Nonlinear Hartree equation as the mean field limit of weakly coupled fermions

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Abstract

We consider a system of N weakly interacting fermions with a real analytic pair interaction. We prove that for a general class of initial data there exists a fixed time T such that the difference between the one particle density matrix of this system and the solution of the non-linear Hartree equation is of order N^{-1} for any time $t \leq T$.

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1 Introduction

The Hartree-Fock theory is a fundamental tool in atomic physics, chemistry, plasma physics and many areas of quantum physics. It is also an important numerical instrument to calculate atomic and molecular structures. Despite numerous applications of the Hartree-Fock theory, many basic theoretical questions remain unsolved. One area where significant progress was made concerns the ground state energy of large atoms and molecules. Consider the simple case of a neutral atom with

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nuclear charge Z. It was first proved by Lieb and Simon [10, 11] that the Hartree-Fock theory gives the correct asymptotic energy to the leading order $Z^{7/3}$ as $Z \to \infty$. The next important step came more than a decade later as Bach [1] proved that the error between the Hartree-Fock and the true atomic energy is less than $Z^{5/3-\delta}$ for some small $\delta > 0$. Similar result with a very different method was announced in [4] and was proved in [5].

The goal of this paper is to justify a time-dependent mean-field theory for the evolution of interacting fermions under a weak pair interaction with initial data localized in a cube of size of order one. The last restriction actually provides the length scale of the system. The interaction potential varies on the same length scale. While one might want to add a background potential, we shall keep the model simple to focus on the many-body interaction effect. We work in $d = 3$ dimensions, but our result holds in any dimension. The Hamiltonian describing such a system is given by

$$H_N := -\frac{\varepsilon^2}{2}\sum_{j=1}^{N}\Delta_{x_j} + \frac{1}{N}\sum_{j,k} U(x_j - x_k) \tag{1.1}$$

acting on $\bigwedge_1^N L^2(\mathbb{R}^3)$, and the Schrödinger equation is given by

$$i\varepsilon\partial_t\psi_t = H_N\psi_t\ . \tag{1.2}$$

Here we have chosen the strength of the interaction between fermions to be of order $1/N$. Examples of such systems with a small coupling constant can be found in astrophysics and plasma physics. For gravitating systems, the strength of the interaction is dictated by the gravitational constant and thus the mean field approximation is suitable. The Coulomb singularity, however, is difficult to control. If one wishes to use (1.1) to model the dynamics of white dwarfs, the kinetic energy has to be further modified to be the relativistic one, according to the famous observation by Chandrasekhar [3], see a rigorous account in [13]. For the plasma physics application, the weak pair potential models combined electron-electron and electron-background interactions.

From now on we will fix a particular relation between ε and N, which is motivated by the following argument. We model a system of N fermions at energy comparable with the ground state energy of the system. The potential energy per particle is of order one. It is well-known that the kinetic energy per particle of N fermions, i.e., $-\frac{1}{2}\varepsilon^2\Delta_{x_j}$, in a cube of size one scales like $\varepsilon^2 N^{2/3}$ in the ground state. In order to keep the kinetic energy per particle of order one, we need to choose $\varepsilon = N^{-1/3}$, a convention we shall use for the rest of this paper. With this choice, the kinetic and the potential energy per particle in H_N are comparable. This is the basic physical criterion to obtain a limiting dynamics (as $N \to \infty$) that captures the nonlinear effect of the interaction. Notice that we have kept the free evolution in the form of $i\varepsilon\partial_t\psi = -\frac{1}{2}\varepsilon^2\Delta\psi$ so that the free evolution has a limit as $\varepsilon \to 0$. The equation (1.2) is formally semiclassical with a mean-field interaction potential at high density. Our choice of scaling is the same as in [14] and [15]. (The interpretation of the origin of this scaling in [14] is somewhat different.)

In order to take the limit $\varepsilon \to 0$, we need to recast the Schrödinger equation using the density matrix. For any wave function $\psi_{N,t}$, define the corresponding density matrix by $\gamma_{N,t} = \pi_{\psi_{N,t}}$, where $\pi_\psi = |\psi\rangle\langle\psi|$ is the orthogonal projection onto ψ. The kernel of $\gamma_{N,t}$ is then given by

$$\gamma_{N,t}(\mathbf{x}, \mathbf{y}) = \psi_{N,t}(\mathbf{x})\overline{\psi_{N,t}(\mathbf{y})} \, . \tag{1.3}$$

The notation $\mathbf{x}$ typically stands for $\mathbf{x} = (x_1, \ldots, x_N)$. Depending on the context sometimes it may denote a shorter vector of x's.

We recall that a self adjoint operator γ is called *density matrix* if $0 \leq \gamma \leq 1$ and $\mathrm{Tr}\ \gamma = 1$. If the density matrix of the system is a one-dimensional projection then we say the system is in a pure state, otherwise it is in a mixed state. The Schrödinger equation (1.2) is equivalent to the Heisenberg equation for the density matrix:

$$i\varepsilon\partial_t\gamma_{N,t} = [H_N, \gamma_{N,t}] \, , \qquad [A, B] = AB - BA \, . \tag{1.4}$$

The n-particle density matrix, $\gamma_{N,t}^{(n)}$, is defined through its kernel

$$\gamma_{N,t}^{(n)}(x_1, .., x_n; y_1, .., y_n) := \int \mathrm{d}x_{n+1}..\mathrm{d}x_N \ \gamma_{N,t}(x_1, .., x_n, x_{n+1}, .., x_N; y_1, .., y_n, x_{n+1}, .., x_N) \tag{1.5}$$

for $1 \leq n \leq N$, and $\gamma_{N,t}^{(n)} := 0$ otherwise. Define the Wigner transform of the one particle density matrix in the scale ε by

$$W_N^{(1)}(x; v) := \frac{1}{(2\pi)^3} \int e^{-iv\cdot\eta}\gamma_N^{(1)}\Big(x + \varepsilon\frac{\eta}{2}, x - \varepsilon\frac{\eta}{2}\Big)\mathrm{d}\eta \, . \tag{1.6}$$

Recall the nonlinear Vlasov equation for a phase space density f:

$$\partial_t f_t(x, v) + v \cdot \nabla_x f_t(x, v) = \nabla_x(U \star \varrho_t) \cdot \nabla_v f_t(x, v) \, , \tag{1.7}$$

where

$$\varrho_t(x) := \int f_t(x, v)\mathrm{d}v$$

is the configuration space density. It was proved by Narnhofer and Sewell [14] that $W_N^{(1)}$ converges weakly to a solution of the Vlasov equation (1.7) provided that the Fourier transform of the potential is compactly supported, in particular U is real analytic. The regularity assumption was substantially relaxed by Spohn [15].

Define the Hartree equation for the time dependent one-particle density matrix ω_t by

$$i\varepsilon\partial_t\omega_t = \Big[-\frac{\varepsilon^2}{2}\Delta + U \star \varrho_t, \omega_t\Big] \tag{1.8}$$

where $\varrho_t(x) := \omega_t(x,x)$. Note that the Vlasov equation (1.7) is the semiclassical approximation of (1.8). One can extend this equation to the Hartree-Fock equation by including the exchange term

$$i\varepsilon\partial_t\omega_t = \Big[-\frac{\varepsilon^2}{2}\Delta + U \star \varrho_t, \omega_t \Big] - \int \Big[U(x-z) - U(y-z) \Big] \omega_t(x,z)\omega_t(z,y) \mathrm{d}z \ . \tag{1.9}$$

Our main result proves that the Hartree equation correctly describes the evolution of the Schrödinger equation (1.4) up to order $O(\varepsilon)$. More precisely, it states that for short semiclassical time the difference between the Wigner transform $W^{(1)}_{N,t}$ of the solution to the Schrödinger equation (1.4) and the Wigner transform of the solution of the Hartree equation (1.8) is of order $O(\varepsilon^3)$ provided that the potential U is real analytic. In other words, all ε^2 corrections come from the difference between the Vlasov equation (1.7) and the Hartree equation (1.8); hence they are related to the accuracy of the semiclassical approximation in the one-body theory. In particular we show that all correlation effects are of order at most $O(\varepsilon^3)$.

In fact, the main correlation effect, the exchange term, is expected to be order ε^3 for smooth potential and ε^2 for the Coulomb potential. Our interpretation of the Hartree-Fock equation resembles the theory concerning the ground state energy for atoms where the Hartree-Fock theory is proved to be correct up to $\varepsilon^{2+\delta}$ smaller than the leading term [1]. The analyticity condition and the short time restriction of our result is unsatisfactory; it nevertheless shows what the correct formulation of the time-dependent Hartree and Hartree-Fock theories should be.

In order to see the effects of the exchange term, i.e. to show that (1.9) approximates the quantum dynamics even better than (1.8), we would need to consider ε^3 correction for the smooth case or the ε^2 correction for the Coulomb potential. Notice that our approach is perturbative and in principle all ε^3 corrections, including the exchange terms, can be calculated. However, there are other sources of ε^3 corrections (see the last two terms in (4.15) in Section 4) which make the exchange correction less prominent. This should be compared with the Coulomb case where all ε^2 corrections are expected to be from the semiclassical approximation to the Hartree equation and the exchange terms.

In a recent paper Graffi et al. [8] proved the convergence of the Wigner transform $W^{(1)}_N$ (of the solution of the Heisenberg equation (1.4)) to the solution of the Vlasov equation under the assumption that the initial wave function is of the semiclassical form $\psi = Ae^{iS/\varepsilon}$. The result also provided error control and the proof is carried out by concise inequalities as opposed to weak convergence method in [14] and [15]. The main restriction is the initial wave functions to be of the semiclassical form. Although this type of wave functions is suitable for bosons, fermionic wave functions are antisymmetric and thus vanish frequently. Notice that in the neighborhood of the zero set of the wave functions, the semiclassical approximation is difficult to apply. In particular, one naive attempt (for fermionic case) is to choose S symmetric and A antisymmetric. But $\int |\nabla A|^2$ will be of order $N^{3/5}$ and this violates a key assumption in this paper.

The recent work of Bardos et al. [2] considers the equation

$$i\partial_t\psi_{N,t} = \Bigg(-\alpha\sum_{j=1}^N \Delta_{x_j} + \frac{1}{N}\sum_{j,k} U(x_j - x_k) \Bigg) \psi_{N,t} \tag{1.10}$$

with an arbitrary $\alpha > 0$ (we have put $\hbar = 1$ which is a constant of order one in this paper). In the limit $N \to \infty$, it was proved that the difference between the one-particle density matrix $\gamma_{N,t}^{(1)} = |\psi_{N,t}\rangle\langle\psi_{N,t}|$ and the solution to the corresponding time-dependent Hartree-Fock equation vanishes in the trace norm provided that the initial data is a Slater determinant (and some other assumptions). Notice that the time scale in (1.10) is of order $\varepsilon = N^{-1/3}$ smaller than (1.2). Thus for initial data considered in [14] [15] and the present article, the one particle dynamics of (1.10) is governed by a free evolution; the effect of the interaction given by U vanishes in the limit $N \to \infty$. We shall make a more detailed comparison in Section 3.

Finally we comment on the method. Our approach is to based on the BBGKY hierarchy and iteration scheme. There are two major elements in the proof. The first one is the control of error term. Since we work on the BBGKY hierarchy for finite N, we need to control the error term in the iteration scheme. Here we used that the trace norm of the density matrix is preserved. The second observation concerns the combinatorics. As usual, the BBGKY hierarchy will produce a $n!$ factor under iteration. However, in the setting of this paper, there are extra sources of $n!$, for example, we will need to take high moments of the interaction:

$$\int |\hat{U}(\xi)||\xi|^m \mathrm{d}\xi \sim C^m m! \tag{1.11}$$

See (1.11) for precise assumption. Since time ordered integration provides only a $1/n!$, we will have to prove that the combined effects of the factorials from all sources is just a single $n!$. See the proof of Lemma 4.1 for details.

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2 Notations

We first fix the notations and recall some definitions. The n-particle density matrix $\gamma_{N,t}^{(n)}$ is defined through the equation (1.5) and clearly satisfies the following normalization

$$\mathrm{Tr}\, \gamma_{N,t}^{(n)} = 1\,. \tag{2.1}$$

It is well-known that the one particle density matrix satisfies the following operator inequality (see [9])

$$0 \leq \gamma_{N,t}^{(1)} \leq \frac{1}{N}\,. \tag{2.2}$$

Therefore, we can write $\gamma_{N,t}^{(1)}$ as

$$\gamma_{N,t}^{(1)} = \frac{1}{N}\sum_{j=1}^{\infty} a_j \pi_j$$

where π_j is the orthogonal projection onto φ_j, and where $a_j \in [0,1]$ for all $j \in \mathbb{N}$ with $\sum_{j=1}^{\infty} a_j = 1$. Note that in the definition of the n-particle density matrices we followed the convention that the trace of the density matrices is normalized. In standard N-body theory an additional $N(N-1)\dots(N-n+1)$ factor would be present in (1.5).

