq \pi(m - \tfrac{1}{4}). \tag{3.20}$$

From published tables (e.g., Abramowitz [8, p.409]) one can check that even for m = 1 these approximate values are already within a few percent of the exact values. By inserting (3.19) into (3.13) and (3.20) into (3.16) we obtain

$$s/\kappa_n^{(-)} \simeq n - \tfrac{1}{4} + (8sd)^{\frac{1}{2}}/\pi, \tag{3.21}$$

and

$$s/\kappa_n^{(+)} \simeq n + \tfrac{1}{4} + (8sd)^{\frac{1}{2}}/\pi. \tag{3.22}$$

Finally we shall consider some special cases. For n = 1 (so $\kappa = s$), Eq.(3.5) obviously has no solution, and Eq.(3.6) or (3.7) has the unique solution sd = 1. We can easily interpret this solution by looking back at fig.1, Section 2, where sd is assumed to be small. When we let d increase, our potential $V(r) = -2s(r + d)^{-1}$ becomes less attractive. Therefore the binding energies will decrease, i.e., the κ_n's will decrease. In fig.1 we see that all κ_n's are smaller than s, with the exception of $\kappa_0^{(+)}$. So it follows that there is no odd solution satisfying $\kappa = s$, and also that the even solution $\kappa = s$ must be the ground-state solution $\kappa_0^{(+)}$.

So we have proved that the even ground-state solution is exactly given by

$$\kappa_0^{(+)} = s, \quad sd = 1. \tag{3.23}$$

For the corresponding bound-state wave function we find

$$u_0^{(+)}(r) = \text{const.}(r+d)\, e^{-r/d}, \qquad \kappa_0^{(+)} = s = 1/d. \tag{3.24}$$

For comparison we give the approximate expression of Eq.(3.22) in the case $sd = 1$, $\kappa_{0\,\text{appr}}^{(+)} \simeq s/1.15$. By taking $n = 2$ in Eq.(3.5) we find in a similar fashion,

$$\kappa_1^{(-)} = s/2, \qquad sd = 2. \tag{3.25}$$

The corresponding odd wave function is given by

$$u_1^{(-)}(r) = \text{const. } r(r+d)\, e^{-r/d}, \quad \kappa_1^{(-)} = s/2 = 1/d. \tag{3.26}$$

In this case we obtain from Eq.(3.21), $\kappa_{1\,\text{appr}}^{(-)} \simeq s/2.02$.

We can make some additional comparisons by taking $n = 2$ in Eq.(3.7) and $n = 3$ in Eq.(3.5). For $sd = 3 + 5^{\frac{1}{2}} \simeq 5.24$ we have $\kappa_0^{(+)} = s/2$, to be compared with the approximate value $\kappa_{0\,\text{appr}}^{(+)} \simeq s/2.31$. When $sd = 3 - 5^{\frac{1}{2}} \simeq 0.76$ we have $\kappa_1^{(+)} = s/2$ and $\kappa_{1\,\text{appr}}^{(+)} \simeq s/2.04$. Finally, when $sd = 3(3 + 3^{\frac{1}{2}})/2 \simeq 7.10$ we get $\kappa_1^{(-)} = s/3$, $\kappa_{1\,\text{appr}}^{(-)} \simeq s/3.15$, and for $sd = 3(3 - 3^{\frac{1}{2}})/2 \simeq 1.90$ we find $\kappa_2^{(-)} = s/3$, $\kappa_{2\,\text{appr}}^{(-)} \simeq s/2.99$. We conclude from these comparisons that the approximate expressions (3.21) and (3.22) are already quite accurate as soon as $\frac{1}{2} < sd < n$.

Now we are going to study the limit of $\kappa_n^{(-)}$ for $sd \to \infty$. In view of Eq.(3.5) we need an expression for the largest zeros of $L_{n-1}^{(1)}(2sd/n)$. Szegö [7, p.132] gives

$$y_{nm} = 4n + O(n^{\frac{1}{3}}), \qquad n \to \infty, \qquad m \text{ fixed}, \tag{3.27}$$

where y_{nm} $(m = 1,2, \ldots)$ are the zeros in <u>decreasing</u> order of $L_n^{(\nu)}(y)$. We deduce from Eq.(3.27) the remarkable fact that

$$\lim_{sd\to\infty} (2s/d)^{-\frac{1}{2}} \kappa_n^{(-)} = 1.$$

Exactly the same limit holds for $\kappa_n^{(+)}$, because on the one hand we have $\kappa_n^{(-)} < \kappa_{n-1}^{(+)}$, and on the other hand,

$$\kappa_0^{(+)} \leq (2s/d)^{\frac{1}{2}}, \tag{3.28}$$

which follows from Eq.(1.8). Therefore

$$\lim_{sd\to\infty} (2s/d)^{-\frac{1}{2}} \kappa_n^{(\pm)} = 1, \tag{3.29}$$

for any fixed n. From this equation we obtain a rough estimate of the accuracy of our approximate expressions (3.21) and (3.22) in the case when $sd >> n$. Clearly we have

$$\lim_{sd\to\infty} (2s/d)^{-\frac{1}{2}} \kappa_{n\,appr}^{(\pm)} = \pi/4, \tag{3.30}$$

for any fixed n. So even in this case the approximate expressions are not too bad.

4. DISCUSSION

In this section we shall discuss some interesting points concerning our results of Sections 2 and 3.

(i) In the first place we note that the odd and even solutions are interlacing, i.e.,

$$\kappa_0^{(+)} > \kappa_1^{(-)} > \kappa_1^{(+)} > \ldots > \kappa_n^{(-)} > \kappa_n^{(+)} > \kappa_{n+1}^{(-)} > \kappa_{n+1}^{(+)} > \ldots \quad (4.1)$$

This a general property, which can be proved for any (sufficiently regular) symmetric potential. Both the sequences $\{\kappa_n^{(+)}\}$ and $\{\kappa_n^{(-)}\}$ are for large n approximately a harmonic progression, i.e., a sequence of terms whose reciprocals form an arithmetic progression. The common difference of this related arithmetic progression is s^{-1}, which follows from Eqs.(2.9), (2.22), (3.21) and (3.22). One might expect that also the sequence

$$\kappa_n^{(-)}, \kappa_n^{(+)}, \kappa_{n+1}^{(-)}, \kappa_{n+1}^{(+)}, \ldots \quad (4.2)$$

will approximate a harmonic progression for large n. However, this is in general not the case. Only when sd is not small, we have from Eqs.(3.21) and (3.22),

$$s/\kappa_{n+1}^{(-)} - s/\kappa_n^{(+)} \approx \tfrac{1}{2}, \quad (4.3)$$

and

$$s/\kappa_n^{(+)} - s/\kappa_n^{(-)} \approx \tfrac{1}{2}. \quad (4.4)$$

So we see that the common difference of the arithmetic progression related to (4.2) is $\frac{1}{2}s^{-1}$ in this case. This can be shown more explicitly by putting

$$\kappa_n^{(-)} \approx s/(n+a),$$

$$\kappa_n^{(+)} \approx s(n+\tfrac{1}{2}+a),$$

where a is a constant, irrelevant for the present discussion. However, when sd is very small, both $\kappa_n^{(-)}$ and $\kappa_n^{(+)}$ are very close to s/n for all n = 1,2, ... , according to Eqs.(2.9) and (2.22). So in this case the sequence (4.2) is far from being harmonic.

In [9] we have found a similar phenomenon for the bound states for the potential $V(x) = c(|x| + d)^{-2}$. In that case, when $c < -\frac{1}{4}$, both $\{\kappa_n^{(+)}\}$ and $\{\kappa_n^{(-)}\}$ are approximately geometric progressions, but only when the potential strength c is sufficiently negative the sequence (4.2) is approximately geometric, too. Therefore we conjecture that the so-called "odd-even staggering" is a generally occurring phenomenon.

(ii) *We compare the odd bound-state solutions given* by Eq.(3.21), with those for the potential

$$V(r) = -2s/r + (2sd)/r^2. \tag{4.5}$$

It is well known that, in the case $2sd = \ell(\ell + 1)$, $\ell = 0, 1, 2, \ldots$, the odd bound-state solutions are given by

$$\kappa = s/m, \qquad m = \ell + 1, \ \ell + 2, \ \ldots .$$

Therefore we have approximately for large sd,

$$s/\kappa_n \simeq n - \tfrac{1}{2} + (2sd)^{\frac{1}{2}}. \tag{4.6}$$

This expression is very similar to the one of Eq.(3.21),

$$s/\kappa_n^{(-)} \simeq n - \tfrac{1}{4} + \frac{2}{\pi}(2sd)^{\frac{1}{2}}. \tag{4.7}$$

The main difference is the appearance of the factor $2/\pi$, which is smaller than 1. We can understand this by noting that

$$-\frac{2s}{r+d} = -\frac{2s}{r} + \frac{2sd}{r^2} - \frac{2sd^2}{r^2(r+d)}. \qquad (4.8)$$

Since the last term on the right-hand side is negative, the potential $-2s/(r+d)$ is more attractive than the potential (4.5), so the κ's corresponding to (4.8) will be bigger than the κ's for the potential (4.5). Indeed we have

$$n - \tfrac{1}{4} + \frac{2}{\pi}(2sd)^{\frac{1}{2}} < n - \tfrac{1}{2} + (2sd)^{\frac{1}{2}}.$$

(iii) The interlacing property (4.1) of the κ_n's does hold for the approximate expressions of Eqs.(3.13) and (3.16) (i.e. if we take the right-hand sides). We can prove this by using a theorem concerning the zeros of the Bessel functions J_ν. First we give the well known interlacing property of these zeros [5, *Vol.2*, p.58],

$$0 < j_{\nu,1} < j_{\nu+1,1} < j_{\nu,2} < j_{\nu+1,2} < j_{\nu,3} \ldots, \quad \nu > -1. \qquad (4.9)$$

Now let sd be such that for some m,

$$j_{1,m} < j_{0,m+1} \leq (8sd)^{\frac{1}{2}} < j_{1,m+1}.$$

Then the right-hand side of Eq.(3.13) is smaller than $n+m+1$, while the right-hand side of Eq.(3.16) is at least $n+m+1$. So in this case Eq.(4.1) is satisfied. The only remaining possibility for sd is, that for some m the inequality

$$j_{0,m} < j_{1,m} \leq (8sd)^{\frac{1}{2}} < j_{0,m+1}$$

holds. In this case we have to prove that

$$\frac{(8sd)^{\frac{1}{2}} - j_{1,m}}{j_{1,m+1} - j_{1,m}} < \frac{(8sd)^{\frac{1}{2}} - j_{0,m}}{j_{0,m+1} - j_{0,m}}. \qquad (4.10)$$

One can easily show that Eq.(4.10) holds by using the fact

that the sequence $j_{1,m+1} - j_{1,m}$ is decreasing to π $(m = 1,2,\ldots)$, whereas the sequence $j_{0,m+1} - j_{0,m}$ is increasing to π. This, in turn, follows from an interesting property of the positive zeros $z_{\nu,n}$ (in ascending order) of any real solution Z_ν of Bessel's differential equation. In the appendix we prove that for $\nu^2 < \frac{1}{4}$ the sequence $\{z_{\nu,n}\}$ is convex, i.e. $\{z_{\nu,n+1} - z_{\nu,n}\}$ is increasing, and that for $\nu^2 > \frac{1}{4}$ the sequence $\{z_{\nu,n}\}$ is concave, i.e. $\{z_{\nu,n+1} - z_{\nu,n}\}$ is decreasing. From the asymptotic behavior of Z_ν it is easily seen that $\{z_{\nu,n+1} - z_{\nu,n}\}$ converges to π for all real ν. In the case $\nu = \pm\frac{1}{2}$, $\{z_{\nu,n+1} - z_{\nu,n}\}$ is neither increasing nor decreasing. We have for all n,

$$z_{\nu,n+1} - z_{\nu,n} = \pi.$$

When ν is purely imaginary, the sequence $\{z_{\nu,n}\}$ is convex. So this holds in particular for the zeros of the modified Bessel function $K_{i\mu}(z)$ (which is real for real μ and z), which have been studied recently [9].

5. SUMMARY

We have obtained explicit approximate expressions for the binding energies for the symmetric shifted Coulomb potential $V(x) = -2s(|x| + d)^{-1}$. For this potential Mehta and Patil [4] have given the binding energies corresponding to the odd wave functions only and for small sd only. In Section 2 we restricted ourselves to $sd << 1$, and in Section 3 we considered the case when sd is not small. We proved that for the ground state, which is even, we have $E_0 = O(s^2 \ell n^2 sd)$ for $s \to 0$, and for all other bound states $E_n = O(s^2)$. Furthermore we have proved that $\lim_{sd\to\infty} E_n d/s = -\frac{1}{2}$ for any fixed n. Explicit approximate expressions for the binding energies have been given in Eqs.(2.10), (2.19), (2.23), (3.13), (3.16), (3.21) and (3.22), valid for various cases. In Eqs.(3.23) - (3.26) ff. we have given some simple <u>exact</u> expressions.

In Section 4 we have discussed some interesting special points. One of these concerns the interlacing of the odd and even solutions. Both $\{\kappa_n^{(+)}\}$ and $\{\kappa_n^{(-)}\}$ are approximately harmonic progressions, but the combined sequence of even and odd solutions is "staggering", except when sd is not small.

APPENDIX

Let Z_ν be any real solution of Bessel's differential equation, and let $z_{\nu,n}$, $n = 1,2, \ldots$, be its positive zeros in ascending order. The function u,

$$u(x) \equiv x^{\frac{1}{2}} Z_\nu(kx), \qquad x > 0,$$

is for $k \neq 0$ a solution of (e.g. Szegö [7], p.17)

$$\frac{d^2u}{dx^2} + (k^2 + \frac{\frac{1}{4} - \nu^2}{x^2})u = 0. \tag{A.1}$$

In this appendix we prove, by applying a theorem of Szegö [7] which is given below, that the sequence $\{z_{\nu,n}\}$ is convex when $\nu^2 < \frac{1}{4}$, i.e. $\{z_{\nu,n+1} - z_{\nu,n}\}$ is increasing, and that $\{z_{\nu,n}\}$ is concave when $\nu^2 > \frac{1}{4}$, i.e. $\{z_{\nu,n+1} - z_{\nu,n}\}$ is decreasing, cf. [7, p.381].

Theorem (Szegö [7], pp. 19 and 20)

Let $\varphi(x)$ be continuous and decreasing in $x_0 < x < X_0$, and let $y(x)$ (not identically zero) be a solution of

$$y'' + \varphi(x)\, y = 0. \tag{A.2}$$

Then $x' < x'' < x'''$ being three consecutive zeros of $y(x)$, we have

$$x'' - x' < x''' - x'', \tag{A.3}$$

that is, the sequence of the zeros of $y(x)$ is convex.

In order to prove $x'' - x' \equiv h < x''' - x''$, we compare Eq. (A.2) with

$$Y'' + \varphi(x - h)\, Y = 0,$$

which has the solution $Y(x) = y(x - h)$. According to a well-known comparison theorem of Sturm's type, $Y(x)$ has a zero in the open interval (x'', x'''). This proves Eq.(A.3).

When $\varphi(x)$ is continuous and <u>increasing</u>, the sequence of the zeros of $y(x)$ is concave. This follows by observing that in this case $\varphi(-x)$ is a decreasing function of x.

The required result is now obtained by taking

$$\varphi(x) = k^2 + (\tfrac{1}{4} - \nu^2)\, x^{-2},$$

cf. Eqs. (A.1) and (A.2).

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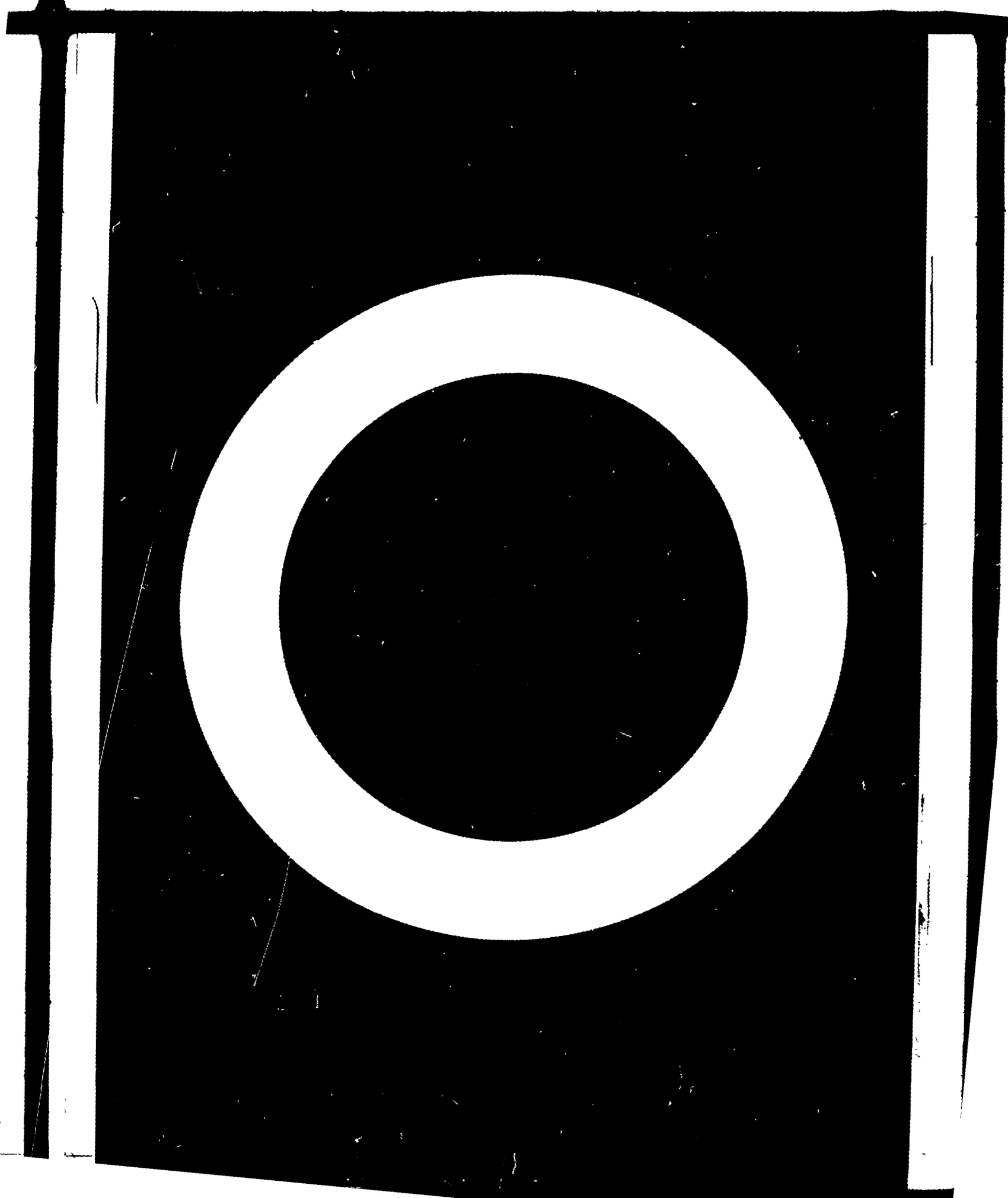

B 2

BOUND STATES FOR r^{-2}LIKE POTENTIALS IN ONE AND THREE DIMENSIONS

We investigate the bound states for a symmetric one-dimensional potential $V(x) = c(|x| + d)^{-2}$ for $|x| > R \geq 0$, $V(x)$ arbitrary for $|x| < R$, and the bound states for its three-dimensional analog. We prove that the number of bound states is finite when $c \geq -\frac{1}{4}$ and infinite when $c < -\frac{1}{4}$. For the borderline case $c = -\frac{1}{4}$ this is a new result. For $R = 0$ we obtain explicit approximate expressions for many binding energies. In this case, when $-\frac{1}{4} \leq c < 0$, there is exactly one bound state in the one-dimensional case and no bound state in the three-dimensional case. The one-dimensional ground-state energy is continuous in c at $c = -\frac{1}{4}$ whereas the excited-state energies are not.

In the case $c < -\frac{1}{4}$ the binding energies form approximately a geometric progression, both for the odd solutions and for the even solutions. The sequence of <u>all</u> binding energies is approximately a geometric progression when $R = 0$ and the potential strength is sufficiently large. However, in general the complete sequence of binding energies shows an odd-even staggering.

1. INTRODUCTION

Recently there has been much interest in bound states for various potentials in non-relativistic quantum mechanics. Many inequalities for the number of two-body bound states as a function of the potential have been established, for which we refer to the review papers by Simon [1] and by Martin [2], and to the recent paper by Glaser et al.[3]. More specifically one can consider a potential λV, $\lambda > 0$, and study the number of bound states and the energies as a function of the coupling constant λ, in particular for $\lambda \to \infty$ (e.g. Chadan [4], Simon [5]) and for $\lambda \to 0$. In one and in two dimensions there is, under certain rather general conditions on the potential V, just one bound state if λ is sufficiently small [6]. For this case, explicit expressions for the ground-state energy up to orders of λ have been deduced by Simon [6], and, for the one-dimensional case only, by Blankenbecler et al.[7] and Klaus [8].

An interesting problem is, how to determine the two classes of hamiltonians $H = -\Delta + V$ for which the number of bound states in finite and infinite, respectively. For local, nonsingular, central potentials V(r) (in three dimensions) which go to zero for $r \to \infty$, it is well known that the bound-state energies can accumulate only at $E = 0$. It is also known that only the tail of the potential is important for the bound-state energies near $E = 0$. Simon [9] proved, by extending certain results in the classical work of Courant and Hilbert [10], that a potential with a tail smaller than $c\,r^{-2}$ with $c < -\frac{1}{4}$ has infinitely many bound states, and that a potential with a tail larger than $c\,r^{-2}$ with $c > -\frac{1}{4}$ has finitely many bound states.

In this paper we deduce explicit approximate expressions for the bound-state energies for the (spherically) symmetric potential $V(r) = c(r+d)^{-2}$ in one and three dimensions in the case when $c + \frac{1}{4}$ is small, and for the one-dimensional ground-state energy for $-\frac{1}{4} \leq c < 0$. More generally, for a potential whose tail equals $c(r+d)^{-2}$, we prove that the number of bound states is finite when $c \geq -\frac{1}{4}$ and infinite when $c < -\frac{1}{4}$. In this way we have extended a result obtained by Simon [9], because in this case d can be negative, and we include the borderline case $c = -\frac{1}{4}$. In the case $c < -\frac{1}{4}$ we have derived approximate explicit expressions for the bound-state energies close to $E = 0$.

In Section 2 some preliminaries are given. In Section 3 we study the three-dimensional case and in Section 4 the one-dimensional case of the pure $c(r+d)^{-2}$ potential. In Section 5 we consider some generalizations, in particular the potentials with tail $c(r+d)^{-2}$. Finally in Section 6 the main results are summarized and discussed. Here we consider the interlacing property of the odd solutions $\kappa_n^{(-)}$ and the even solutions $\kappa_n^{(+)}$, where the κ_n's are the square roots of the binding energies. When $c < -\frac{1}{4}$, the infinite sequences $\{\kappa_n^{(-)}\}$ and $\{\kappa_n^{(+)}\}$ are approximately geometric progressions. This is compared with the case of the symmetric shifted Coulomb potential, for which we have obtained harmonic progressions instead [11]. The sequence $\{\kappa_n^{(-)}, \kappa_n^{(+)}\}$ of all solutions shows staggering in general.

2. PRELIMINARIES

We consider the spherically symmetric three-dimensional

potential

$$V(r) = c(r + d)^{-2}, \tag{2.1}$$

with c real and $d > 0$. A solution $u(r)$ of the $\ell = 0$ radial Schrödinger equation with energy $E = k^2$ has the form

$$(r + d)^{\frac{1}{2}} Z_\nu(kr + kd), \tag{2.2}$$

where Z_ν is any solution of Bessel's differential equation [12] and the order ν follows from

$$\nu^2 = c + \tfrac{1}{4}. \tag{2.3}$$

We shall also consider the symmetric one-dimensional potential

$$V(x) = c(|x| + d)^{-2}. \tag{2.4}$$

Denoting $x > 0$ by r for convenience, we can write any solution of the one-dimensional Schrödinger equation also in the form (2.2). However, the one- and three-dimensional wave functions have to satisfy different boundary conditions.

Since we are interested in bound states, we put $E = -\kappa^2$, $k = i\kappa$, with $\kappa > 0$. Then we have for both the one- and three-dimensional bound-state wave function,

$$u(r) = \text{const.}\ (r + d)^{\frac{1}{2}} K_\nu(\kappa r + \kappa d), \tag{2.5}$$

where K_ν is a modified Bessel function. Some of its properties, useful for our purposes, are

$$K_\nu(z) = K_{-\nu}(z), \tag{2.6}$$

$$K_\nu^*(z) = K_\nu{}^*(z^*), \tag{2.7}$$

and

$$K_\nu(z) \sim (2z/\pi)^{-\frac{1}{2}} e^{-z}, \quad z \to \infty. \tag{2.8}$$

We note that $K_\nu(z)$ has a branch cut along the negative real z-axis. For $\mathrm{Re}\, z > 0$ the following integral representation will be useful [12,13],

$$K_\nu(z) = \int_0^\infty e^{-z \cosh t} \cosh \nu t \, dt, \tag{2.9}$$

which holds for $\mathrm{Re}\, z > 0$ for any ν and, if $\nu = 0$, also for $\mathrm{Re}\, z = 0$. It follows from this expression that, for real positive z, $K_\nu(z)$ is real for real ν as well as for purely imaginary ν.

3. THE THREE DIMENSIONAL CASE

In this case the s-wave bound-states are obtained by imposing the well known boundary condition at the origin, $u(0) = 0$, on the wave function (2.5). This yields the bound-state condition,

$$K_\nu(\kappa d) = 0. \tag{3.1}$$

If $c \geq -\frac{1}{4}$ we have $\nu \geq 0$. It follows from Eq.(2.9) that K_ν has no (real non-negative) zero in this case, cf. also [12].

If, on the other hand, $c < -\frac{1}{4}$, we see from Eq.(2.3) that ν is purely imaginary. It is convenient to use in this case the equality

$$K_\nu(z) = \frac{\pi}{2 \sin \pi\nu} \left(I_{-\nu}(z) - I_\nu(z)\right), \tag{3.2}$$

where

$$I_\nu(z) = \frac{(z/2)^\nu}{\Gamma(1+\nu)} \, {}_0F_1(1+\nu;\, z^2/4). \tag{3.3}$$

We substitute Eqs. (3.2) and (3.3) into Eq.(3.1), put $\kappa d = y$ and $\nu = i\mu$ with $\mu > 0$. We note that $K_{i\mu}(z)$ is a real function. The bound-state condition (3.1) is equivalent to

$$(y/2)^{2i\mu} = \frac{\Gamma(1+i\mu)}{\Gamma(1-i\mu)} \frac{{}_0F_1(1-i\mu;\, y^2/4)}{{}_0F_1(1+i\mu;\, y^2/4)}. \tag{3.4}$$

Since $\Gamma^*(z) = \Gamma(z^*)$ we can write

$$\Gamma(1 + i\mu) / \Gamma(1 - i\mu) = e^{2i\omega}, \tag{3.5}$$

where $\omega = \arg \Gamma(1 + i\mu)$ is a real function of μ. For similar reasons we have

$$\frac{{}_0F_1(1 - i\mu;\ y^2/4)}{{}_0F_1(1 + i\mu;\ y^2/4)} = e^{2i\varphi}, \tag{3.6}$$

where φ is a real function of μ and y^2. We take $\varphi = 0$ when $\mu = 0$ or when $y = 0$. Insertion of Eqs.(3.5) and (3.6) into Eq. (3.4) yields

$$e^{2i\mu \ln(y/2)} = e^{2i\omega + 2i\varphi},$$

or

$$\mu \ln(y/2) = -\pi m + \omega + \varphi. \tag{3.7}$$

We have to investigate for which (integral) values of m Eq.(3.7) has a solution. For this purpose we shall now study the functions ω and φ.

The (generalized) hypergeometric functions ${}_0F_1$, and therefore also φ, can be expanded in a power series in y^2. We obtain

$$\varphi(\mu, y^2) = \mu(1 + \mu^2)^{-1} (y/2)^2 + O(y^4),\ y \to 0. \tag{3.8}$$

In order to find a more explicit expression for ω, we differentiate both sides of Eq.(3.5) with respect to μ and obtain

$$d\omega/d\mu = \tfrac{1}{2}(\psi(1 + i\mu) + \psi(1 - i\mu)) = \mathrm{Re}\ \psi(1 + i\mu) = \mathrm{Re}\ \psi(i\mu). \tag{3.9}$$

Here $\psi(z) \equiv \Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the gamma function. The following two known expressions will be

useful [13],

$$\text{Re}\ \psi(i\mu) = -C + \sum_{n=1}^{\infty} n^{-1}(1 + n^2/\mu^2)^{-1}, \quad |\mu| < \infty$$

$$= -C + \int_0^{\infty} \frac{1 - \cos \mu t}{e^t - 1}\, dt, \qquad |\mu| < \infty . \tag{3.10}$$

Here $C = 0.5772 \ldots$ is Euler's constant. By integrating $d\omega/d\mu$ and noting that $\omega = 0$ when $\mu = 0$ we get

$$\omega(\mu) = -C\mu + \int_0^{\infty} \frac{\mu t - \sin \mu t}{e^t - 1}\, \frac{dt}{t} . \tag{3.11}$$

For $|\mu| \leq 1$ we have from Eq.(3.12) the expansion

$$\omega(\mu) = -C\mu + \sum_{n=1}^{\infty} (-)^{n+1} \mu^{2n+1} \zeta(2n+1)/(2n+1), \quad |\mu| \leq 1, \tag{3.12}$$

where $\zeta(z)$ is Riemann's zeta function. From Eq.(3.10) we have furthermore,

$$\omega(\mu) = -C\mu + \sum_{n=1}^{\infty} (\mu/n - \arctan(\mu/n)), \quad |\mu| < \infty. \tag{3.13}$$

We deduce from the above expressions that $\omega(\mu)$ is negative for small μ and becomes positive when μ increases. From Eqs.(3.9) and (3.10) we have $d^2\omega/d\mu^2 > 0$, so $d\omega/d\mu$ is strictly increasing.

For $\mu \to \infty$ the following <u>asymptotic series</u> is known [13],

$$\text{Re}\ \psi(i\mu) \sim \ell n\, \mu - \sum_{n=1}^{\infty} (-\mu^2)^{-n} B_{2n}/(2n), \tag{3.14}$$

where B_{2n} are Bernoulli's numbers. Since it is permissible to integrate an asymptotic series termwise, we easily get an asymptotic series for ω,

$$\omega(\mu) \sim \mu\, \ell n\, \mu - \mu + c_0 + \sum_{n=1}^{\infty} \frac{(-)^n \mu^{1-2n} B_{2n}}{2n(2n-1)}, \quad \mu \to \infty. \tag{3.15}$$

Here c_0 is the constant of integration, for which we have

obtained $c_0 = \pi/4$.

Now we are in a position to derive the approximate solutions to Eq.(3.7). Let us first restrict ourselves to small μ. Then we have

$$\ell n(y/2) = (-\pi m + \omega + \varphi)/\mu$$
$$\simeq -\pi m/\mu - C + O(y^2). \tag{3.16}$$

For $m = 1,2, \ldots,$ y must be small, so that $O(y^2)$ may be neglected, and the approximate solutions follow at once from Eq.(3.16). For the case $m = 0$ we use the integral representation of Eq.(2.9),

$$K_{i\mu}(y) = \int_0^\infty e^{-y \cosh t} \cos \mu t \, dt. \tag{3.17}$$

It can be seen from this expression that for small μ any solution y of the equation $K_{i\mu}(y) = 0$, if it exists, must be very small. It follows then from Eq.(3.16) that there is no solution at all for $m = 0$. We conclude that for $m = 0$, and a fortiori for $m < 0$, Eq.(3.7) has no solution. (In this connection it may be recalled that for $\mu = 0$ there is no bound state at all). Therefore the ground state corresponds to the case $m = 1$.

So we have proved that, for small μ, <u>all</u> solutions to Eq. (3.1) are given approximately by

$$\kappa_m \simeq (2/d)\, e^{-\pi m/\mu - C}, \quad \mu \text{ small}, \; m = 1,2, \ldots . \tag{3.18}$$

Now we let μ increase to larger values. The solutions κ_m are continuous with respect to μ for $\mu > 0$, so we conclude that, for any $\mu > 0$, <u>all</u> bound states are uniquely determined by the solutions of Eq.(3.7) for $m = 1,2, \ldots$. For each m Eq. (3.7) has a unique solution $y_m = \kappa_m d/2$ and we have

$$\kappa_1 > \kappa_2 > \kappa_3 > \ldots . \tag{3.19}$$

When m/μ is sufficiently large, we see from Eqs.(3.7) and (3.8) that y will be sufficiently small so that φ may be neglected. Therefore we have the explicit expression

$$\kappa_m \simeq (2/d)\, e^{-\pi m/\mu + \omega/\mu}, \quad \mu > 0, \quad m/\mu \text{ large}. \tag{3.20}$$

Note the difference with Eq.(3.18) where ω/μ has been replaced by $-C$. It follows from Eq.(3.20) that

$$\lim_{m\to\infty} \kappa_m/\kappa_{m+1} = e^{\pi/\mu}, \quad \text{for all } \mu > 0, \tag{3.21}$$

so the κ_m's form approximately a geometric progression.

We note that κ_m must be an increasing function of μ. The binding energy will increase with increasing potential strength $|c|$. We can prove this for small μ with the help of Eq.(3.20). We have

$$\frac{d\,\kappa_m}{d\mu} \simeq \left(\frac{\pi m}{\mu^2} + \frac{d}{d\mu}\,\frac{\omega}{\mu}\right)\kappa_m,$$

which is indeed positive for small μ.

Finally we deduce from Eqs.(3.7) and (3.8) the more detailed equality,

$$\lim_{m\to\infty}(\mu\,\ell n(y_m/2) + \pi m - \omega)\exp(2\pi m/\mu) = \mu(1+\mu^2)^{-1}\exp(2\omega/\mu). \tag{3.22}$$

Therefore

$$\lim_{m\to\infty}(\mu\,\ell n(y_m/y_{m+1}) - \pi)\exp(2\pi m/\mu) = \mu(1+\mu^2)^{-1}\exp(2\omega/\mu)(1-\exp(-2\pi/\mu)). \tag{3.23}$$

The right-hand side is for small μ approximately $\mu\exp(-2C)$, whereas for large μ it approaches the number $2\pi\, e^{-2}$.

4. THE ONE DIMENSIONAL CASE

In Section 2 we have seen that the one-dimensional bound-state wave function is given by Eq.(2.5) with $r = x > 0$. Since the potential is symmetric, the bound-state wave functions must be either odd or even. The odd wave functions satisfy $u(0) = 0$ and are therefore for $x > 0$ proportional to the $\ell = 0$ radial solutions for the three-dimensional case which has been studied in Section 3. The corresponding "odd solutions" κ are denoted by $\kappa_m^{(-)}$. These are equal to the solutions κ_m of Eq.(3.1) discussed in the preceding section.

The even wave functions are obtained from Eq.(2.5) by imposing the boundary condition $u'(0) = 0$. In this way we obtain the following bound-state condition,

$$-2\kappa d\, K_\nu'(\kappa d) = K_\nu(\kappa d). \tag{4.1}$$

The so-called even solutions κ of this equation will be denoted by $\kappa_m^{(+)}$. We shall discuss the cases $c < -\frac{1}{4}$ and $c \geq -\frac{1}{4}$ separately.

(i) For $c < -\frac{1}{4}$ the situation is very similar to the three-dimensional case. With the help of Eq.(2.6) and

$$K_\nu' = -K_{1-\nu} - (\nu/(\kappa d))\, K_\nu ,$$

we find that Eq.(4.1) is equivalent to

$$(\tfrac{1}{2} - \nu)\, K_\nu(\kappa d) = \kappa d\, K_{1-\nu}(\kappa d). \tag{4.2}$$

We put $\kappa d = y$ as before, use Eqs.(3.2) and (3.3) and

$$I_{1-\nu}(y) = I_{-1-\nu}(y) + (2\nu/y)\, I_{-\nu} .$$

In this way we obtain the following bound-state condition,

$$(y/2)^{2\nu} = \frac{\Gamma(1+\nu)}{\Gamma(1-\nu)} \frac{(1+2\nu)\,{}_0F_1(1-\nu;y^2/4) - 4\nu\,{}_0F_1(-\nu;y^2/4)}{(1-2\nu)\,{}_0F_1(1+\nu;y^2/4) + 4\nu\,{}_0F_1(\nu;y^2/4)} . \quad (4.3)$$

By again putting $\nu = i\mu$ with $\mu > 0$ we can rewrite Eq.(4.3),

$$(y/2)^{2i\mu} = e^{2i\omega}\, e^{2i\chi} . \quad (4.4)$$

The function ω has been discussed extensively in the preceding section and χ is determined by

$$e^{2i\chi} = \frac{(1+2i\mu)\,{}_0F_1(1-i\mu;y^2/4) - 4i\mu\,{}_0F_1(-i\mu;y^2/4)}{(1-2i\mu)\,{}_0F_1(1+i\mu;y^2/4) + 4i\mu\,{}_0F_1(i\mu;y^2/4)} , \quad (4.5)$$

and by taking $\chi = 0$ when $\mu = 0$. Because we obviously have

$$(e^{2i\chi})^* = e^{-2i\chi},$$

χ is a real function of μ and y^2. It can be expanded in a power series in y^2,

$$\chi(\mu,y^2) = -\arctan(2\mu) + (y/2)^2 \frac{\mu(13+4\mu^2)}{(1+\mu^2)(1+4\mu^2)} + O(y^4), y \to 0. \quad (4.6)$$

We obtain from Eq.(4.4)

$$\mu\, \ell n(y/2) = -\pi m + \omega + \chi. \quad (4.7)$$

This bound-state condition is equivalent to Eq.(4.1). It looks very much like Eq.(3.7) for the three-dimensional case, but there is one important difference. In contrast to Eq.(3.7), the present Eq.(4.7) has a unique solution not only for $m = 1,2, \ldots$, but also for $m = 0$. This $m = 0$ solution is the ground-state, since Eq.(4.7) has no solution for negative values of m.

We prove this as follows. First we take μ small.

In the case $m < 0$, we use the integral representation (3.17) for $K_{i\mu}(y)$, and derive from Eq.(4.1) the following bound-state condition,

$$\int_0^\infty (2y \cosh t - 1)\ e^{-y \cosh t} \cos \mu t \, dt = 0. \tag{4.8}$$

A careful investigation of this equation leads to the conclusion that any solution y must be <u>small</u> if μ is small. (Note that $\exp(-y \cosh t)$ is an extremely rapidly decreasing function of t). But a solution y of Eq.(4.7), which is equivalent to Eq.(4.8), can only be <u>large</u> if m is negative. This implies that there is no solution at all for negative values of m.

For $m = 0$ we have from Eqs.(4.6) and (4.7),

$$\ln(y/2) \simeq -C - 2 + 13(y/2)^2 + \ldots \tag{4.9}$$

This equation does indeed have a unique solution. The point is that y is sufficiently small in order that terms of $O(y^4)$ may be neglected. Since the solution is continuous with respect to μ, we can consider the limit for $\mu \to 0$. A single iteration yields for the ground-state solution y_0,

$$y_0 \simeq 2 \exp\left(-C - 2 + 13\, e^{-2(C+2)}\right) = 0.164 \ldots \tag{4.10}$$

After some more iterations of the approximate Eq.(4.9) we get the more precise value $y_0 \simeq 0.166$.

When we let μ increase to larger values, the ground-state solution will increase continuously. So it is for all $\mu > 0$ defined as the unique solution of Eq.(4.7) with $m = 0$. Of course, the approximate expression (4.10) is no longer valid for large μ.

The discussion of the case $m = 1,2,..$ is similar to the one of Section 3. A solution y of Eq.(4.7) which is small can be approximated by (cf. Eq.(4.6))

$$\mu \ell n(y/2) \simeq -\pi m + \omega - \arctan(2\mu). \tag{4.11}$$

This expression is valid for $m = 1,2,..$ if m/μ is large. A similar approximation for the case when μ is small has been given by Blankenbecler et al.[7] in a different form. Their result contains an error as we shall now show. We deduce from Eq.(4.4) (cf. Eq.(4.11))

$$\tan(\mu \ell n(2/y)) = \frac{2\mu - \tan\omega}{1 + 2\mu \tan\omega} + O(y), \tag{4.12}$$

where

$$\tan\omega = \tan \arg \Gamma(1 + i\mu) = \mathrm{Im}\ \Gamma(1 + i\mu) / \mathrm{Re}\ \Gamma(1 + i\mu).$$

So for small μ we obtain from these expressions,

$$(C + 2)\mu = \tan(\mu \ell n(2/y)) + O(y), \quad y \to 0. \tag{4.13}$$

The right-hand side is the same as in Eq.(2.8) of Blankenbecler et al.[7], but on the left-hand side they only have the term 2μ.

We note that Eqs.(4.12) and (4.13) do hold even with $O(y)$ replaced by $O(y^2)$. However, in order to determine the behavior of the solutions $y = y_m$ for fixed μ, it is preferable to use $\lim_{m\to\infty}$ rather than $O(y)$, cf. Eqs.(3.22) and (3.23). We deduce from Eqs.(4.6) and (4.7) the more detailed equation,

$$\lim_{m\to\infty} [\mu \ell n(y_m/2) + \pi m - \omega + \arctan(2\mu)] \exp(2\pi m/\mu)$$
$$= \mu(1 + \mu^2)^{-1} (1 + 4\mu^2)^{-1} (13 + 4\mu^2) \exp((2\omega - 2\arctan(2\mu))/\mu). \tag{4.14}$$

Therefore

$$\lim_{m\to\infty}[\,\mu\,\ell n(y_m/y_{m+1}) - \pi\,]\,\exp(2\pi m/\mu)$$

$$= \mu(1+\mu^2)^{-1}\,(1+4\mu^2)^{-1}(13+4\mu^2)\exp((2\omega-2\arctan(2\mu))/\mu)(1-\exp(-2\pi/\mu)). \tag{4.15}$$

The right-hand side is for small μ approximately $13\mu\,\exp(-4-2C)$, whereas for large μ it approaches the number $2\pi\,e^{-2}$.

