M2AN - MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

I. GASSER
R. ILLNER
P. A. MARKOWICH
C. SCHMEISER

Semiclassical, $t \to \infty$ asymptotics and dispersive effects for Hartree-Fock systems

M2AN - Modélisation mathématique et analyse numérique, tome 32, nº 6 (1998), p. 699-713
<http://www.numdam.org/item?id=M2AN_1998__32_6_699_0>

MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

(Vol 32, n° 6, 1998, p 699 à 713)

SEMICLASSICAL, $t \to \infty$ ASYMPTOTICS AND DISPERSIVE EFFECTS FOR HARTREE-FOCK SYSTEMS
Dedicated to Helmut Neunzert at the occasion of his 60th birthday

I. GASSER (*), R. ILLNER (**), P. A. MARKOWICH (*) and C. SCHMEISER (***)

Résumé — *On analyse la limite semiclassique et l'asymptotique $t \to \infty$ pour des systèmes des équations de Schrodinger faiblement non linéaire en forme Hartree-Fock En utilisant des techniques de fonction de Wigner, on démontre que la limite semi-classique est représentée par l'équation de Vlasov « self-consistent » En outre, on démontre des estimations du temps pour la densité et le potentiel électrique de Hartree-Fock dans les norms L^p pour $t \to \infty$* © *Elsevier, Paris*

Abstract — *We analyze the semiclassical limit and the "$t \to \infty$ asymptotics" of mildly nonlinear Schrodinger systems of (self-consistent) Hartree-Fock form Using Wigner-function techniques we prove that the semiclassical limit is represented by the self-consistent Vlasov equation Moreover we prove time decay for the position density and for the Hartree-potential in L^p norms as $t \to \infty$* © *Elsevier, Paris*

1. INTRODUCTION

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

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

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

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

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

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

Here $\varepsilon > 0$ denotes the scaled Planck-constant, $\lambda_l^\varepsilon \geq 0$ the occupation number of the state ψ_l^ε, n^ε is the number density of the considered particle system, 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.

Manuscript received April 1, 1997
(*) FB Mathematik MA 6-2, TU-Berlin, Straße des 17 Juni 136, 10623 Berlin, Germany
(**) Department of Mathematics and Statistics, University of Victoria, P.O Box 3045, Victoria, B.C. V8W 3P4, Canada.
(***) Institut fur Angewandte und Numerische Mathematik, TU-Wien, Wiedner Hauptstraße 8-10, 1040 Wien Austria

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 [S], which is not the case for Hartree systems (obtained by setting $V_{ij}^{\varepsilon} := 0$).

In this paper we consider two limits of Hartree-Fock systems. The first one, analyzed in Section 2, is the semiclassical limit $\varepsilon \to 0$. We prove — under suitable assumptions on the data — that the Hartree-Fock exchange term does not give a contribution in the limit $\varepsilon \to 0$, i.e. the semiclassical limit of the Hartree-Fock system is — in a sense made precise in the next section — the selfconsistent Vlasov equation. The same result has already been shown for Hartree systems [LPa, MM]. Clearly, this behaviour is physically plausible, since the Pauli principle is a purely quantum physical notion.

The second limit to be considered is the limit $t \to \infty$ in the purely repulsive case $U \geq 0$. These results, which improve [DF] are contained in Section 3.

Section 4 is concerned with dispersive effects.

2. THE SEMICLASSICAL LIMIT

We define the density matrix ρ^{ε} in the usual way

$$\rho^{\varepsilon}(r, s, t) = \sum_{l=1}^{\infty} \lambda_l^{\varepsilon} \bar{\psi}_l^{\varepsilon}(r, t) \psi_l^{\varepsilon}(s, t), \quad r, s \in \mathbb{R}^d \tag{2.1}$$

and derive the Heisenberg formulation of the Hartree-Fock system:

$$\begin{aligned} - i\varepsilon\rho_t^{\varepsilon} = & - \frac{\varepsilon^2}{2} (\Delta_r - \Delta_s) \rho^{\varepsilon} + (V_E(r) - V_E(s)) \rho^{\varepsilon} \\ & + (V_H^{\varepsilon}(r, t) - V_H^{\varepsilon}(s, t)) \rho^{\varepsilon} \\ & - \int_{\mathbb{R}_z^d} (U(r-z) - U(s-z)) \rho^{\varepsilon}(r, z, t) \rho^{\varepsilon}(z, s, t) \, dz \end{aligned} \tag{2.2a}$$

$$n^{\varepsilon}(x, t) = \rho^{\varepsilon}(x, x, t) \tag{2.2b}$$

$$V_H^{\varepsilon}(x, t) = \int_{\mathbb{R}_z^d} U(x-z) \, n^{\varepsilon}(z, t) \, dz \tag{2.2c}$$

$$\rho^{\varepsilon}(r, s, t=0) = \sum_{l=1}^{\infty} \lambda_l^{\varepsilon} \bar{\varphi}_l^{\varepsilon}(r) \varphi_l^{\varepsilon}(s) =: \rho_I^{\varepsilon}(r, s) . \tag{2.2d}$$

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

$$w^{\varepsilon}(x, v, t) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \rho^{\varepsilon}\left(x + \frac{\varepsilon}{2}\eta, x - \frac{\varepsilon}{2}\eta, t\right) e^{iv \cdot \eta} \, d\eta \tag{2.3}$$

(*cf.* [GMMP], [LPa], [W], where the Fourier transform is defined by

$$\hat{\varphi}(v) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}_x^d} \varphi(x) \, e^{iv \cdot x} \, dx . \tag{2.4}$$

It is the solution of the Wigner-Hartree-Fock equation, obtained from (2.2) by an easy calculation [M]:

$$w_t^\varepsilon + v \,.\, \nabla_x w^\varepsilon + \theta^\varepsilon[V_E]\, w^\varepsilon + \theta^\varepsilon[V_H^\varepsilon]\, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] = 0\,, \tag{2.5a}$$

$$V_H(x,t) = \int_{\mathbb{R}_z^d} U(x-z)\, n^\varepsilon(z,t)\, dz\,, \tag{2.5b}$$

$$n^\varepsilon(x,t) = \int_{\mathbb{R}_v^d} w^\varepsilon(x,v,t)\, dv\,, \tag{2.5c}$$

$$w^\varepsilon(x,v,t=0) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \rho_I^\varepsilon\Big(x+\frac{\varepsilon}{2}\eta,\, x-\frac{\varepsilon}{2}\eta\Big)\, e^{iv\cdot\eta}\, d\eta \tag{2.5d}$$

$$=: w_I^\varepsilon(x,v)\,,$$

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

$$(\theta^\varepsilon[V]\, w)\,(x,v) = \frac{-i}{(2\pi)^d}\int \frac{V\Big(x+\frac{\varepsilon}{2}\eta\Big) - V\Big(x-\frac{\varepsilon}{2}\eta\Big)}{\varepsilon}\, \tilde{w}(x,\eta)\, e^{iv\cdot\eta}\, d\eta\,, \tag{2.6a}$$

