Appendix A
Density Operator and Density Matrix

In this appendix, we introduce density operator as well as density matrix and explain, in brief, some of their important properties relevant to quantum information in general, and to the studies reported in this monograph in particular.

A.1   Completely Random, Pure, and Mixed Systems

Let us consider a beam of silver atoms directly coming out of a hot oven in a Stern–Gerlach type experiment [58]. (This beam can also be called a system/collection/ensemble consisting of subsystems which, in the present case, are silver atoms.) Such a beam can be characterized by

$$p_\uparrow = \frac{N_\uparrow}{N_\uparrow + N_\downarrow} \qquad \text{and} \qquad p_\downarrow = \frac{N_\downarrow}{N_\uparrow + N_{\downarrow 1}}. \qquad (A.1a)$$

Here, $N_\uparrow$ and $N_\downarrow$ are the number of silver atoms in the beam which have their spin up and down (i.e., are in the spin state $|0\rangle$ and $|1\rangle$), respectively. Then, $p_\uparrow$ and $p_\downarrow$ in (A.1a) represent atoms' fractional populations in the two spin states. An unpolarized beam is looked upon to be an even mixture of atoms in the states $|0\rangle \equiv |\uparrow\rangle$ and $|1\rangle \equiv |\downarrow\rangle$. This, in other words, means

$$N_\uparrow = N_\downarrow \qquad \Longrightarrow \qquad p_\uparrow, \quad p_\downarrow = 0.5 \qquad (A.1b)$$

for a beam in which atoms are expected to have their spins oriented randomly in space.

In (A.1), $p_\uparrow$ and $p_\downarrow$ are simply two real numbers. In this equation, there is no information on the relative phase between the spin-up and spin-down kets $|0\rangle$ and $|1\rangle$, respectively. Such a collection of particles is usually referred to as an incoherent,

even mixture of the $|\uparrow\rangle$ and $|\downarrow\rangle$ states. This is called unpolarized because there is no preferred direction for the orientation of the spin of a silver atom and, hence, is characterized by (A.1).

Such a beam, containing particles coming directly out of an oven, is an example of a completely random system. In contrast, a beam that has gone through a selective Stern–Gerlach type measurement [58] is an example of a pure system. This beam is said to be polarized because all members of the collection are characterized by a single common ket ($|0\rangle$ or $|1\rangle$) that describes a state with spin ($\uparrow$ or $\downarrow$) of each atom pointing in some definite direction.

Unpolarized and pure collections are two opposite extremes of a so-called mixed collection. In a mixed beam of silver atoms, for example, a certain fraction—say, 70%—of the members are characterized by the state $|0\rangle$, the remaining 30% by $|1\rangle$. Such a beam is said to be partially polarized. Although states $|0\rangle$ and $|1\rangle$ need not be orthogonal, they are, however, normalized. One can, for example, have 70% of the atoms with their spins in the positive OX direction and 30% of the spin in the negative OZ direction.

Thus, a pure system is defined to be a collection of physical subsystems such that each member is characterized by the same state $|\psi\rangle$. In a mixed system, on the other hand, a fraction of its members with relative population p_1 are in the normalized state $|\psi_1\rangle$, some other fraction with relative population p_2 in the normalized state $|\psi_2\rangle$, and so on. Alternatively, a mixed system can be viewed as a mixture of pure collections. The fractional populations of any mixed system must satisfy the condition

$$\sum_i p_i = 1. \tag{A.2}$$

The number of terms in (A.2) needs not coincide with the dimensionality "d" of the Hilbert space of the system being considered. For example, for a system consisting of spin-$\frac{1}{2}$ particles with $d = 2$, one may have 40% with spins in the positive OZ direction, 30% in the positive OX direction, and the remaining 30% with their spins in the negative OY direction.

State in (2.1), [or (2.2)], on the other hand, is a coherent, linear superposition wherein the phase relation (in the form of the azimuthal angle ϕ) between kets $|0\rangle$ and $|1\rangle$ contains vital information on the spin orientation of a spin-$\frac{1}{2}$ particle. Neither of $p_\uparrow$ and $p_\downarrow$ in (A.1) should, in general, be confused with the probabilities $|C_0|^2$ and $|C_1|^2$ in (2.1b), or r_0^2 and r_1^2 in (2.2a).

A.2   Averaged Value and Representations

According to one of the fundamental postulates [58] of quantum mechanics, the complete information about a system is contained in its wavefunction. But a quantum mechanical wavefunction can describe only a pure system. The density operator formalism, introduced by J. von Neumann [155, 354], is capable of quantitatively describing physical situations with mixed as well as pure collections.

The methods of density operator for mixed and/or pure states of a system were first applied to atomic physics, probably, by Fano [62]. These methods have since then been discussed in varying details in books on quantum mechanics (see, for example, [58]) as well as in the literature (e.g., [60, 61, 68], *etc*) pertaining to the atomic physics.

Suppose, one makes a measurement of some observable, say, Ω on the mixed collection defined in the following Sect. A.1 of this appendix. Then the averaged, measured value (i.e., system/collection average) of Ω for a large number of measurements is given by

$$
\begin{aligned}
[\Omega] &= \sum_i p_i \langle \psi_i | \Omega | \psi_i \rangle \\
&= \sum_{inm} p_i \langle \psi_i | \phi_n \rangle \langle \phi_n | \Omega | \phi_m \rangle \langle \phi_m | \psi_i \rangle \\
&= \sum_{inm} p_i \left[\langle \phi_m | \psi_i \rangle \langle \psi_i | \phi_n \rangle \right] \langle \phi_n | \Omega | \phi_m \rangle .
\end{aligned}
\tag{A.3}
$$

Here, the number of terms to be included in the sums over n (or, m) is just equal to those present in the complete set whose members are the orthonormal basis $\{|\phi_n\rangle,$ $n = 1, 2, \ldots\}$ (or, $\{|\phi_m\rangle, m = 1, 2, \ldots\}$). The number of terms in the sum over i in (A.3) depends, on the other hand, on the decomposition of the mixed collection in pure subsystems. The quantity

$$
\rho \equiv \sum_i p_i \, |\psi_i\rangle \langle \psi_i|
\tag{A.4}
$$

is called the density operator for our mixed system/collection. The (m, n)-th element of this operator's matrix representation in the orthonormal basis $\{|\phi_n\rangle\}$ is

$$
\langle \phi_m | \rho | \phi_n \rangle = \sum_i p_i \langle \phi_m | \psi_i \rangle \langle \psi_i | \phi_n \rangle .
\tag{A.5}
$$

The density operator/matrix contains all the physically significant information about the system under consideration. Now the system-average (A.3) can be written as

$$
\begin{aligned}
[\Omega] &= \sum_{mn} \langle \phi_m | \rho | \phi_n \rangle \langle \phi_n | \Omega | \phi_m \rangle \\
&= \sum_m \langle \phi_m | \rho \, \Omega | \phi_m \rangle \\
&= \mathrm{Tr}(\rho \, \Omega) .
\end{aligned}
\tag{A.6}
$$

As the trace of a matrix is known to be independent of its representation, any complete set $\{|\phi\rangle\}$ can, therefore, be used for calculating $\text{Tr}(\rho\,\Omega)$ in (A.6).

The Hermitian conjugate of the density operator (A.4) is

$$\rho^\dagger = \left(\sum_i p_i \, |\psi_i\rangle\langle\psi_i| \right)^\dagger$$

$$= \sum_i p_i \, |\psi_i\rangle\langle\psi_i| = \rho, \tag{A.7}$$

remembering that each of the probabilities p_i in(A.2) is real. Thus, a physically acceptable density operator/matrix should always be Hermitian.

We further have

$$\text{Tr}(\rho) = \sum_n \langle\phi_n|\rho|\phi_n\rangle$$

$$= \sum_n \langle\phi_n| \left(\sum_i p_i \, |\psi_i\rangle\langle\psi_i| \right) |\phi_n\rangle$$

$$= \sum_{i\,n} p_i \, \langle\phi_n|\,\psi_i\rangle \, \langle\psi_i|\,\phi_n\rangle$$

$$= \sum_i p_i \left(\sum_n \langle\psi_i|\,\phi_n\rangle \, \langle\phi_n|\,\psi_i\rangle \right)$$

$$= \sum_i p_i \, \langle\psi_i|\,\psi_i\rangle = \sum_i p_i \tag{A.8}$$

assuming that the states $|\psi_i\rangle$ are normalized. Then in view of (A.2),

$$\text{Tr}(\rho) = 1. \tag{A.9}$$

Such a density operator is said to be normalized to unit trace. In situations wherein normalization (A.9) does not hold, the system-average of an operator is given by

$$[\Omega] = \frac{\sum_i p_i \, \langle\psi_i|\Omega|\psi_i\rangle}{\sum_i p_i}. \tag{A.10a}$$

Using relations (A.6) and (A.8), one can write

$$[\Omega] = \frac{\text{Tr}\,(\rho\Omega)}{\text{Tr}(\rho)}. \tag{A.10b}$$

Let us now calculate the trace of the square of a density operator, i.e.,

$$\mathrm{Tr}(\rho^2) = \sum_m \langle \phi_m | \rho^2 | \phi_m \rangle$$

$$= \sum_{mn} \langle \phi_m | \rho | \phi_n \rangle \langle \phi_n | \rho | \phi_m \rangle.$$