So we have obtained the following results which are similar to the ones of Section 3, i.e., similar to the results for the odd solutions $\kappa_m^{(-)}$. All solutions of Eq.(4.1) are given by the unique solutions of Eq.(4.7), with $m = 0,1,2,\ldots$, respectively. These solutions $\kappa_m^{(+)}$ are decreasing,

$$\kappa_0^{(+)} > \kappa_1^{(+)} > \kappa_2^{(+)} > \ldots .$$

For small μ we have the approximate expressions,

$$\kappa_m^{(+)} \simeq (2/d)\,e^{-\pi m/\mu - C - 2}, \quad \mu \text{ small}, \quad m = 0,1,2,\ldots, \tag{4.16}$$

whereas for arbitrary $\mu > 0$ and large m we have

$$\kappa_m^{(+)} \simeq (2/d)\,\exp((-\pi m + \omega + \chi)/\mu)$$

$$\simeq (2/d)\,\exp((-\pi m + \omega - \arctan(2\mu))/\mu),\ \mu > 0,\ m/\mu \text{ large}. \tag{4.17}$$

Furthermore, just as for the odd solutions,

$$\lim_{m\to\infty} \kappa_m^{(+)}/\kappa_{m+1}^{(+)} = e^{\pi/\mu}, \quad \text{all } \mu > 0, \tag{4.18}$$

so the $\kappa_m^{(+)}$'s form approximately a geometric progression, too. In Eqs.(4.14) and (4.15) we have given more detailed expressions.

We note that only the ground state remains when we let μ go to zero,

$$\kappa_0^{(+)} \to \simeq (2/d)\, e^{-C-2}, \qquad \mu \to 0, \tag{4.19}$$

$$\kappa_m^{(+)} \to 0, \quad m > 0, \qquad \mu \to 0. \tag{4.20}$$

(ii) We shall now consider the case $-\frac{1}{4} \leq c < 0$, i.e., $0 \leq \nu < \frac{1}{2}$. By considering Eq.(4.1) for $\kappa \to 0$ and for $\kappa \to \infty$ it easily follows that there is <u>at least</u> one bound state for all $d > 0$ (cf. [7]).

We shall prove that there exists <u>exactly one</u> bound state for all $d > 0$. This proof has not been given by Blankenbecler et al. Note that both sides of Eq.(4.1) are positive and monotonic strictly decreasing functions of κ, because

$$(y K_\nu')' = y K_\nu'' + K_\nu' = (y + \nu^2/y) K_\nu > 0, \qquad y > 0, \tag{4.21}$$

where we have used that K_ν satisfies the modified Bessel differential equation. Therefore we have to find a different, equivalent bound-state condition in order to prove that there is <u>only</u> one solution.

For this purpose our Eq.(4.2) is suitable, which we rewrite as

$$f(y) = \tfrac{1}{2} - \nu, \tag{4.22}$$

with $y \equiv \kappa d$ and

$$f(y) \equiv y\, K_{1-\nu}(y)/K_\nu(y). \tag{4.23}$$

We are going to prove that $f'(y) > 0$ for $y > 0$. With the help of Eq.(2.6), the equality

$$K_\nu' = -K_{1-\nu} - (\nu/y) K_\nu, \tag{4.24}$$

and the same relation with ν replaced by $1-\nu$ we derive

$$f'(y) = y(K_{1-\nu}\, K_{1+\nu} - K_\nu^2)/K_\nu^2. \tag{4.25}$$

By substituting the integral representation [13]

$$K_{\nu-\lambda}(y)\; K_{\nu+\lambda}(y) = 2\int_0^\infty K_{2\nu}(2y\cosh t)\cosh(2\lambda t)dt, \quad \mathrm{Re}\, y > 0, \tag{4.26}$$

for the products of the K functions we then prove

$$f'(y) > 0, \quad y > 0. \tag{4.27}$$

Furthermore we have $f(0) = 0$ and $f(y) = O(y)$ for $y \to \infty$, so f is strictly increasing from 0 to ∞. In this way we have proved that Eq.(4.22) has exactly one solution if $0 \leq \nu < \frac{1}{2}$.

Now we shall derive an upper bound to the solution y of Eq.(4.22). From Eq.(2.9) we obtain $(y > 0)$,

$$\begin{aligned} (d/d\nu)\, K_\nu(y) &> 0 \quad \text{if} \quad \nu > 0, \\ &= 0 \quad \text{if} \quad \nu = 0. \end{aligned} \tag{4.28}$$

Therefore $K_\nu(y)$ is a strictly increasing function of ν for $\nu \geq 0$. This implies that

$$K_{1-\nu}(y) > K_\nu(y), \qquad 0 \leq \nu < \tfrac{1}{2}, \quad y > 0, \tag{4.29}$$

so that the solution y of Eq.(4.22) satisfies

$$0 < y < \tfrac{1}{2} - \nu. \tag{4.30}$$

For $\nu \to \frac{1}{2}$, the potential strength c goes to zero and therefore also $y \to 0$, i.e., the binding energy goes to zero. For this case we have proved that

$$\lim_{\nu \uparrow \frac{1}{2}}\; y^{-1}(\tanh(\nu\, \ell n(2/y)) - 2\nu) = 1, \tag{4.31}$$

where we should remember that $y = y(\nu)$ is a function of ν. This result is somewhat more explicit than the one of

Blankenbecler et al. [7, Eq.(2.6)]. Furthermore we have from Eq.(4.3) the approximation,

$$(y/2)^{2\nu} = \frac{\Gamma(1+\nu)}{\Gamma(1-\nu)} \frac{1-2\nu}{1+2\nu} + \frac{\Gamma(1+\nu)}{\Gamma(1-\nu)} \frac{2\nu(13-4\nu^2)}{(1-\nu^2)(1+2\nu)^2}(y/2)^2 + O(y^4), \quad (4.32)$$

for $\nu \to \frac{1}{2}$. Because of the dependence of y on ν, the symbol O in Eq.(4.32) should be handled with care. It is not possible to fix ν and give an approximate formula up to orders of y^2, as we did before in the case $c < -\frac{1}{4}$ (ν imaginary), cf. Eq. (4.12) ff. By using Eq.(4.32) we have obtained for the solution $y = y(\nu)$,

$$\lim_{\nu \uparrow \frac{1}{2}} (1-2\nu)^{-2} (2y(\nu) - (1-2\nu) - (1-2\nu)^2 \ell n(1-2\nu)) = C = 0.5772 \ldots \quad (4.33)$$

This result confirms and extends the corresponding result obtained by Blankenbecler et al.([7], Eq. below (2.6) (corrected for the misprint) and Eq.(2.7)).

The maximum value of κ is attained of course for $\nu = 0$, i.e. for $c = -\frac{1}{4}$ since the attraction is then maximal. It is interesting to calculate the value of κ for this critical potential strength. The bound-state condition Eq.(4.2) for $\nu = 0$ is

$$K_0(\kappa d) = 2\kappa d\, K_1(\kappa d). \quad (4.34)$$

This equation can be solved with the help of tables for Bessel functions, which yields the rough estimate

$$\kappa_0^{(+)} d \lesssim 0.17. \quad (4.35)$$

This is approximately the same result as we have obtained in Eq.(4.10) for the case $\mu \to 0$. Below, in Eq.(4.38) we shall find the more accurate value 0.165721514(2).

We have discussed above the even solutions $\kappa_m^{(+)}$ for the two regions $c < -\frac{1}{4}$ and $c \geq -\frac{1}{4}$. A very interesting phenomenon may be pointed out which occurs at the critical value $c = -\frac{1}{4}$. If we let c increase from below to $-\frac{1}{4}$, an infinite number of bound states disappear abruptly, and only the ground state remains. We have seen that $\kappa_m^{(+)} \to 0$, $m = 1,2,\ldots$, for $c \uparrow -\frac{1}{4}$. However, for $c \downarrow -\frac{1}{4}$ these $\kappa_m^{(+)}$'s are nonexistent, so they are not continuous with respect to c at $c = -\frac{1}{4}$.

We shall now prove that the ground-state solution $\kappa_0^{(+)}$ is continuous with respect to c at $c = -\frac{1}{4}$. In the case $c \uparrow -\frac{1}{4}$, we have from Eq.(4.7) with $m = 0$,

$$\lim_{\mu \to 0} \ell n(y/2) = \lim_{\mu \to 0} (\omega + \chi) / \mu,$$

where $y = \kappa_0^{(+)} d$. It is easy to see that

$$\lim_{\mu \to 0} \chi/\mu = \lim_{\mu \to 0} (e^{2i\chi} - 1) / (2i\mu).$$

We now substitute for $e^{2i\chi}$ the expression of Eq.(4.5) and take the limit for $\mu \to 0$. It is easily seen that the way in which μ goes to zero is irrelevant, so we may also let the real variable $\nu = i\mu$ go to zero. This means that for $c \downarrow -\frac{1}{4}$ we find exactly the same expression as for $c \uparrow -\frac{1}{4}$. After some manipulations, where we use

$$(\nu)_n = \nu(\nu + 1)_{n-1},$$

and

$$\nu\, {}_0F_1(\nu;z) = \nu + z\, {}_1F_2(1;2,1+\nu;z), \tag{4.36}$$

we find the following exact equation for the ground-state solution y, for both cases $c \uparrow -\frac{1}{4}$ and $c \downarrow -\frac{1}{4}$,

$$\ell n(y/2) = -C + \frac{-4+2\,{}_0F_1(1;y^2/4) - {}_0F_1'(1;y^2/4) - y^2\,{}_1F_2'(1;2,1;y^2/4)}{{}_0F_1(1;y^2/4) + y^2\,{}_0F_1(2;y^2/4)}. \quad (4.37)$$

Here we have used the abbreviations, for this occasion only,

$${}_0F_1'(1;y^2/4) \equiv (d/d\nu)\,{}_0F_1(1+\nu;y^2/4)\Big|_{\nu=0},$$

and

$${}_1F_2'(1;2,1;y^2/4) \equiv (d/d\nu)\,{}_1F_2(1;2,1+\nu;y^2/4)\Big|_{\nu=0}.$$

Note that Eq.(4.37) has the same unique solution y as Eq.(4.34), i.e., $K_0(y) = 2y\,K_1(y)$. However, Eq.(4.37) is more suitable for obtaining an accurate value for the solution. We expand the hypergeometric functions on the right-hand side of Eq. (4.37). By means of an iteration procedure we then find for the even ground-state solution,

$$\kappa_0{}^{(+)}d = y_0 = 0.165721514(2), \quad \nu = \mu = 0, \quad c = -\tfrac{1}{4}. \quad (4.38)$$

Let us recall some related results from the above discussion,

$$\kappa_0{}^{(+)}d < \tfrac{1}{2} - \nu, \qquad 0 \le \nu < \tfrac{1}{2}, \quad (4.39)$$

$$\kappa_0{}^{(+)}d \le 0.165721514(2), \quad 0 \le \nu < \tfrac{1}{2}, \quad (4.40)$$

$$\kappa_0{}^{(+)}d \simeq \tfrac{1}{2} - \nu, \qquad \nu \simeq \tfrac{1}{2}. \quad (4.41)$$

We note that Eq.(4.33) gives a more detailed expression for the behavior of $\kappa_0{}^{(+)}d$ near $\nu = \frac{1}{2}$.

5. GENERALIZATIONS

In this section we shall discuss some generalizations of the results of Sections 3 and 4. In the three-dimensional case we take

$$V(r) = c(r+d)^{-2}, \qquad r > R \quad (R > 0,\ R + d > 0), \quad (5.1)$$

and for $0 < r < R$ an arbitrary potential, satisfying

$$\int_0^R | V(r) | r\,dr < \infty . \tag{5.2}$$

In the one-dimensional case we take

$$V(x) = c(|x| + d)^{-2}, \quad |x| > R \ (R > 0,\ R + d > 0), \tag{5.3}$$

and for $|x| < R$ an arbitrary symmetric potential satisfying

$$\int_0^R | V(x) | dx < \infty. \tag{5.4}$$

This condition on the potential is more restrictive than Eq.(5.2). Note that the parameter d may be negative in this section, as long as $R + d > 0$.

We shall prove that also in this case the number of bound states is finite when $c \geq -\frac{1}{4}$, and infinite when $c < -\frac{1}{4}$. In the latter case we shall give explicit approximate expressions for $\kappa_m^{(+)}$ and $\kappa_m^{(-)}$, for large m.

Let us first consider the three-dimensional case. For $\ell > 0$ we can only obtain solutions if d is chosen to be zero. The derivation will be similar to the one of Section 3. We shall restrict ourselves throughout to $\ell = 0$. For $r > R$ the s-wave bound-state wave function is given by Eq.(2.5),

$$u(r) = \text{const.}(r + d)^{\frac{1}{2}} K_\nu(\kappa r + \kappa d), \quad r > R. \tag{5.5}$$

For $0 < r < R$ it satisfies the Volterra integral equation [14,15]

$$u(r) = \kappa^{-1} \sinh \kappa r + \kappa^{-1} \int_0^r \sinh(\kappa r - \kappa r')\, V(r')\, u(r')dr', \tag{5.6}$$

apart from an unimportant normalization constant. It follows that the logarithmic derivative u'/u is a real-analytic function of the energy $k^2 \equiv -\kappa^2$. (Actually, u'/u is real-meromorphic,

so it can accidentally have a pole just at $\kappa = 0$. However the following discussion can easily be adjusted in this exceptional case). We have to match the wave functions for $r < R$ and $r > R$ by requiring u'/u to be continuous at $r = R$. Now we introduce the new variable

$$z \equiv \kappa(R + d),$$

which is more convenient than the variable $y \equiv \kappa d$ which we used before. We then have

$$\lim_{r \downarrow R} u'/u = \kappa K_\nu'(z) / K_\nu(z) + \tfrac{1}{2}(R + d)^{-1}. \tag{5.7}$$

It is therefore convenient to introduce the real-analytic function $A(k^2) \equiv A(-\kappa^2)$ by putting

$$\lim_{r \uparrow R} u'/u = (\tfrac{1}{2} + A) / (R + d). \tag{5.8}$$

In this way we obtain from Eqs.(5.7) and (5.8) the following bound-state condition,

$$A K_\nu(z) = z K_\nu'(z). \tag{5.9}$$

As before, ν is real when $c \geq -\frac{1}{4}$ and ν is imaginary when $c < -\frac{1}{4}$. We convert Eq.(5.9) into

$$(A + \nu) K_\nu(z) = -z K_{1-\nu}(z). \tag{5.10}$$

The solutions κ_m of this equation are just the odd solutions $\kappa_m^{(-)}$ *for the one-dimensional case. The even solutions* $\kappa_m^{(+)}$ follow from a different equation which, however, has exactly the same form as Eq.(5.10). The only difference is in the function A, which is defined by Eq.(5.8) where now $u'(0) = 0$ instead of $u(0) = 0$. This is proved as follows.

The *even bound-state wave function* $u(x)$ *is for* $x > R$ given by (cf.Eq.(5.5))

$$u(x) = \text{const.}(x+d)^{\frac{1}{2}} K_\nu(\kappa x + \kappa d), \quad x > R. \tag{5.11}$$

For $0 < x < R$ it satisfies the Volterra integral equation (apart from an unimportant normalization constant),

$$u(x) = \cosh \kappa x + \kappa^{-1} \int_0^x \sinh(\kappa x - \kappa x')\, V(x')\, u(x')\, dx'. \tag{5.12}$$

It follows that the logarithmic derivative u'/u is again a real-analytic function of the energy at $\kappa = 0$ (in general), just as before in the "odd case". Since the explicit form of this function is irrelevant for our discussion, we may denote it again by A. Obviously the even bound-state condition is then also given by Eq.(5.10).

We note that we must get back the bound-state conditions of Sections 3 and 4 if we let R go to zero Indeed, by taking $A = \infty$ in Eq.(5.10) we obtain Eq.(3.1) for the odd solutions, and by taking $A = -\frac{1}{2}$ we obtain Eq.(4.2) for the even solutions.

In order to find the solutions of Eq.(5.10) we proceed in the same way as before, and obtain the equivalent equation (cf. Eq.(4.3)),

$$(z/2)^{2\nu} = \frac{\Gamma(1+\nu)}{\Gamma(1-\nu)} \frac{(A-\nu)\,{}_0F_1(1-\nu;z^2/4) + 2\nu\,{}_0F_1(-\nu;z^2/4)}{(A+\nu)\,{}_0F_1(1+\nu;z^2/4) - 2\nu\,{}_0F_1(\nu;z^2/4)}. \tag{5.13}$$

It can be shown that this equation can have only a finite number of solutions when ν is a real number, i.e. when $c \geq -\frac{1}{4}$. In the case $c < -\frac{1}{4}$, ν is purely imaginary so we put for convenience $\nu = i\mu$ as before. We rewrite Eq.(5.13) as follows,

$$(z/2)^{2i\mu} = e^{2i\omega}\, e^{2i\xi}. \tag{5.14}$$

The function ω depends only on μ (cf. Eq.(3.13)),

$$\omega(\mu) = \arg \Gamma(1 + i\mu).$$

The function ξ is defined by

$$e^{2i\xi} = \frac{(A-i\mu)\,{}_0F_1(1-i\mu;z^2/4) + 2i\mu\,{}_0F_1(-i\mu;z^2/4)}{(A+i\mu)\,{}_0F_1(1+i\mu;z^2/4) - 2i\mu\,{}_0F_1(i\mu;\,z^2/4)}, \tag{5.15}$$

and by taking $\xi = 0$ when $\mu = 0$. Just as the functions φ and χ of Eqs.(3.6) and (4.5), ξ is real. Since A is a real-analytic function of κ^2, and therefore of $z^2 \equiv \kappa^2(R+d)^2$, we can expand ξ as follows,

$$\xi = \arctan(\mu/A(0)) + O(z^2), \quad z \to 0. \tag{5.16}$$

From Eq.(5.14) we have

$$\mu\,\ell n\,(z/2) = -\pi m + \omega + \xi. \tag{5.17}$$

When m, or m/μ, is sufficiently large, there exist solutions z which are very small. Then we may neglect the term $O(z^2)$ on the right-hand side of Eq.(5.16). So we find the following infinite series of bound-state solutions ($z \equiv \kappa(R+d)$),

$$\kappa_m^{(\pm)} \simeq (2/(R+d))\exp((-\pi m+\omega+\arctan(\mu/A^{(\pm)}(0)))/\mu), \quad m/\mu \text{ large}, \tag{5.18}$$

where we now use the superscripts in $A^{(+)}$ and $A^{(-)}$ to denote the even and the odd case, respectively. By taking $R = 0$ we get back the expressions of Sections 3 and 4. The odd solutions $\kappa_m^{(-)}$ of Eq.(3.20) are recovered by taking $A^{(-)}(0) = \infty$, and the even solutions $\kappa_m^{(+)}$ of Eq.(4.17) by taking $A^{(+)}(0) = -\frac{1}{2}$.

It follows from Eq.(5.18) that the tail of the potential almost completely determines the bound states near the origin. The only effect of the potential for $0 < r < R$ is contained in the constant $A^{(\pm)}(0)$. In particular we have, just as in Sections 3 and 4, for all $\mu > 0$,

$$\lim_{m\to\infty} \kappa_m^{(-)}/\kappa_{m+1}^{(-)} = e^{\pi/\mu}, \tag{5.19}$$

$$\lim_{m\to\infty} \kappa_m^{(+)}/\kappa_{m+1}^{(+)} = e^{\pi/\mu}. \tag{5.20}$$

We note that $\kappa_m^{(\pm)}$ of Eq.(5.18) need not be the m-th or the (m+1)-th κ in the sequence of solutions κ in decreasing order. That is, the counting will in general be different from the counting in Sections 3 and 4. In this connection we note that for $m = 1,2,..$ we have $\kappa_m \to 0$ when $\mu \to 0$. In addition there can be extra bound states which have to be denoted by κ_0, κ_{-1}, κ_{-2}, ... The number of these is finite and depends on the inner part of the potential.

6. SUMMARY AND DISCUSSION

In Section 3 we have deduced the s-wave bound-state energies $E_m = -\kappa_m^2$ for the spherically symmetric three-dimensional potential,

$$V(r) = c(r+d)^{-2}. \tag{6.1}$$

When $c \geq -\frac{1}{4}$ there is no bound state at all, but in the case $c < -\frac{1}{4}$ there are infinitely many bound states. We have obtained (cf. Eqs.(3.18) and (3.20)),

$$\kappa_m \simeq (2/d)\, e^{-\pi m/\mu + \omega/\mu}, \quad m = 1,2,.., \quad m/\mu \text{ large}, \tag{6.2}$$

where $\mu = (-c-\frac{1}{4})^{\frac{1}{2}} > 0$ and $\omega = \arg \Gamma(1+i\mu)$. A more detailed expression for κ_m has been given in Eq.(3.22).

The $\ell = 0$ wave functions are, if we write r for $x > 0$, proportional to the <u>odd</u> wave functions for the one-dimensional symmetric potential,

$$V(x) = c(|x|+d)^{-2}. \tag{6.3}$$

The <u>even</u> bound-state wave functions and the corresponding

energies $-(\kappa_m^{(+)})^2$ for this potential have been investigated in Section 4. For $-\frac{1}{4} \le c < 0$ we have exactly one bound state, $m = 0$. This result has also been obtained by Blankenbecler et al.[7], although they did not give the proof. For $c < -\frac{1}{4}$ we have bound states for $m = 0,1,2, \ldots$. We have proved that $\kappa_0^{(+)}$ is a continuous function of c in particular at $c = -\frac{1}{4}$. For this case ($\mu = 0$, $\nu \equiv (c + \frac{1}{4})^{\frac{1}{2}} = 0$) we have in Eq.(4.38) obtained $y_0 = \kappa_0^{(+)}d = 0.165721514(2)$. This is the solution of Eq.(4.34), and also of Eq.(4.37) which has a very different form. Some relations for $\kappa_0^{(+)}$ in the case $-\frac{1}{4} \le c < 0$ have been given in Eqs. (4.39) - (4.41). In particular for the behavior of $\kappa_0^{(+)}$ for $\nu \to \frac{1}{2}$, i.e. $c \to 0$, we have deduced a precise expression, Eq.(4.33).

The even bound-state solutions with $m = 1,2, \ldots$, which occur for $c < -\frac{1}{4}$, are approximately given by (cf.Eq.(4.17))

$$\kappa_m^{(+)} \simeq (2/d)\exp((-\pi m + \omega - \arctan(2\mu))/\mu), \quad m=1,2,\ldots,m/\mu \text{ large}. \tag{6.4}$$

In Eq.(4.14) we have obtained a more detailed expression.

In Section 5 we considered the more general case of an arbitrary symmetric potential which equals (6.1) or (6.3) only for $r > R$ or $|x| > R$, respectively. We proved that also in this case the number of bound states is finite when $c \ge -\frac{1}{4}$, and infinite when $c < -\frac{1}{4}$. In the latter case we have obtained the approximate expression (cf. Eq.(5.18)),

$$\kappa_m^{(\pm)} \simeq (2/(R+d))\exp((-\pi m + \omega + \arctan(\mu/A^{(\pm)}(0)))/\mu), \quad m/\mu \text{ large}, \tag{6.5}$$

for the odd and the even solutions.

So we have proved that any (spherically) symmetric potential with a tail $c(r+d)^{-2}$ yields, for any $d > -R$, infinitely many bound states when $c < -\frac{1}{4}$ and finitely many when $c \geq -\frac{1}{4}$. In this way we have extended proposition 3 of a paper by Simon [9], which states that the number of bound states is finite for a potential which satisfies $V(r) \geq c\,r^{-2}$ for some $c > -\frac{1}{4}$. Note that the tail $c(r+d)^{-2}$ still yields only finitely many bound states if $c \geq -\frac{1}{4}$, despite the fact that, when d is negative, it is more attractive than the tail cr^{-2}. Our result for the case $c < -\frac{1}{4}$ is in fact equivalent with proposition 2 of [9], which says that, for a potential V with $V(r) < c\,r^{-2}$ $(r > R,\ c < -\frac{1}{4})$, there are infinitely many bound states. The equivalence can be seen by noting that in this case c belongs to the open interval $(-\infty, -\frac{1}{4})$.

We have denoted the ground-state solution in the one-dimensional case by $\kappa_0^{(+)}$, and in the three-dimensional case by κ_1. Our motive for this is that $\kappa_0^{(+)}$ is special since it exists for all $c < 0$, i.e., for arbitrarily small potential strength, while κ_1 (for the three-dimensional case) does not. This is a particular case of a general theorem proved by Simon [6], which has recently been generalized by Klaus [8]. Simon proved that, under the condition

$$\int_{-\infty}^{\infty} (1 + x^2)\,|\,V(x)\,|\,dx < \infty, \quad V \text{ not a.e. zero}, \tag{6.6}$$

$-d^2/dx^2 + \lambda V$ has a bound state for all small positive λ if and only if

$$\int_{-\infty}^{\infty} V(x)\,dx \leq 0.$$

Klaus [8] proved this under the condition (weaker than (6.6))

$$\int_{-\infty}^{\infty} (1 + |x|)\,|V(x)|\,dx < \infty, \quad V \text{ not a.e zero},$$

which had been conjectured by Simon. A similar theorem for the two-dimensional case has also been proved by Simon [6] . An interesting consequence is that, in one and two dimensions, $-\Delta + \lambda V$ has at least one bound state for <u>all</u> $\lambda \neq 0$, if $\int_{-\infty}^{\infty} V(x)\,dx = 0$. If λ is small there is only one bound state [6].

An interesting phenomenon comes to light when we consider the interrelationship between the odd solutions $\kappa_m^{(-)}$ and the even solutions $\kappa_m^{(+)}$. It can be proved that for an arbitrary (nonsingular) symmetric potential these κ's interlace, i.e.,

$$\kappa_0^{(+)} > \kappa_1^{(-)} > \kappa_1^{(+)} > \ldots > \kappa_m^{(-)} > \kappa_m^{(+)} > \kappa_{m+1}^{(-)} > \kappa_{m+1}^{(+)} > \ldots \tag{6.7}$$

Both the sequence $\{\kappa_m^{(-)}\}$ and the sequence $\{\kappa_m^{(+)}\}$ are, for large m, approximately geometric progressions, with common ratio $e^{-\pi/\mu}$. One might expect that also the sequence

$$\kappa_m^{(-)},\ \kappa_m^{(+)},\ \kappa_{m+1}^{(-)},\ \kappa_{m+1}^{(+)},\ \ldots \tag{6.8}$$

will approximate a geometric progression, with common ratio $e^{-\pi/(2\mu)}$, when m is large. However, in general this is not the case. Let us for convenience restrict ourselves to the simple case R = 0. Then we have from Eqs.(6.2) and (6.4), for large m,

$$\kappa_m^{(-)}/\kappa_m^{(+)} \simeq \exp(\mu^{-1} \arctan(2\mu)) > 1, \tag{6.9}$$

and

$$\kappa_m^{(+)}/\kappa_{m+1}^{(-)} \simeq \exp((\pi - \arctan(2\mu))/\mu) > 1. \tag{6.10}$$

Indeed, for large μ both (6.9) and (6.10) approach $e^{\pi/(2\mu)}$, but for small μ the ratio (6.9) becomes e^2, and the ratio (6.10)

becomes $e^{\pi/\mu-2}$. So we see that the sequence (6.8) is approximately a geometric progression only for the case of large μ, that is, for large potential strength.

In this connection it is interesting to note that a similar phenomenon occurs for the case of the symmetric shifted Coulomb potential,

$$V(x) = -2s(|x|+d)^{-1}.$$

Recently we have proved [11] that for this potential both the sequences of the odd solutions $\kappa_n^{(-)}$ and of the even solutions $\kappa_n^{(+)}$ form, for large n, approximately a <u>harmonic</u> progression, i.e., a sequence of terms whose reciprocals form an arithmetic progression. The common difference of this related arithmetic progression turns out to be s^{-1}. For the case of small sd we have deduced,

$$s/\kappa_n^{(-)} \simeq n + 2sd, \quad n = 1,2, \ldots,$$

$$s/\kappa_n^{(+)} \simeq n + (-\ell n(2sd))^{-1}, \quad n = 1,2, \ldots.$$

Clearly the sequence

$$\kappa_n^{(-)}, \kappa_n^{(+)}, \kappa_{n+1}^{(-)}, \kappa_{n+1}^{(+)}, \ldots \tag{6.11}$$

is not a harmonic progression in this case. However, for the case when sd is not small, i.e. for sufficiently large potential strength, we have proved that (6.11) is, for large n, indeed a harmonic progression, approximately. The common difference of its related arithmetic progression is of course just $\frac{1}{2} s^{-1}$.

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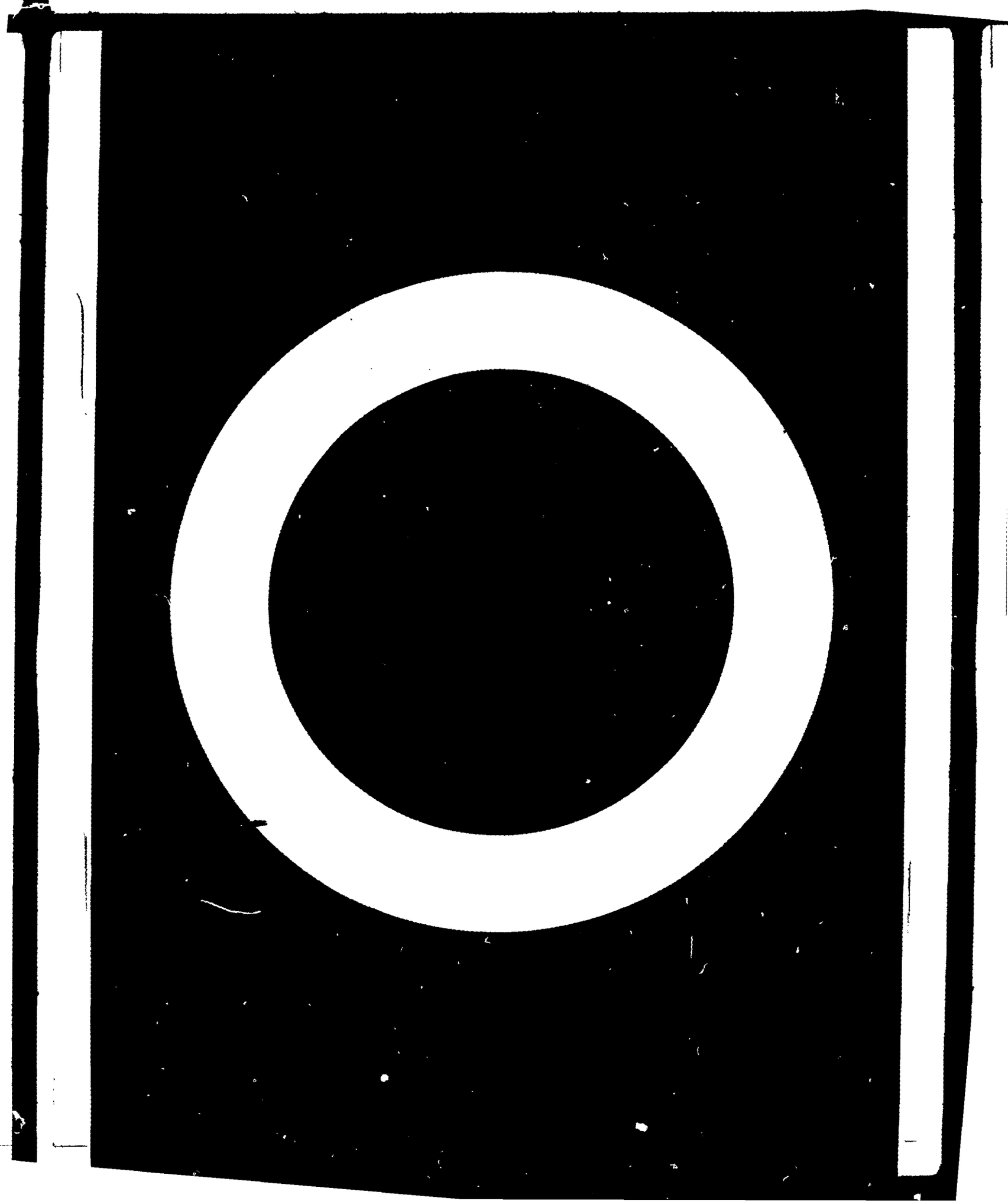

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Coulomb-Scattering States and Partial-Wave Decompositions.

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Summary. — It is customary to split the physical Coulomb-scattering wave function $\psi_C^{(+)}$ into an incoming part ψ_i and a scattered part ψ_s. We derive analytic formulae for the partial-wave projections of ψ_i and ψ_s and discuss the asymptotic convergence of the corresponding partial-wave series. It is found that the above splitting is unsatisfactory. We propose a different splitting of $\psi_C^{(+)}$ into an incoming part and a scattered part which is in close analogy with the standard separation of the scattering wave function for a short-range potential.

1. – Introduction.

It is customary to split the pure Coulomb-scattering wave function $\psi_C^{(+)}(\boldsymbol{k}, \boldsymbol{r})$ into an « incoming part » ψ_i and a « scattered part » ψ_s. See, *e.g.*, ref (1), app. B.4. All these three functions are solutions of Schrödinger's equation, $\psi_C^{(+)}$ is the regular one, ψ_i and ψ_s are irregular.

As solutions of the radial Schrödinger equation the functions F_l, G_l and $u_l^{(\pm)}$ are frequently used (cf. app. B.5 of (1)). Here F_l is the regular solution, G_l and $u_l^{(\pm)}$ are irregular solutions. Besides the radial equation which closely resembles the one-dimensional Schrödinger equation, we shall consider the partial-wave (p.w.) Schrödinger equation which contains the well-known first-derivative term. Because $F_l(r)/r$ and $u_l^{(\pm)}(r)/r$ are solutions of the p.w. Schrödinger equation, one might expect that these functions would be proportional to the p.w. projections of $\psi_C^{(+)}$, ψ_i and ψ_s, which we denote by $\psi_l^{(+)}$, $\psi_{i,l}$ and $\psi_{s,l}$, respectively. It turns out, however, that this expectation does

(1) A. MESSIAH: *Quantum Mechanics*, Vol. I (Amsterdam, 1961).

not quite come true. We shall even find that $\psi_{i,l}$ and $\psi_{s,l}$ are *no* solutions of the p.w. Schrödinger equation. The explanation of this possibly unexpected fact can be found by realizing that only the regular solutions of the Schrödinger equation are eigenfunctions of the Hamiltonian. (Notice that we identify here the Schrödinger equation with the differential equation that is derived from it, as is often done.) So one should discriminate between solutions of the differential equation, on the one hand, and eigenfunctions of the Hamiltonian. on the other hand. It has been realized before that this statement is true in general, but, as the Coulomb potential is so simple, we are able to show it explicitly by means of closed formulae.

We consider the asymptotic behaviour of $\psi_l^{(+)}$, $\psi_{i,l}$, $\psi_{s,l}$ and show then that the p.w. series of $\psi_{i,l}$ is convergent, those of $\psi_l^{(+)}$ and of $\psi_{s,l}$ are divergent, if these series are understood in the usual sense. Convergence can be obtained with the help of Taylor's distribution (2). If we take this distribution aspect into account, we are able to relate $\psi_{i,l}$ with $u_l^{(-)}$ and $\psi_{s,l}$ with $u_l^{(+)}$. It may be that the two procedures « replacing the functions by their asymptotic approximations » and « summing the p.w. series » do not commute. We have not considered the convergence of the p.w. series in general.

The present investigation strengthens the feeling that ψ_i and ψ_s are not the most natural objects to describe the scattering. In our opinion they have no physical interpretation except asymptotically. We conclude that the splitting $\psi_0^{(+)} = \psi_i + \psi_s$ is unsatisfactory. Therefore we propose a different splitting of $\psi_0^{(+)}$ into an incoming part and a scattered part. In ref. (3) we obtained a generalized Lippmann-Schwinger equation in momentum representation. This equation, written out in co-ordinate representation, gives at once the new splitting. It appears that the new states in co-ordinate representation cannot be considered as ordinary functions. This is a new feature. One should realize that in momentum representation the improper scattering states are always distributions, but in co-ordinate representation we are acquainted only with ordinary functions.

The new approach has many applications and admits a more satisfactory physical interpretation. This will be worked out in the near future.

The notation and conventions are explained in sect. **2**. In sect. **3** we derive closed formulae for $\psi_l^{(+)}$, $\psi_{i,l}$ and $\psi_{s,l}$. Here it is found that $\psi_l^{(+)}(kr)$ is proportional to $F_l(kr)/r$, which is known, and that $\psi_{i,l}(kr)$ and $\psi_{s,l}(kr)$ differ in an essential way from $u_l^{(\pm)}(kr)/r$. At the end of sect. **3** the fact that the irregular functions are no eigenfunctions of the Hamiltonian is discussed. This point is illustrated by considering these functions in momentum representation.

Section **4** deals with the new splitting of $\psi_0^{(+)}$. Finally, in sect. **5** we give a short summary and a general discussion.

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(2) J. R. TAYLOR: *Nuovo Cimento*, **23** B, 313 (1974).
(3) H. VAN HAERINGEN: *Coulombian asymptotic states*, preprint (1975).

Appendices A and B give more technical details of certain derivations. As a by-product, an interesting equality relating a finite number of confluent hypergeometric functions ${}_1F_1$ has been obtained (eq. (B.10)).

2. – Notation and conventions.

As usual we take $\hbar = 2m = 1$ (m the reduced mass), the energy is $k^2 > 0$ and the Coulomb potential is given by $V_C(r) = 2k\gamma/r$. Throughout this paper we consider almost only pure Coulomb functions. The appropriate subscript C will mostly be suppressed. To some extent we use the notation of MESSIAH [1]. Deviations from that notation occur because we often prefer Dirac's notation. For example, we write $\langle \boldsymbol{r}|\boldsymbol{k}\rangle$ in place of $(2\pi)^{-\frac{3}{2}} \exp[i\boldsymbol{k}\cdot\boldsymbol{r}]$.

The Coulomb-scattering state is

$$(1)\quad \langle \boldsymbol{r}|\boldsymbol{k}+\rangle \equiv \psi_C^{(+)}(\boldsymbol{k},\boldsymbol{r}) = \\ = (2\pi)^{-\frac{3}{2}} \exp[-\pi\gamma/2]\,\Gamma(1+i\gamma)\exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\,{}_1F_1(-i\gamma;1;ikr-i\boldsymbol{k}\cdot\boldsymbol{r})\,.$$

Here ${}_1F_1$ is the confluent hypergeometric function or Kummer's [4] function Φ. It can be expressed in terms of the function U (*e.g.* [5]), also denoted by Ψ (ref. [4], p. 257):

$$(2)\quad {}_1F_1(-i\gamma;1;z) = \exp[\pi\gamma]/\Gamma(1+i\gamma)\,U(-i\gamma,1,z) - \\ - \exp[\pi\gamma]/\Gamma(-i\gamma)\exp[z]\,U(1+i\gamma,1,-z)\,, \qquad \operatorname{Im} z > 0\,.$$

This defines the splitting $\psi_C^{(+)} = \psi_i + \psi_s$ with

$$(3)\quad \psi_i = (2\pi)^{-\frac{3}{2}} \exp[\pi\gamma/2]\exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\,U(-i\gamma,1,ikr-i\boldsymbol{k}\cdot\boldsymbol{r})\,,$$

$$(4)\quad \psi_s = -(2\pi)^{-\frac{3}{2}} \exp[\pi\gamma/2]\frac{\Gamma(1+i\gamma)}{\Gamma(-i\gamma)}\exp[ikr]\,U(1+i\gamma,1,i\boldsymbol{k}\cdot\boldsymbol{r}-ikr)\,.$$

The difference with eqs. (B.19)-(B.22) of ref. [1] consists merely in the factor $(2\pi)^{-\frac{3}{2}}$. The function U is singular at the origin:

$$(5)\qquad U(a,1,z) = (2C-\psi(a)-\ln z)/\Gamma(a) + \mathcal{O}(|z\ln z|)\,, \qquad z\to 0,$$

where C is Euler's constant and $\psi(a)$ is the logarithmic derivative of the gamma-function.

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[4] A. ERDÉLYI, Editor: *Higher Transcendental Functions*, Vol. 1 (New York, N. Y., 1953).

[5] W. MAGNUS, F. OBERHETTINGER and R. P. SONI: *Formulas and Theorems for the Special Functions of Mathematical Physics* (Berlin, 1966).

At infinity one has

$$U(a, c, z) \sim z^{-a}, \qquad |z| \to \infty. \tag{6}$$

The functions ψ_c and ψ_s are linearly independent so-called irregular solutions of Schrödinger's equation. We define the p.w. projection of a function $f(\boldsymbol{k}, \boldsymbol{r}) \equiv$ $\equiv f(k, r, \hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}})$ by

$$f_l(k, r) \equiv 2\pi \int_{-1}^{1} \mathrm{d}(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) f(\boldsymbol{k}, \boldsymbol{r}) . \tag{7a}$$

This implies in general that

$$f(\boldsymbol{k}, \boldsymbol{r}) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) f_l(k, r) , \tag{7b}$$

where equality is understood in the sense of distributions. For a short-range potential, one has to deal only with the very well-known Dirac δ-function, but in the Coulomb case other distributions play a role, too ([2]). This will be clarified at the end of sect. 3.