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

$$\tilde{w}(x,\eta) = \int_{\mathbb{R}_v^d} w(x,v)\, e^{-iv\cdot\eta}\; dv\,. \tag{2.6b}$$

Ω^ε is the (quadratically) nonlinear operator

$$(\Omega^\varepsilon[w])\,(x,v) := -\varepsilon^{d-1}\, i \iint \Big(U\Big(\varepsilon\Big(z-\frac{\eta}{2}\Big)\Big) - U\Big(\varepsilon\Big(z+\frac{\eta}{2}\Big)\Big)\Big)$$

$$\times\, \tilde{w}\Big(x-\frac{\varepsilon}{2}z+\frac{\varepsilon}{4}\eta,\, z+\frac{\eta}{2}\Big)\, \tilde{w}\Big(x-\frac{\varepsilon}{2}z-\frac{\varepsilon}{4}\eta,\, -z+\frac{\eta}{2}\Big)\, dz e^{iv\cdot\eta}\, d\eta \tag{2.7}$$

The following estimate is basic for carrying out the limit $\varepsilon \to 0+$ in the Hartree-Fock system.

LEMMA 2.1: *Let* $w \in L^2(\mathbb{R}_x^d \times \mathbb{R}_v^d)$, $\varphi \in S(\mathbb{R}_x^d \times \mathbb{R}_v^d)$ *and* $U(-x) = U(x)$ *on* $\mathbb{R}^d$. *Then*

$$\left| \int_{\mathbb{R}_x^d \times \mathbb{R}_v^d} \bar{\varphi}\, \Omega^\varepsilon[w]\, dx\, dv \right| \leq A^\varepsilon(\varphi)\, \|w\|^2_{L^2(\mathbb{R}_x^d\times\mathbb{R}_v^d)}\,, \tag{2.8a}$$

where

$$A^\varepsilon(\varphi) = 2\left(\|\psi\|_{L^1(\mathbb{R}_x^d)} \sup_x \int_{\mathbb{R}_y^d} \psi(x+y)\, |\varepsilon^{d-1}\, U(\varepsilon y)|^2\, dy \right)^{1/2} \tag{2.8b}$$

with $\psi(\eta) := \sup_x |\tilde{\varphi}(x,\eta)|$.

Proof: With the substitution $s=-z+\frac{\eta}{2}$, $r=z+\frac{\eta}{2}$ we obtain

$$\int \Omega^\varepsilon[w]\,\bar{\varphi}\,dx\,dv = i\int [\varepsilon^{d-1}(U(\varepsilon r)-U(\varepsilon s))]\,\tilde{w}\Big(x+\frac{\varepsilon}{2}s, r\Big)\,\tilde{w}\Big(x-\frac{\varepsilon}{2}r, s\Big)\,\bar{\tilde{\varphi}}(x, r+s)\,dr\,ds\,dx\,.$$

We estimate

$$\begin{aligned}\left|\int \Omega^\varepsilon[w]\,\bar{\varphi}\,dx\,dv\right| &\leq \int \psi(r+s)\,[\varepsilon^{d-1}(|U(\varepsilon r)|+|U(\varepsilon s)|)]\\ &\quad\times\left(\int \Big|\tilde{w}\Big(x+\frac{\varepsilon}{2}s, r\Big)\Big|\,\Big|\tilde{w}\Big(x-\frac{\varepsilon}{2}r, s\Big)\Big|\,dx\right)dr\,ds\\ &\leq \int \psi(r+s)\,[\varepsilon^{d-1}(|U(\varepsilon r)|+|U(\varepsilon s)|)]\\ &\quad\times\left(\int |\tilde{w}(x,r)|^2\,dx\right)^{1/2}\left(\int |\tilde{w}(x,s)|^2\,dx\right)^{1/2} dr\,ds\\ &= 2\int \psi(r+s)\,[\varepsilon^{d-1}|U(\varepsilon r)|]\\ &\quad\times\left(\int |\tilde{w}(x,s)|^2\,dx\right)^{1/2}\left(\int |\tilde{w}(x,r)|^2\,dx\right)^{1/2} dr\,ds\end{aligned}$$

and thus

$$\begin{aligned}\left|\int \Omega^\varepsilon[w]\,\bar{\varphi}\,dx\,dv\right| &\leq 2\left(\iint \psi(r+s)\,[\varepsilon^{d-1}|U(\varepsilon r)|]^2\,dr\int |\tilde{w}(x,s)|^2\,dx\,ds\right)^{1/2}\\ &\quad\times\left(\int \psi(r+s)\int |\tilde{w}(x,r)|^2\,dx\,dr\,ds\right)^{1/2}.\end{aligned}$$

The assertion of the Lemma now follows immediately. □

The subsequent Lemma is concerned with *a priori* conserved quantities of the Hartree-Fock system:

LEMMA 2.2: *Let* $U(x)=U(-x)$ *on* $\mathbb{R}^d$ *hold. Then*

$$\int_{\mathbb{R}^d} n^\varepsilon(x,t)\,dx = \int_{\mathbb{R}^d} n_I^\varepsilon(x)\,dx, \quad \forall t\in\mathbb{R}\ (\textit{charge conservation}), \tag{2.9}$$

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

$$E^\varepsilon(t)=E^\varepsilon(0), \quad \forall t\in\mathbb{R}, \tag{2.10}$$

where

$$E^{\varepsilon}(t)=\frac{\varepsilon^{2}}{2}\int_{\mathbb{R}^{d}}\sum_{l=1}^{\infty}\lambda_{l}^{\varepsilon}|\nabla\psi_{l}^{\varepsilon}(x,t)|^{2}\,dx+\int_{\mathbb{R}^{d}}V_{E}(x)\,n^{\varepsilon}(x,t)\,dx$$
$$+\frac{1}{2}\int_{\mathbb{R}^{2d}}U(x-z)\,n^{\varepsilon}(x,t)\,n^{\varepsilon}(z,t)\,dx\,dz$$
$$-\frac{1}{2}\int_{\mathbb{R}^{2d}}U(x-z)\,|\rho^{\varepsilon}(x,z,t)|^{2}\,dx\,dz$$

(energy conservation).

