



A Mixed-Norm Estimate of the Two-Particle Reduced Density Matrix of Many-Body Schrödinger Dynamics for Deriving the Vlasov Equation

Li Chen¹ · Jinyeop Lee² · Yue Li³ · Matthew Liew¹

Received: 2 November 2022 / Accepted: 26 May 2023 / Published online: 7 June 2023
© The Author(s) 2023

Abstract

We re-examine the combined semi-classical and mean-field limit in the N -body fermionic Schrödinger equation with pure state initial data using the Husimi measure framework. The Husimi measure equation involves three residue types: kinetic, semiclassical, and mean-field. The main result of this paper is to provide better estimates for the kinetic and mean-field residue than those in Chen et al. (J Stat Phys 182(2):1–41, <http://arxiv.org/abs/1910.09892v4>, 2021). Especially, the estimate for the mean-field residue is shown to be smaller than the semiclassical residue by a mixed-norm estimate of the two-particle reduced density matrix factorization. Our analysis also updates the oscillation estimate parts in the residual term estimates appeared in Chen et al. (J Stat Phys 182(2):1–41, <http://arxiv.org/abs/1910.09892v4>, 2021).

Keywords Large fermionic system · Vlasov equation · Husimi measure · Schrödinger equation · Mean-field limit · Semi-classical limit

Communicated by Michael Kiessling.

✉ Jinyeop Lee
lee@math.lmu.de

Li Chen
chen@math.uni-mannheim.de

Yue Li
liyue2011008@163.com

Matthew Liew
mliew@mail.uni-mannheim.de

¹ Institut für Mathematik, Universität Mannheim, Mannheim, Germany

² Mathematisches Institut, Ludwig-Maximilians-Universität München, Munich, Germany

³ Department of Mathematics, Nanjing University, Nanjing, China

1 Introduction

In this article, we consider the following N -particle mean-field Schrödinger equation

$$\begin{aligned}
 i\hbar\partial_t \psi_{N,t} &= -\frac{\hbar^2}{2} \sum_{j=1}^N \Delta_{x_j} \psi_{N,t} + \frac{1}{2N} \sum_{i \neq j}^N V(x_i - x_j) \psi_{N,t} \\
 \psi_{N,0} &= \frac{1}{\sqrt{N!}} \det\{e_j(x_i)\}_{i,j=1}^N,
 \end{aligned}
 \tag{1.1}$$

where $\{e_j\}_{j=1}^N$ is a family of orthonormal basis in $L^2(\mathbb{R}^3)$ and Δ_{x_j} is the Laplacian on j -th particle. The initial data in (1.1) is in the form of a Slater determinant, which stays in the antisymmetric subspace $L^2_a(\mathbb{R}^{3N})$ of $L^2(\mathbb{R}^3)$ with $\|\psi_{N,0}\|_2 = 1$, where

$$\begin{aligned}
 L^2_a(\mathbb{R}^{3N}) &:= \{\psi_N \in L^2(\mathbb{R}^{3N}) : \psi_N(x_{\pi(1)}, \dots, x_{\pi(N)}) \\
 &= (\text{sign } \pi) \psi_N(x_1, \dots, x_N) \text{ for all } \pi \in S_N\}.
 \end{aligned}$$

In the above formulation, S_N is the symmetric group.

Note that the number of the terms for interaction is of order N^2 . Hence, with the mean-field constant $1/N$ in front of the interaction, we could think that the size of interaction energy is of order N . Since we are interested in the regime where the size of kinetic energy is similar to the size of interaction energy, we have from Tomas–Fermi theory that $\hbar^2 N^{5/3} = N$. This gives $\hbar = N^{-1/3}$. For more details, we refer to [5, 6, 8].

As it is difficult to solve the Schrödinger equation in (1.1) numerically when the number of particle N is large, we aim to derive its corresponding effective evolution equation. In fact, we consider the k -particle reduced density matrix where its corresponding integral kernel is given by

$$\begin{aligned}
 \gamma_{N,t}^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) \\
 = \frac{N!}{(N-k)!} \int dx_{k+1} \dots dx_N \overline{\psi_{N,t}(y_1, \dots, y_k, x_{k+1}, \dots, x_N)} \psi_{N,t}(x_1, \dots, x_k, x_{k+1}, \dots, x_N),
 \end{aligned}
 \tag{1.2}$$

where $1 \leq k \leq N$. Moreover, we denote the expectation of the one-particle observable as follows,

$$\text{Tr} O \gamma_{N,t}^{(1)} = \langle \psi_{N,t}, O \psi_{N,t} \rangle = \int dx_1 \dots dx_N \overline{\psi_{N,t}(x_1, x_2, \dots, x_N)} (O \psi_{N,t})(x_1, x_2, \dots, x_N).$$

The one-particle reduce density matrix of the initial data given in (1.1) is $\omega_N = \sum_{j=1}^N |e_j\rangle\langle e_j|$, where its corresponding integral kernel is $\omega_N(x; y) = \sum_{j=1}^N \overline{e_j(y)} e_j(x)$.

1.1 Short Review of Mean-Field Limit, $N \rightarrow \infty$

It is well known that the Hartree–Fock equation

$$\begin{aligned}
 i\hbar\partial_t \omega_{N,t} &= \left[-\hbar^2 \Delta + (V * \rho_{N,t}) - X_t, \omega_{N,t} \right], \\
 \rho_{N,t} &= \frac{1}{N} \omega_{N,t}(x; x) \\
 X_t &= \frac{1}{N} V(x - y) \omega_{N,t}(x; y)
 \end{aligned}
 \tag{1.3}$$

is used to approximate the Schrödinger equation in the mean-field limit. Here we use the conventional notation $[A, B] := AB - BA$ for commutator of operators.

The mean field limit result for fixed \hbar has been given in [17] for short time. Under the scaling $\hbar = N^{-1/3}$, the rates of convergence in the trace norm and the Hilbert–Schmidt norm are obtained for arbitrary given time in [8] when the initial data is an approximation of the Slater determinant. Later on, the case with mixed state initial data has been considered in [7, 10]. Furthermore, for Coulomb and Riesz potentials, the rate of convergence is obtained in [40, 41]. We refer more references on this topic to [6, 19, 37–39] and the references therein.

1.2 Short Review of Semi-classical Limit, $\hbar \rightarrow 0$

The Vlasov equation can be obtained via semi-classical limit of the Hartree or the Hartree–Fock equations. It has been first investigated in [32] by using Wigner measure for smooth potentials. Recently, the rates of convergence in the trace norm as well as the Hilbert–Schmidt norm has been studied in [11] with regularity assumptions on the mixed state initial data and a class of regular potentials. The k -particle Wigner measure used in the [11, 32] reads

$$\begin{aligned}
 &W_{N,t}^{(k)}(x_1, p_1, \dots, x_k, p_k) \\
 := &\binom{N}{k}^{-1} \int (dy)^{\otimes k} \gamma_{N,t}^{(k)}\left(x_1 + \frac{\hbar}{2}y_1, \dots, x_k + \frac{\hbar}{2}y_k; x_1 - \frac{\hbar}{2}y_1, \dots, x_k - \frac{\hbar}{2}y_k\right) \\
 &e^{-i\sum_{i=1}^k p_i \cdot y_i}, \tag{1.4}
 \end{aligned}$$

Some of the recent developments in the semi-classical limit are the following: One can find results for the inverse power law potential in [43], for the rate of convergence in the Schatten norm in [30], for the Coulomb potential and mixed states in [42], and for the convergence in the Wasserstein distance in [28, 29]. Relativistic fermionic system has been studied in [16]. Further analyses of the semi-classical limit can be found in [1–3, 6, 20, 34].

1.3 Combined Mean-Field and Semi-classical Limits

Narnhofer and Sewell, and Spohn independently derived Vlasov equation (1.8) from the N -body Schrödinger equation (1.1) with $\hbar = N^{-1/3}$, in [36, 46]. Without assuming $\hbar = N^{-1/3}$, a rate of convergence was obtained in [25] in a weak formulation. The rate of convergence of the combined limits was studied in [22–24] by using the Wasserstein (pseudo-)distance. Under a generalized Husimi measure framework, the authors in [13] obtained the convergence for regular potentials. Recently, the combined limit for the singular potential case with regular mixed state initial data was obtained in [14].

It is well-known that the Wigner measure in (1.4) is not a (proper) probability measure, as there might be some point having negative sign. (We refer, e.g., [12, 26, 27, 33, 45] for further references on Wigner measure.) It has been shown that the Husimi measure, the convolution of the Wigner measure with a Gaussian function, is a nonnegative probability measure [15, 18, 48]. In particular, from [18, p.21], given a specific Gaussian coherent state, the relation between the Husimi measure and Wigner measure is given by the following convolution: for any $1 \leq k \leq N$,

$$m_{N,t}^{(k)} := \frac{N(N-1)\cdots(N-k+1)}{N^k} W_{N,t}^{(k)} * \mathcal{G}^{\hbar}, \tag{1.5}$$

where

$$\mathcal{G}^{\hbar}(q_1, p_1, \dots, q_k, p_k) := \frac{1}{(\pi \hbar)^{3k}} \exp\left(-\frac{\sum_{j=1}^k q_j^2 + p_j^2}{\hbar}\right).$$

The Wigner transform of Hartree (or Hartree–Fock) equation shares the structure of Vlasov equation, see [9, Eq. (6.15)] for example.

In this paper, following the ideas in [13], we study the equation for Husimi measure. Instead of using the classical definition of Husimi measure in (1.5), we consider the following generalized k -particle Husimi measure, which is given for example in [18]: For any $p, q \in \mathbb{R}^3$ and $\psi_{N,t} \in L^2_a(\mathbb{R}^{3N})$, the k -particle Husimi measure is given by

$$m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) = \langle \psi_{N,t}, a^*(f_{q_1,p_1}^{\hbar}) \cdots a^*(f_{q_k,p_k}^{\hbar}) a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \psi_{N,t} \rangle. \tag{1.6}$$

Here $a^*(f_{q,p}^{\hbar})$ and $a(f_{q,p}^{\hbar})$ are standard creation- and annihilation-operator respectively¹ with respect to the coherent state $f_{q,p}^{\hbar}$ given by

$$f_{q,p}^{\hbar}(y) := \hbar^{-\frac{3}{4}} f\left(\frac{y - q}{\sqrt{\hbar}}\right) e^{\frac{i}{\hbar} p \cdot y},$$

where f is any given real-valued function satisfying $\|f\|_2 = 1$.

Remark 1.1 As stated in [18], the k -particle Husimi measure $m_{N,t}^{(k)}$ describes how many fermions are within the k -semi-classical boxes of length $\sqrt{\hbar}$ centered at the phase-spaces $(q_1, p_1), \dots, (q_k, p_k)$.

Remark 1.2 If $f(x) = \pi^{-3/4} e^{-|x|^2/2}$, [15] shows that the k -particle Husimi measure $m_{N,t}^{(k)}$ coincides with the $m_{N,t}^{(k)}$ in (1.5).

1.4 Main Result

Let $\psi_{N,t}$ be the solution to the Schrödinger equation in (1.1) and denote the one-particle Husimi measure of it by $m_{N,t} := m_{N,t}^{(1)}$. From [13, Proposition 2.1], we obtain the following identity:

$$\begin{aligned} & \partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) - \nabla_q \cdot \left(\hbar \operatorname{Im} \langle \nabla_q a(f_{q,p}^{\hbar}) \psi_{N,t}, a(f_{q,p}^{\hbar}) \psi_{N,t} \rangle \right) \\ &= \frac{1}{(2\pi)^3} \nabla_p \cdot \int dw_1 du_1 dw_2 du_2 dq_2 dp_2 \left(f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes 2} \\ & \quad \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \end{aligned} \tag{1.7}$$

where

$$\left(f_{q,p}^{\hbar}(w_1) \overline{f_{q,p}^{\hbar}(u_1)} \right)^{\otimes 2} := f_{q,p}^{\hbar}(w_1) \overline{f_{q,p}^{\hbar}(u_1)} f_{q_2,p_2}^{\hbar}(w_2) \overline{f_{q_2,p_2}^{\hbar}(u_2)}.$$

Remark 1.3 The two-particle reduced density matrix in (1.7) is given in (1.2).

