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On Hartree – Fock Systems

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We show an existence and uniqueness result for mildly nonlinear Schrödinger systems of (self-consistent) Hartree – Fock form. We also shortly resume the already existing results on the semiclassical limit and the asymptotic and dispersive behavior of such systems.

Keywords: Hartree – Fock systems, nonlinear Schrödinger equation, Fermion systems, Pauli principle

1. INTRODUCTION

We consider Hartree – Fock systems in $\mathbb{R}^d$ of the form

$$i\varepsilon\frac{\partial}{\partial t}\psi_l^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi_l^\varepsilon + (V_E(x) + V_H^\varepsilon(x,t))\psi_l^\varepsilon - \sum_{j=1}^{\infty}\lambda_j^\varepsilon V_{lj}^\varepsilon(x,t)\psi_j^\varepsilon, \quad x\in\mathbb{R}^d,\ t\in\mathbb{R},\ l\in\mathbb{N} \tag{1.1a}$$

$$\psi_l^\varepsilon(t=0) = \varphi_l^\varepsilon, \quad l\in\mathbb{N} \tag{1.1b}$$

$$n^\varepsilon(x,t) = \sum_{l=1}^{\infty}\lambda_l^\varepsilon|\psi_l^\varepsilon(x,t)|^2 \tag{1.1c}$$

$$V_H^\varepsilon(x,t) = \int_{\mathbb{R}_z^d} U(x-z)n^\varepsilon(z,t)\,dz \tag{1.1d}$$

$$V_{lj}^\varepsilon(x,t) = \int_{\mathbb{R}_z^d} U(x-z)\psi_l^\varepsilon(z,t)\overline{\psi_j^\varepsilon}(z,t)\,dz. \tag{1.1e}$$

Here $\varepsilon > 0$ denotes the scaled Planck-constant, $\lambda_l^\varepsilon \geq 0$ the occupation number of the state ψ_l^ε and n^ε the number density. V_H^ε is the self-consistent Hartree potential (defined by the interaction potential $U = U(x)$), V_E^ε represents a given exterior potential and V_{lj}^ε stands for the interaction of the l-th and j-th state.The last term in (1.1a) is called the exchange correlation term. The density matrix ρ^ε and the current density J^ε are defined as

$$\rho^\varepsilon(x,y,t) = \sum_{l=1}^{\infty}\lambda_l^\varepsilon\bar{\psi}_l^\varepsilon(x,t)\psi_l^\varepsilon(y,t) \tag{1.1f}$$

$$J^\varepsilon(x,t) = \sum_{l=1}^{\infty}\lambda_l^\varepsilon\bar{\psi}_l^\varepsilon(x,t)\nabla\psi_l^\varepsilon(x,t). \tag{1.1g}$$

Hartree – Fock systems are considered an accurate description of the quantum-mechanical evolution of a Fermion system, since their derivation from many body physics takes into account the

Pauli exclusion principle [16], which is not the case for Hartree systems (obtained by setting $V^{\varepsilon}_{lj} := 0$). An existence analysis for the three dimensional Coulomb case can be found in [2]. The corresponding long time behavior was analysed in [3].

In Section 2 we give an existence and uniqueness result for the system (1.1) for very general interaction potentials in any space dimension and for both the attractive and repulsive case.

Section 3 is a summary of already existing results [4] on the classical limit and the asymptotic and dispersive behavior of the system (1.1).