The regular Coulomb p.w. function $F_l(kr)$ is usually defined (apart from normalization) as the real-valued regular solution of the radial Schrödinger equation. We prefer to use instead

$$\langle r|kl+\rangle = \sqrt{2/\pi}\, i^l \exp[i\sigma_l] F_l(kr)/(kr) . \tag{8}$$

This notation and convention is not new, cf. ref. ([6]). The Coulomb phase shift σ_l is defined by

$$\exp[2i\sigma_l] = \Gamma(l+1+i\gamma)/\Gamma(l+1-i\gamma) .$$

The function $\langle r|kl+\rangle$ is the regular solution of the radial equation including the first-derivative term, which equation will be called the p.w. Schrödinger equation. It arises in a natural way from the p.w. projection of $\langle \boldsymbol{r}|\boldsymbol{k}+\rangle$ and this is also the reason for the occurrence of the factors i^l and $\exp[i\sigma_l]$. The same convention can be used for other potentials V. One requires then that $\langle \boldsymbol{r}|\boldsymbol{k}+\rangle_V$ and $\langle r|kl+\rangle_V$ satisfy eq. (7).

As we said in the introduction, also irregular solutions of the radial Schrödinger equation are in use, notably $G_l(kr)$ and $u_l^{(\pm)}(kr)$ (cf. app. B.5 of ([1])). We prefer to use a new convention and notation. We define $|kl\uparrow\rangle$ and $|kl\downarrow\rangle$ by

$$\langle r|kl\uparrow\rangle = \sqrt{2/\pi}\, i^l u_l^{(+)}(kr)/(kr) , \tag{9}$$

$$\langle r|kl\downarrow\rangle = \sqrt{2/\pi}\, i^l u_l^{(-)}(kr)/(kr) = (-)^l \langle r|kl\uparrow\rangle^* . \tag{10}$$

([6]) J. R. Taylor: *Scattering Theory* (New York, N. Y., 1972).

Notice that in momentum representation no factor $(-)^l$ occurs:

$$\langle p|kl\downarrow\rangle = \langle p|kl\uparrow\rangle^* .$$

The reason for this is that taking the complex conjugate is not a linear operation. The functions in eqs. (9) and (10) are Jost solutions of the p.w. Schrödinger equation. Asymptotically, $\langle r|kl\uparrow\rangle$ is an *outgoing* modified spherical wave and $\langle r|kl\downarrow\rangle$ an incoming one:

$$\langle r|kl\uparrow\rangle \sim \sqrt{2/\pi}\,\frac{1}{kr}\exp\left[ikr - i\gamma\ln(2kr)\right],$$

$$\langle r|kl\downarrow\rangle \sim \sqrt{2/\pi}\,\frac{(-)^l}{kr}\exp\left[-ikr + i\gamma\ln(2kr)\right].$$

Notice that $|kl\uparrow\rangle$ and $|kl\downarrow\rangle$ are defined also for complex values of k, while $|kl+\rangle$ makes sense only for real k. At infinity ($r = \infty$), $\langle r|kl\uparrow\rangle$ is regular if $\mathrm{Im}\ k > 0$ and $\langle r|kl\downarrow\rangle$ is regular if $\mathrm{Im}\ k < 0$.

For the vanishing potential strength one has (cf. app. B.6 of (1))

$$\lim_{\gamma\to 0}\langle r|kl\uparrow\rangle = \sqrt{2/\pi}\,i^l h_l^{(+)}(kr),$$
$$\lim_{\gamma\to 0}\langle r|kl\downarrow\rangle = \sqrt{2/\pi}\,i^l h_l^{(-)}(kr).$$

The following elegant relation holds:

$$\langle r|kl+\rangle = \frac{1}{2i}\left[\exp[2i\sigma_l]\langle r|kl\uparrow\rangle - \langle r|kl\downarrow\rangle\right], \tag{11}$$

which asymptotically becomes ($kr \to \infty$)

$$\langle r|kl+\rangle \sim \frac{\sqrt{2/\pi}}{2ikr}\left[\exp\left[ikr - i\gamma\ln(2kr) + 2i\sigma_l\right] - (-)^l\exp\left[-ikr + i\gamma\ln(2kr)\right]\right].$$

This corresponds completely with the short-range potential formalism. The equation corresponding to eq. (11) in momentum representation can be written down immediately, *i.e.*

$$\langle p|kl+\rangle = \frac{1}{2i}\left[\exp[2i\sigma_l]\langle p|kl\uparrow\rangle - \langle p|kl\downarrow\rangle\right].$$

In this manner we get a convenient standardization of conventions and notations.

3. – Partial-wave projections and expansions.

The main object of this section is to investigate the p.w. projections and the p.w. expansions plus the asymptotic convergence of $\psi_c^{(+)}$, ψ_t and ψ_s. For this purpose, explicit closed formulae will be derived for $\psi_l^{(+)}$, $\psi_{t,l}$ and $\psi_{s,l}$. These functions are defined according to eq. (7*a*). The following integral representations of the functions ${}_1F_1$ and U will be helpful ([6], Ch. VI 6.5):

$$(12) \qquad {}_1F_1(-i\gamma;\,1;\,z) = \frac{\exp[z]}{\Gamma(-i\gamma)\Gamma(1+i\gamma)}\int_0^1 \mathrm{d}t\,\exp[-zt]\,t^{i\gamma}(1-t)^{-1-i\gamma},$$

$$(13) \qquad U(-i\gamma,\,1,\,z) = \big(\exp[z]/\Gamma(-i\gamma)\big)\int_1^\infty \mathrm{d}t\,\exp[-zt]\,t^{i\gamma}(t-1)^{-1-i\gamma},$$

$$(14) \qquad U(1+i\gamma,\,1,\,z) = \big(1/\Gamma(1+i\gamma)\big)\int_0^\infty \mathrm{d}t\,\exp[-zt]\,t^{i\gamma}(1+t)^{-1-i\gamma}.$$

Insert these expressions into eqs. (1), (3) and (4) which give $\psi_c^{(+)}$, ψ_t and ψ_s, respectively. Apply then eq. (7*a*) and utilize eq. (13) for $\psi_{t,l}$, eq. (14) for $\psi_{s,l}$. This yields certain expressions for $\psi_l^{(+)}$, $\psi_{t,l}$ and $\psi_{s,l}$ which contain a double integral. The integration over $x \equiv \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}}$ is easily performed utilizing

$$(15) \qquad \int_{-1}^{1}\mathrm{d}x\,P_l(x)\exp[i\varrho t x] = 2i^l j_l(\varrho t)$$

with $\varrho \equiv kr$. Then one obtains successively

$$(16) \quad \psi_l^{(+)} = \big(\sqrt{2/\pi}\,i^l\exp[-\pi\gamma/2]/\Gamma(-i\gamma)\big)\int_0^1 \mathrm{d}t\,j_l(\varrho t)\exp\{i\varrho(1-t)]\,t^{i\gamma}(1-t)^{-1-i\gamma},$$

$$(17) \quad \psi_{t,l} = \big(\sqrt{2/\pi}\,i^l\exp[\pi\gamma/2]/\Gamma(-i\gamma)\big)\int_1^\infty \mathrm{d}t\,j_l(\varrho t)\exp[i\varrho(1-t)]\,t^{i\gamma}(t-1)^{-1-i\gamma},$$

$$(18) \quad \psi_{s,l} = \big(-\sqrt{2/\pi}\,i^{-l}\exp[\pi\gamma/2]/\Gamma(-i\gamma)\big)\int_0^\infty \mathrm{d}t\,j_l(\varrho t)\exp[i\varrho(1+t)]\,t^{i\gamma}(1+t)^{-1-i\gamma}.$$

Equation (16) is easily reduced with the help of formula 6.625.1 of ([7]). This

([7]) I. S. Gradshteyn and I. M. Ryzhik: *Table of Integrals, Series, and Products* (New York, N. Y., 1965).

yields the expected result

$$\psi_l^{(+)} = \langle r|kl+\rangle = \sqrt{2/\pi}\frac{i(-)^l}{2\varrho}\exp[-\pi\gamma/2]\Gamma(l+1+i\gamma)\mathcal{M}_{-i\gamma,l+\frac{1}{2}}(-2i\varrho)\,, \tag{19}$$

where $\mathcal{M}$ is Buchholz's ([8]) Whittaker function. This derivation is not essentially new. It differs only slightly from that given by MESSIAH ([1]), Ch. XI.10. The integral in eq. (17) can be expressed in terms of a known function with the help of formula 6.625.6 of ([7]). This yields an expression containing Meijer's G-function ([4]). Thus one obtains

$$\psi_{+,l} = \sqrt{2/\pi}\exp[\pi\gamma]\exp[i\varrho - i\gamma\ln(2\varrho)]G^{21}_{23}\left(2i\varrho\,\middle|\,\begin{matrix} i\gamma, & 0 \\ i\gamma, & i\gamma+l,\ i\gamma-l-1\end{matrix}\right). \tag{20}$$

A similar expression can be derived for $\psi_{-,l}$ from eq. (18). Most physicists will not consider Meijer's G-function to be a very «elementary» function. One should like to reduce it to a more transparent expression. We have not been able to perform that in a straightforward way. However, by splitting j_l occurring in eqs. (17) and (18) in the following well-known way:

$$j_l(\varrho) = \frac{1}{2i}\left(h_l^{(+)}(\varrho) - h_l^{(-)}(\varrho)\right), \tag{21}$$

one can obtain an elementary expression for $\psi_{+,l}$. We insert eq. (21) into eqs. (17) and (18) and introduce accordingly the functions ω and χ. That is, we put

$$\psi_{+,l} = \frac{1}{2i}(-\omega_{+,l} + \chi_{+,l})\,, \tag{22}$$

$$\psi_{-,l} = \frac{1}{2i}(\omega_{-,l} - \chi_{-,l})\,, \tag{23}$$

where the four new functions are defined by eqs. (17) and (18) with j_l replaced by $h_l^{(\pm)}$, see appendix A, eqs. (A.1)-(A.4). The fact that $h_l^{(\pm)}(\varrho)$ is equal to $\exp[\pm i\varrho]$ times a polynomial in $1/\varrho$ turns out to be very helpful. In appendix A we prove

$$\omega_{+,l} = \langle r|kl\downarrow\rangle = \sqrt{2/\pi}\exp[\pi\gamma/2]\frac{(-)^l}{\varrho}W_{i\gamma,l+\frac{1}{2}}(2i\varrho)\,, \tag{24}$$

$$\omega_{-,l} = \exp[2i\sigma_l]\langle r|kl\uparrow\rangle = \\ = \sqrt{2/\pi}\exp[\pi\gamma/2]\frac{\Gamma(l+1+i\gamma)}{\Gamma(l+1-i\gamma)}\frac{1}{\varrho}W_{-i\gamma,l+\frac{1}{2}}(-2i\varrho)\,, \tag{25}$$

$$\chi_l = \chi_{+,l} = \chi_{-,l} = \sqrt{2/\pi}\exp[\pi\gamma/2]\frac{\Gamma(2l+1)}{\Gamma(l+1-i\gamma)}\frac{\exp[i\varrho]}{\varrho}\left(\frac{i}{2\varrho}\right)^l \cdot \\ \cdot {}_2F_2(-l,\ i\gamma-l;\ -l,\ -2l;\ -2i\varrho)\,. \tag{26}$$

([8]) H. BUCHHOLZ: *The Confluent Hypergeometric Function* (Berlin, 1969).

In eq. (26) the notation

$$(27)\quad {}_2F_2(-l, i\gamma-l; -l, -2l; -2i\varrho) \equiv \lim_{\varepsilon\to 0} {}_2F_2(\varepsilon^3-l, i\gamma-l; \varepsilon-l, \varepsilon-2l; -2i\varrho)$$

for this truncated confluent hypergeometric series has been borrowed from ref. (4), p. 191. The irregular Whittaker function W is related to U according to

$$(28)\qquad W_{-i\gamma,l+\frac{1}{2}}(z) = \exp[-z/2]\, z^{l+1}\, U(l+1+i\gamma, 2l+2, z)\,.$$

At this point we have sufficient material to discuss the convergence of the p.w. series. As $\psi_{i,l}$ and $\psi_{s,l}$ allow a physical interpretation only for $\varrho\to\infty$, we restrict ourselves to their asymptotic behaviour, symbolically denoted by $\sim$. Our ${}_2F_2$ is a polynomial, so its asymptotic behaviour is just given by the highest power of ϱ. With the help of (cf. eq. (A.10))

$$(-2l)_n = (-)^n \Gamma(2l+1)/\Gamma(2l+1-n)\,,$$

we derive

$${}_2F_2(-l, i\gamma-l; -l, -2l; -2i\varrho) \sim \frac{\Gamma(i\gamma)(2i\varrho)^l}{\Gamma(i\gamma-l)\Gamma(2l+1)}\,,$$

and, utilizing

$$\Gamma(i\gamma-l)\Gamma(l+1-i\gamma) = (-)^l \Gamma(i\gamma)\Gamma(1-i\gamma)\,,$$

we find at once (cf. eq. (A.17))

$$(29)\qquad \chi_l(\varrho) \sim \sqrt{2/\pi}\, \frac{\exp[\pi\gamma/2]}{\Gamma(1-i\gamma)}\, \frac{\exp[i\varrho]}{\varrho}\,.$$

From eqs. (6) and (28) we get the asymptotic expansion of W, and thus eqs. (24) and (25) yield

$$(30)\qquad \omega_{i,l}(\varrho) \sim (-)^l \sqrt{2/\pi}\, \frac{1}{\varrho} \exp[-i\varrho + i\gamma \ln(2\varrho)]\,,$$

$$(31)\qquad \omega_{s,l}(\varrho) \sim \exp[2i\sigma_l] \sqrt{2/\pi}\, \frac{1}{\varrho} \exp[i\varrho - i\gamma \ln(2\varrho)]\,.$$

According to eq. (7) we multiply these p.w. functions by $P_l(x)\ (2l+1)/(4\pi)$ and sum over l (x denoting $\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}}$ as before). The l-dependence in eqs. (29)-(31) is very simple. The well-known completeness relations of the spherical harmonics

$$\sum_{l,m} Y^*_{lm}(\hat{\boldsymbol{r}})\, Y_{lm}(\hat{\boldsymbol{k}}) = \delta(\hat{\boldsymbol{r}}, \hat{\boldsymbol{k}})\,,$$

with self-evident notation, implies

$$\sum_{l=0}^{\infty}(l+\tfrac{1}{2})\,P_l(x)=\delta(1-x)\,. \tag{32}$$

Because $P_l(-x)=(-)^lP_l(x)$ one has

$$\sum_{l=0}^{\infty}(-)^l(l+\tfrac{1}{2})\,P_l(x)=\delta(1+x)\,. \tag{33}$$

Equations (32) and (33) give the summation of the χ_l's and of the $\omega_{s,l}$'s. Eventually we have to evaluate the sum of the $\omega_{s,l}$'s whose l-dependence is asymptotically given by $\exp[2i\sigma_l]$. Now TAYLOR [2] has shown that the sum

$$\sum_{l=0}^{\infty}(l+\tfrac{1}{2})\,P_l(x)\exp[2i\sigma_l] \tag{34}$$

is divergent, considered in the sense of ordinary (δ-function) distributions. TAYLOR introduced test functions $q(x)$ that satisfy

$$q\in C^2[-1,1]\,, \qquad q(1)=0. \tag{35}$$

That is, q is twice continuously differentiable and $q(x)$ vanishes in the forward direction ($x=1:\hat{\boldsymbol{r}}=\hat{\boldsymbol{k}}$). The use of these test functions is physically quite plausible (as discussed in detail by TAYLOR) because measurement in the strict forward direction has no meaning. Let us denote by the symbol $\mathscr{D}$ what we consider distributions defined on Taylor's test functions. Then

$$\delta(1-x)=0,\mathscr{D}, \tag{36}$$

and this in turn means that the summation of the χ_l's yields zero (cf. eqs. (29) and (32)). TAYLOR [2] has proven also that the summation of $\exp[2i\sigma_l]$ in the sense of his distribution gives the Coulomb-scattering amplitude f^{C}. To be precise, he proved

$$\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\,P_l(x)\exp[2i\sigma_l]=\frac{ik}{2\pi}f^{\mathrm{C}}(x),\ \mathscr{D} \tag{37}$$

with

$$f^{\mathrm{C}}(x)=-\frac{\gamma}{2k}\exp[2i\sigma_0]\left(\frac{1-x}{2}\right)^{-1-i\gamma}. \tag{38}$$

Application of all this to eqs. (22) and (23) yields

$$(39)\qquad \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}})\,\psi_{t,l}(kr)\sim\delta(\hat{\boldsymbol{r}},-\hat{\boldsymbol{k}})\sqrt{2/\pi}\,\frac{i}{2kr}\exp[-ikr+i\gamma\ln(2kr)],\mathscr{L},$$

$$(40)\qquad \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}})\,\psi_{s,l}(kr)\sim f^{c}(\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{k}})\sqrt{2/\pi}\,\frac{1}{4\pi r}\exp[ikr-i\gamma\ln(2kr)],\mathscr{L}.$$

One expects that the l.h.s. of eq. (39) be equal to $\psi_t(\boldsymbol{k},\boldsymbol{r})$ and that the l.h.s. of eq. (40) be equal to $\psi_s(\boldsymbol{k},\boldsymbol{r})$. One can check that this is asymptotically correct, in the following (customary) way. Apply eq. (6) directly to eqs. (3) and (4). Because asymptotic expansion then means $kr-\boldsymbol{k}\cdot\boldsymbol{r}\to\infty$, one has to exclude the forward direction in that approach, too. The use of

$$(41)\qquad (2\pi)^{-\frac{1}{2}}\exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\sim\frac{\sqrt{2/\pi}}{2ikr}[\delta(\hat{\boldsymbol{r}},\hat{\boldsymbol{k}})\exp[ikr]-\delta(\hat{\boldsymbol{r}},-\hat{\boldsymbol{k}})\exp[-ikr]]$$

plus eqs. (35) and (36) then gives the desired result, namely $\psi_t(\boldsymbol{k},\boldsymbol{r})$ is asymptotically equal to the r.h.s. of eq. (39) and $\psi_s(\boldsymbol{k},\boldsymbol{r})$ to the r.h.s. of eq. (40). Although this derivation was not the object of this section, it shows the consistency of our approach.

The appearance of the functions χ_l may seem peculiar, for they are no solutions of the p.w. Schrödinger equation (this fact can be derived from their asymptotic behaviour). Because $\omega_{t,l}$ and $\omega_{s,l}$ are known to be solutions, it follows (cf. eqs. (22) and (23)) that $\psi_{t,l}$ and $\psi_{s,l}$ are no solutions of the p.w. Schrödinger equation, either. These latter are the p.w. projections of ψ_t and ψ_s which are well-known solutions of the three-dimensional Schrödinger equation. The reader who distrusts those χ_l's is advised to consult eqs. (B.1)-(B.6) where a very simple derivation of $\chi_{l=0}$ is given, and where it is clearly demonstrated that $\chi_{l=0}$ is no solution of the p.w. Schrödinger equation.

The solution of the above problem can be found in the well-known fact that the irregular functions are no eigenfunctions of the Hamiltonian H, though they are solutions of the differential equation which is derived from the abstract Schrödinger equation $H\psi=k^2\psi$. More precisely, it is known ([1] p. 496) that the operator identity

$$(42)\qquad \Delta=\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r-\frac{\boldsymbol{L}^2}{r^2}$$

holds for any function finite at the point $r=0$. Because the irregular functions are singular at the origin, eq. (42) need not be valid for these functions. See also Chap. IX.2 of ref. ([1]). If we recall that $H=-\Delta+V$, then

([9]) R. G. NEWTON: *Scattering Theory of Waves and Particles* (New York, N. Y., 1966).

it becomes clear that the χ_l's need not be solutions of the p.w. Schrödinger equation. Cf. ref. (9), pp. 329, 330.

A parallel can be found in the following. Since $|kl+\rangle$ is an eigenstate of H, one has

$$H|kl+\rangle = k^2|kl+\rangle\,. \tag{43}$$

Now consider this equation in momentum representation. Take for simplicity $V=0$. Then $H \to p^2$, $|kl+\rangle \to |kl\rangle$ and eq. (43) becomes

$$(p^2-k^2)\langle p|kl\rangle = 0\,,$$

which is correct since $\langle p|kl\rangle = \delta(p-k)/k^2$. On the other hand, we find for $|kl\uparrow\rangle$ in momentum representation ($V=0$)

$$\langle p|kl\uparrow\rangle = (2/\pi)\int_0^\infty \mathrm{d}r\, r^2 j_l(pr) h_l^{(+)}(kr) = \frac{2}{\pi k}\,\frac{(p/k)^l}{p^2-(k+i\varepsilon)^2}\,, \qquad \varepsilon \downarrow 0\,, \tag{44}$$

with the help of formulae 6.521.2 and 8.407.1 of (7) and eq. (A.5). This makes clear that $|kl\uparrow\rangle$ is no eigenstate of H:

$$H|kl\uparrow\rangle \neq k^2|kl\uparrow\rangle\,. \tag{45}$$

The same statement holds for $|kl\downarrow\rangle$. It is expected that eq. (45) be valid for all potentials $V \neq 0$ for which $|kl\uparrow\rangle$ can be defined.

Finally we consider the regular and irregular functions discussed in this section for vanishing potential strength, *i.e.* $\gamma \to 0$. According to (8), p. 23 we have

$$W_{c/2,(c-1)/2}(z) = M_{c/2,(c-1)/2}(z) = z^{c/2}\exp[-z/2]\,,$$

and so (cf. eq. (28))

$$U(0, c, z) \equiv {}_1F_1(0; c; z) \equiv 1\,. \tag{46}$$

Insertion of eq. (46) into eqs. (1)-(4) shows that when $\gamma \to 0$

$$\psi_C^{(+)},\ \psi_i \to \langle \boldsymbol{r}|\boldsymbol{k}\rangle = (2\pi)^{-\frac{3}{2}}\exp[i\boldsymbol{k}\cdot\boldsymbol{r}]\,, \tag{47}$$

$$\psi_s \quad \to 0\,. \tag{48}$$

Furthermore we find

$$\omega_{i,l} \to \sqrt{2/\pi}\, i^l h_l^{(-)}\,,$$
$$\omega_{s,l} \to \sqrt{2/\pi}\, i^l h_l^{(+)}\,,$$
$$\chi_l \quad \to \sqrt{2/\pi}\, i^l h_l^{(+)}\,,$$

so

$$\psi_l^{(+)},\ \psi_{i,l} \to \langle r|kl\rangle = \sqrt{2/\pi}\, i^l j_l(kr)\,, \tag{49}$$

$$\psi_{s,l} \to 0\,. \tag{50}$$

Equations (49) and (50) show the expected fact that the scattered part $\psi_{s,l}$ vanishes when the potential vanishes, and that the incoming part $\psi_{i,l}$ then becomes equal to the free state $\langle r|kl\rangle$. Without the functions χ_l one would obtain unacceptable results in the limit when $\gamma \to 0$, *e.g.* $\psi_{s,l}$ would not vanish.

4. – A different splitting of the scattering wave function.

Although the separation of the regular Coulomb-scattering wave function $\psi_C^{(+)}(\boldsymbol{k}, \boldsymbol{r}) \equiv \langle \boldsymbol{r}|\boldsymbol{k}+\rangle_C$ into ψ_i and ψ_s *is asymptotically satisfactory* (from ψ_s, $r \to \infty$, the scattering amplitude is usually derived), this separation is not in all respects the most natural one. In the nonasymptotic region, neither ψ_i nor ψ_s has a clear physical meaning. Recall that both are singular at the origin (cf. eqs. (3)-(5)).

There exists a different separation of $\langle \boldsymbol{r}|\boldsymbol{k}+\rangle_C$ into an incoming and a scattered part. In ref. [3] we defined Coulombian asymptotic states, in momentum representation denoted by $\langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle_C$. The following equality has been proved [3] (subscript C suppressed):

$$\langle \boldsymbol{p}|\boldsymbol{k}+\rangle = \langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle + \langle \boldsymbol{p}|G_0 V|\boldsymbol{k}+\rangle\,. \tag{51}$$

Here G_0 has argument $(k + i\varepsilon)^2$, $\varepsilon \downarrow 0$. Equation (51) has the form of a generalized Lippmann-Schwinger equation. The asymptotic states may be considered as generalized distributions. The pure Coulomb T-matrix with argument $(k + i\varepsilon)^2$ can serve as a « test function » on which $|\boldsymbol{k}\infty\rangle$ can be properly defined. The fact that $\langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle$ is not an ordinary function need not be disturbing. Recall that the scattering state $\langle \boldsymbol{p}|\boldsymbol{k}+\rangle$ is always a distribution. In co-ordinate representation we have the counterpart of eq. (51)

$$\langle \boldsymbol{r}|\boldsymbol{k}+\rangle = \langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle + \langle \boldsymbol{r}|G_0 V|\boldsymbol{k}+\rangle\,. \tag{52}$$

We remark that this equation seems to conflict with a statement by WEST [10], namely that the Coulomb-scattering wave function is a solution of the homogeneous Lippmann-Schwinger equation. We shall have occasion to discuss this point in a subsequent paper.

It would be interesting to obtain some simple explicit formula for $\langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle$.

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[10] G. B. WEST: *Journ. Math. Phys.*, **8**, 942 (1967).

However, the integral representation $\int d\boldsymbol{p}\langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle$ is not very transparent. We get an idea about the structure of $\langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle$ by observing that

$$(\boldsymbol{p}-\boldsymbol{k})|\boldsymbol{k}\infty\rangle = 0\,. \tag{53}$$

It implies that $|\boldsymbol{k}\infty\rangle$ is a certain generalized improper eigenstate of the momentum operator $\boldsymbol{p}$. The state $\langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle$ is « very similar » to the delta-function $\delta(\boldsymbol{p}-\boldsymbol{k}) = \langle \boldsymbol{p}|\boldsymbol{k}\rangle$, and $\langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle$ is « very similar » to the plane wave $\langle \boldsymbol{r}|\boldsymbol{k}\rangle$. From the explicit expression for $\langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle$ it follows [3] that it contains a certain distortion at $p = k$. Consequently we expect in co-ordinate representation a certain distortion at $r = \infty$. This explains why we can call $\langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle$ an « asymptotically Coulomb-modified improper free state » or, abbreviated, « asymptotic state ».

On account of eq. (53) it looks plausible that $|\boldsymbol{k}\infty\rangle$ contain (almost) no information on the scattering process, and that $G_0V|\boldsymbol{k}+\rangle$ contain therefore (almost) all the scattering information. Moreover we have from [3]

$$G_0V|\boldsymbol{k}+\rangle = G_0T|\boldsymbol{k}\infty\rangle \tag{54}$$

and

$$\langle \boldsymbol{k}'\infty - |T|\boldsymbol{k}\infty\rangle = -f^{\mathrm{C}}(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{k}}')/(2\pi^2)\,, \qquad k' = k. \tag{55}$$

Here f^{C} is the Coulomb-scattering amplitude (cf. eq. (38)), G_0 and T have argument $(k+i\varepsilon)^2$, $\varepsilon \downarrow 0$, and $\langle \boldsymbol{p}|\boldsymbol{k}\infty -\rangle$ is the complex conjugate of $\langle \boldsymbol{p}|\boldsymbol{k}\infty\rangle$ (which is, written more completely, $\langle \boldsymbol{p}|\boldsymbol{k}\infty +\rangle$). Equations (52)-(55) show that $\langle \boldsymbol{r}|G_0V|\boldsymbol{k}+\rangle$ is a proper candidate for the scattered part of $\langle \boldsymbol{r}|\boldsymbol{k}+\rangle$.

For vanishing potential strength we get

$$\lim_{\gamma\to 0}|\boldsymbol{k}\infty\rangle = |\boldsymbol{k}\rangle\,, \tag{56}$$

$$\lim_{\gamma\to 0} G_0V|\boldsymbol{k}+\rangle = 0\,, \tag{57}$$

in agreement with the corresponding short-range formulae.

5. – Summary and discussion.

We obtained in sect. 3 the p.w. projections of $\psi_0^{(+)}$, ψ_i and ψ_s in closed form. See eqs. (22)-(27). An unexpected feature is the appearance of the functions

$$\chi_l(\varrho) = \sqrt{2/\pi}\exp[\pi\gamma/2]\frac{\Gamma(2l+1)}{\Gamma(l+1-i\gamma)}\frac{\exp[i\varrho]}{\varrho}\left(\frac{i}{2\varrho}\right)^l\cdot$$

$$\cdot {}_2F_2(-l, i\gamma-l; -l, -2l; -2i\varrho)\,.$$

These χ_l's are no solutions of the p.w. Schrödinger equation and therefore $\psi_{r,l}$ and $\psi_{s,l}$ are no solutions, although ψ_r and ψ_s are solutions of the three-dimensional Schrödinger equation. There is no contradiction (though it might seem so) because the irregular functions are no eigenfunctions of the Hamiltonian. Apparently they have no physical interpretation. This is discussed at the end of sect. **3**.

We considered the asymptotic behaviour of all occurring functions. The p.w. series are then convergent in the sense of Taylor's distribution ([2]). We found that the p.w. series of the $\psi_{s,l}$'s converges asymptotically to an outgoing distorted spherical wave times the Coulomb-scattering amplitude. This agrees completely with the asymptotic behaviour of the three-dimensional functions ψ_s.

The conclusion we draw from sect. **3** is that the splitting of the physical scattering wave function into two so-called irregular solutions is unsatisfactory. This is already clear from the singular behaviour at the origin of the irregular functions, but the investigation made in sect. **3** reinforces the conclusion.

In sect. **4** we discussed a generalized Lippmann-Schwinger equation for the Coulomb-scattering state in co-ordinate representation, presenting a different and more satisfactory splitting of $\psi_C^{(+)}$ into an incoming part and a scattered part.

Eventually we should like to review these results in a more general context.

It is likely that for other (local) potentials V the three-dimensional scattering wave function can be split up into two irregular solutions of the Schrödinger equation. If this is true, then the present paper suggests that their p.w. projections will turn out to be no solutions of the p.w. Schrödinger equation. However, apart from the Coulomb case no closed formulae seem to be known to check this.

In p.w. space, it follows from the theory of ordinary second-order differential equations that the p.w. Schrödinger equation for a local potential V has (in general) two linearly independent irregular solutions, each with prescribed asymptotic behaviour. There exists just one regular combination of these two. Let us denote these functions by $\langle r|kl\uparrow\rangle_V$, $\langle r|kl\downarrow\rangle_V$ and $\langle r|kl+\rangle_V$, respectively. In analogy with the splitting of the three-dimensional wave function, one has then the splitting (cf. eq. (11))

$$\langle r|kl+\rangle_V = \frac{1}{2i}\left[\exp\left[2i\delta_l(k)\right]\langle r|kl\uparrow\rangle_V - \langle r|kl\downarrow\rangle_V\right], \tag{58}$$

provided that the normalization is appropriate.

Now if V has short range, it is known that $\langle r|kl\uparrow\rangle_V$ and $\langle r|kl\downarrow\rangle_V$ approximate (up to a constant) the « free waves » $h_l^{(\pm)}(kr)$ when $kr \to \infty$. This suggests already that one can split off the free state $\langle r|kl\rangle$, which is then interpreted as the « incoming part », and that the remaining term can be interpreted as the « scattered part ». In this way one obtains an intuitive picture of the p.w.

Lippman-Schwinger equation:

$$\langle r|kl+\rangle_V = \langle r|kl\rangle + \langle r|G_0 V|kl+\rangle_V . \tag{59}$$

When V has long range (*e.g.* the Coulomb potential), eq. (58) still holds but $\langle r|kl\uparrow\rangle_V$ and $\langle r|kl\downarrow\rangle_V$ do not approximate the free waves $h_l^{(\pm)}(kr)$ asymptotically. This suggests that eq. (59) might be not valid then, which is indeed the case for the Coulomb potential. So one has then only the splitting of eq. (58) and this lacks a clear physical interpretation.

The equation:

$$\langle \boldsymbol{r}|\boldsymbol{k}+\rangle_C = \langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle_C + \langle \boldsymbol{r}|G_0 V_C|\boldsymbol{k}+\rangle_C , \tag{52'}$$

where the subscript C for Coulomb is written for this occasion, should be compared with the standard Lippman-Schwinger equation

$$\langle \boldsymbol{r}|\boldsymbol{k}+\rangle_V = \langle \boldsymbol{r}|\boldsymbol{k}\rangle + \langle \boldsymbol{r}|G_0 V|\boldsymbol{k}+\rangle_V , \tag{60}$$

valid for a short-range potential V. To emphasize the analogy, we remark that in eq. (60) $\langle \boldsymbol{r}|\boldsymbol{k}\rangle$ could be replaced by $\langle \boldsymbol{r}|\boldsymbol{k}\infty\rangle_V$, the asymptotic state belonging to V, but these two states are identical if V has short range.

From the physical point of view, a splitting like $\psi_C^{(+)} = \psi_i + \psi_s$, or as in eq. (58), is artificial, though it has been proven very useful in mathematical considerations. The splitting in eqs. (52') and (60) admits a satisfactory physical interpretation. See [3] and the connection with time-dependent Coulomb-scattering theory shown there.

* * *

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APPENDIX A

In this Appendix the expressions for $\omega_{i,l}$, $\omega_{s,l}$, $\chi_{i,l}$ and $\chi_{s,l}$ given in eqs. (24)-(26) will be proved. The p.w. projections of ψ_i and ψ_s have been expressed in eqs. (22) and (23) as

$$\psi_{i,l} = \frac{1}{2i}(-\omega_{i,l} + \chi_{i,l}),$$

$$\psi_{s,l} = \frac{1}{2i}(\omega_{s,l} - \chi_{s,l}) .$$

According to eqs. (17), (18) and (21), the functions ω and χ can and will be defined by

$$\text{(A.1)}\quad \omega_{i,l} = (\sqrt{2/\pi}\, i^l \exp[\pi\gamma/2]/\Gamma(-i\gamma))\int_1^\infty \mathrm{d}t\, h_l^{(-)}(\varrho t)\exp[i\varrho(1-t)]t^{i\gamma}(t-1)^{-1-i\gamma},$$

$$\text{(A.2)}\quad \chi_{s,l} = (\sqrt{2/\pi}\, i^l \exp[\pi\gamma/2]/\Gamma(-i\gamma))\int_1^\infty \mathrm{d}t\, h_l^{(+)}(\varrho t)\exp[i\varrho(1-t)]t^{i\gamma}(t-1)^{-1-i\gamma},$$

$$\text{(A.3)}\quad \chi_{s,l} = (-\sqrt{2/\pi}\, i^{-l}\exp[\pi\gamma/2]/\Gamma(-i\gamma))\int_0^\infty \mathrm{d}t\, h_l^{(-)}(\varrho t)\exp[i\varrho(1+t)]t^{i\gamma}(1+t)^{-1-i\gamma},$$

$$\text{(A.4)}\quad \omega_{s,l} = (-\sqrt{2/\pi}\, i^{-l}\exp[\pi\gamma/2]/\Gamma(-i\gamma))\int_0^\infty \mathrm{d}t\, h_l^{(+)}(\varrho t)\exp[i\varrho(1+t)]t^{i\gamma}(1+t)^{-1-i\gamma}.$$

To ensure convergence of the integrals, the real part of $i\gamma$ has to satisfy certain conditions. These conditions can be relaxed by means of analytical continuation. Now we start with the successive evaluation of the four expressions in eqs. (A.1)-(A.4).

i) First, consider eq. (A.1). The integral there can be expressed in terms of Whittaker's function W, utilizing formula 6.625.10 of (7), in combination with (cf. formula 8.407.1 of (7))

$$K_\nu(i\varrho x) = \tfrac{1}{2}i\pi\exp[\tfrac{1}{2}i\pi\nu]H_\nu^{(1)}(-\varrho x)\,.$$

The relation between the Hankel function $H_{l+\frac{1}{2}}^{(1)}$ and the spherical Hankel functions $h_l^{(1)}$ and $h_l^{(+)}$ is given by (cf. app. B.6 of (1))

$$\text{(A.5)}\qquad h_l^{(+)}(z) = ih_l^{(1)}(z) = i(2z/\pi)^{-\frac{1}{2}}H_{l+\frac{1}{2}}^{(1)}(z)\,,$$

and $h_l^{(-)}$ follows from

$$\text{(A.6)}\qquad h_l^{(\pm)}(-z) = (-)^{l+1}h_l^{(\mp)}(z)\,.$$

Utilizing all this, one obtains (the condition $\mathrm{Re}\, i\varrho > 0$ which has to be met mplies $\sqrt{-\varrho} = i\varrho$)

$$\text{(A.7)}\qquad \int_1^\infty \mathrm{d}t\, h_l^{(-)}(\varrho t)\exp[-i\varrho t]t^{i\gamma}(t-1)^{-1-i\gamma} = i^l\Gamma(-i\gamma)\exp[-i\varrho]/\varrho W_{i\gamma,l+\frac{1}{2}}(2i\varrho).$$

The substitution of eq. (A.7) in eq. (A.1) gives at once

$$\omega_{i,l} = \sqrt{2/\pi}\exp[\pi\gamma/2](-)^l/\varrho W_{i\gamma,l+\frac{1}{2}}(2i\varrho) = \langle r|kl\downarrow\rangle = (-)^l\langle r|kl\uparrow\rangle^*\,,$$

which is just eq. (24).

ii) Next we have to reduce the integral in eq. (A.2). We utilize the fact that $h_l^{(+)}(z)$ is equal to $\exp[iz]$ times a polynomial of $1/z$ (cf. eq. (B.50) of (1)).

The exponential factor $\exp[-i\varrho t]$ in the integrand of the integral in eq. (A.2) then cancels and the remaining integral can be evaluated term by term.

According to eq. (A.5) and [8], p. 214, the following equality holds:

$$h_l^{(\pm)}(z) = l!(-2z)^{-l}\exp[\pm iz]/z\, L_l^{(-2l-1)}(\mp 2iz)\,. \tag{A.8}$$

Here $L_l^{(\alpha)}$ is the generalized Laguerre polynomial which can be expressed in terms of a confluent hypergeometric function

$$L_l^{(\alpha)}(z) = \binom{l+\alpha}{l} {}_1F_1(-l;\, 1+\alpha;\, z)\,. \tag{A.9}$$

Note that Messiah's ([1], eq. (B.13)) $L_l^{(\alpha)}$ *is* $(l+\alpha)!$ *times the r.h.s. of* eq. (A.9). The symbol $\binom{l+\alpha}{l}$ stands for $(1+\alpha)_l/l!$, where $(1+\alpha)_l$ is Pochhammer's symbol. When α is equal to $-2l-1$, it is preferable to write this expression as

$$(1+\alpha)_l = (-)^l\Gamma(-\alpha)/\Gamma(-\alpha-l)\,, \tag{A.10}$$

and thus one obtains

$$L_l^{(-2l-1)}(z) = (-)^l\binom{2l}{l} {}_1F_1(-l;\, -2l;\, z)\,. \tag{A.11}$$

One should realize that in eq. (A.11) the following convention is tacitly understood (cf. eq. (A.15)):

$${}_1F_1(-l;\, -2l;\, z) := \lim_{\varepsilon\to 0} {}_1F_1(\varepsilon^2 - l;\, \varepsilon - 2l;\, z)\,, \tag{A.12}$$

so the Taylor expansion of this ${}_1F_1$ is

$${}_1F_1(-l;\, -2l;\, z) = \sum_{n=0}^{l}(-l)_n/(-2l)_n z^n/n!\,.$$

Utilizing the above relations, we convert the integral in the r.h.s. of eq. (A.2) into

$$\int_1^\infty \ldots \text{ in eq. (A.2)} = \frac{(2l)!}{l!}\frac{\exp[i\varrho]}{\varrho(2\varrho)^l}\int_1^\infty dt \sum_{n=0}^{l}\frac{(-l)_n}{(-2l)_n}\frac{(-2i\varrho t)^n}{n!}t^{i\gamma-l-1}(t-1)^{-1-i\gamma}\,.$$

The finite summation may, of course, be interchanged with the integration. Finally we apply formula 3.191.2 of [7]

$$\int_1^\infty dt\, t^{i\gamma-m}(t-1)^{-1-i\gamma} = B(m, -i\gamma)\,, \tag{A.13}$$

where B denotes the beta-function. Then the integral becomes

$$\text{(A.14)} \qquad \int_1^\infty \ldots = \frac{\Gamma(-i\gamma)\Gamma(2l+1)}{\Gamma(l+1-i\gamma)} \frac{\exp[i\varrho]}{\varrho(2\varrho)^l} \sum_{n=0}^{l} \frac{(i\gamma-l)_n}{(-2l)_n} \frac{(-2i\varrho)^n}{n!} .$$

The finite sum here is a truncated confluent hypergeometric series, which we denote by a ${}_2F_2$:

$$\text{(A.15)} \qquad \sum_{n=0}^{l} \frac{(i\gamma-l)_n}{(-2l)_n} \frac{(-2i\varrho)^n}{n!} \to {}_2F_2(-l, i\gamma-l; -l, -2l; -2i\varrho)$$
$$\lim_{\varepsilon\to 0} {}_2F_2(\varepsilon-l, i\gamma-l; \varepsilon-l, \varepsilon-2l; -2i\varrho) .$$

We borrowed this notation from ref. (4), p. 191. The substitution of eqs. (A.14) and (A.15) in eq. (A.2) yields the desired result, cf. eq. (26).