¹ Definitions of creation- and annihilation-operator is provided in Appendix A.

Our aim is therefore to obtain the convergence from $m_{N,t}$, in weak sense, to the solution of Vlasov equation m_t as follows:

$$\begin{aligned} \partial_t m_t(q, p) &= -p \cdot \nabla_q m_t(q, p) + \nabla_q (V * \varrho_t)(q) \cdot \nabla_p m_t(q, p), \\ m_t(q, p)|_{t=0} &= m_0(q, p), \end{aligned} \tag{1.8}$$

where $\varrho_t = \int dp m_t(q, p)$ and the initial data $m_0(q, p)$ is the one-particle Husimi measure of $\psi_{N,0}$ given in (1.1).

The following assumptions are needed in this paper.

- Assumption H1**
1. (Interaction potential) $V \in L^1(\mathbb{R}^3)$ and $V(-x) = V(x)$. Furthermore it holds $\int dp(1 + |p|^2)|\widehat{V}(p)| < \infty$, where \widehat{V} is its Fourier transform of V .
 2. (Coherent state) $f \in H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ satisfies $\|f\|_2 = 1$, and has compact support in B_{R_1} for a given $R_1 > 0$.
 3. (Initial data) m_N converges weakly to m_0 in $L^1(\mathbb{R}^3)$. Furthermore, it satisfies

$$\int dq dp (|p|^2 + |q|) m_N(q, p) < \infty \tag{1.9}$$

uniformly for all N .

4. (Initial data) ω_N , the one-particle density matrix of $\psi_{N,0}$ satisfies

$$\begin{aligned} \sup_{p \in \mathbb{R}^3} \frac{1}{1 + |p|} \|[e^{ip \cdot x}, \omega_N]\|_{\text{Tr}} &\leq CN\hbar, \\ \|[\hbar \nabla, \omega_N]\|_{\text{Tr}} &\leq CN\hbar, \end{aligned} \tag{1.10}$$

where $\|\cdot\|_{\text{Tr}}$ is the trace norm.

Remark 1.4 The assumptions in (1.10) can be explained by the nature of the semi-classical structure. More details can be found in [8] where mean field limit has been studied.

With the assumptions presented above, our final goal is to obtain the following theorem:

Theorem 1.1 *Let $m_{N,t}$ be the one-particle Husimi measure defined in (1.6) with $\psi_{N,t}$ the solution of Schrödinger equation (1.1), and suppose the aforementioned assumptions hold and m_t is the solution of Vlasov equation in (1.8). Then, for any given $T > 0$, $(m_{N,t})_{N \in \mathbb{N}}$ converges to m_t weakly (*) in $L^p((0, T) \times \mathbb{R}^3 \times \mathbb{R}^3)$ for arbitrary $1 \leq p \leq \infty$.*

Remark 1.5 As a consequence, [47, Theorem 6.9] implies, for $t \geq 0$, that $W_1(m_{N,t}, m_t) \rightarrow 0$ as $N \rightarrow \infty$, where W_1 is 1-Weisserstein distance.

For convenience, we use the Fock space formalism, which will be briefly introduced in Appendix A. By using Husimi transform given in (1.7), the Schrödinger equation for $\psi_{N,t}$ can be rewritten into the Vlasov type equation for $m_{N,t}$ with residual terms. More precisely, from the computations in [13], we have

$$\begin{aligned} &\partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) \\ &= \frac{1}{(2\pi)^3} \nabla_p \cdot \int dq_2 \nabla V(q - q_2) \varrho_{N,t}(q_2) m_{N,t}(q, p) + \nabla_q \cdot \widetilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R}_s + \nabla_p \cdot \mathcal{R}_m, \end{aligned} \tag{1.11}$$

where $\varrho_{N,t}(q) := \int dp m_{N,t}(q, p)$, the kinetic residue $\widetilde{\mathcal{R}}$, the semi-classical residue \mathcal{R}_s and the mean-field residue \mathcal{R}_m are given by

$$\widetilde{\mathcal{R}} := \hbar \text{Im} \langle \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t}, a(f_{q,p}^\hbar) \Psi_{N,t} \rangle,$$

$$\begin{aligned}
 \mathcal{R}_s &:= \frac{1}{(2\pi)^3} \int dw_1 du_1 dw_2 du_2 dq_2 dp_2 \left(f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes 2} \\
 &\quad \left[\int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \\
 \mathcal{R}_m &:= \frac{1}{(2\pi)^3} \int dw_1 du_1 dw_2 du_2 dq_2 dp_2 \left(f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes 2} \\
 &\quad \nabla V(q - q_2) \left[\gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right].
 \end{aligned}
 \tag{1.12}$$

Remark 1.6 The three terms—kinetic residue $\tilde{\mathcal{R}}$, semiclassical residue \mathcal{R}_s , and mean-field residue \mathcal{R}_m —arise due to the following reasons: The kinetic residue $\tilde{\mathcal{R}}$ is bounded by the kinetic energy estimate. This term’s name reflects its connection to the kinetic energy used in establishing the bound. The semiclassical residue \mathcal{R}_s is proven to be small by oscillatory integrals that appear due to the Husimi transform. Similarly, the estimate of mean-field residue \mathcal{R}_m is transformed into the factorization of two-particle reduced density matrix, which is a characteristic of mean-field behavior. Thus, its name denotes its association with mean-field properties.

Under the assumptions of Theorem 1.1, the estimate of the kinetic residue $\tilde{\mathcal{R}}$ can be obtained exactly the same as in [13]. (In the updated arXiv version of [13], the oscillation estimates have been corrected, with which the estimates for the residue terms from BBGKY hierarchy as well as the main result still hold true.) In this paper we give a better estimate for $\tilde{\mathcal{R}}$ in the following proposition.

Proposition 1.1 *Under the assumptions 1, 2, and 3 in H1, the following estimate holds*

$$\left\| \int dp \left| \tilde{\mathcal{R}}(p, \cdot) \right| \right\|_{L^{\frac{5}{4}}(\mathbb{R}^3)} \leq C \hbar^{\frac{1}{2}}.
 \tag{1.13}$$

As a consequence, the following holds:

$$\left| \int dq dp \varphi(q) \phi(p) \nabla_q \cdot \tilde{\mathcal{R}}(q, p) \right| \leq C \hbar^{\frac{1}{2}}.
 \tag{1.14}$$

where C depends on φ, ϕ, f .

The proof will be listed in Sect. 2.

In addition, we obtain the following two propositions for the other two residues:

Proposition 1.2 *Under the assumptions 1, 2, and 3 in H1 and let ϕ, φ be test functions, then the following inequality holds:*

$$\left| \int dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_s(q, p) \right| \leq C \hbar^{\frac{1}{2} + 3(\alpha_2 - 1)},
 \tag{1.15}$$

where $\frac{1}{2} < \alpha_2 < 1$, and C depends on φ, ϕ, f .

Detailed proof will be given in Sect. 3.

Proposition 1.3 *Assuming H1, let $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ be test functions, then the following inequality holds:*

$$\left| \int dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_m(q, p) \right| \leq C \hbar^{\frac{3}{2}(\alpha_1 - \frac{1}{2}) + \frac{3}{2}}
 \tag{1.16}$$

where $\frac{1}{2} < \alpha_1 < 1$, C depends on ϕ, φ, f .

Detailed proof will be given in Sect. 4.

By using a similar idea in the estimate of the semi-classical residue term, as shown in Lemma 4.1, the estimate of the mean-field residue term can be reduced to the corresponding quantities involving

$$\begin{aligned} & \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1)\gamma_{N,t}^{(1)}(u_2; w_2) \\ &= \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \omega_{N,t}(u_1; w_1)\omega_{N,t}(u_2; w_2) \\ & \quad + [\omega_{N,t}(u_1; w_1) - \gamma_{N,t}^{(1)}(u_1; w_1)]\omega_{N,t}(u_2; w_2) \\ & \quad + \gamma_{N,t}^{(1)}(u_1; w_1)[\omega_{N,t}(u_2; w_2) - \gamma_{N,t}^{(1)}(u_2; w_2)] \\ &=: T_1 + T_2 + T_3, \end{aligned} \tag{1.17}$$

where $\omega_{N,t}$ is the solution to Hartree–Fock equation. The terms with T_2 and T_3 can be estimated by the trace norm and Hilbert-Schmidt norm of $\gamma_{N,t}^{(1)} - \omega_{N,t}$, respectively. To control T_1 , we provide a bound of the following mixed norm estimate for two particle density matrix

$$\left(\int dw_1 du_1 \left[\int dw_2 \left| \gamma_{N,t}^{(2)}(w_1, w_2; u_1, w_2) - \omega_{N,t}(w_1; u_1)\omega_{N,t}(w_2; w_2) \right| \right]^2 \right)^{\frac{1}{2}}. \tag{1.18}$$

In [8], the convergence with respect to the trace norm and Hilbert-Schmidt norm of the difference between $\gamma_{N,t}^{(k)}$ and $\omega_{N,t}^{(k)}$ are obtained separately with the help of Wick’s theorem for $k \geq 2$. However, in the current framework the mixed norm estimate as listed in (1.18) needs extra efforts. We trace the strategies given in [8] to reduce it to the estimate of the expectation of the number operator \mathcal{N} along the quantum fluctuation.

The above estimates show that in the sense of distribution $\mathcal{R}_s \sim \hbar^{\frac{1}{2}-}$ and $\mathcal{R}_m \sim \hbar^{\frac{9}{4}-} \sim N^{-\frac{3}{4}-}$, from which one can observe that the semi-classical and mean field residue terms are not of the same order in the combined limit $N^{-1} = \hbar^3$ argument.

This paper is arranged as follows: we prove the estimate for semi-classical residue in Sect. 3, followed by the estimate for mean-field residue in Sect. 4. Then we conclude the proof of Theorem 1.1 in Sect. 5. In the appendices, for reader’s convenience, we list some basic notations and known estimates.

2 Estimate for Kinetic Residue

In this section, we provide the estimate for $\tilde{\mathcal{R}}$ in Proposition 1.1.