2.1 Wigner Transform

The Wigner transform of an N-body density matrix $\gamma_N(\mathbf{x};\mathbf{y})$ is defined by

$$w_N(\mathbf{x};\mathbf{v}) := \frac{1}{(2\pi)^{3N}} \int e^{-i\mathbf{v}\cdot\mathbf{y}} \gamma_N\Big(\mathbf{x} + \frac{\mathbf{y}}{2}, \mathbf{x} - \frac{\mathbf{y}}{2}\Big) \mathrm{d}\mathbf{y}\ . \tag{2.3}$$

From $\mathrm{Tr}\ \gamma_N = 1$ it follows that

$$\int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v}\, w_N(\mathbf{x},\mathbf{v}) = 1. \tag{2.4}$$

Since the velocities of the N particles are of order $N^{1/3} = \varepsilon^{-1}$, we rescale the Wigner transform w_N so that its arguments be typically of order one. Thus we defined the rescaled Wigner transform by

$$W_{N,\varepsilon}(\mathbf{x},\mathbf{v}) = W_N(\mathbf{x},\mathbf{v}) := \varepsilon^{-3N} w_N(\mathbf{x},\mathbf{v}/\varepsilon) = \frac{1}{(2\pi)^{3N}} \int \mathrm{d}\mathbf{y}\ \gamma_N\Big(\mathbf{x} + \frac{\varepsilon\mathbf{y}}{2}, \mathbf{x} - \frac{\varepsilon\mathbf{y}}{2}\Big) e^{-i\mathbf{v}\cdot\mathbf{y}}. \tag{2.5}$$

The factor ε^{-3N} guarantees that the normalization (2.4) holds for the rescaled Wigner transform $W_{N,\varepsilon}(\mathbf{x},\mathbf{v})$ as well. The inverse transform is given by

$$\gamma_N(\mathbf{x},\mathbf{y}) = \int W_{N,\varepsilon}\Big(\frac{\mathbf{x}+\mathbf{y}}{2}, \mathbf{u}\Big) e^{i(\mathbf{x}-\mathbf{y})\cdot\mathbf{u}/\varepsilon} \mathrm{d}\mathbf{u}.$$

In particular, the particle density at the point $\mathbf{x}$ is given by

$$\rho(\mathbf{x}) := \gamma_N(\mathbf{x},\mathbf{x}) = \int W_{N,\varepsilon}(\mathbf{x},\mathbf{u})\mathrm{d}\mathbf{u}.$$

In this paper, we are concerned with the rescaled Wigner transform only, so we shall drop the adjective "rescaled" and the ε index from the notation. The rescaling parameter ε will always be related to the total number of particles as $\varepsilon = N^{-1/3}$.

The time evolution of the Wigner transform $W_N(\mathbf{x},\mathbf{v})$ is given by the Wigner equation

$$\begin{aligned} \partial_t W_N(t;\mathbf{x},\mathbf{v}) &+ \sum_{j=1}^{N} v_j \cdot \nabla_{x_j} W_N(t;\mathbf{x},\mathbf{v}) \\ &= -\frac{i\varepsilon^2}{(2\pi)^{3N}} \int \Big[U\Big(\mathbf{x} + \frac{\varepsilon\mathbf{y}}{2}\Big) - U\Big(\mathbf{x} - \frac{\varepsilon\mathbf{y}}{2}\Big)\Big] e^{i\mathbf{y}\cdot(\mathbf{u}-\mathbf{v})} W_N(t;\mathbf{x},\mathbf{u}) \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{y}, \end{aligned} \tag{2.6}$$

which can be easily derived from the Heisenberg equation (1.4).

It is tempting to consider the Wigner transform as a probability density on the phase space. The problem with this interpretation is that $W_N(\mathbf{x},\mathbf{v})$ is not positive. In order to make the Wigner transform positive we may take convolutions with Gaussian distributions. We can define the *Husimi function* by

$$H_N^{\delta_1,\delta_2} := W_N \star_x G_{\delta_1}^{(N)} \star_v G_{\delta_2}^{(N)}$$

where $\star_x$ denotes the convolution in x-space and

$$G_\delta^{(N)}(\mathbf{z}) := \frac{1}{(\pi\delta^2)^{3N/2}} \exp\Big(-\frac{\mathbf{z}^2}{\delta^2}\Big)$$

is the centered Gaussian distribution in $3N$ dimensions with variance δ. It is easy to check that $H_N^{\delta_1,\delta_2} \geq 0$ if $\delta_1\delta_2 \geq \varepsilon$. The Husimi function is normalized according to

$$\int H_N^{\delta_1,\delta_2}(\mathbf{x},\mathbf{v})\,\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v} = \|\psi_N\|_2^2 = 1$$

and thus can be considered as a probability density on the phase space. The accuracy of the $H_N^{\delta_1,\delta_2} \geq 0$ is of order δ_1 for the space variables and δ_2 for the velocity variables in semiclassical units.

As a side remark, we recall that for $\delta_1 := \delta$, $\delta_2 := \varepsilon\delta^{-1}$ the Husimi function is just the standard *Gaussian coherent state* at scale δ:

$$H_N^{\delta,\varepsilon\delta^{-1}}(\mathbf{x},\mathbf{v}) = C_{N,\delta}(\mathbf{x},\mathbf{v}) := (2\pi\varepsilon)^{-3N}\langle\psi_N, \pi_{\mathbf{x},\mathbf{v}}^\delta\psi_N\rangle$$

where $\pi_{\mathbf{x},\mathbf{v}}^\delta = |\phi_{\mathbf{x},\mathbf{v}}^\delta\rangle\langle\phi_{\mathbf{x},\mathbf{v}}^\delta|$ is the orthogonal projection onto the state

$$\phi_{\mathbf{x},\mathbf{v}}^\delta(\mathbf{z}) = \frac{1}{(\pi\delta^2)^{3N/4}} e^{i\mathbf{z}\cdot\mathbf{v}/\varepsilon} \exp\Big(-\frac{(\mathbf{z}-\mathbf{x})^2}{2\delta^2}\Big).$$

The k-particle Wigner transform $W_N^{(k)}$ is defined to be the Wigner transform of the k particle density matrix $\gamma_N^{(k)}$. Clearly, it can be viewed as the k-particle marginal of W_N since it satisfies

$$\begin{aligned} W_N^{(k)}(x_1,\dots x_k; v_1,\dots v_k) =& \frac{1}{(2\pi)^{3k}}\int \mathrm{d}\mathbf{y}\;\gamma_N^{(k)}\Big(\mathbf{x}+\frac{\varepsilon\mathbf{y}}{2};\mathbf{x}-\frac{\varepsilon\mathbf{y}}{2}\Big)\,e^{-i\mathbf{v}\cdot\mathbf{y}} \\ =& \int W_N(x_1,\dots x_N; v_1,\dots v_N)\mathrm{d}x_{k+1}\dots\mathrm{d}x_N\mathrm{d}v_{k+1}\dots\mathrm{d}v_N \end{aligned} \tag{2.7}$$

The $W_N^{(k)}$ are normalized as

$$\int W_N^{(k)}(\mathbf{x},\mathbf{v})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v} = 1.$$

Notice this definition is consistent with the definition (1.6). We now give some examples of N particle wave functions.

2.2 Some Examples

One of the most important assumptions of our results is that the n-particle Wigner transform $W_N^{(n)}$ of the initial state is factorized in the limit $N \to \infty$. At first glance this assertion might seem surprising, since we are dealing with a system of fermions. In the following we present some typical situation where this condition is indeed fulfilled and we show a very atypical example where factorization is wrong.

The standard examples of many-body fermionic states are the Slater determinants and the quasifree states.

1. Slater determinants. For any orthonormal family $\{\varphi_j, j = 1, \dots, N\}$ define the determinant wave function

$$\psi(\mathbf{x}) = \Big(\bigwedge_{j=1}^{N} \varphi_j \Big)(\mathbf{x}) := \frac{1}{\sqrt{N!}} \sum_{\sigma \in S_N} \operatorname{sgn}(\sigma) \prod_{j=1}^{N} \varphi_j(x_{\sigma_j}) \, .$$

The one particle density matrix is given by

$$\gamma^{(1)}(x, x') = \frac{1}{N} \sum_{j=1}^{N} \varphi_j(x) \overline{\varphi_j(x')} \, .$$

The two-particle density matrix is

$$\begin{aligned} \gamma^{(2)}(x, y, x', y') &= \frac{1}{2N(N-1)} \sum_{k,\ell=1}^{N} \Big[\varphi_k(x)\varphi_\ell(y) - \varphi_k(y)\varphi_\ell(x) \Big] \overline{\Big[\varphi_k(x')\varphi_\ell(y') - \varphi_k(y')\varphi_\ell(x') \Big]} \\ &= \frac{N}{N-1} \Big[\gamma^{(1)}(x, x')\gamma^{(1)}(y, y') - \gamma^{(1)}(x, y')\gamma^{(1)}(y, x') \Big]. \end{aligned} \tag{2.8}$$

2. Quasifree states. An N-particle state ω is called quasifree, if its k-particle density matrices factorize by Wick theorem

$$\omega^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) = \frac{N^k}{N(N-1)\dots(N-k+1)} \det(\omega^{(1)}(x_j, y_j))_{j=1,\dots,k} \, .$$

The unusual prefactor is present due to our choice of normalization. In particular, quasifree states are characterized by their one particle marginals. For example, Slater determinants are pure quasifree states.

The concept of quasifree state can be generalized to grand canonical states with an indefinite particle number. In particular, any normalized density matrix γ on $L^2(\mathbb{R}^3)$, can be realized as a fermionic quantum state whose one particle density matrix is γ. The state can have expected particle number up to $1/\|\gamma\|$. In fact, with $N := \int \mathrm{d}x \mathrm{Tr}\,(\omega a_x^\dagger a_x)$ we have $\gamma(x, y) = N^{-1} \mathrm{Tr}\,(\omega\, a_x^\dagger a_y)$, where $a_x^\dagger$, a_x are fermionic creation and annihilation operators. Thus, for any $\psi \in L^2(\mathbb{R}^3)$,

$$\langle \psi, \gamma\psi \rangle = \frac{1}{N} \mathrm{Tr}\,(\omega a_\psi^\dagger a_\psi) = -\frac{1}{N} \mathrm{Tr}\,(\omega a_\psi a_\psi^\dagger) + \frac{\|\psi\|^2}{N} \le \frac{\|\psi\|^2}{N}, \tag{2.9}$$

where the operators a_ψ and $a^\dagger_\psi$ annihilate and, respectively, create a fermion in the state ψ.

Example 1: Let $\Omega := [0, 2\pi]^3$ and consider the states $\varphi_k(x) = (2\pi)^{-3/2}\, e^{ikx}\chi(x \in \Omega)$ with $|k| \le cN^{1/3}$, $k \in \mathbb{Z}^3$. The number of states is $O(N)$. We consider the pure state $\Psi = \bigwedge \varphi_k$ of the N particle system and we compute the marginals of its Wigner transform. The one particle density matrix is given by

$$\begin{aligned}\gamma^{(1)}(x, x') &= \frac{1}{N} \sum_{k:|k|<cN^{1/3}} \varphi_k(x)\overline{\varphi_k(x')} \\ &= \frac{1}{N} \frac{\chi(x, x' \in \Omega)}{(2\pi)^3} \sum_{k:|k|<cN^{1/3}} e^{ik(x-x')} \sim \chi(x, x' \in \Omega) f((x - x')N^{1/3})\end{aligned} \tag{2.10}$$

with some decaying function f, such that $f(0) = 1$. Its Wigner transform with rescaling parameter $\varepsilon = N^{-1/3}$ is

$$W^{(1)}(x, v) = \frac{\chi(x \in \Omega)}{(2\pi)^6 N} \sum_{k:|k|\le cN^{1/3}} \int dy\; e^{i\varepsilon k y} e^{-ivy} \rightharpoonup \frac{1}{(2\pi)^3}\, \chi(x \in \Omega)\chi(|v| \le c)$$

when $N \to \infty$. Using (2.8) the two particle density matrix can be computed as well. Its Wigner transform is given by

$$\begin{aligned}W^{(2)}(\mathbf{x}, \mathbf{v}) = \frac{N}{(2\pi)^6(N-1)} \int \mathrm{d}\mathbf{y}\; e^{-i\mathbf{v}\cdot\mathbf{y}} \Big\{ &\gamma^{(1)}\left(x_1 + \frac{\varepsilon y_1}{2}, x_1 - \frac{\varepsilon y_1}{2}\right) \gamma^{(1)}\left(x_2 + \frac{\varepsilon y_2}{2}, x_2 - \frac{\varepsilon y_2}{2}\right) \\ &- \gamma^{(1)}\left(x_1 + \frac{\varepsilon y_1}{2}, x_2 - \frac{\varepsilon y_2}{2}\right) \gamma^{(1)}\left(x_2 + \frac{\varepsilon y_2}{2}, x_1 - \frac{\varepsilon y_1}{2}\right) \Big\}\end{aligned} \tag{2.11}$$

Notice that the first term is $W^{(1)}(x_1, v_1)W^{(1)}(x_2, v_2)$ after neglecting the error $N/(N-1) \cong 1$.

The second term is the so called exchange term and it vanishes as $N \to \infty$. By (2.10) this term can be written as

$$W^{(2)}_{\mathrm{ex}}(\mathbf{x}, \mathbf{v}) \cong \frac{\chi(x_1, x_2 \in \Omega)}{(2\pi)^{12} N^2} \sum_{k,\ell} \int \mathrm{d}\mathbf{y}\; e^{-i\mathbf{v}\cdot\mathbf{y}} e^{ik(x_1-x_2)+ik\varepsilon(y_1+y_2)}\, e^{i\ell(x_2-x_1)+i\ell\varepsilon(y_1+y_2)} \tag{2.12}$$

Thus, for an arbitrary function $J(\mathbf{x}, \mathbf{v}) = J_1(\mathbf{x})J_2(\mathbf{v})$ we have

$$\begin{aligned}&\int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v} J(\mathbf{x}, \mathbf{v}) W^{(2)}_{\mathrm{ex}}(\mathbf{x}, \mathbf{v}) \\ &\qquad = \frac{1}{(2\pi)^{12} N^2} \sum_{k,\ell=1}^{N} \int_\Omega \mathrm{d}\mathbf{x} J_1(x_1, x_2)\; e^{i(k-\ell)(x_1-x_2)} \int_\Omega \mathrm{d}\mathbf{y}\; \hat{J}_2(y_1, y_2) e^{i\varepsilon(k+\ell)(y_1+y_2)}\end{aligned} \tag{2.13}$$

For any smooth functions J_1, the $\mathbf{x}$ integration is very small unless $\ell \sim k$. Thus the order of the exchange term is $1/N$. Notice that if we take $J(x,y) \sim |x-y|^{-1}$ then the exchange term becomes of order $N^{-2/3}$, consistent with standard pictures from semiclassical limits of atomic and molecular energies. Indeed, since

$$\int \mathrm{d}\mathbf{x}\, e^{ikx} \frac{1}{|x|} \sim \frac{1}{|k|^2} ,$$

we obtain that in this case

$$W^{(2)}_{\mathrm{ex}}(\mathbf{x},\mathbf{v}) \sim \frac{1}{N^2} \sum_{|k-\ell|=1}^{cN} \frac{1}{(k-\ell)^2} \sim N^{-2/3} .$$

Instead of choosing $\gamma^{(1)}(x,x')$ as in (2.10), we could also define

$$\gamma^{(1)}(x,x') = \frac{1}{N} \sum_{k\in\mathbb{Z}^3} f(k)\varphi_k(x)\overline{\varphi_k(x')} \tag{2.14}$$

for an arbitrary distribution $f(k)$ with $0 \leq f(k) \leq 1$ for all $k \in, \mathbb{Z}^3$, and with $\sum_k f(k) = N$ so that $\gamma^{(1)}(x,x')$ is a density matrix satisfying the conditions (2.1) and (2.2). Typical distributions are of the form $f(k) = g(\varepsilon k)$ for some smooth function g. In this case the one particle density matrix is supported within a distance of order ε from the diagonal, and the exchange term, analogously to (2.12), vanishes in the weak limit $N \to \infty$.