On substituting (A.4)

$$\mathrm{Tr}(\rho^2) = \sum_{mn} \left[\langle \phi_m | \left(\sum_i p_i \, |\psi_i\rangle\langle\psi_i| \right) |\phi_n\rangle \right] \left[\langle \phi_n | \left(\sum_j p_j \, |\psi_j\rangle\langle\psi_j| \right) |\phi_m\rangle \right]$$

$$= \sum_{ijmn} p_i \, p_j \, \langle \phi_m | \psi_i \rangle \langle \psi_i | \phi_n \rangle \langle \phi_n | \psi_j \rangle \langle \psi_j | \phi_m \rangle$$

$$= \sum_{ijm} p_i \, p_j \, \langle \phi_m | \psi_i \rangle \left(\sum_n \langle \psi_i | \phi_n \rangle \langle \phi_n | \psi_j \rangle \right) \langle \psi_j | \phi_m \rangle.$$

Assuming that the pure states $|\psi_i\rangle$ in (A.4) are orthonormal, one obtains

$$\mathrm{Tr}(\rho^2) = \sum_{ijm} p_i \, p_j \, \langle \phi_m | \psi_i \rangle \, \delta_{ij} \, \langle \psi_j | \phi_m \rangle$$

$$= \sum_i p_i^2 \left(\sum_m \langle \psi_i | \phi_m \rangle \langle \phi_m | \psi_i \rangle \right)$$

$$= \sum_i p_i^2 \, \langle \psi_i | \psi_i \rangle$$

$$= \sum_i p_i^2 \leq \left(\sum_i p_i \right)^2 \tag{A.11}$$

in view of the fact that $p_i \geq 0$, always. Thus, relations (A.8) and (A.11) suggest

$$\mathrm{Tr}(\rho^2) \leq [\mathrm{Tr}(\rho)]^2 \tag{A.12}$$

provided the states $|\psi_i\rangle$ representing the i-th subsystem in the density operator (A.4) of the mixed system are orthonormal.

A pure ensemble is specified by $p_i = \delta_{i\,i_0}$ for some specific $|\psi_{i_0}\rangle$. The corresponding density operator

$$\rho = |\psi_{i_0}\rangle\langle\psi_{i_0}| \tag{A.13}$$

is readily obtained from (A.4). Clearly, the density operator for a pure ensemble is idempotent, i.e.,

$$\rho^2 = \rho \tag{A.14a}$$

or, equivalently

$$\rho(\rho - 1) = 0. \tag{A.14b}$$

Hence, for a pure ensemble

$$\text{Tr}(\rho^2) = \text{Tr}(\rho) = 1 \tag{A.15}$$

in view of (A.9). Equations (A.12) and (A.15) suggest that $\text{Tr}(\rho^2)$ has its maximum value of one when the ensemble is pure and normalized; for a mixed ensemble, however, it [*i.e.*, $\text{Tr}(\rho^2)$] is a positive number whose value is less than one.

Let us assume that the complete set $\{|\chi\rangle\}$ diagonalizes the density operator (A.13) for a pure ensemble, that is,

$$\langle \chi_m | \rho | \chi_n \rangle = \rho_m \, \delta_{mn} \tag{A.16a}$$

with ρ_m being one of its eigenvalues. Then relation (A.14) gives

$$\langle \chi_m | \rho^2 | \chi_n \rangle = \langle \chi_m | \rho | \chi_n \rangle$$

$$\text{or,} \quad \sum_k \langle \chi_m | \rho | \chi_k \rangle \langle \chi_k | \rho | \chi_n \rangle = \rho_m \, \delta_{mn}$$

$$\text{or,} \quad \sum_k \rho_m \, \delta_{mk} \, \rho_k \, \delta_{kn} = \rho_m \, \delta_{mn}$$

$$\textit{i.e.,} \quad \rho_m^2 \, \delta_{mn} = \rho_m \, \delta_{mn}$$

$$\text{or,} \quad \rho_m (\rho_m - 1) \delta_{mn} = 0. \tag{A.16b}$$

This suggests that, for $m = n$ (i.e., for diagonal elements), $\rho_m = 0$ or 1. Remembering that $\text{Tr}(\rho) = 1$ for a normalized density matrix and sum of the eigenvalues of a matrix is always equal to its trace, one concludes that, when diagonalized, the normalized density matrix for a pure system has only one non-zero eigenvalue which is always equal to one.[1]

It is obvious from (A.12) and (A.15) that

$$\text{Tr}(\rho^2) = [\text{Tr}(\rho)]^2 = 1 \tag{A.17a}$$

for a pure and normalized system. But for a mixed system

$$0 < \text{Tr}(\rho^2) < [\text{Tr}(\rho)]^2, \quad \text{with} \quad \text{Tr}(\rho^2) < 1. \tag{A.17b}$$

---

[1]The converse of this statement is proved at the end of (A.29).

Let us suppose that $|\varphi\rangle$ is any arbitrary state. Then the expectation value

$$\langle\varphi|\rho|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\psi_i|\varphi\rangle$$

$$= \sum_i p_i |\langle\varphi|\psi_i\rangle|^2 \geq 0 \qquad (A.18)$$

of the density operator (A.4) in this state is a real, non-negative number. An operator whose expectation values are strictly greater than zero for all $|\varphi\rangle \neq 0$, is said to be a positive definite operator; whereas a positive operator can have zero eigenvalues as well. Hence, the density operator ρ—defined in (A.4)—is always, at least, a positive operator.

Different density operators in the form of (A.4), each describing a different mixture of subsystems, can be represented by the same density matrix. Consider, for example [123], a density matrix of the form $\rho = \frac{1}{2}\mathbb{I}_2$, where $\mathbb{I}_2$ is an unit matrix of size (2×2). Some of the possible systems in (A.4) which can be represented by this density matrix are [123]:

1. Mixture of two subsystems

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad \text{with probabilities:} \quad p_1, \; p_2 = \frac{1}{2}; \quad (A.19a)$$

2. Mixture of three subsystems

(a) $\quad |\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; |\psi_2\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \; |\psi_3\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix},$

with probabilities: $\quad p_1, \; p_2, \; p_3 = \frac{1}{3};$ $\qquad (A.19b)$

(b) $\quad |\psi_1\rangle = \frac{1}{\sqrt{281}}\begin{pmatrix} 9 \\ -i10\sqrt{2} \end{pmatrix}, \; |\psi_2\rangle = \frac{1}{\sqrt{194}}\begin{pmatrix} 12 \\ -i5\sqrt{2} \end{pmatrix},$

$|\psi_3\rangle = \frac{1}{\sqrt{17}}\begin{pmatrix} -i3 \\ 2\sqrt{2} \end{pmatrix},$

with probabilities: $\quad p_1 = \frac{281}{900}, \; p_2 = \frac{97}{450}, \; p_3 = \frac{17}{36};$ $\qquad (A.19c)$

etc. Here, each ket represents a column-matrix of size (2×1) (*i.e.*, a rectangular matrix with two rows and one column). One may construct an innumerable number of such examples. In the present example, however, all $|\psi_i\rangle$'s in (A.4), will always have only one column but as many rows as those occurring in the corresponding density matrix ρ.

A.3   Reduced Density Operator and Density Matrix

The concept of reduced density operator and of reduced density matrix is helpful in the analysis of composite quantum systems.

Let us consider two subsystems A and B described jointly by the density operator ρ^{AB}. A complete orthonormal basis set of size d_A for A is $\{|a_i\rangle, i = 1, 2, \ldots, d_A\}$ and that of size d_B for B is $\{|b_j\rangle, j = 1, 2, \ldots, d_B\}$. Then the basis set

$$|\psi_{ij}\rangle \equiv |a_i\rangle \otimes |b_j\rangle \equiv |a_i\, b_j\rangle \equiv |i\, j\rangle \tag{A.20}$$

for the composite system contains $d_A d_B$ members. A typical element of the $(d_A d_B \times d_A d_B)$ density matrix is now given by

$$\langle \psi_{ij}|\rho^{AB}|\psi_{i'j'}\rangle \equiv \langle ij|\rho^{AB}|i'j'\rangle. \tag{A.21}$$

Here, the first set of indices (i, i') refers to the state of the subsystem A and the second set (j, j') to that of the subsystem B. Suppose, an operator Ω_A acts only on the subsystem A. Then a typical matrix element of Ω_A in the basis (A.20) is given by

$$\begin{aligned}
\langle \psi_{ij}|\Omega_A|\psi_{i'j'}\rangle &\equiv \langle ij|\Omega_A|i'j'\rangle \\
&\equiv \langle i|\Omega_A|i'\rangle \langle j|j'\rangle \\
&\equiv \langle i|\Omega_A|i'\rangle \delta_{jj'}.
\end{aligned} \tag{A.22}$$

Let us calculate the trace of $\rho^{AB}\Omega_A$ in the basis set (A.20):

$$\begin{aligned}
\mathrm{Tr}\left(\rho^{AB}\Omega_A\right) &= \sum_{ij} \langle \psi_{ij}|\rho^{AB}\Omega_A|\psi_{ij}\rangle \\
&= \sum_{iji'j'} \langle \psi_{ij}|\rho^{AB}|\psi_{i'j'}\rangle \langle \psi_{i'j'}|\Omega_A|\psi_{ij}\rangle \\
&= \sum_{iji'j'} \langle ij|\rho^{AB}|i'j'\rangle \langle i'|\Omega_A|i\rangle \delta_{jj'} \\
&= \sum_{ii'j} \langle ij|\rho^{AB}|i'j\rangle \langle i'|\Omega_A|i\rangle
\end{aligned} \tag{A.23}$$

Here, we have used (A.22). Let us now define the reduced density matrix

$$\langle i|\rho^A|i'\rangle = \sum_j \langle ij|\rho^{AB}|i'j\rangle. \tag{A.24}$$