Proof of Proposition 1.1 Note that

$$\begin{aligned} & \left| \int dp |\tilde{\mathcal{R}}(q, p)| \right| \leq \hbar \int dp \|\nabla_q a(f_{q,p}^\hbar)\Psi_{N,t}\| \|a(f_{q,p}^\hbar)\Psi_{N,t}\| \\ & \leq \left[\hbar^2 \int dp \langle \nabla_q a(f_{q,p}^\hbar)\Psi_{N,t}, \nabla_q a(f_{q,p}^\hbar)\Psi_{N,t} \rangle \right]^{\frac{1}{2}} \left[\int dp m_{N,t}(q, p) \right]^{\frac{1}{2}} \\ & = \left[\hbar^2 \int dp \langle \nabla_q a(f_{q,p}^\hbar)\Psi_{N,t}, \nabla_q a(f_{q,p}^\hbar)\Psi_{N,t} \rangle \right]^{\frac{1}{2}} \varrho_{N,t}^{\frac{1}{2}} \end{aligned}$$

$$\begin{aligned}
 &= \left[\hbar^{\frac{1}{2}} \int dp \int dw du \nabla_q f \left(\frac{w-q}{\sqrt{\hbar}} \right) \nabla_q f \left(\frac{u-q}{\sqrt{\hbar}} \right) e^{\frac{i}{\hbar} p \cdot (w-u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle \right]^{\frac{1}{2}} \varrho_{N,t}^{\frac{1}{2}}(q) \\
 &= (2\pi)^3 \left[\hbar^{\frac{1}{2}+3} \int dw \hbar^{-1} \left| \nabla f \left(\frac{w-q}{\sqrt{\hbar}} \right) \right|^2 \langle \Psi_{N,t}, a_w^* a_w \Psi_{N,t} \rangle \right]^{\frac{1}{2}} \varrho_{N,t}^{\frac{1}{2}}(q) \\
 &\leq \hbar^2 \left[\int dw \hbar^{-\frac{3}{2}} \left| \nabla f \left(\frac{w-q}{\sqrt{\hbar}} \right) \right|^2 \langle \Psi_{N,t}, a_w^* a_w \Psi_{N,t} \rangle \right]^{\frac{1}{2}} \varrho_{N,t}^{\frac{1}{2}}(q).
 \end{aligned}$$

This implies, by using Hölder inequality, that

$$\begin{aligned}
 &\left(\int dq \left| \int dp \tilde{\mathcal{R}}(q, p) \right|^{\frac{5}{4}} \right)^{\frac{4}{5}} \\
 &\leq \hbar^2 \left[\int dq dw \hbar^{-\frac{3}{2}} \left| \nabla f \left(\frac{w-q}{\sqrt{\hbar}} \right) \right|^2 \langle \Psi_{N,t}, a_w^* a_w \Psi_{N,t} \rangle \right]^{\frac{1}{2}} \left[\int dq \varrho_{N,t}^{\frac{5}{3}}(q) \right]^{\frac{3}{10}} \\
 &\leq C \hbar^2 \|\nabla f\|_2 \langle \Psi_{N,t}, \mathcal{N} \Psi_{N,t} \rangle^{\frac{1}{2}} \leq C \hbar^{\frac{1}{2}}.
 \end{aligned}$$

In the above estimate, we have used the fact that $\|\rho_{N,t}\|_{L^\infty(0,T;L^{\frac{5}{3}}(\mathbb{R}^3))} \leq C$, which is a direct result from Appendix B. Moreover, we obtain

$$\begin{aligned}
 &\left| \int dq dp \varphi(q) \phi(p) \nabla_q \cdot \tilde{\mathcal{R}}(q, p) \right| \\
 &\leq \|\nabla \varphi\|_{L^5(\mathbb{R}^3)} \left(\int dq \left| \int dp \phi(p) \tilde{\mathcal{R}}(q, p) \right|^{\frac{5}{4}} \right)^{\frac{4}{5}} \\
 &\leq \|\nabla \varphi\|_{L^5(\mathbb{R}^3)} \|\phi\|_{L^\infty(\mathbb{R}^3)} \left(\int dq \left| \int dp \tilde{\mathcal{R}}(q, p) \right|^{\frac{5}{4}} \right)^{\frac{4}{5}} \\
 &\leq C \hbar^{\frac{1}{2}}. \quad \square
 \end{aligned}$$

3 Estimate for Semi-classical Residue

In this section, we will estimate the semi-classical residual term under the assumption with $V \in W^{2,\infty}(\mathbb{R}^3)$ in Proposition 1.2, with which give us the insight to compare the rate between semi-classical and mean-field residuals.

Proof of Proposition 1.2 First, recall that

$$\begin{aligned}
 \mathcal{R}_s := &\frac{1}{(2\pi)^3} \int dw_1 du_1 dw_2 du_2 dq_2 dp_2 \left(f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \\
 &\left[\int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2).
 \end{aligned} \tag{3.1}$$

Since $\phi(q), \varphi(p)$ are test functions, we see that

$$\begin{aligned}
 &\left| \int dq dp \phi(q) \varphi(p) \nabla_p \cdot \mathcal{R}_s(q, p) \right| \\
 &= \frac{1}{(2\pi)^3} \left| \int (dq dp)^{\otimes 2} \phi(q) \nabla_p \varphi(p) \cdot \int dw_1 du_1 dw_2 du_2 \left(f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \right|
 \end{aligned}$$

$$\begin{aligned}
 & \left| \int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) \Big| \\
 &= \frac{1}{(2\pi\hbar)^3} \left| \int (dq)^{\otimes 2} dp dw_1 du_1 dw_2 \phi(q) \nabla_p \varphi(p) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
 &\quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \int du_2 dp_2 e^{\frac{i}{\hbar} p_2 \cdot (w_2 - u_2)} f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) f\left(\frac{u_2 - q_2}{\sqrt{\hbar}}\right) \right. \\
 &\quad \left. \left[\int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
 &= \left| \int (dq)^{\otimes 2} dp dw_1 du_1 dw_2 \phi(q) \nabla_p \varphi(p) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
 &\quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \left[\int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \right. \\
 &\quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right|,
 \end{aligned}$$

where we applied the fact that $(2\pi\hbar)^3 \delta_x(y) = \int e^{\frac{i}{\hbar} p \cdot (x-y)} dp$. Then, inserting $\pm \nabla V(q - w_2)$ and we have

$$\begin{aligned}
 &\leq \left| \int (dq)^{\otimes 2} dp dw_1 du_1 dw_2 \phi(q) \nabla \varphi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
 &\quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\
 &\quad \left. \left[\int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - w_2) \right] \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
 &+ \left| \int (dq)^{\otimes 2} dp dw_1 du_1 dw_2 \phi(q) \nabla \varphi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
 &\quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 [\nabla V(q - w_2) - \nabla V(q - q_2)] \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
 &=: I_s + J_s
 \end{aligned}$$

where we used integration by part in the second to last equality.

Before advancing, recalling (B.4), we split the integral and obtain the following estimate, $\forall \alpha_2 \in (\frac{1}{2}, 1)$,

$$\begin{aligned}
 \left| \int dp \nabla \varphi(p) e^{\frac{i}{\hbar} p \cdot (w-u)} \right| &= \left| \int dp \left(\chi_{(w_1 - u_1) \in \Omega_{\hbar}^{\alpha_2}} + \chi_{(w_1 - u_1) \in (\Omega_{\hbar}^{\alpha_2})^c} \right) \nabla \varphi(p) e^{\frac{i}{\hbar} p \cdot (w-u)} \right| \\
 &\leq \tilde{C} \left(\chi_{(w_1 - u_1) \in \Omega_{\hbar}^{\alpha_2}} + \hbar^{(1-\alpha_2)s} \right),
 \end{aligned} \tag{3.2}$$

where \tilde{C} depends on $\|\phi\|_{W^{s+1,\infty}}$ and $\text{supp } \phi$.

Now we want to estimate the term I_s and J_s separately. We begin by estimating I_s ,

$$I_s = \hbar^{\frac{3}{2}} \left| \int dq dp dw_1 du_1 dw_2 \phi(q) \nabla \varphi(p) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right.$$

$$\left(\int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \right) \left[\int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - w_2) \right] \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2).$$

Using $\|D^2V\|_{L^\infty} \leq C$, (3.2), the definition of $\gamma^{(2)}$ with Cauchy-Schwarz inequality, we have

$$\begin{aligned} I_s &\leq C\hbar^{\frac{3}{2}} \int dq |\phi(q)| \int dw_1 du_1 \left(\chi_{(w_1-u_1) \in \Omega_h^{\alpha_2}} + \hbar^{(1-\alpha_2)s} \right) \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\ &\quad (|u_1-q| + |w_1-q|) \int dw_2 |\gamma_{N,t}^{(2)}(w_1, w_2; u_1, w_2)| \\ &\leq C\hbar^{\frac{3}{2}} \int dq |\phi(q)| \int dw_1 du_1 \left(\chi_{(w_1-u_1) \in \Omega_h^{\alpha_2}} + \hbar^{(1-\alpha_2)s} \right) \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\ &\quad (|u_1-q| + |w_1-q|) \left(\int dw_2 \|a_{w_2} a_{w_1} \psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left(\int dw_2 \|a_{w_2} a_{u_1} \psi_{N,t}\|^2 \right)^{\frac{1}{2}} \\ &=: C \left[i_{s,1} + i_{s,2} \right], \end{aligned}$$

where we use $i_{s,1}$ to be the term with $\chi_{(w_1-u_1) \in \Omega_h^{\alpha_2}}$, and $i_{s,2}$ to be the other one.

Due to the symmetric property, we can reduce the estimate for $i_{s,1}$ into the following

$$\begin{aligned} i_{s,1} &\leq 2C\hbar^{\frac{3}{2}} \int dq |\phi(q)| \int dw_1 du_1 \chi_{(w_1-u_1) \in \Omega_h^{\alpha_2}} \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \cdot |u_1-q| \\ &\quad \int dw_2 \|a_{w_2} a_{w_1} \psi_{N,t}\|^2 \\ &\leq C\hbar^{\frac{3}{2}} \|f\left(\frac{u_1-q}{\sqrt{\hbar}}\right)\| \cdot \| |u_1-q| \|_{L^\infty} |\Omega_h^{\alpha_2}| \int dq |\phi(q)| \\ &\quad \int dw_1 \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) \right| \langle \psi_{N,t}, a_{w_1}^* \mathcal{N} a_{w_1} \psi_{N,t} \rangle \\ &\leq C\hbar^{\frac{3}{2}} \hbar^{\frac{1}{2}} \hbar^{3\alpha_2} \hbar^{\frac{3}{2}} \int dw_1 \langle \psi_{N,t}, a_{w_1}^* \mathcal{N} a_{w_1} \psi_{N,t} \rangle \leq C\hbar^{3\alpha_2+3+\frac{1}{2}-6}. \end{aligned} \tag{3.3}$$

Similarly, noticing that $\phi(q)$ has compact support, one obtains the estimate for the term $i_{s,2}$,

$$\begin{aligned} i_{s,2} &\leq 2C\hbar^{\frac{3}{2}} \int dq |\phi(q)| \int dw_1 du_1 \hbar^{(1-\alpha_2)s} \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \cdot |u_1-q| \\ &\quad \int dw_2 \|a_{w_2} a_{w_1} \psi_{N,t}\|^2 \\ &\leq 2C\hbar^{\frac{3}{2}+\frac{3}{2}+\frac{1}{2}} \int d\tilde{u} \chi_{|\tilde{u}| \leq R_1} |f(\tilde{u})| |\tilde{u}| \int dq |\phi(q)| \int dw_1 \hbar^{(1-\alpha_2)s} \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) \right| \\ &\quad \int dw_2 \|a_{w_2} a_{w_1} \psi_{N,t}\|^2 \\ &\leq C\hbar^{\frac{3}{2}+\frac{3}{2}+\frac{1}{2}} \hbar^{(1-\alpha_2)s} \hbar^{\frac{3}{2}} \hbar^{-6} \leq C\hbar^{(1-\alpha_2)s-1} \end{aligned}$$