We point out that the hypergeometric function ${}_2F_2$ in eq. (A.15) can be written in terms of a different hypergeometric function ${}_3F_1$. After the replacement of the summation variable n in eq. (A.15) by $m \quad l-n$, we derive

$$\text{(A.16)} \qquad {}_2F_2(-l, i\gamma-l; -l, -2l; z) =$$
$$= \frac{\Gamma(l+1-i\gamma)}{\Gamma(1-i\gamma)} \frac{z^l}{\Gamma(2l+1)} {}_3F_1(-l, l+1, 1; 1-i\gamma; -1/z) .$$

The substitution of this equality in eq. (26) yields the following simple expression for χ_l:

$$\text{(A.17)} \qquad \chi_l(\varrho) = \sqrt{2/\pi} \frac{\exp[\pi\gamma/2]}{\Gamma(1-i\gamma)} \frac{\exp[i\varrho]}{\varrho} {}_3F_1\left(-l, l+1, 1; 1-i\gamma; \frac{1}{2i\varrho}\right) .$$

iii) We proceed with the evaluation of the integral on the r.h.s. of eq. (A.3). After the substitution of eqs. (A.8) and (A.11) this integral becomes

$$\int_0^\infty \ldots \text{ in eq. (A.3)} = (2l)!/l!\,(2\varrho)^{-l} \exp[i\varrho]/\varrho \cdot$$
$$\cdot \int_0^\infty \mathrm{d}t \sum_{n=0}^{l} \frac{(-l)_n}{(-2l)_n} \frac{(2i\varrho t)^n}{n!} t^{i\gamma-l-1}(1+t)^{-1-i\gamma} .$$

In place of eq. (A.13) we now resort to formula 3.194.3 of (7)

$$\int_0^\infty \mathrm{d}t\, t^{i\gamma+n-l-1}(1+t)^{-1-i\gamma} = B(n-l+i\gamma, l+1-n) .$$

With the help of the equalities

$$\Gamma(n-l+i\gamma) = \Gamma(i\gamma-l)(i\gamma-l)_n ,$$
$$(-l)_n = (-)^n \Gamma(l+1)/\Gamma(l+1-n) ,$$

we find for the integral on the r.h.s. of eq. (A.3) the expression

$$\int_0^\infty \ldots = \frac{\Gamma(i\gamma-l)\Gamma(2l+1)}{\Gamma(1+i\gamma)} \frac{\exp[i\varrho]}{\varrho(2\varrho)^l} \sum_{n=0}^{\infty} \frac{(i\gamma-l)_n}{(-2l)_n} \frac{(-2i\varrho)^n}{n!} .$$

The finite sum on the r.h.s. here is the same ${}_2F_2$ we have defined in eq. (A.15). Insertion of the above expression into eq. (A.3) gives the desired result, *i.e.* it proves eq. (26).

iv) Finally we have to prove eq. (25). To derive the expression given there for $\omega_{s,l}$, it is not necessary to reduce eq. (A.4). Consider eqs. (22) and (23). By virtue of eq. (26) which has just been proved, we have $\chi_{c,l} - \chi_{s,l} = 0$, and therefore

$$\psi_{c,l} + \psi_{s,l} = \psi_l^{(+)} = \langle r|kl+\rangle = \frac{1}{2i}(\omega_{s,l} - \omega_{c,l}) . \tag{A.18}$$

We have already obtained closed formulae for $\psi_l^{(+)}$ and for $\omega_{c,l}$ (cf. eqs. (19) and (24)). By means of these expressions, the required result for $\omega_{s,l}$ can be obtained from eq. (A.18) in the following way.

The expression for $\psi_l^{(+)}$ given in eq. (19) contains the function $\mathscr{M}$. One can express $\mathscr{M}$ in terms of Whittaker's function W (cf. [8], p. 19, eq. (20*a*))

$$\mathscr{M}_{-i\gamma,l+\frac{1}{2}}(-2i\varrho) = M_{-i\gamma,l+\frac{1}{2}}(-2i\varrho)/\Gamma(2l+2) = \exp[\pi\gamma/2] \cdot \left[\frac{1}{\Gamma(l+1+i\gamma)} W_{i\gamma,l+\frac{1}{2}}(2i\varrho) - \frac{(-)^l}{\Gamma(l+1-i\gamma)} W_{-i\gamma,l+\frac{1}{2}}(-2i\varrho)\right] . \tag{A.19}$$

We insert eq. (A.19) into eq. (19) and find

$$\langle r|kl+\rangle = \psi_l^{(+)}(\varrho) = \sqrt{2/\pi}\exp[\pi\gamma/2]/(2i\varrho) \cdot \left[\frac{\Gamma(l+1+i\gamma)}{\Gamma(l+1-i\gamma)} W_{-i\gamma,l+\frac{1}{2}}(-2i\varrho) - (-)^l W_{i\gamma,l+\frac{1}{2}}(2i\varrho)\right] . \tag{A.20}$$

The second term of the expression in brackets here yields an expression equal to $-\omega_{c,l}/(2i)$, according to eq. (24). Comparing with eq. (A.18), we see that the first term will give then $\omega_{s,l}/(2i)$. The expression we get in this way for $\omega_{s,l}$ is just equal to the r.h.s. of eq. (25) and the proof is complete.

In appendix B we shall give a very simple proof of eqs. (24)-(26) in the particular case $l = 0$, and a different, independent proof of eqs. (24) and (25) valid for all $l = 0, 1, \ldots$.

Appendix B

Because the derivation of eqs. (24)-(26) in appendix A is rather involved, though straightforward, it may be interesting to have a second proof. In this appendix such a proof will be provided for eqs. (24) and (25). As a by-product,

we shall find certain equalities that are interesting in their own right, see eqs. (B.7), (B.8), (B.10), (B.15) and (B.16).

First we give a very simple proof of eqs. (24), (25) and (26) for the case $l=0$. Remembering that $P_0=1$ one has to evaluate ($x=\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}$)

$$\int_{-1}^{1}\mathrm{d}x\,\exp\left[i\varrho x\right]U(-i\gamma,1,i\varrho(1-x))$$

and

$$\int_{-1}^{1}\mathrm{d}x\,U(1+i\gamma,1,i\varrho(x-1))\,,$$

according to eqs. (3), (4) and (7*a*). Utilizing the general relations (cf. [5], p. 266)

$$\text{(B.1)}\qquad \frac{\mathrm{d}}{\mathrm{d}z}\left[zU(a,2,z)\right]=(1-a)\,U(a,1,z)\,,$$

$$\text{(B.2)}\qquad \frac{\mathrm{d}}{\mathrm{d}z}\left[z\exp\left[-z\right]U(a+1,2,z)\right]=-\exp\left[-z\right]U(a,1,z)$$

and ([5], p. 288)

$$\text{(B.3)}\qquad U(a,2,z)=\frac{1}{z\Gamma(a)}+\mathcal{O}(|\ln z|)\,,\qquad z\to 0\,,$$

one confirms eqs. (24)-(26) for $l=0$ at once, *i.e.* (cf. eqs. (22), (23) and (28))

$$\text{(B.4)}\quad \omega_{i,l=0}=2i\sqrt{2/\pi}\exp\left[\pi\gamma/2\right]\exp\left[-i\varrho\right]U(1-i\gamma,2,2i\varrho)\,,$$

$$\text{(B.5)}\quad \omega_{s,l=0}=-2i\sqrt{2/\pi}\exp\left[\pi\gamma/2\right]\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\exp\left[i\varrho\right]U(1+i\gamma,2,-2i\varrho)\,,$$

$$\text{(B.6)}\quad \chi_{l=0}=\sqrt{2/\pi}\,\frac{\exp\left[\pi\gamma/2\right]}{\Gamma(1-i\gamma)}\,\frac{\exp\left[i\varrho\right]}{\varrho}\,.$$

It is easy to see that $\exp\left[ikr\right]/r$ is a solution of the $l=0$ p.w. Schrödinger equation without the Coulomb potential, *i.e.* $-(r\chi)''=k^2(r\chi)$ (recall that $\varrho\equiv kr$). This implies that $\chi_{l=0}$ is no solution of the $l=0$ p.w. Schrödinger equation including the Coulomb potential.

The general (second) proof of eqs. (24) and (25) runs as follows. From eqs. (A.8) and (A.11) we have the following convenient expression for Hankel's spherical functions:

$$h_l^{(\pm)}(z)=\left((2l)!/l!\,(2z)^{-l}\right)\left(\exp\left[\pm iz\right]/z\right){}_1F_1(-l;-2l;\mp 2iz)\,.$$

Replacing the summation variable n, arising from the expansion of ${}_1F_1$, by $m\equiv l-n$, we derive (cf. [6], p. 257 (3))

$$h_l^{(\pm)}(z)=i^{\mp l}z^{-1}\exp\left[\pm iz\right]{}_2F_0(-l,l+1;\mp i/(2z))=i^{\mp l}z^{-1}W_{0,l+\frac{1}{2}}(\mp 2iz)\,.$$

Now insert the expression containing the h.f. ${}_2F_0$ into eqs. (A.1) and (A.4), respectively. Utilize further formula 3.384.3 of (7), p. 320 (corrected for the misprint: $2\varrho 1$ must be $2\varrho - 1$). Then eqs. (A.1) plus (24) yield

$$W_{i\gamma,l+\frac{1}{2}}(z) = \sum_{m=0}^{l} \frac{(l+m)!}{(l-m)!} \frac{z^{-\frac{1}{2}m}}{m!} W_{i\gamma-\frac{1}{2}m,\pm\frac{1}{2}(m+1)}(z) \tag{B.7}$$

with the restriction $|\arg z| < \pi$. In the same manner, eqs. (A.4) plus (25) yield

$$W_{-i\gamma,l+\frac{1}{2}}(z) = (-)^{l+1}\Gamma(l+1-i\gamma)/\Gamma(l+1+i\gamma)\cdot \cdot \sum_{m=0}^{l} \frac{(l+m)!}{(l-m)!} \frac{z^{-\frac{1}{2}m}}{m!} \frac{\Gamma(i\gamma-m)}{\Gamma(-i\gamma)} W_{-i\gamma+\frac{1}{2}m,\pm\frac{1}{2}(m+1)}(z) . \tag{B.8}$$

Notice in this context the useful relations ((8), pp. 19, 29, 30)

$$W_{\varkappa,\mu}(z) = W_{\varkappa,-\mu}(z) ,$$
$$W_{\varkappa,\mu}(z) = W^{*}_{\varkappa^{*},\mu}(z^{*}) , \qquad M_{\varkappa,\mu}(z) = M^{*}_{\varkappa^{*},\mu}(z^{*}) , \qquad \text{if } \operatorname{Im}\mu = 0 .$$

If we reverse the arguments leading to eqs. (B.7) and (B.8), it follows that we have an independent second proof of eqs. (24) and (25), once we have proved eqs. (B.7) and (B.8).

Such a proof can be derived from the well-known recurrence relations for the Whittaker functions W, see (8), p. 304. Note the misprint: to the first term of the second equation must be given a minus sign. Then one has

$$W_{\varkappa,\mu+\frac{1}{2}}(z) = W_{\varkappa,\mu-\frac{1}{2}}(z) + 2\mu z^{-\frac{1}{2}} W_{\varkappa-\frac{1}{2},\mu}(z) . \tag{B.9}$$

This equation proves eq. (B.7) in the case $l = 1$. A similar equation can be found as starting point for the proof of eq. (B.8).

We have found, however, a more elegant way to prove eqs. (B.7) and (B.8). Our basic equality is

$$z^{l}\Gamma(l+1+i\gamma)/\Gamma(2l+2)\ {}_1F_1(l+1+i\gamma;\ 2l+2;\ z) = = \sum_{m=0}^{l} \frac{(l+m)!}{(l-m)!} \frac{(-)^m}{m!} \frac{\Gamma(1+i\gamma)}{\Gamma(m+2)} {}_1F_1(1+i\gamma;\ m+2;\ z) . \tag{B.10}$$

One can prove this equation with the help of the Taylor expansion of ${}_1F_1$

$${}_1F_1(a;\ c;\ z) = \sum_{n=0}^{\infty} \big((a)_n/(c)_n\big) z^n/n! , \tag{B.11}$$

utilizing the relation

$$(-)^m(l+m)!/(l-m)! = (-l)_m(l+1)_m , \tag{B.12}$$

interchanging the order of the two summations that arise on the r.h.s. of

eq. (B.10) and applying the well-known equality

$$(B.13) \qquad {}_2F_1(a, b; c; 1) = \Gamma(c)\Gamma(c-a-b)\Gamma^{-1}(c-a)\Gamma^{-1}(c-b)$$

to the hypergeometric functions ${}_2F_1$ with unit argument that one encounters in this process.

Express the confluent hypergeometric functions ${}_1F_1$ occurring in eq. (B.10) in terms of the functions U according to ([5], p. 263)

$$(B.14) \qquad {}_1F_1(a; c; z) = \{\Gamma(c)/\Gamma(c-a)\} \exp[i\pi\eta a]\, U(a, c, z) + \\ + \{\Gamma(c)/\Gamma(a)\} \exp[z] \exp[i\pi\eta(a-c)]\, U(c-a, c, -z)$$

with

$$\eta = \operatorname{sgn}(\operatorname{Im} z), \qquad \operatorname{Im} z \neq 0.$$

With the help of

$$\Gamma(1+i\gamma)/\Gamma(m+1-i\gamma) = (-)^{m+1}\Gamma(i\gamma-m)/\Gamma(-i\gamma)$$

one obtains in this manner from eq. (B.10) the following two equations:

$$(B.15) \qquad z^l U(l+1-i\gamma, 2l+2, z) = \sum_{m=0}^{l} \frac{(l+m)!}{(l-m)!\,m!}\, U(m+1-i\gamma, m+2, z)$$

and

$$(B.16) \qquad z^l U(l+1+i\gamma, 2l+2, z) = (-)^{l+1}\Gamma(l+1-i\gamma)/\Gamma(l+1+i\gamma) \cdot \\ \cdot \sum_{m=0}^{l} \frac{(l+m)!}{(l-m)!\,m!} \cdot \frac{\Gamma(i\gamma-m)}{\Gamma(-i\gamma)}\, U(1+i\gamma, m+2, z).$$

Finally, if we utilize the relation between U and W given in eq. (28), then eq. (B.15) proves eq. (B.7) and eq. (B.16) proves eq. (B.8). This completes the second proof of eqs. (24) and (25).

● RIASSUNTO (*)

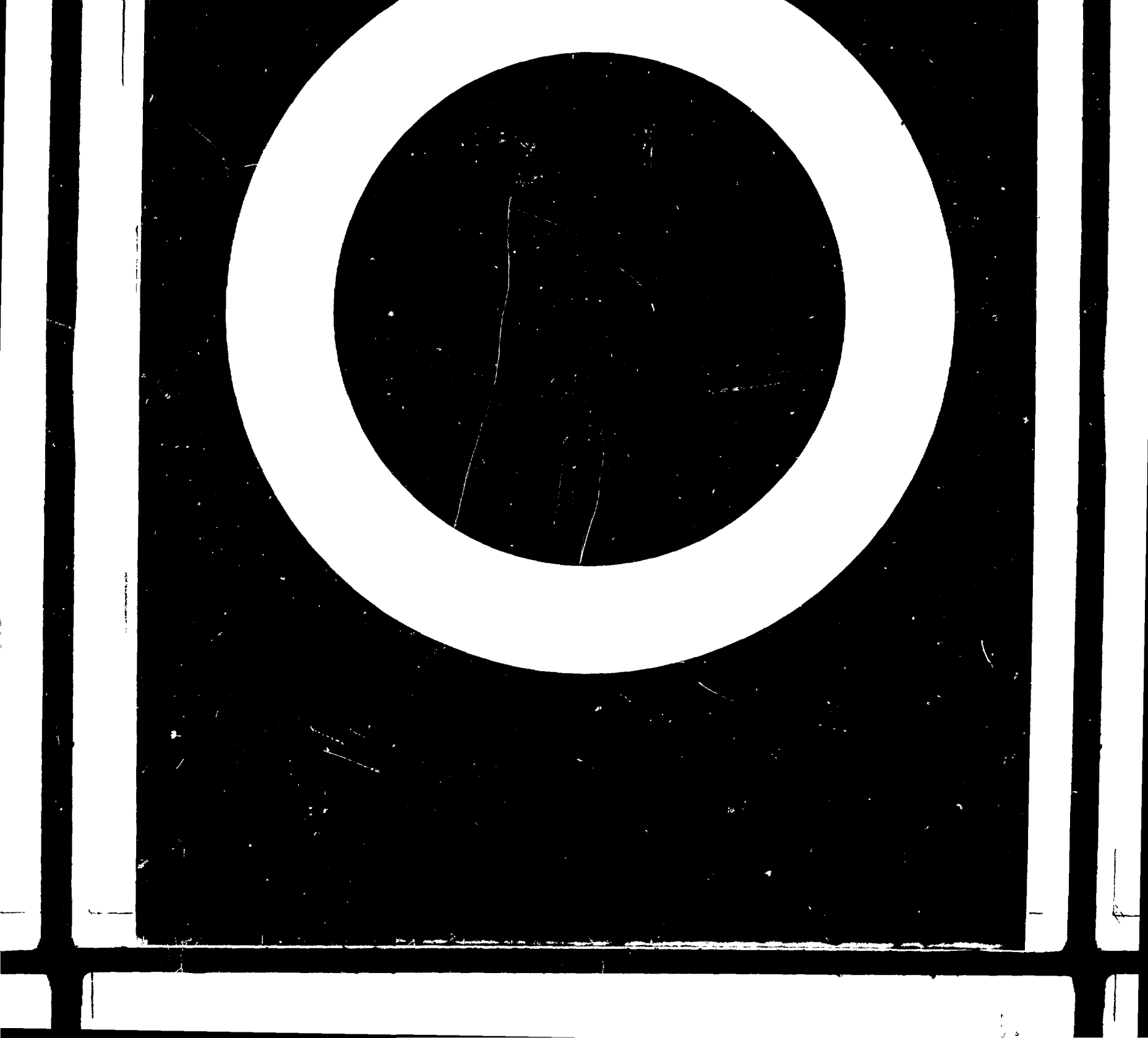
È usuale separare la funzione d'onda fisica $\psi_C^{(+)}$ dello scattering di Coulomb in una parte entrante ψ_i e in una parte diffusa ψ_s. Si deducono formule analitiche per le proiezioni dell'onda parziale di ψ_i e ψ_s e si discute la convergenza asintotica della serie corrispondente di onde parziali. Si trova che questa separazione non è soddisfacente. Si propone una separazione diversa di $\psi_C^{(+)}$ in una parte entrante e una parte diffusa che è in stretta analogia con la separazione normale della funzione d'onda dello scattering per un potenziale a breve raggio.

(*) ***Traduzione a cura della Redazione.***

Кулоновские состояния рассеяния и разложения по парциальным волнам.

Резюме (*). — Обычно волновая функция $\psi_C^{(+)}$ для физического купоновского рассеяния разбивается на падающую часть ψ_i и рассеянную часть ψ_s. Мы выводим аналитическую формулу для парциальных проекций ψ_i и ψ_s и обсуждаем асимптотическую сходимость соответсвующих рядов по парциальным волнам. Получается, что вышеуказанное разделение на ψ_i и ψ_s является неудовлетворительным. Мы предлагаем другое разбиение $\psi_C^{(+)}$ на падающую часть и рассеянную часть. Предложенное разбиение очень похоже на стандартное разделение волновой функции рассеяния для случая короткодействующего потенциала.

(*) *Переведено редакцией.*



𝔅 4

ON AN INHOMOGENEOUS SCHRÖDINGER EQUATION AND ITS SOLUTIONS IN SCATTERING THEORY

We prove that $\psi_{s,\ell}$, the partial-wave projection of the irregular Coulomb wave function ψ_s, is a solution of an inhomogeneous Schrödinger equation. New expressions for $\psi_{s,\ell}$ and ψ_s are obtained in terms of the Coulomb Green functions $G_{C,\ell}$ and G_C, respectively. We discuss irregular solutions, the analogs of ψ_s, for Coulomb-like and short-range potentials. We find that in general these functions do not approach asymptotically the scattering amplitude times an outgoing spherical wave, in contrast to the pure Coulomb function ψ_s.

1. INTRODUCTION

The physical three-dimensional Coulomb scattering wave function $\psi^{(+)}$ is customarily split up into an "incoming part" ψ_i and a "scattered part" ψ_s. Each one of these three functions is a solution of the Schrödinger equation, $\psi^{(+)}$ is regular, ψ_i and ψ_s are irregular. In Ref.1 we have derived closed expressions for $\psi_\ell^{(+)}$, $\psi_{i,\ell}$ and $\psi_{s,\ell}$, the partial wave (p.w.) projections of $\psi^{(+)}$, ψ_i and ψ_s, respectively. We proved that $\psi_{i,\ell}$ and $\psi_{s,\ell}$ are no solutions of the p.w. projected Schrödinger equation.

The function ψ_s approaches asymptotically the Coulomb scattering amplitude times a Coulomb-modified outgoing spherical wave (cf.Eq.(5.1)). The question arises whether there exists also for other potentials a function which

(i) is an irregular solution of the three-dimensional Schrödinger equation, and

(ii) approaches asymptotically the scattering amplitude times an outgoing spherical wave (possibly modified).

In this paper we shall discuss a large class of irregular solutions of the three dimensional Schrödinger equation with a local potential. Their asymptotic behavior is easily obtained when the potential is spherically symmetric. In this case we are able to show that the condition (ii) is not satisfied in general. It seems that the pure Coulomb potential is a remarkable exception in this respect.

In Section 2 we shall prove that $\psi_{s,\ell}$ is a solution of an "inhomogeneous Schrödinger equation", see Eq.(2.3). With the help of this result we deduce in Section 3 a new expression for $\psi_{s,\ell}$,

in terms of the Coulomb Green function $G_{C,\ell}$, Eq.(3.1). In the second part of Section 3 we investigate the behavior of $\psi_{s,\ell}(r)$ for $r \to 0$, starting from different equivalent expressions. When $\ell = 0$ this function diverges like $\ell n\, r$, but for $\ell > 0$ it has a finite limit for $r \to 0$ (Eq.(3.17)).

Summation of the p.w. series with $\psi_{s,\ell}$ leads in a natural way to an expression for $\psi_s(\vec{k},\vec{r})$ in terms of the three dimensional Coulomb Green function G_C, Eq.(4.1). We define in Eq.(4.2) a class of irregular solutions $\psi_w(\vec{k},\vec{r})$ of the three-dimensional Schrödinger equation for a not necessarily spherically symmetric potential in analogy to ψ_s, and study these functions in Section 4. We also discuss here the connection with a line charge distribution on the positive z axis.

The most interesting feature of the Coulomb irregular solution ψ_s is, as we said before, that it approaches asymptotically a Coulomb-modified outgoing spherical wave times the Coulomb scattering amplitude. In Section 5 we discuss the question whether such an irregular solution with a similar asymptotic behavior can be found for other potentials. We successively consider the Coulomb, Coulomb-like, and short-range potentials, first with the "Coulomb-choice" for w, i.e., w(r) proportional to e^{ikr}, and afterwards for other functions w. We have not been able to find an irregular solution ψ_w with the desired property of giving the scattering amplitude. So it seems to be fortuitous that ψ_s yields asymptotically the scattering amplitude. Therefore, although the regular physical wave function $\psi^{(+)}(\vec{k},\vec{r})$ for any local potential can be expressed as the sum of two irregular solutions, $\psi^{(+)} = \psi_i + \psi_s$, this splitting seems to be useful only in the pure Coulomb case.

We shall work throughout in the coordinate representation and restrict ourselves to local potentials. As usual we take $\hbar = 2m = 1$, $E = (k + i\varepsilon)^2$ with $\varepsilon \downarrow 0$, and we suppress the energy dependence of G, G_0 and T. We will often use the subscript C to denote Coulomb quantities.

The p.w. "outgoing" physical scattering state is denoted by $|k\ell +>$, cf. Eq.(11.13) of Taylor [2]. Its connection with Newton's $\psi_\ell^{(+)}$ and φ_ℓ follows from

$$< r \mid k\ell + > \; = (2/\pi)^{\frac{1}{2}}(kr)^{-1}\; i^{\ell}\; \psi_\ell^{(+)}(k,r), \tag{1.1}$$

and (Eq.(12.145) of Ref.3),

$$\psi_\ell^{(+)}(k,r) = k^{\ell+1}\; \varphi_\ell(k,r)\; f_\ell^{-1}(k) \,/\, (2\ell+1)!!, \tag{1.2}$$

where $f_\ell(k)$ is the Jost function. Furthermore we will use the symbols $|\, k\ell \uparrow >$ and $|\, k\ell \downarrow >$ to denote the Jost solutions of the p.w. Schrödinger equation, see Ref.1. We have

$$< r \mid k\ell \uparrow > \; = (2/\pi)^{\frac{1}{2}}\; (kr)^{-1}\; f_\ell(k,r), \tag{1.3}$$

$$2i \mid k\ell + > \; = e^{2i\delta_\ell} \mid k\ell \uparrow > \; - \mid k\ell \downarrow >, \tag{1.4}$$

and

$$< r \mid k\ell + > = (-)^{\ell} < r \mid k\ell - >^{*} \; = (-)^{\ell} < k\ell - \mid r> \, . \tag{1.5}$$

The Coulomb Jost solution is denoted by $< r \mid k\ell \uparrow >_C$, and for $V \equiv 0$ we have [1]

$$< r \mid k\ell \uparrow >_0 \; = (2/\pi)^{\frac{1}{2}}\; i^{\ell}\; h_\ell^{(+)}(kr). \tag{1.6}$$

We shall suppress ℓ when $\ell = 0$. In particular,

$$< r \mid k0 \uparrow >_0 \; = < r \mid k \uparrow >_0 \; = (2/\pi)^{\frac{1}{2}}\; e^{ikr} \,/\, (kr).$$

The subscript 0 to a bra or ket signifies $V = 0$, whereas for a function, e.g. in $f^{*}_{C,0}$, it means $\ell = 0$. The behavior of $< r \mid k\ell + >$ and $< r \mid k\ell \dagger >$ at $r = 0$ follows from

$$\lim_{r\to 0} (\pi/2)^{\frac{1}{2}} (2ikr)^{-\ell} < r \mid k\ell + > (2\ell+1)!/\ell! = f_{\ell}^{-1}(k), \qquad (1.7)$$

and

$$\lim_{r\to 0} (\pi/2)^{\frac{1}{2}} (-2ikr)^{\ell} kr < r \mid k\ell \dagger > \ell!/(2\ell)! = f_{\ell}(k), \qquad (1.8)$$

respectively. These equations are valid for Coulomb-like as well as for (nonsingular) short-range potentials.

For a local central potential $V_{\ell}(r)$ is independent of ℓ. Therefore we shall occasionally suppress the subscript ℓ here.

2. COULOMB FUNCTIONS SATISFYING AN INHOMOGENEOUS SCHRÖDINGER EQUATION

In this section we shall prove that χ_ℓ (see Ref.1) is a solution of the following inhomogeneous differential equation of the Schrödinger type,

$$(k^2 - H_{C,\ell})\, \chi_\ell(kr) = - \langle r \mid V_C \mid k + \rangle_0 \; f^*_{C,0}, \tag{2.1a}$$

that is, written in a more explicit form,

$$\left(k^2 + \frac{1}{r}\frac{d^2}{dr^2} r - \frac{\ell(\ell+1)}{r^2} - \frac{2k\gamma}{r}\right) \chi_\ell(kr)$$

$$= -\frac{2k\gamma}{r} (2/\pi)^{\frac{1}{2}} \frac{e^{ikr}}{kr} \frac{e^{\pi\gamma/2}}{\Gamma(1-i\gamma)}. \tag{2.1b}$$

Here V_C is the Coulomb potential and $f^*_{C,0}$ is the complex conjugate of the Coulomb Jost function for $\ell = 0$ (e.g., Ref.3),

$$f_{C,\ell} = f_{C,\ell}(k) = e^{\pi\gamma/2}\, \Gamma(\ell+1) / \Gamma(\ell+1+i\gamma).$$

The function χ_ℓ has been defined in Ref.1 by

$$\chi_\ell(kr) = e^{2i\sigma_\ell} \langle r \mid k\ell + \rangle_C - 2i\, \psi_{s,\ell}(r), \tag{2.2}$$

where $\langle r \mid k\ell + \rangle_C$ is the Jost solution for the p.w. Schrödinger equation with the Coulomb potential. It follows that if Eq.(2.1) is valid, we also have

$$(k^2 - H_{C,\ell})\, \psi_{s,\ell}(r) = \langle r \mid V_C \mid k + \rangle_0 \; f^*_{C,0} / (2i). \tag{2.3}$$

As we said in the introduction, $\psi_{s,\ell}$ is the p.w. projection of ψ_s (see Eq.(4) of Ref.1),

$$\psi_s(\vec{k},\vec{r}) = -(2\pi)^{-\frac{3}{2}} e^{\pi\gamma/2}\, (\Gamma(1+i\gamma) / \Gamma(-i\gamma))\, e^{ikr}\, U(1+i\gamma, 1, i\vec{k}\cdot\vec{r} - ikr). \tag{2.4}$$

In order to prove Eq.(2.1), we substitute the following

closed expression for χ_ℓ (see Eq.(A.17) of Ref.1),

$$\chi_\ell(kr) = (2/\pi)^{\frac{1}{2}} \frac{\exp(\pi\gamma/2)}{\Gamma(1 - i\gamma)} \frac{\exp(ikr)}{kr} {}_3F_1(-\ell,\ \ell+1,\ 1;\ 1 - i\gamma;\ \frac{1}{2ikr}), \quad (2.5)$$

and introduce the new variables $z = (2ikr)^{-1}$ and $\mu = -i\gamma$. After some manipulations the equation to be proved reduces to

$$-z^3 F''(z) + z(1 - 2z) F'(z) + (\mu + \ell(\ell + 1)z) F(z) = \mu. \quad (2.6)$$

Here

$$F(z) \equiv {}_3F_1(-\ell, \ell + 1, 1; \mu + 1;\ z) = \sum_{n=0}^{\ell} z^n (-\ell)_n (\ell+1)_n / (\mu+1)_n$$

is a polynomial, so the proof of Eq.(2.6) is obtained in a straightforward way.

3. A NEW EXPRESSION FOR $\psi_{s,\ell}$

In this section we shall prove the equation

$$G_{C,\ell}\, V_{C,\ell}\, |\, k\uparrow\rangle_0\, f^*_{C,0} = 2i\, \psi_{s,\ell}, \tag{3.1}$$

where

$$2i\, \psi_{s,\ell} = e^{2i\sigma_\ell}\, |\, k\ell\uparrow\rangle_C - \chi_\ell. \tag{3.2}$$

The left-hand side of (3.1) gives a new expression for $\psi_{s,\ell}$. Further we shall investigate the behavior of $\psi_{s,\ell}(k,r)$ for $r \to 0$, see Eq.(3.17).

Note, however, that

$$G_{C,\ell}\, V_{C,\ell}\, |\, k\downarrow\rangle_0$$

is even not defined. This can be easily deduced from our discussion below (the integral $\int_r^\infty$ in Eq.(3.8) would be divergent in this case), but it also follows from the equality $G_{C,\ell}\, V_{C,\ell} = G_{0,\ell}\, T_{C,\ell}$ and the well-known fact that the half-shell Coulomb T matrix, that is $T_{C,\ell}\, |\, k\ell\rangle$, is not defined.

For the proof of Eq.(3.1) we use

$$\langle r\, |\, G_{C,\ell}\, |\, r'\rangle = (-)^{\ell+1}\, \tfrac{1}{2}\pi k\, \langle r_<\, |\, k\ell +\rangle \langle r_>\, |\, k\ell\uparrow\rangle, \tag{3.3}$$

where $r_<$ is the smaller one and $r_>$ the larger one of the pair r,r'. Such a representation of the Green function holds for any local central potential, as is well known.

A natural and direct way to prove Eq.(3.1) would consist of inserting (3.3) and using the known explicit expressions for the regular and irregular Coulomb wave functions, i.e.,

$$\langle r\, |\, k\ell +\rangle_C = (2/\pi)^{\frac{1}{2}}\, e^{-\pi\gamma/2} (\Gamma(\ell + 1 + i\gamma) / \Gamma(2\ell + 2))$$

$$\times\, (2ikr)^\ell\, e^{-ikr}\, {}_1F_1(\ell + 1 - i\gamma;\, 2\ell + 2;\, 2ikr), \tag{3.4a}$$

and

$$\langle r \,|\, k\ell\uparrow\rangle_C = (2/\pi)^{\frac{1}{2}}\, e^{\pi\gamma/2+ikr}(kr)^{-1}(-2ikr)^{\ell+1}\, U(\ell+1+i\gamma, 2\ell+2, -2ikr). \quad (3.4b)$$

However, it turns out that this approach is somewhat complicated. We have been able to prove Eq.(3.1) in this way only for $\ell = 0$ and for $\ell = 1$. In order to show the complications arising here, we now discuss briefly the $\ell = 0$ case. By using

$$d/dz\ {}_1F_1(-i\gamma; 1; z) = -i\gamma\ {}_1F_1(1 - i\gamma; 2; z),$$

$$d/dz\ e^{-z}\, U(1 + i\gamma, 1, z) = -e^{-z}\, U(1 + i\gamma, 2, z),$$

and

$${}_1F_1(-i\gamma; 1; z) = -i\gamma\ {}_1F_1(1 - i\gamma; 2; z) + (1 + i\gamma)\,{}_1F_1(-i\gamma; 2; z),$$

$$U(1 + i\gamma, 1, z) = U(1 + i\gamma, 2, z) - (1 + i\gamma)\, U(2 + i\gamma, 2, z),$$

we obtain

$$\langle r \,|\, G_C V_C \,|\, k\uparrow\rangle_0 = e^{-\pi\gamma/2}\,\Gamma(1 + i\gamma)\langle r \,|\, k\uparrow\rangle_C + (2/\pi)^{\frac{1}{2}}\, 2i\, e^{ikr}\,\Gamma(1 + i\gamma)$$

$$\times\Big[{}_1F_1(-i\gamma; 1; 2ikr)\ U(1 + i\gamma, 2, -2ikr) + i\gamma\,{}_1F_1(1 - i\gamma; 2; 2ikr)\, U(1 + i\gamma, 1, -2ikr)\Big]. \quad (3.5)$$

The expression between the square brackets can be reduced by noting that the Wronskian W for the functions

$$f(z) \equiv {}_1F_1(-i\gamma;\ 1;\ z)$$

and

$$g(z) \equiv e^{z}\, U(1 + i\gamma,\ 1,\ -z)$$

is equal to

$$W(f,g) \equiv fg' - f'g = z^{-1}\exp(z + i\pi\ \mathrm{sgn}(\mathrm{Im}\, z))\ /\ \Gamma(1 + i\gamma)\ .$$

In this way we get from Eq.(3.5),

$$\langle r \,|\, G_C V_C \,|\, k\uparrow\rangle_0\ \ f^{*}_{C,0} = e^{2i\sigma_0}\langle r \,|\, k\uparrow\rangle_C - (2/\pi)^{\frac{1}{2}}\, e^{\pi\gamma/2}(kr)^{-1} e^{ikr}/\Gamma(1-i\gamma),$$

which is just Eq.(3.1) for $\ell = 0$.

For $\ell > 1$ the above procedure is rather complicated. Therefore we resort to a different approach.

In the preceding section we have proved

$$(k^2 - H_{C,\ell})(2i\,\psi_{s,\ell}) = V_C \,|\, k\uparrow\rangle_0 \; f^*_{C,0}. \tag{3.6}$$

This equation follows from Eq.(3.1), but not vice versa. We shall nevertheless prove Eq.(3.1) with the help of Eq.(3.6). To this end we first observe that the quantity $G_{C,\ell} V_C \,|\, k\uparrow\rangle_0 \; f^*_{C,0}$ is a solution of the same inhomogeneous differential equation,

$$(k^2 - H_{C,\ell})\, G_{C,\ell} V_C \,|\, k\uparrow\rangle_0 \; f^*_{C,0} = V_C \,|\, k\uparrow\rangle_0 \; f^*_{C,0}.$$

Therefore this quantity equals the sum of a particular solution of this equation and some solution of the corresponding homogeneous differential equation. According to Eq.(2.1), $-\chi_\ell$ is a particular solution. Further we know that any solution of the homogeneous differential equation is a linear combination of $|\, k\ell\uparrow\rangle_C$ and $|\, k\ell\downarrow\rangle_C$. Therefore,

$$G_{C,\ell} V_C \,|\, k\uparrow\rangle_0 \; f^*_{C,0} = -\chi_\ell + C_1 \,|\, k\ell\uparrow\rangle_C + C_2 \,|\, k\ell\downarrow\rangle_C. \tag{3.7}$$

We shall prove that $C_2 = 0$ and $C_1 = e^{2i\sigma_\ell}$ by establishing the behavior of the left-hand side for $r \to \infty$ and for $r \to 0$, respectively.

Substitution of (3.3) in the left-hand side of Eq.(3.7) yields

$$\begin{aligned} \langle r \,|\, G_{C,\ell} V_C \,|\, k\uparrow\rangle_0 \; f^*_{C,0} &= (-)^{\ell+1} \tfrac{1}{2}\pi k f^*_{C,0} \\ &\times \Big[\langle r \,|\, k\ell\uparrow\rangle_C \int_0^r \langle r' \,|\, k\ell\uparrow\rangle_C \, V_C(r') \langle r' \,|\, k\uparrow\rangle_0 \; r'^2 dr' \\ &+ \langle r \,|\, k\ell\uparrow\rangle_C \int_r^\infty \langle r' \,|\, k\ell\uparrow\rangle_C \, V_C(r') \langle r' \,|\, k\uparrow\rangle_0 \; r'^2 dr' \Big]. \end{aligned} \tag{3.8}$$

We further use Eq.(1.4) for the Coulomb case,

$$2i\,|k\ell+\rangle_C = e^{2i\sigma_\ell}\,|k\ell+\rangle_C - |k\ell+\rangle_C,$$

and

$$\langle r\,|k\ell+\rangle_C \sim (2/\pi)^{\frac{1}{2}}(kr)^{-1}\exp(ikr - i\gamma\,\ell n(2kr)),\quad r\to\infty. \qquad (3.9)$$

It follows that for $r\to\infty$ the second term on the right-hand side of Eq.(3.8) is negligible. For the first term we find, for $r\to\infty$,

$$-(2/\pi)^{\frac{1}{2}}\,f^{*}_{C,0}(kr)^{-1}\,e^{ikr} + \text{const.}\ r^{-1-i\gamma}\,e^{ikr}.$$

Clearly this implies that we have $C_2 = 0$ in Eq.(3.7).

In order to prove $C_1 = e^{2i\sigma_\ell}$, we consider the expressions in Eq.(3.8) for $r\to 0$. With the help of Eqs.(1.7) and (1.8) one easily verifies that

$$\langle r\,|G_{C,\ell}\,V_C\,|k+\rangle_0 = O(\ell n\,r),\quad r\to 0,\ \text{when}\ \ell = 0,$$
$$= O(1),\quad r\to 0,\ \text{when}\ \ell = 1,2,3,\ \ldots\ . \qquad (3.10)$$

Finally we use Eq.(3.4b), where ([4], p.283, corrected)

$$U(a,c,z) = z^{1-c}\,\Gamma(c-1)/\Gamma(a) + O(|z|^{2-\mathrm{Re}\,c}),\ z\to 0,\ \mathrm{Re}\,c\geq 2,\ c\neq 2, \qquad (3.11)$$

and deduce from Eq.(26) of Ref.1 that

$$\chi_\ell(kr) = (2/\pi)^{\frac{1}{2}}\,e^{\pi\gamma/2}(kr)^{-1}(-2ikr)^{-\ell}\,\Gamma(2\ell+1)/\Gamma(\ell+1-i\gamma),\ r\to 0. \qquad (3.12)$$

With the help of these expressions we obtain $C_1 = e^{2i\sigma_\ell}$. This completes the proof of Eq.(3.1).

The behavior of $\langle r\,|G_{C,\ell}\,V_C\,|k+\rangle_0$ at $r=0$, as given by Eq. (3.10) is somewhat peculiar. The function $\psi_{s,\ell}$ has the same behavior according to Eq.(3.1) that has just been proved. It may be interesting to deduce this behavior of $\psi_{s,\ell}$ at $r=0$ in an in-

dependent manner. We shall do this in two ways, (i) by starting from $\psi_c(\vec{k},\vec{r})$, and (ii) by using an integral representation for $\psi_{s,\ell}$ which we have obtained previously [1]. The second method will give at the same time a more precise expression for $\psi_{s,\ell}$ at $r = 0$.

First we note that Eqs.(3.2) and (3.4) may be used for our purpose, but this approach is not simple for $\ell > 0$. We shall start with $\psi_s(\vec{k},\vec{r})$, a closed form for which has already been given in Eq.(2.4). By using

$$\Gamma(1+i\gamma, 1, z) = -(C+\psi(1+i\gamma)+\pi/2)/(1+i\gamma), \quad z \to 0, \tag{3.16}$$

where C is Euler's constant and ψ the Digamma function, we get

$$\psi_s(\vec{k},\vec{r}) = (2\pi)^{-\frac{3}{2}} e^{ikr+\pi\gamma/2} \Gamma(1+i\gamma)/\Gamma(-i\gamma), \quad kr = \vec{k}\cdot\vec{r}. \tag{3.17}$$

The p.w. projection of ψ_s is given by

$$\psi_{s,\ell}(r) \equiv 2\pi \int_{-1}^{1} P_\ell(x)\, \psi_s(\vec{k},\vec{r})\, dx,$$

with $x = \hat{k}\cdot\hat{r}$. We now use the equalities

$$-\int_{-1}^{1} P_\ell(x)\, \ln(1-x)dx = \ln 2 - 1, \quad \ell = 0$$
$$= -2/(\ell(\ell+1)), \ell = 1,2,3,\ldots, \tag{3.18}$$

that follow easily with the help of (e.g., Ref.4, p.330)

$$\sum_{n=1}^{\infty} (n^{-1}+(n+1)^{-1}) P_n(x) = -1 + \ln 2 - \ln(1-x), \quad -1 \le x < 1. \tag{3.19}$$

In this way we obtain, for $r \to 0$,

$$(\pi/2)^{\frac{1}{2}} e^{-\pi\gamma/2} \Gamma(-i\gamma)\, \psi_{s,\ell}(r) \to \ln r, \quad \ell = 0$$
$$\to -1/(\ell(\ell+1)), \ell = 1,2,3,\ldots. \tag{3.17}$$

This expression not only agrees with Eq.(3.1) but also gives more information.