Proof: (2.9) is obtained by multiplying the Hartree-Fock equation (1.1a) by $\lambda_l^{\varepsilon}\bar{\psi}_l^{\varepsilon}$, integrating by parts, taking imaginary parts and summing over l.

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

$E^{\varepsilon}(t)$ is the total energy, which by effect of Lemma 2.2 is constant in time. We remark that, by a well known calculation (see, e.g. [MM], [LPa]) the kinetic energy can be written as

$$\frac{\varepsilon^{2}}{2}\int_{\mathbb{R}^{d}}\sum_{l=1}^{\infty}\lambda_{l}^{\varepsilon}|\nabla\psi_{l}^{\varepsilon}(x,t)|^{2}\,dx=\int_{\mathbb{R}_{v}^{d}\times\mathbb{R}_{x}^{d}}\frac{|v|^{2}}{2}w^{\varepsilon}(x,v,t)\,dx\,dv\,. \tag{2.11}$$

The following Lemma provides an *a priori* L^2-estimate for the Wigner function w^{ε}:

LEMMA 2.3: *Assume that the initial states* $\{\varphi_l^{\varepsilon}\}_{l=1}^{\infty}$ *are an orthonormal system in* $L^2(\mathbb{R}_x^d)$ *and that* $U(x)=U(-x)$ *on* $\mathbb{R}^d$. *Then*

$$\|w^{\varepsilon}(t)\|^{2}_{L^{2}(\mathbb{R}_{x}^{d}\times\mathbb{R}_{v}^{d})}=\left(\frac{2\pi}{\varepsilon}\right)^{d}\sum_{l=1}^{\infty}(\lambda_{l}^{\varepsilon})^{2},\quad\forall t\in\mathbb{R}\,. \tag{2.12}$$

Proof: Similarly to the proof of (2.9) we show that initially orthogonal states φ_l^{ε}, φ_k^{ε} remain orthogonal for all time under the Hartree-Fock evolution. The result then follows directly from the formulas (2.3), (2.1). □

Also, we remark that the local conservation law

$$n_t^{\varepsilon}+\operatorname{div}J^{\varepsilon}=0 \tag{2.13}$$

holds, where the current density J^{ε} can be calculated from the Wigner function in the usual way

$$J^{\varepsilon}(x,t)=\int_{\mathbb{R}^{d}}v\,w^{\varepsilon}(x,v,t)\,dv \tag{2.14}$$

(see [MM, LPa]). We now make the following assumptions on the data:

(A1) (i) $\forall\varepsilon\in(0,\varepsilon_0],\, l\in\mathbb{N}:\lambda_l^{\varepsilon}\geq 0$;

(ii) $\forall\varepsilon\in(0,\varepsilon_0]:\{\varphi_l^{\varepsilon}\}_{l=1}^{\infty}$ is an ONS in $L^2(\mathbb{R}^d)$;

(iii) $\exists C>0$:

$$\sum_{l=1}^{\infty}\lambda_{l}^{\varepsilon}+\frac{1}{\varepsilon^{d}}\sum_{l=1}^{\infty}(\lambda_{l}^{\varepsilon})^{2}+\varepsilon^{2}\sum_{l=1}^{\infty}\lambda_{l}^{\varepsilon}\|\nabla\varphi_{l}^{\varepsilon}\|^{2}_{L^{2}(\mathbb{R}^{d})}+\int_{\mathbb{R}_{x}^{d}}V_{E}^{+}(x)\,n_{I}^{\varepsilon}(x)\,dx\leq C$$

for $\varepsilon \in (0, \varepsilon_0]$.
On the external potential we assume

(A2) $$V_E \in H^1_{\mathrm{loc}}(\mathbb{R}^d)\,;\ \exists \underline{V} \in \mathbb{R} : V_E(x) \geq \underline{V} \text{ on } \mathbb{R}^d,$$

and on the interaction potential:
(A3) (i) $U(x) = U(-x)$ on $\mathbb{R}^d$
(ii)

$$U \in L^\infty(\mathbb{R}^d) + L^{s,\infty}(\mathbb{R}^d) \quad \text{with} \quad \begin{cases} 2 < s < \infty & \text{if } d = 2, \\ \frac{7}{4} \leq s < \infty & \text{if } d = 3, \\ \frac{d}{2} \leq s < \infty & \text{if } d \geq 4\,; \end{cases}$$

$U \in C_b(\mathbb{R})$ and $U(0) = 0$ if $d = 1$;
(iii) $\nabla U \in L^{\frac{2d+8}{d+8}}(\mathbb{R}^d) + L^{q,\infty}(\mathbb{R}^d)$ with $\frac{2d+8}{d+8} < q < 2$.

For the definition of the 'weak L^p-spaces' $L^{p,\infty}$ we refer to [RS, page 30]. (A1) implies a uniform bound for $n^\varepsilon \in L^\infty(\mathbb{R}_t\,; L^1(\mathbb{R}^d_x))$ for the initial kinetic energy and (with (A3) (i)) on $w^3 \in L^\infty(\mathbb{R}_t\,; L^2(\mathbb{R}^d_x \times \mathbb{R}^d_v))$.

In order to carry out the limit $\varepsilon \to 0$ in the Wigner-Hartree-Fock system we proceed as in [LPa] to establish uniform *a priori* bounds. We start with the initial energy:

PROPOSITION 2.1: $E^\varepsilon(0) \leq C$.

From now on we denote by C generic, not necessarily equal constants which are independent of $\varepsilon \in (0, \varepsilon_0]$.

Proof: The following estimate can be found in [LPa] (*c.f.* the Theorem in the Appendix)

$$\| n^\varepsilon(t) \|_{L^{\frac{d+4}{d+2}}(\mathbb{R}^d_x)} \leq C_0 \| w^\varepsilon(t) \|^\theta_{L^2(\mathbb{R}^d_x \times \mathbb{R}^d_v)} \left(\int_{\mathbb{R}^d_x \times \mathbb{R}^d_v} \frac{|v|^2}{2} w^\varepsilon(t)\, dv\, dx \right) \tag{2.15}$$

where C_0 is also independent of w^ε and

$$\theta = \frac{4}{d+4}.$$

Evaluating at $t = 0$ gives a uniform bound for $n^\varepsilon_I \in L^{\frac{d+4}{d+2}}(\mathbb{R}^d_x)$. The generalized Young inequality [RS, page 32] then yields (together with (A3) (ii)) a uniform bound for $\int_{\mathbb{R}^d_x \times \mathbb{R}^d_z} |U(x-z)|\, n^\varepsilon_I(x)\, n^\varepsilon_I(z)\, dz\, dx$. Since (by the Schwartz inequality)

$$n^\varepsilon(x,t)\, n^\varepsilon(z,t) \geq |\rho^\varepsilon(x,z,t)|^2 \tag{2.16}$$

we obtain a uniform bound for $\int_{\mathbb{R}^d_x \times \mathbb{R}^d_z} |U(x-z)|\, |\rho^\varepsilon_I(x,z)|^2\, dz\, dx$ and the assertion of Proposition 2.1 follows.