To balance the order between $i_{s,1}$ and $i_{s,2}$, the term s is chosen to be

$$s = \left\lceil \frac{3(\alpha_2 - \frac{1}{2})}{1 - \alpha_2} \right\rceil,$$

where $\alpha_2 \in (\frac{1}{2}, 1)$. Therefore, we have

$$I_s \leq C \hbar^{\frac{1}{2} + 3(\alpha_2 - 1)}. \tag{3.4}$$

Now, to estimate J_s , we recall the estimate in (3.2) and obtain

$$\begin{aligned} J_s &\leq C \left| \int (dq)^{\otimes 2} |\phi(q)| \int dw_1 du_1 \left(\chi_{(w_1 - u_1) \in \Omega_{\hbar}^{\alpha_2}} + \hbar^{(1 - \alpha_2)s} \right) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\ &\quad \left. \int dw_2 \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 |w_2 - q_2| \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\ &\leq C \int dq |\phi(q)| \int dw_1 du_1 \left(\chi_{(w_1 - u_1) \in \Omega_{\hbar}^{\alpha_2}} + \hbar^{(1 - \alpha_2)s} \right) \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \\ &\quad \int d\tilde{q} |f(\tilde{q})|^2 h^{\frac{3}{2}} h^{\frac{1}{2}} |\tilde{q}| \int dw_2 |\gamma_{N,t}^{(2)}(w_1, w_2; u_1, w_2)| \\ &\leq C \hbar^2 \int dq |\phi(q)| \int dw_1 du_1 \left(\chi_{(w_1 - u_1) \in \Omega_{\hbar}^{\alpha_2}} + \hbar^{(1 - \alpha_2)s} \right) \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \\ &\quad \left(\int dw_2 \|a_{w_2} a_{w_1} \psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left(\int dw_2 \|a_{w_2} a_{u_1} \psi_{N,t}\|^2 \right)^{\frac{1}{2}} \\ &=: C \left[j_{s,1} + j_{s,2} \right]. \end{aligned}$$

The estimate for $j_{s,1}$ can be exactly done as in (3.3) for $i_{s,1}$, the same for $j_{s,2}$ as in $i_{s,2}$. Therefore we obtain the same rate for J_s as in (3.4) for I_s . This completes the proof. \square

Remark 3.1 The key step in the estimates of semi-classical residue is in (3.3), with which the computational bugs appeared in [13] can both be fixed by the same technique.

4 Estimate for Mean-Field Residue

In this section, we will estimate the mean-field residue by first showing in Lemma 4.1 that the estimate for mean-field residue term can be reduced to the estimate for the term

$$\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \tag{4.1}$$

where we denote

$$\mathbb{T}^{(1)} |\gamma^{(2)} - \gamma^{(1)} \otimes \gamma^{(1)}| (u_1; w_1) := \int dy \left| \gamma^{(2)}(u_1, y; w_1, y) - \gamma^{(1)}(u_1; w_1) \gamma^{(1)}(y; y) \right|.$$

Then, we prove the estimate for (4.1) in Proposition 4.1 and finally summary the estimation for the mean-field residue in Proposition 1.3.

Lemma 4.1 *Let $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$. Then, for $\frac{1}{2} < \alpha_1 < 1$ and $s = \left\lceil \frac{3(\alpha_1 - \frac{1}{2})}{2(1 - \alpha_1)} \right\rceil$, we have*

$$\begin{aligned} & \left| \int dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_m(q, p) \right| \\ & \leq C \|\nabla V\|_{L^\infty} \hbar^{3 + \frac{3}{2}(\alpha_1 - \frac{1}{2}) + \frac{3}{2}} \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}|(u_1; w_1) \right]^2 \right)^{\frac{1}{2}}, \end{aligned} \tag{4.2}$$

where the constant C depends on $\|\varphi\|_\infty, \|\nabla\phi\|_{W^{s,\infty}}, \text{supp } \phi, \|f\|_{L^\infty \cap H^1}, \text{supp } f$.

Proof Recall that, in (1.12), we defined the mean-field residue such that

$$\begin{aligned} \mathcal{R}_m := & \frac{1}{(2\pi)^3} \int dw_1 du_1 dw_2 du_2 dq_2 dp_2 \left(f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \\ & \nabla V(q - q_2) \left[\gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right]. \end{aligned} \tag{4.3}$$

Then one obtains

$$\begin{aligned} & \left| \int dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_m(q, p) \right| \\ & = \frac{1}{(2\pi)^3} \left| \int (dq dp)^{\otimes 2} (dw du)^{\otimes 2} \varphi(q) \nabla\phi(p) \cdot \left(f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \nabla V(q - q_2) \right. \\ & \quad \left. \left[\gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ & = \frac{1}{(2\pi\hbar)^3} \left| \int (dq dw du)^{\otimes 2} \left(f\left(\frac{w - q}{\sqrt{\hbar}}\right) f\left(\frac{u - q}{\sqrt{\hbar}}\right) \right)^{\otimes 2} \left(\int dp \varphi(q) \nabla\phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right) \right. \\ & \quad \left. \nabla V(q - q_2) \left(\int dp_2 e^{\frac{i}{\hbar} p_2 \cdot (w_2 - u_2)} \right) \left[\gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ & = \left| \int (dq)^{\otimes 2} dw_1 du_1 dw_2 f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\ & \quad \left. \left(\int dp \varphi(q) \nabla\phi(p) \cdot e^{\frac{i}{\hbar} p_1 \cdot (w_1 - u_1)} \right) \right. \\ & \quad \left. \nabla V(q - q_2) \left[\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right|, \end{aligned}$$

where we use the weighted Dirac-Delta function in the last equality, i.e.,

$$\frac{1}{(2\pi\hbar)^3} \int dp_2 e^{\frac{i}{\hbar} p_2 \cdot (w_2 - u_2)} = \delta_{w_2}(u_2). \tag{4.4}$$

Now, splitting the domains of w_1 and u_1 into two, namely, with the characteristic functions $\chi_{(w_1 - u_1) \in \Omega_h^{\alpha_1}}$ and $\chi_{(w_1 - u_1) \in (\Omega_h^{\alpha_1})^c}$ whose domain $\Omega_h^{\alpha_1}$ is defined in (B.3), we have

$$\begin{aligned} & \leq \left| \int (dq)^{\otimes 2} \varphi(q) \int dw_1 du_1 dw_2 f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\ & \quad \left. \left(\int dp \chi_{(w_1 - u_1) \in \Omega_h^{\alpha_1}} e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \nabla\phi(p) \right) \cdot \nabla V(q - q_2) \right| \end{aligned}$$

$$\begin{aligned}
 & \left| \left[\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1)\gamma_{N,t}^{(1)}(w_2; w_2) \right] \right| \\
 & + \left| \int (dq)^{\otimes 2} \varphi(q) \int dw_1 du_1 dw_2 f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\
 & \quad \left. \left(\int dp \chi_{(w_1 - u_1) \in (\Omega_{\hbar}^{\alpha_1})^c} e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \nabla \phi(p) \right) \cdot \nabla V(q - q_2) \right. \\
 & \quad \left. \left[\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1)\gamma_{N,t}^{(1)}(w_2; w_2) \right] \right| \\
 & =: J_m + J_m.
 \end{aligned}$$

First, considering the term J_m , by the change of variable $\sqrt{\hbar} \tilde{q}_2 = w_2 - q_2$, we obtain

$$\begin{aligned}
 J_m & = \left| \int dq \varphi(q) \int dw_1 du_1 dw_2 f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
 & \quad \left. \left(\hbar^{\frac{3}{2}} \int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \nabla V(q - w_2 + \sqrt{\hbar} \tilde{q}_2) \right) \right. \\
 & \quad \left. \left(\int dp \chi_{(w_1 - u_1) \in (\Omega_{\hbar}^{\alpha_1})^c} \nabla \phi(p) e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right) \right. \\
 & \quad \left. \left(\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1)\gamma_{N,t}^{(1)}(w_2; w_2) \right) \right| \\
 & \leq C \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \int dw_1 du_1 \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|_{|w_1 - u_1| \leq 2R_1 \sqrt{\hbar}} \chi \\
 & \quad \left| \int dp \chi_{(w_1 - u_1) \in (\Omega_{\hbar}^{\alpha_1})^c} \nabla \phi(p) e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right| \\
 & \quad \int dw_2 \left| \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1)\gamma_{N,t}^{(1)}(w_2; w_2) \right|.
 \end{aligned}$$

where we have used that $\text{supp } f \subset B_{R_1}$. Recall again from Lemma B.4 that we have

$$\left| \int dp \chi_{(w_1 - u_1) \in (\Omega_{\hbar}^{\alpha_1})^c} e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \nabla \phi(p) \right| \leq \|\nabla \phi\|_{W^{s,\infty}} \hbar^{(1-\alpha_1)s}, \tag{4.5}$$

for s to be chosen later. Hence, together with Hölder’s inequality we get

$$\begin{aligned}
 J_m & \leq C \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2} + (1-\alpha_1)s} \\
 & \quad \int dq |\varphi(q)| \left(\int dw_1 du_1 \chi_{|w_1 - u_1| \leq 2R_1 \sqrt{\hbar}} \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|^2 \right)^{\frac{1}{2}} \\
 & \quad \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]_{|w_1 - q| \leq R_1 \sqrt{\hbar}}^2 \chi \right)^{\frac{1}{2}} \\
 & \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2} + (1-\alpha_1)s} \left(\hbar^3 \int d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq 2R_1} |f(\tilde{w}) f(\tilde{u})|^2 \right)^{\frac{1}{2}}
 \end{aligned}$$

$$\begin{aligned}
 & \int dq \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{h}} \right)^{\frac{1}{2}} \\
 & \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3+(1-\alpha)s} \left(\int d\tilde{w}_1 d\tilde{u}_1 |f(\tilde{w}) f(\tilde{u})|^2 \right)^{\frac{1}{2}} \\
 & \quad \hbar^{\frac{3}{2}} \int d\tilde{q}_1 \chi_{|\tilde{q}_1| \leq R_1} \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \\
 & \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3+(1-\alpha)s+\frac{3}{2}} \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} \right. \right. \\
 & \quad \left. \left. - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}.
 \end{aligned}$$

Now, we focus on I_m . Using the fact that $\left| \int dp e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \nabla \phi(p) \right| \leq \|\nabla \phi\|_{L^1}$, we obtain the following estimate:

$$\begin{aligned}
 I_m & \leq C \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \\
 & \int dq |\varphi(q)| \left(\int dw_1 du_1 \chi_{|w_1 - u_1| \leq \hbar^{\alpha_1}} \chi_{|w_1 - u_1| \leq 2R_1 \sqrt{h}} \left| f\left(\frac{w_1 - q}{\sqrt{h}}\right) f\left(\frac{u_1 - q}{\sqrt{h}}\right) \right|^2 \right)^{\frac{1}{2}} \\
 & \quad \hbar^{\frac{3}{2}} \int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{h}} \right)^{\frac{1}{2}} \\
 & \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2}} \left(\hbar^3 \int d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_1 - \frac{1}{2}}} \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq 2R_1} |f(\tilde{w}_1) f(\tilde{u}_1)|^2 \right)^{\frac{1}{2}} \\
 & \quad \int dq \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{h}} \right)^{\frac{1}{2}} \\
 & \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \hbar^3 \left(\int d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_1 - \frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u}_1)|^2 \right)^{\frac{1}{2}} \\
 & \quad \hbar^{\frac{3}{2}} \int d\tilde{q}_1 \chi_{|\tilde{q}_1| \leq R_1} \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}},
 \end{aligned}$$

which together with

$$\int d\tilde{w}_1 |f(\tilde{w}_1)|^2 \int d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_1 - \frac{1}{2}}} |f(\tilde{u}_1)|^2 \leq \|f\|_{L^\infty(\mathbb{R}^3)}^2 \|f\|_{L^2(\mathbb{R}^3)}^2 \hbar^{3(\alpha_1 - \frac{1}{2})},$$

implies immediately that

$$\begin{aligned}
 I_m & \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \hbar^{3+\frac{3}{2}(\alpha_1 - \frac{1}{2})+\frac{3}{2}} \\
 & \quad \times \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}.
 \end{aligned}$$