Finally we will derive the expression (3.1) from the following integral representation for $\psi_{\gamma,\ell}$ (Eq.(3.1) with $\kappa = 1$),

$$\psi_{\gamma,\ell}(r) = -(2/\pi)^{\frac{1}{2}} 2^{-\ell} \cdot \pi\gamma/\Gamma(-\gamma+\ell)^{-1} \int_0^\infty J_\ell(2\sqrt{r}\cdot) \cdot (2\sqrt{r}\cdot)^{2\ell+1} \cdot J_{\gamma+\ell-\frac{1}{2}}(\cdot) \cdot \cdot^{\gamma-\frac{1}{2}} \cdot \quad (3.1)$$

We now the new variable $z = 2\sqrt{r}\cdot$ and see that we have to investigate the following integral for small r,

$$I_\ell(r) \equiv \int_0^\infty J_\ell(z) \cdot e^{-\frac{1}{2}z} (z + 2r)^{-\frac{1}{2}} \cdot (1 + 2r/z)^{-\gamma} \cdot z. \quad (3.1)$$

When $\ell > 1$ we may put $r = 0$ in the integrand because $J_\ell(z) = O(z^\ell)$, $z \to 0$. In this case we obtain

$$\lim_{r\to 0} I_\ell(r) = \int_0^\infty J_\ell(z) \cdot e^{-\frac{1}{2}z} \cdot z^{-\frac{1}{2}} \cdot z = 2^\ell/(\ell+1), \quad \ell = 1, 2, \ldots, \quad (3.1)$$

which follows by using formula (3.1) of [3]. For $\ell = 0$ we have

$$I_0(r) + \ln 2r =$$
$$\int_0^\infty \sin z \cdot e^{-\frac{1}{2}z} \cdot z^{-\frac{1}{2}} (z + 2r)^{-\frac{1}{2}} (1 + 2r/z)^{-\gamma} \cdot z - \int_0^{1-r} (z + 2r)^{-\frac{1}{2}} \cdot z,$$

which expression clearly has a finite limit for $r \to 0$, i.e.

$$I_0(r) = -\ln 2r + O(1), \quad r \to 0. \quad (3.1)$$

By substituting the above results in Eq.(3.1) we obtain the second proof of Eq.(3.1).

4. IRREGULAR SOLUTIONS IN THE GENERAL CASE

In the preceding section we have expressed $\psi_{s,\ell}$ in terms of the Coulomb Green function $G_{C,\ell}$, see Eq.(3.1). By summing the p.w. series for both sides of this equation we obtain

$$\psi_s(\vec{k},\vec{r}) = \int_0^\infty \langle \vec{r} | G_C | \hat{k} r' \rangle V_C(r') \langle r' | k \rangle_0 \, r'^2 dr' \, Y_{\ell,\ell}^*/(2i). \qquad (4.1)$$

In this section we shall discuss irregular solutions ψ_w for a general potential V, not necessarily spherically symmetric. To this end we define, in close analogy to Eq.(4.1),

$$\psi_w(\vec{k},\vec{r}) \equiv \int_0^\infty \langle \vec{r} | G | \hat{k} r' \rangle w(r') \, dr', \qquad (4.2)$$

where $G = (k^2 + \Delta - V)^{-1}$ and the function w is restricted to the extent that the above integral be well defined. For convenience we assume w to be continuously differentiable. By a formal application of G^{-1} it is easily seen that ψ_w satisfies

$$(k^2 + \Delta - V)\psi_w(\vec{k},\vec{r}) = r^{-2} \, w(r) \, \delta(\hat{r},\hat{k}). \qquad (4.3)$$

The Dirac delta function is defined by

$$\int f(\hat{r}) \, \delta(\hat{r},\hat{z}) \, d\hat{r} = f(\hat{k}),$$

where the domain of integration is the surface of the unit sphere.

We will show that ψ_w in general has a logarithmic singularity in the forward direction ($\hat{k} = \hat{r}$). By inserting $G = G_0 + G_0 V G$ in (4.2) one can show that this singularity in general comes from G_0. So we replace G by G_0 in Eq.(4.2) and use

$$\langle \vec{r} | G_0 | \vec{r}' \rangle = -(4\pi)^{-1} | \vec{r} - \vec{r}' |^{-1} \exp(ik | \vec{r} - \vec{r}' |).$$

It follows that the singular part of ψ_w is given by

$$\psi_w = -(4\pi)^{-1} \int_0^\infty w(r') \exp(iky)/y \, dr' + O(1), \quad x \to 1,$$

with $y = (r^2 + r'^2 - 2rr'x)^{\frac{1}{2}}$ and $x = \hat{k}\cdot\hat{r}$ as before. The singularity comes from the integrand at the point $r' = r$. In order to investigate its behavior in this region we introduce the new variable $z = r'/r$. Then one can show that for any positive a,

$$\int_a^1 (1-2xz+z^2)^{-\frac{1}{2}} f(z)\,dz = \mp f(1) \ln(1-x) + O(1), \quad x \to 1, \quad a < 1, \qquad (4.4)$$

for a continuously differentiable function $f(z)$. With the help of Eq.(4.4) we obtain

$$\psi_w = (4\pi)^{-1} w(r) \ln(1-x) + O(1), \quad x \to 1. \qquad (4.5)$$

This expression gives the logarithmic singularity of the irregular solution ψ_w for a general local potential V.

Now we will discuss briefly the singular behavior of ψ_w at $r = 0$. In this case we assume $x \neq 1$. Since $(z^2 - 2xz + 1)^{\frac{1}{2}} \sim z$ for $z \to \infty$ we have

$$\psi_w = -(4\pi)^{-1} \int_1^\infty e^{ikrz} w(rz)\,dz/z + O(1), \quad r \to 0. \qquad (4.6)$$

When w is constant we use

$$\Gamma(0, -ikr) = \int_1^\infty e^{ikrz}\,dz/z = -\ln kr + O(1), \quad r \to 0,$$

where Γ is the incomplete gamma function, and obtain from Eq.(4.6),

$$\psi_w = (4\pi)^{-1} w(0) \ln kr + O(1), \quad r \to 0. \qquad (4.7)$$

When w is proportional to e^{ikr} (cf. Eq.(4.13)) we get exactly the same expression, (4.7).

We note that Eqs.(4.5) and (4.7) can be combined,

$$\psi_w(\vec{k},\vec{r}) = (4\pi)^{-1}\, w(r)\, \ln(kr - \vec{k}\cdot\vec{r}) + O(1), \qquad (4.9)$$

for $\hat{k}\cdot\hat{r} \to 1$ as well as for $r \to 0$. This expression may be compared with Eq.(3.14).

If we now restrict ourselves to spherically symmetric potentials, $\psi_w(\vec{k},\vec{r})$ is a function of k,r and $\hat{k}\cdot\hat{r}$ only. In this case it is possible to consider the p.w. projection of (4.9),

$$\psi_{w,\ell}(k,r) = \int_0^\infty \langle r \mid G_\ell \mid r' \rangle w(r')\, dr'. \qquad (4.10)$$

In order to deduce the behavior of $\psi_{w,\ell}$ at $r = 0$, we use Eq.(4.3) which is valid for any local central potential. Then Eq.(4.9) may be rewritten as

$$\psi_{w,\ell}(k,r) = (-)^{\ell+1}\, \tfrac{1}{2}\pi k \left[\langle r \mid k\ell + \rangle \int_0^r \langle r' \mid k\ell + \rangle w(r')\, dr' + \langle r \mid k\ell + \rangle \int_r^\infty \langle r' \mid k\ell + \rangle w(r')\, dr' \right]. \qquad (4.11)$$

By using Eqs.(1.7) and (1.8) we obtain

$$\psi_{w,\ell}(k,r) \simeq -(2\ell+1)^{-1}\, w(0) \left| r^{-\ell-1} \int_0^r r'^{\ell}\, dr' + r^{\ell} \int_r^{r_0} r'^{-\ell-1}\, dr' \right|, \quad r \to 0, \qquad (4.11')$$

where r_0 is an unimportant constant. Therefore,

$$\psi_{w,\ell}(k,r) = w(0)\, \ln r + O(1), \quad r \to 0, \quad \ell = 0,$$

$$= -w(0)/(\ell(\ell+1)) + o(1), \quad r \to 0, \quad \ell = 1,2,3, \ldots . \qquad (4.12)$$

One easily verifies that the p.w. projection of both sides of Eq.(4.8) yields expressions for $\psi_{w,\ell}$ that are in agreement with Eq.(4.12).

We note that for the Coulomb case, $G = G_C$, ψ_w is just equal to the irregular Coulomb wave ψ_s given by Eq.(2.4) if we choose the function w as

$$w(r) = -i\gamma(2/\pi)^{\frac{1}{2}} f^{*}_{C,0} e^{ikr}. \qquad (4.13)$$

We conclude this section with a remark on the logarithmic singularity of ψ_w, given by Eq.(4.8). We see from Eq.(4.3) that the delta function singularity must be generated by the Laplace operator acting on $\ell n(kr - \vec{k}\cdot\vec{r})$, so

$$\Delta\, \ell n\,(kr - \vec{k}\cdot\vec{r}) = 4\pi\, r^{-2}\, \delta(\hat{r},\hat{k}). \qquad (4.14)$$

It is interesting to note that one can verify that Eq.(4.14) holds with an equality sign.

In order to show this, let us take $\hat{k}$ along the positive z-axis as before. Then the right-hand side of (4.14) describes a uniform line charge density along the positive z-axis. In view of the symmetry in the problem it is natural to use cylindrical coordinates R, z, φ, where $R^2 = r^2 - z^2$. Then we have

$$2\pi\, r^{-2}\, \delta(\hat{r},\hat{z}) = r^{-2}\, \delta(1 - \cos\zeta) = R^{-1}\, \delta(R)\, \theta(z),$$

where θ is the unit step function. Further,

$$kr - \vec{k}\cdot\vec{r} = k(r - z) = k((R^2 + z^2)^{\frac{1}{2}} - z).$$

The electrostatic potential for a uniform charge distribution on the positive z-axis is just proportional to the logarithmic term discussed above. Poisson's equation reads in this case

$$\Delta\, \ell n(\,(R^2 + z^2)^{\frac{1}{2}} - z) = 2\, R^{-1}\, \delta(R)\, \theta(z). \qquad (4.15)$$

This equation shows that (4.14) holds with an equality sign. So we see that the inhomogeneous term in Eq.(4.3) may be compared with a line charge distribution along the positive z-axis with density w(r) or w(z).

5. ON THE CONNECTION WITH THE SCATTERING AMPLITUDE

The function $\psi_S(\vec{k},\vec{r})$ (see Eq.(2.5)) is called the scattered part of the complete physical scattering wave function $\psi^{(+)}(\vec{k},\vec{r})$ for the Coulomb potential because of its asymptotic behavior, which is given by (cf. Eq.(40) of Ref.1)

$$\psi_S(\vec{k},\vec{r}) \sim f^C(\hat{k}\cdot\hat{r})(2\pi)^{-\frac{3}{2}}\, r^{-1}\, e^{ikr-i\gamma\,\ln 2kr}, \quad r\to\infty. \qquad (5.1)$$

Here f^C is the Coulomb scattering amplitude,

$$f^C(x) = -\frac{\gamma}{2k}\, e^{2i\sigma_0}\,(1-x)^{-1-i\gamma}.$$

One may compare (5.1) with the well-known [illegible] formula,

$$\psi^{(+)}(\vec{k},\vec{r}) \sim (2\pi)^{-\frac{3}{2}}\left(e^{i\vec{k}\cdot\vec{r}} + f(\theta)\, e^{ikr}/r\right), \quad r\to\infty.$$

From Eq.(4.1),

$$\psi_S(\vec{k},\vec{r}) = \int_0^\infty \langle \vec{r}\,|\,G_C\,|\,\hat{k}r'\rangle\, V_C(r')\,\langle r'\,|\,k+\rangle_0\, r'^2\, dr'\, [illegible]/(2i),$$

we see that this "scattered part" equals an integral involving the Green operator G_C.

It is interesting to investigate whether Eq.(5.1) can be generalized to other potentials. The problem is, how to find an irregular solution, such that its asymptotic behavior equals the scattering amplitude times a (possibly modified) outgoing spherical wave, just as in Eq.(5.1).

Let us first consider again the p.w. function $\psi_{S,\ell}$ for the pure Coulomb potential. Below we shall consider the generalization to Coulomb-like and other potentials. From Eqs.(3.1) and (3.3) we have, for $r\to\infty$,

$$\psi_{s,\ell}(\ ,r) \sim \tfrac{1}{2}\pi k f^*_{C,0} \langle r \mid k\ell\uparrow\rangle_C \int_C^r \lesssim k\ell - \mid r'\rangle V_C(r') \langle r' \mid k\uparrow\rangle_0 r'^2\, dr'. \quad (5.2)$$

We split the integral in two parts, $\int_0^R + \int_R^r$, where R is so large that the asymptotic behavior of $_C\lesssim k\ell - \mid r'\rangle$ can be used. With the help of Eqs.(1.4) and (3.9) we obtain a term with the asymptotic behavior $-(2/\pi)^{\frac{1}{2}} f^*_{C,0}\, e^{ikr}/(2ikr)$. According to Eq.(3.2),

$$\psi_{s,\ell}(k,r) = (-\chi_\ell + e^{2i\sigma_\ell} \langle r \mid k\ell\uparrow\rangle_C)/(2i),$$

this term is $-\chi_\ell/(2i)$. The rest of $\psi_{s,\ell}$ is proportional to $\langle r \mid k\ell\uparrow\rangle_C$. By using Eq.(3.1) we deduce

$$e^{2i\sigma_\ell} = f^*_{C,0} \lim_{R\to\infty} \left[(2kR)^{i\gamma} - \tfrac{1}{2}\pi k \int_0^R \lesssim k\ell - \mid r\rangle V_C(r) \langle r \mid k\uparrow\rangle_0\, r^2\, dr\right]. \quad (5.3)$$

It is interesting to replace here $\langle r \mid k\uparrow\rangle_0$ by $\langle r \mid q\uparrow\rangle_0$, where as before

$$\langle r \mid q\uparrow\rangle_0 = (2/\pi)^{\frac{1}{2}}\, e^{iqr}/(qr),$$

with $\mathrm{Im}\, q > 0$ and consider the limit for $q \to k$. When $q \neq k$ the integral $\int_0^R \ldots$ is convergent for $R \to \infty$ and may be denoted in this case by $_C\lesssim k\ell - \mid V_{C,\ell} \mid q\uparrow\rangle_0$. We have been able to obtain the following closed expressions,

$$_C\lesssim k\ell - \mid V_{C,\ell} \mid q\uparrow\rangle_0 = \frac{4j\gamma}{\pi q} e^{\pi\gamma/2} \left(\frac{q+k}{q-k}\right)^{i\gamma/2} Q_\ell^{i\gamma}(q/k)$$

$$= -\frac{2}{\pi q} e^{-\pi\gamma/2} \frac{\Gamma(1+i\gamma)\,\Gamma(1-i\gamma)\,\Gamma(\ell+1)}{\Gamma(\ell+1-i\gamma)} \left[P_\ell^{(i\gamma,-i\gamma)}(q/k) - \left(\frac{q+k}{q-k}\right)^{i\gamma} P_\ell^{(-i\gamma,i\gamma)}(q/k)\right]. \quad (5.4)$$

Here $Q_\ell^{i\gamma}$ is Legendre's function of the second kind, and $P_\ell^{(\cdot,\ )}$ is Jacobi's polynomial. In the particular case $\ell = 0$ this expression agrees with Eq.(7) of Ref.6 that we used for the deriva-

tion of the Coulomb off-shell Jost function in closed form.

When $q \sim k$, Eq.(5.4) can be simplified. By inserting

$$P_\ell^{(i\gamma,-i\gamma)}(1) = \Gamma(\ell+1+i\gamma)/(\Gamma(1+i\gamma)\,\Gamma(\ell+1)), \tag{5.5}$$

we obtain

$$\langle k\ell - | V_{C,\ell} | q\,+ \rangle_0 \underset{q\to k}{\sim} -\frac{2}{\pi k} e^{-\pi\gamma/2}\left[e^{2i\sigma_\ell}\Gamma(1-i\gamma) - \Gamma(1+i\gamma)\left(\frac{q+k}{q-k}\right)^{i\gamma}\right]. \tag{5.6}$$

The second term on the right-hand side contains the factor $(q-k)^{-i\gamma}$ and is therefore singular for $q \to k$. It may be compared with the "correction factor" ω of Ref.6, Eq.(2). Note also the similarity with the so-called Coulombian asymptotic state of Ref. 7, Eq.(16), where the typical factor $f^*_{C,0}(p+k)^{i\gamma}(p-k)^{-i\gamma}$ occurs.

This singular term corresponds to that part of the integral on the right-hand side of Eq.(5.3) which contains the (for $R \to \infty$) divergent factor $(2kR)^{i\gamma}$. The other term is continuous for $q \to k$ and this one corresponds just to the "convergent part" of the integral in (5.3).

A natural generalization of the expression $\langle r | G_{C,\ell}\, V_{C,\ell} | k\,+ \rangle_0$ to other central potentials is

$$\psi_\ell(k,r) \equiv \langle r | G_\ell\, V_\ell | k\,+ \rangle_0, \tag{5.7}$$

where G_ℓ is the Green function for V_ℓ. So ψ_ℓ corresponds to the Coulomb function $\psi_{s,\ell}$ of Eq.(3.1) (we have omitted the constant factor $f^*_{C,0}/(2i)$ which is irrelevant here). We first assume that V_ℓ is a Coulomb plus short-range potential, $V_{C,\ell} + V_{s,\ell}$. In order to investigate the asymptotic behavior of ψ_ℓ, we use the expression (cf.Eq.(3.3))

$$\langle r | G_\ell | r' \rangle = -\tfrac{1}{2}\pi k \langle k\ell - | r_< \rangle\langle r_> | k\ell\,+ \rangle.$$

It may be noted that $\langle r | k\ell\,+ \rangle$ has exactly the same asymptotic

behavior as $<r \mid k\ell\uparrow>_C$, which is given by Eq.(3.9). Furthermore we have (cf. Eq.(1.4))

$$2i <k\ell - \mid = e^{2i(\sigma_\ell + \delta_\ell^C)} <k\ell \downarrow \mid - <k\ell \uparrow \mid , \tag{5.8}$$

where δ_ℓ^C is the Coulomb-modified phase shift. We proceed in the same way as in the pure Coulomb case, and find that ψ_ℓ can again be split up in two parts, $\psi_\ell = \psi_\ell^{(1)} + \psi_\ell^{(2)}$, which have different asymptotic behavior. For the first term we get

$$\psi_\ell^{(1)}(r) \sim -(2/\pi)^{\frac{1}{2}}\, e^{ikr}/(kr), \quad r \to \infty, \quad \ell = 0,1,2, \ldots . \tag{5.9}$$

Obviously this is the analog of the function χ_ℓ. Since the right-hand side of (5.9) is independent of ℓ, it follows that the sum of the p.w. series,

$$\sum_{\ell=0}^{\infty} (4\pi)^{-1}(2\ell + 1)\, P_\ell(x)\, \psi_\ell^{(1)}(r),$$

is proportional to $\delta(1 - x)$ for $r \to \infty$.

For the second term we obtain

$$\psi_\ell^{(2)}(r) \sim <r \mid k\ell\uparrow> \lim_{R\to\infty} \Big[(2kR)^{i\gamma} - \tfrac{1}{2}\pi k \int_0^R <k\ell - \mid r'> V(r') <r' \mid k\uparrow>_0\, r'^2 dr'\Big], \quad r \to \infty. \tag{5.10}$$

The integral $\int_0^R$ is divergent for $R \to \infty$. In this limit it has exactly the same singular behavior as for the pure Coulomb case, which can be verified with the help of Eq.(5.8). It is therefore natural to split off the pure Coulomb part. We do this by using the two-potential formalism; in the notation of Ref.8 we have

$$V_\ell \mid k\ell + > = V_{C,\ell} \mid k\ell + >_C + (1 + T_{C,\ell}\, G_{0,\ell})\, t_{Cs,\ell} \mid k\ell + >_C, \tag{5.11a}$$

or

$$<k\ell - \mid V_\ell = {}_C\!<k\ell - \mid V_{C,\ell} + {}_C\!<k\ell - \mid t_{Cs,\ell}(1 + G_{0,\ell}\, T_{C,\ell}). \tag{5.11b}$$

Here $t_{Cs,\ell}$ satisfies the equation

$$t_{Cs,\ell} = V_{s,\ell} + V_{s,\ell}\, G_{C,\ell}\, t_{Cs,\ell},$$

so it is a "short-range operator". Substitution of (5.11) in (5.10) yields

$$\psi_\ell^{(2)}(r) \sim \langle r \mid k\ell + \rangle \left[t_{C,0}^{*-1}\, e^{2i\sigma_\ell} - \tfrac{1}{2}\pi k \,{}_C\langle k\ell - \mid t_{Cs,\ell}(1 + G_{0,\ell} T_{C,\ell}) \mid k + \rangle_0 \right] \quad (5.12)$$

where we have used Eq.(5.3). The phase shift for $V_{C,\ell} + V_{s,\ell}$ is related to $t_{Cs,\ell}$ in the following well-known way,

$${}_C\langle k\ell - \mid t_{Cs,\ell} \mid k\ell + \rangle_C = i(\pi k)^{-1}\, e^{2i\sigma_\ell}(e^{2i\delta_\ell^C} - 1). \quad (5.13)$$

Comparison with Eq.(5.12) shows that the p.w. series $\sum_\ell (4\pi)^{-1}(2\ell + 1)\, P_\ell(x)\, \psi_\ell^{(2)}(r)$ is not proportional to the scattering amplitude in general. Therefore also

$$\psi(\vec{k},\vec{r}) = \sum_{\ell=0}^{\infty} (4\pi)^{-1}(2\ell + 1)\, P_\ell(\hat{k}\cdot\hat{r})\, \psi_\ell(r)$$

has in general not the desired asymptotic behavior (recall that the p.w. series with $\psi_\ell^{(1)}$ is proportional to $\delta(1 - x) = \delta(1 - \hat{k}\cdot\hat{r})$, for $r \to \infty$).

For a short-range potential we obtain for $r \to \infty$, following the same procedure,

$$\psi_\ell(r) \sim -\tfrac{1}{2}\pi k \langle r \mid k\ell + \rangle\langle k\ell - \mid V_\ell \mid k + \rangle_0$$

$$= -\tfrac{1}{2}\pi k \langle r \mid k\ell + \rangle\langle k\ell \mid T_\ell \mid k + \rangle_0. \quad (5.14)$$

In this case the phase shift δ_ℓ is given by

$$\langle k\ell \mid T_\ell \mid k\ell \rangle = i(\pi k)^{-1}\, (e^{2i\delta_\ell} - 1).$$

Apparently the p.w. series with the ψ_ℓ of (5.14) will in general

not be proportional to the scattering amplitude, for $r \to \infty$.

The procedure described above can be repeated for the function $\psi_{w,\ell}$ of Section 4. That is, we replace $\langle r \mid \alpha + \rangle_0$ by a rather arbitrary function w(r) and consider the asymptotic behavior of $\psi_{w,\ell}(r)$, see Eq.(4.9). Again we are not able to find a function w for any potential (except for V_C), such that $\psi_w(\vec{k},\vec{r})$ for $r \to \infty$ approaches the scattering amplitude times an outgoing spherical wave.

So it seems that the pure Coulomb function ψ_s is unique in having the property (5.1). This would mean that the useful property (5.1) of the irregular solution ψ_s is merely a coincidence. Therefore, although the regular physical wave function $\psi^{(+)}(\vec{k},\vec{r})$ for any potential can be expressed as the sum of two irregular solutions, $\psi^{(+)} = \psi_i + \psi_s$, this splitting seems to be useful only in the pure Coulomb case.

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Part C

Simple analytic expressions for the Coulomb off-shell Jost functions

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The off-shell Jost functions have been introduced by Fuda and Whiting. We give simple closed expressions for $f_{C,l}(k,q)$, the off-shell Jost functions for the Coulomb potential, and we derive their connection with the ordinary Coulomb Jost functions $f_{C,l}(k)$.

The concept of a Jost[1] function is well known in the theory of nonrelativistic two-body scattering.[2] Fuda and Whiting[3] have introduced an off-shell generalization of the Jost function $f_l(k)$, which they call the off-shell Jost function $f_l(k,q)$. This function is closely related to the half-off-shell T matrix $T_l(k,q;k^2)$ which plays such an important role in few-body calculations.

For a short-range potential the on-shell limit for $q \to k$ of $f_l(k,q)$ exists and is equal to the ordinary Jost function. This is not true for long-range potentials such as the Coulomb potential. Recently we have derived the $l=0$ Coulomb off-shell Jost function and studied its connection with the Hulthén off-shell Jost function.[4]

In this paper we give an exact closed expression for the Coulomb off-shell Jost function $f_{C,l}(k,q)$ for all l. It follows from this expression that $f_{C,l}(k,q)$ is singular at $q=k$. Below we shall prove that [see Eq. (40.7) of Ref. 4]

$$\lim_{q\to k} \omega f_{C,l}(k,q) = f_{C,l}(k), \quad l = 0, 1, 2, \ldots, \tag{1}$$

with

$$\omega \equiv \left(\frac{q-k}{q+k}\right)^{i\gamma} \frac{\exp(\pi\gamma/2)}{\Gamma(1+i\gamma)}, \tag{2}$$

where γ is Sommerfeld's parameter.

We expect to be able to prove in the near future that a similar relation holds for the off-shell Jost function $f_{C+S,l}(k,q)$ for a potential which is the sum of the Coulomb potential V_C and an arbitrary short-range potential V_S, namely

$$\lim_{q\to k} \omega f_{C+S,l}(k,q) = f_{C+S,l}(k), \tag{3}$$

with the *same* ω of Eq. (2).

Our starting point is an integral representation obtained by Fuda [Ref. 5, Eq. (25)] which we rewrite as follows,

$$f_{C,l}(k,q) = 1 + \tfrac{1}{2}\pi q (q/k)^l \, {}_0\langle ql\,\phi \,|\, V_{C,l} \,|\, kl+\rangle_C f_{C,l}(k). \tag{4}$$

Here $|kl+\rangle_C$ is the (outgoing) Coulomb scattering state and

$$f_{C,l}(k) = \exp(\pi\gamma/2)\Gamma(l+1)/\Gamma(l+1+i\gamma) \tag{5}$$

is the Coulomb Jost function. Furthermore (see Ref. 6),

$${}_0\langle ql\,\phi \,|\, r\rangle = (-)^l \langle r | ql\,\phi\rangle_0 = (2/\pi)^{1/2} i^{-l} h_l^{(+)}(qr).$$

By applying a number of relations existing between various special functions we have been able to derive the following exact expression,

$$\begin{aligned}
{}_0\langle ql\,\phi \,|\, V_{C,l} \,|\, kl+\rangle_C &= {}_C\langle kl- \,|\, V_{C,l} \,|\, ql\,\phi\rangle_0 \\
&= [2i\gamma/(\pi q)] f_{C,l}^{-1}(k)\Gamma(l+1) \\
&\times \sum_{m=0}^{l} [\Gamma(l+m+1)/\Gamma(m+1)](k/q)^m 2^{-l-m} \\
&\times \left[\frac{\Gamma(m-i\gamma)}{\Gamma(l+1+m)\Gamma(l+1-i\gamma)} \right. \\
&\times {}_2F_1(-m-l,\ i\gamma-l;\ 1+i\gamma-m;\ 1-z) \\
&+ (1-z)^{m-i\gamma} \frac{\Gamma(i\gamma-m)}{\Gamma(l+1-m)\Gamma(l+1+i\gamma)} \\
&\left. \times {}_2F_1(m-l,\ -i\gamma-l;\ 1-i\gamma+m;\ 1-z) \right],
\end{aligned} \tag{6}$$

with $z = 2k/(q+k)$. Note that the second term between the square brackets is, apart from the factor $(1-z)^{m-i\gamma}$, just equal to the first term if one replaces m by $-m$ and γ by $-\gamma$.

We point out that both hypergeometric series ${}_2F_1$ occurring in Eq. (6) are terminating ones. Although Eq. (6) looks somewhat complicated, it has the important property that the branch-cut singularity, which is contained in the factor $(1-z)^{-i\gamma}$, can be split off. This has the advantage of revealing the analytic structure of the quantity ${}_0\langle ql\,\phi \,|\, V_{C,l} \,|\, kl+\rangle_C$.

With the help of some further manipulations we have reduced Eq. (6) to the following equivalent, more convenient form,

$$\begin{aligned}
{}_0\langle ql\,\phi \,|\, V_{C,l} \,|\, kl+\rangle_C &= \frac{2}{\pi q} c_{l\gamma} f_{C,l}^{-1}(k) x^{-l} \\
&\times \left[-A_l(x^2;\gamma^2) + x^l \left(\frac{q+k}{q-k}\right)^{i\gamma} P_l^{(-i\gamma,i\gamma)}(u) \right],
\end{aligned} \tag{7}$$

where $x = q/k$, $u = (q^2+k^2)/(2qk)$ and we have used the abbreviation,

$$\begin{aligned}
c_{l\gamma} &\equiv \binom{l+i\gamma}{l}^{-1} \binom{l-i\gamma}{l}^{-1} \\
&= \frac{\Gamma^2(l+1)\Gamma(1+i\gamma)\Gamma(1-i\gamma)}{\Gamma(l+1+i\gamma)\Gamma(l+1-i\gamma)} = \prod_{n=1}^{l} (1+\gamma^2/n^2)^{-1}.
\end{aligned} \tag{8}$$

Furthermore, $P_l^{(-i\gamma,i\gamma)}$ is Jacobi's polynomial and A_l is a certain *polynomial of two variables*. Its degree is, in both variables separately, equal to l and it has real coefficients. For $l=0$, 1, and 2 we have obtained,

$$A_0(x^2;\gamma^2) = 1,$$

$$A_1(x^2;\gamma^2) = \tfrac{1}{2}(x^2 + 1 + 2\gamma^2),$$

$$A_2(x^2;\gamma^2) = \tfrac{1}{8}[3x^4 + 2x^2(1+\gamma^2) + 3 + 2\gamma^2(4+\gamma^2)].$$

For general values of l we have proved the following important properties,

$$A_l(1;\gamma^2) = c_{l\gamma}^{-1}, \tag{9}$$

which gives the on-shell value, and for the case of vanishing potential strength,

$$A_l(x^2;0) = x^l P_l(u),$$

where P_l is Legendre's polynomial. In view of Eqs. (4) and (7) the Coulomb off-shell Jost function is given by

$$f_{C,l}(k,q) = 1 + c_{l\gamma}\left[-A_l(x^2;\gamma^2) + x^l\left(\frac{q+k}{q-k}\right)^{i\gamma} P_l^{(-i\gamma,i\gamma)}(u)\right]. \tag{10}$$

The proof of Eq. (1) now follows from Eqs. (9) and (10) and the equalities

$$P_l^{(-i\gamma,i\gamma)}(1) = \binom{l-i\gamma}{l},$$

$$f_{C,l}(k) = \binom{l-i\gamma}{l} c_{l\gamma} f_{C,0}(k).$$

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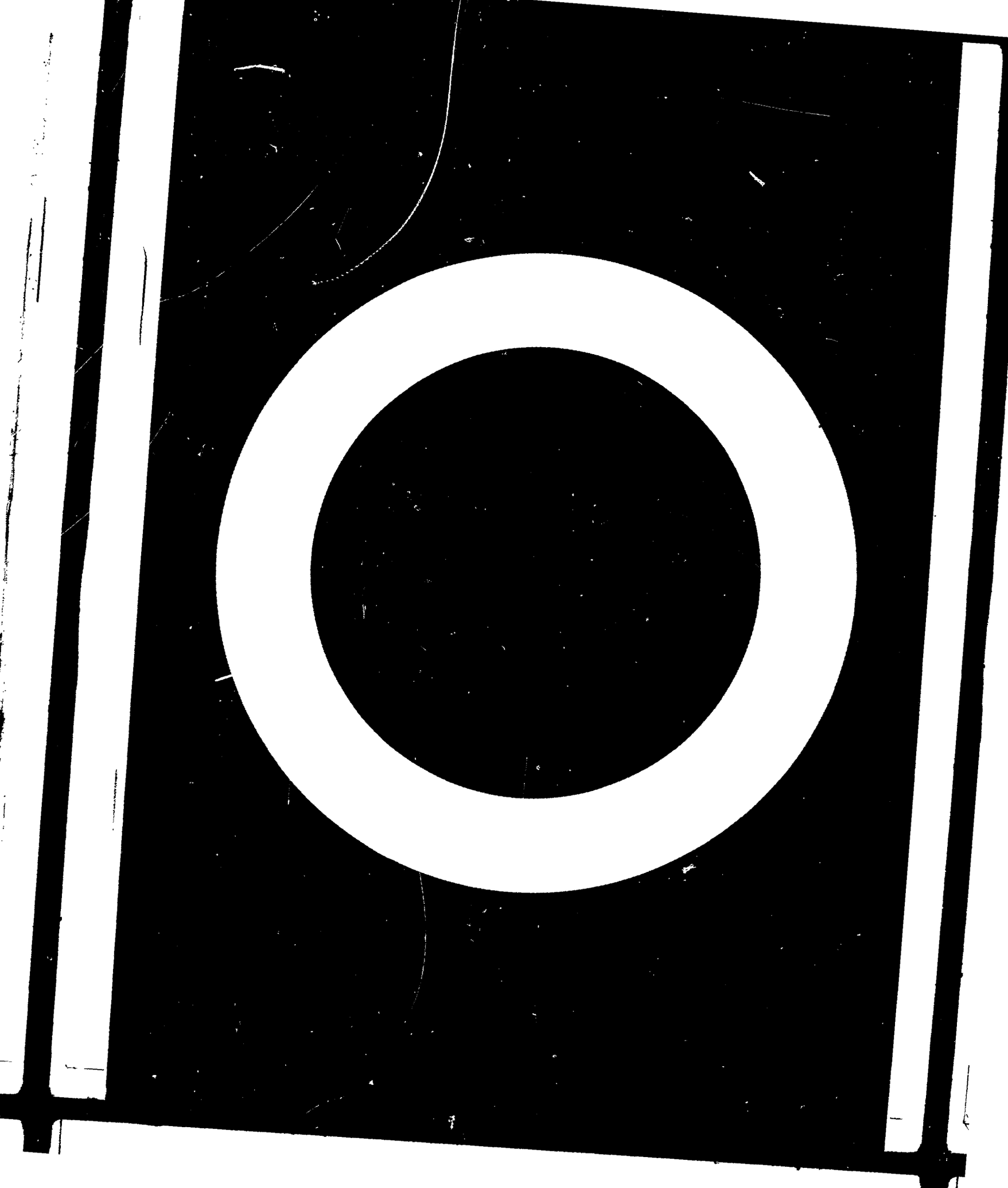

C 2

THE COULOMB AND COULOMB-LIKE OFF-SHELL JOST FUNCTIONS

The off-shell Jost functions are studied for a potential which is the sum of the Coulomb potential and an arbitrary local short-range central potential. We derive their singular on-shell behavior and their connection with the pure Coulomb off-shell Jost functions. For the latter we derive a large variety of interesting explicit analytic expressions which are useful for various purposes.

1. INTRODUCTION

In this paper we investigate the off-shell Jost functions $f_{c\ell}(k,q)$ for the Coulomb potential and the off-shell Jost functions $f_\ell(k,q)$ for a Coulomb plus short-range potential, $V=V_c+V_s$, where V_s is assumed to be local and central. As is now well known, these off-shell Jost functions are interesting in particular in connection with the transition matrices.

In Section 2 we show that $f_{c\ell}(k,q)$ is a basic constituent of $f_\ell(k,q)$. In particular we prove that $f_\ell(k,q)$ has exactly the same singularity in $q=k$ as $f_{c\ell}(k,q)$. In order to obtain the most convenient formula for $f_{c\ell}(k,q)$, a regrouping of certain hypergeometric function expressions has to be performed. By doing this we supply the supplementary proof of the simple formula for $f_{c\ell}(k,q)$ that we have given before [1]. This formula contains Jacobi polynomials and certain polynomials of two variables, A_ℓ.

In Section 3 we derive a large number of interesting expressions for these polynomials A_ℓ. Each of these is useful for different purposes, as is clearly illustrated at the end of Section 3. We shall use the notation of Ref.1.

2. THE OFF-SHELL JOST FUNCTIONS

In this section we will express the off-shell Jost function $f_\ell(k,q)$ for a Coulomb-like potential in terms of the Coulomb off-shell Jost function $f_{c\ell}(k,q)$. By using this expression the on-shell behavior at $q=k$ is easily obtained. Further we shall sketch the derivation of a simple closed expression for $f_{c\ell}(k,q)$.

We start by noting that [2]

$$f_\ell(k,q) = 1 + \tfrac{1}{2}\pi q(q/k)^\ell \; f_\ell(k) \; {}_0\!<q\ell+|\, V_\ell \,|k\ell+>. \qquad (2.1)$$

Here $f_\ell(k)$ is the Jost function and $|k\ell+>$ the "outgoing" scattering state, with energy k^2, for the potential $V_\ell = V_{c\ell} + V_{s\ell}$. We use the Coulomb analog of Eq.(2.1) and apply the two-potential formalism. In this way we get the convenient expression,

$$f_\ell^{-1}(k)\; f_\ell(k,q) = f_{c\ell}^{-1}(k)\; f_{c\ell}(k,q) + {}_c\!<k\ell-|\, V_{s\ell}\, G_\ell \,|\, X_\ell>. \qquad (2.2)$$

Here G_ℓ is the partial-wave Green operator for V_ℓ, and $|\, X_\ell>$ is defined by

$$|\, X_\ell> = \tfrac{1}{2}\pi k \; G_{0\ell}^{-1} \left[(q/k)^{\ell+1} \,|\, q\ell+>_0 \; - \; |\, k\ell+>_0 \right].$$

By inserting

$$<p \,|\, q\ell+>_0 \; = 2(\pi q)^{-1} \,(p/q)^\ell \,(p^2 - q^2)^{-1},$$

we obtain a simple expression for $|\, X_\ell>$ in the momentum representation,

$$<p \,|\, X_\ell> \; = (p/k)^\ell \,(k^2 - q^2) \,/\, (p^2 - q^2). \qquad (2.3)$$

Equation (2.2) is very interesting since it clearly shows that $f_\ell(k,q)$ has exactly the same singularity in $q=k$ as $f_{c\ell}(k,q)$. As a matter of fact, by using Eq.(2.3) we have

$$\lim_{q\to k} \omega \,|\, X_\ell > \;=\; 0, \qquad k > 0,$$

and therefore

$$\lim_{q\to k} \omega\, f_\ell(k,q) \;=\; f_\ell(k), \quad k > 0. \tag{2.4}$$

Here

$$\omega \equiv \left(\frac{q-k}{q+k}\right)^{i\gamma} e^{\pi\gamma/2} \,/\, \Gamma(1+i\gamma) \;=\; f_{c0}(k) \,/\, f_{c0}(k,q).$$

Now we are going to summarily derive explicit expressions for $f_{c\ell}(k,q)$ (cf. Eqs.(4) and (7) of Ref.1). In order to evaluate $_0\!<q\ell+|\,V_{c\ell}\,|\,k\ell+>_c$ which occurs in

$$f_{c\ell}(k,q) \;=\; 1 + \tfrac{1}{2}\pi q (q/k)^\ell f_{c\ell}(k)\; {}_0\!<q\ell+|\,V_{c\ell}\,|\,k\ell+>_c,$$

we use the well-known expressions,

$$_0\!<q\ell+|\,r> \;=\; (2/\pi)^{\frac{1}{2}}\, i^{-\ell}\, h_\ell^{(+)}(qr)$$

$$\;=\; (-)^\ell\, (2/\pi)^{\frac{1}{2}}\, (qr)^{-1}\, e^{iqr}\; {}_2F_0(-\ell,\, \ell+1;\, (2iqr)^{-1}),$$

and

$$<r|\,k\ell+>_c = (2/\pi)^{\frac{1}{2}}\, \ell!\,[f_{c\ell}(k)\,(2\ell+1)!]^{-1} (2ikr)^\ell e^{-ikr}\, {}_1F_1(\ell+1-i\gamma;\, 2\ell+2;\, 2ikr).$$

By using Ref.3, p.278, one obtains

$$_0\!<q\ell+|\,V_{c\ell}\,|\,k\ell+>_c \;=\; 2i\gamma\, \ell!\,[\pi q\, f_{c\ell}(k)\,(2\ell+1)!]^{-1}$$

$$\times \sum_{m=0}^{\ell} (m+1)_\ell\, (k/q)^m\, z^{\ell+1-m}\; {}_2F_1(\ell+1+i\gamma,\, \ell+1-m;\, 2\ell+2;\, z), \tag{2.5}$$

where $z = 2k/(q+k)$. The important step now is to separate off that part which contains the branch-point singularity in $q = k$. To this end we apply two transformations to the hypergeometric function ${}_2F_1$ on the right-hand side of Eq.(2.5) and find (Ref.3, p.47),

$$
{}_2F_1(\ell+1+i\gamma\ ,\ \ell-m+1;\ 2\ell+2;\ z) = (1-z)^{m-i\gamma}
$$

$$
\times\ [\ \Gamma(2\ell+2)\,\Gamma(i\gamma-m)\,/(\Gamma(\ell+1-m)\,\Gamma(\ell+1+i\gamma))\,]\,z^{-2\ell-1}\ {}_2F_1(m-\ell,\ -i\gamma-\ell;\ 1+m-i\gamma;\ 1-z)
$$

$$
+\ [\ \Gamma(2\ell+2)\,\Gamma(m-i\gamma)\,/(\Gamma(\ell+1+m)\,\Gamma(\ell+1-i\gamma))\,]\,z^{-2\ell-1}\ {}_2F_1(-m-\ell,\ i\gamma-\ell;\ 1-m+i\gamma;\ 1-z).
$$

The hypergeometric series for the ${}_2F_1$'s on the right-hand side break off. Therefore these ${}_2F_1$'s can be rewritten in terms of Jacobi polynomials. One has, with $z = 2/(1+x)$,

$$
P_{\ell+m}^{(i\gamma-m,\,-i\gamma-m)}(x) = \binom{\ell+i\gamma}{\ell+m}\, z^{-m-\ell}\ {}_2F_1(-m-\ell,\ i\gamma-\ell;\ 1+i\gamma-m;\ 1-z),
$$

and so

$$
P_{\ell-m}^{(-i\gamma+m,\,i\gamma+m)}(x) = \binom{\ell-i\gamma}{\ell-m} z^{m-\ell}\ {}_2F_1(m-\ell,\ -i\gamma-\ell;\ 1-i\gamma+m;\ 1-z).
$$

When we insert all this in Eq.(2.5) we get a complicated expression. In order to simplify this expression we introduce the polynomials A_ℓ,

$$
A_\ell(q^2/k^2;\ \gamma^2) \equiv \sum_{m=0}^{\ell} \binom{\ell+m}{\ell} (-)^m\, (q/k)^{\ell-m}\ P_{\ell+m}^{(i\gamma-m,\,-i\gamma-m)}(q/k). \tag{2.6}
$$

Furthermore we shall now prove that

$$
\sum_{m=0}^{\ell} \binom{\ell+m}{\ell} \left(\frac{k^2-q^2}{4kq}\right)^m\ P_{\ell-m}^{(m-i\gamma,\,m+i\gamma)}(q/k) = P_\ell^{(-i\gamma,\,i\gamma)}\left(\frac{q^2+k^2}{2qk}\right). \tag{2.7}
$$

For this proof we use

$$
P_n^{(\alpha,\beta)}(\zeta) = \binom{n+\alpha}{n}\, {}_2F_1\,(-n,\ n+1+\alpha+\beta;\ 1+\alpha;\ \tfrac{1}{2}-\tfrac{1}{2}\zeta), \tag{2.8}
$$

and the well-known integral representation,

$$
{}_2F_1\,(a,b;\ c;\ \zeta) = [\Gamma(c)/(\Gamma(b)\Gamma(c-b))]\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-t\zeta)^{-a}dt. \tag{2.9}
$$

The left-hand side of Eq.(2.7) then becomes

$$\Gamma(\ell+1-i\gamma)[\Gamma(-i\gamma-\ell)\,\Gamma^2(\ell+1)]^{-1}\int_0^1 t^{\ell}(1-t)^{-i\gamma-\ell-1}[1-\tfrac{1}{2}t(1-q/k)]^{\ell}$$

$$\times\sum_{m=0}^{\ell}\binom{\ell}{m}[t^{-1}-\tfrac{1}{2}(1-q/k)]^{-m}\,[(k^2-q^2)/(4kq)]^{m}\,dt.$$

By performing the summation and using again Eqs.(2.8) and (2.9) we obtain the desired expression, i.e.,

$$\binom{\ell-i\gamma}{\ell}\,{}_2F_1(-\ell,\ell+1;1-i\gamma;-(q-k)^2/(4kq)) = P_{\ell}^{(-i\gamma,i\gamma)}((q^2+k^2)/(2kq)).$$

This completes the proof of Eq.(2.7).