2. EXISTENCE AND UNIQUENESS OF SOLUTIONS

In this section we investigate the existence and uniqueness of solutions for the system (1.1). Our proof follows the proof in the three dimensional Coulomb case [2] and the existence proof of the corresponding Hartree case [1, 7]. In the following we skip the superscript ε since ε is a fixed parameter in this section. We make the following assumptions

($A1$) (i) $\forall l \in \mathbb{N}$: $\lambda_l \geq 0$;
(ii) $\exists C > 0$:

$$\sum_{l=1}^{\infty} \lambda_l + \varepsilon^2 \sum_{l=1}^{\infty} \lambda_l \|\nabla\varphi_l\|^2_{L^2(\mathbb{R}^d)} + \int_{\mathbb{R}^d_x} V_E^+(x) n_I(x)\, dx \leq C.$$

On the external potential we assume
($A2$) $V_E \in H^1_{\mathrm{loc}}(\mathbb{R}^d)$; $\exists \underline{V} \in \mathbb{R} : V_E(x) \geq \underline{V}$ on $\mathbb{R}^d$, and on the interaction potential:
($A3$) (i) $U(x) = U(-x)$ on $\mathbb{R}^d$

(ii) $U \in L^r(\mathbb{R}^d) + L^{s,\infty}(\mathbb{R}^d)$ with

$$\begin{cases} \max(1, \frac{d}{2}) \leq r \leq \infty & \text{if } d \geq 1, \\ \frac{d}{2} \leq s < \infty & \text{if } d > 2, \\ 1 < s < \infty & \text{if } d = 1, 2; \end{cases}$$

For the definition of the 'weak L^p-spaces' $L^{p,\infty}$ we refer to [RS, page 30]. Obviously, the Coulomb interaction $U(x) = (1/|x|)$ on $\mathbb{R}^3$ satisfies assumption ($A3$).

A crucial tool in the following analysis are the *a priori* conserved quantities. We have

LEMMA 2.1 *Let $U(x) = U(-x)$ on $\mathbb{R}^d$ hold. Then*

$$\int_{\mathbb{R}^d} n(x,t)\, dx = \int_{\mathbb{R}^d} n_I(x)\, dx, \quad \forall t \in \mathbb{R}\ (\textit{charge conservation}), \tag{2.1}$$

where $n_I(x) := \sum_{l=1}^{\infty} \lambda_l |\varphi_l(x)|^2$, and

$$E(t) = E(0), \quad \forall t \in \mathbb{R}, \tag{2.2}$$

where

$$\begin{aligned} E(t) = {} & \frac{\varepsilon^2}{2} \int_{\mathbb{R}^d} \sum_{l=1}^{\infty} \lambda_l |\nabla\psi_l(x,t)|^2\, dx \\ & + \int_{\mathbb{R}^d} V_E(x) n(x,t)\, dx \\ & + \frac{1}{2} \int_{\mathbb{R}^{2d}} U(x-z) n(x,t) n(z,t)\, dxdz \\ & - \frac{1}{2} \int_{\mathbb{R}^{2d}} U(x-z) |\rho(x,z,t)|^2\, dxdz \end{aligned} \tag{2.3}$$

(*energy conservation*).

Proof of Lemma 2.1 Relation (2.2) is obtained by multiplying the Hartree–Fock equation (1.1a) by $\lambda_l \bar{\psi}_l$, integrating by parts, taking imaginary parts and summing over l.

(2.3) is the result of a somewhat more tedious calculation based on multiplying (1.1a) by $\lambda_l \frac{\partial}{\partial t} \bar{\psi}_l$, taking real parts and summing over l. Details can be found in [2] (at least for the Coulomb interaction potential $U(x) = (1/|x|)$ on $\mathbb{R}^3$). ■

Note that if U is not nonnegative, it is *a priori* not clear whether both the kinetic and the potential energy are bounded or not.

