

Time-Dependent Effective One-Particle Equations for  
Large Interacting Fermionic Systems

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## Abstract

On the quantum scale, the dynamics of many-particles in a system are governed by Schrödinger's quantum systems. However, it is computationally costly to simulate if the system consists of a large number of particles. Therefore, the method of deriving an effective equation that captures the macroscopic behavior of the particles is of high interest in the mathematical physics community.

In this thesis, we focus on the derivation of an effective time-dependent equation of a macroscopic system consisting of interacting fermions. In particular, we derive a Vlasov hierarchy from the Schrödinger system with respect to the Husimi measure. Then, we show that under regularized interaction potential, the quantum system converges to the Vlasov equation in terms of semiclassical limit by using the BBGKY method and Bogoliubov transformation independently. Furthermore, we extend the convergence result to the Vlasov-Poisson equation by considering a  $N$ -fermionic Schrödinger system with truncated Coulomb interaction potential.

**Keywords:** Large Fermionic System, Husimi measure, Semiclassical Scale, Schrödinger equation, Coulomb potential, Vlasov-Poisson equation, BBGKY method, Bogoliubov transformation.

## Zusammenfassung

Auf der Quantenebene wird die Teilchendynamik in einem System durch Schrödingers Quantenmechanik beschrieben. Bei einer großen Anzahl Teilchen ist die Simulation eines solchen Systems jedoch sehr rechenaufwändig. Daher ist die Ableitung einer effektiven Gleichung, die das Verhalten von Teilchen auf der Makroebene beschreibt, von hohem Interesse in der mathematischen Physik.

In dieser Doktorarbeit konzentrieren wir uns auf die Bestimmung einer effektiven, zeitabhängigen Gleichung für ein makroskopisches System, bestehend aus Fermionen. Insbesondere leiten wir eine Vlasov-Hierarchie aus dem Schrödinger-System in Form eines Husimi-Maßes her. Anschließend zeigen wir, dass das Quantensystem unter regularisiertem Wechselwirkungspotential mit Hilfe der BBGKY-Methode und der Bogoliubov-Transformation zur Vlasov-Gleichung im semiklassischen Limit konvergiert. Außerdem erweitern wir das Konvergenzresultat von  $N$ -fermionisches Schrödinger-System auf die Vlasov-Poisson-Gleichung, indem wir ein regularisiertes Coulomb-Potential betrachten.

**Schlüsselwörter:** Fermionisches Mehrteilchensysteme, Husimi-Maß, Semiklassische Skalierung, Schrödinger-Gleichung, Coulomb Potential, Vlasov-Poisson Gleichung, BBGKY Verfahren, Bogoliubov Abbildung.

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# Chapter 1

## Introduction

Prior to the 20th century, the physical understanding of the world was thought to be governed by newtonian mechanics. However, as experimental abilities improved at the turn of century, physicists unveiled an increasing number of discrepancies between classical physics and what was observed in their labs. Thus, classical mechanics can no longer adequately explain the phenomenon in both macro- and microscopic level. The first fundamental change was the discovery of *wave-particle duality*, i.e. that light can behave both like particle and wave. The second fundamental change is the probabilistic nature of particles which was shown in the famous ‘Young’s double-slit’ experiment, invalidating the deterministic nature of newtonian physics. From Young’s experiment, it was shown that the collection of identical electrons can behave like a wave. In fact, it evolves in a wave-like equation and one may determine the position of an electron with respect of time, in a certain likelihood, by solving the so-called Schrödinger equation. This set the genesis for the field of quantum mechanics.

In quantum mechanics, physical quantities such as energy, position and momentum are represented by operators in a Hilbert space  $\mathbb{H}$  over complex space. In three dimensional space, the corresponding wave function for the particle is defined as a mapping  $\psi : \mathbb{R}^3 \rightarrow \mathbb{C}$  and its normalization is given by

$$\int_{\mathbb{R}^3} dx |\psi(x)|^2 = 1,$$

for all  $x \in \mathbb{R}^3$ .

Introducing the position and momentum operators on  $\mathbb{H}$  as  $X$  and  $P$  respectively, the *First Quantization* of position and momentum given by the following equations

$$\begin{aligned} X\psi(x) &= x\psi(x), \\ P\psi(x) &= -i\hbar \frac{d}{dx}\psi(x). \end{aligned}$$



Observe that even if  $\psi$  belongs to  $L^2$ -space, the function  $x\psi(x)$  may not be in  $L^2$  space. Moreover,  $\partial^j \psi$  could also fail to be in  $L^2$  space. This means that the operator  $X$  and  $P$  could be unbounded. Therefore, a domain derived from a suitable subspace of  $L^2$  needs to be defined. This could be done with application from spectral theories with certain Hermitian assumption on the Hamiltonian. Nevertheless, this thesis will not itself concern about the unbounded momentum and position operators, instead we assume that the operators in the Hilbert space is bounded.

Furthermore, we observe that the momentum and position operator are self-adjoint, i.e. for all  $\phi, \psi \in L^2$

$$\begin{aligned}\langle \phi, X\psi \rangle_{L^2(\mathbb{R})} &= \langle X\phi, \psi \rangle_{L^2(\mathbb{R})}, \\ \langle \phi, P\psi \rangle_{L^2(\mathbb{R})} &= \langle P\phi, \psi \rangle_{L^2(\mathbb{R})}.\end{aligned}$$

The *Heisenberg uncertainty principle* can be expressed by the following inequality

$$\langle \psi, X^2 \psi \rangle \langle \psi, P^2 \psi \rangle \geq \left( \frac{\hbar}{2} \right)^2. \quad (1.0.1)$$

The left hand side of (1.0.1) can be interpreted as the variance of the observables. The inequality implies that one cannot observe the position of a particle with certainty without giving up the certainty in observing its momentum vice versa.

## 1.1 Many-particles system

Suppose now we have  $N$  particles in a system of the same type (i.e., either bosons or fermions), the Hilbert space of this system is  $L^2(\mathbb{R}^{3N})$ , and that the time-dependent wave function  $\psi_{N,t} \in L^2(\mathbb{R}^{3N})$  has the following normalization

$$1 = \|\psi_{N,t}\|_{L^2}^2 := \int \cdots \int dx_1 \cdots dx_N |\psi_{N,t}(x_1, \dots, x_N)|^2,$$

for all  $t \geq 0$ .

The Hamiltonian for  $N$ -body particles given by

$$H_N = -\frac{\hbar^2}{2} \sum_{j=1}^N \Delta_{x_j} + \frac{\sigma_N}{2} \sum_{i \neq j}^N V(x_i - x_j), \quad (1.1.1)$$

where  $\Delta_{x_j}$  is the Laplacian operator acting on  $j$ -particle and  $\sigma_N$  is the coupling constant that is to be chosen depending on the type of particles.<sup>1</sup> The first term on the left hand side of (1.1.1) corresponds to the kinetic energy of the system and the term  $V$  in the second term is the interaction potential. We will make further

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<sup>1</sup>In fact, for bosons and fermions, the coupling constant  $\sigma_N$  is  $N^{-1}$  and  $N^{-2/3}$  respectively.

assumptions for the term  $V$  later in this thesis.

For all  $t \geq 0$ , the time-dependent Schrödinger equation for  $N$ -identical particles can be expressed by

$$\begin{cases} i\hbar\partial_t\psi_{N,t} = H_N\psi_{N,t}, \\ \psi_{N,0} = \psi_N, \end{cases}$$

where  $\psi_{N,t} \in L^2(\mathbb{R}^{3N})$  and initial data  $\psi_N$  is given.

We assume here that identical particles are indistinguishable. This means that the wave-function should represent the same physical state as the original wave-function if we exchange, for example, position  $x_i$  and  $x_j$ , for  $i \neq j$ . In Hilbert space, this means that the new and old wave-function may differ by a constant that has modulus of 1, i.e., for all  $1 \leq i < j \leq N$ ,

$$\psi_{N,t}(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = \alpha\psi_{N,t}(x_1, \dots, x_j, \dots, x_i, \dots, x_N), \quad (1.1.2)$$

where  $|\alpha| = 1$ . If we switch again the position of any two particles we have  $\alpha^2\psi_{N,t}$ . Therefore,  $\alpha$  can take the value 1 or  $-1$ , depending on the spin of the particle. For example, if a particle is spinless,  $\alpha$  takes a value of 1 and the corresponding Hilbert space for spinless  $N$  particles is the *symmetric* subspace of  $L^2(\mathbb{R}^{3N})$ . This is known as *bosons*. Conversely, if a particle has spin of half of odd-integer (e.g.  $\frac{1}{2}, \frac{3}{2}, \dots$ ), then  $\alpha$  takes the value  $-1$  and its corresponding Hilbert space is an *anti-symmetric* subspace of  $L^2(\mathbb{R}^{3N})$ . The particle of the latter type is known as *fermion*. In this thesis, we will not focus on the spin of particles.

Since particles are assumed to be indistinguishable, the corresponding probability density remains equal, i.e.

$$|\psi_{N,t}(x_1, \dots, x_i, \dots, x_j, \dots, x_N)|^2 = |\psi_{N,t}(x_1, \dots, x_j, \dots, x_i, \dots, x_N)|^2,$$

for both bosons and fermions.

Analyzing the behavior with a large quantity of particles proved to be difficult, as solving the Schrödinger equation with very large  $N$  becomes computationally expensive. Thus, it is highly recommended to approximate the expectation values of observables by employing their corresponding effective evolution equations. To this effect, it is useful to consider a density matrix instead of describing the many particle systems as a whole. In the following, we will briefly introduce the aforementioned density matrix.

Suppose a physical observable can be associated with a self-adjoint operator  $O$  in  $\mathbb{H}$ . The expectation of the observables for a given wave function  $\psi \in L^2(\mathbb{R}^{3N})$  can then be calculated as follows,

$$\langle \psi, O\psi \rangle = \int \dots \int d\mathbf{x} \overline{\psi(\mathbf{x})} (O\psi)(\mathbf{x}),$$

where we denote  $\mathbf{x} := (x_1, \dots, x_N)$ .

Let  $\Gamma$  to be a positive semidefinite trace class operator in  $\mathbb{H}$  with trace equals to one, we define its integral kernel  $\Gamma(x_1, \dots, x_N; y_1, \dots, y_N)$  such that, for any  $\psi \in L^2(\mathbb{R}^{3N})$ ,

$$(\Gamma\psi)(\mathbf{x}) := \int \dots \int (\mathrm{d}y)^{\otimes N} \Gamma(\mathbf{x}; \mathbf{y}) \psi(\mathbf{y}),$$

where we denote  $\mathbf{y} := (y_1, \dots, y_N)$  and  $(\mathrm{d}y)^{\otimes N} := \mathrm{d}y_1 \cdots \mathrm{d}y_N$ . Let  $\{\mathbf{e}^{(j)}\}_{j=1}^N$  be a family of orthonormal bases in  $L^2(\mathbb{R}^{3N})$ ,  $\Gamma$  is called a *pure-state density matrix* when it takes the following form

$$\Gamma = \sum_{j=1}^N |\mathbf{e}^{(j)}\rangle \langle \mathbf{e}^{(j)}|,$$

On the other hand,  $\Gamma$  is called a *mixed-state density matrix* when

$$\Gamma = \sum_{j=1}^N \lambda_j |\mathbf{e}^{(j)}\rangle \langle \mathbf{e}^{(j)}|,$$

where  $\{\lambda_j\}_{j=1}^\infty$  satisfies

$$\sum_{j=1}^\infty \lambda_j = 1 \text{ and } \lambda_1 \geq \lambda_2 \geq \dots \geq 0.$$

The expectation value of an observable associated  $O$  is given by

$$\mathrm{Tr} O\Gamma = \langle \psi, O\psi \rangle \text{ and } \mathrm{Tr} O\Gamma = \sum_{j=1}^N \lambda_j \langle \mathbf{e}^{(j)}, O\mathbf{e}^{(j)} \rangle \quad (1.1.3)$$

for pure and mixed states respectively.<sup>2</sup> In this thesis, we will focus only on pure state.

Furthermore, the total energy is given by

$$\mathcal{E}(\psi) = \mathrm{Tr} H_N \Gamma = \mathrm{Tr} \Gamma H_N,$$

where  $H_N$  is the Hamiltonian defined in (1.1.1).

Assume that the quantum system has only one type of indistinguishable particles, i.e. bosons or fermions. The expectation of observables can be represented such that it depends only on a small number of particles,  $1 \leq k \ll N$ . Namely, denoting the  $k$ -reduced particle density as

$$\gamma^{(k)} = \frac{N!}{(N-k)!} \mathrm{Tr}^{(N-k)} \Gamma, \quad (1.1.4)$$

---

<sup>2</sup>Note here that the convention of inner-product in this thesis is  $\langle A, B \rangle = \int \bar{A}B$ .

and its corresponding integral kernel can be expressed by

$$\gamma^{(k)}(x_1, \dots, x_k; y_1, \dots, y_N) = \frac{N!}{(N-k)!} \int \cdots \int dx_{k+1} \cdots dx_N \Gamma(x_1, \dots, x_N; y_1, \dots, y_k, x_{k+1}, \dots, x_N).$$

The expectation value of any  $k$ -observables  $O^{(k)}$  is written as

$$\text{Tr} \left( O^{(k)} \otimes \mathbb{1}^{(N-k)} \right) \Gamma = \frac{N!}{(N-k)!} \text{Tr} O^{(k)} \gamma^{(k)}.$$

Observe that by the above definition, the  $k$ -reduced particle matrix  $\gamma^{(k)}$  is also a positive semidefinite trace-class operator and that the ‘complete’ trace is

$$\text{Tr} \gamma^{(k)} = \frac{N!}{(N-k)!}.$$

We say that a positive semidefinite operator  $\gamma^{(1)}$  with  $\text{Tr} \gamma^{(1)}$  is admissible if it is the 1-particle reduction of  $\Gamma$  on the  $N$ -particle space. As discussed in [LS09], though  $\gamma^{(1)}$  for  $N$ -bosonic state is admissible, it does not necessary hold for fermionic case. In fact, to summarize Theorem 3.1 and Theorem 3.2 respectively in [LS09], the following statements for bosons and fermions respectively:

1. For all  $N \geq 2$ , there is a bosonic  $N$ -particle density matrix such that  $\gamma^{(1)} = N \text{Tr}^{(N-1)} \Gamma$ .
2. Due to Pauli exclusion principle, there exists a fermionic  $N$ -particle density matrix

$$\gamma^{(1)} = N \text{Tr}^{(N-1)} \Gamma,$$

if and only if

$$\gamma^{(1)} \leq \mathbb{I}. \tag{1.1.5}$$

Denoting observable of  $j$ -th particle as  $O_j = \mathbb{1} \otimes \cdots \otimes O \otimes \cdots \otimes \mathbb{1}$  to be a self-adjoint operator in Hilbert space, the expected value of such observable in terms of one-particle density matrix, i.e.

$$\langle \psi, O_1 \psi \rangle = \text{Tr} O_1 \gamma^{(1)}.$$

The benefit of dealing with a reduced-particle density matrix is that by finding an approximating effective equation that describes the system one avoids having to deal with the  $N$ -particle state  $\psi$ . For the fermionic case, this can lead to the Hartree-Fock equation which will be discussed later in the following section.

### 1.1.1 Large fermionic system

In this subsection, we will focus on the particle system consists of only fermions and briefly introduce its corresponding Hartree-Fock theory and equation. Then, a brief discussion of semiclassical structure will be presented in order to see the relation between the particle density matrix and Wigner measure more clearly.

Observe first that the  $L^2$ -subspace for indistinguishable fermions is the antisymmetric space is defined as

$$\bigwedge^N L^2(\mathbb{R}^3) := \left\{ \psi_{N,t} \in L^2(\mathbb{R}^{3N}) : \psi_{N,t}(x_{\pi(1)}, \dots, x_{\pi(N)}) = \varepsilon(\pi) \psi_{N,t}(x_1, \dots, x_N) \right\}, \quad (1.1.6)$$

for all  $t \geq 0$  and  $\varepsilon(\pi)$  is the sign of odd-permutations. This corresponds to (1.1.2) with  $\alpha = -1$ . In this thesis, we will consider a system of interacting fermions as described by its corresponding Hamiltonian given in (1.1.1). In fact, as discussed in [BBP<sup>+</sup>16, BPS14a, EESY04], it is known that a system of fermions that is initially confined in a volume of order one has kinetic energy of order  $N^{5/3}$  due to the Pauli exclusion principle. This implies that the coupling constant should be chosen as  $N^{-1/3}$  to balance the order of the kinetic energy and the potential energy, the latter is of order  $N^2$ . Thus, the mean-field Hamiltonian acting on  $L_a^2(\mathbb{R}^{3N})$  is given by the following equation:

$$\tilde{H}_N := -\frac{1}{2} \sum_{j=1}^N \Delta_{x_j} + \frac{1}{2N^{1/3}} \sum_{i \neq j}^N V(x_i - x_j).$$

The time-dependent Schrödinger equation is given by

$$i\partial_\tau \psi_{N,\tau} = \tilde{H}_N \psi_{N,\tau},$$

for all  $\psi_{N,\tau} \in L_a^2(\mathbb{R}^{3N})$  and  $\tau \geq 0$ . Since the average kinetic energy for each fermionic particle is of order  $N^{2/3}$ , then its average velocity is of order  $N^{1/3}$ . Therefore, in the mean-field regime, the time evolution of the fermion system is expected to be of order  $N^{-1/3}$ . Rescaling the time variable  $t = N^{1/3}\tau$ , one obtains the following Schrödinger equation for  $N$  fermions:

$$iN^{\frac{1}{3}} \partial_t \psi_{N,t} = \left( \sum_{j=1}^N -\frac{\Delta_j}{2} + \frac{1}{2N^{\frac{1}{3}}} \sum_{i \neq j}^N V(x_i - x_j) \right) \psi_{N,t}, \quad (1.1.7)$$

for all  $\psi_{N,t} \in \bigwedge^N L^2(\mathbb{R}^3)$  and time  $t \in [0, \infty)$ . Denoting the semiclassical scale as,<sup>3</sup>

$$\boxed{\hbar = \frac{1}{N^{1/3}}}, \quad (1.1.8)$$

---

<sup>3</sup>The semiclassical scaling considered here is related to the Planck's constant. Such a scale has been studied extensively for Thomas-Fermi and Hartree-Fock theory (see [LS73]). Other coupling constants for different systems have also been considered and summarized in [BBP<sup>+</sup>16].

and multiply (1.1.7) by  $\hbar^2$  on both side, we obtain

$$i\hbar\partial_t\psi_{N,t} = \left( \sum_{j=1}^N -\frac{\hbar^2}{2}\Delta_j + \frac{1}{2N} \sum_{i \neq j}^N V(x_i - x_j) \right) \psi_{N,t}. \quad (1.1.9)$$

Therefore, the corresponding Hamiltonian that will be considered throughout this thesis is the following:

$$H_N = \sum_{j=1}^N -\frac{\hbar^2}{2}\Delta_j + \frac{1}{2N} \sum_{i \neq j}^N V(x_i - x_j) \quad (1.1.10)$$

*Remark 1.1.1.* Observe that the Hamiltonian given in (1.1.10) yields the Thomas-Fermi energy

$$\mathcal{E}^{\text{TF}}(\rho) = \int dx \frac{3}{5} c_{\text{TF}} \rho(x) + \frac{1}{2} \iint dx dy V(x-y) \rho(x) \rho(y), \quad (1.1.11)$$

where normalized momentum  $\rho \in (L^1(\mathbb{R}^3) \cap L^{\frac{5}{3}}(\mathbb{R}^3))$  is the minimizer of the functional and  $c_{\text{TF}}$  is the Thomas-Fermi constant. See [LS09] for more details.

Denoting  $\gamma_N^{(1)} := \gamma_{N,0}^{(1)}$  as 1-particle density matrix associated with initial state  $\psi_N := \psi_{N,0}$  confined in volume of order 1. Then, choosing the initial data to be Slater determinant, i.e. for any family of orthonormal bases  $\{e_i\}_{i=1}^N \subset L^2(\mathbb{R}^3)$ , one obtains

$$\begin{aligned} \psi_N^{\text{slater}}(x_1, \dots, x_N) &= (N!)^{-\frac{1}{2}} \det\{e_i(x_j)\}_{i,j=1}^N \\ &= \varepsilon(\sigma) \sum_{\sigma \in S_\pi} \prod_{j=1}^N e_{\sigma(j)}(x_j) \end{aligned} \quad (1.1.12)$$

where  $S_\pi$  be the group of odd permutation, and  $\varepsilon(\sigma)$  is the sign function corresponding to the odd permutation. This choice ensures us the  $\psi_N \equiv \psi_N^{\text{slater}}(x_1, \dots, x_N)$  satisfies the antisymmetrized state described in (1.1.6).

Given initial data being Slater determinant, its corresponding 1-particle density function can be written as

$$\omega_N = \sum_{j=1}^N |e_j\rangle\langle e_j|, \quad (1.1.13)$$

where integral kernel is given by  $\sum_{j=1}^N \overline{e_j(y)} e_j(x)$ . Then, one may obtain the following Hartree-Fock energy:

$$\mathcal{E}^{HF}(\omega_N) = \sum_{j=1}^N \int_{\mathbb{R}^3} dx |\nabla e_j(x)|^2 + \frac{1}{2} \iint dx dy \frac{\rho(x)\rho(y) - |\omega(x;y)|^2}{|x-y|}, \quad (1.1.14)$$

where  $\rho(x) := \omega_N(x;x) = \sum_{j=1}^N |e_j|^2$  is the diagonal of the kernel  $\omega$ .

For dynamic case, if we set  $\omega_{N,t} = \sum_{j=1}^N |e_{j,t}\rangle\langle e_{j,t}|$  where  $\{e_{j,t}\}$  is a family of orthonormal base of  $L^2(\mathbb{R})$  for every  $t \geq 0$ . Then, the initial-value problem of Hartree-Fock equation can be written as

$$\begin{cases} i\hbar\partial_t\omega_{N,t} &= [-\hbar^2\Delta + (V * \rho_t) - X_t, \omega_{N,t}], \\ \omega_{N,t}|_{t=0} &= \sum_{j=1}^N |e_j\rangle\langle e_j|, \end{cases} \quad (1.1.15)$$

where  $\rho(x; x) := \frac{1}{N}\omega_{N,t}(x; x)$  is the normalised density of particles at  $x$ , and the exchange operator  $X_t$  has the integral kernel of  $X_t(x; y) = \frac{1}{N}V(x - y)\omega_{N,t}(x; y)$ .

*Remark 1.1.2.* In [BPS14a, Proposition A.1], it is proven that if one assumes  $\int dp (1 + |p|^2)\widehat{V}(p) < \infty$ , then the exchange term  $X_t$  in the Hartree-Fock equation vanishes as  $N$  tends to infinity. Moreover, they also proved that if the initial data for the time-dependent Schrödinger equation from (1.1.9) is Slater-determinant, then the solution is close to factorized form of Slater determinant.

### Semiclassical structure and Wigner measure

In this subsection, we examine the semi-classical structure for Hartree-Fock as presented in [BPS14a]. First, note that the energy minimizer of the Hartree-Fock energy in (1.1.14) is expected to be characterized by a semiclassical structure. In fact, we expect the kernel of reduced particle density to be concentrated close to the diagonal, and decays off-diagonally at  $|x - y| \gg \hbar$ .

Suppose, there are initially  $N$  fermions moving in a box of volume one with a periodic boundary condition. Furthermore, assume the initial condition to be Slater determinant constructed with the plane waves  $e^{ip \cdot x}$ , with  $|p| \leq cN^{1/3}$ , for some constant  $c$  so that the total number of orbitals equals to  $N$ . Now, with this set-up, we define the kernel of the corresponding one-particle reduced density as

$$\omega(x; y) := \sum_{|p| \leq cN^{1/3}} e^{ip \cdot (x-y)}.$$

Letting  $q := \hbar p$  with  $\hbar = N^{-1/3}$ , the kernel can be rewritten as

$$\begin{aligned} \omega(x; y) &= \sum_{|q| \leq c} e^{iq \cdot \frac{x-y}{\hbar}} \\ &\approx \frac{1}{\hbar^3} \int_{\{q \in \mathbb{R}^3; |q| \leq c\}} dq e^{iq \cdot \frac{x-y}{\hbar}}. \end{aligned} \quad (1.1.16)$$

Then, by spherical transformation, we let

$$q_1 = t \cos \theta_1$$

$$q_2 = t \cos \theta_1 \sin \theta_2$$

$$q_3 = t \sin \theta_1 \sin \theta_2.$$

The corresponding Jacobian determinant is hence given by

$$\det J(r, \theta_1, \theta_2) = t^2 \sin \theta_1.$$

Now, choosing  $z$ -axis along  $\frac{x-y}{\hbar}$  and denote  $|\xi| := \left| \frac{x-y}{\hbar} \right|$ , we have that

$$\begin{aligned} \int_{|q| \leq c} e^{iq \cdot \xi} dq &= \int_{\mathbb{R}^3} \mathbb{1}_{|q| \leq c} e^{iq \cdot \xi} dq \\ &= \int_0^c dt \int_0^{2\pi} d\theta_2 \int_0^\pi d\theta_1 e^{i(t \cos \theta_1, t \cos \theta_1 \sin \theta_2, t \sin \theta_1 \sin \theta_2) \cdot \xi} t^2 \sin \theta_1 \\ &= \int_0^c dt \int_0^{2\pi} d\theta_2 \int_0^\pi d\theta_1 e^{it \cos \theta_1 |\xi|} t^2 \sin \theta_1 \\ &= 2\pi \int_0^c \left( \int_0^\pi e^{it \cos \theta_1 |\xi|} \sin \theta_1 d\theta_1 \right) t^2 dt \\ &= 2\pi \int_0^c \left[ -\frac{1}{it|\xi|} e^{it \cos \theta_1 |\xi|} \right]_0^\pi t^2 dt \\ &= 2\pi \int_0^c t \frac{2}{|\xi|} \sin(t|\xi|) dt \\ &= \frac{4\pi}{|\xi|} \int_0^c t \sin(t|\xi|) dt \\ &= \frac{4\pi}{|\xi|^2} \left( \frac{\sin(t|\xi|)}{|\xi|} - c \cos(t|\xi|) \right). \end{aligned}$$

Therefore, we have

$$\omega(x; y) = \frac{1}{\hbar^3} \varphi \left( \frac{x-y}{\hbar} \right), \quad (1.1.17)$$

where we denote

$$\varphi(z) := \frac{4\pi}{|z|^2} \left( \frac{\sin(c|z|)}{|z|} - c \cos(c|z|) \right),$$

for any  $z \in \mathbb{R}^3$ . From equation (1.1.17), if we fix  $\hbar$  and  $N$ , then we observe that  $\omega(x; y)$  decays to zero for  $|x-y| \gg \hbar$ . Therefore, we may make an informed guess that the 1-particle density matrix is approximated to

$$\omega(x; y) \approx \frac{1}{\hbar^3} \varphi \left( \frac{x-y}{\hbar} \right) \chi \left( \frac{x+y}{2} \right), \quad (1.1.18)$$

for appropriate function  $\varphi$  and  $\chi$ , or any linear combination of such kernels. Note here that  $\chi$  fixes the density of the particles in space and that  $\varphi$  determines the momentum distribution as discussed in [BPS14a].



Differentiating the right side of (1.1.18) w.r.t. to  $x$  or  $y$ , we will obtain the constant  $\hbar^{-1}$ . For any test function  $\phi \in C_0^\infty$ , this implies that the commutator  $[\nabla, \omega]$ , is characterized by

$$\begin{aligned} \int [\nabla, \omega](x; y) \phi(y) dy &= \int (\nabla_x \omega(x; y)) \phi(y) dy - \int \omega(x; y) (\nabla_y \phi(y)) dy \\ &= \int (\nabla_x \omega(x; y)) \phi(y) dy + \int (\nabla_y \omega(x; y)) \phi(y) dy \\ &= \int (\nabla_x + \nabla_y) \omega(x; y) \phi(y) dy. \end{aligned}$$

Hence, the integral kernel of  $[\nabla, \omega]$  is

$$[\nabla, \omega](x; y) = (\nabla_x + \nabla_y) \omega(x; y) = \frac{1}{\hbar^3} \varphi\left(\frac{x-y}{\hbar}\right) \nabla \chi\left(\frac{x+y}{2}\right). \quad (1.1.19)$$

Note here that the derivative in the commutator falls onto the  $\chi$  distribution.

*Remark 1.1.3.* Observe that we do not get any factor of  $\hbar^{-1}$  from the derivation in (1.1.19), i.e.

$$\text{Tr} |[\nabla, \omega]| \leqslant CN. \quad (1.1.20)$$

The fact that  $\omega(x; y)$  decays to zero as  $|x - y| \gg \hbar$  suggests that the kernel of  $[x, \omega]$  given by

$$[x, \omega](x, y) = (x - y) \omega(x; y), \quad (1.1.21)$$

is smaller than  $\omega$  by order  $\hbar$ . [BPS14a]

On the other hand, we observe that the  $\varphi$  in (1.1.17) does not decay particularly fast at infinity. Therefore, it is not clear that we can extract  $\hbar$  factor from the difference  $(x - y)$  from the right hand side of (1.1.21). Computing the commutator of reduced density  $\omega$  with a multiplication operator  $e^{ir \cdot x}$  for fixed  $r \in (2\pi)\mathbb{Z}^3$ , we have by definition that

$$[e^{ir \cdot x}, \omega] = \sum_{|p| \leqslant cN^{1/3}} \left( \left| e^{i(r+p) \cdot x} \right\rangle \left\langle e^{ip \cdot x} \right| - \left| e^{ip \cdot x} \right\rangle \left\langle e^{i(r+p) \cdot x} \right| \right).$$

Computing the modulus square of the commutator above gives us

$$|[e^{ir \cdot x}, \omega]|^2 = \overline{[e^{ir \cdot x}, \omega]} [e^{ir \cdot x}, \omega] = \sum_{p \in I_r} |e^{ip \cdot x}\rangle \langle e^{ip \cdot x}|, \quad (1.1.22)$$

where we denote

$$I_r := (2\pi)\mathbb{Z}^3 \cap \left\{ p \in \mathbb{R}^3; \quad |p - r| \leq cN^{1/3} \ \& \ |p| \geq cN^{1/3}, \text{ or } |p - r| \geq cN^{1/3} \ \& \ |p| \leq cN^{1/3} \right\}.$$

Observe that  $||[e^{ir \cdot x}, \omega]|^2 = |[e^{ir \cdot x}, \omega]|$ , one arrives at the following inequality.

$$\text{Tr} |[e^{ir \cdot x}, \omega]| \leq CN\hbar|r|. \quad (1.1.23)$$

Hence, the trace norm of the commutator is smaller, by a factor of  $\hbar$ , than with the norm of operators  $e^{ip \cdot x} \omega$  and  $\omega e^{ip \cdot x}$ . The fact that the kernel  $\omega(x; y)$  is supported near the diagonal allows us to extract additional  $\hbar$ -factor from the trace norm of  $[e^{ir \cdot x}, \omega]$ .