By inserting the above expressions in Eq.(2.5) and using Eqs. (2.6) and (2.7) we obtain

$$\langle q\ell+|V_{c\ell}|k\ell+\rangle_c = 2c_{\ell\gamma}[\pi q\, f_{c\ell}(k)]^{-1}\left[-x^{-\ell}\,A_{\ell}(x^2;\gamma^2)+f_{c0}(k,q)\,P_{\ell}^{(-i\gamma,i\gamma)}(u)\right], \quad (2.10)$$

cf. Eq.(7) of Ref.1. Here $x=q/k$, $u=(q^2+k^2)/(2kq)$,

$$f_{c0}(k,q) = \left(\frac{q+k}{q-k}\right)^{i\gamma},$$

and

$$c_{\ell\gamma} \equiv \Gamma^2(\ell+1)\,\Gamma(1+i\gamma)\,\Gamma(1-i\gamma)/[\Gamma(\ell+1+i\gamma)\,\Gamma(\ell+1-i\gamma)]. \quad (2.11)$$

In the next section we will derive a large number of useful expressions for the polynomials A_{ℓ}.

3. THE TWO-VARIABLE POLYNOMIALS A_ℓ

In this section we shall derive a number of interesting explicit expressions for the polynomials A_ℓ that occur in the formula (2.10) for the Coulomb off-shell Jost functions $f_{c\ell}(k,q)$.

To start with, we have

$$A_\ell \equiv A_\ell(x^2;\gamma^2) = \sum_{n=0}^{\ell} \binom{\ell+n}{\ell} (-)^n \, x^{\ell-n} \, P_{\ell+n}^{(i\gamma-n,-i\gamma-n)}(x) , \qquad (3.1)$$

(Eq.(2.6)) where $x = q/k$. Substitution of

$$P_{\ell+n}^{(i\gamma-n,-i\gamma-n)}(x) = \Gamma(\ell+1+i\gamma)\,[\,\Gamma(\ell+n+1)\,\Gamma(\ell-n+1)\,\Gamma(i\gamma-\ell)\,]^{-1}$$

$$\times \int_0^1 t^{\ell-n}(1-t)^{i\gamma-\ell-1}\,[\,1-\tfrac{1}{2}t(1-x)\,]^{\ell+n}\,dt,$$

yields

$$A_\ell = \Gamma(\ell+1+i\gamma)\,[\,\Gamma^2(\ell+1)\,\Gamma(i\gamma-\ell)\,]^{-1}$$

$$\times \sum_{n=0}^{\ell} \binom{\ell}{n} \int_0^1 (-tx)^{-n}\,[1-\tfrac{1}{2}t(1-x)]^n\,(tx)^{\ell}\,[1-\tfrac{1}{2}t(1-x)]^{\ell}\,(1-t)^{i\gamma-\ell-1}\,dt.$$

The summation is easily carried out. We then get

$$A_\ell = 4^{-\ell}\, i\gamma\, c_{\ell\gamma}^{-1} \int_0^1 (1-t)^{i\gamma-\ell-1}\,[(2-t)^2 - x^2t^2]^{\ell}\,dt, \qquad (3.2a)$$

where $c_{\ell\gamma}$ is given by Eq.(2.11). The polynomials A_ℓ can also be expressed in terms of Gegenbauer polynomials $C_n^{-\ell}$. Indeed, by introducing $\tau = 1 - t$ we get from Eq.(3.2a),

$$A_\ell = \left(\frac{1-x^2}{4}\right)^{\ell} i\gamma\, c_{\ell\gamma}^{-1} \int_0^1 \tau^{i\gamma-\ell-1}\left(1+\tau^2-2\tau\,\frac{x^2+1}{x^2-1}\right)^{\ell} d\tau. \qquad (3.2b)$$

It is well known that

$$(1-2\tau\zeta+\tau^2)^{\lambda} = \sum_{n=0}^{\infty} C_n^{-\lambda}(\zeta)\,\tau^n, \quad |\tau|<1, \quad \lambda \neq 0.$$

Because of

$$C_n^{-\ell} \equiv 0, \quad n = 2\ell+1, \quad 2\ell+2, \quad \ldots ,$$

we can apply the above expansion to Eq.(3.2b), the result being,

$$A_\ell = \left(\frac{1-x^2}{4}\right)^\ell i\gamma\, c_{\ell\gamma}^{-1} \sum_{n=0}^{2\ell} \frac{1}{n-\ell+i\gamma}\, C_n^{-\ell}\left(\frac{x^2+1}{x^2-1}\right). \tag{3.3a}$$

By using

$$C_{\ell-n}^{-\ell}(\zeta) \equiv C_{\ell+n}^{-\ell}(\zeta) \ , \qquad -\ell \le n \le \ell,$$

we recast the above sum in the more convenient form,

$$\sum_{n=0}^{2\ell} \frac{1}{n-\ell+i\gamma} C_n^{-\ell}\left(\frac{x^2+1}{x^2-1}\right) = -i\gamma \sum_{n=0}^{\ell} \frac{\varepsilon_n}{n^2+\gamma^2} C_{\ell\pm n}^{-\ell}\left(\frac{x^2+1}{x^2-1}\right).$$

Here ε_n is the Neumann symbol,

$$\varepsilon_n = \begin{cases} 1 \ , & n = 0 \\ 2 \ , & n = 1, 2, 3, \ldots \ . \end{cases}$$

In this way we obtain from Eq.(3.3a),

$$A_\ell = \left(\frac{1-x^2}{4}\right)^\ell c_{\ell\gamma}^{-1}\ \gamma^2 \sum_{n=0}^{\ell} \frac{\varepsilon_n}{n^2+\gamma^2}\ C_{\ell\pm n}^{-\ell}\left(\frac{x^2+1}{x^2-1}\right). \tag{3.3b}$$

This expression can be rewritten in terms of the Jacobi polynomials $P_\ell^{(n,-n)}$. By using

$$C_n^\lambda\left(\frac{x^2+1}{x^2-1}\right) = (\lambda)_n (n!)^{-1} \left(\frac{x+1}{x-1}\right)^n {}_2F_1\left(\lambda, -n; 1-\lambda-n; \left(\frac{x-1}{x+1}\right)^2\right)$$

$$= (\lambda)_n (n!)^{-1} \left(\frac{x-1}{x+1}\right)^n {}_2F_1\left(\lambda, -n; 1-\lambda-n; \left(\frac{x+1}{x-1}\right)^2\right),$$

we derive the interesting relation,

$$\left(\frac{4x}{1-x^2}\right)^\ell C_{\ell-n}^{-\ell}\left(\frac{x^2+1}{x^2-1}\right) = \frac{\Gamma^2(\ell+1)}{\Gamma(\ell+n+1)\Gamma(\ell-n+1)} \left(\frac{1-x}{1+x}\right)^n P_\ell^{(n,-n)}(\tfrac{1}{2}x+\tfrac{1}{2}x^{-1}), \ |n| \le \ell. \tag{3.3c}$$

By inserting this in (3.3b) we get

$$A_\ell = x^\ell c_{\ell\gamma}^{-1}\, \gamma^2 \sum_{n=0}^{\ell} \frac{\varepsilon_n}{n^2+\gamma^2} \frac{\Gamma^2(\ell+1)}{\Gamma(\ell+n+1)\,\Gamma(\ell-n+1)} \left(\frac{1-x}{1+x}\right)^n P_\ell^{(n,-n)}(\tfrac{1}{2}x+\tfrac{1}{2}x^{-1}). \tag{3.4a}$$

Further we have

$$P_\ell^{(n,-n)}(z) = (\ell+1)_n\, (z+1)^{\frac{1}{2}n}\, (z-1)^{-\frac{1}{2}n}\ P_\ell^{-n}(z),$$

where P_ℓ^{-n} is Legendre's function of the first kind. Substitution of this expression yields

$$A_\ell = x^\ell \, c_{\ell\gamma}^{-1} \, \gamma^2 \sum_{n=0}^{\ell} \frac{\epsilon_n}{n^2+\gamma^2} \, \frac{\Gamma(\ell+1)}{\Gamma(\ell-n+1)} \, P_\ell^{-n}(\tfrac{1}{2}x + \tfrac{1}{2}x^{-1}), \quad 0<x<1. \tag{3.4b}$$

When $x > 1$ the Legendre function here has to be multiplied by $(-)^n$.

From Eq. (3.2a) one can find an expression containing either ${}_2F_1(\ldots;\tfrac{1}{2})$ or ${}_2F_1(\ldots;-1)$ or ${}_2F_1(\ldots;2)$. It turns out that the formula with ${}_2F_1(\ldots;2)$ is the more convenient one. We obtain this formula by using the binomial expansion, which yields

$$A_\ell = 4^{-\ell} \, i\gamma \, c_{\ell\gamma}^{-1} \int_0^1 (1-t)^{i\gamma-\ell-1} \sum_{m=0}^{\ell} \binom{\ell}{m} (2-t)^{2m} \, (-x^2 t^2)^{\ell-m} .$$

By again using the binomial expansion,

$$(2-t)^{2m} = \sum_{n=0}^{2m} \binom{2m}{n} \, 2^n (-t)^{2m-n},$$

the integration can be performed, with the result

$$\int_0^1 (1-t)^{i\gamma-\ell-1} \, t^{2\ell-n} \, dt = \Gamma(2\ell-n+1)\,\Gamma(i\gamma-\ell) \,/\, \Gamma(i\gamma+\ell-n+1).$$

In this way we get

$$A_\ell = 4^{-\ell} \, i\gamma \, c_{\ell\gamma}^{-1} \, (2\ell)! \, [\Gamma(i\gamma-\ell) \,/\, \Gamma(\ell+1+i\gamma)]$$

$$\times \sum_{m=0}^{\ell} \binom{\ell}{m} (-x^2)^{\ell-m} \sum_{n=0}^{2m} (-2m)_n \, (-\ell-i\gamma)_n \, 2^n \,/\, [n!\,(-2\ell)_n] .$$

The sum $\sum_n$ is a terminating hypergeometric series for which we write ${}_2F_1(-2m, -\ell-i\gamma; -2\ell; 2)$. One should be careful here, since the third parameter, -2ℓ, is a nonpositive integer. By using the expression (2.11) for $c_{\ell\gamma}$ we obtain

$$A_\ell = 4^{-\ell} \binom{2\ell}{\ell} \sum_{m=0}^{\ell} \binom{\ell}{m} (-)^m x^{2\ell-2m} \, {}_2F_1(-2m, -\ell-i\gamma; -2\ell; 2).$$

We note that A_ℓ is a function of γ^2 rather than of γ, as can be seen from Eq.(3.3b). So we have, by replacing m by $\ell - n$,

$$A_\ell = 4^{-\ell}\binom{2\ell}{\ell}\sum_{n=0}^{\ell}\binom{\ell}{n}(-)^{\ell-n}\,x^{2n}\,{}_2F_1(2n-2\ell,\,-\ell\pm i\gamma;\,-2\ell;\,2). \qquad (3.5a)$$

The h.f. ${}_2F_1(\ldots;2)$ can be expressed in terms of a Jacobi polynomial with argument 0. By using Ref.3, p.212, we have

$$A_\ell = \frac{(-)^\ell}{\ell!}\sum_{n=0}^{\ell}\frac{(2n)!}{n!}\,\frac{(2\ell-2n)!}{(\ell-n)!}\,(-\tfrac{1}{4}x^2)^n\,P_{2\ell-2n}^{(2n-\ell+i\gamma,\,2n-\ell-i\gamma)}(0), \qquad (3.5b)$$

or

$$A_\ell = \frac{1}{\ell!}\,(\tfrac{1}{4}x^2)^\ell\sum_{n=0}^{\ell}\frac{(2n)!}{n!}\,\frac{(2\ell-2n)!}{(\ell-n)!}\,(-\tfrac{1}{4}x^2)^{-n}\,P_{2n}^{(\ell-2n+i\gamma,\,\ell-2n-i\gamma)}(0). \qquad (3.5c)$$

Now we come to the derivation of the most elegant formula for A_ℓ, i.e., a generalized hypergeometric function ${}_3F_2$ with argument $1-x^2$. From Eq.(3.2a) we have

$$A_\ell = i\gamma\,c_{\ell\gamma}^{-1}\int_0^1 (1-t)^{i\gamma-\ell-1}\,[\,1-t+\tfrac{1}{4}(1-x^2)t^2\,]^\ell\,dt.$$

After substitution of

$$[\,1-t+\tfrac{1}{4}(1-x^2)t^2\,]^\ell = \sum_{n=0}^{\ell}\binom{\ell}{n}(1-t)^{\ell-n}\,t^{2n}\,2^{-2n}(1-x^2)^n,$$

we can perform the integration, the result being

$$\int_0^1 (1-t)^{i\gamma-1-n}\,t^{2n}\,dt = \Gamma(i\gamma-n)\,\Gamma(2n+1)/\Gamma(i\gamma+n+1).$$

In this way we obtain

$$A_\ell = c_{\ell\gamma}^{-1}\sum_{n=0}^{\ell}\frac{(2n)!}{n!}\,\frac{(-\ell)_n}{(1+i\gamma)_n\,(1-i\gamma)_n}\,2^{-2n}(1-x^2)^n. \qquad (3.6a)$$

By using the doubling formula for the gamma function we have

$$(2n)! = (\tfrac{1}{2})_n\,2^{2n}\,n!,$$

and so

$$A_\ell = c^{-1}_{\ell\gamma}\, {}_3F_2(-\ell, 1, \tfrac{1}{2};\ 1 + i\gamma, 1 - i\gamma;\ 1 - x^2). \qquad (3.6b)$$

An alternative expression is

$$A_\ell = \sum_{n=0}^{\ell} \frac{\Gamma(\ell + 1 + i\gamma)}{\Gamma(n + 1 + i\gamma)} \frac{\Gamma(\ell + 1 - i\gamma)}{\Gamma(n + 1 - i\gamma)} \frac{(\tfrac{1}{2})_n\, (x^2 - 1)^n}{\Gamma(\ell + 1)\, \Gamma(\ell + 1 - n)}, \qquad (3.6c)$$

where we have inserted Eq.(2.11). Furthermore we have the terminating hypergeometric series,

$$A_\ell = \frac{(\tfrac{1}{2})_\ell}{\ell!} (x^2 - 1)^\ell \sum_{n=0}^{\ell} \frac{(i\gamma - \ell)_n\, (-i\gamma - \ell)_n}{(\tfrac{1}{2} - \ell)_n} \frac{(1 - x^2)^{-n}}{n!}. \qquad (3.6d)$$

From Eq.(3.6c) one can derive an expression involving a ${}_3F_2$ with argument 1. By inserting

$$(x^2 - 1)^n = \sum_{m=0}^{n} \binom{n}{m} x^{2m} (-)^{n-m}$$

in (3.6c), and introducing the new summation variable $\nu = n - m$, we have

$$\sum_{n=0}^{\ell} \sum_{m=0}^{n} \ldots = \sum_{m=0}^{\ell} \sum_{\nu=0}^{\ell-m} \ldots .$$

It turns out that the sum $\sum_{\nu}$ is a ${}_3F_2(\ldots; 1)$ and thus we obtain

$$A_\ell = \sum_{n=0}^{\ell} \frac{x^{2n}\, (\tfrac{1}{2})_n}{\Gamma(\ell + 1)\, \Gamma(\ell + 1 - n)} \frac{\Gamma(\ell + 1 + i\gamma)\, \Gamma(\ell + 1 - i\gamma)}{\Gamma(n + 1 + i\gamma)\, \Gamma(n + 1 - i\gamma)}$$

$$\times\ {}_3F_2(n - \ell, n + 1, n + \tfrac{1}{2};\ n + 1 + i\gamma, n + 1 - i\gamma;\ 1). \qquad (3.7)$$

We transform this ${}_3F_2$ into a ${}_3F_2$ with different parameters by applying a generalization of Dixon's theorem, see Slater [4], p.52,

$${}_3F_2(n - \ell, n + 1, n + \tfrac{1}{2};\ n + 1 + i\gamma, n + 1 - i\gamma;\ 1)$$

$$= \Gamma\begin{bmatrix} \ell - n + \tfrac{1}{2}, & n + 1 + i\gamma, & n + 1 - i\gamma \\ \tfrac{1}{2}, & \ell + 1, & n + 1 \end{bmatrix} {}_3F_2(i\gamma, -i\gamma, \ell - n + \tfrac{1}{2};\ \tfrac{1}{2}, \ell + 1;\ 1).$$

Then we have from (3.7),

$$A_\ell = \frac{\Gamma(\ell+1+i\gamma)\,\Gamma(\ell+1-i\gamma)}{\Gamma^2(\ell+1)} \sum_{n=0}^{\ell} \frac{x^{2n}}{n!} \frac{(\tfrac{1}{2})_n \Gamma(\ell-n+\tfrac{1}{2})}{\Gamma(\tfrac{1}{2})\Gamma(\ell-n+1)}$$

$$\times\ {}_3F_2(i\gamma, -i\gamma, \ell-n+\tfrac{1}{2};\ \tfrac{1}{2}, \ell+1;\ 1). \qquad (3.8a)$$

Note that the hypergeometric series for this ${}_3F_2$ breaks off when $i\gamma = 0, -1, -2, \ldots$. The case $i\gamma = 0$ corresponds to no Coulomb interaction at all. On the other hand, $i\gamma = -1, -2, -3, \ldots$ occurs for the Coulomb bound states.

It is not difficult to derive from Eq.(3.8a) the corresponding series with *decreasing* powers of x. This expression has almost exactly the same form as (3.8a), namely

$$A_\ell = \frac{\Gamma(\ell+1+i\gamma)\,\Gamma(\ell+1-i\gamma)}{\Gamma^2(\ell+1)} \sum_{n=0}^{\ell} \frac{x^{2\ell-2n}}{n!} \frac{(\tfrac{1}{2})_n \Gamma(\ell-n+\tfrac{1}{2})}{\Gamma(\tfrac{1}{2})\Gamma(\ell-n+1)}$$

$$\times\ {}_3F_2(i\gamma, -i\gamma, n+\tfrac{1}{2};\ \tfrac{1}{2}, \ell+1;\ 1). \qquad (3.8b)$$

By comparing this expression with Eq.(3.5c) we get the interesting equality

$${}_3F_2(i\gamma, -i\gamma, n+\tfrac{1}{2};\ \tfrac{1}{2}, \ell+1;\ 1) = \frac{(-4)^n\,(\ell-n)!\,\ell!\,n!}{\Gamma(\ell+1+i\gamma)\,\Gamma(\ell+1-i\gamma)}\, P_{2n}^{(\ell-2n+i\gamma,\,\ell-2n-i\gamma)}(0).$$

In the particular case when $\ell = 2n$ this expression can be simplified. By using (e.g., Ref.3, p.167)

$$\Gamma(1+\mu)\,P_\nu^{-\mu}(0) = {}_2F_1(-\nu, \nu+1;\ \mu+1;\ \tfrac{1}{2})$$

$$= \Gamma(1+\tfrac{1}{2}\mu)\,\Gamma(\tfrac{1}{2}+\tfrac{1}{2}\mu)\,[\Gamma(1+\tfrac{1}{2}\mu+\tfrac{1}{2}\nu)\,\Gamma(\tfrac{1}{2}+\tfrac{1}{2}\mu-\tfrac{1}{2}\nu)]^{-1},$$

we get

$$P_{2n}^{(i\gamma,-i\gamma)}(0) = 2^{2n}\,\Gamma(\tfrac{1}{2}+\tfrac{1}{2}i\gamma+n)\,[\,\Gamma(\tfrac{1}{2}+\tfrac{1}{2}i\gamma-n)\,\Gamma(2n+1)\,]^{-1}$$

$$= \frac{(-)^n n!}{(\tfrac{1}{2})_n} \binom{n-\tfrac{1}{2}+\tfrac{1}{2}i\gamma}{n} \binom{n-\tfrac{1}{2}-\tfrac{1}{2}i\gamma}{n}, \qquad (3.8c)$$

and so

$$ {}_3F_2(i\gamma, -i\gamma, n+\tfrac{1}{2};\ \tfrac{1}{2}, 2n+1;\ 1) = \frac{\pi\,\Gamma^2(n+1)}{\Gamma(\frac{1}{2}+\frac{1}{2}i\gamma)\,\Gamma(\frac{1}{2}-\frac{1}{2}i\gamma)\,\Gamma(n+1+\frac{1}{2}i\gamma)\,\Gamma(n+1-\frac{1}{2}i\gamma)}, $$

cf. Eq.(2.3.3.13) of Ref.4.

One can see from Eq.(3.6c) in particular that the degree of the polynomial $A_\ell \equiv A_\ell(x^2;\gamma^2)$ is ℓ, both in x^2 and in γ^2,

$$ A_\ell = \sum_{n=0}^{\ell} x^{2\ell-2n}\, D_n^{(\ell)}(\gamma^2), \tag{3.9a} $$

$$ A_\ell = \sum_{n=0}^{\ell} \gamma^{2\ell-2n}\, F_n^{(\ell)}(x^2). \tag{3.9b} $$

Here $D_n^{(\ell)}$ and $F_n^{(\ell)}$ are certain polynomials of degree n. It turns out that Eq.(3.9b) is less suitable for practical applications, so we shall mainly restrict ourselves to the expansion in the $D_n^{(\ell)}$'s. One can also write A_ℓ as

$$ A_\ell = \sum_{n=0}^{\ell} \sum_{m=0}^{n} x^{2\ell-2n}\, \gamma^{2m}\, a_{n,m}^{(\ell)}. \tag{3.10} $$

Here the coefficients $a_{n,m}^{(\ell)}$ are *real positive* numbers, as can be proven with the help of Eq.(3.8).

It is of interest to discuss a number of special cases. In the first place we consider the zero-energy case, $k = 0$. Recalling $x \equiv q/k$ and $\gamma \equiv -s/k$, we have from Eq.(3.6c),

$$ A_\ell \simeq \gamma^{2\ell}(\ell!)^{-2}\, {}_3F_0(-\ell, 1, \tfrac{1}{2}; -x^2/\gamma^2), \quad k \to 0, $$

and so

$$ \lim_{k\to 0} \gamma^{-2\ell} A_\ell = (\ell!)^{-2}\, {}_3F_0(-\ell, 1, \tfrac{1}{2};\ -q^2/s^2). \tag{3.11} $$

On the other hand, for $k \to \infty$ we have $x \to 0$ and $\gamma \to 0$. In this case we get from Eq.(3.8),

$$A_\ell(0;0) = a_{\ell,0}^{(\ell)} = (\tfrac{1}{2})_\ell / \ell! = 4^{-\ell} \binom{2\ell}{\ell}. \tag{3.12}$$

For $x = 1$ one easily derives from Eq.(3.6b)

$$A_\ell(1;\gamma^2) = c_{\ell\gamma}^{-1} = \binom{\ell+i\gamma}{\ell}\binom{\ell-i\gamma}{\ell}. \tag{3.13}$$

The numbers $a_{n,m}^{(\ell)}(n,m = 0, 1, \ldots, \ell)$ can be considered as a matrix, which is triangular because of

$$a_{n,m}^{(\ell)} = 0, \quad n < m.$$

The matrix elements on the principal axis are given by

$$a_{n,n}^{(\ell)} = \frac{4^{n-\ell}(2\ell - 2n)!}{\ell!\, n!\, (\ell - n)!}. \tag{3.14}$$

In particular for $n = \ell$ one has

$$a_{\ell,\ell}^{(\ell)} = F_0^{(\ell)} = (\ell!)^{-2}. \tag{3.15}$$

Equation (3.14) is obtained by considering

$$D_n^{(\ell)}(\gamma^2) = \sum_{m=0}^{n} \gamma^{2m} a_{n,m}^{(\ell)},$$

and

$$D_n^{(\ell)}(\gamma^2) = (-)^n 4^{n-\ell} \frac{(2n)!(2\ell - 2n)!}{\ell!\, n!\, (\ell - n)!} P_{2n}^{(\ell-2n+i\gamma,\,\ell-2n-i\gamma)}(0)$$

$$= (-)^n 4^{-\ell} \binom{2\ell}{\ell}\binom{\ell}{n}\, {}_2F_1(-2n, -\ell \pm i\gamma; -2\ell; 2). \tag{3.16}$$

It is interesting to note the connection of $D_n^{(\ell)}$ with certain known polynomials, namely Krawtchouk's polynomials $k_n(z)$, which depend in addition on a positive variable $p < 1$ and a positive integer N. These polynomials are associated with the binomial distribution in probability theory. According to Refs.5 and 6 one has, with $p = \frac{1}{2}$ and $N = 2\ell$,

$$k_{2n}(i\gamma+\ell) = 4^{-n}\binom{i\gamma+\ell}{2n}\,{}_2F_1(-2n,\, i\gamma-\ell;\; 1+\ell+i\gamma-2n;\; -1)$$

$$= P_{2n}^{(\ell-2n\pm i\gamma,\,\ell-2n\mp i\gamma)}(0) \,. \tag{3.17}$$

Since $k_n(z)$ is defined for an integer variable z only, $D_n^{(\ell)}$ may be considered as a generalization of k_{2n}.

For $\gamma = 0$ we get from Eqs.(3.4a) and (3.6b),

$$A_\ell(x^2;0) = x^\ell\, P_\ell(\tfrac{1}{2}x + \tfrac{1}{2}x^{-1})$$

$$= {}_2F_1(-\ell,\, \tfrac{1}{2};\; 1;\; 1-x^2). \tag{3.18}$$

By using these expressions we obtain

$$a_{n,0}^{(\ell)} = a_{\ell-n,0}^{(\ell)} = D_n^{(\ell)}(0) = 4^{-\ell}\binom{2n}{n}\binom{2\ell-2n}{\ell-n}. \tag{3.19}$$

Further we derive from Eqs.(3.8c) and (3.15),

$$D_n^{(2n)}(\gamma^2) = \binom{n-\frac{1}{2}+\frac{1}{2}i\gamma}{n}\binom{n-\frac{1}{2}-\frac{1}{2}i\gamma}{n}, \tag{3.20}$$

which again shows the dependence on γ^2 rather than on γ. For $x = 0$ we have from Eq.(3.15),

$$A_\ell(0;\gamma^2) = D_\ell^{(\ell)}(\gamma^2) = (-)^\ell\binom{2\ell}{\ell} P_{2\ell}^{(i\gamma-\ell,\,-i\gamma-\ell)}(0) \,. \tag{3.21}$$

In order to obtain explicit expressions for $A_0, A_1, \ldots,$ Eq.(3.6) is very useful. We first recast Eq.(3.6c) in a more explicit form,

$$A_\ell = \binom{\ell+i\gamma}{\ell}\binom{\ell-i\gamma}{\ell}\sum_{n=0}^{\ell}\frac{(-\ell)_n\,(\frac{1}{2})_n}{(1+i\gamma)_n\,(1-i\gamma)_n}\,(1-x^2)^n$$

$$= (\ell!)^{-2}\sum_{\nu=0}^{\ell}(-x^2)^\nu\sum_{n=\nu}^{\ell}\binom{n}{\nu}(-\ell)_n\,(\tfrac{1}{2})_n\prod_{m=n+1}^{\ell}(m^2+\gamma^2). \tag{3.22}$$

Therefore we have

$$D_{\ell-\nu}^{(\ell)}(\gamma^2) = (\ell!)^{-1} \sum_{n=\nu}^{\ell} \left\{ \begin{matrix} n \\ \nu \end{matrix} \right\} \frac{(-)^{n+\nu}(\frac{1}{2})_n}{\Gamma(\ell+1-n)} \prod_{m=n+1}^{\ell} (m^2+\gamma^2). \tag{3.23}$$

In particular,

$$D_0^{(\ell)} = \frac{\Gamma(\ell+\frac{1}{2})}{\ell!\ \Gamma(\frac{1}{2})},$$

$$D_1^{(\ell)} = \frac{\Gamma(\ell-\frac{1}{2})}{\ell!\ \Gamma(\frac{1}{2})} (\gamma^2 + \tfrac{1}{2}\ell),$$

$$D_2^{(\ell)} = \frac{\Gamma(\ell-\frac{3}{2})}{\ell!\ \Gamma(\frac{1}{2})} \tfrac{1}{2} [\gamma^4 + \gamma^2(3\ell-2) + \tfrac{1}{4}\ell(\ell-1)],$$

$$D_3^{(\ell)} = \frac{\Gamma(\ell-\frac{5}{2})}{\ell!\ \Gamma(\frac{1}{2})} \tfrac{1}{6} [\gamma^6 + \gamma^4(\tfrac{15}{2}\ell - 10) + \tfrac{1}{4}\gamma^2(45\ell^2 - 105\ell + 46) + \tfrac{15}{8}\ell(\ell-1)(\ell-2)]. \tag{3.24}$$

Finally we give the first four polynomials A_ℓ in explicit form,

$$A_0 = 1,$$

$$A_1 = \tfrac{1}{2}(x^2 + 1 + 2\gamma^2),$$

$$A_2 = \tfrac{1}{8}[\, 3x^4 + 2x^2(1+\gamma^2) + 3 + 8\gamma^2 + 2\gamma^4 \,],$$

$$A_3 = \tfrac{1}{48}[\, 15x^6 + 3x^4(3+2\gamma^2) + x^2(9 + 14\gamma^2 + 2\gamma^4) + \tfrac{1}{3}(45 + 136\gamma^2 + 50\gamma^4 + 4\gamma^6) \,]. \tag{3.25}$$

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C 3

OFF-SHELL SCATTERING BY COULOMB-LIKE POTENTIALS

We derive closed expressions for and interrelationships between off-shell and on-shell scattering quantities for Coulomb plus short-range potentials. In particular we introduce off-shell Jost states and show how the transition matrices are obtained from these states. We discuss some formulas connecting the coordinate and momentum representatives of certain quantities. For the pure Coulomb case we derive analytic expressions for the Jost state and the off-shell Jost state for $\ell = 0$ in the momentum representation.

1. INTRODUCTION

In this paper we study off-shell scattering by a potential which is the sum of the Coulomb potential and a local central potential of short range. We derive many interesting expressions, notably for the Jost functions, the off-shell Jost functions and the on-shell and off-shell "Jost states". These quantities are closely connected with the transition matrix which plays such an important role in scattering theory.

First, in Section 2, we confine ourselves to a general local short-range central potential. Here we derive many interrelationships between the above quantities. Only a few of these are well known, e.g., the defining expression for the (off-shell) Jost functions in terms of the (off-shell) Jost solutions in the coordinate representation. We give the momentum representation equivalents of these expressions which have a somewhat simpler form.

Some of the equations given in Section 2 are also valid for Coulomb-like potentials. However, some have to be modified for such potentials with a long range. To this end we consider in Section 3 the pure Coulomb case. By working out a number of explicit expressions we pave the way for the treatment of the general case of Coulomb plus short-range potentials, which will be given in Section 4. We also prove the validity of two conjectures made in Ref.1.

Furthermore we derive in Section 3 some interesting analytic expressions, notably for the $\ell = 0$ Coulomb Jost state and the off-shell Jost state in the momentum representation. In these expressions we encounter a certain hypergeometric function which appears in many other Coulomb quantities. Only its argument is different for the various different cases.

We will mainly use the notation of Refs.1 and 2. In particular

the energy is k^2 with $\mathrm{Im}\, k \downarrow 0$ and the energy-dependence of G, G_0 and T will be suppressed. However, instead of the Jost solution $f_\ell(k,r)$ and the off-shell Jost solution $f_\ell(k,q,r)$ of the *radial* differential equations we will use the Jost solution $< r \mid k\ell \uparrow >$ and the off-shell Jost solution $< r \mid kq\ell \uparrow >$ of the partial-wave projected equations. Here q is an off-shell momentum variable for which we assume $\mathrm{Im}\, q \geq 0$. We shall also consider the Hankel transforms of the above Jost solutions. These are denoted by $< p \mid k\ell \uparrow >$ and $< p \mid kq\ell \uparrow >$, respectively. We call $\mid k\ell \uparrow >$ the Jost state and $\mid kq\ell \uparrow >$ the off-shell Jost state.

2. THE SHORT-RANGE POTENTIAL CASE

In this section we confine ourselves to a local central potential $V(r)$, having a short range. Let us first recall Fuda's definition of the off-shell Jost solution [3]: $f_\ell(k,q,r)$ is that solution of the inhomogeneous differential equation

$$\left[k^2+\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}-V(r)\right] f_\ell(k,q,r) = (k^2-q^2)\, i^\ell\, qr\, h_\ell^{(+)}(qr), \tag{2.1}$$

which satisfies the asymptotic condition

$$\lim_{r\to\infty} f_\ell(k,q,r)\; e^{-iqr} = 1.$$

We introduce the "state" $|\, kq\ell\uparrow\rangle$ by

$$\langle r\,|\,kq\ell\uparrow\rangle \;\equiv\; (2/\pi)^{\frac{1}{2}}\,(qr)^{-1}\; f_\ell(k,q,r). \tag{2.2}$$

This may be compared with the "state" $|\, k\ell\uparrow\rangle$ that we introduced before,

$$\langle r\,|\,k\ell\uparrow\rangle \;\equiv\; (2/\pi)^{\frac{1}{2}}\,(kr)^{-1}\; f_\ell(k,r). \tag{2.3}$$

Let $H_\ell = H_{0\ell} + V_\ell$ be the partial-wave Hamiltonian, then we obtain from Eq.(2.1),

$$(k^2 - H_\ell)\,|\,kq\ell\uparrow\rangle = (k^2 - q^2)\,|\,q\ell\uparrow\rangle_0\,, \tag{2.4a}$$

that is,

$$G_\ell^{-1}\,|\,kq\ell\uparrow\rangle = G_{0\ell}^{-1}\,|\,q\ell\uparrow\rangle_0\,. \tag{2.4b}$$

Here $|\,q\ell\uparrow\rangle_0$ is the Jost state corresponding to $V\equiv 0$. In the coordinate representation one has

$$\langle r\,|\,q\ell\uparrow\rangle_0 \;= (2/\pi)^{\frac{1}{2}}\, i^\ell\, h_\ell^{(+)}(qr).$$

Furthermore we denote the scattering state for $V\equiv 0$ and energy k^2 by $|\,k\ell\rangle$, or by $|\,k\rangle$ when no confusion arises, e.g., $T_\ell\,|\,k\ell\rangle = T_\ell\,|\,k\rangle$. It should be noted that Eqs.(2.4) are valid only in the coordinate

representation. We shall call $\langle r \mid kq\ell\uparrow\rangle$ the off-shell Jost solution of the "inhomogeneous Schrödinger equation" corresponding to Eqs.(2.4).

We would like to have a closed expression for $\mid kq\ell\uparrow\rangle$. It is easily seen from Eq.(2.4b) that $G_\ell G_{0\ell}^{-1} \mid q\ell\uparrow\rangle_0$ is a particular solution of an *in*homogeneous differential equation. If one adds to this quantity an arbitrary solution of the corresponding homogeneous differential equation it remains a solution of (2.4). Now we have, again in the coordinate representation only,

$$(k^2 - H_\ell) \mid k\ell\uparrow\rangle = (k^2 - H_\ell) \mid k\ell\downarrow\rangle = 0. \tag{2.5}$$

Furthermore any solution is a linear combination of $\mid k\ell\uparrow\rangle$ and $\mid k\ell\downarrow\rangle$. Therefore, using $G_\ell = G_{0\ell} + G_{0\ell}\, T_\ell\, G_{0\ell}$ we obtain,

$$\mid kq\ell\uparrow\rangle = (1 + G_{0\ell}\, T_\ell) \mid q\ell\uparrow\rangle_0 + c_1 \mid k\ell\uparrow\rangle + c_2 \mid k\ell\downarrow\rangle. \tag{2.6}$$

In order to determine c_1 and c_2 we consider the asymptotic behavior of the right-hand side. By using

$$\langle r \mid G_\ell \mid r' \rangle = -\tfrac{1}{2}\pi k \langle r_> \mid k\ell\uparrow\rangle \langle k\ell - \mid r_< \rangle,$$

we obtain, for $r \to \infty$,

$$\langle r \mid G_{0\ell} T_\ell \mid q\ell\uparrow\rangle_0 = \langle r \mid G_\ell V_\ell \mid q\ell\uparrow\rangle_0 \sim -\tfrac{1}{2}\pi k \langle r \mid k\ell\uparrow\rangle \langle k\ell - \mid V_\ell \mid q\ell\uparrow\rangle_0, \quad r \to \infty.$$

Since $\langle r \mid kq\ell\uparrow\rangle$ has by definition the same asymptotic behavior as $\langle r \mid q\ell\uparrow\rangle_0$, namely,

$$\lim_{r\to\infty} \langle r \mid kq\ell\uparrow\rangle\, qr\, e^{-iqr} = (2/\pi)^{\frac{1}{2}},$$

we find

$$c_1 = \tfrac{1}{2}\pi k \langle k\ell - \mid V_\ell \mid q\ell\uparrow\rangle_0,$$

$$c_2 = 0.$$

It is convenient to rewrite c_1 in terms of the *off-shell Jost func-*

tion $f_\ell(k,q)$. Fuda [4] has given a closed expression which in our notation reads,

$$f_\ell(k,q) = 1 + \tfrac{1}{2}\pi q(q/k)^\ell \; f_\ell(k) \, \langle k\ell - | \, V_\ell \, | \, q\ell + \rangle_0 \, . \tag{2.7a}$$

Some equivalent expressions are

$$f_\ell(k,q) = 1 + \tfrac{1}{2}\pi q(q/k)^\ell \; f_\ell(k) \, \langle k\ell \, | \, T_\ell \, | \, q\ell + \rangle_0 \tag{2.7b}$$

$$= 1 + \tfrac{1}{2}\pi q(q/k)^\ell \; f_\ell(k) \, \langle q\ell + \, | \, T_\ell \, | \, k\ell \rangle \tag{2.7c}$$

$$= 1 + \tfrac{1}{2}\pi q(q/k)^\ell \; f_\ell(k) \, \langle q\ell + \, | \, V_\ell \, | \, k\ell + \rangle . \tag{2.7d}$$

By substituting c_1 in Eq.(2.6) and using (2.7a) we obtain the convenient expression,

$$| \, kq\ell + \rangle = (1 + G_{0\ell} \; T_\ell) \, | \, q\ell + \rangle_0 + | \, k\ell + \rangle \, (k/q)^{\ell+1} \, [f_\ell(k,q) - 1]/f_\ell(k). \tag{2.8}$$

From now on we shall suppress the argument k of the Jost function, so we write f_ℓ instead of $f_\ell(k)$.