In order to state the main existence result we define the following Hilbert space

$$Y = \left\{ \Gamma = (\gamma_m)_{m\in\mathbb{N}} | \gamma_m \in H^1(\mathbb{R}^d) \forall m \in \mathbb{N} \text{ and } \|\Gamma\|_Y = \sqrt{\sum_{m=1}^{\infty} \lambda_m \|\gamma_m\|_{H^1}^2} < \infty \right\}. \tag{2.4}$$

Using this definition it is possible to reformulate problem (1.1) with $\Psi = (\psi_m)_{m\in\mathbb{N}}$ as

$$i\varepsilon\Psi_t = \left[-\frac{\varepsilon^2}{2} + V_E(x) \right] \Psi + F(\Psi) \tag{2.5a}$$

$$\Psi(t=0) = \Psi_0 = (\varphi_m)_{m\in\mathbb{N}} \tag{2.5b}$$

with

$$F(\Psi)(x) = \sum_{l=1}^{\infty} \lambda_l \int_{\mathbb{R}^d} U(x-z) [|\psi_l(z)|^2 \Psi(x) - \Psi(z)\bar{\psi}_l(z)\psi_l(x)] dz. \tag{2.5c}$$

Now we can state our main result

Theorem 2.1 *Let assumption (A1)–(A3) hold. Then, the evolution system (2.5) (and (1.1)) has a unique global solution $\Psi \in C([0,\infty), Y)$.*

We anticipate some lemmas we need in the proof of the above theorem.

We denote by A the operator

$$A\Psi = \left[-\frac{\varepsilon^2}{2}\Delta + V_E \right] \Psi, \qquad D(A) \subset Y. \tag{2.6}$$

The assumption $(A2)$ on V_E suffices to state

Lemma 2.2 *The operator A generates the group e^{iAt}, $t \in \mathbb{R}$ of unitary operators in Y.*

Lemma 2.3 *For every $T > 0$ the map F: $Y \times [0,T] \to Y$ is locally Lipschitz continous in Y uniformly in $t \in [0,T]$.*

Proof of Lemma 2.3 For notational convenience we consider the case $d > 2$ (The cases $d = 1, 2$ differ only in the limiting cases). We are going to show that

$$\|F[\Psi] - F[\tilde{\Psi}]\|_Y \leq c(\Psi, \tilde{\Psi}) \|\Psi - \tilde{\Psi}\|_Y. \tag{2.7}$$

For this purpose we need to estimate

$$\begin{aligned}
&\left\| \int_{\mathbb{R}^d} U(\cdot - z)|\psi_l(z)|^2 dz \psi_s(\cdot) - \int_{\mathbb{R}^d} U(\cdot - z)|\tilde{\psi}_l(z)|^2 dz \tilde{\psi}_s(\cdot) \right\|_{H^1(\mathbb{R}^d)} \\
&\leq \left\| \int_{\mathbb{R}^d} U(\cdot - z)(|\psi_l(z)|^2 - |\tilde{\psi}_l(z)|^2) dz \psi_s(\cdot) \right\|_{H^1(\mathbb{R}^d)} + \left\| \int_{\mathbb{R}^d} U(\cdot - z)|\tilde{\psi}_l(z)|^2 dz (\psi_s(\cdot) - \tilde{\psi}_s(\cdot)) \right\|_{H^1(\mathbb{R}^d)} \\
&\leq \left\| \int_{\mathbb{R}^d} U(\cdot - z)(|\psi_l(z)|^2 - |\tilde{\psi}_l(z)|^2) dz \psi_s(\cdot) \right\|_{L^2(\mathbb{R}^d)} + \left\| \int_{\mathbb{R}^d} \nabla U(\cdot - z)(|\psi_l(z)|^2 - |\tilde{\psi}_l(z)|^2) dz \psi_s(\cdot) \right\|_{L^2(\mathbb{R}^d)} \\
&\quad + \left\| \int_{\mathbb{R}^d} U(\cdot - z)(|\psi_l(z)|^2 - |\tilde{\psi}_l(z)|^2) dz \nabla\psi_s(\cdot) \right\|_{L^2(\mathbb{R}^d)} + \ldots, \quad \forall l, s \in \mathbb{N},
\end{aligned} \tag{2.8}$$