Notice that if we considered the Hilbert-Schmidt(HS) norm of  $[e^{ir \cdot x}, \omega]$  and (1.1.22), one gets

$$||[e^{ir \cdot x}, \omega]||_{HS} = \left( \text{Tr} |[e^{ir \cdot x}, \omega]|^2 \right)^{\frac{1}{2}} \leq (CN\hbar|r|)^{\frac{1}{2}}. \quad (1.1.24)$$

In other words, the HS norm of  $[e^{ir \cdot x}, \omega]$  is smaller, by factor of  $\hbar^{\frac{1}{2}}$ , than HS-norm of  $e^{ip \cdot x} \omega$  and  $\omega e^{ip \cdot x}$ . This is consistent the fact that  $\varphi$  in equation (1.1.18) does not decay fast enough at infinity (follows from the fact that  $\omega$  is a projection corresponding to a characteristic function in momentum space).

Note that in the dynamic case, the corresponding semiclassical structure suggests that reduced particle density operator can be approximated by Weyl-quantization. In particular, the  $k$ -particle Wigner measure is defined as follows

$$\begin{aligned} W_{N,t}^{(k)}(x_1, p_1, \dots, x_k, p_k) \\ = \binom{N}{k}^{-1} \int \dots \int (dy)^{\otimes k} \gamma_{N,t}^{(k)} \left( x_1 + \frac{\hbar}{2} y_1, \dots, x_k + \frac{\hbar}{2} y_k; x_1 - \frac{\hbar}{2} y_1, \dots, x_k - \frac{\hbar}{2} y_k \right) e^{-i \sum_{i=1}^k p_i \cdot y_i}, \end{aligned} \quad (1.1.25)$$

where  $\gamma_{N,t}^{(k)}$  is the kernel of the  $k$ -reduced particle density defined in (2.1.9).

*Remark 1.1.4.* At initial time,  $\gamma_N^{(k)}$  in (1.1.25) is just the initial data of Hartree-Fock  $\omega_N$  when we consider the Slater determinant. As proven in [BPS14a], the solution of Hartree-Fock  $\omega_{N,t}^{(k)}$  is close to  $\gamma_{N,t}^{(k)}$ , the latter characterizes the solution to the Schrödinger equation.

The Weyl-transformation of a given wave function  $\psi_N \in L^2(\mathbb{R}^{3N})$  is defined by the following operator

$$\text{Op}_W^{k,\hbar}[\psi_N](x_1 \dots x_N; y_1, \dots, y_N) := \binom{N}{k}^{-1} \sum_{1 \leq i_1 < \dots < i_k \leq N} \text{Op}_W^{k,\hbar}[\psi_N](x_{i_1}, \dots, x_{i_k}; y_{i_1}, \dots, y_{i_k}), \quad (1.1.26)$$

where its kernel is defined as

$$\text{Op}_W^{k,\hbar}[\psi_N](x_1, \dots, x_k; y_1, \dots, y_k) := \int_{\mathbb{R}^{3k}} (dp)^{\otimes k} \psi_N \left( \frac{x_1 + y_1}{2}, \dots, \frac{x_k + y_k}{2} \right) e^{\frac{i}{\hbar} \sum_{j=1}^k p_j (x_j - y_j)}, \quad (1.1.27)$$

where  $(dp)^{\otimes k} := dp_1 \cdots dp_k$ .

Coming back to equation (1.1.18). If we define  $\Phi(x, p) := \chi \left( |p| \leq (6\pi^2 \rho(x)^{\frac{1}{3}}) \right)$ , where  $\rho$  minimizes (1.1.11). Then, by (1.1.17), one obtains

$$\omega(x; y) = \text{Op}_W^{1,\hbar}[\Phi](x; y).$$

It is remarked in [BPS14a] that the following commutators holds in semiclassical structure,

$$\begin{aligned} [x, \omega] &= -i\hbar \text{Op}_W^{1,\hbar}[\nabla_p \Phi], \\ [\nabla, \omega] &= \text{Op}_W^{1,\hbar}[\nabla_x \Phi]. \end{aligned}$$

Observe that, for a given test function  $\Phi$ , the following hold

$$\begin{aligned} \text{Tr } \Phi[x]\omega &:= \int dx \Phi(x) \omega(x; x) = N \iint dx dp \Phi(x) W_{N,t}(x, p), \\ \text{Tr } \Phi[i\hbar \nabla]\omega &= N \iint dx dp \Phi(p) W_{N,t}(x, p). \end{aligned}$$

With the foundation for Wigner measure established in the preceding discussion, we are now ready to review the existing literature on the topic of effective equations for large fermionic system.

## 1.2 Effective equation for large fermionic system: Literature

In this section, we will discuss the current state of art surrounding the topics of effective equation for large fermionic system. In particular, we will review the existing research from  $N$ -fermionic Schrödinger equation to Vlasov equation. To that effect, we will first give a brief literature review on the Vlasov-Poisson equation.

### 1.2.1 The Vlasov-Poisson equation

As will be shown later in subsection 1.2.2, it is postulated that one is able to derive the Vlasov equation in (1.2.6) from Schrödinger equation when taking the limits. In this subsection, we briefly introduce the Vlasov-Poisson equation and the existing literature surrounding the topic.

The Vlasov-Poisson equation is a combination of Vlasov equation and Poisson's equation for electric charge. In this system, the interaction potential is repulsive, i.e.  $V \geq 0$ . On the other hand, the Vlasov-

Poisson equation can also model galactic dynamics by considering the interaction term as gravitational force, i.e. that the interaction term is attractive  $V \leq 0$ .

In fact, denoting the phase-space as  $(q, p) \in \mathbb{R}^3 \times \mathbb{R}^3$  and let time  $t \in (0, \infty)$ , we consider  $f_t(q, p) := f(t, q, p)$  to be a smooth non-negative probability density function  $f : \Gamma \rightarrow [0, \infty)$ . Denoting the domain  $\Gamma := (0, T] \times \mathbb{R}^3 \times \mathbb{R}^3$  for some fixed  $T > 0$ , the Vlasov-Poisson system with initial data  $f_0$  is given as

$$\begin{cases} \partial_t f_t(q, p) + p \cdot \nabla_q f_t(q, p) + E_t(q) \cdot \nabla_p f_t(q, p) = 0 & \text{in } \Gamma, \\ \varrho_t(q) = \int dp f_t(q, p) & \text{in } (0, \infty) \times \mathbb{R}^3, \\ E_t(q) = \gamma \int dq_2 \varrho_t(q_2) \frac{q - q_2}{|q - q_2|^3} & \text{in } (0, \infty) \times \mathbb{R}^3. \end{cases} \quad (1.2.1)$$

In (1.2.1), the term  $f_t$  represents the density of particles at position  $q$  with momentum  $p$ ,  $\varrho_t$  represents the spatial distribution of particles and  $E_t$  is the electric field (repulsive case)  $\gamma = 1$ , or gravitational field (attractive case)  $\gamma = -1$ .

Note that the Vlasov-Poisson system in (1.2.1) can be rewritten as a transport equation, i.e.

$$\partial_t f_t + \mathbf{b}_t \cdot \nabla_{q,p} f_t = 0,$$

where  $\mathbf{b}_t(q, p) = (p, E_t(q))$  is divergence-free. Furthermore, the vector field  $E_t$  can be written as  $E_t = -\nabla_q V_\varrho$  where the potential  $V_\varrho$  is the solves

$$\begin{cases} \Delta V_\varrho = \gamma \varrho_t & \text{in } \mathbb{R}^3, \\ \lim_{|q| \rightarrow \infty} V_\varrho(q) = 0. \end{cases} \quad (1.2.2)$$

Additionally, if we define Coulomb potential  $V(q) := |q|^{-1}$ , then we have  $E_t(q) = -\gamma \nabla_q (V * \varrho_t)(q)$ . Therefore, we can simplify the systems by the following nonlinear partial differential equation:

$$\partial_t f_t(q, p) + p \cdot \nabla_q f_t(q, p) = \gamma (\nabla V * \varrho_t)(q), \quad (1.2.3)$$

for a given  $f_0$ .

The global existence of classical solution to the Vlasov-Poisson in 3 dimensions is proven in [Pfa92] and [LP91] for a general class of initial data. The uniqueness of the solution is proven in [LP91] for initial datum with strong moment conditions and integrability. Furthermore, the global existence of weak solution is provided in [Ars75] for bounded initial data and kinetic energy. The result is then relaxed to only  $L^p$ -bound for  $p > 1$  in [GT15]. Existence results with symmetric initial data is proven in [Bat77, Dob79, Sch87]. In [Loe06], the uniqueness of the solution is also proven for bounded macroscopic density. For other results on the well-posedness of Vlasov-Poisson equation, we refer to the works in [ACF14, BBC16, HN81] to list a few.

### 1.2.2 The limits from many particles system to Vlasov equation

In section 1.1, we discussed about the computational challenges when one is faced with a many particles system. It is therefore interesting to analyze the mean-field and semiclassical regime for larger fermionic systems. In this subsection, we will discuss the existing literature on the topic of effective equation for large fermionic system.

The analysis of mean-field limit, i.e. from the Schrödinger equation to the Hartree-Fock equation, has been studied extensively. In [EESY04], assuming that the Slater determinant constitutes the initial data and a regular interaction, the convergence is obtained by the use of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy method for short times. In [BPS14a], the rates of convergence in both the trace norm and Hilbert-Schmidt norm for pure states are obtained in the framework of second quantization. The extension to mixed states has been considered in [BJP<sup>+</sup>16] for a positive temperature and for the relativistic case in [BPS14b]. Furthermore, by utilizing the Fefferman-de la Llave decomposition presented in [BBP<sup>+</sup>16, FL86, HS02], the rate of convergence, with more assumptions on the initial data is obtained in [PRSS17] for Coulomb potential and in [Saf17] for inverse power law potential. Further literature on the mean-field limit for fermionic cases can be found in [FK11, Pet14, Pet17, PP16].

The semiclassical limit from the Hartree-Fock equation to the Vlasov equation has also been extensively studied. In [LP93], this is achieved by using the Wigner-Weyl transformation of the density matrix. In [BPSS16], the authors compared the inverse Wigner transform of the Vlasov solution and the solution of the Hartree-Fock equation and obtained the rate of convergence in the trace norm as well as the Hilbert-Schmidt norm with regular assumptions on the initial data. In fact, [BPSS16, Saf20a] utilized the  $k$ -particle Wigner measure defined in (1.1.25)

As suggested in [BPSS16], suppose  $X_t \equiv 0$  in (1.1.15), one obtains

$$\begin{aligned}
i\hbar\partial_t W_{N,t}(x, p) &= \frac{1}{(2\pi)^3} \int dy i\hbar\partial_t \omega_{N,t} \left( x + \frac{\hbar}{2}y; x - \frac{\hbar}{2}y \right) e^{-ip \cdot y} \\
&= \frac{1}{(2\pi)^3} \int dy \left[ \left( -\hbar^2 \Delta_{x+\frac{\hbar}{2}y} + (V * \rho_t)(x + \frac{\hbar}{2}y) \right) \omega_{N,t} \left( x + \frac{\hbar}{2}y; x - \frac{\hbar}{2}y \right) \right. \\
&\quad \left. + \left( \hbar^2 \Delta_{x-\frac{\hbar}{2}y} - (V * \rho_t)(x - \frac{\hbar}{2}y) \right) \omega_{N,t} \left( x + \frac{\hbar}{2}y; x - \frac{\hbar}{2}y \right) \right] e^{-ip \cdot y} \\
&= \frac{\hbar^2}{(2\pi)^3} \int dy \left( -\Delta_{x+\frac{\hbar}{2}y} + \Delta_{x-\frac{\hbar}{2}y} \right) \omega_{N,t} \left( x + \frac{\hbar}{2}y; x - \frac{\hbar}{2}y \right) e^{-ip \cdot y} \\
&\quad + \frac{1}{(2\pi)^3} \int dy \left[ (V * \rho_t)(x + \frac{\hbar}{2}y) - (V * \rho_t)(x - \frac{\hbar}{2}y) \right] \omega_{N,t} \left( x + \frac{\hbar}{2}y; x - \frac{\hbar}{2}y \right) e^{-ip \cdot y}
\end{aligned} \tag{1.2.4}$$

Observe that

$$\begin{aligned}
-\frac{2}{\hbar} \nabla_x \cdot \nabla_y \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) &= -\nabla_x \cdot \left( \nabla_{x+\frac{\hbar}{2}y} \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) \right) \\
&\quad + \nabla_x \cdot \left( \nabla_{x-\frac{\hbar}{2}y} \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) \right) \\
&= -\Delta_{x+\frac{\hbar}{2}y} \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) + \Delta_{x-\frac{\hbar}{2}y} \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) \\
&= \left[ -\Delta_{x+\frac{\hbar}{2}y} + \Delta_{x-\frac{\hbar}{2}y} \right] \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right).
\end{aligned}$$

Moreover, by Taylor's expansion with respect to  $\hbar$  around 0, we get

$$\begin{aligned}
(V * \rho_t)(x + \frac{\hbar}{2} y) &= (V * \rho_t)(x) + \left( \frac{\hbar}{2} y \right) \cdot \nabla (V * \rho_t)(x) + O(\hbar^2), \\
(V * \rho_t)(x - \frac{\hbar}{2} y) &= (V * \rho_t)(x) - \left( \frac{\hbar}{2} y \right) \cdot \nabla (V * \rho_t)(x) + O(\hbar^2).
\end{aligned}$$

This implies that

$$(V * \rho_t)(x + \frac{\hbar}{2} y) - (V * \rho_t)(x - \frac{\hbar}{2} y) = (\hbar y) \cdot \nabla (V * \rho_t)(x) + O(\hbar^2).$$

Then from (1.2.4), we have

$$\begin{aligned}
i\hbar \partial_\tau W_{N,t}(x, p) &= -\frac{2\hbar}{(2\pi)^3} \int dy \left( \nabla_x \cdot \nabla_y \right) \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) e^{-ip \cdot y} \\
&\quad + \frac{\hbar}{(2\pi)^3} \int dy y \cdot \nabla (V * \rho_t)(x) \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) + O(\hbar^2),
\end{aligned} \tag{1.2.5}$$

where  $\tau$  is re-scaled with time  $t$  for convenient purposes. Apply integration by parts w.r.t.  $y$  on equation (1.2.5), we have

$$\begin{aligned}
i\hbar \partial_\tau W_{N,t}(x, p) &= -\frac{2\hbar}{(2\pi)^3} \nabla_x \int dy \nabla_y \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) e^{-ip \cdot y} \\
&\quad + \hbar \nabla (V * \rho_t)(x) \frac{1}{(2\pi)^2} \int dy y \cdot \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) e^{-ip \cdot y} + O(\hbar^2) \\
&= 2\hbar \nabla_x \frac{1}{(2\pi)^2} \int dy \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) \nabla_y e^{-ip \cdot y} \\
&\quad + i\hbar \nabla (V * \rho_t)(x) \frac{1}{(2\pi)^2} \int dy \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) (-i) y e^{-ip \cdot y} + O(\hbar^2) \\
&= -2i\hbar p \cdot \nabla_x W_{N,t}(x, p) \\
&\quad + i\hbar \nabla (V * \rho_t)(x) \cdot \frac{1}{(2\pi)^2} \int dy \omega_{N,t} \left( x + \frac{\hbar}{2} y; x - \frac{\hbar}{2} y \right) \nabla_p e^{-ip \cdot y} + O(\hbar^2)
\end{aligned}$$

$$= -2i\hbar p \cdot \nabla_x W_{N,t}(x, p) + i\hbar \nabla(V * \rho_t)(x) \cdot \nabla_p W_{N,t}(x, p) + O(\hbar^2).$$

Dividing both sides by  $i\hbar$  factor and taking the semi-classical limit, we get the following Vlasov equation

$$\partial_\tau W_{N,t}(x, p) + 2p \cdot \nabla_x W_{N,t}(x, p) = \nabla(V * \rho_t)(x) \cdot \nabla_p W_{N,t}(x, p) + O(\hbar). \quad (1.2.6)$$

As a matter of fact, in [BPSS16], it has been shown that the convergence rate in Hilbert-Schmidt norm from the Hartree-Fock to the Vlasov equation is of order  $\hbar^{2/7}$  for sufficiently regularized initial data as well as the interaction potential satisfies the inequality  $\widehat{V} \in L^1(\mathbb{R}^3, (1 + |p|^4)dp)$ .

The works in this direction have also been extended for the inverse power law potential in [Saf20b], rate of convergence in the Schatten norm in [LS20], Coulomb potential and mixed states in [Saf20a], and convergence in the Wasserstein distance in [Laf19a, Laf19b]. The convergence of the relativistic Hartree dynamic to the relativistic Vlasov equation was considered in [DRS18]. Further analysis of the semiclassical limit from the Hartree-Fock equation to the Vlasov equation can be found in [APPP11, AKN13a, AKN13b, GIMS98, MM93].

We can combine both mean-field and semiclassical limits and directly obtain the convergence from the Schrödinger equation to the Vlasov equation. The notable pioneers in this direction are Narnhofer and Sewell in [NS81] and Spohn in [Spo81]. They proved the limit from the Schrödinger equation to Vlasov, in which the interaction potential  $V$  is assumed to be analytic in [NS81] and  $C^2$  in [Spo81]. The rate of convergence of the combined limit in terms of the Wasserstein pseudo-distance was obtained in [GP17, GPP18, GP19, GP21]. In fact, the authors studied the rate of convergence in terms of the Wasserstein distance by treating the Vlasov equation as a transport equation and applying the Dobrushin estimate with appropriately chosen initial data. Then, the result for the Husimi measure was obtained by convoluting the Wigner measure in the spirit of (2.2.11) with a specifically chosen coherent state. In this thesis, we consider instead a more generalized coherent state. Recently, the combined limit for the singular potential case was obtained in [CLS21] where they showed the derivation of the Vlasov equation using the weighted Schatten norm with a higher moment assumptions, as well as some strong conditions on the initial data.

It is known, however, that the Wigner measure is not a true probability density as it may be negative in certain phase-space. We show this numerically in Figure 1.1 for selected Fock states. In [KRSL07], a *vis-à-vis* comparison of the classical and quantum systems of a nonlinear Duffing resonator shows that the classical system develops a probability density in the traditional sense, while the quantum system yields a negative region in phase space corresponding to the Wigner measure. In fact, it is proven in [Hud74, MKC09, SC83] that the Wigner measure is nonnegative if and only if the pure quantum states are Gaussian. Additionally, in [BW95], it is shown that the Wigner measure is nonnegative only if the wave function is a convex combination of coherent states. The issue of incompatibility between the quantum Wigner and classical regimes remains

an open question [Cas08].

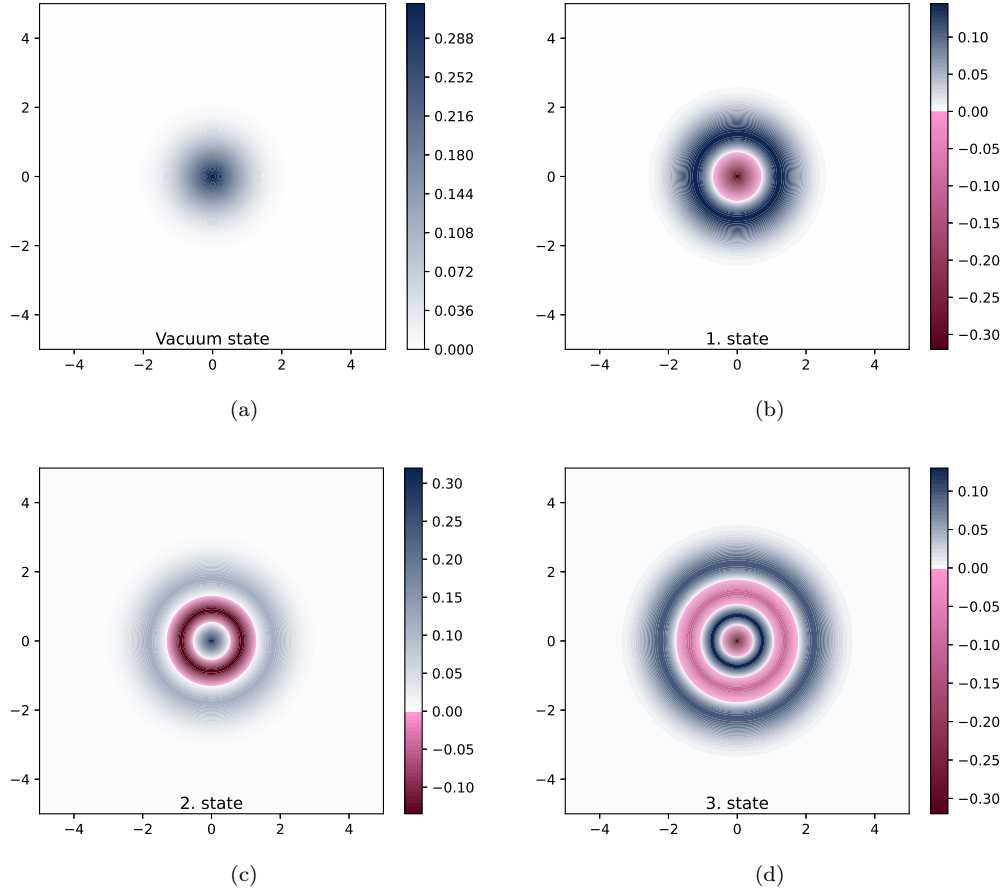


Figure 1.1: Negative Region in Wigner measure.



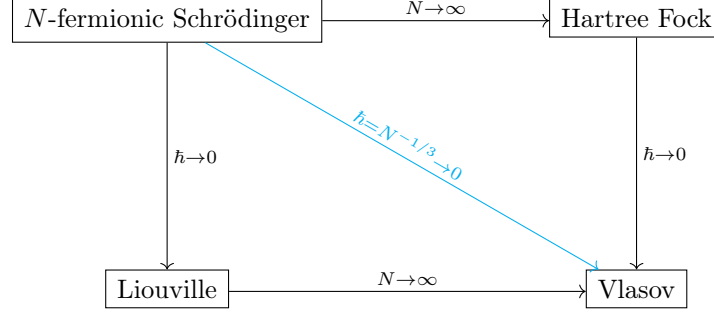


Figure 1.2: Relations of  $N$ -fermionic Schrödinger systems to other mean-field equations [GMP16, GP17, CLL21a].

Nevertheless, it is shown that one can obtain a nonnegative probability measure by taking the convolution of the Wigner measure with a Gaussian function as a mollifier; this is known as the Husimi measure [FLS18, Rob12, Zha08]. As shown later in Lemma 2.2.3, the relation between the Husimi measure and Wigner measure is given by the following convolution with a specific Gaussian coherent state. In particular, let  $\mathbf{m}_{N,t}^{(k)}$  be the  $k$ -particle Husimi measure and  $\mathcal{G}^{\hbar} := (\pi\hbar)^{-3k} \exp(-\hbar^{-1}(\sum_{j=1}^k |q_j|^2 + |p_j|^2))$ , the following equality holds

$$\mathbf{m}_{N,t}^{(k)} = \frac{N(N-1)\cdots(N-k+1)}{N^k} W_{N,t}^{(k)} * \mathcal{G}^{\hbar}, \quad (1.2.7)$$

for any  $1 \leq k \leq N$ . Hence, it is interesting to study the convergence by using Husimi measure. In the next section, we will discuss the motivation and the goals of this thesis.

### 1.3 Main Goals of the Thesis

The smoothing of the Wigner measure shown in (1.2.7) motivates the objective of our study: to obtain the Vlasov-Poisson equation from the Schrödinger equation in terms of the Husimi measure.<sup>4</sup> In particular, this thesis aims to study the time dependent Schrödinger equation for large spinless fermions with the semiclassical scale  $\hbar = N^{-1/3}$  in three dimensions by using the Husimi measure defined by coherent states. In doing so, we will derive the Schrödinger equation into a BBGKY type of hierarchy for the  $k$  particle Husimi measure. Then, the weak limit of Husimi measure is obtained by making use of the weak compactness of the Husimi measure and the uniform estimates for the remainder terms. Then, in similar fashion, we obtain the convergence result with a more relaxed assumption on interaction potential by considering a repulsive interaction that is regularized Coulomb with a polynomial cutoff with respect to  $N$ . Lastly, using the Bogoliubov theory, we show the combined-limit result with a regularized interaction potential.

This thesis will be organized as follows. In chapter 2, we set the foundation of our analysis by introducing

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<sup>4</sup>See Figure 1.2.

Fock Space, Bogoliubov theory, Husimi measure and its relations with Wigner measure, as well as the relevant properties of Husimi measure. On top of that, useful *a priori* estimates such the bound on localized number of particle operator and estimation of oscillation.

With the foundation laid out, we begin in chapter 3 by deriving the Vlasov hierarchy from the convergence from Schrödinger equation and followed by analyzing its corresponding combined convergence to Vlasov equation under the framework that the interaction term is assumed to be  $V \in W^{2,\infty}(\mathbb{R}^3)$ . Building on the Vlasov structure from the preceding chapter, we further study the combined convergence from Schrödinger equation to Vlasov-Poisson equation in chapter 4 by considering the repulsive Coulomb potential with an algebraic cut-off. Lastly, for a different perspective, we explore in chapter 5 the tools developed around Bogoliubov transformation and use it to obtain the combined convergence with the Fourier transformation of interaction term satisfying  $\widehat{V} \in L^1(\mathbb{R}^3; |k|^2 dk)$ .

### Remarks on notations

The following are some helpful remarks on the notations in this thesis:

1. Unless specified, the norm  $\|\cdot\|$  and inner-product  $\langle \cdot, \cdot \rangle$  without subscript will be defined as the norm and inner-product in Fock space.
2. Unless specified, the domain of each integral is always given as whole space  $\mathbb{R}^3$ , i.e.  $\int dx f(x) := \int_{\mathbb{R}^3} dx f(x)$  for any  $x \in \mathbb{R}^3$ .
3. The norm in  $L^p$ -space is denoted as  $\|\cdot\|_p \equiv \|\cdot\|_{L^p(\mathbb{R}^3)}$  for  $1 \leq p \leq \infty$ .
4. For any vectors  $\psi, \phi$  in Hilbert space  $\mathbb{H}$ , the outer product  $|\psi\rangle\langle\phi|$  acting on an operator  $O$  in  $\mathbb{H}$  is defined by  $\langle\phi, O\rangle_{\mathbb{H}}\psi$ .
5. The trace norm will be denoted as  $\|O\|_{\text{Tr}}$ , Hilbert-Schmidt norm as  $\|O\|_{\text{HS}}$ , and operator norm as  $\|O\|_{\text{op}}$  for given bounded operator  $O$ .
6. For any trace class operators  $O, P$ , it holds that  $\|O\|_{\text{op}} \leq \|O\|_{\text{HS}} \leq \|O\|_{\text{Tr}}$ ,  $\|OP\|_{\text{Tr}} \leq \|O\|_{\text{HS}}\|P\|_{\text{Tr}}$  and  $\|OP\|_{\text{HS}} \leq \|O\|_{\text{op}}\|P\|_{\text{HS}}$ . (See [RS80] for more details).
7. For any function  $f, g : \mathbb{R}^3 \rightarrow \mathbb{R}$  and  $k \in \mathbb{N}$ , we denote  $(fg)^{\otimes k}(x_1, \dots, x_k) := \prod_{j=1}^k f(x_j)g(x_j)$ , as well as the notation  $(dx)^{\otimes k} := dx_1 \dots dx_k$ .
8. Let  $A$  and  $B$  to be any bounded operators  $\mathbb{H}$ , the commutator and anti-commutator are defined as  $[A, B] = AB - BA$  and  $\{A, B\} = AB + BA$  respectively.
9. The constant  $C \in \mathbb{R}_{>0}$  is defined as an universal constant, of which its dependencies will be stated only when relevant.

## Chapter 2

# Preliminaries

In this chapter, we will briefly introduce the Fock Space, Bogoliubov transformation and present useful *a priori* estimates that will be used later.

### 2.1 Fock space

In the study of large particle systems, we expect the operators to interact with the different Hilbert spaces of the  $N$ -particle system by creating and annihilating particles. Therefore, to analyze a large particle system, it is convenient for us to build a ‘larger’ Hilbert space that preserves the canonical relations and has the norm  $\|\cdot\|$ . This is known as Fock space.

For a large fermionic system in particular, the corresponding Fock space is defined as

$$\mathcal{F}_a = \mathbb{C} \oplus \bigoplus_{n \geq 1} \bigwedge^n L^2(\mathbb{R}^3),$$

where  $\bigwedge^n L^2$  is the  $L^2$  space equipped with antisymmetric property as defined in (1.1.6). Moreover, the vacuum state is denoted as  $\Omega = 1 \oplus 0 \oplus 0 \oplus \dots 0 \in \mathcal{F}_a$ .

Naturally,  $L^2$  is the subspace of the Hilbert space, and therefore has well-defined inner-product and norm. In particular, for  $\Psi, \Phi \in \mathcal{F}_a$  and  $\phi^{(n)}, \psi^{(n)} \in L^2(\mathbb{R}^{3n})$  to be the state in their respective  $n$ -sector in  $\mathcal{F}_a$ , we define the inner product of  $\mathcal{F}_a$  to be

$$\langle \Phi, \Psi \rangle := \sum_{n \in \mathbb{N}} \langle \phi^{(n)}, \psi^{(n)} \rangle_{L^2},$$

and their norm

$$\|\Psi\| := \sum_{n \in \mathbb{N}} \|\psi^{(n)}\|_{L^2}^2,$$

where we will assume is normalized, i.e.  $\|\Psi\| = 1$ . Next, we define the *number of particle operator*  $\mathcal{N}$ , by

$$(\mathcal{N}\Psi)^{(n)} = n\psi^{(n)}, \quad (2.1.1)$$

for any  $\Psi = \{\psi^{(n)}\}_{n \in \mathbb{N}}$ . Note here that the number operator on vacuum state  $\langle \Omega, \mathcal{N}\Omega \rangle$  is zero since  $a_x \Omega = 0$ .