To balance the order between I_m and J_m , s is chosen to be

$$s = \left\lceil \frac{3(\alpha_1 - \frac{1}{2})}{2(1 - \alpha_1)} \right\rceil,$$

for $\alpha_1 \in [0, 1)$. Therefore, we obtained the desired result:

$$\begin{aligned} & \left| \int dq dp \varphi(q)\phi(p)\nabla_p \cdot \mathcal{R}_m \right| \\ & \leq C \|\varphi\|_{L^\infty} \|\nabla\phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3+\frac{3}{2}(\alpha_1-\frac{1}{2})+\frac{3}{2}} \\ & \quad \times \left(\int dw_1 du_1 \left[\mathbb{T}^{(1)}|\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}(u_1; w_1) \right]^2 \right)^{\frac{1}{2}}. \quad \square \end{aligned}$$

Next, we want to bound the term with the ‘mixed’-norm, i.e.,

$$\int dw_1 du_1 \left[\mathbb{T}^{(1)}|\gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}(u_1; w_1) \right]^2. \tag{4.6}$$

The following proposition provides the estimate of (4.6):

Proposition 4.1 *Let $\gamma_{N,t}^{(k)}$ be k -particle reduced density matrix associated with $\Psi_{N,t}$, $\omega_{N,t}$ be the solution of the Hartree–Fock equation in (1.3). Suppose the assumption for Theorem 1.1 holds. Then the following inequalities hold for all $t \in \mathbb{R}$:*

$$\|\gamma_{N,t}^{(1)} - \omega_{N,t}\|_{HS} \leq C. \tag{4.7}$$

and

$$\|\gamma_{N,t}^{(1)} - \omega_{N,t}\|_{Tr} \leq C\sqrt{N}. \tag{4.8}$$

Furthermore, it holds that

$$\left(\int dw_1 du_1 \left[\mathbb{T}^{(1)}|\gamma_{N,t}^{(2)} - \omega_{N,t} \otimes \omega_{N,t}| \right]^2 (u_1; w_1) \right)^{\frac{1}{2}} \leq CN \tag{4.9}$$

where C depends on t but is independent of N .

The proof of Proposition 4.1 requires the following results from [8], namely:

Lemma 4.2 [8, Lemma 3.1] *Let $d\Gamma(O)$ be the second quantization of any bounded operator O on $L^2(\mathbb{R}^3)$, i.e.*

$$d\Gamma(O) := \int dx dy O(x; y) a_x^* a_y.$$

For any $\Psi \in \mathcal{F}_a$, the following inequalities hold

$$\left\| d\Gamma(O)\Psi \right\| \leq \|O\| \|\mathcal{N}\Psi\|. \tag{4.10}$$

If furthermore O is a Hilbert-Schmidt operator, we have the following bounds:

$$\left\| d\Gamma(O)\Psi \right\| \leq \|O\|_{HS} \|\mathcal{N}^{1/2}\Psi\|, \tag{4.11}$$

$$\left\| \int dx dy O(x; y) a_x a_y \Psi \right\| \leq \|O\|_{HS} \|\mathcal{N}^{1/2}\Psi\|, \tag{4.12}$$

$$\left\| \int dx dy O(x; y) a_x^* a_y^* \Psi \right\| \leq 2 \|O\|_{\text{HS}} (\mathcal{N} + 1)^{1/2} \|\Psi\|. \tag{4.13}$$

Finally, if O is a trace class operator, we obtain

$$\left\| d\Gamma(O)\Psi \right\| \leq 2 \|O\|_{\text{Tr}}, \tag{4.14}$$

$$\left\| \int dx dy O(x; y) a_x a_y \Psi \right\| \leq 2 \|O\|_{\text{Tr}}, \tag{4.15}$$

$$\left\| \int dx dy O(x; y) a_x^* a_y^* \Psi \right\| \leq 2 \|O\|_{\text{Tr}}, \tag{4.16}$$

where $\|O\|_{\text{Tr}} := \text{Tr}|O| = \text{Tr}\sqrt{O^*O}$.

Lemma 4.3 [8, Proposition 3.4] *Suppose the assumption for Theorem 1.1 holds. Then, there exist constants $K, c > 0$ depending only on potential V such that*

$$\sup_{p \in \mathbb{R}^3} \frac{1}{1 + |p|} \text{Tr}|\omega_{N,t}, e^{ip \cdot x}| \leq KN\hbar C(t)$$

$$\text{Tr}|\omega_{N,t}, \hbar \nabla| \leq KN\hbar C(t).$$

Lemma 4.4 [8, Theorem 3.2] *Let $\mathcal{U}_N(t; s)$ be the quantum fluctuation dynamics defined in (A.6) and \mathcal{N} be the number operator. If the assumptions in Lemma 4.3 hold. Then for $\xi_N \in \mathcal{F}_a$ with $\langle \xi_N, \mathcal{N}^k \xi_N \rangle \leq C$ for any $k \geq 1$, we have the following inequality:*

$$\|(\mathcal{N} + 1)^k \mathcal{U}_N(t; 0)\xi_N\| \leq C(k, t). \tag{4.17}$$

Remark 4.1 Here in this paper we only need the result for initial data $\xi_N = \Omega$ where Ω is the vacuum state give in Appendix A.

Now, we are ready to provide the proof of Proposition 4.1.

Proof of Proposition 4.1 The proof of the inequalities (4.7) and (4.8) follows by modifying Theorem 2.1 of [8]. In particular, from Eq. (4.3) in [8], we obtain

$$\|\gamma_{N,t}^{(1)} - \omega_{N,t}\|_{\text{HS}} \leq C \|\mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0)\xi_N\|,$$

$$\|\gamma_{N,t}^{(1)} - \omega_{N,t}\|_{\text{Tr}} \leq C\sqrt{N} \|\mathcal{N} \mathcal{U}_N(t; 0)\xi_N\|,$$

by choosing the appropriate operator O as discussed in [8]. Our results for (4.7) and (4.8) are obtained by applying Lemma 4.4 and taking the assumption that $\|(\mathcal{N} + 1)\xi_N\| \leq C$.

Therefore, it remains to prove for (4.9). As remarked previously, the trace norm and Hilbert-Schmidt norm of the difference between $\gamma_{N,t}^{(k)}$ and $\omega_{N,t}^{(k)}$ are obtained separately with the help of Wick’s theorem for $k \geq 2$ in [8]. For our term, however, we do not directly use Wick’s theorem to compute (4.9) as each terms requires similar but still unique method when taking the estimation.

Simplifying the notation $\mathcal{R}_t := \mathcal{R}_{\mathcal{V}_{N,t}}$, where $\mathcal{R}_{\mathcal{V}_{N,t}}$ is the Bogoliubov transformation given in (A.4), we have, from the definition of a 2-particle reduced density matrix and (A.4). that

$$\gamma_{N,t}^{(2)}(x_1, x_2; y_1, y_2)$$

$$= \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{R}_t^* a_{y_1}^* a_{y_2}^* a_{x_2} a_{x_1} \mathcal{R}_t \mathcal{U}_N(t; 0)\xi_N \rangle$$

$$\begin{aligned}
 &= \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{R}_t^* a_{y_1}^* \mathcal{R}_t \mathcal{R}_t^* a_{y_2}^* \mathcal{R}_t \mathcal{R}_t^* a_{x_2} \mathcal{R}_t \mathcal{R}_t^* a_{x_1} \mathcal{R}_t \mathcal{U}_N(t; 0) \xi_N \rangle \\
 &= \left\langle \xi_N, \mathcal{U}_N^*(t; 0) \left(a^*(\mathbf{u}_{t,y_1}) + a(\bar{\mathbf{v}}_{t,y_1}) \right) \left(a^*(\mathbf{u}_{t,y_2}) + a(\bar{\mathbf{v}}_{t,y_2}) \right) \right. \\
 &\quad \left. \left(a(\mathbf{u}_{t,x_2}) + a^*(\bar{\mathbf{v}}_{t,x_2}) \right) \left(a(\mathbf{u}_{t,x_1}) + a^*(\bar{\mathbf{v}}_{t,x_1}) \right) \mathcal{U}_N(t; 0) \xi_N \right\rangle \\
 &= \left\langle \xi_N, \mathcal{U}_N^*(t; 0) \left[a(\bar{\mathbf{v}}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,x_1}) + a(\bar{\mathbf{v}}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,x_1}) \right. \right. \\
 &\quad + a(\bar{\mathbf{v}}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,x_1}) + a(\bar{\mathbf{v}}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,x_1}) \\
 &\quad + a(\bar{\mathbf{v}}_{t,y_1}) a^*(\mathbf{u}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,x_1}) + a(\bar{\mathbf{v}}_{t,y_1}) a^*(\mathbf{u}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,x_1}) \\
 &\quad + a(\bar{\mathbf{v}}_{t,y_1}) a^*(\mathbf{u}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,x_1}) + a(\bar{\mathbf{v}}_{t,y_1}) a^*(\mathbf{u}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,x_1}) \\
 &\quad + a^*(\mathbf{u}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,x_1}) + a^*(\mathbf{u}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,x_1}) \\
 &\quad + a^*(\mathbf{u}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,x_1}) + a^*(\mathbf{u}_{t,y_1}) a(\bar{\mathbf{v}}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,x_1}) \\
 &\quad \left. \left. + a^*(\mathbf{u}_{t,y_1}) a^*(\mathbf{u}_{t,y_2}) a(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,x_1}) + a^*(\mathbf{u}_{t,y_1}) a^*(\mathbf{u}_{t,y_2}) a^*(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,x_1}) \right] \mathcal{U}_N(t; 0) \xi_N \right\rangle, \tag{4.18}
 \end{aligned}$$

where we use (A.4) in the third equality. Therefore, we obtain, using the fact that $\langle \bar{\mathbf{v}}_{t,x}, \mathbf{u}_{t,y} \rangle = 0$, $\langle \mathbf{u}_{t,x}, \bar{\mathbf{v}}_{t,y} \rangle = 0$, $\langle \bar{\mathbf{v}}_{t,x}, \bar{\mathbf{v}}_{t,y} \rangle = \omega_{N,t}(y; x)$, and CAR,

$$\begin{aligned}
 &\int dx_1 dx_2 dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \left(\gamma_{N,t}^{(2)}(z_1, z_2; x_1, x_2) - \omega_{N,t}(z_1; x_1) \omega_{N,t}(z_2; x_2) \right) \\
 &= \int dx_1 dx_2 dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \left\langle \xi_N, \mathcal{U}_N^*(t; 0) \left[a(\bar{\mathbf{v}}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \right. \right. \\
 &\quad + a(\bar{\mathbf{v}}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,z_2}) + a(\bar{\mathbf{v}}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,z_2}) \\
 &\quad + a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_1}) a^*(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \\
 &\quad + a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) a^*(\mathbf{u}_{t,x_2}) - a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \\
 &\quad + a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) \\
 &\quad + a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,z_2}) + a^*(\bar{\mathbf{v}}_{t,z_1}) a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) \\
 &\quad + a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \\
 &\quad + a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,z_2}) + a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,z_2}) \\
 &\quad + a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) \\
 &\quad - a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_1}) a(\mathbf{u}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) + a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \\
 &\quad - a(\mathbf{u}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) \\
 &\quad - \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle a(\bar{\mathbf{v}}_{t,x_1}) a(\mathbf{u}_{t,z_2}) + \langle \bar{\mathbf{v}}_{t,x_1}, \bar{\mathbf{v}}_{t,z_1} \rangle a(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \\
 &\quad - \langle \mathbf{u}_{t,z_1}, \mathbf{u}_{t,x_2} \rangle a(\bar{\mathbf{v}}_{t,x_1}) a(\mathbf{u}_{t,z_2}) + \langle \mathbf{u}_{t,z_1}, \mathbf{u}_{t,x_2} \rangle a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_1}) - \langle \mathbf{u}_{t,z_1}, \mathbf{u}_{t,x_2} \rangle \langle \bar{\mathbf{v}}_{t,x_1}, \bar{\mathbf{v}}_{t,z_2} \rangle \\
 &\quad + \langle \bar{\mathbf{v}}_{t,x_1}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,z_2}) + \langle \bar{\mathbf{v}}_{t,x_1}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,z_2}) \\
 &\quad - \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_2}) - \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) \\
 &\quad - \langle \mathbf{u}_{t,z_1}, \mathbf{u}_{t,x_2} \rangle a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_2}) - \langle \mathbf{u}_{t,z_1}, \mathbf{u}_{t,x_2} \rangle a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) \\
 &\quad - \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_2} \rangle a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_1}) + \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_1}) \\
 &\quad + \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_2} \rangle a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_1}) - \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_2} \rangle a^*(\bar{\mathbf{v}}_{t,z_1}) a^*(\mathbf{u}_{t,x_1}) \\
 &\quad \left. - \langle \bar{\mathbf{v}}_{t,x_1}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) - \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle \langle \bar{\mathbf{v}}_{t,x_1}, \bar{\mathbf{v}}_{t,z_2} \rangle \right] \mathcal{U}_N(t; 0) \xi_N \right\rangle
 \end{aligned}$$