Example 2: Let ω be a smooth decaying function. We define

$$\varphi_k(x) = \varepsilon^{-3/2}\omega\Big(\frac{x-k}{\varepsilon}\Big) ,$$

where k runs over lattice sites with $|k| \leq c/\varepsilon$, and $\varepsilon = N^{-1/3}$, as always. In other words, $\varphi_k(x)$ represents a state localized inside a sphere of radius ε around the lattice site k. It is a straight-forward exercise to show that the exchange term in the two-particle Wigner transform of $\bigwedge \varphi_k$ is again of order $1/N$. Indeed, we obtain in this case that

$$\begin{aligned}
\int \mathrm{d}\mathbf{x} J(\mathbf{x}) W^{(2)}_{\mathrm{ex}}(\mathbf{x},\mathbf{v}) &= \frac{1}{(2\pi)^6} \sum_{k,\ell=1}^{N} \int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} J(x_1,x_2) e^{-i\mathbf{v}\cdot\mathbf{y}}\, \omega\Big(\frac{x_1-k}{\varepsilon} + \frac{y_1}{2}\Big) \overline{\omega\Big(\frac{x_2-k}{\varepsilon} - \frac{y_2}{2}\Big)} \\
&\qquad\qquad \times \omega\Big(\frac{x_2-\ell}{\varepsilon} + \frac{y_2}{2}\Big) \overline{\omega\Big(\frac{x_1-\ell}{\varepsilon} - \frac{y_1}{2}\Big)} \\
&= \frac{1}{(2\pi)^6 N^2} \sum_{k,\ell=1}^{N} \int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} J(\varepsilon x_1, \varepsilon x_2) e^{-i\mathbf{v}\cdot\mathbf{y}}\, \omega\Big(x_1 - \frac{k}{\varepsilon} + \frac{y_1}{2}\Big) \overline{\omega\Big(x_2 - \frac{k}{\varepsilon} - \frac{y_2}{2}\Big)} \\
&\qquad\qquad \times \omega\Big(x_2 - \frac{\ell}{\varepsilon} + \frac{y_2}{2}\Big) \overline{\omega\Big(x_1 - \frac{\ell}{\varepsilon} - \frac{y_1}{2}\Big)}
\end{aligned} \tag{2.15}$$

Clearly, for any smooth function $J(\mathbf{x})$, only terms with $k = \ell$ give a considerable contribution to the sum; therefore the right hand side of the above equation is bounded by $1/N$.

Example 3: In the last two examples the kernel of the one particle density matrix, $\gamma^{(1)}(x, y)$, is concentrated on the diagonal $|x-y| \lesssim N^{-1/3}$. Suppose now that we are given a one particle density matrix $\gamma(x, y)$ on $[0, 2\pi]^3 \times [0, 2\pi]^3$, which satisfies $0 \le \gamma \le (\text{const.})/N$, $\text{Tr}\, \gamma = 1$ and it is supported near the diagonal. Let

$$\tilde{\gamma}(x, y) := \beta\Big[\gamma(x, y) + \gamma(x+e, y) + \gamma(x, y+e) + \gamma(x+e, y+e)\Big] \tag{2.16}$$

with $e := (0, 0, 2\pi)$. We can choose the constant β so that $\text{Tr}\, \tilde{\gamma} = 1$ and we still have

$$0 \le \tilde{\gamma} \le (\text{const.})/N \ .$$

Thus we constructed a density matrix which is not concentrated on the diagonal. The corresponding quasifree state can be constructed by standard procedure.

This construction can be carried out on the level of the wave functions as well. Let φ_k, $k \in \mathbb{Z}^3$, $|k| \le cN^{1/3}$ be N orthonormal one body wavefunctions supported the cube $[0, 2\pi]^3$ as in Example 1. Then $\gamma := \frac{1}{N}\sum_k |\varphi_k\rangle\langle\varphi_k|$ is supported near the diagonal. Define

$$\tilde{\psi} = \bigwedge_k \psi_k \ , \qquad \text{with} \quad \psi_k(x) := 2^{-1/2}[\varphi_k(x) + \varphi_k(x+e)] \ .$$

Then the one particle density matrix is of the form $\tilde{\gamma}$ from (2.16). It is concetrated around three submanifolds $x = y$ and $x = y \pm e$ and not just along the diagonal $|x-y| \lesssim N^{-1/3}$. In particular, the exchange term is still of order $1/N$.

The fact that the exchange terms are of order $1/N$ in all these three examples tells us that there is a large class of initial data for which $W_N^{(2)}$ is factorized in the weak limit $N \to \infty$. Similar result can be obtained for any n-particle function if n is fixed:

$$\lim_{N\to\infty} W_N^{(n)}(x_1, \ldots, x_n, v_1, \ldots, v_n) = \prod_{j=1}^{n} W_N^{(1)}(x_j, v_j) \ , \tag{2.17}$$

or, more precisely, $|\langle J, W_N^{(n)} - (W_N^{(1)})^{\otimes n}\rangle| \le c/N$, where the constant depends on n and on the smooth test function $J(\mathbf{x}, \mathbf{v})$.

2.3 The Fourier Transform of $W_N(\mathbf{x}, \mathbf{v})$

Instead of working directly with the Wigner function W_N it is often more convenient to work with its Fourier transform, which we define as

$$\mu_N(\boldsymbol{\xi}, \boldsymbol{\eta}) := \text{Tr}\, \gamma_N\, e^{-i(\varepsilon\boldsymbol{\eta}\cdot\hat{\mathbf{p}} + \boldsymbol{\xi}\cdot\hat{\mathbf{x}})}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}} = -i\nabla_{\mathbf{x}}$ are the position and momentum operators on $L^2(\mathbb{R}^{3N})$. Narnhofer and Sewell defined the same quantity with a somewhat different notation (see (3.2) in [14]): the $\boldsymbol{\xi}, \boldsymbol{\eta}$ variables are interchanged and the conjugate is considered. Noting that

$$\left(e^{-i(\varepsilon\boldsymbol{\eta}\cdot\hat{\mathbf{p}}+\boldsymbol{\xi}\cdot\hat{\mathbf{x}})}\psi\right)(\mathbf{x}) = e^{i\frac{\varepsilon}{2}\boldsymbol{\xi}\cdot\boldsymbol{\eta}}e^{-i\boldsymbol{\xi}\cdot\mathbf{x}}\psi(\mathbf{x}-\varepsilon\boldsymbol{\eta}),$$

we have

$$\mu_N(\boldsymbol{\xi},\boldsymbol{\eta}) = \int e^{-i\boldsymbol{\xi}\cdot\mathbf{x}}\gamma_N\Big(\mathbf{x}-\frac{\varepsilon\boldsymbol{\eta}}{2}, \mathbf{x}+\frac{\varepsilon\boldsymbol{\eta}}{2}\Big)\mathrm{d}\mathbf{x} = \int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v}\; W_N(\mathbf{x},\mathbf{v})e^{-i\boldsymbol{\xi}\cdot\mathbf{x}-i\boldsymbol{\eta}\cdot\mathbf{v}}$$

and hence

$$W_N(\mathbf{x},\mathbf{v}) = \frac{1}{(2\pi)^{6N}}\int \mu_N(\boldsymbol{\xi},\boldsymbol{\eta})e^{i\boldsymbol{\xi}\cdot\mathbf{x}+i\boldsymbol{\eta}\cdot\mathbf{v}}\mathrm{d}\boldsymbol{\eta}\mathrm{d}\boldsymbol{\xi}.$$

Notice the operator norm of $e^{-i(\varepsilon\boldsymbol{\eta}\cdot\hat{\mathbf{p}}+\boldsymbol{\xi}\cdot\hat{\mathbf{x}})}$ is equal one. Since γ_N is positive and $\mathrm{Tr}\;\gamma_N = 1$, we have

$$|\mu_N(\boldsymbol{\xi},\boldsymbol{\eta})| = |\mathrm{Tr}\;\gamma_N e^{-i(\varepsilon\mathbf{p}\cdot\boldsymbol{\eta}+\boldsymbol{\xi}\cdot\mathbf{x})}| \leq 1. \tag{2.18}$$

For any $J(\mathbf{x},\mathbf{v})$ with $\|\hat{J}\|_{L_1(\mathrm{d}\boldsymbol{\xi},\mathrm{d}\boldsymbol{\eta})}$ bounded, we have

$$|\langle J, W_N\rangle| = |\langle \hat{J}, \mu_N\rangle| \leq \|\hat{J}\|_{L_1(\mathrm{d}\boldsymbol{\xi},\mathrm{d}\boldsymbol{\eta})}\,, \tag{2.19}$$

where $\langle f, g\rangle := \int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v}\overline{f(\mathbf{x},\mathbf{v})}g(\mathbf{x},\mathbf{v})$. Therefore, one can always extract weak limit points of Wigner transforms.

The time evolution of $\mu_N(\boldsymbol{\xi},\boldsymbol{\eta})$ can be easily derived from (2.6):

$$\begin{aligned}\partial_t\mu_N(t,\boldsymbol{\xi},\boldsymbol{\eta}) &= \sum_{j=1}^N \xi_j\cdot\nabla_{\eta_j}\mu_N(t,\boldsymbol{\xi},\boldsymbol{\eta})\\ &\quad - 2\varepsilon^2\sum_{j<k}^N\int \mathrm{d}q\,\hat{U}(q)\,\sin\Big(\frac{\varepsilon}{2}q(\eta_j-\eta_k)\Big)\;\mu_N(t,\xi_1,\ldots,\xi_j-q,\ldots,\xi_k+q,\ldots,\xi_N;\boldsymbol{\eta}),\end{aligned} \tag{2.20}$$

where we defined $\hat{U}(q) := (2\pi)^{-3}\int \mathrm{d}xe^{-iqx}U(x)$. We denote by $\mu_N^{(k)}$ the Fourier transform of the k particle Wigner function $W_N^{(k)}$. Then we have

$$\begin{aligned}\mu_N^{(k)}(\xi_1\ldots\xi_n;\eta_1\ldots\eta_n) &= \int \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v}\; W_N^{(k)}(\mathbf{x},\mathbf{v})e^{-i\mathbf{x}\cdot\boldsymbol{\xi}-i\mathbf{v}\cdot\boldsymbol{\eta}}\\ &= \mu_N(\xi_1,\ldots,\xi_k,0,\ldots,0;\eta_1,\ldots\eta_k,0,\ldots,0),\end{aligned} \tag{2.21}$$

if $k \leq N$ and $\mu_N^{(k)} = 0$ otherwise. From (2.18)

$$|\mu_N^{(k)}(\boldsymbol{\xi},\boldsymbol{\eta})| \leq 1 \tag{2.22}$$

is valid for all k.