Next we derive a uniform bound for the total kinetic energy:

PROPOSITION 2.2:

$$E^\varepsilon_{kin}(t) = \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_v} \frac{|v|^2}{2} w^\varepsilon(t)\, dv\, dx \leq C, \quad t \in \mathbb{R}_t.$$

Proof: From (2.10), (2.11) we obtain

$$E^{\varepsilon}_{kin}(t) \leqslant E^{\varepsilon}(t=0) - \underline{V}\int_{\mathbb{R}_x} n^{\varepsilon}(t)\,dx$$
$$-\frac{1}{2}\int_{\mathbb{R}^d_x\times\mathbb{R}^d_z} U^{+}(x-z)\,(n^{\varepsilon}(x,t)\,n^{\varepsilon}(z,t) - |\rho^{\varepsilon}(x,z,t)|^2)\,dz\,dx$$
$$+\frac{1}{2}\int_{\mathbb{R}^d_x\times\mathbb{R}^d_z} U^{-}(x-z)\,(n^{\varepsilon}(x,t)\,n^{\varepsilon}(z,t) - |\rho^{\varepsilon}(x,z,t)|^2)\,dz\,dx$$

and (2.15) gives

$$E^{\varepsilon}_{kin}(t) \leqslant C + \frac{1}{2}\int_{\mathbb{R}^d_x\times\mathbb{R}^d_z} |U(x-z)|\,n^{\varepsilon}(x,t)\,n^{\varepsilon}(z,t)\,dz\,dx\,.$$

For $d=1$ the assertion follows. For $d>1$ we again apply the generalized Young inequality

$$\int_{\mathbb{R}^d_x\times\mathbb{R}^d_z} |U(x-z)|\,n^{\varepsilon}(x,t)\,n^{\varepsilon}(z,t)\,dz\,dx \leqslant C(1+\|n^{\varepsilon}(t)\|^2_{L^p(\mathbb{R}^d_x)})$$

with $2=\frac{1}{s}+\frac{2}{p}$ where s is of (A3) (ii). By interpolation we have

$$\|n^{\varepsilon}(t)\|_{L^p(\mathbb{R}^d_x)} \leqslant C\|n^{\varepsilon}(t)\|^{1-\theta_1}_{L^{\frac{d+4}{d+2}}(\mathbb{R}^d_x)}\,,\quad \theta_1 = \frac{\frac{d+4}{d+2}-p}{p\,\frac{2}{d+2}}\,.$$

and (2.15) gives

$$E^{\varepsilon}_{kin}(t) \leqslant C(1+E^{\varepsilon}_{kin}(t)^{2(1-\theta_1)(1-\theta)})$$

and $2(1-\theta_1)(1-\theta) = d\frac{p-1}{p} < 1$ by (A3) (ii). □

We thus obtain a uniform bound for $n^{\varepsilon} \in L^{\infty}(\mathbb{R}_t; L^{\frac{d+4}{d+2}}(\mathbb{R}^d_x))$ from (2.15) and uniform bounds for

$$\int_{\mathbb{R}^d_x\times\mathbb{R}^d_z} |U(x-z)|\,n^{\varepsilon}(x,t)\,n^{\varepsilon}(z,t)\,dz\,dx$$

and

$$\int_{\mathbb{R}^d_x\times\mathbb{R}^d_z} |U(x-z)|\,|\rho^{\varepsilon}(x,z,t)|^2\,dz\,dx$$

in $L^{\infty}(\mathbb{R}_t)$ follow.

Finally we need

LEMMA 2.4: *Let (A3) (i), (iii) hold and assume that $w^{\varepsilon} \in L^{\infty}(\mathbb{R}_t; L^2(\mathbb{R}^d_x\times\mathbb{R}^d_v))$ uniformly as $\varepsilon \to 0$. Then*

$$\Omega^{\varepsilon}[w^{\varepsilon}] = \begin{cases} O(\varepsilon^{d-1-\frac{d}{s}}), & d>1 \\ o(1), & d=1 \end{cases}$$

in $S'(\mathbb{R}^d_x\times\mathbb{R}^d_v\times\mathbb{R}_t)$.

Proof: The assertion for $d = 1$ follows immediately from Lemma 2.1. Thus, we assume $d > 1$ for the following.

At first we observe that the $L^\infty(\mathbb{R}^d)$ part of $U(x)$ gives an $O(\varepsilon^{d-1})$ contribution to $A^\varepsilon(\phi)$ defined in (2.8) (b) and consequently by (2.8) (a) its contribution to $\Omega^\varepsilon[w^\varepsilon]$ in S' is of the same order. Therefore, to complete the proof, it suffices to assume $U \in L^{s,\infty}(\mathbb{R}^d)$ with s as of (A3) (ii).

We denote $Z^\varepsilon(x) := |\varepsilon^{d-1} U(\varepsilon x)|^2$ and estimate the convolution in (2.8b) using the generalized Young inequality:

$$\|\psi * Z^\varepsilon\|_{L^{1/\delta}(\mathbb{R}_x^d)} \leq \|\psi\|_{L^{p_\delta}(\mathbb{R}_x^d)} \|Z^\varepsilon\|_{L^{q,\infty}(\mathbb{R}_x^d)}$$

for $\psi \in L^1(\mathbb{R}_x^d) \cap L^\infty(\mathbb{R}_x^d)$, where $1 < q < \infty$, $0 < \delta < \frac{1}{q}$ and $p_\delta = \frac{q}{q(1+\delta)-1}$. Keeping q fixed and taking δ to zero gives

$$\|\psi * Z^\varepsilon\|_{L^\infty(\mathbb{R}_x^d)} \leq C(\psi) \|Z^\varepsilon\|_{L^{q,\infty}(\mathbb{R}_x^d)} .$$

Since

$$\|Z^\varepsilon\|_{L^{q,\infty}(\mathbb{R}_x^d)} = \varepsilon^{2d-2-\frac{d}{q}} \|U\|^2_{L^{2q,\infty}}$$

we conclude the assertion with $s = 2q$. □

The existence of a unique solution of the Hartree-Fock problem (or, equivalently, the Wigner-Hartree-Fock system) for $\varepsilon > 0$ can easily be shown by generalizing the methods of [CG]. Details are left to the reader. The limit $\varepsilon \to 0$ can now be carried out by applying the methods that lead to Theorem IV.5 in [LPa].