$$=: \sum_{i=1}^{16} A_i + \sum_{j=1}^{16} B_j + C. \tag{4.19}$$

Using the fact that $\|u_t\|_{op}, \|v_t\|_{op} \leq 1, \|v_t\|_{HS} \leq \sqrt{N}, \|\omega_{N,t}\|_{Tr} = N$ and the assumption $\|\xi_N\| \leq 1$, we do the following estimates for the first term from $\{A_i\}_{i=1}^{16}$ and $\{B_i\}_{i=1}^{16}$ separately.

$$\begin{aligned} & |A_1| \\ &= \left| \int dx_1 dx_2 dz_1 dz_2 \langle \xi_N, U_N^*(t; 0) \int d\eta_1 d\eta'_1 a_{\eta_1} a_{\eta'_1} v_t(\eta_1; x_1) O_1(x_1; z_1) u_t(z_1; \eta'_1) \right. \\ &\quad \left. \int d\eta_2 d\eta'_2 a_{\eta_2} a_{\eta'_2} v_t(\eta_2; x_2) O_2(x_2; z_2) u_t(z_2; \eta'_2) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \int d\eta_1 d\eta'_2 \langle \xi_N, U_N^*(t; 0) a_{\eta_1} a(\overline{v_t O_1 u_t}(\eta_1; \cdot)) a(\overline{v_t O_2 u_t}(\cdot; \eta'_2)) a_{\eta'_2} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &\leq \int d\eta_1 \|a^*(\overline{v_t O_1 u_t}(\eta_1; \cdot)) a_{\eta_1}^* \mathcal{U}_N(t; 0) \xi_N\| \int d\eta'_2 \|a(\overline{v_t O_2 u_t}(\cdot; \eta'_2)) a_{\eta'_2} \mathcal{U}_N(t; 0) \xi_N\| \\ &\leq \int d\eta_1 \|v_t O_1 u_t(\eta_1; \cdot)\|_2 \|a_{\eta_1}^* \mathcal{U}_N(t; 0) \xi_N\| \int d\eta'_2 \|v_t O_2 u_t(\cdot; \eta'_2)\|_2 \|a_{\eta'_2} \mathcal{U}_N(t; 0) \xi_N\| \\ &\leq \|v_t O_1 u_t\|_{HS} \left(\int d\eta_1 \|a_{\eta_1}^* \mathcal{U}_N(t; 0) \xi_N\|^2 \right)^{\frac{1}{2}} \|v_t O_2 u_t\|_{HS} \left(\int d\eta'_2 \|a_{\eta'_2} \mathcal{U}_N(t; 0) \xi_N\|^2 \right)^{\frac{1}{2}} \\ &\leq \sqrt{N} \|v_t\|_{op} \|O_1\|_{HS} \|u_t\|_{op} \|v_t\|_{HS} \|O_2\|_{op} \|u_t\|_{op} (\mathcal{N} + 1)^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \| \\ &\leq N \|O_1\|_{HS} \|O_2\|_{op} (\mathcal{N} + 1)^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \|. \end{aligned}$$

Additionally, we have

$$\begin{aligned} & |B_1| \\ &= \left| \int dx_1 dx_2 dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \right. \\ &\quad \left. \langle \overline{v_{t,x_2}}, \overline{v_{t,z_1}} \rangle a(\overline{v_{t,x_1}}) a(u_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \int dx_1 dx_2 dz_1 dz_2 \langle \xi_N, \mathcal{U}_N^*(t; 0), \int d\eta d\eta' a_{\eta} a_{\eta'} \right. \\ &\quad \left. v_t(\eta; x_1) O_1(x_1; z_1) \omega_{N,t}(z_1; x_2) O_2(x_2; z_2) u_t(z_2; \eta') \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \int d\eta d\eta' \langle \xi_N, \mathcal{U}_N^*(t; 0), a_{\eta} a_{\eta'} (v_t O_1 \omega_{N,t} O_2 u_t)(\eta; \eta') \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &\leq \|v_t O_1 \omega_{N,t} O_2 u_t\|_{HS} \|\xi_N\| \|\mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N\| \\ &\leq \|O_1\|_{HS} \|O_2\|_{op} \|\mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N\|. \end{aligned}$$

The estimates for the rest of the terms can be done with similar steps After getting the bound of each terms, we have obtained the following estimates:

$$\left| \sum_{i=1}^{16} A_i \right| \leq N \|O_1\|_{HS} \|O_2\|_{op} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\|,$$

$$\left| \sum_{j=1}^{16} B_j \right| \leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left(N \|(\mathcal{N} + 1)^{1/2} \mathcal{U}_N(t; 0) \xi_N\| + \sqrt{N} \|(\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N\| \right) \leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|(\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N\|. \tag{4.20}$$

Lastly, the final term is estimated as follows:

$$\begin{aligned} |C| &= \left| \int dx_1 dx_2 dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_1} \rangle \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_2} \rangle \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \int dx_2 \langle \xi_N, \mathcal{U}_N^*(t; 0) (O_1 \omega_{N,t} O_2 \omega_{N,t})(x_2; x_2) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &\leq \|O_1 \omega_{N,t} O_2 \omega_{N,t}\|_{\text{Tr}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{U}_N(t; 0) \xi_N \rangle \\ &\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}}. \end{aligned}$$

As a summary, we have

$$\begin{aligned} \left| \text{Tr} O(\gamma_{N,t}^{(2)} - \omega_{N,t} \otimes \omega_{N,t}) \right| &\leq \left| \sum_{i=1}^{16} A_i \right| + \left| \sum_{j=1}^{16} B_j \right| + |C| \\ &\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|(\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N\|, \end{aligned} \tag{4.21}$$

which implies that, for O_1 and O_2 being Hilbert-Schmidt and trace class operators, we get

$$\begin{aligned} &\left(\int dx_1 dy_1 \left[\int dx_2 \left| \gamma_{N,t}^{(2)}(x_1, x_2; y_1, x_2) - \omega_{N,t}(x_1; y_1) \omega_{N,t}(x_2; x_2) \right|^2 \right] \right)^{\frac{1}{2}} \\ &\leq N \|(\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N\|. \end{aligned} \tag{4.22}$$

Applying Lemma 4.4, we obtain the inequalities in Proposition 4.1 as desired. □

Finally, we have the following estimate for the mixed-norm. Since it is one of the main contributions of this paper, we write it as a theorem.

Theorem 4.1 *Suppose the assumptions given in Proposition 4.1 hold. Then, we have the following estimate*

$$\left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \leq C_t N, \tag{4.23}$$

where the constant C_t depends on potential V and time t .

Proof of Theorem 4.1 Inserting the intermediate terms

$$\begin{aligned} &\gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \\ &= \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \omega_{N,t}(u_1; w_1) \omega_{N,t}(u_2; w_2) \\ &\quad + [\omega_{N,t}(u_1; w_1) - \gamma_{N,t}^{(1)}(u_1; w_1)] \omega_{N,t}(u_2; w_2) \\ &\quad + \gamma_{N,t}^{(1)}(u_1; w_1) [\omega_{N,t}(u_2; w_2) - \gamma_{N,t}^{(1)}(u_2; w_2)] \\ &=: T_1 + T_2 + T_3, \end{aligned} \tag{4.24}$$

the estimate in (4.23) is then reduced into the estimates of the following terms.

- $\left(\int dw_1 du_1 \left[\mathbb{T}^{(1)} |\gamma_{N,t}^{(2)} - \omega_{N,t}^{(1)} \otimes \omega_{N,t}^{(1)}|(u_1; w_1) \right]^2 \right)^{\frac{1}{2}},$
- $\|\omega_{N,t} - \gamma_{N,t}^{(1)}\|_{\text{HS}} \|\omega_{N,t}\|_{\text{Tr}},$
- $\|\gamma_{N,t}^{(1)}\|_{\text{HS}} \|\omega_{N,t} - \gamma_{N,t}^{(1)}\|_{\text{Tr}}.$

Proposition 4.1 implies immediately (4.23) considering the fact that $\|\omega_{N,t}\|_{\text{Tr}} \leq N$. □

Proof of Proposition 1.3 Direct corollary from Theorem 4.1. □

5 Proof of Theorem 1.1

In this section, we prove the main theorem. As have been mentioned in the introduction. We will show that, for any $T > 0$, the sequence $m_{N,t}$ is weakly compact and that any accumulation point m_t is exactly the solution of the Vlasov equation. For this purpose, we need the following lemma.

Lemma 5.1 *Let $m_{N,t}$ be weak solution of the reformulated Schrödinger equation (1.11) and $\rho_{N,t}(q) := \int dp m_{N,t}(p, q)$. Then there exists a subsequence of $m_{N,t}$ (without relabeling for convenience) and function m_t such that as $N \rightarrow \infty$*

$$m_{N,t} \xrightarrow{*} m_t \text{ in } L^\infty(0, T; L^s(\mathbb{R}^3 \times \mathbb{R}^3)), \quad s \in [1, \infty], \tag{5.1}$$

$$\nabla V * \rho_{N,t} \rightarrow \nabla V * \rho_t \text{ in } L^r(0, T; L^r(\mathbb{R}^3)), \quad r \in (1, \infty), \tag{5.2}$$

where $\rho_t = \int dp m_t$.

Proof The estimates in Appendix B imply

$$\|m_{N,t}\|_{L^\infty(0,T;L^1(\mathbb{R}^3 \times \mathbb{R}^3))} + \|m_{N,t}\|_{L^\infty(0,T;L^\infty(\mathbb{R}^3 \times \mathbb{R}^3))} \leq C, \tag{5.3}$$

where C appeared in this section denotes a positive constant independent of N . And combining interpolation inequality, we have

$$\|m_{N,t}\|_{L^\infty(0,T;L^s(\mathbb{R}^3 \times \mathbb{R}^3))} \leq C, \quad s \in [1, \infty].$$

Therefore, (5.1) is a direct consequence of the above inequality and the moment estimates in Proposition B.1.