3 The BBGKY Hierarchy and the Main Result

The family of marginals $\{W_N^{(n)}\}_{n=1,..,N}$ satisfies a hierarchy of equations, usually called the BBGKY hierarchy, which can be derived from (2.20) (also using the symmetry of $W_N^{(n)}$):

$$\begin{aligned}
&\partial_t W_N^{(n)}(t;x_1,\dots,x_n,v_1,\dots,v_n) + \sum_{j=1}^n v_j \cdot \nabla_{x_j} W_N^{(n)}(t;x_1,\dots x_n,v_1,\dots v_n) \\
&\quad = -\frac{i\varepsilon^3}{(2\pi)^{3n}} \sum_{1\le j<k\le n} \int \varepsilon^{-1}\left[U\Big(x_j+\frac{\varepsilon y_j}{2}-x_k-\frac{\varepsilon y_k}{2}\Big)-U\Big(x_j-\frac{\varepsilon y_j}{2}-x_k+\frac{\varepsilon y_k}{2}\Big)\right] \\
&\qquad \times e^{i\sum_{j=1}^n y_j(u_j-v_j)} W_N^{(n)}(t;x_1,\dots,x_n,u_1,\dots,u_n)\mathrm{d}u_1\mathrm{d}y_1\dots\mathrm{d}u_n\mathrm{d}y_n \\
&\qquad -\frac{i(1-n\varepsilon^3)}{(2\pi)^{3n}}\sum_{j=1}^n \int \varepsilon^{-1}\left[U\Big(x_j+\frac{\varepsilon y_j}{2}-x_{n+1}\Big)-U\Big(x_j-\frac{\varepsilon y_j}{2}-x_{n+1}\Big)\right] e^{i\sum_{j=1}^n y_j(u_j-v_j)} \\
&\qquad \times W_N^{(n+1)}(t;x_1,\dots,x_n,x_{n+1},u_1,\dots,u_n,u_{n+1})\mathrm{d}u_1\mathrm{d}y_1\dots\mathrm{d}u_n\mathrm{d}y_n\mathrm{d}u_{n+1}\mathrm{d}x_{n+1}.
\end{aligned} \tag{3.1}$$

The main goal of this paper is to compare solutions of this hierarchy of equation with tensor products of solutions of the one particle Hartree equation (1.8) which can be rewritten in terms of the one particle Wigner transform as

$$\partial_t W_t(x,v)+v\cdot\nabla_x W_t(x,v) = -\frac{i}{(2\pi)^3}\int \mathrm{d}y\mathrm{d}u\,\frac{1}{\varepsilon}\,\Big((U\star\rho_t)(x+\frac{\varepsilon y}{2})-(U\star\rho_t)(x-\frac{\varepsilon y}{2})\Big)\,W_t(x,u)\,e^{iu\cdot y}. \tag{3.2}$$

Let us denote by $\widetilde{W}^{(n)}(t,\mathbf{x},\mathbf{v})$ the n particle Wigner transform constructed taking tensor products of solutions of (3.2), that is

$$\widetilde{W}^{(n)}(t,\mathbf{x},\mathbf{v}) = \prod_{j=1}^n W_t(x_j,v_j).$$

Moreover we denote by

$$\begin{aligned}
H_{\ell,N}^{\delta_1,\delta_2}(t,\mathbf{x},\mathbf{v}) &= \Big(G_{\delta_1}^{(\ell)}\star_x G_{\delta_2}^{(\ell)}\star_v W_N^{(\ell)}(t)\Big)(\mathbf{x},\mathbf{v}) \qquad \text{and} \\
\widetilde{H}_{\ell,N}^{\delta_1,\delta_2}(t,\mathbf{x},\mathbf{v}) &= \Big(G_{\delta_1}^{(\ell)}\star_x G_{\delta_2}^{(\ell)}\star_v \widetilde{W}^{(\ell)}(t)\Big)(\mathbf{x},\mathbf{v})
\end{aligned} \tag{3.3}$$

the Husimi functions associated with the solution $W_N^{(\ell)}(t)$ of (3.1) and with $\widetilde{W}^{(\ell)}(t)$, respectively. Here we used, as in Section 2.1, the notation

$$G_\delta^{(n)}(\mathbf{z}) = \left(\frac{1}{\pi\delta^2}\right)^{3n/2} e^{-\frac{\mathbf{z}^2}{\delta^2}}\,. \tag{3.4}$$

The main result of this paper can be stated as follows.

Theorem 3.1. *Let U be a radial symmetric real valued potential and assume that there is a constant κ_1 so that*

$$\|U\|_m = \int |\hat{U}(\xi)||\xi|^m d\xi \le \kappa_1^m m! \tag{3.5}$$

for all $m \in \mathbb{N}$. Suppose that, for $k \le 2\log N$,

$$\left|\left\langle O^{(k)}, W_N^{(k)}(0) - \widetilde{W}^{(k)}(0)\right\rangle\right| \le \frac{1}{N}\sup_{\mathbf{x},\mathbf{v}} |O^{(k)}(\mathbf{x},\mathbf{v})|. \tag{3.6}$$

Then, for any fixed ℓ, δ_1 and δ_2, we have

$$\limsup_{N\to\infty} \sup_{\mathbf{x},\mathbf{v}} \left| \left(H_{\ell,N}^{\delta_1,\delta_2} - \widetilde{H}_{\ell,N}^{\delta_1,\delta_2}\right)(t,\mathbf{x},\mathbf{v})\right| \cdot N < \infty \tag{3.7}$$

uniformly for all $t < \frac{1}{4}(\sqrt{1+1/(7\kappa_1^2)} - 1)$.

Remarks .

1) Condition (3.5) holds for bounded, real analytic functions $U(x)$. The symmetry condition is physically natural. The proof can easily be modified to include non-symmetric potentials as well.

2) It is clear from the proof (see Section 4) that the theorem is still true, with N in (3.7) replaced by $N^{-1+\kappa}$ with an arbitrary small $\kappa > 0$, if we allow δ_1, δ_2 and ℓ depend on N as long the conditions
$$\ell(N) = o(\sqrt{\log N})\ , \qquad [\delta_j(N)]^{-2} = o(\sqrt{\log N}), \qquad j = 1,2, \tag{3.8}$$
are satisfied.

3) It is also clear from the proof (see Section 4) that the theorem is still true if we replace the accuracy $1/N$ both in (3.6) and (3.7) by $N^{-\kappa}$ with $0 < \kappa \le 1$. It follows that if the exchange term $W_{\rm ex}^{(n)}$ (see Section 2.2) of the initial data is of order $N^{-\kappa}$, then it remain of the same order for all sufficiently small times.

The proof of this theorem is given in Section 4 below: it is based on a perturbative expansion of solutions of the BBGKY Hierarchy. For technical reasons, instead of expanding solutions of (3.1), it turns out to be more convenient to work with the Fourier transforms $\mu_N^{(\ell)}(\boldsymbol{\xi},\boldsymbol{\eta})$ of the $W_N^{(\ell)}(\mathbf{x},\mathbf{v})$ (see Section 2.3 for the definition of $\mu_N^{(\ell)}$). Eq. (3.1) is equivalent to the following hierarchy of equations for the marginals $\mu_N^{(n)}$:

$$\partial_t \mu_N^{(n)}(t,\boldsymbol{\xi},\boldsymbol{\eta}) = \sum_{j=1}^n \xi_j \cdot \nabla_{\eta_j} \mu_N^{(n)}(t,\boldsymbol{\xi},\boldsymbol{\eta})$$

$$- 2\varepsilon^2 \sum_{1\le j<k\le n} \int \mathrm{d}q \hat{U}(q) \sin\left(\frac{\varepsilon\, q\cdot(\eta_j-\eta_k)}{2}\right) \mu_N^{(n)}(t,\xi_1,\ldots,\xi_j-q,\ldots\xi_k+q,\ldots,\xi_n,\boldsymbol{\eta}) \tag{3.9}$$

$$- (1-n\varepsilon^3)\sum_{j=1}^n \int \mathrm{d}q \hat{U}(q)\,\frac{2}{\varepsilon}\sin\left(\frac{\varepsilon q\cdot \eta_j}{2}\right) \mu_N^{(n+1)}(t,\xi_1,\ldots\xi_j-q,\ldots\xi_n,q,\boldsymbol{\eta},0)$$

3.1 Vlasov hiearchy

The classical Vlasov hierarchy is the semiclassical approximation of the BBGKY hierarchy. It is obtained from (3.1) by formally setting $\varepsilon \to 0$ and approximate the potential difference by gradient. Using

$$U\Big(x_j + \frac{\varepsilon y_j}{2} - x_{n+1}\Big) - U\Big(x_j - \frac{\varepsilon y_j}{2} - x_{n+1}\Big) = \nabla U(x_j - x_{n+1})\varepsilon y_j + O(\varepsilon^2) \tag{3.10}$$

and

$$i y_j e^{i y_j (v_j - u_j)} = -\nabla_{u_j} e^{i y_j (v_j-u_j)},$$

we can perform an integration by parts, then integrate out $\mathrm{d}u_1\mathrm{d}y_1\ldots\mathrm{d}u_n\mathrm{d}y_n$ to collect delta functions $\prod_1^n \delta(u_j - v_j)$. Neglecting lower order terms, we obtain formally

$$\partial_t \widetilde{W}^{(n)}(t;x_1,\ldots x_n,v_1,\ldots v_n) + \sum_{j=1}^n v_j\cdot\nabla_{x_j}\widetilde{W}^{(n)}(t;x_1,\ldots,x_n,v_1,\ldots,v_n) \tag{3.11}$$

$$= \sum_{j=1}^n \int \nabla U(x_j - x_{n+1})\nabla_{v_j}\widetilde{W}^{(n+1)}(t;x_1,\ldots,x_n,x_{n+1},v_1,\ldots,v_n,u_{n+1})\mathrm{d}u_{n+1}\mathrm{d}x_{n+1}$$

for the weak limit

$$\widetilde{W}^{(n)}(t,\mathbf{x},\mathbf{v}) := \lim_{N\to\infty} W_N^{(n)}(t,\mathbf{x},\mathbf{v})\ . \tag{3.12}$$

The main result of [14] and [15] proves that this limit exists, it solves the Vlasov hierarchy (3.11) and the solution is unique. Therefore $\widetilde{W}^{(n)} = w_t^{\otimes(n)}$ where w_t satisfies the Vlasov equation (1.7).

3.2 Other Scalings

Theorem 3.1 identifies the limit dynamics of the Wigner transform at scale $\varepsilon = N^{-1/3}$. One may define the Wigner transform at a different scale ν by

$$W_{N,\nu}^{(1)}(x;v) := \frac{1}{(2\pi)^3}\int e^{-iv\cdot y}\gamma_N^{(1)}\Big(x+\nu\frac{y}{2}, x-\nu\frac{y}{2}\Big)\mathrm{d}y\ . \tag{3.13}$$

The following lemma shows, however, that under a natural energy conditions, $W^{(1)}_{N,\nu}$ cannot converge to a non-trivial function unless $\nu \sim \varepsilon$. Similar statement is true for higher order marginals. It justifies our choice of scaling in Section 2.1 in order to derive a dynamics for a nondegenerate limiting distribution.

Lemma 3.2. *Let* $\varepsilon := N^{-1/3}$.

(i) Suppose the kinetic energy of a state Ψ *is comparable with the ground state kinetic energy of* N *fermions in a box of size one, i.e.*

$$\Big\langle \Psi, \Big(\sum_{j=1}^N -\Delta_{x_j} \Big) \Psi \Big\rangle \le C_1 N^{5/3} \; . \tag{3.14}$$

Let $O \in \mathcal{S}(\mathbb{R}^3_x \times \mathbb{R}^3_v)$ *be a Schwarz function with support in* $\{|v| \ge \lambda\}$ *for some* $\lambda > 0$. *Then*

$$|\langle O, H_{N,\nu}\rangle| \le \Big[C_1 \Big(\frac{\nu}{\lambda\varepsilon}\Big)^2 + O(\nu\lambda^{-2})\Big] \|O\|_\infty \; , \tag{3.15}$$

with $H_{N,\nu} := W^{(1)}_{N,\nu} \star_x G_{\sqrt{\nu}} \star_v G_{\sqrt{\nu}}$, *in particular, the one particle Husimi function of* Ψ *at scale* ν *vanishes outside of the* $\{v = 0\}$ *hyperplane if* $\nu \ll \varepsilon$.

(ii) Suppose that the average mean square displacement of Ψ *is of order one, i.e.*

$$\Big\langle \Psi, \frac{1}{N} \Big(\sum_{j=1}^N x_j^2 \Big) \Psi \Big\rangle \le C_2 \; . \tag{3.16}$$

Let $O \in \mathcal{S}(\mathbb{R}^3_x \times \mathbb{R}^3_v)$ *be a Schwarz function with support in* $\{|v| \le \lambda\}$ *for some* $\lambda > 0$. *Then*

$$|\langle O, H_{N,\nu}\rangle| \le \textit{(const.)} C_2 \|O\|_\infty \Big(\frac{\lambda\varepsilon}{\nu}\Big)^{6/5} \tag{3.17}$$

with a universal constant.

Proof. (i) Since $|O(x,v)| \le \|O\|_\infty v^2 \lambda^{-2}$ and the Husimi function is positive, we obtain

$$|\langle O, H_{N,\nu}\rangle| \le \frac{\|O\|_\infty}{\lambda^2} \langle v^2, H_{N,\nu}\rangle = \frac{\|O\|_\infty}{\lambda^2} \int u^2 G_{\sqrt{\nu}}(v-u) \varrho_\nu(v) \mathrm{d}v\mathrm{d}u = \frac{\|O\|_\infty}{\lambda^2} \int (v^2 + c\nu) \varrho_\nu(v) \mathrm{d}v \; ,$$

where $\varrho_\nu(v) := \int W(x,v)\mathrm{d}x$ is the momentum distribution and c is a universal constant. Since $\int \varrho_\nu(v)\mathrm{d}v = 1$ and by (3.14)

$$\int v^2 \varrho_\nu(v)\mathrm{d}v = \nu^2 \,\mathrm{Tr}(-\Delta)\gamma \le C_1 \, \nu^2 N^{2/3} = C_1(\nu/\varepsilon)^2 \; ,$$

we obtain (3.15).

(ii) We apply the Lieb-Thirring inequality [12] in the Fourier space

$$\int \varrho(v)^{5/3} \mathrm{d}v \le (\text{const.}) \Big\langle \Psi, \Big(\sum_{j=1}^{N} x_j^2 \Big) \Psi \Big\rangle \tag{3.18}$$

with a universal constant, where $\varrho(v) = N \int |\widehat{\Psi}(v, v_2, \dots, v_N)|^2 \mathrm{d}v_2 \dots \mathrm{d}v_N$ is the one particle momentum density of the antisymmetric function Ψ. After rescaling we obtain $\varrho_\nu(v) = (\varepsilon/\nu)^3 \varrho(v/\nu)$, hence $\int \varrho_\nu^{5/3} \le (\text{const.}) C_2 (\varepsilon/\nu)^2$ from (3.16) and (3.18). Therefore

$$\begin{aligned} |\langle O, H_{N,\nu} \rangle| &\le \|O\|_\infty \int \mathrm{d}x \mathrm{d}v \; \chi(|v| \le \lambda) H_{N,\nu}(x, v) \\ &= \|O\|_\infty \int \mathrm{d}u \mathrm{d}v \; \chi(|u| \le \lambda) G_{\sqrt{\nu}}(v - u) \varrho_\nu(v) \\ &\le (\text{const.}) \|O\|_\infty \|\chi(|\cdot| \le \lambda)\|_{5/2} \|G_{\sqrt{\nu}}\|_1 \|\varrho_\nu\|_{5/3} \\ &\le (\text{const.}) C_2 \|O\|_\infty \Big(\frac{\lambda \varepsilon}{\nu} \Big)^{6/5} \end{aligned} \tag{3.19}$$

by Young's inequality. □

This lemma shows that the weak limits of $W^{(1)}_{N,\nu}$ are zero if $\nu \gg \varepsilon$, in particular if the Wigner transform is unscaled, $\nu = 1$. It may, nevertheless, be reasonable to investigate how well Hartree or Hartree-Fock evolutions approximate the true dynamics compared to the actual size of W in a different topology.