This definition facilitates rewriting of (A.23) in the following form

$$\text{Tr}\left(\rho^{AB}\Omega_A\right) = \sum_{i\,i'} \langle i|\rho^A|i'\rangle \langle i'|\Omega_A|i\rangle$$

$$= \sum_{i} \langle i|\rho^A\Omega_A|i\rangle$$

$$= \text{Tr}\left(\rho^A\Omega_A\right) = [\Omega_A] \qquad (A.25)$$

Thus, according to the last of (A.25), the average value of the one-particle operator Ω_A may be obtained with the reduced density operator ρ^A [see, (A.26)] whose $(i,\,i')$-th matrix elements (A.24) are derivable from those of the density operator ρ^{AB} defined for the composite quantum system formed from the subsystems A and B. The important distinction between ρ^{AB} and ρ^A is that while the former refers to the composite system as a whole, the latter refers to a component (namely, subsystem A) of the composite quantum system. The operator Ω_A operates only on this part of the whole system. Hence, one can write

$$\rho^A \equiv \text{Tr}_B\left(\rho^{AB}\right) \qquad (A.26)$$

with its $(i,\,i')$-th matrix element given by (A.24). Also,

$$\rho^B \equiv \text{Tr}_A\left(\rho^{AB}\right), \qquad (A.27a)$$

with

$$\langle j|\rho^B|j'\rangle = \sum_{i} \langle i\,j|\rho^{AB}|i\,j'\rangle. \qquad (A.27b)$$

Here, ρ^A in (A.26) and ρ^B in (A.27) are the reduced density operators for the respective subsystems A and B constituting the composite system $A \otimes B$ whose density operator is ρ^{AB}. The operators ρ^A and ρ^B are, of course, defined over the respective bases sets $\{|a_i\rangle\}$ and $\{|b_j\rangle\}$. Further, it is obvious from expressions [(A.24), (A.27b)] that [Tr_B, Tr_A] in [(A.26), (A.27a)] denote, respectively, the sum of the diagonal elements—associated with the respective subsystems [B, A]—of the density matrix of the composite system ρ^{AB}. This, in other words, means that if one is interested, for example, in the development of the subsystem A only, the pertinent density operator is ρ^A, which has no reference to the indices associated with its companion subsystem B. In this way, unwanted indices are eliminated. Further, dimensions of the matrices representing the reduced density operators [ρ^A, ρ^B] are [$d_A \times d_A, d_B \times d_B$].

A.4   Miscellaneous

(1) Matrix representations of the density matrix (A.4) will obviously be different in different orthonormal basis. If λ_i's are the eigenvalues of the density operator in (A.4) in the orthonormal basis $\{|i\rangle, \ i = 1, 2, \ldots\}$, then a spectral representation of ρ for the present basis is given by

$$\rho = \sum_i \lambda_i \ |i\rangle\langle i| \tag{A.28a}$$

and, hence,

$$\rho^2 = \sum_i \lambda_i^2 \ |i\rangle\langle i|. \tag{A.28b}$$

It is obvious from these relations that

$$\mathrm{Tr}\,(\rho) = \sum_i \lambda_i = 1, \tag{A.29a}$$

where the last result holds for any normalized density matrix [or, from (A.9)]; and

$$\mathrm{Tr}\,(\rho^2) = \sum_i \lambda_i^2. \tag{A.29b}$$

Equations (A.29) reinforces the statements of (A.12)–(A.15). Equation (A.29a) further shows that if only one, say m-th, of the eigenvalues is non-zero with $\lambda_m = 1$, then (A.28a) reduces to $\rho = |m\rangle\langle m|$, i.e., the system represented by the density operator ρ is in a pure state $|m\rangle$.

(2) A state of a system in quantum mechanics can be represented in more than one equivalent ways, e.g., by a state vector, wave function, density operator, or by a density matrix. For example, in view of the discussions presented in this appendix, the density operator and density matrix for first of the four Bell states (2.17) are

$$\rho_{\psi+} \equiv \begin{cases} |\psi^+\rangle\langle\psi^+| = \tfrac{1}{2}\Big(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|\Big) \quad \text{and} \\[2mm] \dfrac{1}{2}\begin{pmatrix} 0\ 0\ 0\ 0 \\ 0\ 1\ 1\ 0 \\ 0\ 1\ 1\ 0 \\ 0\ 0\ 0\ 0 \end{pmatrix}. \end{cases}$$

$$\tag{A.30a}$$

respectively. Here, while $(|0\rangle, |1\rangle)$ are the bases for each of the two qubits in the state $|\psi^+\rangle$; but, the matrix representation of $\rho_{\psi+}$ is in the basis $(|00\rangle, |01\rangle, |10\rangle, |11\rangle)$. One can, however, calculate the matrix representation of $\rho_{\psi+}$ in the bases taken in $(|11\rangle, |10\rangle, |01\rangle, |00\rangle)$, or in some other order as well. Similarly, one obtains

$$
\rho_{\psi-} \equiv
\begin{cases}
|\psi^-\rangle\langle\psi^-| = \frac{1}{2}\Big(|01\rangle\langle01| - |01\rangle\langle10| - |10\rangle\langle01| + |10\rangle\langle10|\Big) \\[6pt]
\frac{1}{2}
\begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & -1 & 0 \\
0 & -1 & 1 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
\end{cases}
$$

$$(A.30b)$$

$$
\rho_{\phi+} \equiv
\begin{cases}
|\phi^+\rangle\langle\phi^+| = \frac{1}{2}\Big(|00\rangle\langle00| + |00\rangle\langle11| + |11\rangle\langle00| + |11\rangle\langle11|\Big) \\[6pt]
\frac{1}{2}
\begin{pmatrix}
1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1
\end{pmatrix},
\end{cases}
$$

$$(A.30c)$$

and

$$
\rho_{\phi-} \equiv
\begin{cases}
|\phi^-\rangle\langle\phi^-| = \frac{1}{2}\Big(|00\rangle\langle00| - |00\rangle\langle11| - |11\rangle\langle00| + |11\rangle\langle11|,\Big) \\[6pt]
\frac{1}{2}
\begin{pmatrix}
1 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 1
\end{pmatrix}.
\end{cases}
$$

$$(A.30d)$$

for the remaining three Bell states (2.17b) and (2.17c).

(3) Suppose we have a composite system consisting of n parts such that $\Omega^{(u)}$ represents an operator for the u-th part of this system. If $\Omega^{(u)}$ is defined in the Hilbert space H_u of dimensions d_u, then operator

$$
\Omega \equiv \sum_{u=1}^{n} \Omega^{(u)} \tag{A.31a}
$$

for this composite system of n parts is given by

$$\Omega = \Omega^{(1)} \otimes I^{(2)} \otimes I^{(3)} \otimes \cdots \otimes I^{(n-1)} \otimes I^{(n)} +$$
$$I^{(1)} \otimes \Omega^{(2)} \otimes I^{(3)} \otimes \cdots \otimes I^{(n-1)} \otimes I^{(n)} +$$
$$\cdots\cdots\cdots \tag{A.31b}$$
$$I^{(1)} \otimes I^{(2)} \otimes I^{(3)} \otimes \cdots \otimes \Omega^{(n-1)} \otimes I^{(n)} +$$
$$I^{(1)} \otimes I^{(2)} \otimes I^{(3)} \otimes \cdots \otimes I^{(n-1)} \otimes \Omega^{(n)}.$$

Here, $I^{(u)}$ is a unit operator defined in the Hilbert space of the u-th part of the composite system. Operator Ω in (A.31a) is defined in the Hilbert space

$$H \equiv H_1 \otimes H_2 \otimes \cdots \otimes H_n \tag{A.32a}$$

of size

$$d \equiv d_1 d_2 d_3 \cdots d_n. \tag{A.32b}$$

Thus, the u-th term $I^{(1)} \otimes I^{(2)} \otimes I^{(3)} \otimes \cdots \otimes I^{(u-1)} \otimes \Omega^{(u)} \otimes I^{(u+1)} \otimes \cdots \otimes I^{(n)}$ in (A.31b) represents $\Omega^{(u)}$ in the $(d \times d)$-dimensional Hilbert space (A.32) of the composite system Ω defined by (A.31a).

For example, (2.6) and (2.8) contain expressions for the three Cartesian components of the Pauli spin operator [58] in the matrix and Dirac notations, respectively. After multiplying the right-hand side of each of the two equations by $\frac{1}{2}$, these can be looked upon also as representations of the three Cartesian components of an operator for angular momentum $\frac{1}{2}$ in the $(|0\rangle, |1\rangle)$ bases. According to (A.31) and (A.32), the angular momentum operator for a composite system of two spin-$\frac{1}{2}$ particles is then

$$\boldsymbol{\sigma} \equiv \frac{1}{2}\left(\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)}\right) = \frac{1}{2}\left(\boldsymbol{\sigma}^{(1)} \otimes I^{(2)} + I^{(1)} \otimes \boldsymbol{\sigma}^{(2)}\right), \tag{A.33}$$

where each of $I^{(1)}$ and $I^{(2)}$ is an unit operator defined in the (2×2)-dimensional Hilbert space of the first and the second spin-$\frac{1}{2}$ particles, respectively. Using (2.6), one now obtains

$$\sigma_x = \frac{1}{2} \begin{cases} \left(\sigma_x^{(1)} \otimes I^{(2)} + I^{(1)} \otimes \sigma_x^{(2)}\right), \\ \left(|1\rangle\langle 0| + |0\rangle\langle 1|\right)^{(1)} \otimes \left(|0\rangle\langle 0| + |1\rangle\langle 1|\right)^{(2)} + \\ \left(|0\rangle\langle 0| + |1\rangle\langle 1|\right)^{(1)} \otimes \left(|1\rangle\langle 0| + |0\rangle\langle 1|\right)^{(2)}, \\ \left(|00\rangle + |11\rangle\right)\left(\langle 01| + \langle 10|\right) + \left(|10\rangle + |01\rangle\right)\left(\langle 00| + \langle 11|\right), \\ \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \end{cases} \tag{A.34a}$$

$$\sigma_y = \frac{1}{2} \begin{cases} \left(\sigma_y^{(1)} \otimes I^{(2)} + I^{(1)} \otimes \sigma_y^{(2)}\right), \\ -i\left(|00\rangle - |11\rangle\right)\left(\langle 01| + \langle 10|\right) + i\left(|10\rangle + |01\rangle\right)\left(\langle 00| - \langle 11|\right), \\ \begin{pmatrix} 0 & -i & -i & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}, \end{cases}$$

(A.34b)

and

$$\sigma_z = \begin{cases} \frac{1}{2}\left(\sigma_z^{(1)} \otimes I^{(2)} + I^{(1)} \otimes \sigma_z^{(2)}\right), \\ |00\rangle\langle 00| - |11\rangle\langle 11|, \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \end{cases}$$

(A.34c)

for the matrix representations [in the $(|00\rangle, |01\rangle, |10\rangle, |11\rangle)$ bases] of the three Cartesian components of the angular momentum operator $\boldsymbol{\sigma}$ in (A.33) for a composite system of two spin-$\frac{1}{2}$ particles. Furthermore, two times of each of the three operators in (A.34) are applicable to any bipartite system of two qubits as well.