and, in analogy, we estimate in the exchange correlation part

$$\left\| \int_{\mathbb{R}^d} U(\cdot - z)\psi_l(z)\bar{\psi}_s(z)dz\psi_s(\cdot) - \int_{\mathbb{R}^d} U(\cdot - z)\tilde{\psi}_l(z)\bar{\tilde{\psi}}_s(z)dz\tilde{\psi}_s(\cdot)\right\|_{H^1(\mathbb{R}^d)}$$
$$\leq \left\| \int_{\mathbb{R}^d} U(\cdot - z)\psi_l(z)\bar{\psi}_s(z)dz(\psi_s(\cdot) - \tilde{\psi}_s(\cdot))\right\|_{L^2(\mathbb{R}^d)}$$
$$+ \left\| \int_{\mathbb{R}^d} U(\cdot - z)(\psi_l(z) - \tilde{\psi}_l(z))\bar{\psi}_s(z)dz\tilde{\psi}_s(\cdot)\right\|_{L^2(\mathbb{R}^d)}$$
$$+ \left\| \int_{\mathbb{R}^d} U(\cdot - z)\tilde{\psi}_l(z)(\bar{\psi}_s(z) - \bar{\tilde{\psi}}_s(z))dz\tilde{\psi}_s(\cdot)\right\|_{L^2(\mathbb{R}^d)}$$
$$\leq \ldots, \quad \forall l, s \in \mathbb{N}. \tag{2.9}$$

Using

$$\left||\psi_l(z)|^2 - |\tilde{\psi}_l(z)|^2\right| \leq |\psi_l(z) - \tilde{\psi}_l(z)||\psi_l(z) + \tilde{\psi}_l(z)| \tag{2.10}$$

and (as an example)

$$\int_{\mathbb{R}^d} \nabla_x U(x - z)\psi_l(z)\bar{\psi}(z)dz = -\int_{\mathbb{R}^d} \nabla_z U(x - z)\psi_l(z)\bar{\psi}(z)dz = \int_{\mathbb{R}^d} U(x - z)\nabla_z(\psi_l(z)\bar{\psi}(z))dz \tag{2.11}$$

we are able to estimate the many terms having similar structure. It turns out that there are basically two types of L^2 norms to be estimated,

$$\left\| \int_{\mathbb{R}^d} U(\cdot - z)a(z)b(z)dzc(\cdot)\right\|_{L^2(\mathbb{R}^d)}, \quad a, b \in L^p(\mathbb{R}^d),\ 2 \leq p \leq \frac{2d}{d-2},\ c \in L^2(\mathbb{R}^d), \tag{2.12}$$

and

$$\left\| \int_{\mathbb{R}^d} U(\cdot - z)a(z)b(z)dzc(\cdot)\right\|_{L^2(\mathbb{R}^d)}, \quad a, c \in L^p(\mathbb{R}^d),\ 2 \leq p \leq \frac{2d}{d-2},\ b \in L^2(\mathbb{R}^d). \tag{2.13}$$

In the first case, considering the weak L^s part of the interaction potential U only and using the generalized Young inequality we have

$$\left\| \int_{\mathbb{R}^d} U(\cdot - z)a(z)b(z)dzc(\cdot)\right\|_{L^{2-\delta}(\mathbb{R}^d)} \leq \|U\|_{L^{s,\infty}(\mathbb{R}^d)}\|a\|_{L^p(\mathbb{R}^d)}\|b\|_{L^p(\mathbb{R}^d)}\|c\|_{L^2(\mathbb{R}^d)} \tag{2.14}$$

for all $\delta \in (0, \delta_0]$ and some $2 \leq p \leq (2d/d-2)$. Passing to the limit $\delta \to 0$ we obtain the estimate for the L^2 norm. For the strong L^r part of U we use the Young inequality and obtain the estimate directly. In the second case we have

$$\left\| \int_{\mathbb{R}^d} U(\cdot - z)a(z)b(z)dzc(\cdot)\right\|_{L^2} \leq \|U\|_{L^{s,\infty}(\mathbb{R}^d)}\|a\|_{L^p(\mathbb{R}^d)}\|b\|_{L^2(\mathbb{R}^d)}\|c\|_{L^p(\mathbb{R}^d)} \tag{2.15}$$

for some $2 \leq p \leq (2d/d-2)$. The strong L^r part of U can be estimated in the same way. Collecting all the terms and summing over l and s we obtain the result

$$\|F[\Psi] - F[\tilde{\Psi}]\|_Y^2 \leq c(U)[\|\Psi\|_Y^4 + \|\tilde{\Psi}\|_Y^4]\|\Psi - \tilde{\Psi}\|_Y^2. \tag{2.16}$$