Bardos et al. [2] have recently studied the equation (1.10) and showed that the Hartree-Fock equation approximates the dynamics in the trace norm. In order to study (1.10) one first needs to choose the parameter α. Denote by $H_{N,\alpha} = -\alpha \Delta_N + (1/N) \sum_{i<j} U(x_i - x_j)$ the Hamiltonian corresponding to (1.10), and consider an initial state $\gamma_{N,0}$. Here we assume the two body potential U to have bounded derivative. Let $\gamma_{N,t}$ be the time evolution of $\gamma_{N,0}$. We are interested in an estimate for the mean squared distance between two particles at an arbitrary fixed time t. Define the quantities

$$\begin{aligned} u_t &:= \big[\mathrm{Tr} \; \gamma_{N,t} \, (x_1 - x_2)^2 \big]^{1/2}, \\ v_t &:= \big[\mathrm{Tr} \; \gamma_{N,t} \, (p_1 - p_2)^2 \big]^{1/2} , \end{aligned}$$

where $p_j := -i \nabla_{x_i}$. For typical interacting initial states the mean square distance between the particles is of order one, $u_0 = O(1)$, the kinetic energy per particle is of order $N^{2/3}$, due to Fermi statistics, therefore $v_0 \le (const.) N^{1/3}$. The next lemma shows that v_0 is exactly of order $N^{1/3}$ for any fermionic state localized within an order one distance from the center of mass; in particular there cannot be strong velocity correlation between the particles. Then in Lemma 3.4 we show how to use the lower bound on v_0 to give a lower bound on the mean square displacement u_t^2.

Lemma 3.3. *Let γ be a fermionic N-particle density matrix, $Tr\,\gamma = 1$, satisfying*

$$Tr\,\Big[\gamma\,\frac{1}{N}\sum_{j=1}^N (x_j-\bar{X})^2\Big] \le K\,, \qquad \bar{X} := \frac{1}{N}\sum_{j=1}^N x_j\,. \tag{3.20}$$

Then

$$Tr\,\gamma\;(p_1-p_2)^2 \ge (const.)N^{2/3}$$

with a positive constant depending on K.

Remark. By the symmetry of γ and a Schwarz inequality

$$\begin{aligned}\mathrm{Tr}\,\Big[\gamma\,\frac{1}{N}\sum_{j=1}^N (x_j-X)^2\Big] &= \mathrm{Tr}\,\gamma\Big(\frac{1}{N}\sum_{j=1}^N (x_1-x_j)\Big)^2\\ &\le \frac{N-1}{N}\,\mathrm{Tr}\,\gamma\,(x_1-x_2)^2\,,\end{aligned} \tag{3.21}$$

so the condition (3.20) is satisfied if $\mathrm{Tr}\,\gamma\,(x_1-x_2)^2 \le K$.

Lemma 3.4. *Let $C := \|\nabla U\|_\infty$ and let u_0, v_0 be the initial mean squared distance between two particles in position and momentum space, respectively. Then for any $0\le t\le v_0/(8C)$*

$$u_t^2 \ge u_0^2 + \alpha^2\,v_0^2t^2 - (const.)\alpha t\Big(u_0v_0 + u_0t + \alpha v_0 t^2\Big)\,, \tag{3.22}$$

where the constant depends only on C.

The proofs of these lemmas are deferred to the Appendix.

According to Lemma 3.3 and the subsequent remark, if the initial inter-particle distance u_0 is of order one, then $v_0 \ge (const.)N^{1/3}$. In this case Lemma 3.4 shows that if we want u_t to remain of order one for $t>0$ uniformly as $N\to\infty$, then we have to assume that $\alpha = O(\varepsilon) = O(N^{-1/3})$. Otherwise the interaction between the particles typically vanishes as $U(x_1-x_2)\to 0$ for $|x_1-x_2|\to\infty$.

When $\alpha=\varepsilon$, we can rewrite the Schrödinger equation (1.10) as

$$i\varepsilon\partial_t\psi_{N,t} = \Big(-\varepsilon^2\sum_{j=1}^N \Delta_{x_j} + \frac{\varepsilon}{N}\sum_{j,k} U(x_j-x_k)\Big)\psi_{N,t}. \tag{3.23}$$

This equation is the same as (1.2) except the extra ε factor in front of the interaction. Since (1.2) converges to the Vlasov equation, (3.23) converges to a free evolution.

Although some of these conclusions are partly based on initial data considered in [14], [15] or Section 2.2, this behavior is expected for a general reasonable interacting physical system. While one may be able to consider some initial data so that the one particle density matrix $\gamma^{(1)}_{N,t}$ (for the dynamics (1.10)) is not given by a free evolution in the $N\to\infty$ limit, we do not know if there is a natural class of such initial data.

4 Proof of the Main Result

As explained in Section 3 the proof of our main result, Theorem 3.1, is based on a perturbative expansion of solutions $\mu_N^{(\ell)}(t,\boldsymbol{\xi},\boldsymbol{\eta})$ of the BBGKY hierarchy in the form (3.9). We will compare $\mu_N^{(\ell)}(t,\boldsymbol{\xi},\boldsymbol{\eta})$ with tensor products of a solution of the Hartree equation (3.2), which, after Fourier transform can be written in the form

$$\partial_t\mu_t(\xi,\eta) = \xi\cdot\nabla_\eta\mu_t(\xi,\eta) - \int \mathrm{d}q\, \hat{U}(q)\frac{2}{\varepsilon}\sin\Big(\frac{\varepsilon q\eta}{2}\Big)\,\mu_t(\xi-q,\eta)\mu_t(q,0) \tag{4.1}$$

with a given initial condition μ_0. In the following we will use the notation

$$\tilde{\mu}_t^{(\ell)}(\boldsymbol{\xi},\boldsymbol{\eta}) = \prod_{j=1}^{\ell}\mu_t(\xi_j,\eta_j) \tag{4.2}$$

for ℓ-particle tensor products of a solution μ_t of (4.1). We remark that global existence, uniqueness and regularity of the solution of (4.1) have been established in [6, 7].

For any n-particle observable $O^{(n)}(\boldsymbol{\xi},\boldsymbol{\eta})$, with $\boldsymbol{\xi} = (\xi_1,\ldots,\xi_n)$, $\boldsymbol{\eta} = (\eta_1,\ldots,\eta_n)$, we define the norms

$$\|O^{(n)}\|_{\boldsymbol{\alpha}} = \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\,|O^{(n)}(\boldsymbol{\xi},\boldsymbol{\eta})|\prod_{j=1}^{n}(|\xi_j|+|\eta_j|)^{\alpha_j} \tag{4.3}$$

for $\boldsymbol{\alpha} = (\alpha_1,\ldots,\alpha_n)\in\mathbb{N}^n$. Moreover we use the notation

$$\langle O^{(n)},\mu^{(n)}\rangle = \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\,\overline{O}^{(n)}(\boldsymbol{\xi},\boldsymbol{\eta})\,\mu^{(n)}(\boldsymbol{\xi},\boldsymbol{\eta}). \tag{4.4}$$

The following lemma is the main ingredient in the proof of Theorem 3.1.

Lemma 4.1. *Assume there exists a constant κ_1 so that*

$$\|U\|_m = \int |\hat{U}(\xi)||\xi|^m\mathrm{d}\xi \le \kappa_1^m m! \tag{4.5}$$

for all $m\in\mathbb{N}$. Fix positive integers ℓ, n and suppose that, for all $k\le(n+\ell)$,

$$\Big|\langle O,\mu_N^{(k)}(0)-\tilde{\mu}_0^{(k)}\rangle\Big| \le \frac{1}{N}\|O\|_0. \tag{4.6}$$

Consider an observable $O^{(\ell)}$ with

$$\|O^{(\ell)}\|_{\boldsymbol{\alpha}} \le C_0^\ell\,\kappa_2^{|\boldsymbol{\alpha}|}\alpha_1!\ldots\alpha_\ell!\,,\quad \forall\,\boldsymbol{\alpha}\in\mathbb{N}^\ell, \tag{4.7}$$

then we have

$$\Big|\langle O^{(\ell)},\mu_N^{(\ell)}(t)-\tilde{\mu}_t^{(\ell)}\rangle\Big| \le \frac{2}{\kappa_1}(2C_0)^\ell\,(2\kappa_t)^n + \frac{C_0^\ell}{N}\Big(1+\frac{3\kappa_t}{\kappa_1}(\ell+2)^2\Big(\frac{1}{1-\kappa_t}\Big)^{\ell+3}\Big), \tag{4.8}$$

where we put $\kappa_t = 9\kappa_1 t(1+2t)(\kappa_1+\kappa_2)$ and assumed that $\kappa_t<1$.

Proof. From (3.9), expanding around the free evolution, we find

$$
\begin{aligned}
\mu_N^{(\ell)}(t,\boldsymbol{\xi},\boldsymbol{\eta}) &= \mu_N^{(\ell)}(0,\boldsymbol{\xi},\boldsymbol{\eta}+t\boldsymbol{\xi}) \\
&\quad - \varepsilon^3 \sum_{1\le j<k\le \ell} \int_0^t \mathrm{d}s \int \mathrm{d}q\, \hat{U}(q)\, \frac{2}{\varepsilon} \sin\left(\frac{\varepsilon q\cdot((\eta_j-\eta_k)+(t-s)(\xi_j-\xi_k))}{2}\right) \\
&\qquad \times \mu_N^{(\ell)}(s,\xi_1,\dots,\xi_j-q,\dots,\xi_k+q,\dots,\xi_n;\boldsymbol{\eta}+(t-s)\xi) \\
&\quad - (1-\ell\varepsilon^3)\sum_{j=1}^{\ell} \int_0^t \mathrm{d}s \int \mathrm{d}q\, \hat{U}(q) \frac{2}{\varepsilon}\sin\left(\frac{\varepsilon q\cdot(\eta_j+(t-s)\xi_j)}{2}\right) \\
&\qquad \times \mu_N^{(\ell+1)}(s,\xi_1,\dots,\xi_j-q,\dots,\xi_\ell,q;\boldsymbol{\eta}+(t-s)\boldsymbol{\xi},0).
\end{aligned}
\tag{4.9}
$$

Next we insert this expansion in the expectation $\langle O^{(\ell)},\mu_N^{(\ell)}\rangle$ and we find, moving the free evolution from the μ to the observable,

$$
\begin{aligned}
\langle O^{(\ell)},\mu_N^{(\ell)}(t)\rangle &= \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\, \overline{O^{(\ell)}}(\boldsymbol{\xi},\boldsymbol{\eta}-t\boldsymbol{\xi})\mu_N^{(\ell)}(0,\boldsymbol{\xi},\boldsymbol{\eta}) \\
&\quad - \varepsilon^3 \sum_{1\le j<k\le\ell} \int_0^t \mathrm{d}s \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta} \int \mathrm{d}q\, \hat{U}(q)\overline{O^{(\ell)}}(\boldsymbol{\xi},\boldsymbol{\eta}-(t-s)\boldsymbol{\xi})\, \frac{2}{\varepsilon}\sin\left(\frac{\varepsilon q\cdot(\eta_j-\eta_k)}{2}\right) \\
&\qquad \times \mu_N^{(\ell)}(s,\xi_1,\dots,\xi_j-q,\dots,\xi_k+q,\dots,\xi_n;\boldsymbol{\eta}) \\
&\quad - (1-\ell\varepsilon^3)\sum_{j=1}^{\ell}\int_0^t \mathrm{d}s \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\int \mathrm{d}q\, \hat{U}(q)\overline{O^{(\ell)}}(\boldsymbol{\xi},\boldsymbol{\eta}-(t-s)\boldsymbol{\xi})\frac{2}{\varepsilon}\sin\left(\frac{\varepsilon q\cdot\eta_j}{2}\right) \\
&\qquad \times \mu_N^{(\ell+1)}(s,\xi_1,\dots\xi_j-q,\dots\xi_\ell,q;\boldsymbol{\eta},0).
\end{aligned}
\tag{4.10}
$$

Now we define the following two operators acting on the observable $O^{(\ell)}$:

$$
(AO^{(\ell)})(\boldsymbol{\xi},\boldsymbol{\eta}) = -\varepsilon^3 \sum_{1\le j<k\le\ell}\int \mathrm{d}q\,\hat{U}(q)\,\frac{2}{\varepsilon}\sin\left(\frac{\varepsilon q\cdot(\eta_j-\eta_k)}{2}\right) O^{(\ell)}(\xi_1,\dots,\xi_j+q,\dots,\xi_k-q,\dots,\xi_\ell;\boldsymbol{\eta})
\tag{4.11}
$$

and

$$
(BO^{(\ell)})(\boldsymbol{\xi},\xi_{\ell+1};\boldsymbol{\eta},\eta_{\ell+1}) = -\sum_{j=1}^{\ell}\hat{U}(\xi_{\ell+1})\delta(\eta_{\ell+1})\frac{2}{\varepsilon}\sin\left(\frac{\varepsilon\xi_{\ell+1}\cdot\eta_j}{2}\right)O^{(\ell)}(\xi_1,\dots,\xi_j+\xi_{\ell+1},\dots\xi_\ell;\boldsymbol{\eta}).
\tag{4.12}
$$

Moreover, we denote by $(S_tO^{(\ell)})(\boldsymbol{\xi},\boldsymbol{\eta}) := O^{(\ell)}(\boldsymbol{\xi},\boldsymbol{\eta}-t\boldsymbol{\xi})$ the free evolution of the observable $O^{(\ell)}$.