When the potential has a short range the off-shell Jost function and solution are continuous in $q = k$, (cf. Ref.3)

$$\lim_{q \to k} \; f_\ell(k,q) = f_\ell , \tag{2.9}$$

$$\lim_{q \to k} \; | \, kq\ell + \rangle = | \, k\ell + \rangle . \tag{2.10}$$

By taking the limit $q \to k$ in Eq.(2.8) we obtain

$$| \, k\ell + \rangle = (1 + G_{0\ell} \; T_\ell) \, | \, k\ell + \rangle_0 \, f_\ell . \tag{2.11}$$

We multiply both sides of this equation by V_ℓ and get

$$V_\ell \, | \, k\ell + \rangle = T_\ell \, | \, k\ell + \rangle_0 \, f_\ell . \tag{2.12}$$

This equality turns out to be very useful below.

Multiplying Eq.(2.8) by V_ℓ and using Eq.(2.12) we obtain

$$V_\ell \mid kq\ell\uparrow\rangle = T_\ell \mid q\ell\uparrow\rangle_0 + T_\ell \mid k\ell\uparrow\rangle_0 (k/q)^{\ell+1} [f_\ell(k,q) - 1]. \qquad (2.13)$$

Further we get some closed formulas for the Jost function from Eqs.(7) by taking $q = k$. We have

$$f_\ell = f_\ell(k,k) = 1 + \tfrac{1}{2}\pi k \, f_\ell \langle k\ell- \mid V_\ell \mid k\ell\uparrow\rangle_0,$$

and therefore

$$f_\ell^{-1} = 1 - \tfrac{1}{2}\pi k \langle k\ell- \mid V_\ell \mid k\ell\uparrow\rangle_0 = 1 - \tfrac{1}{2}\pi k \langle k\ell \mid T_\ell \mid k\ell\uparrow\rangle_0$$

$$= 1 - \tfrac{1}{2}\pi k \langle k\ell\downarrow \mid V_\ell \mid k\ell+\rangle = 1 - \tfrac{1}{2}\pi k \langle k\ell\downarrow \mid T_\ell \mid k\ell\rangle. \qquad (2.14)$$

By using Eq.(2.12) we obtain from Eq.(2.14),

$$f_\ell = 1 + \tfrac{1}{2}\pi k \langle k\ell \mid V_\ell \mid k\ell\uparrow\rangle = 1 + \tfrac{1}{2}\pi k \langle k\ell\downarrow \mid V_\ell \mid k\ell\rangle. \qquad (2.15)$$

We shall need the connection between $\langle p \mid k\ell\uparrow\rangle$ and $\langle p \mid V \mid k\ell\uparrow\rangle$. From Eq.(2.11) we have

$$\mid k\ell\uparrow\rangle f_\ell^{-1} = \mid k\ell\uparrow\rangle_0 + G_{0\ell} \, T_\ell \mid k\ell\uparrow\rangle_0$$

$$= \mid k\ell\uparrow\rangle_0 + G_{0\ell} \, V_\ell \mid k\ell\uparrow\rangle f_\ell^{-1}. \qquad (2.16)$$

Therefore

$$\langle p \mid k\ell\uparrow\rangle = \langle p \mid k\ell\uparrow\rangle_0 \, f_\ell + \langle p \mid G_{0\ell} \, V_\ell \mid k\ell\uparrow\rangle. \qquad (2.17)$$

The free "state" $\langle p \mid k\ell\uparrow\rangle_0$ is given explicitly by

$$\langle p \mid k\ell\uparrow\rangle_0 = \frac{2}{\pi k} \frac{(p/k)^\ell}{p^2 - k^2}, \qquad \mathrm{Im}\, k > 0. \qquad (2.18)$$

By inserting this in Eq.(2.17) one easily obtains

$$\langle p \mid V_\ell \mid k\ell\uparrow\rangle = (k^2 - p^2) \langle p \mid k\ell\uparrow\rangle + 2(\pi k)^{-1} (p/k)^\ell f_\ell, \qquad (2.19)$$

which is the relation we wanted.

The connection between the *off-shell* quantities, corresponding to the one of Eq.(2.19), can be obtained from Eqs.(2.8), (2.13) and (2.19),

$$\langle p \mid V_\ell \mid kq\ell\uparrow\rangle = (k^2 - p^2)\langle p \mid kq\ell\uparrow\rangle + 2(\pi q)^{-1}(p/q)^\ell [f_\ell(k,q) - (k^2-q^2)/(p^2-q^2)]. \quad (2.20)$$

It is interesting to consider the limit of $\langle p \mid k\ell\uparrow\rangle$ for $p\to\infty$. This limit could be used for an alternative definition of f_ℓ (cf. Refs.5 and 6). By using the fact that $\langle r \mid k\ell\uparrow\rangle = O(r^{-\ell-1})$ as $r\to 0$, we obtain

$$\langle p \mid V_\ell \mid k\ell\uparrow\rangle = (2/\pi)^{\frac{1}{2}} i^{-\ell} \int_0^\infty j_\ell(pr)\, V_\ell(r) \langle r \mid k\ell\uparrow\rangle r^2\, dr$$

$$\simeq c\, p^{\ell-2} \int_0^\infty j_\ell(x)\, V_\ell(x/p)\, x^{1-\ell}\, dx, \quad p\to\infty.$$

In this way we find that

$$\lim_{p\to\infty} p^{-\ell} \langle p \mid V_\ell \mid k\ell\uparrow\rangle = 0, \quad (2.21)$$

when the potential is nonsingular, i.e.,

$$V(r) = O(r^{-\alpha}), \quad \alpha < 2, \quad r\to 0.$$

It is easily seen from Eqs.(2.19) and (2.21) that

$$f_\ell = \tfrac{1}{2}\pi k^{\ell+1} \lim_{p\to\infty} p^{2-\ell} \langle p \mid k\ell\uparrow\rangle. \quad (2.22)$$

This may be compared with the usual definition of f_ℓ,

$$f_\ell \equiv (\pi/2)^{\frac{1}{2}} (2/i)^\ell \, (\ell!/(2\ell)!) \lim_{r\to 0} (kr)^{\ell+1} \langle r \mid k\ell\uparrow\rangle. \quad (2.23)$$

Similar equations hold for the *off-shell* Jost function and solution. The analog of Eq.(2.23) is [3]

$$f_\ell(k,q) = (\pi/2)^{\frac{1}{2}} (2/i)^\ell (\ell!/(2\ell)!) \lim_{r\to 0} (qr)^{\ell+1} \langle r \mid kq\ell\uparrow\rangle. \quad (2.24)$$

The off-shell analog of Eq.(2.22) follows by using Eq.(2.8). We have (cf. Eq.(2.21))

$$\lim_{p\to\infty} p^{2-\ell} \langle p \mid G_{0\ell}\, T_\ell \mid q\ell\uparrow\rangle_0 = \lim_{p\to\infty} p^{-\ell} \langle p \mid T_\ell \mid q\ell\uparrow\rangle_0 = 0,$$

and so we obtain from (2.8),

$$f_\ell(k,q) = \tfrac{1}{2}\pi q^{\ell+1} \lim_{p\to\infty} p^{2-\ell} \langle p \mid kq\ell\uparrow\rangle. \quad (2.25)$$

This expression can also be derived with the help of Eq.(2.20).

It is interesting to note that Eq.(2.25) is obtained in a different way, by using Eq.(2.24) in the expression

$$\langle p \mid kq\ell\uparrow\rangle = (2/\pi)^{\frac{1}{2}} i^{-\ell} \int_0^\infty j_\ell(pr) \langle r \mid kq\ell\uparrow\rangle r^2\, dr, \quad (2.26)$$

and applying the equality

$$\int_0^\infty j_\ell(x)\, x^{1-\lambda}\, dx = \pi^{\frac{1}{2}} 2^{-\lambda} \Gamma(1 + \tfrac{1}{2}\ell - \tfrac{1}{2}\lambda)/\Gamma(\tfrac{1}{2} + \tfrac{1}{2}\ell + \tfrac{1}{2}\lambda),$$

$$0 < \mathrm{Re}\,\lambda < \ell+2. \quad (2.27)$$

On the other hand, we shall now derive Eq.(2.24) from Eq.(2.25). We have

$$\langle r \mid kq\ell\uparrow\rangle = (2/\pi)^{\frac{1}{2}} i^\ell \lim_{\varepsilon\downarrow 0} \int_0^\infty j_\ell(pr) \langle p \mid kq\ell\uparrow\rangle e^{-\varepsilon p} p^2\, dp, \quad (2.28)$$

where $e^{-\varepsilon p}$ has been inserted to guarantee the convergence of the integral. It turns out that, when r goes to zero, $\langle p \mid kq\ell\uparrow\rangle$ may be replaced by its asymptotic value, which is given by Eq.(2.25). Then we obtain from (2.28), using the new variable of integration $x = pr$,

$$\lim_{r\to 0} (qr)^{\ell+1} \langle r \mid kq\ell\uparrow\rangle = f_\ell(k,q)\, (2/\pi)^{3/2}\, i^\ell \times \lim_{\varepsilon\downarrow 0} \int_0^\infty j_\ell(x)\, x^\ell\, e^{-\varepsilon x/r}\, dx. \quad (2.29)$$

In order to evaluate the integral here, we note that

$$\int_0^\infty e^{-\alpha x} J_\mu(\beta x)\, x^\nu dx = (\alpha^2+\beta^2)^{-\frac{1}{2}-\frac{1}{2}\nu}\, \Gamma(1+\mu+\nu)\, P_\nu^{-\mu}(\alpha(\alpha^2+\beta^2)^{-\frac{1}{2}}),$$

$$\alpha > 0, \quad \beta > 0, \quad \mathrm{Re}(1+\mu+\nu) > 0. \tag{2.30}$$

Here $P_\nu^{-\mu}(\zeta)$ is the Legendre function of the first kind "on the cut": $-1 < \zeta < 1$. Its value for $\zeta = 0$ is given by

$$\Gamma(1+\mu)\, P_\nu^{-\mu}(0) = {}_2F_1(-\nu, \nu+1; \mu+1; \tfrac{1}{2}) = \frac{\Gamma(1+\frac{1}{2}\mu)\,\Gamma(\frac{1}{2}+\frac{1}{2}\mu)}{\Gamma(1+\frac{1}{2}\mu+\frac{1}{2}\nu)\,\Gamma(\frac{1}{2}+\frac{1}{2}\mu-\frac{1}{2}\nu)}. \tag{2.31}$$

By using this expression we get

$$\lim_{\varepsilon \downarrow 0} \int_0^\infty e^{-\varepsilon x} J_\mu(x)\, x^\nu\, dx = 2^\nu\, \Gamma(\tfrac{1}{2}+\tfrac{1}{2}\mu+\tfrac{1}{2}\nu) / \Gamma(\tfrac{1}{2}+\tfrac{1}{2}\mu-\tfrac{1}{2}\nu),$$

$$\mathrm{Re}(1+\mu+\nu) > 0,$$

and so

$$\lim_{\varepsilon \downarrow 0} \int_0^\infty e^{-\varepsilon x} j_\ell(x)\, x^\ell\, dx = \pi^{\frac{1}{2}}\, 2^{\ell-1}\, \Gamma(\ell+\tfrac{1}{2}) = \pi\, 2^{-\ell-1} (2\ell)! / \ell! \tag{2.32}$$

By inserting this in Eq.(2.29) we just obtain Eq.(2.24).

We note that the above limiting procedures constitute in fact a generalization of the well-known Riemann-Lebesgue lemma, i.e.,

$$\lim_{y \to \pm\infty} \int f(x)\, e^{ixy}\, dx = 0,$$

where f is any summable function.

3. THE COULOMB CASE

Some of the expressions derived in the preceding section do not hold when the potential has a Coulomb range. Especially Eqs.(2.9), (2.10), (2.14) and (2.15) need modification. In this section we shall derive the analogs of these equations for the case of the pure Coulomb potential. Further we shall develop some explicit expressions, in terms of hypergeometric functions, for the particular case when $\ell = 0$. In the next section we shall derive interesting formulas for the case when the potential is the sum of the Coulomb potential and a short-range potential, by using the results obtained in Sections 2 and 3.

In the first place we note that the important equations (2.11) and (2.12) *do* hold for the Coulomb case, i.e.,

$$| k\ell \uparrow >_c = (1 + G_{0\ell}\, T_{c\ell}) \, | k\ell \uparrow >_0 \; f_{c\ell}, \tag{3.1}$$

and so

$$V_{c\ell} \, | k\ell \uparrow >_c = T_{c\ell} \, | k\ell \uparrow >_0 \; f_{c\ell}. \tag{3.2}$$

We shall prove Eq.(3.1) in an independent way. To start with, we observe that the *existence* of the quantity $G_{0\ell} T_{c\ell} \, | k\ell \uparrow >_0 = G_{c\ell} V_{c\ell} \, | k\ell \uparrow >_0$ is easily confirmed by using

$$< r \, | \, G_{c\ell} \, | \, r' > = -\tfrac{1}{2}\pi k < r_> \, | \, k\ell \uparrow >_c \, \lesssim k\ell - | \, r_< >. \tag{3.3}$$

One can also show in this way that $G_{0\ell} \, T_{c\ell} \, | k\ell \uparrow >_0$ is *not* defined, i.e. that it contains a divergent integral.

In order to prove Eq.(3.1), we note that its right-hand side equals some solution ψ of the equation $(k^2 - H_{c\ell})\psi = 0$ (in the coordinate representation). Further, by using Eq.(3.3) and by considering the asymptotic behavior $(r \to \infty)$ of the right-hand side of (3.1), we find that it must be proportional to $| k\ell \uparrow >_c$. The next

step is to consider the behavior for small r. By again using (3.3) one has

$$\langle r \mid G_{c\ell}\, V_{c\ell} \mid k\ell\, + \rangle_0 = O(\ell n\, r), \quad \ell = 0, \quad r \to 0,$$

$$= O(r^{-\ell}), \quad \ell > 0, \quad r \to 0. \tag{3.4}$$

Therefore

$$\lim_{r\to 0} r^{\ell+1} \langle r \mid G_{0\ell}\, T_{c\ell} \mid k\ell\, + \rangle_0 = 0, \quad \ell = 0,1, \ldots .$$

By using Eq.(2.23) the proof of Eq.(3.1) now follows easily.

In a previous paper [2] we have derived the Coulomb analog of Eq.(2.9), by using an explicit expression for $f_{c\ell}(k,q)$. The following equality holds,

$$\lim_{q\to k} \omega\, f_{c\ell}(k,q) = f_{c\ell}, \quad k > 0. \tag{3.5}$$

Here

$$\omega \equiv \left(\frac{q-k}{q+k}\right)^{i\gamma} \frac{e^{\pi\gamma/2}}{\Gamma(1+i\gamma)} = f_{c0}/f_{c0}\ (k,q), \quad \mathrm{Im}\, q > 0. \tag{3.6}$$

The Coulomb analog of Eq.(2.10) is now easily obtained by using Eqs.(2.8), (3.1) and (3.5),

$$\lim_{q\to k} \omega \mid kq\ell\, + \rangle_c = \mid k\ell\, + \rangle_c, \quad k > 0. \tag{3.7}$$

It is interesting to note that we are now able to prove the validity of two conjectures from a preceding paper [1]. The first one, Eq.(40.ℓ), is in fact just (3.7). The second one, Eq.(40.k), is easily proved by using Eqs.(40.h) - (40.j) of Ref.1 and Eq.(2.8).

We note that Eqs.(a) and (d) of (2.7) are valid in the Coulomb case, whereas Eqs.(b) and (c) are not. By using Eqs.(2.7a) and (3.5) we have obtained the interesting equality,

$$f_{c\ell}^{-1} = \lim_{q\to k} (\omega^{-1} - \tfrac{1}{2}\pi k\ {}_c\langle k\ell - \mid V_{c\ell} \mid q\ell\, + \rangle_0), \quad k > 0. \tag{3.8}$$

Obviously this can be considered as a Coulomb analog of the short-range potential formulas given in Eq.(2.14).

It would be interesting to have available explicit expressions for the above quantities. Only a few such formulas are known. The quantities $<r \mid k\ell\uparrow>_c$ and $f_{c\ell}(k)$ for $\ell = 0,1,2, \ldots$ have been known since a long time. We have obtained a number of interesting analytic expressions for $f_{c\ell}(k,q)$, $\ell = 0,1,2, \ldots$, see Ref.7. Further $<p \mid T_{c\ell} \mid p'>$ is known in closed form for $\ell = 0$ [8] and for $\ell = 1$ [9] only. Below we shall derive analytic expressions for $<p \mid k\ell\uparrow>_c$, $<p \mid kq\ell\uparrow>_c$, and for $<p \mid T_{c\ell} \mid q\ell\uparrow>_0$, in the case $\ell = 0$ only.

Before we start with the derivations we would like to make some remarks on the interrelationships between the above quantities. It is important to note that $<p \mid T_{c\ell} \mid q\ell\uparrow>_0$ can be considered as the general object from which all other quantities can be obtained in a *simple* way. This is true as well for Coulomb-like potentials, and of course also for short-range potentials. Indeed, by taking $q = k$ we have $<p \mid T_{c\ell} \mid k\ell\uparrow>_0$ from which $<p \mid k\ell\uparrow>_c$ follows with the help of Eqs.(2.12) and (2.19). Once $<p \mid k\ell\uparrow>_c$ is known, $<p \mid kq\ell\uparrow>_c$ is obtained by using Eq.(2.8). The ordinary off-shell Coulomb T matrix $<p \mid T_{c\ell} \mid p'>$ follows from $<p \mid T_{c\ell} \mid q\ell\uparrow>_0$ by noting that

$$2i\, T_{c\ell} \mid p'\ell> = T_{c\ell} \mid p'\ell\uparrow>_0 + (-)^{\ell}\, T_{c\ell} \mid (-p')\ell\uparrow>_0 . \qquad (3.9)$$

Furthermore, $f_{c\ell}(k,q)$ can be obtained from $<p \mid kq\ell\uparrow>_c$ and $f_{c\ell}$ from $<p \mid k\ell\uparrow>_c$ by using Eqs.(2.25) and (2.22), respectively. Finally we note that application of the Coulombian asymptotic states (see Ref. 10) to $<p \mid T_{c\ell} \mid q\ell\uparrow>_0$ and $<p \mid T_{c\ell} \mid p'>$ yields $f_{c\ell}(k,q)$ and $<p \mid k\ell+>_c$, respectively. Since, therefore, $<p \mid T_{c\ell} \mid q\ell\uparrow>_0$ appears to be the object of central importance, we are interested in the general structure of an analytic expression for this quantity.

For the moment we restrict ourselves to the case $\ell = 0$ and we suppress ℓ. Let us first recall the expression for $\langle p \mid T_c \mid p' \rangle$ given in Ref.8,

$$\langle p \mid T_c \mid p' \rangle = ik(\pi pp')^{-1} \left[F_{i\gamma}(aa') + F_{i\gamma}((aa')^{-1}) - F_{i\gamma}(a/a') - F_{i\gamma}(a'/a) \right]. \quad (3.10)$$

Here

$$F_{i\gamma}(z) \equiv {}_2F_1(1, i\gamma;\ 1 + i\gamma;\ z)$$

and

$$a \equiv (p - k)/(p + k), \quad a' \equiv (p' - k)/(p' + k).$$

By using a well-known integral representation for the hypergeometric function,

$$F_{i\gamma}(z) = i\gamma \int_0^1 t^{i\gamma - 1} (1 - tz)^{-1}\, dt, \quad (3.11)$$

we are able to evaluate

$$\langle p \mid T_c \mid q \uparrow \rangle_0 = \int_0^\infty \langle p \mid T_c \mid p' \rangle \langle p' \mid q \uparrow \rangle_0\ p'^2\, dp',$$

where (cf. Eq.(2.18))

$$\langle p \mid q \uparrow \rangle_0 = 2(\pi q)^{-1} (p^2 - q^2)^{-1}, \quad \mathrm{Im}\, q > 0.$$

After a number of manipulations we arrive at

$$\langle p \mid T_c \mid q \uparrow \rangle_0 = -2k(\pi pq)^{-1} \left[F_{i\gamma}(ab) - F_{i\gamma}(b/a) - F_{i\gamma}(a) + F_{i\gamma}(1/a) \right], \quad (3.12)$$

with

$$b \equiv (q - k)\,/\,(q + k).$$

Equation (3.9) provides us with a check on this result. It can be seen by inspection that we have indeed

$$\lim_{q \to p'} \left(\langle p \mid T_c \mid q \uparrow \rangle_0 + \langle p \mid T_c \mid (-q) \uparrow \rangle_0 \right) = 2i \langle p \mid T_c \mid p' \rangle, \quad (3.13)$$

note that $b \to 1/b$ when q is replaced by $-q$.

Further we clearly have from (3.12),

$$\lim_{q\to k} \langle p \mid T_c \mid q\uparrow\rangle_0 = \langle p \mid T_c \mid k\uparrow\rangle_0 = 2(\pi p)^{-1}\left[F_{i\gamma}(a) - F_{i\gamma}(1/a)\right]. \quad (3.14)$$

By using Eq.(3.1) one easily obtains

$$\langle p \mid V_c \mid k\uparrow\rangle_c = 2(\pi p)^{-1} f_c \left[F_{i\gamma}(a) - F_{i\gamma}(1/a)\right], \quad (3.15)$$

and with the help of Eq.(2.19),

$$\langle p \mid k\uparrow\rangle_c = 2(\pi p)^{-1} (p^2 - k^2)^{-1} f_c \left[p/k - F_{i\gamma}(a) + F_{i\gamma}(1/a)\right]. \quad (3.16)$$

Finally we note that $\langle p \mid kq\uparrow\rangle_c$ can now easily be given. We only need to insert the known expressions for the terms on the right-hand side of Eq.(2.8). In particular we have

$$f_c(k,q) = b^{-i\gamma}. \quad (3.17)$$

Let us for completeness write out this expression for the Hankel transform of the Coulomb off-shell Jost solution for $\ell = 0$,

$$\langle p \mid kq\uparrow\rangle_c = \frac{2}{\pi q(p^2 - q^2)} + \frac{2k}{\pi pq(p^2 - k^2)}$$

$$\times \left[F_{i\gamma}(ab) - F_{i\gamma}(b/a) - p/k + b^{-i\gamma}\{p/k - F_{i\gamma}(a) + F_{i\gamma}(1/a)\}\right]. \quad (3.18)$$

By using Eq.(2.13) or Eq.(2.20) we have

$$\langle p \mid V_c \mid kq\uparrow\rangle_c = 2k(\pi pq)^{-1}\left[F_{i\gamma}(b/a) - F_{i\gamma}(ab) + b^{-i\gamma}\{F_{i\gamma}(a) - F_{i\gamma}(1/a)\}\right]. \quad (3.19)$$

By taking here the limit $q \to k$ we get, with $\omega = f_c b^{i\gamma}$,

$$\lim_{q\to k} \omega \langle p \mid V_c \mid kq\uparrow\rangle_c = \langle p \mid V_c \mid k\uparrow\rangle_c.$$

Such a relation holds in fact for all ℓ. Indeed, with the help of Eqs.(2.19), (2.20), (3.5) and (3.7) the proof of

$$\lim_{q\to k} f_c\, b^{i\gamma} \langle p \mid V_{c\ell} \mid kq\ell\uparrow\rangle_c = \langle p \mid V_{c\ell} \mid k\ell\uparrow\rangle_c, \quad \ell = 0,1,2,\ldots, \quad (3.20)$$

is easily obtained.

A final remark concerning the generalization of the $\ell = 0$ expression for $< p \mid T_c \mid q \uparrow >_0$ to general values of ℓ is appropriate here. In view of Eq.(3.12) it can be expected that $< p \mid T_{c\ell} \mid q^{\ell} \uparrow >_0$, where $\ell = 0,1,2, \ldots,$ can be expressed in terms of simple functions and the hypergeometric function $F_{i\gamma}$ with *exactly* the same arguments as in (3.12), notably ab, b/a, a and 1/a.

4. THE COULOMB-LIKE POTENTIAL CASE

In this section we assume that the potential is the sum of the Coulomb potential and a short-range potential, $V = V_c + V_s$. We shall discuss the necessary modifications of the equations given in Section 2, by using the appropriate results obtained in Section 3. In particular we will derive the analogs of Eqs.(2.9), (2.10) and (2.14).

We shall use the well-known two potential formalism. The T operator corresponding to $V = V_c + V_s$ is given by

$$T = T_c + (1 + T_c G_0)\, t_{cs} (1 + G_0 T_c), \tag{4.1}$$

where t_{cs} is the solution of

$$t_{cs} = V_s + V_s G_c\, t_{cs}. \tag{4.2}$$

The partial-wave analogs of these equations have exactly the same form. For the partial-wave "outgoing" scattering state $|k\ell +>$ the following equation can be obtained,

$$|k\ell +> = |k\ell +>_c + G_{c\ell}\, t_{cs\ell}\, |k\ell +>_c . \tag{4.3}$$

In order to derive relations for the "Jost states", we use Eqs.(2.11) and (2.12). These are also valid for a Coulomb-like potential. We insert (4.1) in (2.11),

$$|k\ell \uparrow> f_\ell^{-1} = (1 + G_{0\ell}\, T_\ell)\, |k\ell \uparrow>_0 ,$$

and obtain

$$|k\ell \uparrow> f_\ell^{-1} = |k\ell \uparrow>_c f_{c\ell}^{-1} + G_{c\ell}\, t_{cs\ell}\, |k\ell \uparrow>_c f_{c\ell}^{-1}$$

$$= (1 + G_{c\ell}\, t_{cs\ell})\, |k\ell \uparrow>_c f_{c\ell}^{-1}. \tag{4.4}$$

Further by inserting (4.1) in (2.12),

$$V_\ell \mid k\ell\uparrow > f_\ell^{-1} = T_\ell \mid k\ell\uparrow >_0 ,$$

we get

$$V_\ell \mid k\ell\uparrow > f_\ell^{-1} = V_{c\ell} \mid k\ell\uparrow >_c f_{c\ell}^{-1} + G_{0\ell}^{-1} G_{c\ell}\, t_{cs\ell} \mid k\ell\uparrow >_c f_{c\ell}^{-1}. \qquad (4.5)$$

We are now going to derive a connection between the Jost function f_ℓ and the Coulomb Jost function $f_{c\ell}$. To this end we write Eq.(4.3) in the coordinate representation. In the resulting equation we insert the equality (cf. Eq.(3.3))

$$< r \mid G_{c\ell} \mid r' > \; = -\tfrac{1}{2}\pi k \; < r_< \mid k\ell + >_c \; {}_c\!< k\ell\downarrow \mid r_> >.$$

We note that ${}_c\!< k\ell\downarrow \mid t_{cs\ell} \mid k\ell + >_c$ is a well-defined quantity since $t_{cs\ell}$ is a short-range operator. By using

$$< r \mid t_{cs\ell} \mid k\ell + >_c \; = O(r^{\ell-\alpha}), \quad \alpha < 2, \quad r \to 0,$$

we obtain from Eq.(4.3)

$$< r \mid k\ell + > = < r \mid k\ell + >_c - \tfrac{1}{2}\pi k \; < r \mid k\ell + >_c \; {}_c\!< k\ell\downarrow \mid t_{cs\ell} \mid k\ell + >_c + O(r^{\ell+2-\alpha}), \; r \to 0.$$

The Jost functions can be obtained from the scattering states by considering their small-r behavior. We have (e.g., Refs. 5 and 6)

$$\lim_{r\to 0} r^{-\ell} \; < r \mid k\ell + > \; = f_\ell^{-1} (2/\pi)^{\frac{1}{2}} \, (2ik)^\ell \, \ell!/(2\ell+1)! \; . \qquad (4.6)$$

With the help of this relation one obtains

$$f_\ell^{-1} = f_{c\ell}^{-1} - \tfrac{1}{2}\pi k \, f_{c\ell}^{-1} \; {}_c\!< k\ell\downarrow \mid t_{cs\ell} \mid k\ell + >_c ,$$

as can be seen by inspection. We rewrite this equation in the more convenient form,

$$f_{c\ell} \, f_\ell^{-1} = 1 - \tfrac{1}{2}\pi k \; {}_c\!< k\ell\downarrow \mid t_{cs\ell} \mid k\ell + >_c \; . \qquad (4.7a)$$

If we take here $V_c \to 0$ we get back one of the expressions of Eq. (2.14), since in this case $t_{cs\ell} \to T_{s\ell}$ and $f_{c\ell} \to 1$. Just as in (2.14)

there are three different equivalent expressions, namely

$$f_{c\ell}\, f_\ell^{-1} = 1 - \tfrac{1}{2}\pi k\ {}_c\!<k\ell +\,|\, V_{s\ell}\,|\, k\ell +>_c \tag{4.7b}$$

$$= 1 - \tfrac{1}{2}\pi k\ <k\ell -\,|\, V_{s\ell}\,|\, k\ell +>_c \tag{4.7c}$$

$$= 1 - \tfrac{1}{2}\pi k\ {}_c\!<k\ell -\,|\, t_{cs\ell}\,|\, k\ell +>_c. \tag{4.7d}$$

These are easily derived with the help of Eqs.(4.1) and (4.3).

In order to derive the analog of Eq.(2.15), we first multiply both sides of Eq.(4.4) by $V_{s\ell}$. This yields

$$V_{s\ell}\,|\, k\ell +> f_\ell^{-1} = t_{cs\ell}\,|\, k\ell +>_c f_{c\ell}^{-1}. \tag{4.8}$$

By inserting this equation in (4.7d) we get

$$f_{c\ell}^{-1}\, f_\ell = 1 + \tfrac{1}{2}\pi k\ {}_c\!<k\ell -\,|\, V_{s\ell}\,|\, k\ell +>$$

$$= 1 + \tfrac{1}{2}\pi k\ <k\ell +\,|\, V_{s\ell}\,|\, k\ell +>_c. \tag{4.9}$$

Obviously this is the two-potential analog of Eq.(2.15).

It is interesting to consider the analog of Eq.(3.8), i.e.,

$$f_\ell^{-1} = \lim_{q\to k}(\omega^{-1} - \tfrac{1}{2}\pi k\ <k\ell -\,|\, V_\ell\,|\, q\ell +>_0),\quad k > 0. \tag{4.10}$$

In order to prove this equation, we first note that one has from Eqs.(4.1) - (4.3),

$$<k\ell -\,|\, V_\ell = {}_c\!<k\ell -\,|\, V_{c\ell} + {}_c\!<k\ell -\,|\, t_{cs\ell}(1 + G_{0\ell}\, T_{c\ell}). \tag{4.11}$$

We insert this expression in (4.10) and use

$$\lim_{q\to k}\,(1 + G_{0\ell}\, T_{c\ell})\,|\, q\ell +>_0 = |\, k\ell +>_c f_{c\ell}^{-1}. \tag{4.12}$$

By applying finally Eqs.(3.8) and (4.7d) the proof of Eq.(4.10) is completed.

Now we turn to the *off-shell* Jost function. In Eq.(2.7a) the following general formula

$$f_\ell(k,q) = 1 + \tfrac{1}{2}\pi q(q/k)^\ell \; f_\ell \, {}^{(-)}\langle k\ell \uparrow | V_\ell | q\ell \uparrow \rangle_0 \qquad (4.13)$$

has been given [4]. This equation is also valid for a Coulomb-like potential. By inserting Eq.(4.11) in (4.13), and by using (4.13) for the pure Coulomb case, we obtain

$$[f_\ell(k,q) - 1]\, f_\ell^{-1} = [f_{C\ell}(k,q) - 1]\, f_{C\ell}^{-1}$$

$$+ \tfrac{1}{2}\pi q(q/k)^\ell \; {}_C^{(-)}\langle k\ell | t_{CS\ell}(1 + G_{0\ell}\, T_{C\ell}) | q\ell \uparrow \rangle_0 . \qquad (4.14)$$

Herewith we have obtained a useful relation between the Coulomb off-shell Jost function and the off-shell Jost function for a Coulomb-like potential. Indeed, from Eq.(4.14) one obtains, by using Eqs.(4.12) and (3.5), the analog of the pure Coulomb formula (3.5),

$$\lim_{q\to k} \omega\, f_\ell(k,q) = f_\ell, \quad k > 0. \qquad (4.15)$$

Here ω is given by Eq.(3.6).

Finally we are going to prove

$$\lim_{q\to k} \omega\, | kq\ell \uparrow \rangle = | k\ell \uparrow \rangle, \quad k > 0. \qquad (4.16)$$

This is just the Coulomb-like analog of the pure Coulomb formula (3.7). From Eqs.(2.8) and (2.11) we obtain

$$| kq\ell \uparrow \rangle \underset{q\to k}{\longrightarrow} | k\ell \uparrow \rangle \; f_\ell^{-1} \; f_\ell(k,q).$$

Application of Eq.(4.15) then completes the proof of Eq.(4.16).

So we see that the singular behavior of the off-shell Jost function and of the off-shell Jost state in $q = k$ is just the same as for the pure Coulomb potential. This result is as might

be expected, since this singularity is generated by the asymptotic part of the potential only.

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Fuda's off-shell Jost function for Coulomb, Hulthén, and Eckart potentials and limiting relations

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We study the off-shell Jost function $f(k,q)$, introduced by Fuda, for the Coulomb, the Hulthén, and two modified Eckart potentials. A simple closed expression for the $l = 0$ Coulomb off-shell Jost function has been obtained. This function is discontinuous at $q = k$. Its on-shell limiting behavior is given by the singular factor $(q-k)^{-i\gamma}$ where γ is the Sommerfeld parameter. We also discuss the off-shell Jost solution $f(k,q,r)$ which is an off-shell generalization of the Jost solution $f(k,r)$. We consider the Hulthén potential as a screened Coulomb potential, let the screening parameter a go to infinity, and derive the limiting behavior of the Jost solution, the Jost function, the off-shell Jost function, and the half-shell T matrix for the Hulthén potential as $a \to \infty$. We obtain discontinuities given by the singular factor $a^{i\gamma}$. For comparison, we introduce two modifications of an Eckart potential which can be considered to be a screened r^{-2} potential and derive a number of limiting relations in analogy to those for the Hulthén-Coulomb pair of potentials.

I. INTRODUCTION

The concepts of Jost[1] function and Jost solution are very well known in the theory of nonrelativistic two-body scattering by a spherically symmetric potential.[2-4] Their usefulness in the study of the Schrödinger equation may be recognized from some of their properties: the phase of the Jost function is the negative of the phase shift for the physical wave function. For a local potential, the Jost function is identical to the Fredholm determinant and its zeros determine the bound-state energies of the two-body system.

For many-particle systems one needs off-shell quantities, in particular the off-shell T matrix. The on-shell restriction of the T matrix is proportional to the two-particle scattering amplitude. Fuda and Whiting[5] have introduced and studied a generalization of the Jost function which they call the off-shell Jost function $f_l(k,q)$. It is a function of the wave number k and an off-shell momentum q. These authors have discussed its usefulness in off-shell scattering. In particular, they have proved a simple relation connecting the half-shell T matrix $T_l(k,q;k^2)$ and the off-shell Jost function, see Eq. (16). Further, they have discussed an off-shell extension of the Jost solution. This is a solution $f_l(k,q,r)$ with prescribed asymptotic behavior e^{ikr}, $r \to \infty$, of an inhomogeneous "Schrödinger equation." We shall call this function $f_l(k,q,r)$ the off-shell Jost solution.

Recently Fuda[6] has developed a momentum-space formulation of the off-shell Jost function and derived two integral representations for it. Finally we note that very recently Pasquier and Pasquier[7,8] have studied an off-shell generalization of the Jost formalism in a more general context.

For some particular potentials the Jost function and the Jost solution are known in closed form, see Newton,[2] Chap. 14. In the case of s waves ($l = 0$) the off-shell T matrix $T(p,q;k^2)$ has been obtained for a small number of potentials only. Most of these explicit expressions are in terms of generalized hypergeometric functions[9,10] ${}_mF_n$.

Fuda[11] has derived $T_{l=0}$ for the exponential potential in terms of ${}_1F_2$ and ${}_2F_3$, while Bahethi and Fuda[12] have given an expression for the case of the Hulthén potential in terms of ${}_3F_2$ and ${}_4F_3$. Finally Fuda and Whiting[5] have simplified these expressions. For the Coulomb potential, van Haeringen and van Wageningen[13] have derived the $l=0$ T matrix in terms of ${}_2F_1$.

In the case $l>0$, no closed expression for T_l is known for the exponential and Hulthén potentials. van Haeringen[14] has obtained the $l=1$ Coulomb T matrix, also in terms of the Gaussian hypergeometric function ${}_2F_1$. This expression is much more complicated than the Coulomb $T_{l=0}$ expression.

The s-wave off-shell Jost function and solution for the exponential potential and for the Hulthén potential have been given by Fuda and Whiting.[5] Fuda and Girard[15] have derived integral representations for the s wave, off-shell Jost function, and half-off-shell T matrix for a superposition of Yukawa potentials. Some work has also been done on other potentials, cf. the references quoted by Fuda and Girard.[15]

In this paper we extend these investigations on off-shell Jost functions and solutions, in particular to the Coulomb case. Here we meet special difficulties, which are due to the long range of the

Coulomb potential.

In Sec. II we study the off-shell Jost solution and function for the Coulomb potential for arbitrary values of l. For $l=0$ we obtain a very simple closed expression for the Coulomb off-shell Jost function $f_C(k,q)$, see Eq. (24). In connection with the derivation of the $l=0$ off-shell Jost function for the Hulthén potential, we pay attention to a statement concerning the hypergeometric function ${}_3F_2$ which is of general interest. It is formulated as follows: any Saalschützian ${}_3F_2$ of argument 1, with one of its three first parameters equal to 1, can be summed in terms of Γ functions.

The Hulthén potential goes over into the Coulomb potential when the so-called screening parameter a goes to infinity. We investigate whether or not the limits for $a\to\infty$ of the Hulthén Jost functions and solutions are equal to the Coulomb Jost function and solution, respectively. We establish the type of singularity for those cases for which this limit is nonexistent. It is given by $a^{i\gamma}$, where γ is the Sommerfeld parameter.[16]

Further, we investigate the continuity of the off-shell Jost solutions and functions with respect to the off-shell variable q at $q=k$. According to Fuda and Whiting,[5] the off-shell Jost function and solution are continuous at $q=k$ with limit equal to the ordinary Jost function and solution, if the potential has a short range. We prove that the Coulomb off-shell Jost function is not continuous but singular at $q=k$ and we also show that the source of the singularity lies in the factor $(q-k)^{-i\gamma}$.

Finally, we take a third and a fourth limit into consideration. Besides $a\to\infty$ and $q\to k$ we also consider $r\to\infty$ and $r\to 0$. A survey of our main results for these limiting relations may be found in Eqs. (40)–(41), and in Fig. 1.

In the final part of Sec. III we prove an interesting limiting relation for the half-shell Hulthén T matrix, see Eq. (48). In Sec. IV we consider a potential from the Eckart[17] class and two modifications, and we derive some limiting relations. In Sec. V we give a summary and a short discussion.

We shall mainly use the notation of Newton[2] and of Fuda and Whiting.[5]

II. COULOMB AND HULTHÉN FUNCTIONS

The Jost[1] solution $f_l(k,r)$ is that solution of the radial Schrödinger equation,

$$\left(k^2+\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V(r)\right)f_l(k,r)=0\,, \tag{1}$$

which satisfies the asymptotic condition

$$\lim_{r\to\infty} f_l(k,r)e^{-ikr}=1\,. \tag{2}$$

This function $f_l(k,r)$ is well defined if the potential $V(r)$ is not singular and satisfies

$$V(r)=O(r^{-\alpha})\,,\quad \alpha>1\,,\quad r\to\infty\,.$$

In the Coulomb case ($\alpha=1$), a different asymptotic behavior has to be prescribed, because there is no solution of Eq. (1) satisfying Eq. (2) in this case. Then one may define $f_{C,l}$ such that

$$\lim_{r\to\infty} f_{C,l}(k,r)e^{-ikr+i\gamma\ln(2kr)}=1\,, \tag{3}$$

where γ is Sommerfeld's parameter. The factor $(2k)^{i\gamma}$ in Eq. (3) is usually included for convenience. The Coulomb potential is given by

$$V_C(r)=2k\gamma/r\,.$$

The Coulomb Jost solution can be given in several equivalent closed forms, e.g.,

$$f_{C,l}(k,r)=e^{i\gamma/2+\pi\gamma/2}(-2ikr)^{l+1}\times U(l+1+i\gamma,2l+2,-2ikr) \tag{4}$$

$$=e^{ikr-i\gamma\ln(2kr)}\,{}_2F_0(l+1+i\gamma,i\gamma-l;(2ikr)^{-1})\,. \tag{5}$$

Here U is an irregular solution of the confluent hypergeometric differential equation,[18] and ${}_2F_0$ is a generalized hypergeometric function. Note that Eq. (3) is easily read off from Eq. (5) since

$$\lim_{z\to 0}{}_2F_0(a,b;z)=1\,.$$

The Jost *function* is defined by[19] [Newton,[2] Eqs. (12.140) and (12.142)]

$$f_l(k)\equiv\lim_{r\to 0} f_l(k,r)(-2ikr)^l\,1\,1/(2l)\,1\,. \tag{6}$$

This definition is also valid in the Coulomb case. By using (Ref. 18, p.288)

$$\lim_{z\to 0} z^{c-1}U(a,c,z)=\Gamma(c-1)/\Gamma(a)\,,\quad \mathrm{Re}\,c>1\,,$$

one obtains from Eq. (4) the well-known expression

$$f_{C,l}(k)=e^{\pi\gamma/2}\Gamma(l+1)/\Gamma(l+1+i\gamma) \tag{7}$$

for the Coulomb Jost function.