■

Proof of Theorem 2.1 We split the proof into two parts. First we prove the existence of a local (in time) solution. Then, we deduce the existence of a global solution by using the conserved quantities.

Lemmas 2.1 and 2.2 guarantee the existence of a $T_M > 0$ such that the Eq. (2.5) has a unique solution on $[0, T_M)$ and that

$$\lim_{t \to T_M} \|\Psi\|_Y = \infty$$

if $T_M < \infty$ (see semigroup theory in [14]). The global (in time) existence follows by using the conserved quantities. Assumption $(A1)$ provides bounded total initial density and energy. Lemma 2.1 gives bounded total density at every time. Also, for $U \geq 0$ we obtain immediately $\|\Psi(t)\|_Y < \infty, \forall t > 0$, since using Schwartz inequality we have

$$n^\varepsilon(x,t)n^\varepsilon(z,t) \geq |\rho^\varepsilon(x,z,t)|^2. \tag{2.17}$$

In the case of non nonnegative interaction potential the boundedness of the Y norm of Ψ is also true but needs an explanation. In fact, we have

$$\begin{aligned}\|n\|_{L^{\frac{p}{2}}(\mathbb{R}^d)} &\leq \sum_{l=1}^{\infty} \lambda_l^\varepsilon |\psi_l^\varepsilon(x)|^2_{L^p(\mathbb{R}^d)} \\ &\leq \sum_{l=1}^{\infty} \lambda_l^\varepsilon |\psi_l^\varepsilon(x)|^2_{H^1(\mathbb{R}^d)}, \ 2 \leq p \leq \frac{2d}{d-2},\end{aligned} \tag{2.18}$$

and (again for the weak L^s part of the interaction potential)

$$\begin{aligned}&\left|\int_{\mathbb{R}_z^d}\int_{\mathbb{R}_x^d} U(x-z)n(z)n(x)dxdz\right| \\ &\qquad \leq \|U\|_{L^{s,\infty}(\mathbb{R}^d)}\|n\|^2_{L^{\frac{p}{2}}(\mathbb{R}^d)},\end{aligned} \tag{2.19}$$

for some $2 \leq p \leq (2d/d-2)$. The same holds for the strong L^r part of the interaction potential. Therefore, not only the total energy is conserved, but also the kinetic and potential energies are bounded uniformly in time and as a consequence $\|\Psi(t)\|_Y < \infty$, $\forall t > 0$. ■

3. OTHER PROPERTIES OF HARTREE–FOCK SYSTEMS

In this section we collect other interesting properties of the system (1.1). We only give a description of the results. Details of the following results can be found in [4]. The superscript ε is important in this section, especially in the first part. The results are valid for $d > 1$, for $d = 1$ special assumptions are needed (see [4]).

3.1. The Classical Limit

In this section we describe the results on the classical limit of the Hartree–Fock systems. The appropriate formulation to perform the classical limit is the Wigner formalism, which we shortly describe.