Equation (4.10) can be rewritten as

$$
\begin{aligned}
\langle O^{(\ell)},\mu_N^{(\ell)}(t)\rangle &= \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\, (S_t\overline{O^{(\ell)}})(\boldsymbol{\xi},\boldsymbol{\eta})\mu_N^{(\ell)}(0,\boldsymbol{\xi},\boldsymbol{\eta}) \\
&+ \int_0^t \mathrm{d}s \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\, (AS_{t-s}\overline{O^{(\ell)}})(\boldsymbol{\xi},\boldsymbol{\eta})\mu_N^{(\ell)}(s,\boldsymbol{\xi},\boldsymbol{\eta}) \\
&+ (1-\ell\varepsilon^3)\int_0^t \mathrm{d}s \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\mathrm{d}\xi_{\ell+1}\mathrm{d}\eta_{\ell+1}\, (BS_{t-s}\overline{O^{(\ell)}})(\boldsymbol{\xi},\xi_{\ell+1},\boldsymbol{\eta},\eta_{\ell+1})\mu_N^{(\ell+1)}(s,\boldsymbol{\xi},\xi_{\ell+1},\boldsymbol{\eta},\eta_{\ell+1}),
\end{aligned}
\tag{4.13}
$$

or, in a more compact form, as

$$
\begin{aligned}
\langle O^{(\ell)},\mu_N^{(\ell)}(t)\rangle = \langle S_t O^{(\ell)},\mu_N^{(\ell)}(0)\rangle &+ \int_0^t \mathrm{d}s\langle AS_{t-s}O^{(\ell)},\mu_N^{(\ell)}(s)\rangle \\
&+ (1-\ell\varepsilon^3)\int_0^t \mathrm{d}s\langle BS_{t-s}O^{(\ell)},\mu_N^{(\ell+1)}(s)\rangle,
\end{aligned}
\tag{4.14}
$$

where we used that the operators A, B and S_t commute with the complex conjugation (note that, since $U(x)$ is symmetric and $\hat{U}(q)$ is real). Next we iterate this relation n times. We find

$$
\begin{aligned}
\langle O^{(\ell)},\mu_N^{(\ell)}(t)\rangle &= \langle S_t O^{(\ell)},\mu_N^{(\ell)}(0)\rangle \\
&+ \sum_{m=1}^{n-1}\int_0^t \mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\ldots\int_0^{s_{m-1}}\mathrm{d}s_m\langle S_{s_m}BS_{s_{m-1}-s_m}B\ldots BS_{t-s_1}O^{(\ell)},\mu_N^{(\ell+m)}(0)\rangle \\
&+ \int_0^t \mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\ldots\int_0^{s_{n-1}}\mathrm{d}s_n\langle BS_{s_{n-1}-s_n}B\ldots BS_{t-s_1}O^{(\ell)},\mu_N^{(\ell+n)}(s_n)\rangle \\
&+ \sum_{m=1}^{n}\int_0^t \mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\ldots\int_0^{s_{m-1}}\mathrm{d}s_m\langle AS_{s_{m-1}-s_m}B\ldots BS_{t-s_1}O^{(\ell)},\mu_N^{(\ell+m-1)}(s_m)\rangle \\
&- \varepsilon^3\sum_{m=1}^{n}(\ell+m-1)\int_0^t \mathrm{d}s_1\int_0^{s_1}\mathrm{d}s_2\ldots\int_0^{s_{m-1}}\mathrm{d}s_m\langle BS_{s_{m-1}-s_m}B\ldots BS_{t-s_1}O^{(\ell)},\mu_N^{(\ell+m)}(s_m)\rangle\ .
\end{aligned}
\tag{4.15}
$$

Using (2.22) we have, for any time t and any observable $O^{(k)}$,

$$
|\langle O^{(k)},\mu_N^{(k)}(t)\rangle| \le \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\,|O^{(k)}(\boldsymbol{\xi},\boldsymbol{\eta})|. \tag{4.16}
$$

So, in order to control the error terms on the last three lines of (4.15) we need to estimate the quantities

$$
\begin{aligned}
K_{\ell,n} &:= \int \Big| \Big(\prod_{k=1}^{n} S_{s_k}\, B\, S_{-s_k}\, S_t O^{(\ell)} \Big)(\xi_1, \ldots, \xi_{n+\ell}; \eta_1, \ldots, \eta_{n+\ell}) \Big| \, \mathrm{d}\boldsymbol{\xi}\, \mathrm{d}\boldsymbol{\eta} \qquad \text{and} \\
M_{\ell,n} &:= \int \Big| \Big(S_{s_n} A S_{-s_n} \prod_{k=1}^{n-1} S_{s_k}\, B\, S_{-s_k}\, S_t O^{(\ell)} \Big)(\xi_1, \ldots, \xi_{n+\ell-1}; \eta_1, \ldots, \eta_{n+\ell-1}) \Big| \, \mathrm{d}\boldsymbol{\xi}\, \mathrm{d}\boldsymbol{\eta}.
\end{aligned}
\tag{4.17}
$$

We begin by $K_{\ell,n}$. By the definition of the operator B (see (4.12)) we have, for general $m \in \mathbb{N}$ and $s \in \mathbb{R}$,

$$
\begin{aligned}
(S_s\, B\, S_{-s}\, O^{(m)})(\xi_1, \ldots, \xi_{m+1}; \eta_1, \ldots, \eta_{m+1}) &= \frac{2}{\varepsilon} \sum_{j=1}^{m} \hat{U}(\xi_{m+1}) \, \sin\Big(\frac{\varepsilon}{2} (\eta_j - s\xi_j) \xi_{m+1} \Big) \\
&\quad \times \delta(\eta_{m+1} - s\xi_{m+1})\, O^{(m)}(\xi_1, \ldots, \xi_j + \xi_{m+1}, \ldots, \xi_m; \eta_1, \ldots, \eta_j + s\xi_{m+1}, \ldots, \eta_m)\,.
\end{aligned}
\tag{4.18}
$$

Since $|\sin x| \le |x|$, we obtain the bound

$$
\begin{aligned}
K_{\ell,n} \le \int \mathrm{d}\xi_1 \ldots \mathrm{d}\xi_{n+\ell} \mathrm{d}\eta_1 \ldots \mathrm{d}\eta_{n+\ell-1} |\hat{U}(\xi_{\ell+n})|\, |\xi_{\ell+n}| \sum_{j=1}^{\ell+n-1} |\eta_j - s_n \xi_j| \\
\times \Big| \Big(\prod_{k=1}^{n-1} S_{s_k}\, B\, S_{-s_k}\, S_t O^{(\ell)} \Big)(\xi_1, \ldots, \xi_{n+\ell-1}; \eta_1, \ldots, \eta_{n+\ell-1}) \Big|.
\end{aligned}
\tag{4.19}
$$

Applying equation (4.18) once again we find

$$
\begin{aligned}
K_{\ell,n} \le \int & \mathrm{d}\xi_1 \ldots \mathrm{d}\xi_{n+\ell} \mathrm{d}\eta_1 \ldots \mathrm{d}\eta_{n+\ell-1} |\hat{U}(\xi_{\ell+n})| |\xi_{\ell+n}|\, |\hat{U}(\xi_{\ell+n-1})|\, |\xi_{\ell+n-1}|\, \delta(\eta_{n+\ell-1} - s_{n-1}\xi_{n+\ell-1}) \\
& \times \Big(\sum_{j_1=1}^{\ell+n-1} |\eta_{j_1} - s_n \xi_{j_1}| \Big) \sum_{j_2=1}^{n+\ell-2} |\eta_{j_2} - s_{n-1} \xi_{j_2}| \\
& \times \Big| \Big(\prod_{k=1}^{n-2} S_{s_k}\, B\, S_{-s_k}\, S_t O^{(\ell)} \Big)(\xi_1, .., \xi_{j_2} + \xi_{n+\ell-1}, .., \xi_{n+\ell-2}; \eta_1, .., \eta_{j_2} + s_{n-1}\xi_{n+\ell-1}, .. \eta_{n+\ell-2}) \Big|.
\end{aligned}
\tag{4.20}
$$

After shifting the variables $\xi_{j_2} \to \xi_{j_2} - \xi_{n+\ell-1}$, $\eta_{j_2} \to \eta_{j_2} - s_{n-1}\xi_{n+\ell-1}$ and computing the integral over $\eta_{n+\ell-1}$ (using the delta-function) we get

$$K_{\ell,n} \leq \int \mathrm{d}\xi_1 \dots \mathrm{d}\xi_{n+\ell} \mathrm{d}\eta_1 \dots \mathrm{d}\eta_{n+\ell-2} |\hat{U}(\xi_{\ell+n})||\xi_{\ell+n}|\, |\hat{U}(\xi_{\ell+n-1})|\, |\xi_{\ell+n-1}| \\ \times \Big(\sum_{j_1=1}^{\ell+n-2} |\eta_{j_1} - s_n \xi_{j_1}| + 2(s_{n-1} - s_n)|\xi_{n+\ell-1}| \Big) \Big(\sum_{j_2=1}^{n+\ell-2} |\eta_{j_2} - s_{n-1}\xi_{j_2}| \Big) \\ \times \Big| \Big(\prod_{k=1}^{n-2} S_{s_k}\, B\, S_{-s_k}\, S_t O^{(\ell)} \Big)(\xi_1, \dots, \xi_{n+\ell-2}; \eta_1, \dots \eta_{n+\ell-2}) \Big| . \tag{4.21}$$

After n such iterations we arrive to the estimate

$$K_{\ell,n} \leq \int \mathrm{d}\xi_1 \dots \mathrm{d}\xi_{n+\ell}\, \mathrm{d}\eta_1 \dots \mathrm{d}\eta_\ell \prod_{k=1}^{n} |\hat{U}(\xi_{\ell+k})|\, |\xi_{\ell+k}| \\ \times \prod_{k=1}^{n} \Big(\sum_{i=1}^{\ell} |\eta_i + (t - s_k)\xi_i| + 2 \sum_{j=\ell+1}^{\ell+k-1} (s_{j-\ell} - s_k)|\xi_j|) \Big) |O^{(\ell)}(\boldsymbol{\xi}, \boldsymbol{\eta})| . \tag{4.22}$$

Using that $|s_i - s_j| \leq t$ for all i, j we get the bound

$$K_{\ell,n} \leq \int \mathrm{d}\xi_1 \dots \mathrm{d}\xi_{n+\ell}\, \mathrm{d}\eta_1 \dots \mathrm{d}\eta_\ell \prod_{k=1}^{n} |\hat{U}(\xi_{\ell+k})|\, |\xi_{\ell+k}| \\ \times \prod_{k=1}^{n} \Big(\sum_{i=1}^{\ell} (|\eta_i| + t|\xi_i|) + 2t \sum_{j=\ell+1}^{\ell+k-1} |\xi_j|) \Big) |O^{(\ell)}(\boldsymbol{\xi}, \boldsymbol{\eta})| . \tag{4.23}$$

Let us use the notation

$$x_1 := \sum_{i=1}^{\ell} (|\eta_i| + t|\xi_i|) ; \quad x_j := 2t|\xi_{\ell+j-1}| \quad \text{for } j = 2, \dots, n . \tag{4.24}$$

The integrand on the right hand side of equation (4.22) is dominated by

$$\Big(\prod_{k=1}^{n} |\hat{U}(\xi_{\ell+k})|\, |\xi_{\ell+k}| \Big) \cdot |O^{(\ell)}(\xi_1, \dots, \xi_\ell; \eta_1, \dots, \eta_\ell)| \cdot \prod_{k=1}^{n} \sum_{j=1}^{k} x_j , \tag{4.25}$$

which, in turn, is bounded by

$$\Big(\prod_{k=1}^{n} |\hat{U}(\xi_{k+1})|\, |\xi_{k+1}| \Big) \cdot |O^{(\ell)}(\xi_1, \dots, \xi_\ell; \eta_1, \dots, \eta_\ell)| \cdot \Big(\sum_{j=1}^{n} \frac{n - j + 1}{n} x_j \Big)^n , \tag{4.26}$$

where we estimated the product by its arithmetic mean in power n. Next we use the binomial expansion

$$\Big(\sum_{j=1}^{n}\frac{n-j+1}{n}x_j\Big)^n = n!\sum_{\alpha_1+\ldots+\alpha_n=n}\prod_{j=1}^{n}\frac{\left(\frac{n-j+1}{n}x_j\right)^{\alpha_j}}{\alpha_j!}\,,$$

and we note that, because of the assumption (4.7), we have

$$\begin{aligned}
&\int |O^{(\ell)}(\xi_1,\ldots,\xi_\ell;\eta_1,\ldots,\eta_\ell)|\left(\sum_{i=1}^{\ell}|\eta_i|+t|\xi_i|\right)^{\alpha}\mathrm{d}\xi\,\mathrm{d}\eta\\
&\qquad\le(1+t)^{\alpha}\sum_{\alpha_1+\ldots+\alpha_\ell=\alpha}\frac{\alpha!}{\prod\alpha_i!}\int|O^{(\ell)}(\xi_1,\ldots,\xi_\ell;\eta_1,\ldots,\eta_\ell)|\prod_{i=1}^{\ell}(|\eta_i|+|\xi_i|)^{\alpha_i}\,\mathrm{d}\xi\,\mathrm{d}\eta\\
&\qquad\qquad\le C_0^{\ell}(1+t)^{\alpha}\,\kappa_2^{\alpha}\,\alpha!\sum_{\alpha_1+\ldots+\alpha_\ell=\alpha}1\le C_0^{\ell}\,(1+t)^{\alpha}\,\kappa_2^{\alpha}\,\frac{(\alpha+\ell)!}{\ell!}\,.
\end{aligned}\tag{4.27}$$