Furthermore, Proposition B.1 implies $\| |p|^2 m_{N,t} \|_{L^\infty(0,T;L^1(\mathbb{R}^3 \times \mathbb{R}^3))} \leq C$, together with (5.3), we arrive at $\|\rho_{N,t}\|_{L^\infty(0,T;L^s(\mathbb{R}^3))} \leq C$ for $s \in [1, \frac{5}{3}]$. Hence there exists a subsequence of $\rho_{N,t}$ (which is not re-labeled for convenience) such that

$$\rho_{N,t} \xrightarrow{*} \rho_t \text{ in } L^\infty(0, T; L^s(\mathbb{R}^3)), \quad s \in \left(1, \frac{5}{3}\right].$$

Owing to $V \in W^{2,\infty}(\mathbb{R}^3)$ and Young’s convolution inequality, we have for a.e. $t \in (0, T)$,

$$\|\nabla^2 V * \rho_{N,t}\|_{L^\infty(\mathbb{R}^3)} \leq \|\nabla^2 V\|_{L^\infty(\mathbb{R}^3)} \|\rho_{N,t}\|_{L^1(\mathbb{R}^3)} \leq C.$$

Similarly, we obtain that

$$\|\nabla V * \rho_{N,t}\|_{L^\infty(0,T;W^{1,\infty}(\mathbb{R}^3))} \leq C. \tag{5.4}$$

By means of (1.11), we get

$$\partial_t \rho_{N,t} = \partial_t \int dp m_{N,t}(p, q) = -\nabla_q \cdot \int dp p m_{N,t}(p, q) + \nabla_q \cdot \int dp \tilde{\mathcal{R}}.$$

It is easy to see that $\partial_t(\nabla V * \rho_{N,t})$ satisfies the following equation:

$$\partial_t(\nabla V * \rho_{N,t}) = -\nabla_q \cdot \left(\nabla V \otimes_* \int dp p m_{N,t}(p, q) \right) + \nabla_q \cdot \left(\nabla V \otimes_* \int dp \tilde{\mathcal{R}} \right),$$

where $(u \otimes_* v)_{ij} = u_i * v_j$ for $(u, v) \in \mathbb{R}^3 \times \mathbb{R}^3$. Noticing that

$$\left\| \int dp p m_{N,t}(p, q) \right\|_{L^\infty(0,T;L^s(\mathbb{R}^3))} \leq C, \quad s \in \left[1, \frac{5}{4} \right],$$

we derive for any test function $\tilde{\varphi}(q) \in W^{1,3}(\mathbb{R}^3)$ and a.e. $t \in (0, T)$,

$$\begin{aligned} & \left| \int_{\mathbb{R}^3} dq \nabla_q \cdot \left(\nabla V \otimes_* \int dp p m_{N,t}(p, q) \right) \tilde{\varphi}(q) \right| \\ & \leq C(V) \left\| \int dp p m_{N,t}(p, q) \right\|_{L^1(\mathbb{R}^3)} \|\nabla \tilde{\varphi}(q)\|_{L^3(\mathbb{R}^3)}. \end{aligned}$$

For the second term, applying Proposition 1.1, we have

$$\begin{aligned} \left| \int dq \nabla_q \cdot \left(\nabla V \otimes_* \int dp \tilde{\mathcal{R}} \right) \tilde{\varphi}(q) \right| & \leq C(V) \left\| \int dp \tilde{\mathcal{R}} \right\|_{L^{\frac{5}{4}}(\mathbb{R}^3)} \|\nabla \varphi(q)\|_{L^3(\mathbb{R}^3)} \\ & \leq C\hbar \|\nabla \varphi(q)\|_{L^3(\mathbb{R}^3)}. \end{aligned}$$

The estimates above show that

$$\|\partial_t(\nabla V * \rho_{N,t})\|_{L^\infty(0,T;W^{-1,\frac{3}{2}}(\mathbb{R}^3))} \leq C. \tag{5.5}$$

The inequalities (5.4) and (5.5) allow us to apply Aubin–Lions lemma (e.g. in [4, 31]) to infer that (5.2). We mention here that the application of Aubin–Lions lemma is proceeded in a sequence of growing balls, and the convergent subsequence is obtained through diagonal rule. \square

Proof of Theorem 1.1 With the help of (5.1), (5.2), Propositions 1.1, 1.2 and 1.3, we can take limit $N \rightarrow \infty$ in the weak formulation of the reformulated Schrödinger equation (1.11). More precisely, for any $\phi, \varphi \in C_0^\infty(\mathbb{R}^3)$ and $\eta \in C_0^\infty[0, T)$, $m_{N,t}$ satisfies the following equation

$$\begin{aligned} & \int_0^T dt \int dq dp m_{N,t}(p, q) [\partial_t \eta \varphi(q) \phi(p) + p \cdot \eta(t) \nabla_q \varphi(q) \phi(p) \\ & \quad - \frac{1}{(2\pi)^3} \nabla V * \rho_{N,t} \eta(t) \varphi(q) \cdot \nabla_p \phi(p)] \\ & = \int_0^T dt \eta(t) \int dq dp (\nabla \varphi(q) \phi(p) \tilde{\mathcal{R}} + \varphi(q) \nabla \phi(p) (\mathcal{R}_s + \mathcal{R}_m)) \\ & \quad - \eta(0) \int dq dp \varphi(q) \phi(p) m_{N,0}. \end{aligned}$$

Since the sums and products of functions of the form $\eta(t)\varphi(q)\phi(p)$ are dense in $C_0^\infty([0, T) \times \mathbb{R}^3 \times \mathbb{R}^3)$, we have showed that the limit of the subsequence is a weak solution of the Vlasov equation. On the other hand, the assumption 1 in H1 implies that $V \in W^{2,\infty}$, from which

one obtains that the Vlasov equation has a unique weak solution as in [21, Theorem 1.1]. Therefore, the whole sequence $m_{N,t}$ converges weakly. Hence the proof of Theorem 1.1 is completed. \square

Acknowledgements We acknowledge support from the Deutsche Forschungsgemeinschaft through Grant CH 955/4-1. Yue Li supported by National Natural Science Foundation of China (12071212). Jinyeop Lee received funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy (EXC-2111-390814868).

Funding Open Access funding enabled and organized by Projekt DEAL.

Data Availability Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

Declarations

Conflicts of interest The authors declare that they have no conflict of interest.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article’s Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article’s Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

Appendices

Appendix A: Second Quantization

The Fock space formalism and some results from Bogoliubov theory for the proof of this paper are listed in the following.² In particular, as in [9], we will introduce the fermionic Fock space over Hilbert spaces as the following direct sum:

$$\mathcal{F}_a := \mathbb{C} \oplus \bigoplus_{n \geq 1} L_a^2(\mathbb{R}^{3n}).$$

By convention, we say that the vacuum state, denoted as $\Omega = \{1, 0, 0, \dots\}$, belongs to \mathbb{C} . For all $\Psi = \{\psi^{(n)}\}_{n \in \mathbb{N}} \in \mathcal{F}_a$ and $\psi^{(n)} \in L_a^2(\mathbb{R}^{3n})$, we define the number of particle operator on the n -th sector by $(\mathcal{N}\Psi)^{(n)} = n\psi^{(n)}$.

As in [9], the creation and annihilation operators acting on $\Psi \in \mathcal{F}_a$ is defined as follows: for any $f \in L^2(\mathbb{R}^3)$

$$(a^*(f)\Psi)^{(n)}(x_1, \dots, x_n) := \sum_{j=1}^n \frac{(-1)^j}{\sqrt{n}} f(x_j) \psi^{(n-1)}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n),$$

$$(a(f)\Psi)^{(n)}(x_1, \dots, x_n) := \sqrt{n+1} \int dx \overline{f(x)} \psi^{(n+1)}(x, x_1, \dots, x_n),$$

² See [35] for more pedagogic treatment on the topics.

where $\psi^{(n)} \in L^2(\mathbb{R}^{3n})$ for any $n \in \mathbb{N}$. Additionally, for convenient purposes, the creation and annihilation operators will be represented by its operator-value distribution, a_x^* and a_x respectively, so that

$$a^*(f) = \int dx f(x) a_x, \quad a(f) = \int dx \overline{f(x)} a_x.$$

Therefore, the canonical anticommutator relation(CAR) is written as

$$\{a_x^*, a_y\} = \delta_{x=y}, \quad \{a_x^*, a_y^*\} = \{a_x, a_y\} = 0,$$

for any $x, y \in \mathbb{R}^3$.

Observe that for given any $\Psi, \Phi \in \mathcal{F}_a$, it holds that

$$\langle \Psi, \mathcal{N}\Phi \rangle = \int dx \langle a_x \Psi, a_x \Phi \rangle.$$

Therefore, we write the number of particles operator as $\mathcal{N} = \int dx a_x^* a_x$. Similarly, the integral kernel of the k -particle reduced density matrix is written as follows:

$$\gamma^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) = \langle \Psi, a_{y_1}^* \dots a_{y_k}^* a_{x_k} \dots a_{x_1} \Psi \rangle. \tag{A.1}$$

Moreover, the Hamiltonian acting on $\Psi \in \mathcal{F}_a$ can be written as

$$\mathcal{H}_N := \frac{\hbar^2}{2} \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \int dx dy V(x - y) a_x^* a_y^* a_y a_x, \tag{A.2}$$

where V is the interaction potential. We will denote the operator of the kinetic term as

$$\mathcal{K} = \hbar^2 \int dx \nabla_x a_x^* \nabla_x a_x. \tag{A.3}$$

As presented in [8, 44], for any $t \geq 0$, there exists a unitary transformation $\mathcal{R}_{\mathcal{V}_{N,t}} : \mathcal{F}_a \rightarrow \mathcal{F}_a$ such that

$$\begin{aligned} \mathcal{R}_{\mathcal{V}_{N,t}}^* a_x \mathcal{R}_{\mathcal{V}_{N,t}} &= a(u_{t,x}) + a^*(\bar{v}_{t,x}), \\ \mathcal{R}_{\mathcal{V}_{N,t}}^* a_x^* \mathcal{R}_{\mathcal{V}_{N,t}} &= a^*(u_{t,x}) + a(\bar{v}_{t,x}), \end{aligned} \tag{A.4}$$

where $v_{t,x} := \sum_{j=1}^N |\bar{e}_{j,t}\rangle \langle e_{j,t}|$ and $u_{t,x} := \mathbb{1} - \sum_{j=1}^N |e_{j,t}\rangle \langle e_{j,t}|$, for any orthonormal basis $\{e_{j,t}\}_{j=1}^N \subset L^2(\mathbb{R}^3)$.

Then, for $t \geq 0$, the solution of the Schrödinger equation is given as

$$\Psi_{N,t} = e^{-\frac{i}{\hbar} \mathcal{H}_N t} \mathcal{R}_{\mathcal{V}_{N,0}} \Omega = \mathcal{R}_{\mathcal{V}_{N,t}} \mathcal{U}_N(t; 0) \Omega, \tag{A.5}$$

where $\mathcal{R}_{\mathcal{V}_{N,t}}$ is a unitary Bogoliubov mapping and \mathcal{U}_N is the quantum fluctuation dynamics defined as follows,

$$\mathcal{U}_N(t; s) := \mathcal{R}_{\mathcal{V}_{N,t}}^* e^{-\frac{i}{\hbar} \mathcal{H}_N(t-s)} \mathcal{R}_{\mathcal{V}_{N,s}}. \tag{A.6}$$

Appendix B: A Priori Estimates

In this appendix, we present in this section a sequence of estimates from [13] that will prove useful to our calculation. First, we have the following properties of k -particle Husimi measures from [13, Lemma 2.2]

Lemma B.1 Let $m_{N,t}^{(k)}$ be the k -particle Husimi measure as defined in (1.6). Then, the following properties hold:

1. $m_{N,t}^{(k)}(q, p, \dots, q_k, p_k)$ is symmetric,
2. $\frac{1}{(2\pi)^{3k}} \int (dq dp)^{\otimes k} m_{N,t}^{(k)}(q, p, \dots, q_k, p_k) = \frac{N(N-1)\dots(N-k+1)}{N^k}$,
3. $\frac{1}{(2\pi\hbar)^3} \int dq_k dp_k m_{N,t}^{(k)}(q, p, \dots, q_k, p_k) = (N - k + 1)m_{N,t}^{(k-1)}(q, p, \dots, q_{k-1}, p_{k-1})$,
4. $0 \leq m_{N,t}^{(k)}(q, p, \dots, q_k, p_k) \leq 1$ a.e.,

where $1 \leq k \leq N$.