Appendix B
Density Matrix and State Multipoles for a Photon Beam

In the theoretical considerations developed in the Chap. 3 and thereafter, the ionizing radiation γ_r has always been assumed to be in a definite state of its polarization (i.e., LP, RCP, LCP, or UP). However, in many experiments, the incident electromagnetic wave may be either partially or arbitrarily polarized. A light beam of any kind of polarization is properly described by three Stokes' parameters [61, 76]. The present appendix contains such description of γ_r used in (1.1)–(1.8) and shows as to how it can easily be introduced in the density matrices derived in this monograph to study entanglement properties of states of qubits generated in these processes when ionizing radiation γ_r has an arbitrary polarization. This appendix also gives the description of a photon beam in terms of its state multipoles (or statistical tensors) [61,68,173,355]. The following description is applicable when the incident radiation is being treated in the $E1$ approximation.

Let us represent by $\langle 1m_r| \rho_r |1m_r' \rangle$ an element of the density operator ρ_r, introduced in (3.3) for describing the ionizing radiation γ_r in the spherical bases states $|10\rangle$, $|1, +1\rangle$, and $|1\text{-}1\rangle$ defined on page 7 in Chap. 1. In order to describe an uncorrelated system of (arbitrarily polarized photon + polarized target), before the absorption of γ_r by $\mathfrak{T}$ takes place, expression (3.4b) for the density operator everywhere in this monograph be replaced by

$$\rho_i = \sum_{m_r\, m_r'} |0;\, 1m_r\rangle\langle 1m_r|\, \rho_r\, |1m_r'\rangle\langle 0;\, 1m_r'|. \tag{B.1a}$$

If, on the other hand, the target $\mathfrak{T}$ too is unpolarized before absorbing the photon, then the density operator

$$\rho_i = \frac{1}{n_{d_0}} \sum_{d_0\, m_r\, m_r'} |0;\, 1m_r\rangle\langle 1m_r|\, \rho_r\, |1m_r'\rangle\langle 0;\, 1m_r'|, \tag{B.1b}$$

in place of (3.4c), represents the uncorrelated (arbitrarily polarized γ_r + unpolarized $\mathfrak{T}$)-system.

On using in (B.1a) and (B.1b) the density operator (3.3c) for a photon in a state $|1m_r\rangle$ of definite polarization, one reproduces the respective expressions (3.4b) and (3.4c) for the density operator ρ_i. However, for an electromagnetic wave with arbitrary polarization, the photon density matrix ρ_r is well represented in terms of the Stokes' parameters $(I_r, \eta_1, \eta_2, \eta_3)$ by [61, 173, 355]

$$\begin{array}{ccc} |+1\rangle & |0\rangle & |-1\rangle \end{array}$$

$$\rho_r = \frac{1}{2} I_r \begin{pmatrix} 1+\eta_2 & 0 & -\eta_3+i\eta_1 \\ 0 & 0 & 0 \\ -\eta_3-i\eta_1 & 0 & 1-\eta_2 \end{pmatrix} \tag{B.2}$$

In this equation, ρ_r has been calculated in the $(|1+1\rangle, |10\rangle, |1\text{-}1\rangle)$ basis. Further in (B.2), I_r is the total intensity of the arbitrarily polarized radiation incident on the target $\mathfrak{T}$ along the OZ-axis of our SF. If $I_r(\beta_r)$ is the intensity of this same beam transmitted by a Nicol prism oriented at an angle β_r with respect to the OX-axis of the SF, the remaining three Stokes' parameters are given by [61, 173, 355]

$$\eta_1 = \frac{1}{I_r}\Big[I_r(\pi/4) - I_r(3\pi/4)\Big], \tag{B.3a}$$

$$\eta_2 = \frac{1}{I_r}\Big[I_r(+) - I_r(-)\Big], \tag{B.3b}$$

$$\eta_3 = \frac{1}{I_r}\Big[I_r(0) - I_r(\pi/2)\Big]. \tag{B.3c}$$

In (B.3), $I_r(+)$ and $I_r(-)$ are the intensities of the electromagnetic wave (of total intensity I_r) transmitted along the OZ-axis by the polarization filters, which fully transmit only photons of positive and negative helicities, respectively. Hence, for an incident electromagnetic wave

$$\left.\begin{array}{ll} \text{LP along the } OX\text{-axis:} & \eta_1, \eta_2 = 0, \eta_3 = +1; \\ \text{LP along the } OY\text{-axis:} & \eta_1, \eta_2 = 0, \eta_3 = -1; \\ \text{RCP (i.e., positive helicity):} & \eta_1 = 0, \eta_2 = +1, \eta_3 = 0; \\ \text{LCP (i.e., negative helicity):} & \eta_1 = 0, \eta_2 = -1, \eta_3 = 0. \end{array}\right\} \tag{B.4}$$

The density operator for a photon beam can be expanded in terms of the tensor operators $T(1)_{KQ}$ as follows [61, 68, 173, 355]

$$\rho_r = \sum_{KQ} \left\langle T(1)_{kQ}^\dagger \right\rangle T(1)_{KQ} \tag{B.5a}$$

with state multipoles (or statistical tensors) given by

$$\left\langle T(1)^\dagger_{kQ}\right\rangle = \sqrt{2K+1}\sum_{m_r\,m'_r}(-1)^{1-m_r}$$

$$\begin{pmatrix}1 & 1 & K\\ m_r & -m'_r & -Q\end{pmatrix}\langle 1m_r|\rho_r|1m'_r\rangle. \tag{B.5b}$$

The state multipoles for a beam of electromagnetic radiation in a pure state of polarization are readily obtained [172] by substituting the corresponding density matrix (3.3c) in (B.5b). However, in order to calculate state multipoles for an UP electromagnetic wave, one needs to use [172]

$$\rho_r = \frac{1}{2}\Big(|1+1\rangle\langle 1+1| + |1-1\rangle\langle 1-1|\Big), \tag{B.6}$$

in place of (3.3c), in (B.5b). Table B.1 [172] contains state multipoles for an LP photon beam with its electric field vector, or for RCP, LCP, or UP radiation propagating, along the OZ-axis of the SF. These results are same as those given in [172, 173].

Table B.2 [172], on the other hand, contains state multipoles for an arbitrarily polarized electromagnetic wave propagating along the OZ-axis. Entries in this table are identical to those calculated by Kleinman et al. [355].

Furthermore [172], state multipoles (or statistical tensors) given in Table B.1 for RCP, LCP, or UP γ_r propagating along the OZ-axis can also be gotten by substituting the appropriate values (B.4) of the Stokes' parameters in Table B.2. This procedure, however, cannot give us state multipoles in Table B.1 for radiation LP along the OZ-axis (i.e., for $m_r = 0$). For, both Stokes' parameters in (B.4) and

Table B.1 State multipoles for an electromagnetic wave in a pure polarization state.

Polarization of the electromagnetic wave	Monopole moment $(K=0)$	Orientation vector[a] $(K=1)$	Alignment tensor[b] $(K=2)$
LP ($m_r = 0$)[c]	$\left\langle T(1)^\dagger_{00}\right\rangle = \frac{1}{\sqrt{3}}$	$\left\langle T(1)^\dagger_{10}\right\rangle = 0$	$\left\langle T(1)^\dagger_{20}\right\rangle = -\sqrt{\frac{2}{3}}$
RCP ($m_r = +1$)[c]	$\left\langle T(1)^\dagger_{00}\right\rangle = \frac{1}{\sqrt{3}}$	$\left\langle T(1)^\dagger_{10}\right\rangle = \frac{1}{\sqrt{2}}$	$\left\langle T(1)^\dagger_{20}\right\rangle = \frac{1}{\sqrt{6}}$
LCP ($m_r = -1$)[c]	$\left\langle T(1)^\dagger_{00}\right\rangle = \frac{1}{\sqrt{3}}$	$\left\langle T(1)^\dagger_{10}\right\rangle = -\frac{1}{\sqrt{2}}$	$\left\langle T(1)^\dagger_{20}\right\rangle = \frac{1}{\sqrt{6}}$
UP[d]	$\left\langle T(1)^\dagger_{00}\right\rangle = \frac{1}{\sqrt{3}}$	$\left\langle T(1)^\dagger_{10}\right\rangle = 0$	$\left\langle T(1)^\dagger_{20}\right\rangle = \frac{1}{\sqrt{6}}$

[a] Its each of the remaining two components $\left[ie,\left\langle T(1)^\dagger_{1\,\pm 1}\right\rangle\right]$, not given in this table, are zero

[b] Its each of the remaining four components $\left[ie,\left\langle T(1)^\dagger_{2\,\pm 1}\right\rangle,\left\langle T(1)^\dagger_{2\,\pm 2}\right\rangle\right]$, not given in this table, are zero

[c] The density operator is given by (3.3c)

[d] The density operator is given by (B.6)

Table B.2 State multipoles for an electromagnetic wave of arbitrary polarization.