This, together with the assumption (4.5), implies that

$$\begin{aligned}
K_{\ell,n}&\le C_0^{\ell}\,n!\sum_{\alpha_1+\ldots+\alpha_n=n}\kappa_2^{\alpha_1}(1+t)^{\alpha_1}\,\kappa_1^{2n-\alpha_1-1}(2t)^{n-\alpha_1}\frac{(\alpha_1+\ell)!}{\alpha_1!\ell!}\prod_{j=2}^{n}(\alpha_j+1)\Big(\frac{n-j+1}{n}\Big)^{\alpha_j}\\
&\le C_0^{\ell}\,\kappa_1^{n-1}((1+t)\kappa_1+2t\kappa_2)^n\frac{(n+\ell)!}{\ell!}\prod_{j=2}^{n}\Big(\frac{1}{1-\frac{n-j+1}{n}}\Big)^2\\
&\le C_0^{\ell}\frac{(n+\ell)!}{\ell!}\,\kappa_1^{n-1}(\kappa_1+\kappa_2)^n(1+2t)^n\Big(\frac{n^{n-1}}{(n-1)!}\Big)^2\le n!\binom{n+\ell}{\ell}C_0^{\ell}\kappa_1^{-1}\left[9\kappa_1(\kappa_1+\kappa_2)(1+2t)\right]^n.
\end{aligned}\tag{4.28}$$

Analogously we can bound $M_{\ell,n}$. Using the definition of A we find

$$\begin{aligned}
M_{\ell,n}\le\varepsilon^3\int\mathrm{d}q\,|\hat U(q)|\,|q|\,&\sum_{j<k}|(\eta_j-s_n\xi_j)-(\eta_k-s_n\xi_k)|\\
&\cdot\Big|\Big(\prod_{r=1}^{n-1}S_{s_r}\,B\,S_{-s_r}\,S_tO^{(\ell)}\Big)(\xi_1,\ldots,\xi_{\ell+n-1};\eta_1,\ldots,\eta_{\ell+n-1})\Big|\,\mathrm{d}\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{\eta}\,,
\end{aligned}\tag{4.29}$$

and since

$$\sum_{j<k}|\eta_j-s_n\xi_j-(\eta_k-s_n\xi_k)|\le(\ell+n-2)\sum_{j=1}^{\ell+n-1}|\eta_j-s_n\xi_j|\,,$$

we get the bound

$$M_{\ell,n}\le\varepsilon^3(\ell+n-2)K_{\ell,n}\,.\tag{4.30}$$

Inserting (4.28) and (4.30) in (4.15) and performing the integration over the s variables, we find

$$\begin{aligned}
&\Big|\langle O^{(\ell)}, \mu_N^{(\ell)}(t)\rangle - \Big\{\langle S_t O^{(\ell)}, \mu_N^{(\ell)}(0)\rangle + \\
&\quad + \sum_{m=1}^{n-1} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \ldots \int_0^{s_{m-1}} \mathrm{d}s_m \langle S_{s_m} B S_{s_{m-1}-s_m} B \ldots B S_{t-s_1} O^{(\ell)}, \mu_N^{(\ell+m)}(0)\rangle\Big\}\Big| \\
&\qquad\qquad \leq \binom{n+\ell}{\ell} C_0^\ell \kappa_1^{-1}\, \kappa_t^n + 2\kappa_1^{-1} C_0^\ell \varepsilon^3 \sum_{m=1}^{n} (\ell+m) \binom{m+\ell}{m} \kappa_t^m\,,
\end{aligned} \tag{4.31}$$

where we introduced $\kappa_t := 9t\kappa_1(\kappa_1+\kappa_2)(1+2t)$. Next we want to compare $\langle O^{(\ell)}, \mu_N^{(\ell)}(t)\rangle$ with $\langle O^{(\ell)}, \tilde{\mu}_t^{(\ell)}\rangle$, where $\tilde{\mu}_t^{(\ell)}$ was defined in (4.2). Using that $\mu_t(\xi,\eta)$ is a solution of the 1-particle Hartree Equation (4.1) we find that $\tilde{\mu}_t^{(\ell)}$ satisfies the following hierarchy of equation:

$$\begin{aligned}
\partial_t \tilde{\mu}_t^{(\ell)}(\boldsymbol{\xi},\boldsymbol{\eta}) =& \,\boldsymbol{\xi}\cdot\nabla_{\boldsymbol{\eta}} \tilde{\mu}_t^{(\ell)}(\boldsymbol{\xi},\boldsymbol{\eta}) \\
&- \sum_{j=1}^{\ell} \int \mathrm{d}q \hat{U}(q) \frac{2}{\varepsilon} \sin\Big(\frac{\varepsilon q\cdot \eta_j}{2}\Big)\, \tilde{\mu}_t^{(\ell+1)}(\xi_1,\ldots,\xi_j - q,\ldots,\xi_n, q; \boldsymbol{\eta}, 0).
\end{aligned} \tag{4.32}$$

One can then expand the expectation $\langle O^{(\ell)}, \tilde{\mu}_t^{\ell}\rangle$ in a series, exactly as we did for $\langle O^{(\ell)}, \mu_N^{\ell}(t)\rangle$. Clearly one finds

$$\begin{aligned}
\langle O^{(\ell)}, \tilde{\mu}_t^{(\ell)}\rangle =& \,\langle S_t O^{(\ell)}, \tilde{\mu}_0^{(\ell)}\rangle \\
&+ \sum_{m=1}^{n-1} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \ldots \int_0^{s_{m-1}} \mathrm{d}s_m \langle S_{s_m} B S_{s_{m-1}-s_m} B \ldots B S_{t-s_1} O^{(\ell)}, \tilde{\mu}_0^{(\ell+m)}\rangle \\
&+ \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \ldots \int_0^{s_{n-1}} \mathrm{d}s_n \langle B S_{s_{n-1}-s_n} B \ldots B S_{t-s_1} O^{(\ell)}, \tilde{\mu}_{s_n}^{(\ell+m)}\rangle.
\end{aligned} \tag{4.33}$$

The error term on the last line can be bounded as before (equation (2.22) holds with $\mu_N^{(k)}$ replaced by $\tilde{\mu}^{(k)}$ as well). We have

$$\begin{aligned}
&\Big|\langle O^{(\ell)}, \tilde{\mu}_t^{(\ell)}\rangle - \Big\{\langle S_t O^{(\ell)}, \tilde{\mu}_0^{(\ell)}\rangle + \\
&\quad + \sum_{m=1}^{n-1} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \ldots \int_0^{s_{m-1}} \mathrm{d}s_m \langle S_{s_m} B S_{s_{m-1}-s_m} B \ldots B S_{t-s_1} O^{(\ell)}, \tilde{\mu}_0^{(\ell+m)}\rangle\Big\}\Big| \\
&\qquad\qquad \leq \binom{n+\ell}{\ell} C_0^\ell \kappa_1^{-1}\, \kappa_t^n\,.
\end{aligned} \tag{4.34}$$

Combining (4.31) and (4.34) we find

$$
\begin{aligned}
\left|\langle O^{(\ell)}, (\mu_N^{(\ell)}(t) - \tilde{\mu}_t^{(\ell)})\rangle\right| &\leq 2\binom{n+\ell}{\ell} C_0^\ell \kappa_1^{-1}\, \kappa_t^n + 2\varepsilon^3 C_0^\ell \kappa_1^{-1} \sum_{m=1}^{n} (\ell+m)\binom{m+\ell}{m} \kappa_t^m \\
&+ \left|\langle S_t O^{(\ell)}, (\mu_N^{(\ell)}(0) - \tilde{\mu}_0^{(\ell)})\rangle\right| \\
&+ \sum_{m=1}^{n-1} \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \ldots \int_0^{s_{m-1}} \mathrm{d}s_m \left|\langle S_{s_m} B S_{s_{m-1}-s_m} B \ldots B S_{t-s_1} O^{(\ell)}, (\mu_N^{(\ell+m)}(0) - \tilde{\mu}_0^{(\ell+m)})\rangle\right| .
\end{aligned}
\tag{4.35}
$$

Using the assumption (4.6) and equation (4.28) to bound $\|S_{s_m} B S_{s_{m-1}-s_m} B \ldots B S_{t-s_1} O^{(\ell)}\|_0$ we find

$$
\left|\langle O^{(\ell)}, \mu_N^\ell(t) - \tilde{\mu}_t^\ell\rangle\right| \leq 2\binom{n+\ell}{\ell} C_0^\ell \kappa_1^{-1}\, \kappa_t^n + C_0^\ell \varepsilon^3 + 3\varepsilon^3 C_0^\ell \kappa_1^{-1} \sum_{m=1}^{n} (\ell+m)\binom{m+\ell}{m} \kappa_t^m . \tag{4.36}
$$

Using that

$$
\binom{n+\ell}{n} \leq 2^{n+\ell},
$$

and that

$$
\sum_{m=1}^{\infty} (\ell+m)\binom{m+\ell}{m} \kappa_t^m \leq (\ell+2)^2\, \kappa_t \sum_{m=0}^{\infty} \binom{m+\ell+2}{m} \kappa_t^m = (\ell+2)^2\, \kappa_t \left(\frac{1}{1-\kappa_t}\right)^{\ell+3} , \tag{4.37}
$$

the claim of Lemma 4.1 follows. □

In order to apply this lemma to prove Theorem 3.1, we need to estimate the $\boldsymbol{\alpha}$-norm of some product of Gaussian functions in the $\boldsymbol{\xi}$- and in the $\boldsymbol{\eta}$-space. This is the aim of the following lemma.

Lemma 4.2. *For $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_\ell)$, $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_\ell)$ we set*

$$
F_{\delta_1,\delta_2}^{(\ell)}(\boldsymbol{\xi}, \boldsymbol{\eta}) := e^{-\frac{\delta_1^2 \boldsymbol{\xi}^2}{4}}\, e^{-\frac{\delta_2^2 \boldsymbol{\eta}^2}{4}} . \tag{4.38}
$$

Then there exist universal constants C_1 and C_2 such that for arbitrary $\kappa > 0$

$$
\|F_{\delta_1,\delta_2}^{(\ell)}\|_{\boldsymbol{\alpha}} \leq \left(\frac{C_1}{\delta_1^3 \delta_2^3}\right)^{\ell} C_2^{\ell/(\delta^2\kappa^2)}\, \kappa^{|\boldsymbol{\alpha}|} \alpha_1! \ldots \alpha_\ell! \,, \tag{4.39}
$$

where $\delta^{-1} := \delta_1^{-1} + \delta_2^{-1}$, and $|\boldsymbol{\alpha}| = \alpha_1 + \cdots + \alpha_\ell$.

Proof. We have

$$
\begin{aligned}
\|F^{(\ell)}_{\delta_1,\delta_2}\|_{\boldsymbol{\alpha}} &= \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\, |F^{(\ell)}_{\delta_1,\delta_2}(\boldsymbol{\xi},\boldsymbol{\eta})| \prod_{j=1}^{\ell}(|\xi_j|+|\mu_j|)^{\alpha_j} = \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\, e^{-\frac{\delta_1^2\boldsymbol{\xi}^2}{4}}\, e^{-\frac{\delta_2^2\boldsymbol{\eta}^2}{4}} \prod_{j=1}^{\ell}(|\xi_j|+|\eta_j|)^{\alpha_j} \\
&\leq \prod_{j=1}^{\ell} 2^{\alpha_j}\Big\{ \int \mathrm{d}\xi_j e^{-\frac{\delta_1^2\xi_j^2}{4}}|\xi_j|^{\alpha_j} \int \mathrm{d}\eta_j e^{-\frac{\delta_2^2\eta_j^2}{4}} + \int \mathrm{d}\xi_j e^{-\frac{\delta_1^2\xi_j^2}{4}} \int \mathrm{d}\eta_j e^{-\frac{\delta_2^2\eta_j^2}{4}}|\eta_j|^{\alpha_j}\Big\} \\
&= \left(\frac{C_1}{\delta_1^3\delta_2^3}\right)^{\ell} \prod_{j=1}^{\ell}\left(\frac{4}{\delta}\right)^{\alpha_j} \Gamma\left(\frac{\alpha_j+3}{2}\right),
\end{aligned}
\tag{4.40}
$$

for a universal constant C_1. Here we put $\delta = (\delta_1^{-1}+\delta_2^{-1})^{-1}$. Simple estimate shows that

$$
\Gamma\left(\frac{\alpha_j+3}{2}\right) \leq \frac{D_1^{\alpha_j+1}}{\alpha_j^{\alpha_j/2}}\, \alpha_j!\,, \tag{4.41}
$$

thus

$$
\|F^{(\ell)}_{\delta_1,\delta_2}\|_{\boldsymbol{\alpha}} \leq \left(\frac{C_1}{\delta_1^3\delta_2^3}\right)^{\ell} \prod_{j=1}^{\ell}\left(\frac{D_2}{\delta^2\alpha_j}\right)^{\alpha_j/2} \alpha_j!\,, \tag{4.42}
$$

where C_1, D_2 are universal constants. Elementary calculation shows that

$$
\left(\frac{D_2}{\delta^2\alpha_j}\right)^{\alpha_j/2} \leq C_2^{1/(\delta^2\kappa^2)}\kappa^{\alpha_j} \tag{4.43}
$$

for a sufficiently large universal constant C_2. $\square$

We are now ready to proceed with the proof of our main result, Theorem 3.1.