Now we turn to the *off-shell* Jost solution and the *off-shell* Jost function, introduced by Fuda and Whiting.[5] The off-shell Jost solution $f_l(k,q,r)$ is that solution of the so-called inhomogeneous Schrödinger equation

$$\left(k^2+\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V(r)\right)f_l(k,q,r)=(k^2-q^2)\,i^l qr h_l^{(+)}(qr)\,, \tag{8}$$

which satisfies the asymptotic condition

$$\lim_{r\to\infty} f_l(k,q,r)e^{-ikr}=1\,. \tag{9}$$

Here $h_l^{(+)}$ is the spherical Hankel function,[16] for which the following useful equality holds,

$$i^l z h_l^{(+)}(z) = e^{iz}\, {}_2F_0(l+1, -l; (2iz)^{-1}). \tag{10}$$

We have found that one can also define for the Coulomb potential an off-shell Jost solution which satisfies Eqs. (8) and (9). We shall denote this solution by $f_{C,l}(k,q,r)$. It is remarkable that its asymptotic behavior is the same as for a short-range potential. Recall from Eq. (3) that the ordinary Coulomb Jost solution $f_{C,l}(k,r)$ has a more complicated asymptotic behavior. In particular, one may expect that

$$\lim_{q\to k} f_{C,l}(k,q,r) \neq f_{C,l}(k,r)\,, \tag{11}$$

in contrast to the short-range case, where the equality holds, see Eq. (13) below.

The off-shell Jost function is defined by Fuda and Whiting[5,19] with

$$f_l(k,q) \equiv \lim_{r\to 0} f_l(k,q,r)\,(-2iqr)^l\, l!/(2l)!\,. \tag{12}$$

Note that this definition is completely analogous to the definition of $f_l(k)$ in Eq. (6). It also holds for the Coulomb case, just as Eq. (6) did.

Fuda and Whiting have studied the off-shell Jost solution, the off-shell Jost function, and some related functions for general short-range potentials. Some of their results, relevant for this paper, are

$$\lim_{q\to k} f_l(k,q,r) = f_l(k,r)\,, \tag{13}$$

$$\lim_{q\to k} f_l(k,q) = f_l(k)\,, \tag{14}$$

$$f_l(k,-q) = f_l^*(k,q) \quad (k \text{ and } q \text{ real})\,, \tag{15}$$

and

$$T_l(k,q;k^2) = \left(\frac{k}{q}\right)^l \frac{f_l(k,q) - f_l(k,-q)}{i\pi q f_l(k)}\,. \tag{16}$$

These authors have also derived $f_l(k,q,r)$ and $f_l(k,q)$ in closed form for the square-well potential and, for $l=0$ only, for the exponential potential and the Hulthén potential.

We shall discuss now some functions for the Hulthén potential V_H and compare these with the corresponding functions for the Coulomb potential V_C. We use the subscripts H and C, respectively, and we restrict ourselves to the $l=0$ case and omit l.

The Hulthén potential is given by

$$V_H(r) = V_0 e^{-r/a}/(1-e^{-r/a})\,.$$

V_H can be considered as a screened Coulomb potential with screening parameter a. For $a\to\infty$, V_H goes over into V_C. More precisely,

$$\lim_{\substack{a\to\infty \\ V_0\to 0 \\ aV_0\to 2k\gamma}} V_0 \frac{e^{-r/a}}{1-e^{-r/a}} = \frac{2k\gamma}{r} = V_C(r)\,. \tag{17}$$

The Jost solution and the Jost function for V_H are known in closed form (for $l=0$ only), see Newton[2] Chap. 14.4,

$$f_H(k,r) = e^{ikr}\, {}_2F_1(A,B;C;e^{-r/a})\,, \tag{18}$$

$$f_H(k) = {}_2F_1(A,B;C;1)$$

$$= \Gamma(C)/[\Gamma(1+A)\Gamma(1+B)]\,, \tag{19}$$

with

$$A = -iak + ia(k^2+V_0)^{1/2}\,,$$

$$B = -iak - ia(k^2+V_0)^{1/2}\,,$$

$$C = 1 - 2iak = 1 + A + B\,.$$

The expressions of Fuda and Whiting for the off-shell Jost solution and the off-shell Jost function are as follows:

$$f_H(k,q,r) = e^{i\sigma r}\left(1 + \frac{ABe^{-r/a}}{(1+\sigma)(C+\sigma)}\, {}_3F_2(1,1+A+\sigma,1+B+\sigma;2+\sigma,1+C+\sigma;e^{-r/a})\right), \tag{20}$$

$$f_H(k,q) = \frac{\Gamma(1+\sigma)\Gamma(C+\sigma)}{\Gamma(1+A+\sigma)\Gamma(1+B+\sigma)}\,, \tag{21}$$

with

$$\sigma = iak - iaq\,.$$

The derivation of Eq. (21) from Eq. (20) has been given by Bahethi and Fuda.[12] We now give a slightly different but essentially equivalent derivation because it is of general interest.

The ${}_3F_2$ of Eq. (20) is of the Saalschützian type.[9,10] Every Saalschützian ${}_3F_2$ of argument 1, with one of its three first parameters equal to 1, can be summed in terms of Γ functions. In order to find these Γ functions explicitly one can proceed as follows: According to a well-known theorem by Dixon,[9] any well-poised ${}_3F_2$ of unit argument can be summed in terms of Γ functions. A generalization of Dixon's theorem is (Slater,[9] p.52)

$${}_3F_2(a,b,c;e,f;1) = \frac{\Gamma(e)\Gamma(f)\Gamma(s)}{\Gamma(a)\Gamma(b+s)\Gamma(c+s)} \times {}_3F_2(e-a,f-a,s;b+s,c+s;1)\,, \quad \mathrm{Re}s>0,\ \mathrm{Re}a>0 \tag{22}$$

with

$$s \equiv e + f - a - b - c .$$

For a Saalschützian ${}_3F_2$ we have $s = 1$. $a = s = 1$ if and only if both ${}_3F_2$'s of Eq. (22) are Saalschützian. In this case, they can be summed in terms of Γ functions, which is easily seen if one uses the general formula

$$z\frac{\alpha\beta\cdots}{\gamma\delta\cdots}\,{}_mF_n(1,\alpha+1,\beta+1,\ldots;\gamma+1,\delta+1,\ldots;z) = -1 + {}_mF_n(1,\alpha,\beta,\ldots;\gamma,\delta,\ldots;z) . \quad (23)$$

By applying Eqs. (22) and (23) to the ${}_3F_2$ of Eq. (20) (with $c = 1$), Eq. (21) is readily obtained.

In the first place, we are interested in the behavior of $f_H(k)$, $f_H(k,r)$, $f_H(k,q)$, and $f_H(k,q,r)$ as the screening parameter a goes to infinity. Do these four functions approach their Coulomb analogs, as one might hope in view of Eq. (17)? The Coulomb analogs of the two first functions, $f_C(k)$ and $f_C(k,r)$, are given by Eqs. (4) and (7). We have been able to derive a closed expression for $f_C(k,q)$ which is extremely simple,

$$f_C(k,q) = \left(\frac{q+k}{q-k}\right)^{i\gamma} . \quad (24)$$

Here k is real positive and q is complex with $\mathrm{Im}q > 0$. One obtains $f_C(k,q)$ for real positive k and q by taking the limit $\mathrm{Im}q \to 0+$ which yields

$$f_C(k,q) = e^{\pi\gamma}\left|\frac{q+k}{q-k}\right|^{i\gamma} \quad \text{if } 0<q<k ,$$

$$= \left|\frac{q+k}{q-k}\right|^{i\gamma} \quad \text{if } 0<k<q .$$

In contrast fo $f_C(k,q)$, $f_C(k,q,r)$ is quite complicated. The function $f_C(k,q,r)$ can be expressed by an indefinite integral involving the Whittaker function W. We omit this expression since it does not seem to be very useful.

III. LIMITING RELATIONS

In this section, we shall consider the limits of various functions which have been discussed in Sec. II, for $a \to \infty$, for $q \to k$, for $r \to \infty$, and for $r \to 0$, respectively.

In the first place, we consider the limit of the functions f_H for the Hulthén potential, for $a \to \infty$ and $V_0 \to 0$ in such a way that their product remains constant, $a\,V_0 \to 2k\gamma$ [cf. Eq. (17)]. In this connection we rewrite the Hulthén potential as

$$V_H(r) = \frac{2k\gamma}{a}\,\frac{e^{-r/a}}{1-e^{-r/a}} = \frac{2k\gamma/a}{e^{r/a}-1} . \quad (25)$$

The four parameters A, B, C, and σ are functions of a. We have, for $a \to \infty$,

$$1 + A + \sigma \sim -ia(q-k) + 1 + i\gamma ,$$

$$1 + B + \sigma \sim -ia(q+k) + 1 - i\gamma ,$$

$$1 + C + \sigma = -ia(q+k) + 2 ,$$

$$2 + \sigma = -ia(q-k) + 2 .$$

We use the following property of the Γ function,

$$\frac{\Gamma(z+\alpha)}{\Gamma(z+\beta)} = z^{\alpha-\beta}\left[1 + O(z^{-1})\right] , \quad z \to \infty , \quad |\arg(z)| < \pi . \quad (26)$$

Then we obtain from Eq. (19)

$$\lim_{a\to\infty}(2ak)^{-i\gamma} f_H(k) = i^{-i\gamma}/\Gamma(1+i\gamma) = f_C(k) , \quad (27)$$

and from Eq. (21),

$$\lim_{a\to\infty} f_H(k,q) = f_C(k,q) . \quad (28)$$

From Eq. (27), we see that the usual (on-shell) Hulthén Jost function has no limit for $a \to \infty$, since it is proportional to $a^{i\gamma}$ for $a \to \infty$. Remarkably enough, Eq. (28) shows that the *off-shell* Hulthén Jost function *does* have as its limit the off-shell Coulomb Jost function.

Further, we consider $f_H(k,r)$ for $a \to \infty$ [see Eq. (18)]. It is known that[18]

$$\lim_{c\to\infty} z^{-\lambda}\,{}_2F_1(\lambda,b;c;1-c/z) = U(\lambda,\lambda-b+1,z) . \quad (29)$$

By applying the Euler transformation

$${}_2F_1(\lambda,b;c;\zeta) = (1-\zeta)^{-\lambda}\,{}_2F_1[\lambda,c-b;c;\zeta/(\zeta-1)] , \quad (30)$$

we get

$$\lim_{c\to\infty} c^{-\lambda}\,{}_2F_1(\lambda,b+c;c;1-z/c) = U(\lambda,\lambda+b+1,z) . \quad (31)$$

From this equality, we derive

$$\lim_{a\to\infty}(-2iak)^{-i\gamma}\,{}_2F_1(i\gamma, C-1-i\gamma; C; e^{-r/a}) = U(i\gamma, C, -2ikr) .$$

Finally, it is known that

$$U(\lambda,c,z) = z^{1-c}U(\lambda+1-c,2-c,z) , \quad (32)$$

and so we obtain from Eq. (31)

$$\lim_{a\to\infty}(2ak)^{-i\gamma}e^{ikr}\,{}_2F_1(i\gamma,-i\gamma-2iak;1-2iak;e^{-r/a}) = -2ikr\,i^{-i\gamma}e^{ikr}U(1+i\gamma,2,-2ikr) , \quad (33)$$

which is equivalent to

$$\lim_{a\to\infty}(2ak)^{-i\gamma} f_H(k,r) = f_C(k,r) , \quad (34)$$

according to Eqs. (4) and (18). So we have proved *that the Hulthén Jost solution*, just as the Hulthén Jost function, has no limit for $a \to \infty$.

We have seen in Eq. (27) that the limit for $a \to \infty$ of the *off-shell* Hulthén Jost *function* is equal to

$f_C(k,q)$. Therefore, we conjecture that the analogous relation for the off-shell Jost *solutions*, namely,

$$\lim_{a\to\infty} f_H(k,q,r) = f_C(k,q,r), \quad q \neq k, \tag{35}$$

will turn out to be true.

Let us now consider the limit for $q \to k$ of the off-shell Jost solutions and functions. In the short-range case, in particular for the Hulthén potential, it is known that

$$\lim_{q\to k} f(k,q) = f(k),$$

$$\lim_{q\to k} f(k,q,r) = f(k,r).$$

In the Coulomb case we have proved that $f_C(k,q)$ is not continuous at $q=k$. We have from Eq. (24),

$$\lim_{q\to k} \left(\frac{q-k}{q+k}\right)^{i\gamma} \frac{e^{\pi\gamma/2}}{\Gamma(1+i\gamma)} f_C(k,q) = f_C(k). \tag{36}$$

Therefore, we conjecture that the following equality will turn out to hold for the off-shell Coulomb Jost solution,

$$\lim_{q\to k} \left(\frac{q-k}{q+k}\right)^{i\gamma} \frac{e^{\pi\gamma/2}}{\Gamma(1+i\gamma)} f_C(k,q,r) = f_C(k,r). \tag{37}$$

We summarize the results obtained so far. For completeness we also give well-known relations and our conjectures. We use the abbreviations,

$$\alpha \equiv (2ak)^{-i\gamma}, \tag{38}$$

$$\omega \equiv \left(\frac{q-k}{q+k}\right)^{i\gamma} \frac{e^{\pi\gamma/2}}{\Gamma(1+i\gamma)} = \frac{f_C(k)}{f_C(k,q)}, \quad \mathrm{Im}q > 0. \tag{39}$$

It is known that

$$\lim_{r\to 0} f_H(k,r) = f_H(k), \tag{40a}$$

$$\lim_{r\to 0} f_H(k,q,r) = f_H(k,q), \tag{40b}$$

$$\lim_{r\to 0} f_C(k,r) = f_C(k), \tag{40c}$$

$$\lim_{q\to k} f_H(k,q) = f_H(k), \tag{40d}$$

$$\lim_{q\to k} f_H(k,q,r) = f_H(k,r). \tag{40e}$$

We have proved

$$\lim_{r\to 0} f_C(k,q,r) = f_C(k,q), \tag{40f}$$

$$\lim_{q\to k} \omega f_C(k,q) = f_C(k), \tag{40g}$$

$$\lim_{a\to\infty} \alpha f_H(k) = f_C(k), \tag{40h}$$

$$\lim_{a\to\infty} f_H(k,q) = f_C(k,q), \quad q \neq k, \tag{40i}$$

$$\lim_{a\to\infty} \alpha f_H(k,r) = f_C(k,r). \tag{40j}$$

Our conjectures are

$$\lim_{a\to\infty} f_H(k,q,r) = f_C(k,q,r), \quad q \neq k, \tag{40k}$$

$$\lim_{q\to k} \omega f_C(k,q,r) = f_C(k,r). \tag{40l}$$

We found it convenient to arrange these twelve limiting relations of Eq. (40) schematically, see Fig. 1 [note that $f_H(k)$, $a\to\infty$ occurs twice].

So we see that difficulties occur in the two limits $a\to\infty$ and $q\to k$. The third limit $r\to 0$ is, in general, well defined. We note in particular that it may be interchanged with $\lim a\to\infty$ and with $\lim q\to k$, e.g.,

$$\lim_{r\to 0}\lim_{a\to\infty} f_H(k,q,r) = \lim_{a\to\infty}\lim_{r\to 0} f_H(k,q,r) = f_C(k,q),$$

and

$$\lim_{r\to 0}\lim_{q\to k} f_H(k,q,r) = \lim_{q\to k}\lim_{r\to 0} f_H(k,q,r) = f_H(k).$$

We can take a fourth limit into our considerations, namely, $\lim r\to\infty$. Of course, the asymptotic behavior of the Jost solutions is well known, because it is part of their definition. We shall give one interesting example, which involves the interchange of $\lim r\to\infty$ and $\lim a\to\infty$. From Eq. (40j), we have

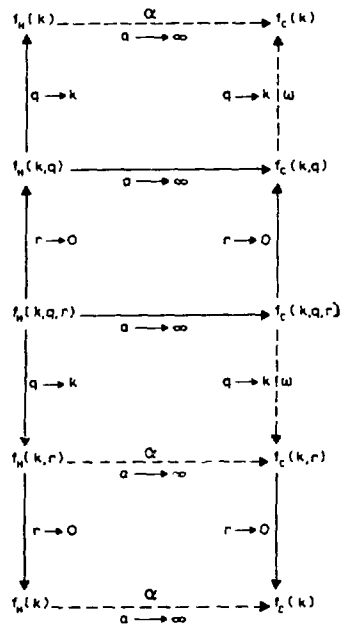

FIG. 1. Limiting relations for various functions. A full arrow indicates that the corresponding limit exists. For a dashed arrow, the limit does not exist, but a factor α or ω, respectively, is involved, see text.

$$\lim_{a\to\infty}(2ak)^{-i\gamma}f_H(k,r)=f_C(k,r)\,,$$

and from Eq. (3),

$$\lim_{r\to\infty}(2kr)^{i\gamma}e^{-ikr}f_C(k,r)=1\,.$$

It follows from these two equations and Eq. (2) that

$$\lim_{r\to\infty}\lim_{a\to\infty}(r/a)^{i\gamma}e^{-ikr}f_H(k,r)=1\,. \tag{41}$$

These two limits cannot be interchanged, because

$$\lim_{a\to\infty}\lim_{r\to\infty}(r/a)^{i\gamma}e^{-ikr}f_H(k,r)$$

is not defined. Instead we have

$$\lim_{a\to\infty}\lim_{r\to\infty}e^{-ikr}f_H(k,r)=1\,.$$

The off-shell Jost function has an analytic continuation into the complex q plane. From our closed form, Eq. (24), we have for the Coulomb off-shell Jost function, for real positive k and complex q,

$$f_C^*(k,q^*)=f_C(k,-q)\,. \tag{42}$$

This is a generalization of Fuda's relation for real q, see Eq. (15).

One should compare Eq. (42) with similar equations for the ordinary Jost function, see Eqs. (12.30) and (12.32a) of Newton.[2] It appears natural to define a "minus" Jost function f_- by

$$f_-(k,q)=f(k,-q)\,. \tag{43}$$

For a short-range potential, the half-off-shell T matrix can be expressed in terms of the off-shell Jost function, as Fuda and Whiting have shown, see our Eq. (16). We rewrite this equation as follows,

$$i\pi q f(k)\,\langle q|T|k\rangle=f(k,q)-f^*(k,q)\,, \tag{44}$$

where the T operator has energy variable k^2.

In virtue of Eq. (40.9) we have for $q\neq k$,

$$\lim_{a\to\infty}f_H(k,q)=f_C(k,q)\,,$$

so

$$\lim_{a\to\infty}f_H^*(k,q)=f_C^*(k,q)\,. \tag{45}$$

Therefore, the limit for $a\to\infty$ of $f_H(k)\langle q|T_H|k\rangle$ exists for $q\neq k$. This implies that $\langle q|T_H|k\rangle$ has no limit for $a\to\infty$. Now, it is well known that the following equality holds,

$$\langle q|T_H|k\rangle=\langle q|V_H|k+\rangle_H\,, \tag{46}$$

where $|k+\rangle_H$ is the (outgoing) Hulthén $l=0$ scattering state. The Coulomb analog of Eq. (46) is not valid, since the Coulomb half-shell T matrix is not defined. However, $\langle q|V_C|k+\rangle_C$ is a well-defined quantity, for which we have been able to find the following closed form,

$$\langle q|V_C|k+\rangle_C=\frac{1}{i\pi q f_C(k)}\lim_{\eta\to0+}\left[\left(\frac{q+i\eta+k}{q+i\eta-k}\right)^{i\gamma}-\text{c.c.}\right],\qquad k>0\,,$$

$$=\lim_{\eta\to0+}\frac{f_C(k,q+i\eta)-f_C^*(k,q+i\eta)}{i\pi q f_C(k)},\qquad k>0\,. \tag{47}$$

From Eqs. (44)–(47), we derive the following interesting equality,

$$f_C(k)\langle q|V_C|k+\rangle_C=\lim_{a\to\infty}f_H(k)\langle q|V_H|k+\rangle_H$$

$$=\lim_{a\to\infty}f_H(k)\langle q|T_H|k\rangle\,. \tag{48}$$

IV. MODIFIED ECKART POTENTIALS AND LIMITING RELATIONS

It is very likely that all troubles with nonexistent limits we have encountered in Sec. III merely arise from the Coulomb tail. In order to investigate this point, one may study a screened $r^{-\alpha}$ type potential with $\alpha>1$. We feel that all limits of our scheme will be valid if V_C is replaced by a (nonsingular) potential of the form

$$V_\alpha(r)=O(r^{-\alpha}),\quad \alpha>1,\quad r\to\infty\,,$$

and V_H by an exponentially screened V_α potential. A convenient candidate for such a potential is

$$V_E(r)=\frac{2}{a^2}\frac{e^{-r/a}}{(1-e^{-r/a})^2}\,. \tag{49}$$

This is a member of the Eckart[17] class. Obviously we have

$$\lim_{a\to\infty}V_E(r)=2/r^2\,. \tag{50}$$

The $l=0$ Jost solution for $V_E(r)$ is well known,[1]

$$f_E(k,r)=e^{ikr}\left(1+\frac{2}{(1-2iak)(e^{r/a}-1)}\right). \tag{51}$$

However, we have an annoying complication which should be avoided in this investigation. Since $V_E(r)$ is singular at the origin,

$$V_E(r)\simeq 2/r^2,\quad r\to0\,,$$

the usual definition of the Jost function is meaningless. This problem may be disposed of in either of two ways, by not considering V_E but one of the potentials $V_E^{(1)}$, $V_E^{(2)}$ defined below.

In the first approach we define

$$V_E^{(1)}(r)\equiv V_E(r)-2/r^2\,. \tag{52}$$

Then the ($l=0$) Jost solution $f_E(k,r)$ is just the $l=1$ Jost solution for $V_E^{(1)}$: $f_E(k,r)=f_{E,1}^{(1)}(k,r)$, since the term $2/r^2$ equals the centrifugal-barrier term for $l=1$. So we can find the $l=1$ Jost function simply by applying Eq. (6),

$$f^{(1)}_{E,l}(k) = \lim_{r\to 0} -ikrf_E(k,r) = \frac{2iak}{2iak-1}\,. \tag{53}$$

Remarkably enough, for this nonsingular potential $V^{(1)}_E$, we did *not* succeed in finding the $l=0$ Jost solution, but the $l=1$ Jost solution (and $l=1$ Jost function).

In the second approach, we define

$$V^{(2)}_E(r) \equiv V_E(r+d) = \frac{2}{a^2}\,\frac{\exp[-(r+d)/a]}{\{1-\exp[-(r+d)/a]\}^2}\,, \tag{54}$$

with $d>0$. Obviously, $f_E(k,r+d)$ is a solution of the $l=0$ radial Schrödinger equation. Therefore, the Jost solution for $V^{(2)}_E$ is

$$\begin{aligned} f^{(2)}_E(k,r) &= e^{-ikd}f_E(k,r+d) \\ &= e^{ikr}\left(1+\frac{2(1-2iak)^{-1}}{\exp[(r+d)/a]-1}\right). \end{aligned} \tag{55}$$

The $l=0$ Jost function for $V^{(2)}_E$ is then given by

$$f^{(2)}_E(k) = f^{(2)}_E(k,0) = 1+\frac{2(1-2iak)^{-1}}{\exp(d/a)-1}\,. \tag{56}$$

Now we consider the limits of the above quantities for $a\to\infty$. We have

$$\begin{aligned} &\lim_{a\to\infty} V^{(1)}_E = 0\,, \\ &\lim_{a\to\infty} V^{(2)}_E = 2(r+d)^{-2}\,, \\ &\lim_{a\to\infty} f^{(1)}_{E,l}(k,r) = ikrh^{(+)}_l(kr) = e^{ikr}[1-(ikr)^{-1}]\,, \\ &\lim_{a\to\infty} f^{(1)}_{E,l}(k) = 1\,, \end{aligned} \tag{57}$$

$$\lim_{a\to\infty} f^{(2)}_E(k,r) = e^{ikr}\{1-[ik(r+d)]^{-1}\}, \tag{58}$$

$$\lim_{a\to\infty} f^{(2)}_E(k) = 1-(ikd)^{-1}\,. \tag{59}$$

It follows from these expressions that the limits of $f^{(1)}$ and $f^{(2)}$ do indeed correspond to the limits of $V^{(1)}_E$ and $V^{(2)}_E$, respectively.

Fuda has obtained an expression for the off-shell Jost function for a short-range potential [Ref. 6, Eq. (25)]. In the notation of Ref. 20, it reads

$$f_l(k,q) = 1+\tfrac{1}{2}\pi q(q/k)^l\,{}_0\langle ql\,|\,V_l\,|\,kl+\rangle f_l(k)\,, \tag{60}$$

where

$${}_0\langle ql\,|\,r\rangle \equiv (2/\pi)^{1/2}i^{-l}h^{(+)}_l(qr)\,.$$

We find from Eq. (60) that the off-shell Jost functions $f^{(1)}_E$ and $f^{(2)}_E$ are continuous at $q=k$. Moreover, the limits $a\to\infty$ and $q\to k$ may be interchanged. We conjecture that the same holds for the off-shell Jost solutions. If this is true, a diagram can be given similar to Fig. 1 where now, however, all of the limits are valid.

So we have indeed succeeded in proving (except for the off-shell Jost solutions) that, for the above screened r^{-2}-type potentials, the screening can be turned off without any discontinuity problem, in contrast to the situation for the (Hulthén) screened r^{-1} potential.

V. SUMMARY AND DISCUSSION

We have studied in Sec. II the off-shell Jost solution and function for the Coulomb potential for arbitrary values of l. For $l=0$, we have obtained a very simple closed expression for the off-shell Coulomb Jost function $f_C(k,q)$, see Eq. (24).

The Hulthén potential goes over into the Coulomb potential when the screening parameter a goes to infinity. In Sec. III we have investigated whether or not the limits for $a\to\infty$ of the Hulthén Jost functions and solutions are equal to the Coulomb Jost functions and solutions, respectively. The limits of the ordinary (on-shell) Jost function and solution do not exist. We have proved that in both cases the singularity is due to the factor $a^{i\nu}$. Further, we have proved that for the Coulomb case the off-shell Jost function is not continuous at $q=k$. Here, the singularity is given by the factor $(q-k)^{-i\nu}$. We also have derived some relations for the limits $r\to\infty$ and $r\to 0$. The main results have been summarized in Eqs. (40)–(41) and in Fig. 1. In the final part of Sec. III we have given an interesting limiting relation, for $a\to\infty$, of the half-shell Hulthén T matrix, see Eq. (48).

The different kinds of singularities which we have found in Sec. III should be attributed to the long range of the Coulomb potential. In earlier studies of the Coulomb T matrix we have seen singularities of a similar type.[13,21] It is very likely that, with a screened $r^{-\alpha}$ potential with $\alpha>1$, no singularity will turn out to exist. With the aim of giving an illustrative and interesting example, we have studied in Sec. IV a potential of the Eckart[17] class, which may be considered as a screened r^{-2} potential. Its Jost solution is well known and has a simple form. However, this Eckart potential is singular at the origin, $V(r) \simeq 2r^{-2}$, $r\to 0$, which makes the usual definition of the Jost function meaningless.

One way of avoiding this complication consists in subtraction of the singular term, which can in this particular case be interpreted as a centrifugal-barrier term for $l=1$.

A second method is generally useful for an arbitrary potential. The central idea here is that the Jost solution for a shifted potential function follows in an easy way from the ordinary Jost solution. To be specific, let $f(k,r)$ be the $l=0$ Jost solution for any potential $V(r)$. Then $e^{-ikd}f(k,r+d)$ is the Jost solution for the shifted potential $V(r+d)$ (where d is some real param-

eter). This follows easily from the defining differential equation. By the same reasoning, $e^{-iqd}f(k,q,r+d)$ is the off-shell Jost solution for the shifted potential $V(r+d)$. Obviously, the above statements hold only for the $l=0$ case.

By applying this method to any potential $V(r)$ which is (too) singular at $r=0$, we obtain a potential which is regular at $r=0$, if we choose d to be positive. Therefore, it has a Jost solution which is sufficiently regular at $r=0$ that the corresponding Jost *function* is well defined [namely, by the limit of $f(k,r)$ for $r\to 0$].

For the two modified Eckart potentials, obtained in the above-described way, we have made an investigation similar to the one of Sec. III. We have shown that the limits for $a\to\infty$ of the Jost functions corresponding to the screened potentials exist and do indeed correspond to the Jost functions of the unscreened potentials.

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Synopses

Synopsis

This dissertation consists of an analytic study of the Coulomb interaction in nonrelativistic quantum mechanics and some related topics. We investigate in a number of self-contained articles various interesting and important properties of the Coulomb potential. Some of these properties are shared by other potentials which also play a role in quantum mechanics. For such related interactions a comparative study is made.

The great physical importance of the Coulomb interaction follows from the observation that it acts between any pair of charged particles. Since moreover Coulomb's law, describing the force as a function of the distance between two particles, has the same mathematical form as Newton's law of gravitation, it is not surprising that this law has received a great deal of attention.

Apart from being important in physics the Coulomb potential is also mathematically of great interest. This is mainly due to the following two characteristic properties. In the first place, the Coulomb Hamiltonian shows in addition to the usual spherical symmetry an extra symmetry, which is closely connected with the invariant vector of Lenz in the classical conic section orbits. The main axis of such a conic section orbit is fixed in space. In the second place, the Coulomb potential and more generally any Coulomb-like potential has a long range. This means that such a potential diminishes rather slowly for increasing distance. The long range generates singularities in certain quantities which play an important role in quantum mechanical scattering theory, notably in the off-shell transition matrix. This so-called T matrix has a branch-point singularity in the half-shell and on-shell points, which requires the application of a certain renormalization procedure. Furthermore, the Coulomb T matrix has an essential singularity in the zero-energy point. This singularity is connected with the infinite number of bound-state poles which accumulate at the origin of the complex energy plane.

In this thesis we pay attention in particular to the off-shell transition matrix for Coulomb plus short-range potentials. Here the short-range potentials are taken to be local as well as nonlocal, separable. We develop analytic expressions involving hypergeometric functions for many quantities. Especially for the case of rational separable potentials we are able to derive relatively simple expressions for the T matrix and for the effective range function.

The principal difficulties in the description of proton-deuteron scattering and break-up reactions, due to the Coulomb interaction, are studied by working out a simple model. These problems concern the two-particle renormalization procedure and the essential singularity at zero energy discussed before.

We study the bound states for the Coulomb plus Yamaguchi potential, for the symmetric shifted Coulomb potential, and for local potentials with an inverse-distance-squared asymptotic behavior.

Further we investigate so-called irregular solutions of the three-dimensional and radial Schrödinger equations. These are closely connected with the Jost solutions. We study for the Coulomb, Hulthén and Eckart potentials the Jost solutions, off-shell Jost solutions, Jost functions, and off-shell Jost functions.

A large variety of simple analytic expressions is obtained for the Coulomb off-shell Jost functions for all values of the angular momentum quantum number. Further we give for some Coulomb Jost states analytic expressions involving hypergeometric functions.

We develop for Coulomb plus short-range potentials a large number of interesting relations between various quantities that play an important role in off-shell scattering theory.

Synopsis

Deze dissertatie bestaat uit een analytische studie van de Coulomb wisselwerking in de niet-relativistische quantummechanica en een aantal hiermee samenhangende onderwerpen. In een aantal onafhankelijke artikelen onderzoeken we diverse belangwekkende en belangrijke eigenschappen van de Coulomb potentiaal. Sommige van deze eigenschappen heeft de Coulomb potentiaal gemeen met andere potentialen die eveneens een rol spelen in de quantummechanica. Voor dergelijke verwante potentialen wordt een vergelijkende studie verricht.

De grote fysische betekenis van de Coulomb wisselwerking volgt uit de constatering dat zij werkt tussen elk paar geladen deeltjes. Bovendien heeft de wet van Coulomb, die de kracht als functie van de afstand tussen twee deeltjes beschrijft, dezelfde wiskundige vorm als de zwaartekrachtwet van Newton. Het is dan ook niet verwonderlijk dat aan deze wet veel aandacht is besteed.

De Coulomb potentiaal is niet alleen belangrijk in de natuurkunde, maar ook wiskundig gezien zeer interessant. Dit is voornamelijk te danken aan de volgende twee karakteristieke eigenschappen. Ten eerste vertoont de Coulomb Hamiltoniaan behalve de gewone bolsymmetrie een extra symmetrie, die in verband staat met de invariante vector van Lenz in de klassieke kegelsnede-banen. De hoofdas van zo'n kegelsnede-baan ligt vast in de ruimte. Ten tweede heeft de Coulomb potentiaal en meer algemeen elke Coulomb plus korte-dracht potentiaal een lange dracht. Dit betekent dat zo'n potentiaal tamelijk langzaam afneemt voor toenemende afstand. De lange dracht veroorzaakt singulariteiten in bepaalde grootheden die een belangrijke rol spelen in de quantummechanische verstrooiingstheorie, met name in de off-shell overgangsmatrix. Deze zogenaamde T matrix heeft een vertakkingspunt-singulariteit in de half-shell en on-shell punten, hetgeen toepassing van een bepaalde renormalisatieprocedure vereist. Verder heeft de Coulomb T matrix in het energienulpunt een essentiële singulariteit, die in direct verband staat met het oneindig groot aantal gebonden toestanden. De hiermee corresponderende polen verdichten zich in de oorsprong van het complexe energievlak.

In dit proefschrift besteden we vooral aandacht aan de off-shell overgangsmatrix voor Coulomb plus korte-dracht potentialen. Hierbij worden zowel lokale als niet-lokale, separeerbare, potentialen beschouwd. We ontwikkelen voor diverse grootheden analytische uitdrukkingen waarin hypergeometrische functies voorkomen. In het bijzonder voor het geval van rationale separeerbare potentialen zijn we in staat relatief eenvoudige uitdrukkingen af te leiden voor de T matrix en voor de effectieve dracht functie.

De voornaamste moeilijkheden in de beschrijving van proton-deuteron verstrooiings- en break-up reacties, veroorzaakt door de Coulomb wisselwerking, worden bestudeerd aan de hand van een eenvoudig model. Het gaat hierbij in feite om de bovengenoemde twee-deeltjes renormalisatieprocedure en de essentiële singulariteit in het energienulpunt.

We bestuderen de gebonden toestanden voor de Coulomb plus Yamaguchi potentiaal, voor de symmetrische verschoven Coulomb potentiaal, en voor lokale potentialen die asymptotisch omgekeerd evenredig zijn met het kwadraat van de afstand.

Verder worden de zogenaamde irreguliere oplossingen van de driedimensionale en radiale Schrödingervergelijkingen onderzocht. Deze staan in nauw verband met de Jost oplossingen. Voor de Coulomb, Hulthén en Eckart potentialen bestuderen we de Jost oplossingen, off-shell Jost oplossingen, Jost functies en off-shell Jost functies.

We leiden een groot aantal eenvoudige analytische uitdrukkingen af voor de Coulomb off-shell Jost functies voor alle waarden van het impulsmomentquantumgetal. Verder geven we voor enkele Coulomb Jost toestanden analytische uitdrukkingen waarin hypergeometrische functies voorkomen.

Voor Coulomb plus korte-dracht potentialen ontwikkelen we een groot aantal interessante relaties tussen diverse grootheden die een belangrijke rol spelen in de off-shell verstrooiingstheorie.

КРАТКОЕ СОДЕРЖАНИЕ

Настоящая диссертация состоит из аналитического исследования кулоновского взаимодействия в нерелятивистской квантовой механике и некоторых связанных с этим тем. В нескольких самостоятельных статьях мы исследуем различные важные и представляющие интерес свойства кулоновского потенциала. Некоторые свойства, характерные для кулоновского потенциала, присущи также другим потенциалам, играющим важную роль в квантовой механике. Для таких родственных взаимодействий производится сравнительное исследование.

Вывод о большом физическом значении кулоновского взаимодействия можно сделать из наблюдения, что такое взаимодействие действительно для любой пары заряженных частиц. Поскольку закон Кулона, описывающий силу как функцию расстояния между двумя частицами, имеет то же самое математическое выражение, что и закон тяготения Ньютона, то совсем неудивительно проявление к этому закону повышенного интереса.

Кулоновский потенциал не только имеет большое значение в физике, но и чрезвычайно интересен с математической точки зрения, главным образом, благодаря двум следующим характерным свойствам. Во-первых, кроме обычной сферической симметрии кулоновские гамильтонианы обнаруживают дополнительную симметрию, которая тесно связана с инвариантным вектором Ленца в классических орбитах конического сечения. Главная ось такой орбиты конического сечения закреплена в пространстве. Во-вторых, кулоновский и вообще любой подобный кулоновскому потенциал отличается дальнодействующим характером. Это значит, что для увеличивающегося расстояния такой потенциал убывает довольно медленно. Дальнодействие вызывает сингулярности в определенных величинах, которые играют существенную роль в квантомеханической теории рассеяния, особенно, в случае матрицы перехода, лежащей вне поверхности энергии. Эта т.н. Т-матрица имеет сингулярность точки ветвления в полуповерхностной и наповерхностной точках, что требует применения определенного метода перенормировки. Кроме того, кулоновская Т-матрица имеет в точке нулевой энергии важную сингулярность,

находящуюся в прямой связи с бесконечным числом связанных состояний, соответствующие полюса которых собираются в исходной точке комплексной плоскости энергии.

Особое внимание в этой диссертации уделяется матрице перехода, лежащей вне поверхности энергии, для кулоновского плюс короткодействующего потенциалов, причем рассматриваются как локальные, так и нелокальные, сепарабельные потенциалы. Мы выводим аналитические выражения, в которых встречаются гипергеометрические функции для многих величин. Особенно в случае сепарабельных потенциалов можно вывести довольно простые выражения для Т-матрицы и для функции эффективной дальности действия.

Основные трудности в описании рассеяния протонов дейтронами и реакций развала, вызванных кулоновским взаимодействием, исследуются путем разработки простой модели. Суть дела фактически заключается в методе перенормировки двух частиц и важной сингулярности при нулевой энергии.

Исследуются связанные состояния для кулоновского плюс ямагушинского потенциалов, для симметричного смещенного кулоновского потенциала и локальных потенциалов с асимптотикой, обратно пропорциональной квадрату расстояния.

Далее мы исследуем т.н. иррегулярные решения трехмерных и радиальных уравнений Шрёдингера. Они вплотную приближаются к решениям Джоста. Для кулоновского, хултенского и экартовского потенциалов мы исследуем решения Джоста, решения Джоста в случае выхода за поверхность энергии, функции Джоста и функции Джоста в случае выхода за поверхность энергии.

Нами получено большое число простых аналитических выражений для кулоновских внеповерхностных функций Джоста для всех значений квантового числа орбитального момента. Для некоторых кулоновских состояний мы даем также аналитические выражения, включающие гипергеометрические функции.

Мы разрабатываем для кулоновского плюс короткодействующего потенциалов большое количество интересных соотношений между различными величинами, которые играют важную роль в теории рассеяния вне поверхности энергии.

梗　概

この学位論文は、非相対論的量子力学におけるクーロン相互作用の解析的研究と、それに関係のあるいくつかの主題とを取扱うものである。私は一連の論文において、クーロン・ポテンシャルのいろいろな興味ある重要な性質を調べてきた。クーロン・ポテンシャルのこれらの種の性質は、量子力学においてやはり一役を演ずる他のポテンシャルの性質と共通するものである。ここではそのような互に関連のあるポテンシャルについての比較研究を行う。

クーロン相互作用の物理学における重要性は、クーロンの力で任意の一対の荷電粒子間に働くという事実に存する。しかも、力を二つの粒子間の距離の函数として与えるクーロンの法則はニュートンの重力法則と同じ数学形式を持っている。だからクーロンの法則が多くの注意を惹いてきたのも決して異とするに足りない。

クーロン・ポテンシャルは物理学において重要なばかりではなく、数学的にしても非常に面白い。その理由は、主として次の二つの特性による。すなわち、第一に、クーロン・ハミルトン演算子は、通常の球対称のほかに、古典円錐曲線軌道の主軸は空間に固定している。第二に、クーロン・ポテンシャル、いやもっと一般的にクーロン・プラス・近距離ポテンシャルは常に遠達力をもっている。すなわち、このようなポテンシャルは距離が増大するにつれてかなり緩やかに減少する。この遠達力は、量子力学的散乱理論で重要なある種の量、例えば吋-shell遷移行列における特異点の原因をなすものである。このいわゆる下列は、

half-shell points ならびに on-shell points で分岐点特異点 (branch-point singularity) を持っており、そのため何らかのくりこみの方法を用いることが必要となる。さらに、クーロン・T行列はエネルギー零点において真性特異点を有しており、これが無限に多い束縛状態をもたらす。これらの状態に対応する極は、複素エネルギー面の原点に密集している。

この学位論文において、私は、特にクーロン・プラス・近距離ポテンシャルに対する off-shell 還元核を取扱う。ただし、局所的と非局所的と両方の、可能なポテンシャルを考える。そして種々の量に対して、超幾何函数を用いた解析式を展開しよう。特に有理分離可能ポテンシャルの場合に T行列ならびに有効距離函数に対して比較的簡単な式を導くことをホそう。

クーロン相互作用による陽子－重陽子の散乱および解体の反応を叙述する場合の主な困難を、一つの単純なモデルによって示す。この問題は、事実上、上述の二粒子間のくりこみ方法とエネルギー零点での真性特異点との問題である。

それから、束縛状態を、クーロン・プラス・山口ポテンシャルの場合、対称的な変位クーロン・ポテンシャルの場合、また漸近的に距離の二乗に逆比例する局所的ポテンシャルの場合について研究する。

さらに三次元のシュレーディンガー方程式の径部分のいわゆる非正則解のことを調べる。これは Jost 解と密接な関係を持っている。クーロン・ポテン Hulthén ポテンシャル、および Eckart ポテンシャルに

対して、それぞれ Jost 解、off-shell Jost 解、Jost 函数ならびに off-shell Jost 函数を検討しよう。

クーロン・off-shell Jost 函数に対して、角運動量[illegible]数のあらゆる値にわたって成立する一連の簡単な[illegible]形式を導き出そう。また若干のクーロン・Jost 状態[illegible]して、幾可函数を用いた解析式を与えよう。

最後に、クーロン・プラス・近距離ポテンシャルに対して off-shell 散乱理論で重要な諸量[illegible]に存在する多数の興味深い関係を導き出そう。