Monopole moment ($K = 0$)	Orientation vector ($K = 1$)	Alignment tensor ($K = 2$)
$\left\langle T(1)^{\dagger}_{00} \right\rangle = \frac{1}{\sqrt{3}} I_r$	$\left\langle T(1)^{\dagger}_{10} \right\rangle = \frac{1}{\sqrt{2}} I_r \eta_2$	$\left\langle T(1)^{\dagger}_{20} \right\rangle = \frac{1}{\sqrt{6}} I_r$
	$\left\langle T(1)^{\dagger}_{1\pm1} \right\rangle = 0$	$\left\langle T(1)^{\dagger}_{2\pm1} \right\rangle = 0$
		$\left\langle T(1)^{\dagger}_{2\pm2} \right\rangle = \frac{1}{2}\left(-\eta_3 \pm i \eta_1 \right) I_r$

state multipoles in the Table B.2 are for electromagnetic wave LP along the OX- or OY-axis.

The inverse of (B.5b) is

$$\langle 1m_r | \rho_r | 1m_r' \rangle = (-1)^{1-m_r} \sum_{KQ} \sqrt{2K+1}$$

$$\times \begin{pmatrix} 1 & 1 & K \\ m_r & -m_r' & -Q \end{pmatrix} \left\langle T(1)^{\dagger}_{kQ} \right\rangle. \tag{B.7}$$

On substituting (B.7) for the matrix elements of the photon density operator ρ_r, one readily expresses the density operator ρ_i in (B.1) in terms of the state multipoles of the arbitrarily polarized ionizing photon γ_r. If one is interested in studying entanglement between the particles produced in any of the processes (1.1)–(1.8), wherein an inner-shell vacancy is created due to the absorption of an arbitrarily polarized γ_r, the consequent expression for ρ_i should be used in deriving the corresponding density matrix. However, this change will not at all affect the Coulombic entanglement discussed in this monograph, The entanglement generated in the absence of SDIs is always independent of the polarization of the ionizing radiation. Use of [(B.1), (B.7)] should, on the other hand, certainly have an effect on the fine-structure entanglement because it very much involves polarization of the γ_r used in (1.1)–(1.8) on account of the fact that the presence of the SDIs couples the non-local correlation with both the kinematics and dynamics of these processes.

Appendix C
Decoherence and Dissipation of Quantum Entanglement

This appendix contains a very brief, elementary and qualitative description of decoherence and dissipation of entanglement in a state of a system due to its interaction with ambient external environment.

The first time a student comes across the word coherence in physics is, probably, in the context of electromagnetic waves when phenomena like interference (in, e.g., young's double slit experiment, etc.) and/or Fraunhofer and Fresnel diffractions are introduced to him/her in optics [356]. Two electromagnetic waves are said to be coherent if the phase difference between them does not change with time; otherwise, they are considered to be incoherent waves. Electromagnetic radiations produced in the spontaneous decay of excited states of atoms or molecules in the solid, liquid, or gas phase of matter are known to be incoherent; whereas, laser or maser generated in induced (i.e., stimulated) decay of an excited state are the well known examples of coherent electromagnetic waves. Another popular example is a coherent state in quantum optics [25, 27].

Superpositions of two or more electromagnetic waves, or of states in quantum mechanics, can also be of two kinds: Namely (see, for example, [76, 356]), coherent or incoherent superpositions. A coherent superposition consists of addition of complex amplitudes with appropriate multiplying constants which may even be complex. In an incoherent superposition, on the other hand, intensities (i.e., square of the modulus of amplitudes) are added with appropriate weights. Coherent superposition generates interference of amplitudes which gives rise, for example, to a stable pattern of maxima and minima in the above-mentioned phenomena of interference and diffraction in optics, provided [76, 356] superposed waves are also coherent. Such interference terms can, of course, never be present in an incoherent superposition.

Both, time-dependent and time-independent Schrödinger equations in quantum mechanics are linear as well as homogeneous (see, for example, [58, 59]). These two properties mean that a linear combination (i.e., a superposition) of their solutions

is also a solution of the respective Schrödinger equation. Of the two kinds of superpositions mentioned in the preceding paragraph, separable states like (2.27), (2.39a), etc. represent an incoherent superposition of the product states. Similarly, (A.4) too is an example of an incoherent superposition. On the other hand, the simplest possible coherent superposition in quantum mechanics is, probably, the one-particle state (2.1). This state gives rise to terms whose coefficients are $C_0C_1^*$ and $C_0^*C_1$, in addition to those multiplied by $|C_0|^2$ and $|C_1|^2$, when probability for finding a result on measuring an observable of the system represented by the state (2.1) is to be calculated. The former two (i.e., $C_0C_1^*$ and $C_0^*C_1$) are known as interference terms representing local coherence inherently present in any linear superposition [e.g., like (2.1)] of one (or more)-particle states. The incoherent state (2.27), on the other hand, is a statistical mixture, which can never give rise to any interference terms similar to those which may be generated by a coherent superposition.

An entangled state is also a coherent superposition of the product states of more than one particle. For example, Bell states (2.17) are four different coherent superpositions of the products ($|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$) of the states of two qubits (e.g., photons, two-level atoms, spin-$\frac{1}{2}$ particles). Similar is the case with the bipartite states [e.g., (4.13), (5.14), (6.10b), etc.] discussed in various chapters of this monograph. In an entangled state, correlation is present among its constituent particles [i.e., between two qubits in (2.17)] as well. These particles may or may not be interacting among themselves and may be located at places far away from each other. Such a non-local correlation is also called distributed coherence. Thus, both local and non-local coherences are present in an entangled state. The former exists for each particle constituting the system; while, the non-separability of the state of this system is due to the non-local correlation/distributed coherence. It has already been mentioned at several places in this monograph that non-diagonal elements of a density matrix represents coherence effects. Thus, the non-diagonal elements in the matrix representation of an entangled state contain both local and non-local coherence. It is, nevertheless, possible that local coherence may be present also in a separable state. (For a more detailed discussion of local and non-local coherence in a bipartite entangled state of two qubits, see, for example, [53].)

Hence, in a density matrix form [e.g., (A.30), *etc*] of a linear superposition [e.g., (2.17), *etc*], the non-diagonal terms arise due to coherence (or, interference); whereas diagonal terms represent probabilities for the outcome of a measurement of an observable performed on a coherent superposition of states. Sometimes, depending upon the observable being measured, the diagonal elements are called populations as well. It is obvious from the discussion given herein that coherence in states like (2.1), (2.17), *etc*, is a consequence of the phases of various terms present in a superposition; whereas these phases play no role whatsoever in determining the populations represented by these states.

Coherence is considered to be a major resource in quantum mechanics. Chapter 2 explains, in brief, the importance of entangled state, i.e., the availability of non-local coherence, in quantum information. However, due to the presence of noisy backgrounds and interaction with the ambient external environment, an entangled

state always tends to lose its both local and non-local coherences. Such loss of coherence for reasons external to a system is known as decoherence (see, for example, [357–361]). Thus, decoherence affects the phase relationship among the terms present in a coherent superposition of states. This, in other words, means that value of the exponent ϕ may be affected by decoherence of a single qubit state (2.2b) if it is subjected to a noisy environment. Hence, decoherence is the decay of the off-diagonal matrix elements of the density matrix of a system due to its coupling to an ambient external environment. There have recently been several studies of decoherence, including dynamics of dis-entanglement (see, for examples, reviews [160, 348, 351]).

On the other hand, changes in the diagonal elements (i.e., populations) in a density matrix representation of a coherent superposition of a state of a system due to its interaction with the external ambient environment is known as dissipation. Thus, in dissipation, magnitudes—rather than phases—of the various terms present in a coherent superposition change if a system represented by this state is experiencing a noisy external background. References [180–182], *etc*, are some of the studies of both decoherence and dissipation in quantum information.

Appendix D
A Computer Programme for Calculating 3-j, 6-j, and 9-j Symbols in Powers of Prime Numbers

It is obvious from discussions given in Chaps. 3–10 of this monograph that calculations of the density matrices needed for studying entanglement properties of various bipartite states of flying particles generated in the processes (1.1)–(1.8) capable of taking place in an atom or a linear molecule require a large number of 3-j, 6-j, and/or 9-j symbols [65]. Most of the books on quantum mechanics (e.g., [58, 59]), angular momentum (e.g., [65–68, 187]), atomic physics (e.g., [10, 60, 184]), nuclear physics (e.g., [64]), for example, contain tables of 3-j, 6-j, and/or 9-j symbols in one form or the other—specifically, for smaller values of the angular momentum quantum numbers. Among these, and several others, the excellent book by Rotenberg et al. [187] is exclusively dedicated to the tables of 3-j and 6-j symbols. In addition, a number of different computer programmes for calculating all or some of these n-j (i.e., 3-j, 6-j, and/or 9-j) symbols are also readily available in the literature (see, for example, [68]). One may, then, wonder as to what is the need for writing a new computer code for calculating these n-j symbols and then including it in the present monograph?