THEOREM 2.1: *Let (A1), (A2), (A3) hold. Then, for every sequence $\varepsilon \to 0$ there exists a subsequence (denoted by the same symbol) such that*

$$w_I^\varepsilon \to w_I^0 \geq 0 \quad \text{in } L^2(\mathbb{R}_x^d \times \mathbb{R}_v^d) \text{ weakly}, \tag{2.17a}$$

$$w^\varepsilon \to w^0 \geq 0 \quad \text{in } L^\infty(\mathbb{R}_t ; L^2(\mathbb{R}_x^d \times \mathbb{R}_v^d)) \text{ weak-}*, \tag{2.17b}$$

$$n^\varepsilon \to n^0 = \int w^0 \, dv \quad \text{in } L^\infty(\mathbb{R}_t ; L^{\frac{d+4}{d+2}}(\mathbb{R}_x^d)) \text{ weak-}*, \tag{2.17c}$$

$$J^\varepsilon \to J^0 = \int v w^0 \, dv \quad \text{in } L^\infty(\mathbb{R}_t ; L^{\frac{d+4}{d+3}}(\mathbb{R}_x^d)) \text{ weak-}*, \tag{2.17d}$$

$$\nabla V_H^\varepsilon \to \nabla V_H^0 = \int_{\mathbb{R}^d} \nabla_z U(x-z) \, n^0(z,t) \, dz \quad \text{in} \quad L^\infty(\mathbb{R}_t ; L^2(\mathbb{R}_x^d)) \text{ weak-}*, \tag{2.17e}$$

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

$$w_t^0 + v \cdot \nabla_x w^0 - \nabla_x V_H^0 \cdot \nabla_v w^0 = 0 \quad \text{in } \mathbb{R}_x^d \times \mathbb{R}_v^d \times \mathbb{R}_t \tag{2.18a}$$

$$w^0(t=0) = w_I^0 . \tag{2.18b}$$

Remark 2.1: The important case of the Coulomb interaction in 3 dimensions

$$U(x) = \frac{1}{|x|}, \quad x \in \mathbb{R}^3 \tag{2.19}$$

is contained in the assumptions. We then have $q = \frac{3}{2}$ and $s = 3$ in (A3). The limiting problem (2.18), (2.17c), (2.17e) is the Vlasov-Poisson equation [LPe], [LPa].

Remark 2.2: The case of the Poisson interaction $U(x) = |x|$ in 1 dimension is not included because of (A3) (iii), which was imposed in order to be able to treat the (relatively uninteresting) 1-dimensional case analogously to the case $d > 1$. However, the assumption $U \in C_b(\mathbb{R})$ can easily be replaced by at most polynomial growth at ∞ and continuity at 0.

Remark 2.3: Both the attractive case ($U \leqslant 0$) and the repulsive case ($U \geqslant 0$) are covered by Theorem 2.1.

Remark 2.4: The cases of ε-independent occupation probabilities λ_l^ε and of finitely many states (i.e. $\lambda_l^\varepsilon = 0$ for $l > N$) is not included because of (A1) (iii). While it can be dealt with rather easily in the Hartree case with a smooth interaction potential U (cf. [LPa]), it creates difficulties for the Hartree-Fock problem when the complete semiclassical information is sought. Then the Schrödinger problem (1.1) has to be dealt with as a fully coupled system of N equations and methods as presented in [GMMP] have to be applied (passage to the semiclassical limit in the Wignermatrix of the Schrödinger system). Serious mathematical difficulties then occur at points in (x, t)-space where the spectral decomposition of the Hartree interaction potential matrix V_{lj}^ε degenerates. To our knowledge, this problem has not been solved yet.

However, the semiclassical limit of $w^\varepsilon(t)$ (and consequently of $n^\varepsilon(t)$ and $J^\varepsilon(t)$) can still be computed. Therefore, assume that $U \in C^{1,\beta}(\mathbb{R})$ for some $0 < \beta \leqslant 1$. A simple modification of the proof of Lemma 2.1 shows that (2.8a) also holds with

$$A^\varepsilon(\varphi) = 2\left(\|\psi\|_{L^1(\mathbb{R}_x^d)} \sup_x \int_{\mathbb{R}_y^d} \psi(x+y)\, |\varepsilon^{d-1}(U(\varepsilon y) - U(0))|^2\, dy \right)^{1/2}.$$

Thus, by the regularity of U and since $\nabla U(0) = 0$ we obtain

$$A^\varepsilon(\phi) = O(\varepsilon^{d+\beta}) \quad \text{in } S(\mathbb{R}_x^d \times \mathbb{R}_v^d). \tag{2.20}$$

Instead of the uniform bound on $\frac{1}{\varepsilon^d} \sum_{l=1}^\infty (\lambda_l^\varepsilon)^2$ in (iii) assume now that $\sum_{l=1}^\infty (\lambda_l^\varepsilon)^2$ is bounded uniformly in ε (e.g. finitely many states only). Lemma 2.3 then implies $\|w^\varepsilon(t)\|_{L^2(\mathbb{R}_x^d \times \mathbb{R}_v^d)} = O\left(\frac{1}{\varepsilon^d}\right)$ and Lemma 2.1 (with (2.20) instead of (2.8b)) gives

$$\Omega^\varepsilon[w^\varepsilon] = O(\varepsilon^\beta) \quad \text{in } S'(\mathbb{R}_x^d \times \mathbb{R}_v^d).$$

The other terms in (2.5a) and (2.5c) can be taken to the limit as in [LP]. Thus, Theorem 2.1 also applies for smooth interaction potential (instead of (A3)) without the uniform L^2-bound on w^ε, however the topologies for the limit process (2.17) have to be changed accordingly.

3. ASYMPTOTIC BEHAVIOUR AS $t \to \infty$ IN THE REPULSIVE CASE

In this section we investigate the time decay properties of the Hartree-Fock-System (2.5). We shall assume vanishing external potential $V_E \equiv 0$.