Such a formalism allows us to describe states where the number of particle is not fixed. In particular, the state in  $\mathcal{F}_a$  characterize a superposition of states with varying number of particles. For example,  $n$ -th sector of the state is characterized by  $\psi^{(n)}$ . As such, the expectation of the number of particles for the state in  $n$ -th sector is  $\|\psi^{(n)}\|_{L^2}^2$ . Note that in Husimi measure, its symmetric property preserves the number of the states.

Next, we will introduce the creation and annihilation operators in  $\mathcal{F}_a$ .

**Definition 2.1.1** (Creation and Annihilation Operators). *For any  $f \in L^2(\mathbb{R}^3)$ , we define the creation and annihilation operators, as*

1. **Creation operator:**  $a^*(f) : \bigwedge^n L^2(\mathbb{R}^3) \longrightarrow \bigwedge^{n+1} L^2(\mathbb{R}^3)$  such that,

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

where the hat indicates missing component.

2. **Annihilation operator:**  $a(f) : \bigwedge^n L^2(\mathbb{R}^3) \longrightarrow \bigwedge^{n-1} L^2(\mathbb{R}^3)$  such that,<sup>1</sup>

$$(a(f)\Psi)^{(n-1)}(x_1, \dots, x_{n-1}) = \sqrt{n} \int dx_n \overline{f(x_n)} \psi^{(n)}(x_1, \dots, x_n).$$

*Remark 2.1.1.* Note here that  $a^*(f)$  is the adjoint of  $a(f)$ .

*Remark 2.1.2.* When applying on a vacuum state  $\Omega$ , we have that  $a^*(f)\Omega = f$  and  $a(f)\Omega = 0$ .

For systems of fermions, the creation and annihilation operators adhere to Canonical Anticommutator Relation (CAR). For completeness, we will present the proof as follows.

**Lemma 2.1.1** (Canonical Anticommutator Relation). *For any operators  $A$  and  $B$  in Hilbert space  $\mathbb{H}$ , we define the Anticommutator as  $\{A, B\} := AB + BA$ . Then, the following identities holds*

1.  $\{a(f), a(g)\} = 0$ ,

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<sup>1</sup>Taking the convention that  $\bigwedge^{-1} L^2(\mathbb{R}^3) = \{0\}$ .

$$2. \{a^*(f), a^*(g)\} = 0,$$

$$3. \{a(f), a^*(g)\} = \langle f, g \rangle_{L^2},$$

for any  $f, g \in L^2(\mathbb{R}^3)$ .

*Proof.* 1. We need to show that  $a(f)a(g)\Psi = a(g)a(f)\Psi$  for any  $\Psi \in \mathcal{F}_a$ . Consider the  $n$ -sector, by definition we have

$$\begin{aligned} (a(f)a(g)\Psi)^{(n-2)}(x_1, \dots, x_{n-2}) &= \sqrt{n-1}\sqrt{n} \int dx_n \overline{f(x_n)} \int dx_{n-1} \overline{g(x_{n-1})} \psi^{(n)}(x_1, \dots, x_{n-1}, x_n) \\ &= -\sqrt{n-1}\sqrt{n} \iint dx_n dx_{n-1} \overline{g(x_n)} \overline{f(x_{n-1})} \psi^{(n)}(x_1, \dots, x_n, x_{n-1}) \\ &= -(a(g)a(f)\Psi)^{(n)}(x_1, \dots, x_{n-2}), \end{aligned}$$

where we used the antisymmetric property of  $\Psi$  in second equality.

2. From Remark 2.1.1, we exploit the fact that creation operator is adjoint of annihilation operator and that  $(AB)^* = B^*A^*$ ,

$$\{a^*(f), a^*(g)\} = a^*(f)a^*(g) + a^*(g)a^*(f) = (a(g)a(f) + a(f)a(g))^* = (\{a(f), a(g)\})^* = 0.$$

3. From Remark 2.1.2, testing against the vacuum state  $\Omega$  yields,

$$\begin{aligned} \{a(f), a^*(g)\}\Omega &= (a(f)a^*(g) + a^*(g)a(f))\Omega \\ &= a(f)g = \int dx \overline{f(x)}g(x) \\ &= \langle f, g \rangle. \end{aligned}$$

Now consider any test function  $\Psi$  in  $n$ -th sector, we want to show that  $a(f)a^*(g)\Psi + a^*(g)a(f)\Psi = \langle f, g \rangle\Psi$ . From definition of creation and annihilation operators,

$$\begin{aligned} (a(f)a^*(g)\Psi)^{(n)}(x_1, \dots, x_n) &= \frac{1}{\sqrt{n+1}} \left[ a(f) \left( \sum_{j=1}^{n+1} (-1)^{j-1} g(y_j) \psi^{(n)}(y_1, \dots, \hat{y}_j, \dots, y_{n+1}) \right) \right] (x_1, \dots, x_n) \\ &= \int dx_{n+1} \overline{f(x_{n+1})} \sum_{j=1}^{n+1} (-1)^{j-1} g(x_j) \psi^{(n)}(x_1, \dots, \hat{x}_j, \dots, x_{n+1}) \\ &= (-1)^{2n} \langle f, g \rangle \psi^{(n)}(x_1, \dots, x_n) \\ &\quad + \int dx_{n+1} \overline{f(x_{n+1})} \sum_{j=1}^n (-1)^{j-1} g(x_j) \psi^{(n)}(x_1, \dots, \hat{x}_j, \dots, x_{n+1}) \end{aligned}$$

$$\begin{aligned}
&= \langle f, g \rangle_{L^2} \psi^{(n)}(x_1, \dots, x_n) \\
&\quad + \sum_{j=1}^n (-1)^{2j-1} g(x_j) \int dy \overline{f(y)} \psi^{(n)}(x_1, \dots, \hat{x}_j, \dots, x_n, y) \\
&= (\langle f, g \rangle_{L^2} \Psi - a^*(g) a(f) \Psi)^{(n)}(x_1, \dots, x_n).
\end{aligned}$$

■

Next, we observe that creation and annihilation operators defined for fermions are bounded operators:

**Lemma 2.1.2.** *For any function  $f \in L^2$ , let  $a^*(f)$  and  $a(f)$  be the creation and annihilation operators defined in Definition 2.1.1, then we have*

$$1. \|a^*(f)\| \leq \|f\|_2,$$

$$2. \|a(f)\| \leq \|f\|_2.$$

*Proof.* Suppose any function  $\Psi \in \mathcal{F}_a$  such that  $\|\Psi\| = 1$ . Then by CAR,

$$\begin{aligned}
\|a^*(f)\Psi\|^2 &= \langle a^*(f)\Psi, a^*(f)\Psi \rangle = \langle \Psi, a(f)a^*(f)\Psi \rangle \\
&= \langle \Psi, \|f\|_{L^2}^2 \Psi \rangle - \langle \Psi, a^*(f)a(f)\Psi \rangle \\
&= \|f\|_{L^2}^2 \|\Psi\|^2 - \|a^*(f)\Psi\|^2 \\
&\leq \|f\|_{L^2}^2.
\end{aligned}$$

Similarly

$$\|a(f)\Psi\|^2 = \|f\|_{L^2}^2 \|\Psi\|^2 - \|a(f)\Psi\|^2 \leq \|f\|_{L^2}^2.$$

■

It is convenient in this thesis to introduce operator-value distribution  $a_x^*$  and  $a_x$  for the creation and annihilation operator respectively. Namely, corresponding to the definition given in Definition 2.1.1, we will henceforth represent the creation and annihilation operator as follows,

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

for any  $f \in L^2$ . For all  $f, g \in L^2$ , the CAR can be rewritten as

$$\{a_x, a_y\} = 0, \quad \{a_x^*, a_y^*\} = 0, \quad \text{and} \quad \{a_x, a_y^*\} = \delta_{y=x}, \quad (2.1.2)$$

where  $\delta_{y=x} = \delta(y-x)$  is the dirac-delta.

With the help of creation and annihilation operators, we introduce the second quantization formalism which allows us to conveniently represent the many-body operators in Fock space.

**Definition 2.1.2.** Let  $h$  be a self-adjoint single-particle operator defined on  $L^2(\mathbb{R}^3)$ . Then its second quantization is an operator on  $\mathcal{F}_a$  defined as,

$$d\Gamma(h) = \bigoplus_{n \geq 0} \sum_{i=1}^n h_i \psi^{(n)},$$

where  $\Psi \in \mathcal{F}_a$  and  $\psi^{(n)} \in L^2(\mathbb{R}^{3n})$ .

*Remark 2.1.3.* In  $n$ -sector, we have  $(d\Gamma(h)\Psi)^{(n)} = \sum_{i=1}^n h_i \psi^{(n)}$ .

*Remark 2.1.4.* Note that some other literature may write the second quantization for given any orthogonal basis  $\{f_j\}_{j \in \mathbb{N}}$ , i.e.  $d\Gamma(h) = \sum_{j,k \geq 1} \langle f_j, h f_k \rangle a_j^* a_k$ . [Nam20]

Heuristically, suppose the self-adjoint operator  $h$  has an integral kernel, for  $\Psi, \phi \in \mathcal{F}_a$  we observe that,

$$\begin{aligned} \langle \phi, d\Gamma(h)\Psi \rangle &= \sum_{n \geq 0} \sum_{i=1}^n \langle \Phi^{(n)}, h_i \psi^{(n)} \rangle \\ &= \sum_{n \geq 0} \int \cdots \int dx (dx)^{\otimes (n-1)} \overline{\Phi^{(n)}(x, x_1, \dots, x_n)} \int dy h(x, y) \psi^{(n)}(y, x_1, \dots, x_n) \\ &= \sum_{n \geq 0} \int \cdots \int dx dy (dx)^{\otimes (n-1)} \overline{\Phi^{(n)}(x, x_1, \dots, x_n)} \int h(x, y) \psi^{(n)}(y, x_1, \dots, x_n) \\ &= \iint dx dy \sum_{n \geq 0} \int \cdots \int (dx)^{\otimes (n-1)} h(x; y) \overline{a_x \Phi^{(n-1)}(x_2, \dots, x_n)} a_y \psi^{(n-1)}(x_2, \dots, x_n) \\ &= \iint dx dy h(x; y) \langle a_x \phi, a_y \Psi \rangle \\ &= \left\langle \phi, \iint dx dy h(x; y) a_x^* a_y \Psi \right\rangle, \end{aligned} \tag{2.1.3}$$

which implies that

$$d\Gamma(h) = \iint dx dy h(x; y) a_x^* a_y. \tag{2.1.4}$$

Thus, we can rewrite the number operator defined in (2.1.1) as by replacing  $h$  to identity operator  $\mathbb{1}$  in (2.1.4), i.e.

$$d\Gamma(\mathbb{1}) = \int dx a_x^* a_x =: \mathcal{N}. \tag{2.1.5}$$

Observe here we can extend the single-body operator defined in (2.1.4) into many-bodies operator. In fact, let  $h^{(k)}$  be an operator on the Hilbert Space  $\bigwedge^k L^2(\mathbb{R}^3)$ , then we may have the following second-quantization representation,

$$\mathrm{d}\Gamma(h^{(k)}) = \int \cdots \int (\mathrm{d}x \mathrm{d}y)^{\otimes k} h^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) a_{x_1}^* \cdots a_{x_k}^* a_{y_k} \cdots a_{y_1}, \quad (2.1.6)$$

where  $h^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k)$  is the integral kernel of the operator  $h^{(k)}$ . Thus, we may also write the corresponding number of particle operator,

**Lemma 2.1.3.** *For every normalized state  $\Psi_N \in \mathcal{F}_a$  on  $N$ -sector, and the number of particles operator defined in (2.1.5). Then, the following equality holds*

$$\int \cdots \int (\mathrm{d}x)^{\otimes k} a_{x_1}^* \cdots a_{x_k}^* a_{x_k} \cdots a_{x_1} = \mathcal{N}(\mathcal{N} - 1) \cdots (\mathcal{N} - k + 1). \quad (2.1.7)$$

*Proof.* Let  $k = 2$ , we compute

$$\begin{aligned} \iint \mathrm{d}x_1 \mathrm{d}x_2 a_{x_1}^* a_{x_2}^* a_{x_2} a_{x_1} &= - \iint \mathrm{d}x_1 \mathrm{d}x_2 a_{x_1}^* a_{x_2}^* a_{x_1} a_{x_2} \\ &= \iint \mathrm{d}x_1 \mathrm{d}x_2 a_{x_1}^* a_{x_1} a_{x_2}^* a_{x_2} - \iint \mathrm{d}x_1 \mathrm{d}x_2 \delta_{x_1=x_2} a_{x_1}^* a_{x_2} \\ &= \mathcal{N}^2 - \int \mathrm{d}x_1 a_{x_1}^* a_{x_1} \\ &= \mathcal{N}(\mathcal{N} - 1). \end{aligned}$$

■

We extend the Hamilton operator appeared in (1.1.9) acting on  $L_a^2(\mathbb{R}^{3N})$  to an operator acting on the Fock space  $\mathcal{F}_a$  by  $(\mathcal{H}_N \Psi)^{(n)} = \mathcal{H}_N^{(n)} \psi^{(n)}$  with

$$\mathcal{H}_N^{(n)} = \sum_{j=1}^n -\frac{\hbar^2}{2} \Delta_{x_j} + \frac{1}{2N} \sum_{i \neq j}^n V(x_i - x_j).$$

From the similar calculation in (2.1.3) we can rewrite the Hamiltonian as follows

$$\mathcal{H}_N = \frac{\hbar^2}{2} \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \iint \mathrm{d}x \mathrm{d}y V(x - y) a_x^* a_y^* a_y a_x. \quad (2.1.8)$$

*Remark 2.1.5.* Observe here that the operator  $\mathcal{H}_N$  defined above preserves the number of particle, i.e. it commutes with the number operator  $\mathcal{N}$ .

Naturally, we may also write the reduced particle densities discussed in Section 1.1 by its second quantization form. In fact, for any normalized  $\Psi_{N,t} \in \mathcal{F}_a$  in  $N$ -sector, we define the  $k$ -particle density  $\gamma_{N,t}^{(k)}$  having the kernel

$$\gamma_{N,t}^{(k)}(x_1, \dots, x_k; y_1 \dots y_k) = \langle \Psi_{N,t}, a_{y_1}^* \cdots a_{y_k}^* a_{x_k} \cdots a_{x_1} \Psi_{N,t} \rangle, \quad (2.1.9)$$



where  $1 \leq k \leq N$ . Recall from (1.1.4) that the trace of  $\gamma_{N,t}^{(k)}$  is  $N!/(N-k)!$ .

The main benefits of using the second quantization formalism is not only that it simplifies the analysis for many-particles operators, it helps to find the estimates by counting the number of particles.

### Bogoliubov transformation

With the framework given, the Cauchy problem for the Schrödinger equation is given as

$$\begin{cases} i\hbar\partial_t \Psi_{N,t} = \mathcal{H}_N \Psi_{N,t}, \\ \Psi_{N,0} = \Psi_N^{\text{Slater}}, \end{cases} \quad (2.1.10)$$

for all  $\Psi_{N,t} \in \mathcal{F}_a$  and  $\|\Psi_{N,t}\| = 1$  for  $t \in [0, T]$ .

Note that the solution to the Schrödinger equation in (2.1.10) is  $\Psi_{N,t} = e^{-\frac{i}{\hbar}\mathcal{H}_N t} \Psi_N$ , where we let  $\Psi_N^{\text{Slater}}$  be the initial data characterized by the Slater determinant, given as

$$\Psi_N^{\text{Slater}} := 0 \oplus \cdots \oplus 0 \oplus \psi_N^{\text{Slater}} \oplus 0 \cdots \oplus 0 = a^*(e_1) \cdots a^*(e_N) \Omega, \quad (2.1.11)$$

where  $\psi_N^{\text{Slater}} \in L^2(\mathbb{R}^{3N})$  and orthonormal bases  $\{e_j\}_{j=1}^N$  as defined in (1.1.12).

As the right-hand side of (2.1.11) shows, the initial state is obtained by applying an isomorphic mapping to the vacuum state  $\Omega$ . Introduced by Bogoliubov in [Bog47], it is stated that the approximation of the Hamiltonian for a many-particle system with weak interaction can be described by a quadratic Hamiltonian in Fock space by using a special class of unitary operators that preserve the canonical commutation relation algebra for a bosonic gas. For fermionic cases, the treatment with respect to Bogoliubov theory has also been shown in [BPS14a, NNS16, Sol09] to name a few.

Following [BPS14a], we briefly discuss the Bogoliubov theory here by first defining generalized annihilation and creation operators as

$$A(f, g) = a(f) + a^*(\bar{g}), \quad A^*(f, g) = a^*(f) + a(\bar{g}),$$

for any  $f, g \in L^2(\mathbb{R}^3)$ , then we have, for any  $f_1, g_1, f_2, g_2 \in L^2(\mathbb{R}^3)$ , that

$$\{A(f_1, g_1), A^*(f_2, g_2)\} = \langle (f_1, g_1), (f_2, g_2) \rangle_{L^2 \oplus L^2} \quad (2.1.12)$$

due to the CAR.

Next, let  $\mathcal{J} : L^2 \oplus L^2 \rightarrow L^2 \oplus L^2$  be an anti-unitary operator such that<sup>2</sup>

$$\mathcal{J} := \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix},$$

where  $J : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$  be an antilinear operator such that  $Jf = \bar{f}$ . Then, we define a mapping  $\mathcal{V} : L^2 \oplus L^2 \rightarrow L^2 \oplus L^2$  such that, for all  $(f_1, g_1), (f_2, g_2) \in (L^2 \oplus L^2)$ , it satisfies

$$\{A(\mathcal{V}(f_1, g_1)), A^*(\mathcal{V}(f_2, g_2))\} = \langle (f_1, g_1), (f_2, g_2) \rangle,$$

as well as

$$A^*(\mathcal{V}(f, g)) = A(\mathcal{V}(\bar{g}, \bar{f})). \quad (2.1.13)$$

By [Sol09, Theorem 9.2], the linear bounded isomorphism  $\mathcal{V} : L^2 \oplus L^2 \rightarrow L^2 \oplus L^2$  is a Bogoliubov transformation if and only if it satisfies

$$\mathcal{V}\mathcal{V}^* = \mathbb{1}_{L^2 \oplus L^2} = \mathcal{V}^*\mathcal{V} \text{ and } \mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}. \quad (2.1.14)$$

Consequently, given any linear maps  $u, v : L^2 \rightarrow L^2$  and denoting  $\bar{u} := JuJ$ , the fermionic Bogoliubov map  $\mathcal{V} : L^2 \oplus L^2 \rightarrow L^2 \oplus L^2$  is a unitary map given by

$$\mathcal{V} = \begin{pmatrix} u & \bar{v} \\ v & \bar{u} \end{pmatrix}, \quad (2.1.15)$$

where  $u$  and  $v$  have to satisfy

$$u^*u + v^*v = 1, \text{ and } u^*\bar{v} + v^*\bar{u} = 0. \quad (2.1.16)$$

Then, by [Sol09, Theorem 9.5], we say that the Bogoliubov transformation is implementable if there exists a unitary transformation  $\mathcal{R}_{\mathcal{V}} : \mathcal{F}_a \rightarrow \mathcal{F}_a$  such that, for all  $F \in L^2 \oplus L^2$ ,

$$\mathcal{R}_{\mathcal{V}}^* A(f, g) \mathcal{R}_{\mathcal{V}} = A(\mathcal{V}(f, g)), \quad (2.1.17)$$

if and only if the Bogoliubov map  $\mathcal{V}^*\mathcal{V}$  given in (2.1.15) is a trace class. The latter can be obtained by having  $v$  be a Hilbert-Schmidt operator in our framework.<sup>3</sup> In fact, denoting  $u_x(y) := u(y; x)$  and  $\bar{u}_x(y) := \bar{u}(y; x)$ ,

---

<sup>2</sup>Note here that  $\mathcal{J} = \mathcal{J}^{-1} = \mathcal{J}^*$ , and  $A^*(f, g) = A(\mathcal{J}(f, g))$ . [NNS16]

<sup>3</sup>This is known as the Shale-Stinespring condition. [Rui78]

we have

$$\begin{aligned}\mathcal{R}_\mathcal{V}^* A(f, g) \mathcal{R}_\mathcal{V} &= A(\mathcal{V}(f, g)) = A \left( \begin{pmatrix} \mathbf{u} & \bar{\mathbf{v}} \\ \mathbf{v} & \bar{\mathbf{u}} \end{pmatrix} (f, g) \right) \\ &= \int dx \left( (a(\mathbf{u}_x) + a^*(\bar{\mathbf{v}}_x)) \bar{f}(x) + \int dx \left( a(\bar{\mathbf{v}}_x) + a^*(\mathbf{u}_x) \right) \bar{g}(x) \right).\end{aligned}\tag{2.1.18}$$

On other hand, we have

$$\mathcal{R}_\mathcal{V}^* A(f, g) \mathcal{R}_\mathcal{V} = \int dx \mathcal{R}_\mathcal{V}^* a_x \mathcal{R}_\mathcal{V} \bar{f}(x) + \int dx \mathcal{R}_\mathcal{V}^* a_x^* \mathcal{R}_\mathcal{V} \bar{g}(x).$$

This implies that the following properties hold

$$\begin{aligned}\mathcal{R}_\mathcal{V}^* a_x \mathcal{R}_\mathcal{V} &= a(\mathbf{u}_x) + a^*(\bar{\mathbf{v}}_x) \\ \mathcal{R}_\mathcal{V}^* a_x^* \mathcal{R}_\mathcal{V} &= a^*(\mathbf{u}_x) + a(\bar{\mathbf{v}}_x).\end{aligned}\tag{2.1.19}$$

Let  $\gamma_\Psi$  be the 1-particle reduced density associated with some  $\Psi \in \mathcal{F}_a$  defined with the integral kernel as

$$\gamma_\Psi(x; y) := \langle \Psi, a_y^* a_x \Psi \rangle.$$

Note that  $\text{Tr } \gamma = \langle \Psi, \mathcal{N} \Psi \rangle = N$ . We define the pairing density  $\alpha_\Psi$  as a one-particle operator with an integral kernel

$$\alpha_\Psi(x; y) := \langle \Psi, a_y a_x \Psi \rangle$$

and that  $\overline{\alpha_\Psi(x; y)} = \langle \Psi, a_x^* a_y^* \Psi \rangle$ .

Now, we observe that

$$\begin{aligned}\langle \Psi, A^*(f_2, g_2) A(f_1, g_1) \Psi \rangle &= \langle \Psi, (a^*(f_2) + a(\bar{g}_2)) (a(f_1) + a^*(\bar{g}_1)) \Psi \rangle \\ &= \iint dx dy \left[ \langle \Psi, a_y^* a_x \Psi \rangle \overline{f_1(x)} f_2(y) + \langle \Psi, a_y^* a_x^* \Psi \rangle \overline{g_1(x)} f_2(y) \right. \\ &\quad \left. + \langle \Psi, a_y a_x \Psi \rangle \overline{f_1(x)} g_2(y) + \langle \Psi, a_y a_x^* \Psi \rangle \overline{g_1(x)} g_2(y) \right] \\ &= \left\langle (f_1, g_1), \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ -\bar{\alpha}_\Psi & 1 - \bar{\gamma}_\Psi \end{pmatrix} (f_2, g_2) \right\rangle = \langle (f_1, g_1), \Gamma_\Psi(f_2, g_2) \rangle,\end{aligned}$$

where we defined the generalized 1-particle reduced density as

$$\Gamma_\Psi := \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ -\bar{\alpha}_\Psi & 1 - \bar{\gamma}_\Psi \end{pmatrix}.\tag{2.1.20}$$

As we are considering the case of the pure state, we have  $\alpha_\Psi = 0$ . Let  $\Psi = \mathcal{R}_\mathcal{V} \Omega$ , where  $\mathcal{R}_\mathcal{V}$  is the unitary

map of the Bogoliubov transformation  $\mathcal{V}$ ; then, we have from 1-particle reduced density that

$$\begin{aligned}
\gamma_\Psi(x; y) &= \langle \mathcal{R}_\mathcal{V} \Omega, a_y^* a_x \mathcal{R}_\mathcal{V} \Omega \rangle \\
&= \langle \Omega, \mathcal{R}_\mathcal{V}^* a_y^* \mathcal{R}_\mathcal{V} \mathcal{R}_\mathcal{V}^* a_x \mathcal{R}_\mathcal{V} \Omega \rangle \\
&= \langle \Omega, [a^*(u_y) + a(\bar{v}_y)] [a(u_x) + a^*(\bar{v}_x)] \Omega \rangle \\
&= (\bar{v}v)(x; y) = \omega(x; y),
\end{aligned} \tag{2.1.21}$$

where we use (2.1.19), (2.1.2) and  $a_x \Omega = 0$ . Similarly, we can show that  $\alpha_\Psi = \bar{v}u$ . As  $\text{Tr } \gamma_\Psi = N$ , (2.1.21) implies that  $v$  is a Hilbert-Schmidt operator and therefore is implementable.

As discussed in [BPS14a, PRSS17], for the Bogoliubov transformation to be implementable, we set that  $v_{N,t} = \sum_{j=1}^N |\bar{e}_{t,j}\rangle \langle e_{t,j}|$  for any orthonormal basis  $\{e_{t,j}\}_{j=1}^N \subset L^2(\mathbb{R}^3)$  and that  $u_{N,t} := \mathbb{1} - \omega_{N,t}$ . In this setting, the mapping  $\mathcal{V}$  defined in (2.1.15) is an implementable Bogoliubov transformation with a generalized 1-particle reduced density matrix given as

$$\Gamma_{\mathcal{V}_{N,t}} = \begin{pmatrix} \omega_{N,t} & 0 \\ 0 & \mathbb{1} - \bar{\omega}_{N,t} \end{pmatrix}, \tag{2.1.22}$$

for any  $t \geq 0$ .<sup>4</sup> Furthermore, the initial data with the Slater determinant can be expressed with  $\mathcal{R}_{\mathcal{V}_{N,0}} \Omega$ ; i.e.,

$$0 \oplus \cdots \oplus 0 \oplus (N!)^{-1/2} \det\{e_i(x_j)\}_{i,j=1}^N \oplus 0 \oplus \cdots \oplus 0 = \mathcal{R}_{\mathcal{V}_{N,0}} \Omega. \tag{2.1.23}$$

Observe that, for  $t \geq 0$ , the solution of the Schrödinger equation given as

$$\Psi_{N,t} = e^{-\frac{i}{\hbar} \mathcal{H}_N t} \mathcal{R}_{\mathcal{V}_{N,0}} \Omega = \mathcal{R}_{\mathcal{V}_{N,t}} \mathcal{U}_N(t; 0) \Omega, \tag{2.1.24}$$

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

$$\mathcal{U}_N(t; s) := R_{\mathcal{V}_{N,t}}^* e^{-\frac{i}{\hbar} \mathcal{H}_N (t-s)} R_{\mathcal{V}_{N,s}}. \tag{2.1.25}$$

Since  $\mathcal{V}_{N,t}$  and  $\mathcal{R}_{\mathcal{V}_{N,t}}$  are unitary mapping, then from (2.1.17), it implies

$$\mathcal{R}_{\mathcal{V}_{N,t}} a^\#(f) \mathcal{R}_{\mathcal{V}_{N,t}}^* = \mathcal{R}_{\mathcal{V}_{N,t}}^* a^\#(f) \mathcal{R}_{\mathcal{V}_{N,t}}^* = \mathcal{R}_{\mathcal{V}_{N,t}}^* a^\#(f) \mathcal{R}_{\mathcal{V}_{N,t}},$$

for any  $f \in L^2(\mathbb{R}^3)$  and  $a^\#$  denotes both creation and annihilation operator. Furthermore, as discussed in

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<sup>4</sup>Note that here, we write  $\mathcal{R}_{\mathcal{V}_{N,t}}$  instead of  $\mathcal{R}_\mathcal{V}$  as defined in (2.1.17) to emphasize its dependence on  $N$  and  $t$ .

[BPS14a], by (2.1.23) and the property

$$\mathcal{R}_{\mathcal{V}_{N,t}}^* a^*(e_i) \mathcal{R}_{\mathcal{V}_{N,t}} = \begin{cases} a(e_i), & \text{for } i \leq N, \\ a^*(e_i), & \text{for } i > N, \end{cases}$$

where  $\{e_i\}_{i \in \mathbb{N}}$  is an orthonormal system on  $L^2(\mathbb{R}^3)$ , the mapping  $\mathcal{R}_{\mathcal{V}_{N,t}}$  is surjective and preserves the algebraic structure of the CAR.

For a more structured and pedagogical treatment of Bogoliubov theory, we refer the readers to [BPS16, Nam20, Sol09].

## 2.2 Husimi measure

In chapter 1.2.2, we have discussed that the Wigner measure is not a true probability distribution, as part of it may lie in the negative region.<sup>5</sup> To overcome this problem, one may ‘smoothen’ the Wigner measure by using a Gaussian function, which yields a probability measure known as Husimi measure.

As with [FLS18], we formally define the Husimi measure by first defining the coherent state.

**Definition 2.2.1** (Coherent State). *For  $p, q, y \in \mathbb{R}^3$  and  $\hbar$  be the semiclassical scale, the coherent state is defined as*

$$f_{q,p}^\hbar(y) = \hbar^{-\frac{3}{4}} f\left(\frac{y-q}{\sqrt{\hbar}}\right) e^{\frac{i}{\hbar} p \cdot y}, \quad (2.2.1)$$

where the function  $f$  any real-valued function with normalization  $\|f\|_2 = 1$ .

Note here that the function  $f$  defined above is allowed to be any real-valued function. Furthermore, as the function  $f$  defined above is a very well localized function in practice [FLS18], we will make the following assumption throughout the thesis

**Assumption H1.** *The real-valued function  $f \in H^1(\mathbb{R}^3)$  satisfies  $\|f\|_2 = 1$ , and has compact support.*

**Lemma 2.2.1** (Projection of the coherent state, ). *Assume H1. For  $f_{q,p}^\hbar$  defined as in definition 2.2.1, we have the following projection*

$$\frac{1}{(2\pi\hbar)^3} \iint dq dp |f_{q,p}^\hbar\rangle \langle f_{q,p}^\hbar| = \frac{1}{(2\pi\hbar)^3} \iint dq dp \langle f_{q,p}^\hbar, \cdot \rangle f_{q,p}^\hbar(y) = \mathbb{1}. \quad (2.2.2)$$

Additionally, it will be desirable for us to define here the  $\hbar$ -weighted Fourier transformation,

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<sup>5</sup>Known as ‘quasiprobability’ distribution, Wigner measure can be negative depending on the state. See Figure 1.1

**Definition 2.2.2** ( $\hbar$ -weighted Fourier transform). *Let  $f$  be any real-valued function in  $L^2(\mathbb{R}^3)$ . We define the  $\hbar$ -weighted Fourier transform of  $f$  to be,*

$$\mathcal{F}_\hbar[f](p) := \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int_{\mathbb{R}^3} dx f(x) e^{-\frac{i}{\hbar} p \cdot x},$$

and we denote the corresponding inverse transform by  $\mathcal{F}_\hbar^{-1}$ .