First, the book cited in [187] was published more than fifty years ago. It has been out of print since long and, consequently, it is presently available only at few places (e.g., libraries, universities, etc.) in the world. Moreover, Rotenberg et al. [187] have given tables only for 3-j and 6-j symbols, but none for 9-j symbols. The expressions for the density matrices derived herein and elsewhere (e.g., [56, 57]) contain, on the other hand, also the 9-j symbols, in addition to the 3-j and 6-j symbols. To the best of our knowledge, there are no computer codes for calculating an n-j symbol (or, square of it, for that matter) in powers of prime numbers. Almost all of the available programmes compute values of these symbols in decimal forms which results in the considerable loss of accuracy. Moreover, in an analytical calculation, it is far more convenient to use a value of an n-j symbol in terms of prime numbers than in a decimal form. It is for these and other such

reasons that computer programmes which calculate square of a n-j symbol in terms of powers of prime numbers have been written in Chandra's [362] group.

Although this [362] computer programme can not be claimed to be either elegant or optimum, its accuracy has, however, been checked by various methods. For example, results obtained from this programme for a 3-j symbol and a 6-j symbol agree with those given in [67,187].[1] A 9-j symbol, on the other hand was calculated using two independent expressions (D.4) and (D.5) given on pages 275 and 276 herein. These two methods gave identical results which, in addition, agreed also with their values in [67]. This programme for n-j symbols was subsequently used for calculating density matrices needed for studying both Coulombic entanglement and fine-structure entanglement.

D.1   Methods of Calculation

A 3-j symbol has been computed after suitably modifying the expression originally derived by Racah [363] for Clebsch–Gordon coefficients and written in a symmetrical form by Edmonds $\big($see (3.6.11) and (3.7.3) in [65]$\big)$. Accordingly, one can write [65, 187]

$$\begin{pmatrix} A & B & C \\ a & b & c \end{pmatrix} = (-1)^{A-B-c} \, (2C+1)^{-\frac{1}{2}} \Big(Aa \, Bb | AB \, C-c \Big) \qquad \text{(D.1a)}$$

$$= (-1)^{A-B-c} \, \Delta\big(A, B, C\big) \, \delta_{0, a+b+c}$$

$$\times \sqrt{(A+a)!(A-a)!(B+b)!(B-b)!(C+c)!(C-c)!}$$

$$\times \Sigma_{k \geq 0} \, (-1)^k \Big[k!(A+B-C-k)!(A-a-k)!(B+b-k)!$$

$$\times (C-B+a+k)!(C-A-b+k)! \Big]^{-1}. \qquad \text{(D.1b)}$$

Here,

$$\Delta\big(A, B, C\big) = \left[\frac{(A+B-C)!(A-B+C)!(-A+B+C)!}{(A+B+C+1)!} \right]^{\frac{1}{2}}. \qquad \text{(D.2)}$$

In (D.1b), one needs to sum over all those positive integral values of k for which arguments of none of the factorials functions present in the denominator of this

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[1] All the tables given by Rotenberg et al. [187] contain values of the squares of 3-j and of 6-j symbols in prime numbers; whereas, those given in [67] have n-j symbols in both prime numbers and in decimals forms.

expression becomes negative [see, for example, footnote (3) on page 277 in the present Appendix D].

A 6-j symbol, used in this monograph, is related to Racah's W-coefficient [363] by [67, 187]

$$\left\{ \begin{array}{ccc} A & B & C \\ D & E & F \end{array} \right\} = (-1)^{A+B+D+E} W(ABED; CF). \tag{D.3a}$$

This can finally be written as [65, 67, 68]

$$\left\{ \begin{array}{ccc} A & B & C \\ D & E & F \end{array} \right\} = \Delta(ABC)\, \Delta(AEF)\, \Delta(DBF)\, \Delta(DEC)$$

$$\times \Sigma_{k \geq 0} (-1)^k \, (k+1)! \Big[(k-A-B-C)!(k-A-E-F)!(k-D-B-F)!$$

$$\times (k-D-E-C)!(A+B+D+E-k)!(B+C+E+F-k)!$$

$$\times (C+A+F+D-k)! \Big]^{-1}. \tag{D.3b}$$

Similar to (D.1b), the upper limit for the positive integer k in the sum (D.3b) is determined so that none of the factorials in this expression is negative.

There are various equivalent expressions (see, for example, [64, 65, 67, 68, 364]) available in the literature for computing a 9-j symbol. It can be written as a sum of the product of six 3-j symbols, sum of a triple product of 6-j symbols, or in the form of an algebraic expression. The two expressions used herein are

$$\left\{ \begin{array}{ccc} A & B & C \\ D & E & F \\ G & H & J \end{array} \right\} = \Sigma_{k \geq 0} (-1)^{2k} \, (2k+1) \left\{ \begin{array}{ccc} A & D & G \\ H & J & k \end{array} \right\}$$

$$\left\{ \begin{array}{ccc} B & E & H \\ D & k & F \end{array} \right\} \left\{ \begin{array}{ccc} C & F & J \\ k & A & B \end{array} \right\} \tag{D.4}$$

in terms of 6-j symbols {e.g., (6.4.3) in [65]} and the following algebraic relation

$$\left\{ \begin{array}{ccc} A & B & C \\ D & E & F \\ G & H & J \end{array} \right\} = (-1)^{C+F-J} \frac{\Delta'(DAG)\, \Delta'(BEH)\, \Delta'(JGH)}{\Delta'(DEF)\, \Delta'(BAC)\, \Delta'(JCF)}$$

$$\times \Sigma_{p \geq 0} \, \Sigma_{q \geq 0} \, \Sigma_{r \geq 0} \frac{(-1)^{p+q+r}}{p!\,q!\,r!} \frac{(2F-p)!\,(2A-r)!}{(2H+1+q)!\,(A+D+G+1-r)!}$$

$$\times \frac{(D+E-F+p)!\,(C+J-F+p)!}{(E+F-D-p)!\,(C+F-J-p)!}$$

$$\times \frac{(E + H - B + q)!\,(G + H - J + q)!}{(B + E - H - q)!\,(G + J - H - q)!}$$

$$\times \frac{(B + C - A + r)!}{(A + D - G - r)!\,(A + C - B - r)!}$$

$$\times \frac{(A + D + J - H - q - r)!}{(D + H - B - F + p + q)!\,(B - F - A + J + p + r)!} \quad \text{(D.5a)}$$

with

$$\Delta'(A, B, C) = \left[\frac{(A + B - C)!(A - B + C)!(A + B + C + 1)!}{(-A + B + C)!} \right]^{\frac{1}{2}}. \quad \text{(D.5b)}$$

originally obtained by Jucys and Bandzaitis [364] and reproduced in [(A-6)–(A-8)] in [68]. In the three sums present in (D.5a), only those positive integral values of each of p, q, and r are to be considered for which argument of none of the factorials present therein is negative.

D.2   A Short Description of the Programme

The programme `threenj` consists of a master driver which reads the input data and directs the flow of the whole programme through its eight subroutines.[2] This driver programme also writes the results calculated. Details of the working of the programme are described in its comment cards. In the following, we give, in alphabetical order, a brief description of each of the 10 parts of the present programme `threenj`. A complete listing of this programme is available from the Springer's website <http://extra.springer.com>.

D.2.1   Subroutine `delta`

This subroutine is called in each of the three subroutines `ninej_JB` (Sect. D.2.5), `sixj` (Sect. D.2.9), and `threej` (Sect. D.2.10). It is needed for calculating

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[2]The driver of `threenj` calls the subroutines of this programme in the following sequence:
(*i*) `primnum`, (*ii*) `gamafun`, (*iii*) `threej`, (*iv*) `printr`, (*v*) `sixj`, (*vi*) `printr`, (*vii*) `nine_JB`, (*viii*) `printr`, (*ix*) `nine_6j`, (*x*) `printr`.
The `logical function`, in addition to the subroutine `printr`, is used by each of `threej`, `sixj`, `nine_JB`, and `nine_6j`.

$\Delta(A\ B\ C)$ [in `threej` and `sixj`] or $\Delta'(A\ B\ C)$ [in `ninej_JB`], defined in (D.2) or (D.5b), respectively. The value of the input integer "iselect" decides as to which of the two deltas is to be calculated:

If "iselect" $= 1$, $\Delta(A\ B\ C)$ of (D.2) is computed;

if "iselect" $= 2$, $\Delta'(A\ B\ C)$ of (D.5b) will be calculated.

Delta, calculated in the subroutine `delta`, is printed if "iprint(4)" is a non-zero integer.

D.2.2   The Driver

It reads the input data, controls the flow of the programme, and prints results. The input data is described in the Sect. D.3 (page 280). On the other hand, the output of a test run is available from the web page <http://extra.springer.com> which contains also a complete listing of the present programme `threenj`.

D.2.3   Subroutine `gamafun`

This is a subroutine for calculating Gamma functions in terms of prime numbers and their powers.[3] Gamma functions are calculated for all the integers in the range from n $=$ 1 to prime(nprim). The calculated Gamma functions are stored in the 2-dimensional integer matrix "gamma.[4]" This matrix is passed to other parts of the programme `threenj` through a common block.

Matrix "gamma" is printed if "iprint(2)" is a non-zero integer.

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[3]Note [259] that $\Gamma(n) = (n-1)!$; $0! = 1$; n! $= \pm\infty$ when n is a *negative* integer.