The Wigner transform of the density matrix is the Fourier transform of the function $\rho^\varepsilon(x+(\varepsilon/2)\eta, x-(\varepsilon/2)\eta, t)$ with respect to η, *i.e.*,

$$\begin{aligned}w^\varepsilon(x,v,t) &:= \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \\ &\qquad \rho^\varepsilon\left(x+\frac{\varepsilon}{2}\eta, x-\frac{\varepsilon}{2}\eta, t\right)e^{iv\cdot\eta}\,d\eta\end{aligned} \tag{3.1}$$

(*cf.* [5, 8, 17]), where the Fourier transform is defined by

$$\hat{\varphi}(v) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}_x^d} \varphi(x)e^{iv\cdot x}\,dx. \tag{3.2}$$

The Wigner transform is the solution of the Wigner–Hartree–Fock equation, obtained from (1.1) by an easy calculation [11]:

$$\begin{aligned}&w_t^\varepsilon + v\cdot\nabla_x w^\varepsilon + \theta^\varepsilon[V_E]w^\varepsilon \\ &\qquad + \theta^\varepsilon[V_H^\varepsilon]w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] = 0,\end{aligned} \tag{3.3a}$$

$$V_H(x,t) = \int_{\mathbb{R}_z^d} U(x-z)n^\varepsilon(z,t)\,dz, \tag{3.3b}$$

$$n^\varepsilon(x,t) = \int_{\mathbb{R}_v^d} w^\varepsilon(x,v,t)\,dv, \tag{3.3c}$$

$$\begin{aligned}&w^\varepsilon(x,v,t=0) \\ &\quad = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \rho_I^\varepsilon\left(x+\frac{\varepsilon}{2}\eta, x-\frac{\varepsilon}{2}\eta\right)e^{iv\cdot\eta}\,d\eta \\ &\quad =: w_I^\varepsilon(x,v),\end{aligned} \tag{3.3d}$$

For a given potential $V = V(x)$ the pseudo-differential operator $\theta^{\varepsilon}[V]$ is defined by

$$(\theta^{\varepsilon}[V]w)(x,v) = \frac{-i}{(2\pi)^d}\int \frac{V(x+\frac{\varepsilon}{2}\eta) - V(x-\frac{\varepsilon}{2}\eta)}{\varepsilon} \tilde{w}(x,\eta)\mathrm{e}^{iv\cdot\eta}\,d\eta, \tag{3.4a}$$

where $\tilde{w}$ denotes the inverse Fourier transform of $w = w(x,v)$ with respect to v:

$$\tilde{w}(x,\eta) = \int_{\mathbb{R}_v^d} w(x,v)\mathrm{e}^{-iv\cdot\eta}\,dv. \tag{3.4b}$$

Ω^{ε} is the (quadratically) nonlinear operator

$$\begin{aligned}(\Omega^{\varepsilon}[w])(x,v) &:= -\varepsilon^{d-1} i \int\int \left(U\left(\varepsilon\left(z-\frac{\eta}{2}\right)\right) - U\left(\varepsilon\left(z+\frac{\eta}{2}\right)\right)\right)\\ &\cdot \tilde{w}\left(x-\frac{\varepsilon}{2}z+\frac{\varepsilon}{4}\eta,\ z+\frac{\eta}{2}\right)\\ &\tilde{w}\left(x-\frac{\varepsilon}{2}z-\frac{\varepsilon}{4}\eta,\ -z+\frac{\eta}{2}\right) dz\mathrm{e}^{iv\cdot\eta}\,d\eta\end{aligned} \tag{3.5}$$

Under additional assumptions on the interaction potential (and on its gradient) and on the initial data it is possible to carry out the limit $\varepsilon \to 0$.

Theorem 3.1 *Let (A1), (A2), (A3) of* [4] *hold. Then, for every sequence $\varepsilon \to 0$ there exists a subsequence (denoted by the same symbol) such that*

$$w_I^{\varepsilon} \to w_I^0 \geq 0 \quad in\, L^2(\mathbb{R}_x^d \times \mathbb{R}_v^d)\ weakly, \tag{3.6a}$$

$$w^{\varepsilon} \to w^0 \geq 0 \quad in\, L^{\infty}(\mathbb{R}_t; L^2(\mathbb{R}_x^d \times \mathbb{R}_v^d))\ weak - *, \tag{3.6b}$$