From the Definition 2.2.2, we may also derive the corresponding dirac-delta ‘function’. In fact, for any  $G, F \in L^2(\mathbb{R}^3)$ ,

$$\int_{\mathbb{R}^3} dy G(y) F(y) = \int_{\mathbb{R}^3} dy G(y) \frac{1}{(2\pi\hbar)^3} \iint_{\mathbb{R}^{3,2}} dp dv F(v) e^{\frac{i}{\hbar} p \cdot (y-v)}, \quad (2.2.3)$$

Thus, the dirac-delta distribution corresponding to the  $\hbar$ -weighted Fourier transform is,

$$\delta_y(v) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} dp e^{\frac{i}{\hbar} p \cdot (y-v)}. \quad (2.2.4)$$

Now, we are ready to define the Husimi measure. Similar to [Del16, FLS18], we define it as

**Definition 2.2.3** (Husimi Measure). *Let  $f_{q_k, p_k}^\hbar$  to be the coherent state defined in definition 2.2.1, the  $k$ -particle Husimi measure is defined as*

$$m_N^{(k)}(q_1, p_1, \dots, q_k, p_k) = \langle \psi_N, a^*(f_{q_1, p_1}^\hbar) \cdots a^*(f_{q_k, p_k}^\hbar) a(f_{q_k, p_k}^\hbar) \cdots a(f_{q_1, p_1}^\hbar) \psi_N \rangle, \quad (2.2.5)$$

where  $\psi_N \in L_a^2(\mathbb{R}^{3N})$ . Moreover, we also define the time-dependent Husimi measure  $m_{N,t}^{(k)}$ , by replacing  $\Psi_N$  with  $\psi_{N,t}$ .

*Remark 2.2.1.* It should be obvious here that the Husimi measure defined above is non-negative due to the inner-product, as opposed to the possibility of having negative region in Wigner measure as demonstrated in Figure 1.1.

Observe here that by the second quantization convention, the Husimi measure can be expressed by

$$\begin{aligned} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) &= \int \cdots \int (dw du)^{\otimes k} \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes k} \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle \\ &= \int \cdots \int (dw du)^{\otimes k} \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes k} \gamma_{N,t}^{(k)}(u_1, \dots, u_k; w_1, \dots, w_k), \end{aligned} \quad (2.2.6)$$

for any  $\Psi_{N,t} \in \mathcal{F}_a$ , where we use the notations

$$(dw du)^{\otimes k} := dw_1 du_1 \cdots dw_k du_k, \text{ and } \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes k} := \prod_{j=1}^k f_{q_j, p_j}^\hbar(w_j) \overline{f_{q_j, p_j}^\hbar(u_j)}.$$

*Remark 2.2.2.* Observe that if the initial data is described by Slater determinant as in (1.1.13), then the Husimi measure at initial time is

$$m_N^{\text{Slater}}(q, p) = \sum_{j=1}^N \iint dw_1 du_1 f_{q,p}^{\hbar}(w_1) \overline{e_j(w_1)} e_j(u_1) \overline{f_{q,p}^{\hbar}(u_1)}, \quad (2.2.7)$$

for any family of orthonormal basis  $\{e_j\}_{j=1}^N$  in  $L^2(\mathbb{R}^3)$ .

The relation between the Husimi measure and the number of particles operator can be expressed as follows, for the 1-particle Husimi measure  $m_{N,t} := m_{N,t}^{(1)}$ ,

$$\begin{aligned} \iint dq dp m_{N,t}(q, p) &= \iint dq dp \iint dw_1 du_1 f_{q,p}^{\hbar}(w_1) \gamma_{N,t}^{(1)}(w_1; u_1) \overline{f_{q,p}^{\hbar}(u_1)} \\ &= \hbar^{-\frac{3}{2}} \int dq \iint dw_1 du_1 f\left(\frac{w_1 - q_1}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q_1}{\sqrt{\hbar}}\right) \left(\int dp e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)}\right) \gamma_{N,t}^{(1)}(w_1; u_1) \\ &= (2\pi\hbar)^3 \hbar^{-\frac{3}{2}} \iint dq_1 dw_1 \left| f\left(\frac{w_1 - q_1}{\sqrt{\hbar}}\right) \right|^2 \gamma_{N,t}^{(1)}(w_1; w_1) \\ &= (2\pi\hbar)^3 \int d\tilde{q} |f(\tilde{q})|^2 \int dw_1 \gamma_{N,t}^{(1)}(w_1; w_1) \\ &= (2\pi)^3, \end{aligned}$$

where we use the Dirac-delta  $\delta_x(y) := \int e^{\frac{i}{\hbar} p \cdot (x-y)} dp$ .

Next, we prove the following properties of  $k$ -particle Husimi measure  $m_N^{(k)}$

**Lemma 2.2.2** (Properties of  $k$ -particle Husimi measure). *Suppose  $\|\psi_{N,t}\|_2 = 1 = \|\Psi_{N,t}\|$  for  $t \geq 0$ . Then, the following properties hold true for  $m_{N,t}^{(k)}$ :*

1.  $m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k)$  is symmetric,
2.  $\frac{1}{(2\pi)^{3k}} \int \dots \int (dq dp)^{\otimes k} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) = \frac{N(N-1)\dots(N-k+1)}{N^k}$ ,
3.  $\frac{1}{(2\pi\hbar)^3} \iint dq_k dp_k m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) = (N-k+1) m_{N,t}^{(k-1)}(q_1, p_1, \dots, q_{k-1}, p_{k-1})$ , and
4.  $0 \leq m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \leq 1$  a.e.,

where  $1 \leq k \leq N$ .

*Proof.* 1. *Symmetry* Not that from the second quantization definition of Husimi measure in (2.2.3), we have

$$\begin{aligned} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) &= \langle \psi_{N,t}, a^*(f_{q_1,p_1}^{\hbar}) \cdots a^*(f_{q_k,p_k}^{\hbar}) a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \psi_{N,t} \rangle \\ &= \langle a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \psi_{N,t}, a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \psi_{N,t} \rangle \\ &= \|a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \psi_{N,t}\|_2^2. \end{aligned} \quad (2.2.8)$$

Therefore any permutation of the pair  $(q_j, p_j)$  will be even.

2 and 3. Observe first that

$$\begin{aligned}
\int \cdots \int (dp)^{\otimes k} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} &= \int \cdots \int (dp)^{\otimes k} \prod_{j=1}^k f_{q_j, p_j}^{\hbar}(w_j) \overline{f_{q_j, p_j}^{\hbar}(u_j)} \\
&= \hbar^{-\frac{3}{2}k} \prod_{j=1}^k f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) f\left(\frac{u_j - q_j}{\sqrt{\hbar}}\right) \left( \int dp_j e^{-\frac{i}{\hbar} p_j \cdot (w_j - u_j)} \right) \quad (2.2.9) \\
&\stackrel{(2.2.4)}{=} (2\pi)^{3k} \hbar^{(3-\frac{3}{2})k} \prod_{j=1}^k f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) f\left(\frac{u_j - q_j}{\sqrt{\hbar}}\right) \delta_{w_j}(u_j).
\end{aligned}$$

Therefore, from the definition of Husimi measure,

$$\begin{aligned}
&\frac{1}{(2\pi)^{3k}} \int \cdots \int (dq dp)^{\otimes k} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\
&= \frac{1}{(2\pi)^{3k}} \int \cdots \int (dq dw du)^{\otimes k} \left[ \int \cdots \int (dp)^{\otimes k} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \right] \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle \\
&= \int \cdots \int (dq dw du)^{\otimes k} \hbar^{(3-\frac{3}{2})k} \prod_{j=1}^k f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) f\left(\frac{u_j - q_j}{\sqrt{\hbar}}\right) \delta_{w_j}(u_j) \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle \\
&= \int \cdots \int (dq dw)^{\otimes k} \hbar^{(3-\frac{3}{2})k} \prod_{j=1}^k \left| f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) \right|^2 \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{w_k} \cdots a_{w_1} \Psi_{N,t} \rangle \\
&= \int \cdots \int (d\tilde{q} dw)^{\otimes k} \hbar^{3k} \prod_{j=1}^k |f(\tilde{q}_j)|^2 \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{w_k} \cdots a_{w_1} \Psi_{N,t} \rangle \\
&= \frac{1}{N^k} \prod_{j=1}^k \int d\tilde{q}_j |f(\tilde{q}_j)|^2 \int \cdots \int dw_1 \cdots dw_k \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{w_k} \cdots a_{w_1} \Psi_{N,t} \rangle \\
&\stackrel{(2.1.7)}{=} \frac{1}{N^k} \int \cdots \int dw_1 \cdots dw_k \langle \Psi_{N,t}, \mathcal{N}(\mathcal{N}-1) \cdots (\mathcal{N}-k+1) \Psi_{N,t} \rangle \\
&= \frac{N(N-1) \cdots (N-k+1)}{N^k}. \quad (2.2.10)
\end{aligned}$$

4. Observe that  $m_N^{(k)} \geq 0$  is obtained directly by its definition. To prove,  $m_N^{(k)} \leq 1$  observe from (2.2.8) and Lemma 2.1.2, we have

$$\begin{aligned}
m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) &= \left\| a(f_{q_k, p_k}^{\hbar}) \cdots a(f_{q_1, p_1}^{\hbar}) \psi_N \right\|_2^2 \\
&\leq \prod_{j=1}^k \|f_{q_j, p_j}^{\hbar}\|_2^2 \|\psi_N\|_2^2 \leq 1.
\end{aligned}$$

■



The relation between Husimi measure that of Wigner discussed at (1.2.7) is that one can think of Husimi as the ‘smoothing’ of Wigner by a Gaussian function. In fact, for a specific chosen coherent state, we have the following equality.

**Lemma 2.2.3** (Relation between Wigner and Husimi.). *Suppose  $m_{N,t}^{(k)}$  be the Husimi measure and let  $f(x) = \pi^{-3/4} e^{-|x|^2/2}$ . Then, we have for  $1 \leq k \leq N$ ,*

$$m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) = \frac{N(N-1) \cdots (N-k+1)}{N^k} (W_{N,t}^{(k)} * \mathcal{G}^{\hbar})(q_1, p_1, \dots, q_k, p_k), \quad (2.2.11)$$

where  $\mathcal{G}^{\hbar} = (\pi\hbar)^{-3k} \exp(-\hbar^{-1}(\sum_{j=1}^k |q_j|^2 + |p_j|^2))$  and  $W_{N,t}^{(k)}$  is the Wigner transform of  $k$ -particle density matrix defined in (1.1.25).

*Remark 2.2.3.* The lemma above implies that the Husimi measure  $m_{N,t}^{(k)}$  defined in (2.2.6) coincides with  $\mathbf{m}_{N,t}^{(k)}$  in (1.2.7).

*Proof.* We will prove for the cases for  $k = 1$ , i.e.,

$$m_{N,t}^{(1)}(q_1, p_1) = (W_{N,t}^{(1)} * \mathcal{G}_1^{\hbar})(q_1, p_1).$$

From (2.1.9), we can rewrite  $m_{N,t}^{(1)}$  as follows,

$$\begin{aligned} m_{N,t}^{(1)}(q_1, p_1) &= (\pi\hbar)^{-\frac{3}{2}} \iint dw du e^{-\frac{1}{2\hbar}(|q_1-w|^2 + |q_1-u|^2)} \gamma_t(w; u) e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \\ &= (\pi\hbar)^{-\frac{3}{2}} \iint dw du e^{-\frac{1}{2\hbar}(|q_1-w|^2 + |q_1-u|^2)} \gamma_t(w; u) e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \end{aligned} \quad (2.2.12)$$

We want to then compare the above to the convolution

$$\begin{aligned} (W_{N,t}^{(1)} * \mathcal{G}_1^{\hbar})(q_1, p_1) &= \iint dz dv W_{N,t}^{(1)}(z, v) \mathcal{G}_1^{\hbar}(q_1 - z, p_1 - v) \\ &= \hbar^3 (\pi\hbar)^{-3} \iint dz dv \int dy \gamma_t\left(z + \frac{\hbar}{2}y; z - \frac{\hbar}{2}y\right) e^{-iv \cdot y} e^{-\frac{|q_1-z|^2 + |p_1-v|^2}{\hbar}} \end{aligned}$$

By change of variable, one obtains

$$\begin{cases} w &= z + \frac{\hbar}{2}y, \\ u &= z - \frac{\hbar}{2}y. \end{cases} \Rightarrow dw du = \det(J) dz dy,$$

where the Jacobian determinant is

$$\det(J) = \det \begin{bmatrix} \frac{\partial w}{\partial z} & \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} & \frac{\partial u}{\partial y} \end{bmatrix} = -\hbar^3.$$

To continue, we have then

$$\begin{aligned} & (W_{N,t}^{(1)} * \mathcal{G}_1^{\hbar})(q_1, p_1) \\ &= -\hbar^3 (\pi \hbar)^{-3} \hbar^{-3} \iint dw du \int dv \gamma_t(w; u) e^{-\frac{i}{\hbar} v \cdot (w-u)} e^{-\frac{|(q_1-u)+(q_1-w)|^2}{4\hbar}} e^{-\frac{|p_1-v|^2}{\hbar}}. \end{aligned}$$

Letting  $\tilde{v} = p_1 - v$ , then we have

$$= (\pi \hbar)^{-3} \iint dw du \gamma_t(w; u) e^{\frac{i}{\hbar} p_1 \cdot (w-u)} e^{-\frac{|(q_1-u)+(q_1-w)|^2}{4\hbar}} \int d\tilde{v} e^{-\frac{1}{\hbar} (|\tilde{v}|^2 - i(w-u) \cdot \tilde{v})}$$

Observe that, for all  $w, u, v \in \mathbb{R}^3$ ,

$$\int_{\mathbb{R}^3} d\tilde{v} e^{-\frac{|\tilde{v}|^2}{\hbar} + \frac{i}{\hbar} (w-u) \cdot \tilde{v}} = (\pi \hbar)^{\frac{3}{2}} e^{\frac{i^2 |w-u|^2}{4\hbar}} = (\pi \hbar)^{\frac{3}{2}} e^{-\frac{|w-u|^2}{4\hbar}}. \quad (2.2.13)$$

Therefore, we have

$$\begin{aligned} &= (\pi \hbar)^{-\frac{3}{2}} \iint dw du \gamma_t(w; u) e^{\frac{i}{\hbar} p \cdot (w-u)} e^{-\frac{|(q-u)+(q-w)|^2}{4\hbar}} e^{-\frac{|w-u|^2}{4\hbar}} \\ &= (\pi \hbar)^{-\frac{3}{2}} \iint dw du \gamma_t(w; u) e^{\frac{i}{\hbar} p \cdot (w-u)} e^{-\frac{|q-w|^2 + |q-u|^2}{2\hbar}} \end{aligned}$$

where we used by Parallelogram identity in the last equality, i.e.,

$$\begin{aligned} |(q-w) + (q-u)|^2 + |w-u|^2 &= |(q-w) + (q-u)|^2 + |-w+u|^2 \\ &= |(q-w) + (q-u)|^2 + |(q-w) - (q-u)|^2 \\ &= 2|q-w|^2 + 2|q-u|^2. \end{aligned}$$

We then finally have

$$\begin{aligned} (W_{N,t}^{(1)} * \mathcal{G}_1^{\hbar})(q_1, p_1) &= (\pi \hbar)^{-\frac{3}{2}} \iint dw du \gamma_t(w; u) e^{\frac{i}{\hbar} p \cdot (w-u)} e^{-\frac{|q-w|^2 + |q-u|^2}{2\hbar}} \\ &= m_{N,t}^{(1)}(q_1; p_1), \end{aligned}$$

by (2.2.12). The case  $k \geq 2$  can be proven inductively. ■

## 2.3 *A priori* estimates

In this part, we give the bounds of number operators and their corresponding localized version, both of which are used extensively in estimating the remainder terms in (3.2.1) and (3.2.3).

**Lemma 2.3.1.** *Let  $\Psi_{N,t} \in \mathcal{F}_a$  be the solution to Schrödinger equation in (2.1.10) with initial data  $\|\Psi_N\| = 1$ , the number operator  $\mathcal{N}$  defined in (2.1.5). Then, for finite  $1 \leq k \leq N$ , we have*

$$\left\langle \Psi_{N,t}, \frac{\mathcal{N}^k}{N^k} \Psi_{N,t} \right\rangle \leq 1.$$

*Proof.* Since  $\Psi_{N,t}$  satisfies the Schrödinger equation, then for  $k \geq 1$ ,

$$i\hbar \frac{d}{dt} \langle \Psi_{N,t}, \mathcal{N}^k \Psi_{N,t} \rangle = \langle \Psi_{N,t}, [\mathcal{N}^k, \mathcal{H}_N] \Psi_{N,t} \rangle = k \langle \Psi_{N,t}, \mathcal{N}^{k-1} [\mathcal{N}, \mathcal{H}_N] \Psi_{N,t} \rangle = 0,$$

where we used the fact that  $\mathcal{H}_N$  is self-adjoint and  $[\mathcal{H}_N, \mathcal{N}] = 0$ . Therefore, integrating the above equation with respect to time, gives us

$$\left\langle \Psi_{N,t}, \frac{\mathcal{N}^k}{N^k} \Psi_{N,t} \right\rangle = \left\langle \Psi_N, \frac{\mathcal{N}^k}{N^k} \Psi_N \right\rangle = \frac{N(N-1) \cdots (N-k+1)}{N^k} \leq 1,$$

for any  $1 \leq k \leq N$ . ■

*Remark 2.3.1.* The expectation of the number operator is the total mass of Husimi measure. In fact, observe that

$$\langle \Psi_{N,t}, \mathcal{N} \Psi_{N,t} \rangle = \int dx \langle \Psi_{N,t}, a_x^* a_x \Psi_{N,t} \rangle = \int dx \langle \Psi_{N,t}, a_x^* \mathbb{1} a_x \Psi_{N,t} \rangle,$$

Then, by (2.2.2)

$$\begin{aligned} &= \frac{1}{(2\pi\hbar)^3} \iint dq dp \int dx \left\langle \Psi_{N,t}, a_x^* f_{q,p}^\hbar(x) \left( \int dy a_y \overline{f_{q,p}^\hbar(y)} \right) \Psi_{N,t} \right\rangle \\ &= \frac{1}{(2\pi\hbar)^3} \iint dq dp \langle \Psi_{N,t}, a^*(f_{q,p}^\hbar) a(f_{q,p}^\hbar) \Psi_{N,t} \rangle \\ &= \frac{1}{(2\pi\hbar)^3} \iint dq dp m_{N,t}^{(1)}(q, p) \\ &= N, \end{aligned}$$

where we use Lemma 2.2.2 in the last equality. Moreover, if we repeat the projection above for  $k$ -times, we get

$$\begin{aligned} &\frac{1}{(2\pi)^{3k}} \int \cdots \int (dq dp)^{\otimes k} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\ &\leq \left\langle \Psi_{N,t}, \frac{\mathcal{N}^k}{N^k} \Psi_{N,t} \right\rangle \leq 1, \end{aligned} \tag{2.3.1}$$

where  $1 \leq k \leq N$  and  $t \geq 0$ .

More importantly, we have the following estimates for localized number operators.

**Lemma 2.3.2** (Bound on localized number operator). *Let  $\Psi_N \in \mathcal{F}_a$  such that  $\|\Psi_N\| = 1$ , and  $R$  be the radius of a ball such that the volume is 1. Then, for all  $1 \leq k \leq N$ , we have*

$$\int \cdots \int (dq dx)^{\otimes k} \left\langle \Psi_N, \left( \prod_{n=1}^k \chi_{|x_n - q_n| \leq \sqrt{\hbar} R} \right) a_{x_1}^* \cdots a_{x_k}^* a_{x_k} \cdots a_{x_1} \Psi_N \right\rangle \leq \hbar^{-\frac{3}{2}k}, \quad (2.3.2)$$

where  $\chi$  is a characteristic function

*Proof.* Consider first the case where  $k = 1$ . For every  $1 \leq j \leq k$ , we have

$$\begin{aligned} & \int dx_j \left( \int dq_j \chi_{|x_j - q_j| \leq \sqrt{\hbar} R} \right) \langle \Psi_N, a_{x_j}^* a_{x_j} \Psi_N \rangle \\ &= \hbar^{\frac{3}{2}} \langle \Psi_N, \mathcal{N} \Psi_N \rangle = \hbar^{\frac{3}{2}-3} \left\langle \Psi_N, \frac{\mathcal{N}}{N} \Psi_N \right\rangle \leq \hbar^{-\frac{3}{2}}, \end{aligned}$$

where we used Lemma 2.3.1. Analogously, for  $2 \leq k \leq N$ ,

$$\begin{aligned} & \int (dx)^{\otimes k} \left( \prod_{n=1}^k \int dq_n \chi_{|x_n - q_n| \leq \sqrt{\hbar} R} \right) \langle \Psi_N, a_{x_1}^* \cdots a_{x_k}^* a_{x_k} \cdots a_{x_1} \Psi_N \rangle \\ & \leq \hbar^{\frac{3}{2}k} \langle \Psi_N, \mathcal{N}^k \Psi_N \rangle = \hbar^{\frac{3}{2}k-3k} \left\langle \Psi_N, \frac{\mathcal{N}^k}{N^k} \Psi_N \right\rangle \leq \hbar^{\frac{3}{2}k-3k}, \end{aligned}$$

where we applied Lemma 2.3.1 again. ■

Next, we present the following important estimate which is similar to van der Corput lemma, i.e.

**Lemma 2.3.3** (Estimate of oscillation). *For  $\varphi(p) \in C_0^\infty(\mathbb{R}^3)$  and*

$$\Omega_\hbar := \{x \in \mathbb{R}^3; \max_{1 \leq j \leq 3} |x_j| \leq \hbar^\alpha\}, \quad (2.3.3)$$

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

$$\left| \int_{\mathbb{R}^3} dp e^{\frac{i}{\hbar} p \cdot x} \varphi(p) \right| \leq C \hbar^{(1-\alpha)s}, \quad (2.3.4)$$

where  $C$  depends on the compact support and the  $C^s$ -norm of  $\varphi$ .

*Proof.* We will prove the lemma in a single-variable environment. That is, we let the momentum and space to be  $p = (p_1, p_2, p_3)$  and  $x = (x_1, x_2, x_3)$  such that  $x_j, p_j \in \mathbb{R}$  for all  $j \in \{1, 2, 3\}$ . Then, for arbitrary  $x \in \mathbb{R}^3 \setminus \Omega_\hbar$ , one of the  $x_j$ s is bigger than  $\hbar^\alpha$ . Without loss of generality, we assume that  $|x_1| > \hbar^\alpha$  and  $x_2, x_3 \in \mathbb{R}$ . Let  $\text{supp } \varphi \subset B_r(0) \subset \mathbb{R}^3$ , we can rewrite the left hand of (2.3.4) into the following,

$$\left| \int_{-r}^r dp_1 \int_{-r}^r dp_2 \int_{-r}^r dp_3 e^{\frac{i}{\hbar} (p_1 x_1 + p_2 x_2 + p_3 x_3)} \varphi(p) \right|$$

$$= \left| \int_{-r}^r dp_2 e^{\frac{i}{\hbar} p_2 x_2} \int_{-r}^r dp_3 e^{\frac{i}{\hbar} p_3 x_3} \int_{-r}^r dp_1 e^{\frac{i}{\hbar} p_1 x_1} \varphi(p) \right|$$

Observe that since

$$-i \frac{\hbar}{x_1} \frac{d}{dp_1} e^{\frac{i}{\hbar} p_1 x_1} = e^{\frac{i}{\hbar} p_1 x_1},$$

we have after  $s$  times integration by parts in  $p_1$ ,

$$\begin{aligned} & \left| \int_{-r}^r dp_1 \int_{-r}^r dp_2 \int_{-r}^r dp_3 e^{\frac{i}{\hbar} (p_1 x_1 + p_2 x_2 + p_3 x_3)} \varphi(p) \right| \\ &= \left| \left( -i \frac{\hbar}{x_1} \right)^s \int_{-r}^r dp_2 e^{\frac{i}{\hbar} p_2 x_2} \int_{-r}^r dp_3 e^{\frac{i}{\hbar} p_3 x_3} \int_{-r}^r dp_1 e^{\frac{i}{\hbar} p_1 x_1} \partial_{p_1}^s \varphi(p) \right| \\ &\leq C \frac{\hbar^s}{|x_1|^s} \leq C \hbar^{(1-\alpha)s}, \end{aligned}$$

where  $s$  indicates the number of time that integration by parts has been performed. ■

## Chapter 3

# Vlasov hierarchy

We begin the study of the convergence from time dependent Schrödinger equation for large spinless fermions with the semiclassical scale  $\hbar = N^{-1/3}$  in three dimensions by considering the interaction potential as follows.

**Assumption H2.**  $V$  is a real-valued function such that  $V(-x) = V(x)$  and  $V \in W^{2,\infty}(\mathbb{R}^3)$ .

Furthermore, we will derive in this chapter the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY)-type hierarchy from the Schrödinger equation in terms of the  $k$ -particle Husimi measure defined by coherent states. In addition, uniform estimates for the remainder terms in the aforementioned hierarchy are derived in order to show that in the semiclassical regime the weak limit of the Husimi measure is exactly the solution of the Vlasov equation. The work in this chapter is based on our article in [CLL21a] which has been published in *Journal of Statistical Physics*.

### 3.1 Main Results

As discussed in chapter 1.2.1, it is well known that in the mean field semiclassical regime, the dynamic of (2.1.10) can be approximated by a one particle Vlasov equation. Namely, for all  $q, p \in \mathbb{R}^3$

$$\partial_t m_t(q, p) + p \cdot \nabla_q m_t(q, p) = \nabla(V * \rho_t)(q) \cdot \nabla_p m_t(q, p), \quad (3.1.1)$$

with initial data  $m_0(q, p)$ , where  $m_t(q, p)$  is the time dependent one particle probability density function, and  $\rho_t(q) = \int m_t(q, p) dp$ . Although (3.1.1) is a non-linear equation, such equation would be more suitable to analyze than the increasingly large systems of Schrödinger equation. The well-posedness of the above Vlasov problem is given by Drobrushin [Dob79] for smooth  $V$ .

**Theorem 3.1.1.** *Let Assumptions H1 and H2 hold,  $\Psi_{N,t}$  be the solution of Schrödinger equation (2.1.10),  $m_{N,t}^{(k)}$  be the Husimi measure defined in (2.2.3). If the initial 1-particle Husimi measure  $m_N^{(1)} := m_N^{Slater}$ ,*

where  $m_N^{\text{Slater}}$  is defined in (2.2.7), satisfies

$$\iint dq_1 dp_1 (|p_1|^2 + |q_1|) m_N^{(1)}(q_1, p_1) \leq C. \quad (3.1.2)$$

Then, for all  $t \geq 0$ , the  $k$ -particle Husimi measure at time  $t$ ,  $m_{N,t}^{(k)}$  has a weakly convergent subsequence which converges to  $m_t^{(k)}$  in  $L^1(\mathbb{R}^6)$ , where  $m_t^{(k)}$  is a weak solution of the following infinite hierarchy in the sense of distribution, i.e. it satisfies for all  $k \geq 1$  that

$$\begin{aligned} & \partial_t m_t^{(k)}(q_1, p_1, \dots, q_k, p_k) + \mathbf{p}_k \cdot \nabla_{\mathbf{q}_k} m_t^{(k)}(q_1, p_1, \dots, q_k, p_k) \\ &= \frac{1}{(2\pi)^3} \nabla_{\mathbf{p}_k} \cdot \iint dq_{k+1} dp_{k+1} \nabla V(q_j - q_{k+1}) m_t^{(k+1)}(q_1, p_1, \dots, q_{k+1}, p_{k+1}). \end{aligned} \quad (3.1.3)$$

By using [Vil03, Theorem 7.12], we have the following corollary,

**Corollary 3.1.1.** *Suppose assumptions H1 and H2 hold. Assume further that the initial data of (3.1.3) can be factorized, i.e. for all  $k \geq 1$ ,*

$$\|m_N^{(k)} - m_0^{\otimes k}\|_{L^1} \rightarrow 0, \quad \text{as } N \rightarrow \infty. \quad (3.1.4)$$

Then, if the infinite hierarchy (3.1.3) has a unique solution and  $m_t$  is the solution to the classical Vlasov equation in (3.1.1), it holds that

$$W_1(m_{N,t}^{(1)}, m_t) \rightarrow 0, \quad \text{as } N \rightarrow \infty,$$

for  $t \geq 0$ .

*Remark 3.1.1.* In the pioneering work by Spohn [Spo81], he considered

$$\begin{aligned} & r_n^{(N)}(\xi_1, \eta_1, \dots, \xi_N, \eta_N, t) \\ &= \text{tr} \left[ e^{-iH_N t} |\psi_N\rangle \langle \psi_N| e^{iH_N t} \prod_{j=1}^N \exp\left\{i(N^{-1/3} \xi_j p_j + \eta_j x_j)\right\} \right] \end{aligned}$$

with  $p_j = -i\nabla_j$  and obtained the following Vlasov hierarchy,

$$\begin{aligned} & \frac{\partial}{\partial t} r_n^{(N)}(\xi_1, \eta_1, \dots, \xi_n, \eta_n, t) = \sum_{j=1}^n \eta_j \frac{\partial}{\partial \xi_j} r_n^{(N)}(\xi_1, \eta_1, \dots, \xi_n, \eta_n, t) \\ & + \sum_{j=1}^n \int \hat{V}(dk) k \cdot \xi_j r_{n+1}^{(N)}(\xi_1, \eta_1, \dots, \xi_j, \eta_j + k, \dots, \xi_n, \eta_n, 0, -k, t), \end{aligned}$$

which is slightly different from Vlasov hierarchy for Husimi measure given in (3.1.3), or the version in (3.2.3) before taking the limit. The benefit of the hierarchy in (3.2.3) is that one observes directly the mean field and semiclassical structure in the remainder terms. The explicit formulation is helpful in getting estimates for the remainder terms in (3.2.3). Moreover if one can handle singular potentials (or even the Coulomb potential) for both terms separately, one expects that this new approach can be applied to obtain the limit from many body Schrödinger to Vlasov with singular potentials in the future. Since the mean field limit with singular potential has been studied with convergence rate, for example in [BPS16], then we can utilize similar ideas to handle one of the remainder term which includes the mean field structure. In parallel, we can apply the techniques in semiclassical limit, for example in [Saf20b], to get estimates for the other remainder term.

