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

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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 $\psi_l^\varepsilon$, $n^\varepsilon$ is the number density of the considered particle system, $V_H^\varepsilon$ is the self-consistent Hartree potential (defined by the interaction potential $U = U(x)$), $V_E^\varepsilon$ represents a given exterior potential and $V_{lj}^\varepsilon$ stands for the interaction of the $l$-th and $j$-th state.

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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 $V^{\varepsilon}_{lj} := 0$).

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 $\rho^{\varepsilon}$ 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 $\eta$, 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 $v$:

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

$\Omega^\varepsilon$ 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*

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

*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

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

We estimate

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

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 $w^\varepsilon$:

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 $\varphi_l^\varepsilon$, $\varphi_k^\varepsilon$ 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 $J^\varepsilon$ 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 $w^\varepsilon$ 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 $\delta$ 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 $\infty$ 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 $\varepsilon$-independent occupation probabilities $\lambda_l^\varepsilon$ 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 $V_{lj}^\varepsilon$ 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 $\varepsilon$ (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 $w^\varepsilon$, 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) $U = U_0(|x|) \geqslant 0$.

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

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

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:*

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

*with c independent of t.*

*Proof:* Using the equation (2.5a) we obtain

$$\begin{aligned} &\frac{d}{dt} \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |x - vt|^2 \, w^\varepsilon(t) \, dx \, dv \\ &= - \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |x - vt|^2 \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv \\ &= 2\, t \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} x \cdot v \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv \\ &\quad - t^2 \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} |v|^2 \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv \,. \end{aligned}$$

An easy but tedious calculation gives

$$\begin{aligned} &2\, t \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} x \cdot v \{ \Theta^\varepsilon[V_H^\varepsilon] \, w^\varepsilon + \Omega^\varepsilon[w^\varepsilon] \} \, dx \, dv = \\ &t \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_v^d} z \cdot \nabla U(z) \{ n^\varepsilon(x - z) \, n^\varepsilon(x) - |\rho^\varepsilon(x - z, x)|^2 \} \, dz \, dx \,. \end{aligned}$$

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

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

It is (again an easy but tedious calculation)

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

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

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

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 $1-a=\frac{d}{2}\left(1-\frac1q\right)$, $\frac1s=\frac2q+\frac12$, $1+\frac1r=\frac1q+\frac{\alpha}{d}$ and $c$ independent of $\varepsilon$. 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

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

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

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

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

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

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

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

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

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 $\dfrac{v\cdot(x-x_0)}{(\delta + |x-x_0|^\alpha)^{1/\alpha}}$ gives the identity:

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

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

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

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

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 $\varepsilon$ 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.

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