From [13, Lemma 2.6] and [13, Proposition 2.3], we have the following estimate for the kinetic energy as well as the moment estimate of the 1-particle Husimi measure respectively:

Lemma B.2 Assume $V \in W^{1,\infty}(\mathbb{R}^3)$, then the kinetic energy is bounded as follows:

$$\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \rangle \leq \langle \Psi_N, \frac{\mathcal{K}}{N} \Psi_N \rangle + Ct^2, \tag{B.1}$$

where \mathcal{K} is defined in (A.3) and the constant C depends on $\|\nabla V\|_\infty$.

Proposition B.1 For $t \geq 0$, we have the following finite moments:

$$\int dq dp (|q| + |p|^2) m_{N,t}(q, p) \leq C(1 + t^3), \tag{B.2}$$

where $C > 0$ is a constant that depends on initial data $\int dq dp (|q| + |p|^2) m_N(q, p)$.

Next, we will present the oscillation estimate from [13, Lemma 2.5] which will be used frequently in our proof:

Lemma B.3 (Bound on localized number operator) Let $\psi_N \in \mathcal{F}_a^{(N)}$ such that $\|\psi_N\| = 1$, and R be the radius of a ball such that the volume is 1. Then we have

$$\int dq dx \langle \psi_N, \chi_{|x-q| \leq \sqrt{\hbar}R} a_x^* a_x \psi_N \rangle \leq C(R)\hbar^{-\frac{3}{2}},$$

where χ is a characteristic function.

Lemma B.4 (Estimate of oscillation) For $\varphi \in C_0^\infty(\mathbb{R}^3)$ and

$$\Omega_h^\alpha := \{x \in \mathbb{R}^3; \max_{1 \leq j \leq 3} |x_j| \leq h^\alpha\}, \tag{B.3}$$

it holds for every $\alpha \in (0, 1)$, $s \in \mathbb{N}$, and $x \in \mathbb{R}^3 \setminus \Omega_h^\alpha$,

$$\left| \int_{\mathbb{R}^3} dp e^{\frac{i}{\hbar} p \cdot x} \varphi(p) \right| \leq C\hbar^{(1-\alpha)s}, \tag{B.4}$$

where C depends on the compact support and the C^s -norm of φ .

References

1. Amour, L., Khodja, M., Nourrigat, J.: The classical limit of the Heisenberg and time-dependent Hartree–Fock equations: the Wick symbol of the solution. *Math. Res. Lett.* **20**(1), 119–139 (2013)
2. Amour, L., Khodja, M., Nourrigat, J.: The semiclassical limit of the time dependent Hartree–Fock equation: the Weyl symbol of the solution. *Anal. PDE* **6**(7), 1649–1674 (2013)

3. Athanassoulis, A., Paul, T., Pezzotti, F., Pulvirenti, M.: Strong semiclassical approximation of Wigner functions for the Hartree dynamics. In: *Atti della Accademia Nazionale dei Lincei, Classe di Scienze Fisiche, Matematiche e Naturali, Rendiconti Lincei Matematica E Applicazioni*, 22 (2011)
4. Aubin, J.-P.: Analyse mathématique-un theoreme de compacite. *C. R. Hebdomad. Seanc. Acad. Sci.* **256**(24), 5042 (1963)
5. Bach, V., Breteaux, S., Petrat, S., Pickl, P., Tzaneteas, T.: Kinetic energy estimates for the accuracy of the time-dependent Hartree–Fock approximation with Coulomb interaction. *J. Math. Pures Appl.* **105**(1), 1–30 (2016)
6. Benedikter, N.: Effective dynamics of interacting fermions from semiclassical theory to the random phase approximation. *J. Math. Phys.* **63**(8), 081101 (2022)
7. Benedikter, N., Porta, M., Schlein, B.: Mean-field dynamics of fermions with relativistic dispersion. *J. Math. Phys.* **55**(2), 021901 (2014)
8. Benedikter, N., Porta, M., Schlein, B.: Mean-field evolution of fermionic systems. *Commun. Math. Phys.* **331**(3), 1087–1131 (2014)
9. Benedikter, N., Porta, M., Schlein, B.: *Effective Evolution Equations from Quantum Dynamics*, vol. 7. Springer, New York (2016)
10. Benedikter, N., Jakšić, V., Porta, M., Saffirio, C., Schlein, B.: Mean-field evolution of fermionic mixed states. *Commun. Pure Appl. Math.* **69**(12), 2250–2303 (2016)
11. Benedikter, N., Porta, M., Saffirio, C., Schlein, B.: From the Hartree dynamics to the Vlasov equation. *Arch. Ration. Mech. Anal.* **221**(1), 273–334 (2016)
12. Bröcker, T., Werner, R.F.: Mixed states with positive Wigner functions. *J. Math. Phys.* **36**(1), 62–75 (1995)
13. Chen, L., Lee, J., Liew, M.: Combined mean-field and semiclassical limits of large fermionic systems. *J. Stat. Phys.* **182**(2), 1–41 (2021). [arXiv:1910.09892v4](https://arxiv.org/abs/1910.09892v4)
14. Chong, J.J., Lafleche, L., Saffirio, C.: From many-body quantum dynamics to the Hartree–Fock and Vlasov equations with singular potentials (2021). [arXiv:2103.10946](https://arxiv.org/abs/2103.10946)
15. Combesure, M., Robert, D.: *Coherent States and Applications in Mathematical Physics*. Springer, Heidelberg (2012)
16. Dietler, E., Rademacher, S., Schlein, B.: From Hartree dynamics to the relativistic Vlasov equation. *J. Stat. Phys.* **172**(2), 398–433 (2018)
17. Elgart, A., Erdős, L., Schlein, B., Yau, H.-T.: Nonlinear Hartree equation as the mean field limit of weakly coupled fermions. *J. Math. Pures Appl.* **83**(10), 1241–1273 (2004)
18. Fournais, S., Lewin, M., Solovej, J.P.: The semi-classical limit of large fermionic systems. *Calc. Variat. Partial Diff. Equ.* **57**(4), 105 (2018)
19. Fröhlich, J., Knowles, A.: A microscopic derivation of the time-dependent Hartree–Fock equation with Coulomb two-body interaction. *J. Stat. Phys.* **145**(1), 23 (2011)
20. Gasser, I., Illner, R., Markowich, P.A., Schmeiser, C.: Semiclassical, $t \rightarrow \infty$ asymptotics and dispersive effects for Hartree–Fock systems. *ESAIM Math. Model. Numer. Anal. Mod. Math. Anal. Num.* **32**(6), 699–713 (1998)
21. Golse, F.: Mean-field limits in statistical dynamics. (2022). [arXiv:2201.02005](https://arxiv.org/abs/2201.02005)
22. Golse, F., Paul, T.: The Schrödinger equation in the mean-field and semiclassical regime. *Arch. Ration. Mech. Anal.* **223**(1), 57–94 (2017)
23. Golse, F., Paul, T.: Mean-field and classical limit for the n-body quantum dynamics with Coulomb interaction. *Commun. Pure Appl. Math.* (2021)
24. Golse, F., Paul, T., Pulvirenti, M.: On the derivation of the Hartree equation in the mean field limit: Uniformity in the Planck constant. *J. Funct. Anal.* **275**(7), 1603–1649 (2018)
25. Graffi, S., Martinez, A., Pulvirenti, M.: Mean-field approximation of quantum systems and classical limit. *Math. Models Methods Appl. Sci.* **13**(01), 59–73 (2003)
26. Hudson, R.: When is the Wigner quasi-probability density non-negative? *Rep. Math. Phys.* **6**(2), 249–252 (1974)
27. Kenfack, A., Życzkowski, K.: Negativity of the Wigner function as an indicator of non-classicality. *J. Opt. B* **6**(10), 396 (2004)
28. Lafleche, L.: Global semiclassical limit from Hartree to Vlasov equation for concentrated initial data. [arXiv:1902.08520](https://arxiv.org/abs/1902.08520) (2019)
29. Lafleche, L.: Propagation of moments and semiclassical limit from Hartree to Vlasov equation. *J. Stat. Phys.* **177**(1), 20–60 (2019)
30. Lafleche, L., Saffirio, C.: Strong semiclassical limit from Hartree and Hartree–Fock to Vlasov–Poisson equation. [arXiv:2003.02926](https://arxiv.org/abs/2003.02926) (2020)
31. Lions, J.-L.: *Quelques Méthodes de Résolution des Problemes aux Limites non Linéaires*. Dunod, Paris (1969)
32. Lions, P.-L., Paul, T.: Sur les mesures de Wigner. *Rev. Mat. Iberoam.* **9**(3), 553–618 (1993)

33. Mandilara, A., Karpov, E., Cerf, N.J.: Extending Hudson's theorem to mixed quantum states. *Phys. Rev. A* **79**, 062302 (2009)
34. Markowich, P.A., Mauser, N.J.: The classical limit of a self-consistent quantum-Vlasov equation in 3d. *Math. Models Methods Appl. Sci.* **3**, 109–124 (1993)
35. Nam, P.T.: *Mathematical Quantum Mechanics II*. Lecture Notes (2020)
36. Narnhofer, H., Sewell, G.L.: Vlasov hydrodynamics of a quantum mechanical model. *Commun. Math. Phys.* **79**(1), 9–24 (1981)
37. Petrat, S.: *Derivation of Mean-field Dynamics for Fermions*. PhD thesis, LMU Munich (2014)
38. Petrat, S.: Hartree corrections in a mean-field limit for fermions with Coulomb interaction. *J. Phys. A* **50**(24), 244004 (2017)
39. Petrat, S., Pickl, P.: A new method and a new scaling for deriving fermionic mean-field dynamics. *Math. Phys. Anal. Geom.* **19**, 1–51 (2016)
40. Porta, M., Rademacher, S., Saffirio, C., Schlein, B.: Mean field evolution of fermions with Coulomb interaction. *J. Stat. Phys.* **166**(6), 1345–1364 (2017)
41. Saffirio, C.: Mean-field evolution of fermions with singular interaction. In: *Workshop on Macroscopic Limits of Quantum Systems*. Springer, New York, pp. 81–99 (2017)
42. Saffirio, C.: From the Hartree equation to the Vlasov–Poisson system: strong convergence for a class of mixed states. *SIAM J. Math. Anal.* **52**(6), 5533–5553 (2020)
43. Saffirio, C.: Semiclassical limit to the Vlasov equation with inverse power law potentials. *Commun. Math. Phys.* **373**(2), 571–619 (2020)
44. Solovej, J.P.: *Many body quantum mechanics* (2009)
45. Soto, F., Claverie, P.: When is the Wigner function of multidimensional systems nonnegative? *J. Math. Phys.* **24**(1), 97–100 (1983)
46. Spohn, H.: On the Vlasov hierarchy. *Math. Methods Appl. Sci.* **3**(1), 445–455 (1981)
47. Villani, C.: *Topics in Optimal Transportation*. American Mathematical Society, London (2003)
48. Zhang, P.: *Wigner Measure and Semiclassical Limits of Nonlinear Schrödinger Equations*. American Mathematical Society, London (2008)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.