*Remark 3.1.2.* Although the results in this article does not yield a convergent rate, the main purpose of this article is to present an alternative approach and framework, namely to rewrite the Schrödinger equation into a BBGKY type of hierarchy, and to derive estimates for the remainder terms that appear in the new hierarchy.

*Remark 3.1.3.* In Corollary 3.1.1, the convergence is stated in terms of 1-Wasserstein distance. For completeness, we give its definition as defined in [Vil03]

$$W_1(\mu, \nu) := \max_{\pi \in \Pi(\mu, \nu)} \int |x - y| \, d\pi(x, y), \quad (3.1.5)$$

where  $\mu$  and  $\nu$  are probability measures and  $\Pi(\mu, \nu)$  the set of all probability measures with marginals  $\mu$  and  $\nu$ . The Wasserstein distance, also known as Monge-Kantorovich distance, is a distance on the set of probability measures. In fact, if we interpret the metric in  $L^p$  space as the distance that measures two densities “vertically”, the Wasserstein distance measures the distance between two densities “horizontally” [San15].

*Remark 3.1.4.* The assumptions for initial data (3.1.2) and (3.1.4) can be realized by choosing  $\Psi_N$  to be the Slater-determinant. That is, for all orthonormal basis  $\{\varphi_j\}_{j=1}^\infty$ , the initial data is given as

$$\Psi_N(q_1, \dots, q_N) = \frac{1}{\sqrt{N!}} \det\{\varphi_j(q_i)\}_{1 \leq i, j \leq N}, \quad (3.1.6)$$

*Remark 3.1.5.* Assumptions H1 and H2 are expected to be weakened to the situation that  $f \in H^1(\mathbb{R}^3)$ ,  $|x|f(x) \in L^2(\mathbb{R}^3)$ , and  $V$  to be Coulomb potential. These will be our future projects.

*Remark 3.1.6.* In this context, we have applied the BBGKY hierarchy, the intermediate mean field approximation Hartree Fock system has not been benefited. With Hartree Fock approximation, one can do direct factorization in the equation for  $m_{N,t}^{(1)}$ . In this direction, we expect to derive the rate of convergence in an appropriate distance between the Husimi measure and the solution of the Vlasov equation.



The arrangement of this chapter is the following. In section 3.2, we give the main strategy of the proof. Followed by the corresponding kinetic energy operator, which will be contributed to do compactness argument for the Husimi measure. We leave the computation of the hierarchy to section 3.3.1. Furthermore, the uniform estimates for remainder terms in the hierarchy, which is another main contribution of this thesis, are provided in section 3.3.2.

### 3.1.1 The BBGKY method

Denoting  $f_{N,t}$  to be a time-dependent probability density measure on the  $N$ -particles phase-space  $\mathbb{R}^{3N}$ , the dimension of  $F_{N,t}$  increases as  $N$  tends to infinity, causing the number of variables in  $F_{N,t}$  to also tend to infinity. To solve this, one would instead look at the first marginal of  $F_{N,t}$ , denoted as  $F_{N,t}^{(1)}$ . However, as one observes later, the computation of  $F_{N,t}^{(1)}$  involves second marginal  $F_{N,t}^{(2)}$  as the pairwise interaction of the particles, while the second marginal involves the third, and so on.

Nevertheless, under the assumption that  $F_{N,t}^{(j)} \rightarrow F_t^{(j)}$  as  $N \rightarrow \infty$  (in certain sense) for all  $j \geq 1$ , then one obtains the following limits with respect of  $N$ :

$$\begin{aligned} \frac{N-j}{N} \int dx_{j+1} K(x_\ell; x_{j+1}) F_{N,t}^{(j+1)} &\longrightarrow \int dx_{j+1} V(x_\ell - x_{j+1}) F_t^{(j+1)}, \\ \frac{1}{N} K(x_\ell; x_k) F_{N,t}^{(j)} &\longrightarrow 0, \end{aligned}$$

where  $\ell \in \{1, \dots, j\}$ ,  $k \in \{j+1, \dots, N\}$  and  $K$  is a kernel that represents the interaction term. This implies that the mean field hierarchy is

$$\partial_t F_t^{(j)} + \sum_{i=1}^j \operatorname{div}_{x_i} \int dx_{j+1} K(x_i; x_{j+1}) F_t^{(j+1)} = 0, \quad (3.1.7)$$

for all  $j \geq 1$ . Assuming a regular  $K$  and initial data of (3.1.7) is factorized, e.g.  $F_{N,0} = (f^{\text{in}})^{\otimes N}$  where  $f^{\text{in}}$  is an initial data, then one obtains

$$F_{N,t}^{(j)} \longrightarrow F_t^{(j)} = f^{\otimes j},$$

where  $f$  be the solution of mean-field partial differential equation with initial data  $f^{\text{in}}$ . Details of existence and uniqueness of (3.1.7) can be found in [CGP12] and [Pet72] respectively.

## 3.2 Proof strategy through BBGKY type hierarchy for Husimi measure

We first start from the many particle Schrödinger equation and derive an approximated hierarchy of time dependent Husimi measure by direct computation. Compare to the BBGKY hierarchy of Liouville equation in the classical sense, it has two families of remainder terms, which are determined by the  $N$  particle wave function from Schrödinger equation. In order to take a convergent subsequence of the  $k$ -particle Husimi measure, we derive the uniform estimates for number operator and the kinetic energy. Together with an additional estimate for localized number operator, we can show that the remainder terms are of order  $\hbar^{\frac{1}{2}-\delta}$ , for arbitrary small  $\delta$ . Then the desired result will be obtained by the uniqueness of solution to the infinite hierarchy.

### 3.2.1 Reformulation: Hierarchy of time dependent Husimi measure

In this subsection, we begin by examining the dynamics of  $k$ -particle Husimi measure by using the  $N$ -body fermionic Schrödinger. The proofs of the following propositions are provided in section 3.3.1.

**Proposition 3.2.1.** *Suppose  $\Psi_{N,t} \in \mathcal{F}_a$  is anti-symmetric  $N$ -particle state satisfying the Schrödinger equation in (2.1.10). Moreover, if  $V(-x) = V(x)$  then we have the following equation for  $k = 1$ ,*

$$\begin{aligned} & \partial_t m_{N,t}^{(1)}(q_1, p_1) + p_1 \cdot \nabla_{q_1} m_{N,t}^{(1)}(q_1, p_1) \\ &= \frac{1}{(2\pi)^3} \nabla_{p_1} \cdot \iint dq_2 dp_2 \nabla V(q_1 - q_2) m_{N,t}^{(2)}(q_1, p_1, q_2, p_2) + \nabla_{q_1} \cdot \mathcal{R}_1 + \nabla_{p_1} \cdot \tilde{\mathcal{R}}_1, \end{aligned} \quad (3.2.1)$$

where the remainder terms  $\mathcal{R}_1$  and  $\tilde{\mathcal{R}}_1$ , are given by

$$\begin{aligned} \mathcal{R}_1 &:= \hbar \operatorname{Im} \langle \nabla_{q_1} a(f_{q_1, p_1}^{\hbar}) \Psi_{N,t}, a(f_{q_1, p_1}^{\hbar}) \Psi_{N,t} \rangle, \\ \tilde{\mathcal{R}}_1 &:= \frac{1}{(2\pi)^3} \cdot \operatorname{Re} \iint dw du \iint dy dv \iint dq_2 dp_2 \int_0^1 ds \\ & \quad \nabla V(su + (1-s)w - y) f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} f_{q_2, p_2}^{\hbar}(y) \overline{f_{q_2, p_2}^{\hbar}(v)} \langle a_y a_w \Psi_{N,t}, a_v a_u \Psi_{N,t} \rangle \\ & \quad - \frac{1}{(2\pi)^3} \iint dq_2 dp_2 \nabla V(q_1 - q_2) m_{N,t}^{(2)}(q_1, p_1, q_2, p_2), \end{aligned} \quad (3.2.2)$$

**Proposition 3.2.2.** *For every  $1 \leq i, j \leq k$  and  $q_j, p_j \in \mathbb{R}^3$ , denote  $\mathbf{q}_k = (q_1, \dots, q_k)$  and  $\mathbf{p}_k = (p_1, \dots, p_k)$ .*

Under the assumption in Proposition 3.2.1, then for  $1 < k \leq N$ , we have the following hierarchy

$$\begin{aligned}
& \partial_t m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) + \mathbf{p}_k \cdot \nabla_{\mathbf{q}_k} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\
&= \frac{1}{(2\pi)^3} \nabla_{\mathbf{p}_k} \cdot \iint dq_{k+1} dp_{k+1} \nabla V(q_j - q_{k+1}) m_{N,t}^{(k+1)}(q_1, p_1, \dots, q_{k+1}, p_{k+1}) \\
&\quad + \nabla_{\mathbf{q}_k} \cdot \mathcal{R}_k + \nabla_{\mathbf{p}_k} \cdot \tilde{\mathcal{R}}_k + \hat{\mathcal{R}}_k,
\end{aligned} \tag{3.2.3}$$

where the remainder terms are denoted as

$$\begin{aligned}
\mathcal{R}_k &:= \hbar \operatorname{Im} \langle \nabla_{\mathbf{q}_k} (a(f_{q_k, p_k}^{\hbar}) \cdots a(f_{q_1, p_1}^{\hbar})) \Psi_{N,t}, a(f_{q_k, p_k}^{\hbar}) \cdots a(f_{q_1, p_1}^{\hbar}) \Psi_{N,t} \rangle, \\
(\tilde{\mathcal{R}}_k)_j &:= \frac{1}{(2\pi)^3} \operatorname{Re} \int \cdots \int (dw du)^{\otimes k} \int dy \left[ \int_0^1 ds \nabla V(su_j + (1-s)w_j - y) \right] \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
&\quad \iint d\tilde{q} d\tilde{p} f_{\tilde{q}, \tilde{p}}^{\hbar}(y) \int dv \overline{f_{\tilde{q}, \tilde{p}}^{\hbar}(v)} \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_v \Psi_{N,t} \rangle \\
&\quad - \frac{1}{(2\pi)^3} \iint dq_{k+1} dp_{k+1} \nabla V(q_j - q_{k+1}) m_{N,t}^{(k+1)}(q_1, p_1, \dots, q_{k+1}, p_{k+1}), \\
\hat{\mathcal{R}}_k &:= \frac{\hbar^2}{2} \operatorname{Im} \int \cdots \int (dw du)^{\otimes k} \sum_{j \neq i}^k \left[ V(u_j - u_i) - V(w_j - w_i) \right] \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
&\quad \langle a_{w_k} \cdots a_{w_1} \Psi_{N,t}, a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle
\end{aligned} \tag{3.2.4}$$

### 3.2.2 Finite moments of Husimi measure

To prove that the second moment in  $p$  of the Husimi measure is finite, we first show that the kinetic energy is bounded from above. Recall that the definition of the kinetic energy operator  $\mathcal{K}$ , i.e.,

$$\mathcal{K} = \frac{\hbar^2}{2} \int dx \nabla_x a_x^* \nabla_x a_x,$$

and the kinetic energy associated with  $\Psi_N \in \mathcal{F}_a$  is given as  $\langle \Psi_N, \mathcal{K} \Psi_N \rangle$ .

**Lemma 3.2.1.** *Assume  $V \in W^{1,\infty}$ , then the kinetic energy is bounded in the following*

$$\left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle \leq 2 \left\langle \Psi_N, \frac{\mathcal{K}}{N} \Psi_N \right\rangle + Ct^2, \tag{3.2.5}$$

where  $C$  depends on  $\|\nabla V\|_{\infty}$ .

*Proof.* From the Schrödinger equation, we get

$$i\hbar \frac{d}{dt} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle = \langle \Psi_{N,t}, [\mathcal{K}, \mathcal{H}] \Psi_{N,t} \rangle. \tag{3.2.6}$$

Note that since the commutator between kinetic and interaction term is given as

$$\begin{aligned}
[\mathcal{K}, \mathcal{H}] &= \frac{\hbar^2}{4} \left[ \int dx \nabla_x a_x^* \nabla_x a_x, \iint dy dz V(y-z) a_y^* a_z^* a_z a_y \right] \\
&= \frac{\hbar^2}{4} \iint dx dy \nabla_x V(x-y) \left( \nabla_x a_x^* a_y^* a_y a_x - a_x^* a_y^* a_y \nabla_x a_x \right) \\
&= \frac{\hbar^2}{2N} \operatorname{Im} \iint dx dy \nabla_x V(x-y) (\nabla_x a_x^* a_y^* a_y a_x)
\end{aligned}$$

Then, from (3.2.6), we have that

$$\frac{1}{N} \frac{d}{dt} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle = \frac{\hbar}{2N^2} \operatorname{Im} \iint dx dy \nabla_x V(x-y) \langle \Psi_{N,t}, \nabla_x a_x^* a_y^* a_y a_x \Psi_{N,t} \rangle.$$

Now, observe that

$$\begin{aligned}
& \left| \frac{\hbar}{2N^2} \iint dx dy \nabla_x V(x-y) \langle \Psi_{N,t}, \nabla_x a_x^* a_y^* a_y a_x \Psi_{N,t} \rangle \right| \\
& \leq \frac{\hbar}{2N^2} \|\nabla V\|_{L^\infty} \iint dx dy \|a_y \nabla_x a_x \Psi_{N,t}\| \|a_y a_x \Psi_{N,t}\| \\
& \leq C \frac{\hbar}{2N^2} \left( \iint dx dy \langle \Psi_{N,t}, \nabla_x a_x^* a_y^* a_y \nabla_x a_x \Psi_{N,t} \rangle \right)^{\frac{1}{2}} \left( \iint dx dy \langle \Psi_{N,t}, a_x^* a_y^* a_y a_x \Psi_{N,t} \rangle \right)^{\frac{1}{2}} \\
& = C \left( \frac{\hbar^2}{N} \int dx \left\langle \Psi_{N,t}, \nabla_x a_x^* \frac{\mathcal{N}}{N} \nabla_x a_x \Psi_{N,t} \right\rangle \right)^{\frac{1}{2}} \left\langle \Psi_{N,t}, \frac{\mathcal{N}^2}{N^2} \Psi_{N,t} \right\rangle^{\frac{1}{2}} \\
& \leq C \left( \left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle \right)^{\frac{1}{2}},
\end{aligned}$$

Thus, we have

$$\frac{d}{dt} \left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle \leq C \left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle^{\frac{1}{2}}.$$

Integrating both sides with respect to time  $t$  and we obtain the desired inequality. ■

**Proposition 3.2.3.** *For  $t \geq 0$ , assume H1 and let  $m_{N,t}^{(k)}$  to be the  $k$ -particle Husimi measure. Denoting the phase-space vectors  $\mathbf{q}_k = (q_1, \dots, q_k)$  and  $\mathbf{p}_k = (p_1, \dots, p_k)$ , we have the following finite moments,*

$$\int \cdots \int (dq dp)^{\otimes k} (|\mathbf{q}_k| + |\mathbf{p}_k|^2) m_{N,t}^{(k)}(q_1, \dots, p_k) \leq C(1+t^3)$$

where  $C$  is a constant dependent on  $k$ ,  $\iint dq_1 dp_1 (|q_1| + |p_1|^2) m_N^{(1)}(q_1, p_1)$ , and  $\|\nabla V\|_\infty$ .

*Proof.* We first consider the case where  $k = 1$ . Observe that we may rewrite the kinetic energy as follows

$$\begin{aligned}
\frac{1}{N} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle &= \frac{\hbar^2}{N} \int dw \langle \Psi_{N,t}, \nabla_w a_w^* \nabla_w a_w \Psi_{N,t} \rangle \\
&= \frac{\hbar^2}{N} (2\pi\hbar)^{-3} \iint dq_1 dp_1 \iint dw du f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, \nabla_w a_w^* \nabla_u a_u \Psi_{N,t} \rangle \\
&= \frac{\hbar^2}{(2\pi)^3} \iint dq_1 dp_1 \iint dw du \nabla_w f_{q_1, p_1}^\hbar(w) \overline{\nabla_u f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle \\
&= \frac{\hbar^2}{(2\pi)^3} \iint dq_1 dp_1 \iint dw du (-\nabla_{q_1} + i\hbar^{-1} p_1) f_{q_1, p_1}^\hbar(w) \cdot (-\nabla_{q_1} - i\hbar^{-1} p_1) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle,
\end{aligned}$$

where we used the fact that

$$\nabla_w f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) = -\nabla_{q_1} f\left(\frac{w - q_1}{\sqrt{\hbar}}\right).$$

To continue, we have

$$\begin{aligned}
\frac{1}{N} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle &= \frac{1}{(2\pi)^3} \iint dq_1 dp_1 |p_1|^2 m_{N,t}^{(1)}(q_1, p_1) \\
&\quad + \frac{\hbar^2}{(2\pi)^3} \iint dq_1 dp_1 \iint dw du \nabla_{q_1} f_{q_1, p_1}^\hbar(w) \cdot \nabla_{q_1} \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle \\
&\quad + \frac{2i}{(2\pi)^3} \text{Im} \iint dq_1 dp_1 \iint dw du p_1 \cdot \nabla_{q_1} f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle.
\end{aligned} \tag{3.2.7}$$

Since kinetic energy is real-valued, if we take the real part of (3.2.7), the last term in the right hand side vanishes since it is purely imaginary, yielding

$$\begin{aligned}
\frac{1}{N} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle &= \frac{1}{(2\pi)^3} \iint dq_1 dp_1 |p_1|^2 m_{N,t}^{(1)}(q_1, p_1) \\
&\quad + \frac{\hbar^2}{(2\pi)^3} \text{Re} \iint dq_1 dp_1 \iint dw du \nabla_{q_1} f_{q_1, p_1}^\hbar(w) \cdot \nabla_{q_1} \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle.
\end{aligned}$$

Note that by (2.2.3), we have

$$\begin{aligned}
&\frac{\hbar^2}{(2\pi)^3} \iint dq_1 dp_1 \iint dw du \nabla_{q_1} f_{q_1, p_1}^\hbar(w) \cdot \nabla_{q_1} \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle \\
&= \hbar^{2+3} \iint dq_1 dw \hbar^{-\frac{3}{2}} \left| \nabla_{q_1} f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \right|^2 \langle \Psi_{N,t}, a_w^* a_w \Psi_{N,t} \rangle \\
&= \hbar \int d\tilde{q} |\nabla f(\tilde{q})|^2 \left\langle \Psi_{N,t}, \frac{\mathcal{N}}{N} \Psi_{N,t} \right\rangle \\
&= \hbar \int d\tilde{q} |\nabla f(\tilde{q})|^2,
\end{aligned} \tag{3.2.8}$$

where we recall that  $\hbar^3 = N^{-1}$ . Thus, taking the real part of (3.2.7), we have that

$$\left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle = \frac{1}{(2\pi)^3} \iint dq_1 dp_1 |p_1|^2 m_{N,t}^{(1)}(q_1, p_1) + \hbar \int dq |\nabla f(q)|^2, \quad (3.2.9)$$

which means,

$$\frac{1}{(2\pi)^3} \iint dq_1 dp_1 |p_1|^2 m_{N,t}^{(1)}(q_1, p_1) \leq \left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle. \quad (3.2.10)$$

Therefore, (3.2.10) tells us that the second moment of the 1-particle Husimi measure in momentum space is finite if the kinetic energy is finite.

Now, we turn our focus on the moment with respect to position space. From (3.2.1), we get

$$\begin{aligned} & \partial_t \iint dq_1 dp_1 |q_1| m_{N,t}^{(1)}(q_1, p_1) = \iint |q_1| \partial_t m_{N,t}^{(1)}(q_1, p_1) \\ &= \iint dq_1 dp_1 |q_1| \left( -p_1 \cdot \nabla_{q_1} m_{N,t}^{(1)}(q_1, p_1) + \frac{1}{(2\pi)^3} \nabla_{p_1} \cdot \iint dw du \iint dx dy \iint dq_2 dp_2 \int_0^1 ds \right. \\ & \quad \left. \nabla V(su + (1-s)w - x) f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} f_{q_2, p_2}^{\hbar}(x) \overline{f_{q_2, p_2}^{\hbar}(y)} \langle a_x a_w \Psi_{N,t}, a_y a_u \Psi_{N,t} \rangle + \nabla_{q_1} \cdot \mathcal{R}_1 \right). \end{aligned} \quad (3.2.11)$$

where  $R_1$  is the remainder term in (3.2.2).

To check that the surface integral of middle term of (3.2.11) when taking integration by part will vanish when  $p$  is evaluated at far field. In fact, we will check for the  $L^1$  integrability, i.e.

$$\begin{aligned} & \frac{1}{(2\pi)^3} \iint dq_1 dp_1 |q_1| \nabla_{p_1} \cdot \iint dw_1 du_1 \iint dq_2 dp_2 \iint dw_2 du_2 \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) \\ & \quad f_{q_1, p_1}^{\hbar}(w_1) \overline{f_{q_1, p_1}^{\hbar}(u_1)} f_{q_2, p_2}^{\hbar}(w_2) \overline{f_{q_2, p_2}^{\hbar}(u_2)} \langle a_{w_2} a_{w_1} \Psi_{N,t}, a_{u_2} a_{u_1} \Psi_{N,t} \rangle \\ &= C \hbar^{3-1} \iint dq_1 d\tilde{p} |q_1| \nabla_{\tilde{p}} \cdot \iint dw_1 du_1 \int dw_2 \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) \\ & \quad f\left(\frac{w_1 - q_1}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q_1}{\sqrt{\hbar}}\right) e^{i\tilde{p} \cdot (w_1 - u_1)} \int dq_2 \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \langle a_{w_2} a_{w_1} \Psi_{N,t}, a_{w_2} a_{u_1} \Psi_{N,t} \rangle \\ &= C \hbar^2 \hbar^{\frac{3}{2}} \|f\|_2^2 \iint dq_1 d\tilde{p} |q_1| \nabla_{\tilde{p}} \cdot \iint dw_1 du_1 \int dw_2 \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) \\ & \quad f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) e^{i\tilde{p} \cdot (w_1 - u_1)} \langle a_{w_2} a_{w_1} \Psi_{N,t}, a_{w_2} a_{u_1} \Psi_{N,t} \rangle \end{aligned}$$

Then, note that since

$$\begin{aligned}
& \hbar^{2+\frac{3}{2}} \iint dw_1 du_1 \left| \int dw_2 \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) f\left(\frac{w_1 - q_1}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q_1}{\sqrt{\hbar}}\right) \langle a_{w_1} \Psi_{N,t}, a_{w_2}^* a_{w_2} a_{u_1} \Psi_{N,t} \rangle \right| \\
& \leq \hbar^{2+\frac{3}{2}} \|\nabla V_N\|_\infty \iint dw_1 du_1 \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\| \|a_{w_2} a_{u_1} \Psi_{N,t}\| \\
& \leq \hbar^{2+\frac{3}{2}} \|\nabla V_N\|_\infty \iint dw_1 du_1 \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \\
& \leq \hbar^{2+\frac{3}{2}} \|\nabla V_N\|_\infty \left[ \iint dw_1 du_1 \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|^2 \right]^{\frac{1}{2}} \iint dw_1 dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \\
& \leq \hbar^{5-6} \|\nabla V_N\|_\infty \int d\tilde{q} |f(\tilde{q})|^2 \\
& \leq C_N.
\end{aligned} \tag{3.2.12}$$

This implies that, for any fixed  $N \in \mathbb{N}$ , the function in (3.2.12) is bounded  $L^1$  in both  $w_1$  and  $u_1$ . Then by Riemann-Lebesgue Lemma, the surface integral from applying divergence theorem for the middle term vanishes when evaluating  $|p_1| \rightarrow \infty$ .

Thus, integration-by-parts with respect to  $p_1$ , and then with respect to  $q_1$  in (3.2.11), we obtain

$$\begin{aligned}
& \partial_t \iint dq_1 dp_1 |q_1| m_{N,t}^{(1)}(q_1, p_1) \\
& \leq \iint dq_1 dp_1 \nabla_{q_1} |q_1| \cdot \left( p_1 m_{N,t}^{(1)}(q_1, p_1) + \mathcal{R}_1 \right) \\
& = \iint dq_1 dp_1 \frac{q_1}{|q_1|} \cdot \left( p_1 m_{N,t}^{(1)}(q_1, p_1) + \mathcal{R}_1 \right) \\
& \leq \iint dq_1 dp_1 \left( |p_1| m_{N,t}^{(1)}(q_1, p_1) + |\mathcal{R}_1| \right),
\end{aligned}$$

Note that by Young's product inequality, we have

$$\begin{aligned}
\iint dq_1 dp_1 |p_1| m_{N,t}^{(1)}(q_1, p_1) & \leq \iint dq_1 dp_1 (1 + |p_1|^2) m_{N,t}^{(1)}(q_1, p_1) \\
& \leq (2\pi)^3 \left( 1 + 2 \left\langle \Psi_N, \frac{\mathcal{K}}{N} \Psi_N \right\rangle + Ct^2 \right),
\end{aligned}$$

where we used (3.2.10) and Lemma 3.2.1 in the last inequality. Next, we want to bound the term associated with  $\mathcal{R}_1$ ,

$$\iint dq_1 dp_1 |\mathcal{R}_1| \leq \hbar \iint dq_1 dp_1 \left| \langle \nabla_{q_1} a(f_{q_1, p_1}^\hbar) \Psi_{N,t}, a(f_{q_1, p_1}^\hbar) \Psi_{N,t} \rangle \right|.$$

Observe that we have,

$$\begin{aligned}
& \hbar \iint dq_1 dp_1 \left| \langle \nabla_{q_1} a(f_{q_1, p_1}^h) \Psi_{N, t}, a(f_{q_1, p_1}^h) \Psi_{N, t} \rangle \right| \leq \hbar \iint dq_1 dp_1 \|\nabla_{q_1} a(f_{q_1, p_1}^h) \Psi_{N, t}\| \|a(f_{q_1, p_1}^h) \Psi_{N, t}\| \\
& \leq \hbar \left[ \iint dq_1 dp_1 \langle \nabla_{q_1} a(f_{q_1, p_1}^h) \Psi_{N, t}, \nabla_{q_1} a(f_{q_1, p_1}^h) \Psi_{N, t} \rangle \right]^{\frac{1}{2}} \left[ \iint dq_1 dp_1 \langle \Psi_{N, t}, a^*(f_{q_1, p_1}^h) a(f_{q_1, p_1}^h) \Psi_{N, t} \rangle \right]^{\frac{1}{2}} \\
& = \left[ \hbar^2 \iint dq_1 dp_1 \iint dw du \nabla_{q_1} f_{q_1, p_1}^h(w) \cdot \nabla_{q_1} \overline{f_{q_1, p_1}^h(u)} \langle \Psi_{N, t}, a_w^* a_u \Psi_{N, t} \rangle \right]^{\frac{1}{2}} (2\pi)^{\frac{3}{2}} \\
& \leq (2\pi)^3 \sqrt{\hbar} \left[ \int d\tilde{q} |\nabla f(\tilde{q})|^2 \right]^{\frac{1}{2}},
\end{aligned}$$

where we used (3.2.8), Lemma 2.2.2. Thus, we have that

$$\partial_t \iint dq_1 dp_1 |q_1| m_{N, t}^{(1)}(q_1, p_1) \leq (2\pi)^3 \left( 1 + 2 \left\langle \Psi_N, \frac{\mathcal{K}}{N} \Psi_N \right\rangle + Ct^2 + C\sqrt{\hbar} \right) \leq C(1 + t^2). \quad (3.2.13)$$

which gives the estimate for first moment after integrating with respect to time  $t$ .

We now consider the case of  $2 \leq k \leq N$ . In this computation, we make use of the properties of  $k$ -particle Husimi measure. Namely, that the  $m_{N, t}^{(k)}$  is symmetric and satisfies the following equation

$$\begin{aligned}
\frac{1}{(2\pi)^3} \iint dq_k dp_k m_{N, t}^{(k)}(q_1, p_1, \dots, q_k, p_k) &= \frac{(N - k + 1)}{N} m_{N, t}^{(k-1)}(q_1, p_1, \dots, q_{k-1}, p_{k-1}) \\
&\leq m_{N, t}^{(k-1)}(q_1, p_1, \dots, q_{k-1}, p_{k-1}).
\end{aligned} \quad (3.2.14)$$

Observe that for fixed  $1 \leq k \leq N$ .

$$\begin{aligned}
& \int \cdots \int (dq dp)^{\otimes k} \sum_{j=1}^k |p_j|^2 m_{N, t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\
&= \sum_{j=1}^k \iint dq_j dp_j |p_j|^2 \int \cdots \int dq_1 dp_1 \cdots \widehat{dq_j dp_j} \cdots dq_k dp_k m_{N, t}^{(k)}(q_1, p_1, \dots, q_k, p_k).
\end{aligned}$$

Then, by using the symmetricity of  $m_{N, t}^{(k)}$  and change of variables, we get

$$\begin{aligned}
&= k \iint dq dp |p|^2 \int \cdots \int (dq dp)^{\otimes k-1} m_{N, t}^{(k)}(q, p, q_1, p_1, \dots, q_{k-1}, p_{k-1}) \\
&= (2\pi)^{3(k-1)} k \frac{(N-1) \cdots (N-k+1)}{N^{k-1}} \iint dq dp |p|^2 m_{N, t}^{(1)}(q, p) \\
&\leq (2\pi)^{3k} k \left( 1 + 2 \left\langle \Psi_N, \frac{\mathcal{K}}{N} \Psi_N \right\rangle + Ct^2 \right) \leq C(1 + t^2),
\end{aligned}$$

where we denoted  $(dq dp)^{\otimes k-1} = dq_1 dp_1 \cdots dq_{k-1} dp_{k-1}$ .



Similar strategy is used to obtain the first moment with respect to  $\mathbf{q}_k$ . That is

$$\begin{aligned}
& \int \cdots \int (dq dp)^{\otimes k} \sum_{j=1}^k |q_j| m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\
&= (2\pi)^{3(k-1)} k \frac{(N-1) \cdots (N-k+1)}{N^{k-1}} \iint dq dp |q| m_{N,t}^{(1)}(q, p) \\
&\leq (2\pi)^{3(k-1)} k \iint dq dp |q| m_{N,t}^{(1)}(q, p) \leq C(1+t^3).
\end{aligned}$$

This yields the desired conclusion. ■

### 3.2.3 Uniform estimates for the remainder terms

In this subsection, we give uniform estimates for the error terms that appear in (3.2.1) and (3.2.3). They are all bounded of order  $\hbar^{\frac{1}{2}-\delta}$  for arbitrary small  $\delta > 0$ . The proofs of all the following propositions will be provided in section 3.3.2.