$$n^{\varepsilon} \to n^0 = \int w^0\,dv \quad in\ L^{\infty}(\mathbb{R}_t; L^{\frac{d+4}{d+2}}(\mathbb{R}_x^d))\ weak - *, \tag{3.6c}$$

$$J^{\varepsilon} \to J^0 = \int v w^0\,dv \quad in\ L^{\infty}(\mathbb{R}_t; L^{\frac{d+4}{d+3}}(\mathbb{R}_x^d))\ weak - *, \tag{3.6d}$$

$$\nabla V_H^{\varepsilon} \to \nabla V_H^0 = \int_{\mathbb{R}^d} \nabla_z U(x-z) n^0(z,t)dz \quad in\ L^{\infty}(\mathbb{R}_t; L^2(\mathbb{R}_x^d))\ weak - *, \tag{3.6e}$$

$$\Omega^{\varepsilon}[w^{\varepsilon}] \to 0 \quad in\, S'(\mathbb{R}_x^d \times \mathbb{R}_v^d \times \mathbb{R}_t) \tag{3.6f}$$

where $(w^0, n^0, E^0 = \nabla V_H^0)$ are weak solutions of the self consistent Vlasov equation:

$$w_t^0 + v\cdot\nabla_x w^0 - \nabla_x V_H^0 \cdot \nabla_v w^0 = 0\ in\ \mathbb{R}_x^d \times \mathbb{R}_v^d \times \mathbb{R}_t \tag{3.7a}$$

$$w^0(t=0) = w_I^0. \tag{3.7b}$$

The contribution of the exchange correlation part originating from the Pauli principle does not give any contribution in the classical limit in which no such principle exists. Therefore, the result is physically reasonable and expected.

In three dimensions with Coulomb interaction the limiting classical problem is the Vlasov-Poisson system, which also represents the limiting problem if we start from the Hartree system only (without exchange correlation part) [8, 9, 12].

3.2. Long Time Behavior

In this section we report on the asymptotic behavior in the repulsive case ($U \geq 0$) and without external potential $V_E = 0$. In the non (totally) repulsive case or if $V_E \neq 0$ the following result cannot be expected. For simplicity, we give the result for the interaction potential $U(x) = (1/|x|)$ only.

Theorem 3.2 *Under the assumptions of* [4] *the following decay estimates hold*:

(i) $\|n^\varepsilon\|_{L^q(\mathbb{R}^d_x)} = c\,t^{-(1-a)}$,
(ii) $\| J^\varepsilon\|_{L^s(\mathbb{R}^d_x)} = c\,t^{-(1/2)(1-a)}$,
(iii) $\|V_H\|_{L^r(\mathbb{R}^d_x)} = c\,t^{-(1-a)}$,
(iv) *with* $1-a = (d/2)(1-(1/q))$, $(1/s) = (2/q)+(1/2)$, $1+(1/r) = (1/q)+(1/d)$, $1 \le q \le (d/d-2)$, $1 \le s < (2d/3d-4)$ *and* $max(1, (d/2d+1)) \le r < d$.

Note that results along the lines of the ones presented (and in the more general in [4]) entirely based on the Schrödinger formalism restricted to the $3d$ Coulomb case and finitely many coupled states can be found in [3, 13]. Decay results for the Hartree case with Coulomb interaction can be found in [7].

3.3. A Dispersive Identity

Let $x_0 \in \mathbb{R}^d$ fixed, set $\delta = 0$ or $\delta = 1$ and $\alpha > 0$. Then multiplying (3.3a) by $(v \cdot (x-x_0)/(\delta + |x-x_0|^\alpha)^{(1/\alpha)})$ gives the identity:

$$\begin{aligned}
&\int_{T_1}^{T_2}\int_{\mathbb{R}^d_x}\int_{\mathbb{R}^d_v} w^\varepsilon(x,v,t)[(|v|^2(\delta+|x-x_0|^\alpha)-\\
&((x-x_0)\cdot v)^2|x-x_0|^{\alpha-2})/\\
&(\delta+|x-x_0|^\alpha)^{1+\frac{1}{\alpha}}]\,dvdxdt\\
&-\int_{T_1}^{T_2}\int_{\mathbb{R}^d_x}((x-x_0)\\
&\cdot\nabla V_E/(\delta+|x-x_0|^\alpha)^{1/\alpha})n^\varepsilon(x,t)\,dxdt\\
&+\int_{T_1}^{T_2}\int_{\mathbb{R}^d_x}\int_{\mathbb{R}^d_z}((x-x_0)\\
&\cdot\nabla U(x-z)/(\delta+|x-x_0|^\alpha)^{1/\alpha})\\
&\quad(|\varrho^\varepsilon(x,z,t)|^2 - n^\varepsilon(x,t)n^\varepsilon(z,t))\,dzdxdt\\
&=\int_{\mathbb{R}^d_x}((x-x_0)/(\delta+|x-x_0|^\alpha)^{1/\alpha})\\
&\cdot(J^\varepsilon(x,T_1)-J^\varepsilon(x,T_2))\,dx
\end{aligned} \tag{3.8}$$

for all $-\infty < T_1 < T_2 < \infty$. Integral identities of this type were obtained in [10] for the free transport equation, in [13] for the Vlasov-Poisson and Wigner-Poisson systems and in [6] for a large class of equations.

A lengthy calculation shows that the first term on the left hand side of (3.8) is nonnegative. For example in the case $d = 3$ and $\delta = 0$ it is equal to

$$\begin{aligned}
\varepsilon^2\sum_{l=1}^\infty \lambda_l^\varepsilon \int_{T_1}^{T_2}\Bigg[\int_{\mathbb{R}^3}\bigg(&\frac{|\nabla\psi_l^\varepsilon(x,t)|^2}{|x-x_0|}\\
&-\frac{|(x-x_0)\cdot\nabla\psi_l^\varepsilon(x,t)|^2}{|x-x_0|^3}\bigg)dx\\
&+8\pi|\psi_l^\varepsilon(x_0,t)|^2\Bigg]\,dt
\end{aligned} \tag{3.9}$$

(see [10] also for the other cases). Now let's assume that $V_E \equiv 0$ (no exterior field) and that the interaction potential is radial $U = U_0(|x|)$ with $U_0'(r) \le 0$. Then, an easy calculation using $\varrho^\varepsilon(x,z,t) = \overline{\varrho^\varepsilon(z,x,t)}$ and (2.17) shows that also the third term in (3.8) is nonnegative. Thus, the identity (3.8) gives the bound for the first term on its left hand side:

$$\| J^\varepsilon(T_1)\|_{L^1(\mathbb{R}^d_x)} + \| J^\varepsilon(T_2)\|_{L^1(\mathbb{R}^d_x)}.$$

Energy conservation shows that $\| J^\varepsilon(t)\|_{L^1(\mathbb{R}^d_x)}$ is uniformly bounded in ε and t. Thus, we conclude for $d = 3$ and all $x_0 \in \mathbb{R}^3$:

$$\begin{aligned}
\varepsilon^2\sum_{l=1}^\infty \lambda_l^\varepsilon \int_{-\infty}^{\infty}\int_{\mathbb{R}^3}\bigg(&\frac{|\nabla\psi_l^\varepsilon(x,t)|^2}{|x-x_0|}\\
&-\frac{|(x-x_0)\cdot\nabla\psi_l^\varepsilon(x,t)|^2}{|x-x_0|^3}\bigg)dx\\
&+\varepsilon^2\int_{-\infty}^{\infty} n^\varepsilon(x_0,t)\,dt \le C = C(E^\varepsilon_{kin}(0))
\end{aligned} \tag{3.10}$$

(just as for the free Schrödinger equation). Similar estimates can be obtained for dimensions different from 3.

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