Also, we assume that a global unique strong solution of the Hartree-Fock-System exists. The assumptions of the previous section are sufficient for this; we remark that the (A1) (iii) can be weakened. In addition we impose the following assumptions on the interaction potential:

(A3) (iv) $U = U_0(|x|) \geq 0$.

(v) $U_0'(r) \leq -\frac{\alpha}{r} U_0(r), \quad r > 0, \alpha > 0$.

Also, for the sake of clarity of the presentation we consider the case $d \geq 2$.

Note that results along the lines of the ones presented below entirely based on the Schrödinger formalism restricted to the $3d$ Coulomb case and finitely many coupled states can be found in [DF, P]. Decay results for the Hartree case with Coulomb interaction can be found in [ILZ].

We state

LEMMA 3.1: *The following relation holds:*

$$0 \leq \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |x - vt|^2 \, w^\varepsilon(t) \, dx \, dv \leq \begin{cases} c(1 + t^{2-\alpha}), & \alpha < 2 \\ c, & \alpha \geq 2 \end{cases} \tag{3.1}$$

with c independent of t.

Proof: Using the equation (2.5a) we obtain

$$\frac{d}{dt} \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |x - vt|^2 \, w^\varepsilon(t) \, dx \, dv$$

$$= - \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |x - vt|^2 \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv$$

$$= 2\, t \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} x \cdot v \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv$$

$$- t^2 \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |v|^2 \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv \, .$$

An easy but tedious calculation gives

$$2\, t \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} x \cdot v \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv =$$

$$t \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} z \cdot \nabla U(z) \{ n^\varepsilon(x - z) \, n^\varepsilon(x) - |\rho^\varepsilon(x - z, x)|^2 \} \, dz \, dx \, .$$

Now, combining the energy conservation (2.10) with $V_E \equiv 0$ and (2.11) gives

$$\frac{d}{dt} \left[\frac{1}{2} \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |v|^2 \, w^\varepsilon \, dx \, dv + \frac{1}{2} \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} U(x - z) \{ n^\varepsilon(x) \, n^\varepsilon(z) - |\rho^\varepsilon(x, z)|^2 \} \, dx \, dz \right] = 0 \, .$$

With the relation

$$\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} v^2 \, w^\varepsilon \, dx \, dv + \frac{1}{2} \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |v|^2 \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv = 0 \, , \tag{3.2}$$

obtained by multiplying the equation (2.5a) by $\frac{1}{2}|v|^2$ and integrating over $\mathbb{R}_x^d \times \mathbb{R}_v^d$, we conclude

$$-t^2 \int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} |v|^2 \{\Theta^\varepsilon[V_H^\varepsilon]\, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon]\}\, dx\, dv$$

$$= -t^2 \frac{d}{dt}\int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} U(x-z)\{n^\varepsilon(x)\, n^\varepsilon(z) - |\rho^\varepsilon(x,z)|^2\}\, dx\, dz\,.$$

Therefore

$$\frac{d}{dt}\left[\int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} |x-vt|^2\, w^\varepsilon\, dx\, dv + g(t)\right]$$

$$= + t\int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} (x-z)\,\nabla U(x-z)\{n^\varepsilon(x)\, n^\varepsilon(z) - |\rho^\varepsilon(x,z)|^2\}\, dx\, dz + \frac{2}{t}\, g(t)$$

with

$$g(t) = t^2 \int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} U(x-z)\{n^\varepsilon(x)\, n^\varepsilon(z) - |\rho^\varepsilon(x,z)|^2\}\, dx\, dz$$

holds. Using the assumptions on the interaction potential we have

$$x\cdot\nabla_x U + \alpha U = r\cdot U'(r) + \alpha U \leqslant 0\,.$$

We obtain

$$\frac{d}{dt}\left[\int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} |x-vt|^2\, w^\varepsilon\, dx\, dv + g(t)\right] \leqslant \begin{cases} \dfrac{2-\alpha}{t}\, g(t), & \alpha < 2 \\ 0, & \alpha \geqslant 2\,. \end{cases} \tag{3.3}$$

It is (again an easy but tedious calculation)

$$0 \leqslant \sum_{i=1}^{\infty} \lambda_i^\varepsilon \|(x + i\varepsilon t\nabla_x)\, \psi_i^\varepsilon(x,t)\|^2_{L^2(\mathbb{R}_x^d)} = \int_{\mathbb{R}_x^d}\int_{\mathbb{R}_v^d} |x-vt|^2\, w^\varepsilon\, dx\, dv\,.$$

Therefore we can apply Gronwall's lemma to (3.3) and arrive at (3.1). □

We need also

LEMMA 3.2: *Let* $V_E \equiv 0$ *and* $\sum_{i=1}^{\infty} \lambda_i^\varepsilon \|x\varphi_i^\varepsilon\|_{L^2(\mathbb{R}_x^d)} < \infty$. *The estimate*

$$\sum_{i=1}^{\infty} \lambda_i^\varepsilon \|x\psi_i^\varepsilon(t)\|_{L^2(\mathbb{R}_x^d)} < \infty$$

holds for the wavefunctions corresponding to the solution of problem (2.5).

Proof: It is

$$\sum_{i=1}^{\infty} \lambda_i^\varepsilon \|x\psi_i^\varepsilon(x,t)\|^2_{L^2(\mathbb{R}_x^d)} = \int_{\mathbb{R}_x^d} |x|^2\, n(x,t)\, dx$$

and

$$\begin{aligned}\frac{d}{dt}\int_{\mathbb{R}_x^d}|x|^2\, n(x,t)\,dx &= 2\int_{\mathbb{R}_x^d} x\cdot J^\varepsilon(x,t)\,dx\\ &= 2\,\varepsilon\,\mathrm{Im}\left\{\sum_{j=1}^{\infty}\lambda_i^\varepsilon\int_{\mathbb{R}_x^d} x\cdot\nabla_x\psi_j^\varepsilon\,\bar\psi_j^\varepsilon\,dx\right\}\\ &\leqslant 2\left[\sum_{i=1}^{\infty}\lambda_i^\varepsilon\,\varepsilon^2\int_{\mathbb{R}_x^d}|\nabla\psi_i^\varepsilon|^2\,dx\right]^{\frac12}\left[\int_{\mathbb{R}_x^d}|x|^2\,n^\varepsilon(x,t)\,dx\right]^{\frac12}\\ &\leqslant 2\sqrt{E^\varepsilon(0)}\,\sqrt{\int_{\mathbb{R}_x^d}|x|^2\,n^\varepsilon(x,t)\,dx}\,.\end{aligned}$$

Then the result follows applying the Gronwall's lemma. □

This result is needed in order to apply the well known.