**Proposition 3.2.4.** *Let Assumption H1 holds, then for  $1 \leq k \leq N$ , we have the following bound for  $\mathcal{R}_k$  in (3.2.1) and (3.2.3). For arbitrary small  $\delta > 0$ , the following estimate holds for any test function  $\Phi \in C_0^\infty(\mathbb{R}^{6k})$ ,*

$$\left| \int \cdots \int (dq dp)^{\otimes k} \Phi(q_1, p_1, \dots, q_k, p_k) \nabla_{\mathbf{q}_k} \cdot \mathcal{R}_k \right| \leq C \hbar^{\frac{1}{2}-\delta},$$

where  $C$  depends on  $\|D^{s(\delta)}\Phi\|_\infty$  and  $k$ .

**Proposition 3.2.5.** *Let Assumption H1 and H2 hold, then we have the following bound for  $\tilde{\mathcal{R}}_1$  in (3.2.2). For arbitrary small  $\delta > 0$ , the following estimate holds for any test function  $\Phi \in C_0^\infty(\mathbb{R}^6)$ ,*

$$\left| \iint dq_1 dp_1 \Phi(q_1, p_1) \nabla_{p_1} \cdot \tilde{\mathcal{R}}_1 \right| \leq C \hbar^{\frac{1}{2}-\delta}, \tag{3.2.15}$$

where  $C$  depends on  $\|D^{s(\delta)}\Phi\|_\infty$ .

**Proposition 3.2.6.** *Suppose that Assumption H1 and H2 hold. Denote the remainders terms  $\tilde{\mathcal{R}}_k$  and  $\hat{\mathcal{R}}_k$  as in (3.2.4). Then for  $1 \leq k \leq N$  and arbitrary small  $\delta > 0$ , the following estimates hold for any test function  $\Phi \in C_0^\infty(\mathbb{R}^{6k})$ ,*

$$\left| \int \cdots \int (dq dp)^{\otimes k} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \hat{\mathcal{R}}_k \right| \leq C \hbar^{3-\delta}, \tag{3.2.16}$$

and

$$\left| \int \cdots \int (dq dp)^{\otimes k} \Phi(q_1, p_1, \dots, q_k, p_k) \nabla_{\mathbf{p}_k} \cdot \tilde{\mathcal{R}}_k \right| \leq C \hbar^{\frac{1}{2}-\delta}, \tag{3.2.17}$$

where  $C$  depends on  $\|D^{s(\delta)}\Phi\|_\infty$  and  $k$ .

### 3.2.4 Convergence to infinite hierarchy

In this subsection, we prove that the  $k$ -particle Husimi measure  $m_{N,t}^{(k)}$  has subsequence that converges weakly (as  $N \rightarrow \infty$ ) to a limit  $m_t^{(k)}$  in  $L^1$ , which is a solution of the infinite hierarchy in the sense of distribution.

The weak compactness of  $k$ -particle Husimi measure  $m_{N,t}^{(k)}$  can be proved by the use of Dunford-Pettis theorem.<sup>1</sup> In particular, we have the following result.

**Proposition 3.2.7.** *Let  $\{m_{N,t}^{(k)}\}_{N \in \mathbb{N}}$  be the  $k$ -particle Husimi measure, then there exists a subsequence  $\{m_{N_j,t}^{(k)}\}_{j \in \mathbb{N}}$  that converges weakly in  $L^1(\mathbb{R}^{3 \times R^3})$  to a function  $(2\pi)^{3k} m_t^{(k)}$ , i.e. for all  $\Phi \in L^\infty(\mathbb{R}^3 \times R^3)$ , it holds*

$$\frac{1}{(2\pi)^{3k}} \int \cdots \int (dq dp)^{\otimes k} m_{N_j,t}^{(k)} \Phi \rightarrow \int \cdots \int (dq dp)^{\otimes k} m_t^{(k)} \Phi,$$

when  $j \rightarrow \infty$  for arbitrary fixed  $k \geq 1$ .

*Proof.* To apply Dunford-Pettis theorem, we need to check that it is uniformly integrable and bounded. From Lemma 2.2.2 and the finite moment in Proposition 3.2.3 imply

$$\left\| m_{N,t}^{(k)} \right\|_{L^\infty} \leq 1, \quad \left\| (|\mathbf{q}_k| + |\mathbf{p}_k|) m_{N,t}^{(k)} \right\|_{L^1} \leq C(t).$$

where  $\mathbf{q}_k := (q_1, \dots, q_k)$ ,  $\mathbf{p}_k := (p_1, \dots, p_k)$  and  $C(t)$  is a time-dependent constant. Now, we will check the uniform integrability, i.e. for any  $\varepsilon > 0$ , by taking  $r = \varepsilon^{-1} (2\pi)^{3k} C(t)$  we have that

$$\frac{1}{(2\pi)^{3k}} \int \cdots \int_{|\mathbf{q}_k| + |\mathbf{p}_k| \geq r} (dq dp)^{\otimes k} m_{N,t}^{(k)} \leq \frac{1}{r} \frac{1}{(2\pi)^{3k}} \int \cdots \int (dq dp)^{\otimes k} (|\mathbf{q}_k| + |\mathbf{p}_k|) m_{N,t}^{(k)} \leq \varepsilon. \quad (3.2.18)$$

Furthermore, for arbitrary  $\varepsilon > 0$ , by taking  $\delta = \varepsilon$ , we have that for all  $E \subset \mathbb{R}^{6k}$  with  $\text{Vol}(E) \leq \delta$ , it holds

$$\int \cdots \int_E m_{N,t}^{(k)} \leq \left\| m_{N,t}^{(k)} \right\|_{L^\infty} \text{Vol}(E) \leq \varepsilon,$$

which means that there is no concentration for the  $k$ -particle Husimi measure.

It is shown in Lemma 2.2.2 that the boundedness of  $k$ -particle Husimi measure in  $L^1$ , i.e.

$$\left\| m_{N,t}^{(k)} \right\|_{L^1} \leq (2\pi)^{3k}.$$

Then applying directly Dunford-Pettis Theorem one obtain that  $k$ -particle Husimi measure is weakly compact in  $L^1$ . ■

**Proof of Theorem 3.1.1 and Corollary 3.1.1.** Cantor's diagonal procedure shows that we can take the same convergent subsequence of  $m_{N,t}^{(k)}$  for all  $k \geq 1$ . Then by the error estimates obtained in Propositions

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<sup>1</sup>See Theorem 4.30 in [Bre10] for more details.

3.2.4, 3.2.5, and 3.2.6, we can obtain that the limit satisfies the infinite hierarchy (3.1.3) in the sense of distribution, by directly taking the limit in the weak formulation of (3.2.1) and (3.2.3).

Observe that the estimates for the remainder terms also show that any convergent subsequence of  $m_{N,t}^{(k)}$  converges weakly in  $L^1$  to the solution of the infinite hierarchy. Therefore, if the infinite hierarchy has a unique solution, then the sequence  $m_{N,t}^{(k)}$  itself converges weakly to the solution of the infinite hierarchy.

As for Corollary 3.1.1, one only need to combine the facts that the infinite hierarchy has a unique solution and that the tensor products of the solution of the Vlasov equation (3.1.1),  $m_t^{\otimes k}$  is a solution of the infinite hierarchy.

Lastly, by Theorem 7.12 in [Vil03], we would obtain the convergence in 1-Wasserstein metric.  $\blacksquare$

### 3.3 Completion of the reformulation and estimates in the proof

#### 3.3.1 Proof of the reformulation in section 3.2.1

In this subsection we supply the proofs for the reformulation of Schrödinger equation into a hierarchy of  $k$  ( $1 \leq k \leq N$ ) particle Husimi measure. The reformulation shares similar structure to the classical BBGKY hierarchy.

*Proof of Proposition 3.2.1.* First, observe that taking the time derivative on the Husimi measure, we have

$$\begin{aligned}
& 2i\hbar\partial_t m_{N,t}^{(1)}(q_1, p_1) \\
&= \left( \hbar^2 \iiint dw du dx f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \nabla_x a_x^* \nabla_x a_x \Psi_{N,t} \rangle \right. \\
&\quad \left. - \hbar^2 \iiint dw du dx \overline{f_{q_1, p_1}^\hbar(w)} f_{q_1, p_1}^\hbar(u) \langle \Psi_{N,t}, \nabla_x a_x^* \nabla_x a_x a_u^* a_w \Psi_{N,t} \rangle \right) \\
&\quad + \left( \frac{1}{N} \iint dw du \iint dx dy f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, V(x-y) a_w^* a_u a_x^* a_y^* a_y a_x \Psi_{N,t} \rangle \right. \\
&\quad \left. - \frac{1}{N} \iint dw du \iint dx dy \overline{f_{q_1, p_1}^\hbar(w)} f_{q_1, p_1}^\hbar(u) \langle \Psi_{N,t}, V(x-y) a_x^* a_y^* a_y a_x a_u^* a_w \Psi_{N,t} \rangle \right) \\
&=: I_1 + II_1.
\end{aligned}$$

Now, focus on  $I_1$ , we have

$$\begin{aligned}
I_1 &= \hbar^2 \iiint dw du dx f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, a_w^* a_u \nabla_x a_x^* \nabla_x a_x \Psi_{N,t} \rangle \\
&\quad - \hbar^2 \iiint dw du dx f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N,t}, \nabla_x a_x^* \nabla_x a_x a_w^* a_u \Psi_{N,t} \rangle,
\end{aligned}$$

where the last equality is just change of variable on the complex conjugate term. Then, from CAR, observe

we have that

$$\begin{aligned}
-a_w^* a_u a_x^* \Delta_x a_x &= a_w^* a_x^* a_u \Delta_x a_x - \delta_{u=x} a_w^* \Delta_x a_x \\
&= a_x^* a_w^* \Delta_x a_x a_u - \delta_{u=x} a_w^* \Delta_x a_x \\
&= \Delta_x a_x^* a_w^* a_x a_u - \delta_{u=x} a_w^* \Delta_x a_x \\
&= -\Delta_x a_x^* a_x a_w^* a_u + \delta_{w=x} \Delta_x a_x^* a_u - \delta_{u=x} a_w^* \Delta_x a_x,
\end{aligned}$$

where integration by parts and CAR of the operator have been used several times. Putting this back, we cancel out the the second term and get

$$\begin{aligned}
I_1 &= \hbar^2 \iiint dw du dx f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N, t}, (\delta_{w=x} \Delta_x a_x^* a_u - \delta_{u=x} a_w^* \Delta_x a_x) \Psi_{N, t} \rangle \\
&= \hbar^2 \iint dw du \left( \Delta_w f_{q_1, p_1}^\hbar(w) \right) \overline{f_{q_1, p_1}^\hbar(u)} \langle \Psi_{N, t}, a_w^* a_u \Psi_{N, t} \rangle \\
&\quad - \hbar^2 \iint dw du f_{q_1, p_1}^\hbar(w) \left( \Delta_u \overline{f_{q_1, p_1}^\hbar(u)} \right) \langle \Psi_{N, t}, a_w^* a_u \Psi_{N, t} \rangle.
\end{aligned} \tag{3.3.1}$$

Now, observe the following

$$\begin{aligned}
\nabla_u \overline{f_{q_1, p_1}^\hbar(u)} &= \nabla_u \left( \hbar^{-\frac{3}{4}} f \left( \frac{u - q_1}{\sqrt{\hbar}} \right) e^{-\frac{i}{\hbar} p_1 \cdot u} \right) \\
&= \hbar^{-\frac{3}{4}} \nabla_u f \left( \frac{u - q_1}{\sqrt{\hbar}} \right) e^{-\frac{i}{\hbar} p_1 \cdot u} + \hbar^{-\frac{3}{4}} f \left( \frac{u - q_1}{\sqrt{\hbar}} \right) \nabla_u e^{-\frac{i}{\hbar} p_1 \cdot u} \\
&= -\hbar^{-\frac{3}{4}} \nabla_{q_1} f \left( \frac{u - q_1}{\sqrt{\hbar}} \right) e^{-\frac{i}{\hbar} p_1 \cdot u} - i \hbar^{-1} p_1 \cdot \hbar^{-\frac{3}{4}} f \left( \frac{u - q_1}{\sqrt{\hbar}} \right) e^{-\frac{i}{\hbar} p_1 \cdot u} \\
&= (-\nabla_{q_1} - i \hbar^{-1} p_1) \overline{f_{q_1, p_1}^\hbar(u)},
\end{aligned}$$

and furthermore,

$$\begin{aligned}
\Delta_u \overline{f_{q_1, p_1}^\hbar(u)} &= \nabla_u \cdot \nabla_u \overline{f_{q_1, p_1}^\hbar(u)} \\
&= \nabla_u \cdot (-\nabla_{q_1} - i \hbar^{-1} p_1) \overline{f_{q_1, p_1}^\hbar(u)} \\
&= (-\nabla_{q_1} - i \hbar^{-1} p_1) \cdot (-\nabla_{q_1} - i \hbar^{-1} p_1) \overline{f_{q_1, p_1}^\hbar(u)} \\
&= \left( \Delta_{q_1} + 2i \hbar^{-1} p_1 \cdot \nabla_{q_1} - \hbar^{-2} p_1^2 \right) \overline{f_{q_1, p_1}^\hbar(u)}.
\end{aligned} \tag{3.3.2}$$

and similarly

$$\Delta_w f_{q_1, p_1}^\hbar(w) = \left( \Delta_{q_1} - 2i \hbar^{-1} p_1 \cdot \nabla_{q_1} - \hbar^{-2} p_1^2 \right) f_{q_1, p_1}^\hbar(w), \tag{3.3.3}$$

we obtain by putting these back into (3.3.1),

$$\begin{aligned}
I_1 = & \hbar^2 \left[ \left\langle \Delta_{q_1} \int dw \overline{f_{q_1,p_1}^\hbar(w)} a_w \Psi_{N,t}, \int du \overline{f_{q_1,p_1}^\hbar(u)} a_u \Psi_{N,t} \right\rangle \right. \\
& - \left\langle \int dw \overline{f_{q_1,p_1}^\hbar(w)} a_w \Psi_{N,t}, \Delta_{q_1} \int du \overline{f_{q_1,p_1}^\hbar(u)} a_u \Psi_{N,t} \right\rangle \Big] \\
& - 2i\hbar p_1 \cdot \left[ \left\langle \nabla_{q_1} \int dw \overline{f_{q_1,p_1}^\hbar(w)} a_w \Psi_{N,t}, \int du \overline{f_{q_1,p_1}^\hbar(u)} a_u \Psi_{N,t} \right\rangle \right. \\
& \left. + \left\langle \int dw \overline{f_{q_1,p_1}^\hbar(w)} a_w \Psi_{N,t}, \nabla_{q_1} \int du \overline{f_{q_1,p_1}^\hbar(u)} a_u \Psi_{N,t} \right\rangle \right] \\
= & 2i\hbar^2 \operatorname{Im} \langle \Delta_{q_1} a(f_{q_1,p_1}^\hbar) \Psi_{N,t}, a(f_{q_1,p_1}^\hbar) \Psi_{N,t} \rangle - 2i\hbar p_1 \cdot \nabla_{q_1} m_{N,t}^{(1)}(q_1, p_1).
\end{aligned} \tag{3.3.4}$$

Since the Husimi measure is actually a real-valued function, we have that

$$\partial_t m_{N,t}^{(1)}(q_1, p_1) + p_1 \cdot \nabla_{q_1} m_{N,t}^{(1)}(q_1, p_1) = \operatorname{Re} \left( \frac{II_1}{2i\hbar} \right) + \hbar \operatorname{Im} \langle \Delta_{q_1} a(f_{q_1,p_1}^\hbar) \Psi_{N,t}, a(f_{q_1,p_1}^\hbar) \Psi_{N,t} \rangle. \tag{3.3.5}$$

Now, we turn our focus on  $II_1$ , i.e.,

$$\begin{aligned}
II_1 = & \frac{1}{N} \iint dw du \iint dx dy \overline{f_{q_1,p_1}^\hbar(w)} f_{q_1,p_1}^\hbar(u) \langle \Psi_{N,t}, V(x-y) a_w^* a_u^* a_x^* a_y^* a_y a_x \Psi_{N,t} \rangle \\
& - \frac{1}{N} \iint dw du \iint dx dy \overline{f_{q_1,p_1}^\hbar(w)} f_{q_1,p_1}^\hbar(u) \langle \Psi_{N,t}, V(x-y) a_x^* a_y^* a_y a_x a_u^* a_w \Psi_{N,t} \rangle.
\end{aligned}$$

Observe that

$$\begin{aligned}
a_w^* a_u^* a_x^* a_y^* a_y a_x &= a_x^* a_y^* a_y a_x a_w^* a_u \\
&+ \delta_{w=y} a_x^* a_y^* a_x a_u - \delta_{w=x} a_x^* a_y^* a_y a_u \\
&+ \delta_{u=x} a_w^* a_y^* a_y a_x - \delta_{u=y} a_w^* a_x^* a_y a_x.
\end{aligned}$$

The first term and the complex conjugate term vanishes under changes of variable,  $u$  to  $w$  and  $w$  to  $u$ .

Therefore, since from assumption  $V(x) = V(-x)$ , we have

$$\begin{aligned}
II_1 &= \frac{1}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \langle \Psi_{N, t}, V(x-w) a_x^* a_w^* a_x a_u \Psi_{N, t} \rangle \\
&\quad - \frac{1}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \langle \Psi_{N, t}, V(x-u) a_w^* a_x^* a_u a_x \Psi_{N, t} \rangle \\
&\quad + \frac{1}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \langle \Psi_{N, t}, V(u-y) a_w^* a_y^* a_y a_u \Psi_{N, t} \rangle \\
&\quad - \frac{1}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \langle \Psi_{N, t}, V(w-y) a_w^* a_y^* a_y a_u \Psi_{N, t} \rangle \\
&= \frac{1}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \left( V(u-x) - V(w-x) \right) \langle \Psi_{N, t}, a_w^* a_x^* a_x a_u \Psi_{N, t} \rangle \\
&\quad + \frac{1}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \left( V(u-y) - V(w-y) \right) \langle \Psi_{N, t}, a_w^* a_y^* a_y a_u \Psi_{N, t} \rangle \\
&= \frac{2}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \left( V(u-y) - V(w-y) \right) \langle \Psi_{N, t}, a_w^* a_y^* a_y a_u \Psi_{N, t} \rangle.
\end{aligned} \tag{3.3.6}$$

Now, note that mean value theorem gives

$$V(u-y) - V(w-y) = \int_0^1 ds \nabla V(s(u-y) + (1-s)(w-y)) \cdot (u-w), \tag{3.3.7}$$

and observe that since,  $V(s(u-y) + (1-s)(w-y)) = V(su + (1-s)w - y)$ , we can have from (3.3.6) the following

$$\begin{aligned}
II_1 &= \frac{2}{N} \iiint dw dx dy f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \left( \int_0^1 ds \nabla V(su + (1-s)w - y) \right) \cdot (u-w) \cdot \\
&\quad \langle \Psi_{N, t}, a_w^* a_y^* a_y a_u \Psi_{N, t} \rangle \\
&= \frac{2i\hbar}{N} \iiint dw dx dy \int_0^1 ds \nabla V(su + (1-s)w - y) \cdot \nabla_{p_1} \left( f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \right) \langle \Psi_{N, t}, a_w^* a_y^* a_y a_u \Psi_{N, t} \rangle \\
&= \frac{2i\hbar}{N} \iiint dw dx dy \int_0^1 ds \nabla V(su + (1-s)w - y) \cdot \nabla_{p_1} \left( f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \right) \langle a_w a_y \Psi_{N, t}, a_u a_y \Psi_{N, t} \rangle,
\end{aligned} \tag{3.3.8}$$

where we use the fact that

$$\nabla_{p_1} \left( f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \right) = \frac{i}{\hbar} (w-u) \cdot f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)}. \tag{3.3.9}$$

Then we get

$$II_1 = \frac{2i\hbar}{N} \iiint dw dx dy \int_0^1 ds \nabla V(su + (1-s)w - y) \cdot \nabla_{p_1} \left( f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} \right) \langle a_w a_y \Psi_{N, t}, a_u a_y \Psi_{N, t} \rangle. \tag{3.3.10}$$

Applying the following projection

$$\frac{1}{(2\pi\hbar)^3} \iint dq_2 dp_2 |f_{q_2, p_2}^\hbar\rangle \langle f_{q_2, p_2}^\hbar| = \mathbb{1}, \quad (3.3.11)$$

onto  $a_y \Psi_{N,t}$ , we get

$$a_y \Psi_{N,t} = \frac{1}{(2\pi\hbar)^3} \iint dq_2 dp_2 f_{q_2, p_2}^\hbar(y) \int dv \overline{f_{q_2, p_2}^\hbar(v)} a_v \Psi_{N,t}.$$

Putting this back into (3.3.10), we get the following

$$\begin{aligned} II_1 = & \frac{2i\hbar}{N} \frac{1}{(2\pi\hbar)^3} \iint dw du \iint dy dv \iint dq_2 dp_2 \int_0^1 ds \nabla V(su + (1-s)w - y) \\ & \cdot \nabla_{p_1} \left( f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \right) f_{q_2, p_2}^\hbar(y) \overline{f_{q_2, p_2}^\hbar(v)} \langle a_w a_y \Psi_{N,t}, a_u a_v \Psi_{N,t} \rangle. \end{aligned} \quad (3.3.12)$$

Recall that  $\hbar^3 = N^{-1}$ , we have

$$\begin{aligned} II_1 = & \frac{2i\hbar}{(2\pi)^3} \iint dw du \iint dy dv \iint dq_2 dp_2 \int_0^1 ds \nabla V(su + (1-s)w - y) \\ & \cdot \nabla_{p_1} \left( f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \right) f_{q_2, p_2}^\hbar(y) \overline{f_{q_2, p_2}^\hbar(v)} \langle a_w a_y \Psi_{N,t}, a_u a_v \Psi_{N,t} \rangle. \end{aligned} \quad (3.3.13)$$

Therefore, we have the last term in (3.3.5) as

$$\begin{aligned} \text{Re} \frac{II_1}{2i\hbar} = & \frac{1}{(2\pi)^3} \text{Re} \iint dw du \iint dy dv \iint dq_2 dp_2 \int_0^1 ds \nabla V(su + (1-s)w - y) \\ & \cdot \nabla_{p_1} \left( f_{q_1, p_1}^\hbar(w) \overline{f_{q_1, p_1}^\hbar(u)} \right) f_{q_2, p_2}^\hbar(y) \overline{f_{q_2, p_2}^\hbar(v)} \langle a_w a_y \Psi_{N,t}, a_u a_v \Psi_{N,t} \rangle, \end{aligned}$$

thus we have derived the equation for  $m_{N,t}^{(1)}(q_1, p_1)$ . ■

We have proved the reformulation from Schrödinger equation into 1-particle Husimi measure. We also observed that it contains a resemblance to the classical Vlasov equation. Next we want to prove the similar result for  $2 \leq k \leq N$ .

*Proof of Proposition 3.2.2.* Now we focus on the case where  $2 \leq k \leq N$ . As in the proof for the case of  $k = 1$ , we first observe that for every  $k \in \mathbb{N}$ ,

$$\begin{aligned} & 2i\hbar \partial_t m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\ = & \left( -\hbar^2 \int \dots \int (dw du)^{\otimes k} \int dx \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes k} \Delta_x \langle \Psi_{N,t}, a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_x \Psi_{N,t} \rangle \right. \\ & \left. + \hbar^2 \int \dots \int (dw du)^{\otimes k} \int dx \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes k} \Delta_x \langle \Psi_{N,t}, a_x^* a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} \Psi_{N,t} \rangle \right) \end{aligned}$$

$$\begin{aligned}
& + \left( \frac{1}{N} \int \dots \int (dw du)^{\otimes k} \iint dx dy V(x-y) \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \langle \Psi_{N,t}, a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_y^* a_y a_x \Psi_{N,t} \rangle \right. \\
& \left. - \frac{1}{N} \int \dots \int (dw du)^{\otimes k} \iint dx dy V(x-y) \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \langle \Psi_{N,t}, a_x^* a_y^* a_y a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} \Psi_{N,t} \rangle \right) \\
& =: I_2 + II_2,
\end{aligned} \tag{3.3.14}$$

where the tensor product denotes  $(dw du)^{\otimes k} = dw_1 \dots dw_k du_1 \dots du_k$ .

We first focus on the  $I_2$  part of (3.3.14), i.e.,

$$\begin{aligned}
I_2 = & -\hbar^2 \int \dots \int (dw du)^{\otimes k} \int dx \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \Delta_x \langle \Psi_{N,t}, a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_x \Psi_{N,t} \rangle \\
& + \hbar^2 \int \dots \int (dw du)^{\otimes k} \int dx \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \Delta_x \langle \Psi_{N,t}, a_x^* a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} \Psi_{N,t} \rangle.
\end{aligned} \tag{3.3.15}$$

Observe that we have

$$\begin{aligned}
a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_x = & (-1)^{4k} a_x^* a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} \\
& + a_x^* \left( \sum_{j=1}^k (-1)^j \delta_{x=w_j} a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^* \right) a_{u_k} \dots a_{u_1} \\
& - a_{w_1}^* \dots a_{w_k}^* \left( \sum_{j=1}^k (-1)^j \delta_{x=u_j} a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1} \right) a_x,
\end{aligned} \tag{3.3.16}$$

where the *hat* indicates exclusion of that element.

Putting this back into (3.3.15), we obtain

$$\begin{aligned}
I_2 = & \hbar^2 \int \dots \int (dw du)^{\otimes k} \int dx \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \cdot \Delta_x \left\langle \Psi_{N,t}, a_{w_1}^* \dots a_{w_k}^* \left( \sum_{j=1}^k (-1)^j \delta_{x=u_j} a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1} \right) a_x \Psi_{N,t} \right\rangle \\
& - \hbar^2 \int \dots \int (dw du)^{\otimes k} \int dx \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \cdot \Delta_x \left\langle \Psi_{N,t}, a_x^* \left( \sum_{j=1}^k (-1)^j \delta_{x=w_j} a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^* \right) a_{u_k} \dots a_{u_1} \Psi_{N,t} \right\rangle \\
= & \hbar^2 \sum_{j=1}^k (-1)^j \int \dots \int (dw du)^{\otimes k} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \cdot \left( \Delta_{u_j} \langle \Psi_{N,t}, a_{w_1}^* \dots a_{w_k}^* (a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1}) a_{u_j} \Psi_{N,t} \rangle \right. \\
& \left. - \Delta_{w_j} \langle \Psi_{N,t}, a_{w_j}^* (a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^*) a_{u_k} \dots a_{u_1} \Psi_{N,t} \rangle \right).
\end{aligned} \tag{3.3.17}$$



Note that, if we want to move the missing  $a_{u_j}$  or  $a_{w_j}^*$  back to their original position after applying the delta function, we have for fixed  $j$

$$\begin{aligned} (-1)^j a_{w_1}^* \cdots a_{w_k}^* [a_{u_k} \cdots \widehat{a_{u_j}} \cdots a_{u_1}] a_{u_j} &= \frac{(-1)^j}{(-1)^{j-1}} a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \\ &= (-1)^1 a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1}, \\ (-1)^j a_{w_j}^* [a_{w_1}^* \cdots \widehat{a_{w_j}^*} \cdots a_{w_k}^*] a_{u_k} \cdots a_{u_1} &= (-1)^1 a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1}. \end{aligned}$$

Therefore, continuing from (3.3.17), we have

$$I_2 = -\hbar^2 \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} [\Delta_{u_j} - \Delta_{w_j}] \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle. \quad (3.3.18)$$

Now, by integration by parts on (3.3.18) and note that the Laplacian acting on the coherent state would be similar to (3.3.2) and (3.3.3), i.e., for fixed  $j$  where  $1 \leq j \leq k$

$$\begin{aligned} \Delta_{u_j} \left( \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} &= (\Delta_{q_j} + 2i\hbar^{-1} p_j \cdot \nabla_{q_j} - \hbar^{-2} p_j^2) \left( \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k}, \\ \Delta_{w_j} \left( f_{q,p}^{\hbar}(w) \right)^{\otimes k} &= (\Delta_{q_j} - 2i\hbar^{-1} p_j \cdot \nabla_{q_j} - \hbar^{-2} p_j^2) \left( f_{q,p}^{\hbar}(w) \right)^{\otimes k}. \end{aligned}$$

Thus, we have similar for when  $k = 1$ , the kinetic part as

$$\begin{aligned} I_2 &= -2i\hbar \sum_{j=1}^k p_j \cdot \nabla_{q_j} \int \cdots \int (dw du)^{\otimes k} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \langle \Psi_{N,t}, a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle \\ &\quad + 2\hbar^2 \operatorname{Im} \sum_{j=1}^k \langle \Delta_{q_j} a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t}, a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t} \rangle \\ &= -2i\hbar \mathbf{p}_k \cdot \nabla_{\mathbf{q}_k} \langle a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t}, a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t} \rangle \\ &\quad + 2i\hbar^2 \operatorname{Im} \sum_{j=1}^k \langle \Delta_{q_j} a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t}, a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t} \rangle. \end{aligned} \quad (3.3.19)$$

Therefore it follows that

$$\begin{aligned} I_2 &= -2i\hbar \mathbf{p}_k \cdot \nabla_{\mathbf{q}_k} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\ &\quad + 2i\hbar^2 \operatorname{Im} \sum_{j=1}^k \langle \Delta_{q_j} a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t}, a(f_{q_k,p_k}^{\hbar}) \cdots a(f_{q_1,p_1}^{\hbar}) \Psi_{N,t} \rangle. \end{aligned} \quad (3.3.20)$$

Now, we turn our focus on part  $II_2$  of (3.3.14),

$$\begin{aligned}
& II_2 \\
&= \frac{1}{N} \int \dots \int (dw du)^{\otimes k} \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes k} \iint dx dy V(x-y) \langle \Psi, a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_y^* a_y a_x \Psi \rangle \\
&\quad - \frac{1}{N} \int \dots \int (dw du)^{\otimes k} \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes k} \iint dx dy V(x-y) \langle \Psi, a_x^* a_y^* a_y a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} \Psi \rangle.
\end{aligned} \tag{3.3.21}$$