[4]For example, for "nprim" $= 10$, this subroutine will calculate first ten prime numbers (excluding 1), namely: 2, 3, 5, 7, 11, 13, 17, 19, 23, 29. Then, the Γ functions are calculated for the first thirty integers, *ie*, 1, 2, 3, 4, . . ., 29, 30. Thus, elements gama(1, i) $= 0$ (with i $= 1$–10) contain the value of $\Gamma(1)(= 0! = 1 = 2^0 \times 3^0 \times 5^0 \times \ldots 29^0)$. Similarly, gama (2, i) $= 0$ (with i $= 1$–10) give the value of $\Gamma(2)(= 1! = 1 = 2^0 \times 3^0 \times 5^0 \times \ldots 29^0)$; gama (3, 1) $= 1$, gama (3, i) $= 0$ (with i $= 2$–10) give the value of $\Gamma(3)$ ($= 2! = 2 = 2^1 \times 3^0 \times 5^0 \times \ldots 29^0$); gama(4, 1) $= 1$, gama(4, 2) $= 1$, gama (4, i) $= 0$ (with i $= 3$–10) give the value of $\Gamma(4)$ ($= 3! = 6 = 2^1 \times 3^1 \times 5^0 \times \ldots 29^0$). Further, gama(29, 1) $= 25$, gama(29, 2) $= 13$, gama(29, 3) $= 6$, gama(29, 4) $= 4$, gama(29, 5) $= 2$, gama(29, 6) $= 2$, gama(29, 7) $= 1$, gama(29, 8) $= 1$, gama(29, 9) $= 1$, gama(29, 10) $= 0$, give the value of $\Gamma(29)$ ($= 28! = 2^{25} \times 3^{13} \times 5^6 \times 7^4 \times 11^2 \times 13^2 \times 17^1 \times 19^1 \times 23^1 \times 29^0$). Lastly, gama(30, 1) $= 25$, gama(30, 2) $= 13$, gama(30, 3) $= 6$, gama(29, 4) $= 4$, gama(30, 5) $= 2$, gama(30, 6) $= 2$, gama(30, 7) $= 1$, gama(30, 8) $= 1$, gama(30, 9) $= 1$, gama(30, 10) $= 1$, is the value of $\Gamma(30)$ ($= 29! = 2^{25} \times 3^{13} \times 5^6 \times 7^4 \times 11^2 \times 13^2 \times 17^1 \times 19^1 \times 23^1 \times 29^1$). Thus, gama($j, i$) is the power of the i-th prime number present in $\Gamma(j)$.

D.2.4   Function `logical function`

This function tests whether the three angular momenta (say, j1, j2, j3) of a 3n-j symbol satisfy the well-known triangular condition (i.e., |j1 - j2| $\leq$ j3 $\leq$ j1 + j2) applicable [63–68] to their vector addition in quantum mechanics. It is called at various places in the subroutine `threenj` in order to avoid those calls of the subroutines `ninej_JB`, `ninej_6j`, `sixj`, and `threej` wherein any of the 3-j, 6-j, or 9-j symbols identically vanishes.

Value of the logical variable "ltc," calculated in this function, is printed if iprint(7) is a non-zero integer.

D.2.5   Subroutine `ninej_JB`

This is a subroutine for calculating square of a 9-j symbol using the algebraic expression (D.5). Its output is in powers of prime numbers. The input arguments are: "j1" = 2*A, "j2" = 2*B, "j12" = 2*C, "j3" = 2*D, "j4" = 2*E, "j34" = 2*F, "j13" = 2*G, "j24" = 2*H, and "jj" = 2*J, i.e., TWICE of the actual values of angular momenta. Hence, each of the nine input arguments is always a positive and real integer. The respective triads (j1, j2 j12), (j3, j4, j34), and (j13, j24, jj) of the angular momenta form the first, second, and third rows of a 9-j symbol [see, for example, left-hand sides of (D.4) and of (D.5a)]. The integer variables "sign9j," "n9j," "sum9j," and the integer array "v9j" contain this subroutine's output.

The driver, discussed in the Sect. D.2.2, will call the subroutine `ninej_JB` if input integer "i9" = 1, or $\geq$ 3.

A 9-j symbol, calculated in this subroutine is printed if "iprint(9)" is a non-zero integer.

A "*" symbol in front of a printed value of a 9-j symbol means that its negative square root is to be used.

D.2.6   Subroutine `ninej_6j`

This subroutine uses the relation (D.4) for computing square of a 9-j symbol in terms of the prime numbers. Its input arguments are exactly the same as in the case of the subroutine `ninej_JB`, discussed in the immediately preceding Sect. D.2.5.

The subroutine `ninej_6j` is called by the driver (see the Sect. D.2.2) of the present programme `threenj` if the input integer "i9" $\geq$ 2.

A 9-j symbol, calculated in the subroutine `ninej_6j`, is printed if "iprint(10)" is a non-zero integer.

A "*" symbol in front of a printed value of a 9-j symbol means that its negative square root is to be used.

Thus, if "i9" > 2, a required 9-j symbol will be calculated by using the relation (D.4) as well as the algebraic expression (D.5). This provides a very good check for each of the three subroutines sixj (Sect. D.2.9), ninej_JB (Sect. D.2.5), and ninej_6j (Sect. D.2.6), provided the last two subroutines compute identical values for a given 9-j symbol.

D.2.7 Subroutine `primnum`

This subroutine calculates first "nprim" prime numbers. These prime numbers are stored in the 1-dimensional, integer array called "prim." [See footnotes (2) and (4).] Both "nprim" and the array "prim" are passed to other parts of the programme through a common block.

Array "prim" is printed if "iprint(1)" is a non-zero integer.

D.2.8 Subroutine `printr`

The driver (Sect. D.2.2) as well as each of the four subroutines ninej_JB (Sect. D.2.5), nine_6j (Sect. D.2.6), sixj (Sect. D.2.9), and threej (Sect. D.2.10) calls the subroutine printr for printing a 3-j, 6-j, and/or 9-j symbol calculated in the present programme threenj.

D.2.9 Subroutine `sixj`

This subroutine computes the square of a 6-j symbol in terms of the powers of prime numbers. The definition used is that given in (D.3). Its input arguments ("j1" = 2*A, "j2" = 2*B, "j3" = 2*C, "l1" = 2*D, "l2" = 2*E, and "l3" = 2*F) are TWICE of the actual values of angular momenta for which a 6-j symbol is required. Hence, each of these six input arguments is always a positive and real integer. The output of sixj is given by the integers "sign6j," "n6j," "sum6j," and the integer array "v6j." A "*" sign means that a negative square root of a computed value is to be used.

A 6-j symbol, calculated in the subroutine sixj, is printed if "iprint(6)" is a non-zero integer.

D.2.10 Subroutine `threej`

The square of a 3-j symbol is computed in this subroutine in terms of prime numbers and their powers. It is defined in (D.1) and (D.2). The input arguments of the present subroutine are: "j1" = 2*A, "j2" = 2*B, "j3" = 2*C, "m1" = 2*a, "m2" = 2*b, and "m3" = 2*c, i.e., TWICE of the actual angular momenta and of their projections. Hence, arguments ("j1, j2, j3, m1, m2, m3") of threej are always

real integers. Here, "j1, j2, j3" are necessarily non-negative; whereas -j1 $\leq$ m1 $\leq$ j1, -j2 $\leq$ m2 $\leq$ j2, -j3 $\leq$ m3 $\leq$ j3 such that (m1 + m2 + m3) = 0. The output of this subroutine is contained in the integer variables "sign3j, n3j, sum3j," and in the integer array "v3j." Results preceded by a '*' (for "sign3j" < 0) means that one should use negative of the square root of the computed value.

A 3-j symbol, calculated in the subroutine `threej`, is printed if "iprint(3)" is a non-zero integer.

D.3   Input

The whole of the input information needed for a successful run of `threenj` is read in the `driver` segment of this programme. Some of it (i.e., integer variable "nprim," and integer array "iprint") is passed to the other parts of the programme `threenj` through a common block; whereas the remaining in the form of the arguments of the various subroutines already described herein.

1. nprim (1 $\leq$ nprim $\leq$ 100)   Described in the Sects. D.2.3 and D.2.7.
2. irpt (1 $\leq$ irpt $\leq$ 11)   Controls the re-looping of the
                                        programme `threenj`:
irpt = 1, input for the statement number 10 is read;
irpt = 2-4, input for the statement number 30 (for a 3-j symbol) is read;
irpt = 5-7, input for the statement number 60 (for a 6-j symbol)is read;
irpt = 8-10, input for the statement number 90 (for a 9-j symbol)is read;
irpt = 11, programme `threenj` ends.
3. iprint(i)   Controls the printing in various
                                        subroutines.
4. (j1, j2, j3, m1, m2, m3)   Described in the Sect. D.2.10.
5. (j1, j2, j3, l1, l2, l3)   Described in the Sect. D.2.9.
6. (j1, j2, j12, j3, j4, j34, j13, j24, jj)   Described in the Sects. D.2.5
                                        and D.2.6.
7. i9   Described in the Sects. D.2.5 and D.2.6.

D.4   Programme Listing

It is available from Springer's web page <http://extra.springer.com>.

D.5   Test Run Output

It too is available from Springer's web page <http://extra.springer.com>.

Appendix E
A Generic Computer Programme
for the Coefficient A's Needed in the Calculation
of the Density Matrix for Fine-Structure
Entanglement in 2-DPI

This appendix is a brief write-up of the computer code `coefficient_A` used [188] for calculating the coefficient A's present in the density matrix (7.19) needed for studying fine-structure entanglement between the spins of a photoelectron e_p and Auger electron e_a generated in the 2-DPI process (1.3). This is a generic programme as it can readily be adapted for calculating density matrices needed for similar studies of entanglement between two electronic qubits, which may be generated in the 2-DPI process taking place in a linear molecular target or in 1-DPI (1.2) in an atom or a molecule. Furthermore, the following programme `coefficient_A` can readily be generalized also to the two-step process (1.4) for studying the hybrid, fine-structure entanglement between the spin of photoelectron e_p and polarization of the emitted fluorescence γ_d.