LEMMA 3.3: *Let $u^\varepsilon\in H^1(\mathbb{R}^d)$ such that $xu^\varepsilon\in L^2(\mathbb{R}^d)$. Then*

$$\|u^\varepsilon\|_{L^p}\leqslant C(p,d)\,\|G(-t)\,u^\varepsilon\|_{L^2}^{a}\,\|(x+i\varepsilon t\nabla_x)\,u^\varepsilon\|_{L^2}^{1-a}\,t^{a-1}\,\varepsilon^{a-1}$$

where $G(t)$ is the unitary group generated by the homogeneous linear Schrödinger equation, $2\leqslant p\leqslant\frac{2d}{d-2}$ and a is given by $1-a=d\left(\frac12-\frac1p\right)$.

The proof of this lemma can be found in [ILZ] or [GV].

At this point we can state our decay result.

THEOREM 3.1: *Under the assumptions of this section the following decay estimates hold:*

(i) $\|n^\varepsilon\|_{L^q(\mathbb{R}_x^d)}=\begin{cases}c(t\varepsilon)^{-2(1-a)}, & \alpha\geqslant 2\\ c(t\varepsilon)^{-\alpha(1-a)}, & \alpha<2\end{cases}$

(ii) $\|J^\varepsilon\|_{L^s(\mathbb{R}_x^d)}=\begin{cases}c(t\varepsilon)^{-(1-a)}, & \alpha\geqslant 2\\ c(t\varepsilon)^{-\frac{\alpha}{2}(1-a)}, & \alpha<2\end{cases}$

(iii) $\|V_H\|_{L^r(\mathbb{R}_x^d)}=\begin{cases}c(t\varepsilon)^{-2(1-a)}, & \alpha\geqslant 2\\ c(t\varepsilon)^{-\alpha(1-a)}, & \alpha<2\end{cases}$

with $1-a=\frac d2\left(1-\frac1q\right)$, $\frac1s=\frac2q+\frac12$, $1+\frac1r=\frac1q+\frac{\alpha}{d}$ and c independent of ε. It is

$$1\leqslant q\leqslant\frac{d}{d-2},\quad 1\leqslant s<\frac{2d}{3d-4}\quad\text{and}\quad\max\left(1,\frac{d}{2d+\alpha}\right)\leqslant r<\frac{d}{\alpha}.$$

Proof: Following [ILZ] and using the Lemmas 3.1-3.3 we estimate

$$\begin{aligned}\|n^\varepsilon(t)\|_{L^{\frac p2}(\mathbb{R}_x^d)}&\leqslant\sum_{i=1}^{\infty}\lambda_i^\varepsilon\,\|\psi_i^\varepsilon\|_{L^p(\mathbb{R}_x^d)}^2\leqslant C(p,d)\,t^{-2(1-a)}\,\varepsilon^{-2(1-a)}\\ &\quad\times\sum_{i=1}^{\infty}\lambda_i^\varepsilon\,\|G(-t)\,\psi_i^\varepsilon(t)\|_{L^2(\mathbb{R}_x^d)}^{2a}\,\|(x+i\varepsilon t\nabla)\,\psi_i^\varepsilon(t)\|_{L^2(\mathbb{R}_x^d)}^{2(1-a)}\\ &\leqslant C(p,d)\,t^{-2(1-a)}\,e^{-2(1-a)}\\ &\quad\times\left(\sum_{i=1}^{\infty}\lambda_i^\varepsilon\,\|\varphi_i^\varepsilon\|_{L^2(\mathbb{R}_x^d)}^2\right)^{a}\left(\sum_{m=1}^{\infty}\lambda_m^\varepsilon\,\|(x+i\varepsilon t\nabla)\,\psi_m^\varepsilon(t)\|_{L^2(\mathbb{R}_x^d)}^2\right)^{1-a}\end{aligned}$$

and the decay result of the density follows. The decay result for the current is obtained using

$$\|J^\varepsilon(t)\|_{L^s(\mathbb{R}^d_x)} \leq \sum_{i=1}^{\infty} \lambda_i^\varepsilon \, \varepsilon \, \|\bar{\psi}_i^\varepsilon \nabla \psi_i^\varepsilon\|_{L^s(\mathbb{R}^d_x)} \leq \sum_{i=1}^{\infty} \lambda_i^\varepsilon \, \varepsilon \, \|\nabla \psi_i^\varepsilon\|_{L^2(\mathbb{R}^d_x)} \, \|\psi_i^\varepsilon\|_{L^{\frac{q}{2}}(\mathbb{R}^d_x)}$$

$$\leq \sqrt{\|n^\varepsilon(t)\|_{L^q(\mathbb{R}^d_x)}} \,,$$

since $\varepsilon \|\nabla \psi_i^\varepsilon\|_{L^2(\mathbb{R}^d_x)}$ is uniformly bounded by the energy conservation (2.10) (with $V_E = 0$). The estimate (iii) follows using the Sobolev inequality

$$\left| \int_{\mathbb{R}^d_y} V_H(y)\, h(y)\, dy \right| \leq \left| \int_{\mathbb{R}^d_y} \int_{\mathbb{R}^d_x} \frac{n^\varepsilon(x)\, h(y)}{|x-y|^\alpha}\, dx\, dy \right| \leq c \|n^\varepsilon\|_{L^q(\mathbb{R}^d_y)} \|h\|_{L^{r'}(\mathbb{R}^d_x)}$$

with $\frac{1}{r'} + \frac{1}{q} + \frac{\alpha}{d} = 2$. Therefore,

$$\|V_H\|_{L^r(\mathbb{R}^d_y)} \leq c \|n^\varepsilon\|_{L^q(\mathbb{R}^d_y)}$$

and the assertion follows. □

4. A DISPERSIVE IDENTITY

Let $x_0 \in \mathbb{R}^d$ fixed with $d > 1$, set $\delta = 0$ or $\delta = 1$ and $\alpha > 0$. Then multiplying (2.5a) by $\frac{v \cdot (x - x_0)}{(\delta + |x - x_0|^\alpha)^{1/\alpha}}$ gives the identity:

$$\int_{T_1}^{T_2} \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_v} w^\varepsilon(x, v, t) \frac{|v|^2 (\delta + |x - x_0|^\alpha) - ((x - x_0) \cdot v)^2 |x - x_0|^{\alpha - 2}}{(\delta + |x - x_0|^\alpha)^{1 + \frac{1}{\alpha}}}\, dv\, dx\, dt$$