For  $1 \leq k \leq N$ , observe that from the CAR, we have

$$\begin{aligned}
& a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_y^* a_y a_x - (-1)^{8k} a_x^* a_y^* a_y a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} \\
&= -a_{w_1}^* \dots a_{w_k}^* \left( \sum_{j=1}^k (-1)^j \delta_{x=u_j} a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1} \right) a_y^* a_y a_x \\
&\quad - a_x^* a_{w_1}^* \dots a_{w_k}^* \left( \sum_{j=1}^k (-1)^j \delta_{y=u_j} a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1} \right) a_y a_x \\
&\quad + a_x^* a_y^* \left( \sum_{j=1}^k (-1)^j \delta_{y=w_j} a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^* \right) a_{u_k} \dots a_{u_1} a_x \\
&\quad + a_x^* a_y^* a_y \left( \sum_{j=1}^k (-1)^j \delta_{x=w_j} a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^* \right) a_{u_k} \dots a_{u_1}.
\end{aligned} \tag{3.3.22}$$

From (3.3.21), we have that

$$\begin{aligned}
& \iint dx dy V(x-y) (a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1} a_x^* a_y^* a_y a_x - a_x^* a_y^* a_y a_x a_{w_1}^* \dots a_{w_k}^* a_{u_k} \dots a_{u_1}) \\
&= \iint dx dy V(x-y) \left[ -a_{w_1}^* \dots a_{w_k}^* \left( \sum_{j=1}^k (-1)^j \delta_{x=u_j} a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1} \right) a_y^* a_y a_x \right. \\
&\quad - a_x^* a_{w_1}^* \dots a_{w_k}^* \left( \sum_{j=1}^k (-1)^j \delta_{y=u_j} a_{u_k} \dots \widehat{a_{u_j}} \dots a_{u_1} \right) a_y a_x \\
&\quad + a_x^* a_y^* a_y \left( \sum_{j=1}^k (-1)^j \delta_{x=w_j} a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^* \right) a_{u_k} \dots a_{u_1} \\
&\quad \left. + a_x^* a_y^* a_y \left( \sum_{j=1}^k (-1)^j \delta_{x=w_j} a_{w_1}^* \dots \widehat{a_{w_j}^*} \dots a_{w_k}^* \right) a_{u_k} \dots a_{u_1} \right] \\
&=: J_1 + J_2 + J_3 + J_4.
\end{aligned}$$

Note that summing  $J_1$  and  $J_4$ , we have

$$\begin{aligned}
J_1 + J_4 &= - \sum_{j=1}^k (-1)^j \int dy \left[ (V(u_j - y) a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots \widehat{a_{u_j}} \cdots a_{u_1} a_y^* a_y a_{u_j}) \right. \\
&\quad \left. - (V(w_j - y) a_{w_j}^* a_y^* a_{w_1}^* \cdots \widehat{a_{w_j}} \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1}) \right] \\
&= \sum_{j=1}^k \left[ \int dy V(u_j - y) a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} a_y^* a_y - V(0) a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \right] \\
&\quad - \sum_{j=1}^k \left[ \int dy V(w_j - y) a_y^* a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} - V(0) a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \right],
\end{aligned}$$

where the terms with  $V(0)$  cancel one another. For the remaining term, we use again CAR to obtain

$$\begin{aligned}
&= \sum_{j=1}^k \int dy (V(u_j - y) - V(w_j - y)) a_y^* a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} a_y \\
&\quad + \sum_{j=1}^k \sum_{i=1}^k (-1)^i \int dy V(u_j - y) \delta_{u_i=y} a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots \widehat{a_{u_i}} \cdots a_{u_1} a_y \\
&\quad - \sum_{j=1}^k \sum_{i=1}^k (-1)^i \int dy V(w_j - y) \delta_{w_i=y} a_y^* a_{w_1}^* \cdots \widehat{a_{w_i}^*} \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} \\
&= \sum_{j=1}^k \int dy (V(u_j - y) - V(w_j - y)) a_y^* a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} a_y \\
&\quad - \sum_{j=1}^k \sum_{i=1}^k (V(u_j - u_i) - V(w_j - w_i)) a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1}.
\end{aligned}$$

On the other hand, the sum of  $J_2$  and  $J_3$  yield

$$J_2 + J_3 = \sum_{j=1}^k \int dx (V(x - u_j) - V(x - w_j)) a_x^* a_{w_1}^* \cdots a_{w_k}^* a_{u_k} \cdots a_{u_1} a_x.$$

By change of variable and using the fact that  $V(-x) = V(x)$ , we have from (3.3.21) that

$$\begin{aligned}
H_2 &= \frac{2}{N} \int \cdots \int (dw du)^{\otimes k} \int dy \sum_{j=1}^k \left[ V(y - u_j) - V(w_j - y) \right] \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
&\quad \cdot \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t} \rangle \\
&\quad - \frac{1}{N} \int \cdots \int (dw du)^{\otimes k} \sum_{j \neq i}^k \left[ V(u_j - u_i) - V(w_j - w_i) \right] \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
&\quad \cdot \langle a_{w_k} \cdots a_{w_1} \Psi_{N,t}, a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle
\end{aligned} \tag{3.3.23}$$

Applying mean value theorem on the first term on right hand side, we have that

$$\begin{aligned}
& \frac{2}{N} \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \int dy (V(y - u_j) - V(w_j - y)) \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t} \rangle \\
& = \frac{2}{N} \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \int dy \left[ \int_0^1 ds \nabla V(su_j + (1-s)w_j - y) \right] \cdot (u_j - w_j) \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t} \rangle \\
& = \frac{2i\hbar}{N} \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \int dy \left[ \int_0^1 ds \nabla V(su_j + (1-s)w_j - y) \right] \cdot \nabla_{p_j} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t} \rangle.
\end{aligned} \tag{3.3.24}$$

As in the case of  $k = 1$ , we apply the projection (3.3.11) onto  $a_y \Psi_{N,t}$  and get further

$$\begin{aligned}
& \frac{2i\hbar}{N} \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \int dy \left[ \int_0^1 ds \nabla V(su_j + (1-s)w_j - y) \right] \cdot \nabla_{p_j} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} \mathbb{1} a_y \Psi_{N,t} \rangle \\
& = \frac{2i\hbar}{N} \frac{1}{(2\pi\hbar)^3} \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \int dy \left[ \int_0^1 ds \nabla V(su_j + (1-s)w_j - y) \right] \cdot \nabla_{p_j} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \iint d\tilde{q} d\tilde{p} f_{\tilde{q},\tilde{p}}^{\hbar}(y) \int dv \overline{f_{\tilde{q},\tilde{p}}^{\hbar}(v)} \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_v \Psi_{N,t} \rangle.
\end{aligned} \tag{3.3.25}$$

Therefore, dividing both equations by  $2i\hbar$ , we have the following equation

$$\begin{aligned}
& \partial_t m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) + \mathbf{p}_k \cdot \nabla_{\mathbf{q}_k} m_{N,t}^{(k)}(q_1, p_1, \dots, q_k, p_k) \\
& = \hbar \operatorname{Im} \sum_{j=1}^k \langle \Delta_{q_j} a(f_{q_k, p_k}^{\hbar}) \cdots a(f_{q_1, p_1}^{\hbar}) \Psi_{N,t}, a(f_{q_k, p_k}^{\hbar}) \cdots a(f_{q_1, p_1}^{\hbar}) \Psi_{N,t} \rangle \\
& \quad + \frac{1}{(2\pi)^3} \sum_{j=1}^k \int \cdots \int (dw du)^{\otimes k} \int dy \left[ \int_0^1 ds \nabla V(su_j + (1-s)w_j - y) \right] \cdot \nabla_{p_j} \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \iint d\tilde{q} d\tilde{p} f_{\tilde{q},\tilde{p}}^{\hbar}(y) \int dv \overline{f_{\tilde{q},\tilde{p}}^{\hbar}(v)} \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_v \Psi_{N,t} \rangle \\
& \quad + \frac{i\hbar^2}{2} \int \cdots \int (dw du)^{\otimes k} \sum_{j \neq i}^k \left[ V(u_j - u_i) - V(w_j - w_i) \right] \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \\
& \quad \cdot \langle a_{w_k} \cdots a_{w_1} \Psi_{N,t}, a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle.
\end{aligned} \tag{3.3.26}$$

for  $1 \leq k \leq N$ ,  $\mathbf{p}_k = (p_1, \dots, p_k)$  and recalling  $\hbar^3 = N^{-1}$ . At this point we finish the computation of the

hierarchy for Husimi measure. ■

### 3.3.2 Proof of the uniform estimates in section 3.2.3

This subsection provide the proof of estimates for the error terms that appeared in the equations for  $m_{N,t}^{(k)}$ . Note that in all the proofs below, we suppose, without loss of generality, that the test function  $\Phi \in C_0^\infty(\mathbb{R}^{6k})$  is factorized in phase-space by family of test functions in  $C_0^\infty(\mathbb{R}^3)$  space.

#### Proof of Proposition 3.2.4

*Proof.* For fixed  $k$ , we denote the vector  $\mathbf{x}_k = (x_1, \dots, x_k)$  for each  $x_j \in \mathbb{R}^3$  with  $j = 1, \dots, k$ . Then we estimate the integral as follows

$$\begin{aligned}
& \left| \int \dots \int (dq dp)^{\otimes k} \nabla_{\mathbf{q}_k} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \mathcal{R}_k \right| \\
& \leq \hbar \left| \sum_{j=1}^k \int \dots \int (dq dp)^{\otimes k} \nabla_{q_j} \Phi(q_1, p_1, \dots, q_k, p_k) \right. \\
& \quad \cdot \left. \langle \nabla_{q_j} (a(f_{q_k, p_k}^{\hbar}) \dots a(f_{q_1, p_1}^{\hbar})) \Psi_{N,t}, a(f_{q_k, p_k}^{\hbar}) \dots a(f_{q_1, p_1}^{\hbar}) \Psi_{N,t} \rangle \right| \\
& = \hbar^{1-\frac{3}{2}k} \left| \sum_{j=1}^k \int \dots \int (dq dp)^{\otimes k} \nabla_{q_j} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \int \dots \int (dw du)^{\otimes k} \prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_{\hbar}^c} + \chi_{(w_n - u_n) \in \Omega_{\hbar}} \right) \right. \\
& \quad \cdot \left. \nabla_{q_j} f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) e^{\frac{i}{\hbar} p_n \cdot (w_n - u_n)} \langle a_{w_k} \dots a_{w_1} \Psi_{N,t}, a_{u_k} \dots a_{u_1} \Psi_{N,t} \rangle \right| \\
& \leq \hbar^{1-\frac{3}{2}k} \sum_{j=1}^k \int \dots \int (dq dw du)^{\otimes k} \left| \int \dots \int (dp)^{\otimes k} \prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_{\hbar}} + \chi_{(w_n - u_n) \in \Omega_{\hbar}^c} \right) \nabla_{q_j} \Phi \cdot e^{\frac{i}{\hbar} p_n \cdot (w_n - u_n)} \right| \\
& \quad \cdot \left| \nabla_{q_j} f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) \right| \left| f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \|a_{w_k} \dots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \dots a_{u_1} \Psi_{N,t}\| \\
& = \hbar^{\frac{1}{2}-\frac{3}{2}k} \sum_{j=1}^k \int \dots \int (dq dw du)^{\otimes k} \left| \int \dots \int (dp)^{\otimes k} \prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_{\hbar}} + \chi_{(w_n - u_n) \in \Omega_{\hbar}^c} \right) \nabla_{q_j} \Phi \cdot e^{\frac{i}{\hbar} p_n \cdot (w_n - u_n)} \right| \\
& \quad \cdot \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{\hbar}}\right) \right| \\
& \quad \cdot \|a_{w_k} \dots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \dots a_{u_1} \Psi_{N,t}\|, \tag{3.3.27}
\end{aligned}$$

where  $\Omega_{\hbar}$  is defined as in (2.3.3) and used the fact that

$$\nabla_{q_j} f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) = -\frac{1}{\sqrt{\hbar}} \nabla f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right).$$

Now, the product term  $\prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_h} + \chi_{(w_n - u_n) \in \Omega_h^c} \right)$  in (3.3.27) includes a summation of  $C(k)$  terms of the following type

$$\chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h} \chi_{(w_{\ell+1} - u_{\ell+1}) \in \Omega_h^c} \cdots \chi_{(w_k - u_k) \in \Omega_h^c}, \quad (3.3.28)$$

where  $\ell \in \{1, \dots, k\}$ . Thus, to continue from (3.3.27), we have

$$\begin{aligned} & \left| \int \cdots \int (dq dp)^{\otimes k} \nabla_{\mathbf{q}_k} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \mathcal{R}_k \right| \\ & \leq C h^{\frac{1}{2} - \frac{3}{2}k} \sum_{j=1}^k \max_{0 \leq \ell \leq k} \int \cdots \int (dq dw du)^{\otimes k} \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{h}}\right) f\left(\frac{u_n - q_n}{\sqrt{h}}\right) \right| \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{h}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{h}}\right) \right| \\ & \quad \cdot \left| \int \cdots \int (dp)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h} \chi_{(w_{\ell+1} - u_{\ell+1}) \in \Omega_h^c} \cdots \chi_{(w_k - u_k) \in \Omega_h^c} \right) \nabla_{q_j} \Phi \cdot e^{\frac{i}{h} \mathbf{p}_k \cdot (\mathbf{w}_k - \mathbf{u}_k)} \right| \\ & \quad \cdot \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \\ & \leq C h^{\frac{1}{2} - \frac{3}{2}k} \sum_{j=1}^k \max_{0 \leq \ell \leq k} \int \cdots \int (dq dw du)^{\otimes k} \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{h}}\right) f\left(\frac{u_n - q_n}{\sqrt{h}}\right) \right| \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{h}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{h}}\right) \right| \\ & \quad \cdot \left| \int \cdots \int (dp)^{\otimes \ell} \chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h} e^{\frac{i}{h} \sum_{m=1}^\ell \mathbf{p}_m \cdot (\mathbf{w}_m - \mathbf{u}_m)} \right. \\ & \quad \cdot \left. \int \cdots \int (dp)^{\otimes (k-\ell)} \chi_{(w_{\ell+1} - u_{\ell+1}) \in \Omega_h^c} \cdots \chi_{(w_k - u_k) \in \Omega_h^c} e^{\frac{i}{h} \sum_{m=k-\ell}^\ell \mathbf{p}_m \cdot (\mathbf{w}_m - \mathbf{u}_m)} \nabla_{q_j} \Phi \right| \\ & \quad \cdot \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \end{aligned}$$

Applying Lemma 2.3.3 onto the  $(k - \ell)$  terms, we have

$$\begin{aligned} & \leq C \sum_{j=1}^k \max_{0 \leq \ell \leq k} h^{\frac{1}{2} - \frac{3}{2}k + (1-\alpha)(k-\ell)s} \int \cdots \int (dq dw du)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h} \right) \\ & \quad \cdot \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{h}}\right) f\left(\frac{u_n - q_n}{\sqrt{h}}\right) \right| \cdot \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{h}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{h}}\right) \right| \\ & \quad \cdot \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\|. \end{aligned}$$

For a fixed  $\ell$ , observe that since  $f$  is compact supported, by using Hölder's inequality in  $w$  and  $u$  variables, we have

$$\begin{aligned} & \int \cdots \int (dq dw du)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h} \right) \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{h}}\right) f\left(\frac{u_n - q_n}{\sqrt{h}}\right) \right| \\ & \quad \cdot \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{h}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{h}}\right) \right| \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \end{aligned}$$

$$\begin{aligned}
&= \int \cdots \int (dq dw du)^{\otimes k} (\chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h}) \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{h}}\right) f\left(\frac{u_n - q_n}{\sqrt{h}}\right) \right| \\
&\quad \cdot \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{h}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{h}}\right) \right| \prod_{m=1}^k \chi_{|w_m - q_m| \leq \sqrt{h}R} \chi_{|u_m - q_m| \leq \sqrt{h}R} \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \\
&\leq \int \cdots \int (dq)^{\otimes k} \left[ \int \cdots \int (dw du)^{\otimes k} (\chi_{(w_1 - u_1) \in \Omega_h} \cdots \chi_{(w_\ell - u_\ell) \in \Omega_h}) \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{h}}\right) f\left(\frac{u_n - q_n}{\sqrt{h}}\right) \right|^2 \right. \\
&\quad \cdot \left. \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{h}}\right) \right|^2 \left| f\left(\frac{u_j - q_j}{\sqrt{h}}\right) \right|^2 \right]^{\frac{1}{2}} \left[ \int \cdots \int (dw)^{\otimes k} \prod_{m=1}^k \chi_{|w_m - q_m| \leq \sqrt{h}R} \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\|^2 \right]^{\frac{1}{2}}.
\end{aligned}$$

By change of variables and then applying Lemma 2.3.2, we have

$$\begin{aligned}
&= h^{\frac{3}{2}k} \left[ \int \cdots \int (d\tilde{w} d\tilde{u})^{\otimes k} (\chi_{|\tilde{w}_1 - \tilde{u}_1| \leq h^{\alpha+\frac{1}{2}}} \cdots \chi_{|\tilde{w}_\ell - \tilde{u}_\ell| \leq h^{\alpha+\frac{1}{2}}}) \prod_{n \neq j}^k |f(\tilde{w}_n)| |f(\tilde{u}_n)|^2 \right. \\
&\quad \cdot \left. |\nabla f(\tilde{w}_j)|^2 |f(\tilde{u}_j)|^2 \right]^{\frac{1}{2}} \int \cdots \int (dq dw)^{\otimes k} \prod_{m=1}^k \chi_{|w_m - q_m| \leq \sqrt{h}R} \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\|^2 \\
&\leq \left[ \int \cdots \int (d\tilde{w} d\tilde{u})^{\otimes k} (\chi_{|\tilde{w}_1 - \tilde{u}_1| \leq h^{\alpha+\frac{1}{2}}} \cdots \chi_{|\tilde{w}_\ell - \tilde{u}_\ell| \leq h^{\alpha+\frac{1}{2}}}) \prod_{n \neq j}^k |f(\tilde{w}_n)| |f(\tilde{u}_n)|^2 |\nabla f(\tilde{w}_j)|^2 |f(\tilde{u}_j)|^2 \right]^{\frac{1}{2}}. \quad (3.3.29)
\end{aligned}$$

Observe now that by using Hölder inequality with respect to  $\tilde{u}$ , we get, for every  $1 \leq n \leq k$ ,

$$\begin{aligned}
&\int d\tilde{w}_n |f(\tilde{w}_n)|^2 \int d\tilde{u}_n \chi_{|\tilde{w}_n - \tilde{u}_n| \leq h^{\alpha+\frac{1}{2}}} |f(\tilde{u}_n)|^2 \\
&\leq \int d\tilde{w}_n |f(\tilde{w}_n)|^2 \left( \int d\tilde{u}_n \chi_{|\tilde{w}_n - \tilde{u}_n| \leq h^{\alpha+\frac{1}{2}}} \right)^{\frac{2}{3}} \left( \int d\tilde{u}_n |f(\tilde{u}_n)|^6 \right)^{\frac{1}{3}} \\
&\leq C h^{2\alpha+1} \left( \int d\tilde{w}_n |f(\tilde{w}_n)|^2 \right) \left( \int d\tilde{u}_n |f(\tilde{u}_n)|^6 \right)^{\frac{1}{3}} \\
&\leq C h^{2\alpha+1}, \quad (3.3.30)
\end{aligned}$$

where we have used the fact that  $f \in H^1$ , it is also embedded in the  $L^6$  space. Similarly,

$$\begin{aligned}
&\iint d\tilde{w}_j d\tilde{u}_j \chi_{|\tilde{w}_j - \tilde{u}_j| \leq h^{\alpha+\frac{1}{2}}} |\nabla f(\tilde{w}_j)|^2 |f(\tilde{u}_j)|^2 \\
&= \int d\tilde{w}_j |\nabla f(\tilde{w}_j)|^2 \int d\tilde{u}_j \chi_{|\tilde{w}_j - \tilde{u}_j| \leq h^{\alpha+\frac{1}{2}}} |f(\tilde{u}_j)|^2 \\
&\leq \int d\tilde{w}_j |\nabla f(\tilde{w}_j)|^2 \left( \int d\tilde{u}_j \chi_{|\tilde{w}_j - \tilde{u}_j| \leq h^{\alpha+\frac{1}{2}}} \right)^{\frac{2}{3}} \left( \int d\tilde{u}_j |f(\tilde{u}_j)|^6 \right)^{\frac{1}{3}} \\
&\leq C h^{2\alpha+1}.
\end{aligned}$$

Putting this back into (3.3.29), we have

$$\begin{aligned} & \int \dots \int (dq dw du)^{\otimes k} (\chi_{(w_1 - u_1) \in \Omega_{\hbar}} \dots \chi_{(w_{\ell} - u_{\ell}) \in \Omega_{\hbar}}) \prod_{n \neq j}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \\ & \cdot \left| \nabla f\left(\frac{w_j - q_j}{\sqrt{\hbar}}\right) \right| \left| f\left(\frac{u_j - q_j}{\sqrt{\hbar}}\right) \right| \|a_{w_k} \dots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \dots a_{u_1} \Psi_{N,t}\| \\ & \leq C \hbar^{(\alpha + \frac{1}{2})\ell}. \end{aligned}$$

Then, from (3.3.28), we have

$$\begin{aligned} \left| \int \dots \int (dq dp)^{\otimes k} \nabla_{\mathbf{q}_k} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \mathcal{R}_k \right| & \leq C \sum_{j=1}^k \max_{0 \leq \ell \leq k} \hbar^{\frac{1}{2} - \frac{3}{2}k + (1-\alpha)(k-\ell)s + (\alpha + \frac{1}{2})\ell} \\ & = Ck \max_{0 \leq \ell \leq k} \hbar^{\frac{1}{2} - \frac{3}{2}k + (1-\alpha)(k-\ell)s + (\alpha + \frac{1}{2})\ell}. \end{aligned} \quad (3.3.31)$$

Therefore, by picking  $s = \left\lceil \frac{1+2\alpha}{2(1-\alpha)} \right\rceil$  we arrive immediately that

$$\left| \int \dots \int (dq dp)^{\otimes k} \nabla_{\mathbf{q}_k} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \mathcal{R}_k \right| \leq C \hbar^{\frac{1}{2} + (\alpha-1)k}.$$

Therefore, for all  $\delta \ll 1$ , we choose  $\frac{1}{2} < \alpha < 1$  such that  $(\alpha - 1)k \leq -\delta$ . ■

### Proof of Proposition 3.2.5

*Proof.* Let  $\Phi$  be an arbitrary test function, then the remainder term  $\tilde{\mathcal{R}}_1$  can be written explicitly into

$$\begin{aligned} & \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \tilde{\mathcal{R}}_1 \right| \\ & = \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \left( \iint dw du \iint dy dv \iint dq_2 dp_2 \right. \right. \\ & \quad \cdot \left[ \int_0^1 ds \nabla V(su + (1-s)w - y) - \nabla V(q_1 - q_2) \right] \\ & \quad \cdot f_{q_1, p_1}^{\hbar}(w) \overline{f_{q_1, p_1}^{\hbar}(u)} f_{q_2, p_2}^{\hbar}(y) \overline{f_{q_2, p_2}^{\hbar}(v)} \langle a_w a_y \Psi_{N,t}, a_u a_v \Psi_{N,t} \rangle \Big) \Big| \\ & = \frac{1}{\hbar^3} \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \iint dw du \iint dy dv \iint dq_2 dp_2 \right. \\ & \quad \cdot \left[ \int_0^1 ds \nabla V(su + (1-s)w - y) - \nabla V(q_1 - q_2) \right] e^{\frac{i}{\hbar} p_1 \cdot (w-u)} e^{\frac{i}{\hbar} p_2 \cdot (y-v)} \\ & \quad \cdot f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} f\left(\frac{y - q_2}{\sqrt{\hbar}}\right) \overline{f\left(\frac{v - q_2}{\sqrt{\hbar}}\right)} \langle a_w a_y \Psi_{N,t}, a_u a_v \Psi_{N,t} \rangle \Big|. \end{aligned}$$



Then, utilizing (2.2.3), we may get

$$\begin{aligned}
& (2\pi)^3 \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \iint dw du \iint dy dq_2 \right. \\
& \quad \cdot \left[ \int_0^1 ds \nabla V(su + (1-s)w - y) - \nabla V(q_1 - q_2) \right] \\
& \quad \cdot f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} e^{\frac{i}{\hbar} p_1 \cdot (w - u)} \left| f\left(\frac{y - q_2}{\sqrt{\hbar}}\right) \right|^2 \langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle \Big| \\
& = (2\pi)^3 \hbar^{\frac{3}{2}} \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \iint dw du \iint dy d\tilde{q}_2 \right. \\
& \quad \cdot \left[ \int_0^1 ds \nabla V(su + (1-s)w - y) - \nabla V(q_1 - y + \sqrt{\hbar} \tilde{q}_2) \right] \\
& \quad \cdot f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} e^{\frac{i}{\hbar} p_1 \cdot (w - u)} |f(\tilde{q}_2)|^2 \langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle \Big|.
\end{aligned}$$

Then, we insert a term, namely  $\nabla V(q_1 - y)$  and use triangle inequality to obtain

$$\begin{aligned}
& \leq (2\pi)^3 \hbar^{\frac{3}{2}} \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \iint dw du \iint dy d\tilde{q}_2 \right. \\
& \quad \cdot \int_0^1 ds \left( \nabla V(su + (1-s)w - y) - \nabla V(q_1 - y) \right) \\
& \quad \cdot f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} e^{\frac{i}{\hbar} p_1 \cdot (w - u)} |f(\tilde{q}_2)|^2 \langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle \Big| \\
& + (2\pi)^3 \hbar^{\frac{3}{2}} \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \iint dw du \iint dy d\tilde{q}_2 \left( \nabla V(q_1 - y) - \nabla V(q_1 - y + \sqrt{\hbar} \tilde{q}_2) \right) \right. \\
& \quad \cdot f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} e^{\frac{i}{\hbar} p_1 \cdot (w - u)} |f(\tilde{q}_2)|^2 \langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle \Big| \\
& =: I_3 + II_3,
\end{aligned}$$

where we have used change of variable  $\sqrt{\hbar} \tilde{q}_2 = (y - q_2)$  in the second term above.

We first focus on  $II_3$ . We begin by splitting the integral on momentum, by using Lemma 2.3.3, it follows

$$\begin{aligned}
II_3 & = (2\pi)^3 \hbar^{\frac{3}{2}} \left| \iint dq_1 dp_1 \nabla_{p_1} \Phi(q_1, p_1) \cdot \iint dw du \iint dy d\tilde{q}_2 \left( \chi_{(w-u) \in \Omega_h^c} + \chi_{(w-u) \in \Omega_h} \right) \right. \\
& \quad \cdot \left( \nabla V(q_1 - y) - \nabla V(q_1 - y + \sqrt{\hbar} \tilde{q}_2) \right) f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} \\
& \quad \cdot e^{\frac{i}{\hbar} p_1 \cdot (w - u)} |f(\tilde{q}_2)|^2 \langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle \Big| \\
& \leq (2\pi)^3 \hbar^{\frac{3}{2} + \frac{1}{2}} \int dq_1 \iint dw du \int dy \left( \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w - u)} \chi_{(w-u) \in \Omega_h^c} \nabla_{p_1} \Phi(q_1, p_1) \right| \right. \\
& \quad \left. + \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w - u)} \chi_{(w-u) \in \Omega_h} \nabla_{p_1} \Phi(q_1, p_1) \right| \right) \cdot \left| f\left(\frac{w - q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u - q_1}{\sqrt{\hbar}}\right)} \right|
\end{aligned}$$

$$\begin{aligned}
& \cdot \left( \int d\tilde{q}_2 |\tilde{q}_2| |f(\tilde{q}_2)|^2 \right) |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \\
& \leq C h^{\frac{3}{2} + \frac{1}{2}} \int dq_1 \iint dw du \int dy \left( \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h^c} \nabla_{p_1} \Phi(q_1, p_1) \right| \right. \\
& \quad \left. + \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h} \nabla_{p_1} \Phi(q_1, p_1) \right| \right) \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \\
& \quad \cdot |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \\
& =: i_{31} + ii_{31},
\end{aligned} \tag{3.3.32}$$

where we used the fact that  $\nabla V$  is Lipschitz continuous,  $f$  has compact support, and the definition of  $\Omega_h$  in (2.3.3).