Proof of Theorem 3.1. First we note that the assumption (3.6) is equivalent to the assumption (4.6) in Lemma 4.1 after taking Fourier transform. On the other hand, with the notation $\delta W^{(\ell)}(t) := W_N^{(\ell)}(t) - \widetilde{W}^{(\ell)}(t)$ we have

$$
\begin{aligned}
\left(H^{\delta_1,\delta_2}_{\ell,N} - \widetilde{H}^{\delta_1,\delta_2}_{\ell,N}\right)(t,\mathbf{x},\mathbf{v}) &= \int \mathrm{d}\mathbf{x}'\mathrm{d}\mathbf{v}'\, G^{(\ell)}_{\delta_1}(\mathbf{x}-\mathbf{x}')G^{(\ell)}_{\delta_2}(\mathbf{v}-\mathbf{v}')\delta W^{(\ell)}(t,\mathbf{x}',\mathbf{v}') \\
&= \left(\frac{1}{2\pi}\right)^{6\ell} \int \mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{\eta}\, e^{i(\mathbf{x}\cdot\boldsymbol{\xi}+\mathbf{v}\cdot\boldsymbol{\eta})} e^{-\frac{\delta_1^2\boldsymbol{\xi}^2}{4}}\, e^{-\frac{\delta_2^2\boldsymbol{\eta}^2}{4}}\, \delta\mu^{(\ell)}(t,\boldsymbol{\xi},\boldsymbol{\eta})\,.
\end{aligned}
\tag{4.44}
$$

In the following we use the notation

$$
\tilde{F}^{(\ell)}_{\delta_1,\delta_2}(\boldsymbol{\xi},\boldsymbol{\eta}) := \left(\frac{1}{2\pi}\right)^{6\ell} e^{i(\mathbf{x}\cdot\boldsymbol{\xi}+\mathbf{v}\cdot\boldsymbol{\eta})} \exp\Big(-\frac{\delta_1^2\boldsymbol{\xi}^2}{4} - \frac{\delta_2^2\boldsymbol{\eta}^2}{4}\Big).
$$

From Lemma 4.2 we find, for an arbitrary $\kappa_2 > 0$,

$$\|\tilde{F}^{(\ell)}_{\delta_1,\delta_2}\|_{\boldsymbol{\alpha}} \leq \left(\frac{C_1}{2\pi\delta_1^3\delta_2^3}\right)^{\ell} C_2^{\ell/(\delta^2\kappa_2^2)}\ \kappa_2^{|\boldsymbol{\alpha}|}\alpha_1!\dots\alpha_\ell! \tag{4.45}$$

where the constants C_1 and C_2 are universal. From Lemma 4.1 and from Eq. (4.44) it follows that

$$\begin{aligned}\left|\left(H^{\delta_1,\delta_2}_{\ell,N} - \widetilde{H}^{\delta_1,\delta_2}_{\ell,N}\right)(t,\mathbf{x},\mathbf{v})\right| \leq\ & 2\kappa_1^{-1}\left(\frac{C_1}{\pi\delta_1^3\delta_2^3}\right)^{\ell} C_2^{\ell/(\delta^2\kappa_2^2)}\ (2\kappa_t)^n \\ & + \frac{1}{N}\left(\frac{C_1}{2\pi\delta_1^3\delta_2^3}\right)^{\ell} C_2^{\ell/(\delta^2\kappa_2^2)}\left(1 + \frac{3\kappa_t}{\kappa_1}(\ell+2)^2\left(\frac{1}{1-\kappa_t}\right)^{\ell+3}\right)\end{aligned}$$

for any $\kappa_2 > 0$ and $n \leq 2\log N - \ell$. Here, as in Lemma 4.1, we use the notation $\kappa_t = 9\kappa_1(\kappa_1 + \kappa_2)t(1+2t)$. Since $t < \frac{1}{4}(\sqrt{1 + 1/(7\kappa_1^2)} - 1)$, we can fix $\kappa_2 > 0$ such that $2\kappa_t \leq e^{-1}$. Then choosing $n = \log N$ we find

$$\left|\left(H^{\delta_1,\delta_2}_{\ell,N} - \widetilde{H}^{\delta_1,\delta_2}_{\ell,N}\right)(t,\mathbf{x},\mathbf{v})\right| \leq \frac{C_{\ell,\delta_1,\delta_2}}{N}, \tag{4.46}$$

where $C_{\ell,\delta_1,\delta_2}$ is independent of N. Thus, for any fixed ℓ, δ_1, δ_2 we get

$$\limsup_{N\to\infty}\ \sup_{\mathbf{x},\mathbf{v}\in\mathbb{R}^{3\ell}}\left|\left(H^{\delta_1,\delta_2}_{\ell,N} - \widetilde{H}^{\delta_1,\delta_2}_{\ell,N}\right)(t,\mathbf{x},\mathbf{v})\right| \cdot N \leq C_{\ell,\delta_1,\delta_2}. \tag{4.47}$$

$\square$

A Proof of Lemma 3.3 and 3.4

Proof of Lemma 3.3. We can restrict ourselves to pure states. Let Ψ be a normalized fermionic wavefunction. For any $X \in \mathbb{R}^3$ define

$$\Psi_X(y_1,\dots,y_{N-1}) := \Psi\big(y_1 + \bar{X}, y_2 + \bar{X}, \dots, y_{N-1} + \bar{X}, \bar{X} - (y_1 + \ldots + y_{N-1})\big)\ ,$$

where $\bar{X} := X/N$. Clearly Ψ_X is antisymmetric and $\int \|\Psi_X\|^2 \mathrm{d}X = 1$. By the Lieb-Thirring inequality in the Fourier space (3.18)

$$\int \varrho_X(v)^{5/3}\,\mathrm{d}v \leq (const.)\|\Psi_X\|^{4/3}\Big\langle\Psi_X, \Big(\sum_{j=1}^{N-1} y_j^2\Big)\Psi_X\Big\rangle\ , \tag{A.48}$$

where $\varrho_X := \varrho_{\Psi_X}$ is the momentum distribution of the one-particle marginal of Ψ_X with the normalization $\int \varrho_X = (N-1)\|\Psi_X\|^2$ (see the proof of Lemma 3.2). Simple calculation shows that

$$\int \mathrm{d}X\,\Big\langle\Psi_X, \Big(\sum_{j=1}^{N-1} y_j^2\Big)\Psi_X\Big\rangle = \frac{N-1}{N}\Big\langle\Psi, \sum_{j=1}^{N}(x_j - \bar{X})^2\ \Psi\Big\rangle\ . \tag{A.49}$$

For an arbitrary $\rho(v) \in L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3)$ we have

$$\begin{aligned} \int_{|v|\geq \ell} \mathrm{d}v\, \rho(v) &\leq \frac{1}{\ell^2} \int_{|v|\geq \ell} \mathrm{d}v\, v^2 \rho(v) \leq \frac{1}{\ell^2} \int \mathrm{d}v\, v^2 \rho(v), \\ \int_{|v|\leq \ell} \mathrm{d}v\, \rho(v) &\leq \ell^3 \left(\frac{1}{\ell^3} \int_{|v|\leq \ell} \mathrm{d}v\, \rho^{5/3}(v) \right)^{3/5} \leq \ell^{6/5} \|\rho\|_{5/3}. \end{aligned} \tag{A.50}$$

This implies that

$$\int \mathrm{d}v\, \rho(v) \leq \frac{1}{\ell^2} \int \mathrm{d}v\, v^2 \rho(v) + \ell^{6/5} \|\rho\|_{5/3}. \tag{A.51}$$

Optimizing with respect to ℓ we easily obtain $\int v^2 \varrho(v) \mathrm{d}v \geq (const.) \|\varrho\|_1^{8/3} / \|\varrho\|_{5/3}^{5/3}$ with a positive constant. Applying this inequality for ϱ_X, using (A.48) and the normalization $\|\varrho_X\|_1 = (N-1)\|\Psi_X\|^2$, we have

$$\int v^2 \varrho_X(v)\, \mathrm{d}v \geq \frac{(const.)(N-1)^{8/3} \|\Psi_X\|^4}{\left\langle \Psi_X, \left(\sum y_j^2 \right) \Psi_X \right\rangle}\,.$$

Integrating X, using a Schwarz inequality and (A.49) we obtain

$$\iint v^2 \varrho_X(v)\, \mathrm{d}v\, \mathrm{d}X \geq (const.) N^{8/3} \frac{\left(\int \|\Psi_X\|^2 \, \mathrm{d}X \right)^2}{\int \left\langle \Psi_X, \left(\sum y_j^2 \right) \Psi_X \right\rangle \mathrm{d}X} \geq (const.) N^{5/3}$$

if $N \geq 2$. Finally we conclude by the identity

$$\iint v^2\ \varrho_X(v)\, \mathrm{d}v\, \mathrm{d}X = \int \mathrm{d}X \left\langle \Psi_X, \Big(\sum_{j=1}^{N-1} (p_j - p_N)^2 \Big) \Psi_X \right\rangle = (N-1) \langle \Psi, (p_1 - p_2)^2 \Psi \rangle\ ,$$

where we again used the symmetry of Ψ. $\square$

Proof of Lemma 3.4. First we want to prove that v_t remains of order $N^{1/3}$ for all finite times. To this end we compute

$$\begin{aligned} [iH_{N,\alpha}, (p_1 - p_2)^2] = &-\frac{1}{N} \sum_{m\geq 3} \Big((p_1 - p_2) \cdot (\nabla U(x_1 - x_m) - \nabla U(x_2 - x_m)) \\ &\qquad + (\nabla U(x_1 - x_m) - \nabla U(x_2 - x_m)) \cdot (p_1 - p_2) \Big) \\ &-\frac{2}{N} \Big((p_1 - p_2) \cdot \nabla U(x_1 - x_2) + \nabla U(x_1 - x_2) \cdot (p_1 - p_2) \Big), \end{aligned}$$

which implies, using $C = \|\nabla U\|_\infty$, and applying the Schwarz inequality, that

$$|\partial_t v_t^2| = \left|\mathrm{Tr}\,\left(\gamma_{N,t}[iH_{N,\alpha},(p_1-p_2)^2]\right)\right| \leq 8C\, v_t.$$

Integrating the last equation we obtain

$$v_0 - 4Ct \leq v_t \leq v_0 + 4Ct \tag{A.52}$$

for all $t > 0$. Next we derive an upper bound for the quantity u_t. Here we use

$$[iH_{N,\alpha},(x_1-x_2)^2] = 2\alpha\Big((p_1-p_2)\cdot(x_1-x_2) + (x_1-x_2)\cdot(p_1-p_2)\Big),$$

and from (A.52) we find that

$$|\partial_t u_t^2| \leq 4\alpha\, v_t\, u_t \leq 4\,\alpha\,(v_0 + 4Ct)\, u_t, \tag{A.53}$$

hence, for $t \leq v_0/8C$,

$$u_t \leq u_0 + 3\,\alpha\, v_0\, t. \tag{A.54}$$

Finally we want to estimate the quantity u_t from below. To this end we compute the second derivative of u_t using that

$$\begin{aligned}[iH_{N,\alpha},[iH_{N,\alpha},(x_1-x_2)^2]] = 8\alpha^2(p_1-p_2)^2 - \frac{4\alpha}{N}\sum_{m\geq 3}(\nabla U(x_1-x_m) - \nabla U(x_2-x_m))\cdot(x_1-x_2) \\ - \frac{8\alpha}{N}\nabla U(x_1-x_2)\cdot(x_1-x_2).\end{aligned}$$

Applying the Schwarz inequality, using $C = \|\nabla U\|_\infty$ and equations (A.52), (A.54), we find

$$\begin{aligned}\partial_t^2 u_t^2 &\geq 8\,\alpha^2\, v_t^2 - 8C\,\alpha\, u_t \\ &\geq 2\alpha^2\, v_0^2 - 8C\,\alpha\,(u_0 + 3\,\alpha\, v_0 t)\ ,\end{aligned}$$

for $t \leq v_0/8C$. Integrating this equation twice with the help of (A.53), one easily finds (3.22). □

References

[1] V. Bach: *Error bound for the Hartree-Fock energy of atoms and molecules.* Comm. Math. Phys. **147** (1992), no. 3, 527–548.

[2] C. Bardos, F. Golse, A. Gottlieb, and N. Mauser: *Mean field dynamics of fermions and the time-dependent Hartree-Fock equation.* J. Math. Pures Appl. (9) **82** (2003), 665–683.

[3] S. Chandrasekhar: *On stars, their evolution and their stability.* Rev. Mod. Phys. **56** (1984), 137–147.

[4] C. Fefferman and L. Seco: *On the energy of a large atom.* Bull. Amer. Math. Soc. (N.S.) **23** (1990), no. 2, 525–530.

[5] C. Fefferman and L. Seco: *On the Dirac and Schwinger corrections to the ground-state energy of an atom.* Adv. Math. **107** (1994), no. 1, 1–185.

[6] J. Ginibre and G. Velo: *The classical field limit of scattering theory for non-relativistic many-boson systems. I and II.* Commun. Math. Phys. **66**, 37–76 (1979) and **68**, 45-68 (1979).

[7] J. Ginibre and G. Velo: *On a class of nonlinear Schrödinger equations with nonlocal interactions.* Math. Z. **170**, 109–145 (1980)

[8] S. Graffi, A. Martinez, and M. Pulvirenti: *Mean-field approximation of quantum systems and classical limit.* Math. Models Methods Appl. Sci. **13** (2003), no. 1, 59–73.

[9] E. H. Lieb: *Density functional for Coulomb systems.* International J. Quantum Chem., **24** (1983), 243–277.

[10] E. H. Lieb and B. Simon: *The Hartree-Fock theory for Coulomb systems.* Comm. Math. Phys. **53** (1977), no. 3, 185–194.

[11] E. H. Lieb and B. Simon: *The Thomas-Fermi theory of atoms, molecules and solids.* Advances in Math. **23** (1977), no. 1, 22–116.

[12] E. H. Lieb, W. Thirring: *Inequalities for moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities.* In: Studies in Mathematical Physics (E. Lieb, B. Simon, A. Wightman eds.) Princeton University Press, 269–330 (1975).

[13] E H. Lieb and H.-T. Yau: *The Chandrasekhar theory of stellar collapse as the limit of quantum mechanics.* Comm. Math. Phys. **53** (1987), 147–174.

[14] H. Narnhofer and G. L. Sewell: *Vlasov hydrodynamics of a quantum mechanical model.* Commun. Math. Phys. **79** (1981), 9–24.

[15] H. Spohn: *On the Vlasov hierarchy.* Math. Methods Appl. Sci. **3** (1981), no. 4, 445–455.

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