E.1   Method of Calculation

For a given set of values of the integer variables $(S_p, S_a, N_{S_p}, N_{S_a}, m_r)$ [(7.19b)], programme `coefficient_A` calculates A's in terms of the products of spherical harmonics $\left[Y_{L_p}^{M_{L_p}}(\hat{\boldsymbol{k}}_p)\right]^* \left[Y_{L_a}^{M_{L_a}}(\hat{\boldsymbol{k}}_a)\right]^*$ as well as of the photoionization and Auger decay amplitudes $P_e(J_{1+}{}^* j_p;\ J_0\ 1;\ j_t;\ \ell_p)\ \left[P_e(J_{1+}{}^* j_p';\ J_0\ 1; j_t';\ \ell_p')\right]^*$ and $A_e(J_{2+}\ j_a;\ J_{1+}{}^*;\ \ell_a)\ \left[A_e(J_{2+}\ j_a';\ J_{1+}{}^*;\ \ell_a')\right]^*$, respectively. For the spherical harmonics, the phase convention used is the one given in (2.5.29) in Edmond's book [65] or, for examples, (1)–(5) on page 59 in [365]; whereas the latter two amplitudes are defined by the respective (7.20). This programme substitutes neither the trigonometric [i.e., in terms of the spherical angles (θ_p, ϕ_p) of $\hat{\boldsymbol{k}}_p$, or (θ_a, ϕ_a) of $\hat{\boldsymbol{k}}_a$] nor numerical values of a spherical harmonics $\left[Y_{L_p}^{M_{L_p}}(\hat{\boldsymbol{k}}_p)\right]^*$ or of $\left[Y_{L_a}^{M_{L_a}}(\hat{\boldsymbol{k}}_a)\right]^*$. It, on the other hand, determines values of (L_p, M_{L_p}) and (L_a, M_{L_a}) for which the two required spherical harmonics are to be used. The advantage of doing this is

that on substituting these A's in the expression (7.19a), one is free to compute the density matrix $\langle J_{2+}; \mu_p\,\hat{\boldsymbol{u}}_p\,\boldsymbol{k}_p; \mu_a\,\hat{\boldsymbol{u}}_a\,\boldsymbol{k}_a|\,\rho^{(2\text{-DPI})}\,|J_{2+}; \mu'_p\,\hat{\boldsymbol{u}}_p\,\boldsymbol{k}_p; \mu'_a\,\hat{\boldsymbol{u}}_a\,\boldsymbol{k}_a\rangle$ for any experimental geometry (i.e., directions $\hat{\boldsymbol{k}}_p$ and $\hat{\boldsymbol{k}}_a$) one desires without having to recalculate the A's for that specific 2-DPI process (1.3). Thus, need for calculating A's for each new $\hat{\boldsymbol{k}}_p$ and/or $\hat{\boldsymbol{k}}_a$ is completely the eliminated.

Similarly, it is more likely than not that more than one amplitudes $P_e(J_{1+^*}\,j_p; J_0\,1; j_t; \ell_p)$ [each with a different set of values of the quantum numbers (ℓ_p, j_p, j_t)] and $A_e(J_{2+}\,j_a; J_{1+^*}; \ell_a)$ [differing in ℓ_a, j_a] contribute to the photoionization (1.3a)] and Auger decay (1.3b), respectively. In view of these possibilities, although the programme coefficient_A does inform its user as to which of the $P_e(J_{1+^*}\,j_p; J_0\,1; j_t; \ell_p)$ and $A_e(J_{2+}\,j_a; J_{1+^*}; \ell_a)$ is to be used where; it, however, does not require numerical/algebraic values of either amplitudes. These values are used when A's are substituted in (7.19a) for the final calculation of the density matrix. This feature of coefficient_A makes it possible to compute the density matrix (7.19a) for the same participating transitions but in different atoms without requiring recalculation of A's. In other words, the A's obtained from the programme coefficient_A are only transition, but neither atom nor geometry, specific.

However, in spite of the above-discussed two features of the programme coefficient_A, one still requires to compute A's for each different polarization (specified by $m_r = -1, 0, +1$) of the incident photon γ_r used for ionization of the atomic target $\mathfrak{T}$ in the 2-DPI process (1.3).

For the calculation of the various n-j (i.e., 3-j, 6-j, and/or 9-j) symbols, present in the expression (7.19b), coefficient_A uses the subroutines given in the programme threenj (but without its driver part) described in the Appendix D on pages 273–280.

E.2 A Short Description of the Programme

The programme coefficient_A contains twelve subroutines, including a block_data and a driver. Out of these, nine (namely: delta, gamafun, logical_function, ninej_JB, ninej_6j, primnum, printr, sixj, threej) are those needed to calculate a 3n-j symbol and have already been explained in the Appendix D. In the following, therefore, the remaining three parts of the present programme are explained.

E.2.1 The Driver

It reads the input data, i.e., "nprim," "iprint," and "irpt" (each explained in the Sect. D.3 on page 280); all the ten elements of the array "iwrite" (explained in the source code of the subroutine main of the present programme). In addition, the values of the

parameters $(S_p, S_a, N_{S_p}, N_{S_a}, m_r)$,[1] needed to specify an $A^{S_p \, S_a}_{N_{S_p} \, N_{S_a}} (m_r; \hat{\boldsymbol{k}}_p \, \hat{\boldsymbol{k}}_a)$ in (7.19), are also read in this driver part of the programme `coefficient_A`. It then calls the subroutine `main`.

E.2.2 `block data`

This part of the present programme stores the variables corresponding to the total angular momenta (J_0, J_{1+*}, J_{2+}) of $(\mathfrak{T}, \mathfrak{T}^{1+*}, \mathfrak{T}^{2+})$ as well as values (ℓ_p, ℓ_a) of the orbital angular momenta of the partial waves of (photoelectron e_p, Auger electron e_a) participating in the 2-DPI process (1.3).

In this `block_data`, (nl1v, nl2v) are the number of the values of (ℓ_p, ℓ_a), which need to be taken in to account for a given 2-DPI process (1.3). These values of (ℓ_p, ℓ_a) are stored in the integer arrays (l1v, l2v).

In the given version of the programme `coefficient_A`, each of the arrays (l1v, l2v) has been declared to have dimension 05. This can, however, readily be changed according to one's requirements. If either or both of (nl1v, nl2v) have values less than the declared dimensions of (l1v, l2v), then the remaining elements of these two arrays are filled with some un-physical value (e.g., say, -1), which neither of the partial waves (ℓ_p, ℓ_a) can ever have.

E.2.3 Subroutine `main`

This subroutine is the main part of the present programme `coefficient_A`. It performs the following tasks:

1. Determines the possible values of all the variables [other than those (i.e., S_p, S_a, N_{S_p}, N_{S_a}, m_r) read in the driver (Sect. E.2.1) or stored (i.e., $J_0, J_{1+*}, J_{2+}, \ell_p, \ell_a$ in the `block data` (Sect. E.2.2)).
2. Calculates all the 3n-j symbols contributing to (7.19b).
3. Multiplies the product of these 3n-j symbols with appropriate spherical harmonics $\left[Y^{M_{L_p}}_{L_p} (\hat{\boldsymbol{k}}_p) \right]^*$, $\left[Y^{M_{L_a}}_{L_a} (\hat{\boldsymbol{k}}_a) \right]^*$ [after determining the proper values of (L_p, M_{L_p}) and of (L_a, M_{L_a})] and by the photoionization amplitudes

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[1]Recall that each of S_p, S_a, N_{S_p}, N_{S_a}, and m_r is always an integer. Their values are: $m_r = 0$ [for LP ionizing radiation γ_r], or $+1$ (-1) [for CP ionizing radiation γ_r with negative (positive) helicity] in (7.19). $N_{S_p} = 0$ (for $S_p = 0$); $-1, 0, +1$ (for $S_p = +1$). $N_{S_a} = 0$ (for $S_a = 0$); -1, $0, +1$ (for $S_a = +1$). Programme `coefficient_A` does not need any information about either the unit vectors $(\hat{\boldsymbol{k}}_p, \hat{\boldsymbol{k}}_a)$, or amplitudes (P_e, A_e).

$$\left[P_e(J_{1+*} \; j_p; \; J_0 \; 1; \; j_t; \; \ell_p), \; \left[P_e(J_{1+*} \; j_p'; \; J_0 \; 1; \; j_t'; \; \ell_p') \right]^* \right] \text{ as well as Auger}$$

decay amplitudes $\left[A_e(J_{2+} \; j_a; \; J_{1+*}; \; \ell_a), \; \left[A_e(J_{2+} \; j_a'; \; J_{1+*}; \; \ell_a') \right]^* \right]$ belonging

to the appropriate values of $[(j_p \; j_t \; \ell_p), \; (j_p' \; j_t' \; \ell_p')]$ and $[(j_a \; \ell_a), \; (j_p' \; \ell_a')]$, respectively.

4. These products are then added to obtain the final expression for a desired $A_{N_{S_p} \; N_{S_a}}^{S_p \; S_a}(m_r; \; \hat{\boldsymbol{k}}_p \; \hat{\boldsymbol{k}}_a)$ according to the definitions given in (7.19) and (7.20).

5. Complete calculation in this programme is performed in integer algebra.

E.3   Input

The integer variables ("nprim," and "iprint") are read in the beginning of the driver part (i.e., Sect. E.2.1) of the programme coefficient_A. Integer variables $[S_p,\ S_a, N_{S_p}, N_{S_a}, m_r]$ (see footnote (1) on page 283), "irpt," and all the ten elements of the array "iwrite" are supplied in the second read statement of the driver. A value of the integer variable "irpt" decides the flow of the programme coefficient_A in its driver part.

E.4   Programme Listing

Folder *programme_coefficient_A*, available at the web page <http://extra.springer.com> contains a complete listing of the present programme coefficient_A.

E.5   Test Run Output

Folder *programme_coefficient_A*, available at the web page <http://extra.springer.com> contains output of a test run of coefficient_A. The test run given therein corresponds to the 2-DPI transition (7.21).

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