$$- \int_{T_1}^{T_2} \int_{\mathbb{R}^d_x} \frac{(x - x_0) \cdot \nabla V_E}{(\delta + |x - x_0|^\alpha)^{1/\alpha}} n^\varepsilon(x, t)\, dx\, dt$$

$$+ \int_{T_1}^{T_2} \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_z} \frac{(x - x_0) \cdot \nabla U(x - z)}{(\delta + |x - x_0|^\alpha)^{1/\alpha}} (|\rho^\varepsilon(x, z, t)|^2 - n^\varepsilon(x, t)\, n^\varepsilon(z, t))\, dz\, dx\, dt$$

$$= \int_{\mathbb{R}^d_x} \frac{(x - x_0)}{(\delta + |x - x_0|^\alpha)^{1/\alpha}} \cdot (J^\varepsilon(x, T_1) - J^\varepsilon(x, T_2))\, dx \tag{4.1}$$

for all $-\infty < T_1 < T_2 < \infty$. Integral identities of this type were obtained in [LPe1] for the free transport equation and in [P] for the Vlasov-Poisson and Wigner-Poisson systems.

A lengthy calculation shows that the first term on the left hand side of (4.1) is nonnegative. For example in the case $d = 3$ and $\delta = 0$ it is equal to

$$\varepsilon^2 \sum_{l=1}^{\infty} \lambda_l^\varepsilon \int_{T_1}^{T_2} \left[\int_{\mathbb{R}^3} \left(\frac{|\nabla \psi_l^\varepsilon(x,t)|^2}{|x-x_0|} - \frac{|(x-x_0)\cdot \nabla \psi_l^\varepsilon(x,t)|^2}{|x-x_0|^3} \right) dx + 8\pi |\psi_l^\varepsilon(x_0,t)|^2 \right] dt \tag{4.2}$$

(see [LPe1] also for the other cases). Assume now that $V_E \equiv 0$ (no exterior field) and that the interaction potential is radial $U = U_0(|x|)$ with $U_0'(r) \leqslant 0$. Then, an easy calculation using $\rho^\varepsilon(x,z,t) = \overline{\rho^\varepsilon(z,x,t)}$ and (2.16) shows that also the third term in (4.1) is nonnegative. Thus, the identity (4.1) gives the bound for the first term on its left hand side:

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

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

$$\varepsilon^2 \sum_{l=1}^{\infty} \lambda_l^\varepsilon \int_{-\infty}^{\infty} \int_{\mathbb{R}^3} \left(\frac{|\nabla \psi_l^\varepsilon(x,t)|^2}{|x-x_0|} - \frac{|(x-x_0)\cdot \nabla \psi_l^\varepsilon(x,t)|^2}{|x-x_0|^3} \right) dx\, dt + \varepsilon^2 \int_{-\infty}^{\infty} n^\varepsilon(x_0,t)\, dt \leqslant C = C(E_{kin}^\varepsilon(0)) \tag{4.3}$$

(just as for the free Schrödinger equation). Similar estimates can be obtained for dimensions different from 3. Other applications of the dispersive identity (4.1) are also possible.

ACKNOWLEDGEMENTS

This research was supported by grant Nr. A7487 of the Natural Science and Engineering Research Council of Canada. The first and the third author were supported by grant Nr. MA 1662/1-1 and 1-2 of the german 'Deutsche Forschungsgemeinschaft'. The last author was supported by grant Nr. P11308-MAT of the austrian 'Found zur Förderung der Wissenschaft und Forschung'. We would like to thank Dr. Raimund Wegener who alerted us to the problems posed by the Hartree Fock systems. I. Gasser, P. A. Markowich and C. Schmeiser would also like to acknowledge the hospitality of the University of Victoria, where this research was started.

REFERENCES

[CG] J. M. CHADAM and R. T. GLASSEY, *Global existence of solutions to the Cauchy problem for time dependent Hartree equations,* J.M.P. 16(5), pp. 1122-1130, 1975.

[DF] J. P. DIAS and M. FIGUEIRA, *Conservation laws and time decay for the solutions of some nonlinear Schrödinger-Hartree equations and systems,* J. Math. Anal. Appl. **84,** pp. 486-508, 1981.

[GMMP] P. GERARD, P. A. MARKOWICH, N. J. MAUSER and F. POUPAUD, *Homogenization limits and Wigner transforms,* Comm. Pure Appl. Math. **50**, No. 4, pp. 323-379, 1997.

[GV] J. GINIBRE and G. VELO, *On a class of nonlinear Schrödinger equations. II. Scattering theory, general case,* J. Funct. Anal. **32,** pp. 33-71, 1979.

[ILZ] R. ILLNER, P. F. ZWEIFEL and H. LANGE, *Uniqueness and asymptotic behaviour of solutions of the Wigner-Poisson and the Schrödinger-Poisson Systems, M^2AS* **17,** pp. 349-376, 1994.

[LPa] P. L. LIONS et T. PAUL, *Sur les mesures de Wigner,* Revista Matematica Iberoamericana 9, pp. 553-618, 1993.

[LPe] P. L. LIONS et B. PERTHAME, *Global solutions of Vlasov-Poisson type equations,* preprint n. 8824, Ceremade, 1995.

[LPe1] P. L. LIONS et B. PERTHAME, *Lemme de moments, de moyenne et de dispersion,* C. R. Acad. Sci. Paris, 314, Serie 1, pp. 801-806, 1992.

[M] P. A. MARKOWICH, *On the equivalence of the Schrödinger and the Quantum Liouville equation, M^2AS* 11, pp. 459-469, 1989.

[MM] P. A. MARKOWICH and N. J. MAUSER, *The classical limit of a self-consistent quantum-Vlasov equation in 3d, M^3AS* 3, pp. 109-124, 1993.

[P] B. PERTHAME, *Time decay, propagation of low moments and dispersive effects of kinetic equations,* Com. PDE **21**, No. 3-4, pp. 659-686, 1996.

[RS] M. REED and B. SIMON, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness,* Academic Press, New York, 1975.

[S] J. C. SLATER, *A simplification of the Hartree-Fock method,* Phys. Rev. 81(3), pp. 385-390, 1951.

[W] E. WIGNER, *On the Quantum Correction for the Thermodynamic Equilibrium,* Phys. Rev. **40,** pp. 749-759, 1932.