The next step is to use Lemmata 2.3.2 and 2.3.3 to bound the terms  $i_{31}$  and  $ii_{31}$ . Then we examine what the appropriate terms  $\alpha$  and  $s$  should be. By Lemma 2.3.3, we may bound the term  $i_{31}$ , i.e.,

$$\begin{aligned}
i_{31} & \leq C h^{\frac{3}{2} + \frac{1}{2} + (1-\alpha)s} \int dq_1 \iint dw du \int dy \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \\
& \leq C h^{\frac{3}{2} + \frac{1}{2} + (1-\alpha)s} \int dq_1 \iint dw du \int dy \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\|.
\end{aligned}$$

Since we assume that  $f$  is compactly supported, by Hölder inequality with respect to  $w$  and  $u$ , we have we have that

$$\begin{aligned}
i_{31} & \leq C h^{\frac{3}{2} + \frac{1}{2} + (1-\alpha)s} \int dq_1 \left( \iint dw du \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \right|^2 \left| f\left(\frac{u-q_1}{\sqrt{\hbar}}\right) \right|^2 \right)^{\frac{1}{2}} \\
& \quad \cdot \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \left( \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^2 \right)^{\frac{1}{2}} \\
& = C h^{3 + \frac{1}{2} + (1-\alpha)s} \int dq_1 \left( \int d\tilde{w} |f(\tilde{w})|^2 \right) \\
& \quad \cdot \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \left( \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^2 \right)^{\frac{1}{2}},
\end{aligned}$$

where we used the change of variable  $\sqrt{\hbar}\tilde{w} = w - q_1$  in the last inequality. Now, since  $\|f\|_2$  is normalized, we continue to have

$$\begin{aligned}
& \leq C h^{3 + \frac{1}{2} + (1-\alpha)s} \int dq_1 \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \left( \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^2 \right)^{\frac{1}{2}} \\
& \leq C h^{3 + \frac{1}{2} + (1-\alpha)s} \int dq_1 \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \left( \int dy \|a_w a_y \Psi_{N,t}\|^2 \right) \left( \int dy \|a_u a_y \Psi_{N,t}\|^2 \right) \right)^{\frac{1}{2}} \\
& = C h^{3 + \frac{1}{2} + (1-\alpha)s} \int dq_1 \iint dy dw \chi_{|w-q_1| \leq \sqrt{\hbar}R} \|a_w a_y \Psi_{N,t}\|^2
\end{aligned}$$

$$= C\hbar^{3+\frac{1}{2}+(1-\alpha)s} \int dy \iint dq_1 dw \left\langle a_y \Psi_{N,t}, \chi_{|w-q_1| \leq \sqrt{\hbar}R} a_w^* a_w a_y \Psi_{N,t} \right\rangle$$

by Lemma 2.3.2

$$\begin{aligned} i_{31} &\leq C\hbar^{3-\frac{3}{2}+\frac{1}{2}+(1-\alpha)s} \int dy \langle a_y \Psi_{N,t}, a_y \Psi_{N,t} \rangle \\ &= C\hbar^{(1-\alpha)s-1} \left\langle \Psi_{N,t}, \frac{\mathcal{N}}{N} \Psi_{N,t} \right\rangle \leq C\hbar^{(1-\alpha)s-1}. \end{aligned} \quad (3.3.33)$$

On the other hand, from  $ii_{31}$  we have

$$\begin{aligned} ii_{31} &\leq C\hbar^{\frac{3}{2}+\frac{1}{2}} \int dq_1 \iint dw du \int dy \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h} \nabla_{p_1} \Phi(q_1, p_1) \right| \\ &\quad \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \\ &\leq C\hbar^{\frac{3}{2}+\frac{1}{2}} \int dq_1 \iint dw du \int dy \int dp_1 \chi_{(w-u) \in \Omega_h} |\nabla_{p_1} \Phi(q_1, p_1)| \\ &\quad \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \\ &\leq C\hbar^{\frac{3}{2}+\frac{1}{2}} \int dq_1 \iint dw du \int dy \chi_{(w-u) \in \Omega_h} \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \end{aligned}$$

Since  $f$  is assumed to be compactly supported, we have

$$\begin{aligned} &\leq C\hbar^{\frac{3}{2}+\frac{1}{2}} \int dq_1 \left( \iint dw du \chi_{(w-u) \in \Omega_h} \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right|^2 \right)^{\frac{1}{2}} \\ &\quad \cdot \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \left( \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^2 \right)^{\frac{1}{2}}, \end{aligned}$$

where we use Cauchy-Schwarz inequality and Hölder inequality.

Next, by change of variables as well as Hölder inequality in respect of  $y$ , we have

$$\begin{aligned} &\leq C\hbar^{3+\frac{1}{2}} \left( \iint d\tilde{w} d\tilde{u} \chi_{|\tilde{w}-\tilde{u}| \leq \hbar^{\alpha+\frac{1}{2}}} \left| f(\tilde{w}) \overline{f(\tilde{u})} \right|^2 \right)^{\frac{1}{2}} \\ &\quad \cdot \int dy \iint dq_1 dw \chi_{|w-q_1| \leq \sqrt{\hbar}R} \langle a_y \Psi_{N,t}, a_w^* a_w a_y \Psi_{N,t} \rangle \\ &\leq C\hbar^{-1} \left( \int d\tilde{w} |f(\tilde{w})|^2 \int d\tilde{u} \chi_{|\tilde{w}-\tilde{u}| \leq \hbar^{\alpha+\frac{1}{2}}} |f(\tilde{u})|^2 \right)^{\frac{1}{2}}, \end{aligned} \quad (3.3.34)$$

where we applied Lemma 2.3.2. Observe from (3.3.30), we get

$$ii_{31} \leq C\hbar^{\alpha-\frac{1}{2}}.$$

Now we compare power of  $\hbar$  with the one in (3.3.33). Namely,

$$\alpha - \frac{1}{2} = (1 - \alpha)s - 1. \quad (3.3.35)$$

Therefore, we choose  $s = \left\lceil \frac{1+2\alpha}{2(1-\alpha)} \right\rceil$  such that  $II_3$  is of order  $\hbar^{\alpha-\frac{1}{2}}$ . Now, focus on  $I_3$ , we use similar strategy as with  $II_3$ .

$$\begin{aligned} I_3 &\leq C\hbar^{\frac{3}{2}} \int dq_1 \iint dw du \int dy \int_0^1 ds \left| \nabla V(su + (1-s)w - y) - \nabla V(q_1 - y) \right| \\ &\quad \cdot \left( \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h^c} \nabla_{p_1} \Phi(q_1, p_1) \right| + \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h} \nabla_{p_1} \Phi(q_1, p_1) \right| \right) \\ &\quad \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \left( \int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \right) |\langle a_w a_y \Psi_{N,t}, a_u a_y \Psi_{N,t} \rangle| \\ &\leq C\hbar^{\frac{3}{2}} \int dq_1 \iint dw du \int dy \int_0^1 ds |su + (1-s)w - q_1| \left( \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h^c} \nabla_{p_1} \Phi(q_1, p_1) \right| \right. \\ &\quad \left. + \left| \int dp_1 e^{\frac{i}{\hbar} p_1 \cdot (w-u)} \chi_{(w-u) \in \Omega_h} \nabla_{p_1} \Phi(q_1, p_1) \right| \right) \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \\ &\quad \cdot \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \\ &=: i_{32} + i\bar{i}_{32} \end{aligned} \quad (3.3.36)$$

Again, by Lemma 2.3.3 and the bounds for number operator and localized number operator, we have for  $i_{32}$  that

$$\begin{aligned} i_{32} &\leq C\hbar^{\frac{3}{2}+(1-\alpha)s} \int dq_1 \iint dw du \int_0^1 ds |su + (1-s)w - q_1| \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \\ &\quad \cdot \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \\ &\leq C\hbar^{3+\frac{1}{2}+(1-\alpha)s} \int dq_1 \left( \iint d\tilde{w} d\tilde{u} \int_0^1 ds |s\tilde{u} + (1-s)\tilde{w}|^2 \cdot \left| f(\tilde{w}) \overline{f(\tilde{u})} \right|^2 \right)^{\frac{1}{2}} \\ &\quad \cdot \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \left( \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^2 \right)^{\frac{1}{2}} \\ &\leq C\hbar^{3+\frac{1}{2}+(1-\alpha)s} \left( \iint d\tilde{w} d\tilde{u} \int_0^1 ds |s\tilde{u} + (1-s)\tilde{w}|^2 \cdot \left| f(\tilde{w}) \overline{f(\tilde{u})} \right|^2 \right)^{\frac{1}{2}} \\ &\quad \cdot \int dy \iint dq_1 dw \chi_{|w-q_1| \leq \sqrt{\hbar}R} \langle a_y \Psi_{N,t}, a_w^* a_w a_y \Psi_{N,t} \rangle \\ &\leq C\hbar^{(1-\alpha)s-1}, \end{aligned}$$

where we used Lemma 2.3.2 and the bounds for number operator. Similarly, for  $ii_{32}$ , we have

$$\begin{aligned}
ii_{32} &\leq C\hbar^{\frac{3}{2}} \int dq_1 \iint dw du \int dy \int_0^1 ds |su + (1-s)w - q_1| \int dp_1 |\chi_{(w-u) \in \Omega_h} \nabla_{p_1} \Phi(q_1, p_1)| \\
&\quad \cdot \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \\
&\leq C\hbar^{\frac{3}{2}} \int dq_1 \iint dw du \int dy \int_0^1 ds |su + (1-s)w - q_1| \chi_{(w-u) \in \Omega_h} \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right| \\
&\quad \cdot \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \\
&\leq C\hbar^{\frac{3}{2}} \int dq_1 \left( \iint dw du \int_0^1 ds |su + (1-s)w - q_1|^2 \left| f\left(\frac{w-q_1}{\sqrt{\hbar}}\right) \overline{f\left(\frac{u-q_1}{\sqrt{\hbar}}\right)} \right|^2 \chi_{(w-u) \in \Omega_h} \right)^{\frac{1}{2}} \\
&\quad \cdot \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^{\frac{1}{2}} \\
&\leq C\hbar^{3+\frac{1}{2}} \left( \iint d\tilde{w} d\tilde{u} \int_0^1 ds |s\tilde{u} + (1-s)\tilde{w}|^2 \left| f(\tilde{w}) \overline{f(\tilde{u})} \right|^2 \chi_{|\tilde{w}-\tilde{u}| \leq \hbar^{\alpha+\frac{1}{2}}} \right)^{\frac{1}{2}} \\
&\quad \cdot \int dq_1 \left( \iint dw du \chi_{|w-q_1| \leq \sqrt{\hbar}R} \chi_{|u-q_1| \leq \sqrt{\hbar}R} \int dy \|a_w a_y \Psi_{N,t}\| \|a_u a_y \Psi_{N,t}\| \right)^{\frac{1}{2}}.
\end{aligned}$$

By Lemma 2.3.2 and the bounds for number operator, we have

$$\leq C\hbar^{-1} \left( \iint d\tilde{w} d\tilde{u} \int_0^1 ds |s\tilde{u} + (1-s)\tilde{w}|^2 \left| f(\tilde{w}) \overline{f(\tilde{u})} \right|^2 \chi_{|\tilde{w}-\tilde{u}| \leq \hbar^{\alpha+\frac{1}{2}}} \right)^{\frac{1}{2}}.$$

Then, by using similar computation in (3.3.30) and the assumption that  $f$  is compactly supported, we may get

$$ii_{32} \leq C\hbar^{\alpha-\frac{1}{2}}.$$

Therefore,  $II_3$  and  $I_3$  together, we have the bound of order  $\hbar^{\alpha-\frac{1}{2}}$  for  $\alpha \in (\frac{1}{2}, 1)$ . ■

### Proof of Proposition 3.2.6

*Proof.* To calculate the bound in (3.2.16) for  $\widehat{\mathcal{R}}_k$ . It has automatically an  $1/N$  as a factor, therefore, we expect it has better estimates than the other remainder terms. More precisely, we can split the integrals as before,

$$\begin{aligned}
&\left| \frac{1}{2N} \int \dots \int (dq dp)^{\otimes k} (dw du)^{\otimes k} \Phi(q_1, p_1, \dots, q_k, p_k) \sum_{j \neq i}^k \left[ V(u_j - u_i) - V(w_j - w_i) \right] \right. \\
&\quad \cdot \left. \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \langle a_{w_k} \dots a_{w_1} \Psi_{N,t}, a_{u_k} \dots a_{u_1} \Psi_{N,t} \rangle \right|
\end{aligned}$$

$$\begin{aligned}
&= \left| \frac{1}{2N} \int \cdots \int (dq dp)^{\otimes k} (dw du)^{\otimes k} \Phi(q_1, p_1, \dots, q_k, p_k) \sum_{j \neq i}^k \left[ V(u_j - u_i) - V(w_j - w_i) \right] \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \right. \\
&\quad \cdot \left. \prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_{\hbar}^c} + \chi_{(w_n - u_n) \in \Omega_{\hbar}} \right) \langle a_{w_k} \cdots a_{w_1} \Psi_{N,t}, a_{u_k} \cdots a_{u_1} \Psi_{N,t} \rangle \right|,
\end{aligned}$$

where  $\Omega_{\hbar}$  is defined as in (2.3.3). Since  $V \in W^{2,\infty}$  and recall  $\hbar^3 = N^{-1}$ , we have

$$\begin{aligned}
&\leq C(k) \|V\|_{\infty} \hbar^{3-\frac{3}{2}k} \int \cdots \int (dq dw du)^{\otimes k} \prod_{n=1}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \\
&\quad \cdot \left| \prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_{\hbar}^c} + \chi_{(w_n - u_n) \in \Omega_{\hbar}} \right) \int \cdots \int (dp)^{\otimes k} e^{\frac{i}{\hbar} \sum_{m=1}^k p_m \cdot (w_m - u_m)} \Phi(q_1, \dots, p_k) \right| \\
&\leq C \hbar^{3-\frac{3}{2}k} \max_{0 \leq \ell \leq k} \int \cdots \int (dq dw du)^{\otimes k} \prod_{n=1}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \\
&\quad \cdot \left| \int \cdots \int (dp)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} \cdots \chi_{(w_{\ell} - u_{\ell}) \in \Omega_{\hbar}} \chi_{(w_{\ell+1} - u_{\ell+1}) \in \Omega_{\hbar}^c} \cdots \chi_{(w_k - u_k) \in \Omega_{\hbar}^c} \right) \nabla_{q_j} \Phi \cdot e^{\frac{i}{\hbar} \mathbf{p}_k \cdot (\mathbf{w}_k - \mathbf{u}_k)} \right| \\
&= C \hbar^{3-\frac{3}{2}k} \max_{0 \leq \ell \leq k} \int \cdots \int (dq dw du)^{\otimes k} \left| \int \cdots \int (dp)^{\otimes \ell} \chi_{(w_1 - u_1) \in \Omega_{\hbar}} \cdots \chi_{(w_{\ell} - u_{\ell}) \in \Omega_{\hbar}} e^{\frac{i}{\hbar} \sum_{m=1}^{\ell} p_m \cdot (w_m - u_m)} \right. \\
&\quad \cdot \left. \int \cdots \int (dp)^{\otimes (k-\ell)} \chi_{(w_{\ell+1} - u_{\ell+1}) \in \Omega_{\hbar}^c} \cdots \chi_{(w_k - u_k) \in \Omega_{\hbar}^c} e^{\frac{i}{\hbar} \sum_{m=\ell+1}^k p_m \cdot (w_m - u_m)} \nabla_{q_j} \Phi(q_1, p_1, \dots, q_k, p_k) \right| \\
&\quad \cdot \prod_{n=1}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\|,
\end{aligned}$$

where we apply similar argument in (3.3.28) in the last inequality. Note here that the constant  $C$  above is dependent on  $k$ . Applying Lemma 2.3.3 we have

$$\begin{aligned}
&\leq C \max_{0 \leq \ell \leq k} \hbar^{3-\frac{3}{2}k+(1-\alpha)(k-\ell)s} \int \cdots \int (dq dw du)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} \cdots \chi_{(w_{\ell} - u_{\ell}) \in \Omega_{\hbar}} \right) \\
&\quad \cdot \prod_{n=1}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \\
&= C \max_{0 \leq \ell \leq k} \hbar^{3-\frac{3}{2}k+(1-\alpha)(k-\ell)s} \int \cdots \int (dq dw du)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} \cdots \chi_{(w_{\ell} - u_{\ell}) \in \Omega_{\hbar}} \right) \\
&\quad \cdot \prod_{n=1}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| \chi_{|w_n - q_n| \leq \sqrt{\hbar}R} \chi_{|u_n - q_n| \leq \sqrt{\hbar}R} \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} \Psi_{N,t}\| \\
&\leq C \max_{0 \leq \ell \leq k} \hbar^{3-\frac{3}{2}k+(1-\alpha)(k-\ell)s} \int \cdots \int (dq)^{\otimes k} \left[ \int \cdots \int (dw du)^{\otimes k} \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} \cdots \chi_{(w_{\ell} - u_{\ell}) \in \Omega_{\hbar}} \right) \right. \\
&\quad \cdot \left. \prod_{n=1}^k \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right|^2 \right]^{\frac{1}{2}} \left[ \int \cdots \int (dw)^{\otimes k} \prod_{n=1}^k \chi_{|w_n - q_n| \leq \sqrt{\hbar}R} \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\|^2 \right] \\
&= C \max_{0 \leq \ell \leq k} \hbar^{3+(1-\alpha)(k-\ell)s} \int \cdots \int (dq)^{\otimes k} \left[ \int \cdots \int (d\tilde{w} d\tilde{u})^{\otimes k} \left( \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha+\frac{1}{2}}} \cdots \chi_{|\tilde{w}_{\ell} - \tilde{u}_{\ell}| \leq \hbar^{\alpha+\frac{1}{2}}} \right) \right]
\end{aligned}$$

$$\begin{aligned} & \cdot \prod_{n=1}^k |f(\tilde{w}_n) f(\tilde{u}_n)|^2 \Big]^\frac{1}{2} \left[ \int \cdots \int (dw)^{\otimes k} \prod_{n=1}^k \chi_{|w_n - q_n| \leq \sqrt{\hbar} R} \|a_{w_k} \cdots a_{w_1} \Psi_{N,t}\|^2 \right] \\ & \leq C \max_{0 \leq \ell \leq k} \hbar^{3 - \frac{3}{2}k + (1-\alpha)(k-\ell)s + (\alpha + \frac{1}{2})\ell}, \end{aligned}$$

where, as in the proof of Proposition 3.2.4, we applied Lemma 2.3.2 and (3.3.30). Therefore, we obtain the desired result by choosing  $s = \left\lceil \frac{1+2\alpha}{2(1-\alpha)} \right\rceil$ .

Next, we switch to estimate (3.2.17) for  $\tilde{\mathcal{R}}_k$ . Repeated the steps in the proof of Proposition 3.2.5, we have

$$\begin{aligned} & \left| \int \cdots \int (dq dp)^{\otimes k} \nabla_{\mathbf{p}_k} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \tilde{\mathcal{R}}_k \right| \\ &= \left| \sum_{j=1}^k \int \cdots \int (dq dp)^{\otimes k} (dw du)^{\otimes k} \nabla_{p_j} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \iint dy dv \iint dq_{k+1} dp_{k+1} \right. \\ & \quad \cdot \int_0^1 ds [\nabla V(su_j + (1-s)w_j - y) - \nabla V(q_j - y) + \nabla V(q_j - y) - \nabla V(q_j - q_{k+1})] \\ & \quad \cdot \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} f_{q_{k+1}, p_{k+1}}^{\hbar}(y) \overline{f_{q_{k+1}, p_{k+1}}^{\hbar}(v)} \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_v \Psi_{N,t} \rangle \Big|. \end{aligned}$$

Applying the  $\hbar$ -weighted Dirac-delta function as in (2.2.3), we have

$$\begin{aligned} &= (2\pi)^3 \hbar^{3 - \frac{3}{2}} \left| \sum_{j=1}^k \int \cdots \int (dq dp)^{\otimes k} (dw du)^{\otimes k} \nabla_{p_j} \Phi(q_1, p_1, \dots, q_k, p_k) \cdot \iint dy dq_{k+1} \right. \\ & \quad \cdot \int_0^1 ds [\nabla V(su_j + (1-s)w_j - y) - \nabla V(q_j - y) + \nabla V(q_j - y) - \nabla V(q_j - q_{k+1})] \\ & \quad \cdot \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes k} \left| f \left( \frac{y - q_{k+1}}{\sqrt{\hbar}} \right) \right|^2 \langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t} \rangle \Big| \\ &\leq (2\pi)^3 \hbar^{3 - \frac{3}{2}k} \sum_{j=1}^k \int \cdots \int (dq dw du)^{\otimes k} \prod_{n=1}^k \left| \int \cdots \int (dp)^{\otimes k} \nabla_{p_j} \Phi(q_1, p_1, \dots, q_k, p_k) e^{\frac{i}{\hbar} p_n \cdot (w_n - u_n)} \right| \iint dy d\tilde{q}_{k+1} \\ & \quad \cdot \left( \int_0^1 ds |\nabla V(su_j + (1-s)w_j - y) - \nabla V(q_j - y)| + |\nabla V(q_j - y) - \nabla V(q_j - y + \sqrt{\hbar} \tilde{q}_{k+1})| \right) \\ & \quad \cdot \left| f \left( \frac{w_n - q_n}{\sqrt{\hbar}} \right) f \left( \frac{u_n - q_n}{\sqrt{\hbar}} \right) \right| |f(\tilde{q}_{k+1})|^2 |\langle a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}, a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t} \rangle|. \end{aligned}$$

Using the fact that  $\nabla V$  is Lipchitz continuous and that  $f$  is compactly supported, we have

$$\begin{aligned} &\leq (2\pi)^3 \hbar^{3 - \frac{3}{2}k} \sum_{j=1}^k \int \cdots \int (dq dw du)^{\otimes k} \prod_{n=1}^k \left| \int \cdots \int (dp)^{\otimes k} \nabla_{p_j} \Phi(q_1, p_1, \dots, q_k, p_k) e^{\frac{i}{\hbar} p_n \cdot (w_n - u_n)} \right| \iint dy d\tilde{q}_{k+1} \\ & \quad \cdot \left( \int_0^1 ds |su_j + (1-s)w_j - q_j| + |\sqrt{\hbar} \tilde{q}_{k+1}| \right) \left| f \left( \frac{w_n - q_n}{\sqrt{\hbar}} \right) f \left( \frac{u_n - q_n}{\sqrt{\hbar}} \right) \right| |f(\tilde{q}_{k+1})|^2 \\ & \quad \cdot \chi_{|w_n - q_n| \leq \sqrt{\hbar} R} \chi_{|u_n - q_n| \leq \sqrt{\hbar} R} \|a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t}\| \end{aligned}$$

$$=: I_4 + II_4$$

Focusing on  $I_4$ , we split the integral as follows

$$\begin{aligned} I_4 = & (2\pi)^3 \hbar^{3-\frac{3}{2}k} \sum_{j=1}^k \int \cdots \int (dq dw du)^{\otimes k} \left| \prod_{n=1}^k \left( \chi_{(w_n - u_n) \in \Omega_h^c} + \chi_{(w_n - u_n) \in \Omega_h} \right) \int \cdots \int (dp)^{\otimes k} \nabla_{p_j} \Phi(q_1, p_1, \dots, q_k, p_k) \right. \\ & \cdot e^{\frac{i}{\hbar} \sum_{m=1}^k p_m \cdot (w_m - u_m)} \left| \iint dy d\tilde{q}_{k+1} \int_0^1 ds |su_j + (1-s)w_j - q_j| \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| |f(\tilde{q}_{k+1})|^2 \right. \\ & \cdot \chi_{|w_n - q_n| \leq \sqrt{\hbar}R} \chi_{|u_n - q_n| \leq \sqrt{\hbar}R} \|a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t}\|. \end{aligned}$$

where  $\Omega_h$  is defined as in (2.3.3). We do similar computations for  $II_4$ ,

$$\begin{aligned} II_4 = & (2\pi)^3 \hbar^{3-\frac{3}{2}k} \sum_{j=1}^k \int \cdots \int (dq dw du)^{\otimes k} \left| \prod_{n=1}^k \int \cdots \int (dp)^{\otimes k} \left( \chi_{(w_n - u_n) \in \Omega_h^c} + \chi_{(w_n - u_n) \in \Omega_h} \right) \nabla_{p_j} \Phi(q_1, p_1, \dots, q_k, p_k) \right. \\ & \cdot e^{\frac{i}{\hbar} p_n \cdot (w_n - u_n)} \left| \iint dy d\tilde{q}_{k+1} \left| \sqrt{\hbar} \tilde{q}_{k+1} \right| \left| f\left(\frac{w_n - q_n}{\sqrt{\hbar}}\right) f\left(\frac{u_n - q_n}{\sqrt{\hbar}}\right) \right| |f(\tilde{q}_{k+1})|^2 \right. \\ & \cdot \chi_{|w_n - q_n| \leq \sqrt{\hbar}R} \chi_{|u_n - q_n| \leq \sqrt{\hbar}R} \|a_{w_k} \cdots a_{w_1} a_y \Psi_{N,t}\| \|a_{u_k} \cdots a_{u_1} a_y \Psi_{N,t}\|. \end{aligned}$$

Repeating the proof of Proposition 3.2.5, namely in (3.3.36) and (3.3.32), as well as the proof for estimate (3.2.16), we eventually obtain

$$I_4 + II_4 \leq C \max_{0 \leq \ell \leq k} \hbar^{\frac{1}{2} - \frac{3}{2}k + (1-\alpha)(k-\ell)s + (\alpha + \frac{1}{2})\ell},$$

where the constant  $C$  depends on  $k$ . As before, we choose  $s = \left\lceil \frac{1+2\alpha}{2(1-\alpha)} \right\rceil$  and choose  $\alpha \in (\frac{1}{2}, 1)$  such that  $(\alpha - 1)k \leq -\delta$ , and we obtain the desired estimates.  $\blacksquare$



## Chapter 4

# Vlasov-Poisson equation

In this chapter we study the convergence from Schrödinger equation to Vlasov-Poisson equation by considering the following mollification of repulsive Coulomb potential,

**Assumption H3.** For any  $x \in \mathbb{R}^3$ , let  $V(x) = |x|^{-1}$  and its mollification given by

$$V_N(x) = (V * \mathcal{G}_{\beta_N})(x) \quad (4.0.1)$$

with  $\mathcal{G}_{\beta_N}(x) := \frac{1}{(2\pi\beta_N^2)^{3/2}} e^{-(x/\beta_N)^2}$ .

Heuristically, the  $\beta_N$  in regularized potential defined in (4.0.1) can be understood as a low-pass filter. Another interpretation of the mollification above is that, instead of point particles, we are considering spherical particles with vanishing radius. This method of starting from mollified Coulomb potential and remove the mollification when taking  $N \rightarrow \infty$  has been applied by many researches, for example in [HJ15, Laz16, LP17], to derive the Vlasov-Poisson equation from  $N$  body classical dynamics. In [CLS11], such a regularized potential has also been considered for the bosonic case in the quantum settings.

Therefore, in this chapter, we will show the convergence from Schrödinger equation to Vlasov-Poisson equation. The work in this chapter is based on our article in [CLL21b] which has been accepted in *Annales Henri Poincaré*.

### 4.1 Main result

The Hamiltonian acting on  $\mathcal{F}_a$  we are considering in this chapter is given as

$$\mathcal{H}_N = \frac{\hbar^2}{2} \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \iint dx dy V_N(x-y) a_x^* a_y^* a_y a_x, \quad (4.1.1)$$

and the Cauchy problem for the Schrödinger equation in Fock space is given by

$$\begin{cases} i\hbar\partial_t\Psi_{N,t} = \mathcal{H}_N\Psi_{N,t}, \\ \Psi_{N,0} = \Psi_N^{\text{Slater}}, \end{cases} \quad (4.1.2)$$

for all  $\Psi_{N,t} \in \mathcal{F}_a$  and  $\|\Psi_{N,t}\| = 1$  for  $t \in [0, T]$ .

In this section, we provide our main result, proof strategies, and the *a priori* estimates. The complete proof will be presented in Section 4.1.3. In the following, we denote  $\nabla_q f$  and  $\nabla_p f$  to be the gradients of  $f$  with respect to the position and momentum variables respectively.

**Theorem 4.1.1.** *Suppose that  $V_N$  is the regularized Coulomb potential given in (4.0.1) with  $\beta_N := N^{-\epsilon}$  and  $0 < \epsilon < \frac{1}{24}$  hold. For any fixed  $T > 0$ , let  $\Psi_{N,t} \in \mathcal{F}_a$ ,  $t \in [0, T]$ , be the solution to the Schrödinger equation (4.1.2) with the Slater determinant as the initial data. Let  $m_{N,t}$  be the 1-particle Husimi measure defined in (2.2.6), where  $f$  is a compact supported positive-valued function in  $H^1(\mathbb{R}^3)$  with  $\|f\|_{L^2} = 1$ . Moreover, let  $m_N^{\text{Slater}}$  be the initial 1-particle Husimi measure with its  $L^1$ -weak limit  $m_0$  and there exists a constant  $C > 0$  independent of  $N$  such that*

$$\iint dq dp (|p|^2 + |q|) m_N(q, p) \leq C. \quad (4.1.3)$$

*Then,  $m_{N,t}$  has a weak- $\star$  convergent subsequence in  $L^\infty((0, T]; L^1(\mathbb{R}^3 \times \mathbb{R}^3))$  with limit  $m_t$ , where  $m_t$  is, in the sense of distribution, the solution of the Vlasov-Poisson equation with repulsive Coulomb potential,*

$$\begin{cases} \partial_t m_t(q, p) + p \cdot \nabla_q m_t(q, p) = \nabla_q (|\cdot|^{-1} * \varrho_t)(q) \cdot \nabla_p m_t(q, p), \\ m_t(q, p)|_{t=0} = m_0(q, p), \end{cases} \quad (4.1.4)$$

where  $\varrho_t(q) := \int dp m_t(q, p)$ .

*Remark 4.1.1.* Since the total energy is conserved in this problem, the assumption of repulsive interacting potential is important to give uniform estimates both for kinetic energy and potential energy.<sup>1</sup> In fact, the result in Theorem 4.1.1 holds also for attractive singular potential if the kinetic energy can be bounded uniformly in  $N$ .

*Remark 4.1.2.* It is proven in Proposition 3.2.3 that the first moment of the Husimi measure  $m_{N,t}$  is uniformly bounded. Therefore, by Theorem 7.12 in [Vil03], the convergence stated in theorem also holds in terms of the 1-Wasserstein metric.<sup>2</sup>

*Remark 4.1.3.* In [GP17], the rate of convergence from Schrödinger to the Vlasov equation in the pseudo-metric is obtained for the interaction potential  $V \in C^{1,1}$ . In addition, the authors commented that their

<sup>1</sup>See Lemma 3.2.1 below

<sup>2</sup>The 1-Wasserstein metric is defined as  $W_1(\mu, \nu) := \max_{\pi \in \Pi(\mu, \nu)} \int |x - y| d\pi(x, y)$ , where  $\mu$  and  $\nu$  are probability measures and  $\Pi(\mu, \nu)$  the set of all probability measures with marginals  $\mu$  and  $\nu$ . [Vil03]

result can be extended for the truncated Coulomb interaction, but with order higher than  $C/\sqrt{\ln N}$  for some constant  $C > 0$ . In Theorem 4.1.1, the mollification of the Coulomb interaction can be handled with polynomial truncation.

*Remark 4.1.4.* The global existence of classical solution to the Vlasov-Poisson equation in 3-dimension is proven in [Pfa92] and [LP91] for a general class of initial data. The uniqueness of the solution is proven in [LP91] for initial datum with strong moment conditions and integrability. In [Loe06], the uniqueness of the solution is also proven for bounded macroscopic density. Furthermore, the global existence of weak solutions is provided in [Ars75] for bounded initial data and kinetic energy. The result is then relaxed to only  $L^p$ -bound for  $p > 1$  in [GT15]. Result on existence with symmetric initial data is proven in [Bat77, Dob79, Sch87]. For other results, we refer to the works given in [ACF14, BBC16, HN81] to list a few.

### 4.1.1 Proof strategies

As in chapter 5, recall again that from Proposition 3.2.1, we obtain the following reformulation of Schrödinger equation given (2.1.10), i.e.,

$$\begin{aligned} & \partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) - \nabla_q \cdot (\hbar \operatorname{Im} \langle \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t}, a(f_{q,p}^\hbar) \Psi_{N,t} \rangle) \\ &= \frac{1}{(2\pi)^3} \nabla_p \cdot \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \\ & \quad \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \end{aligned} \quad (4.1.5)$$

where we denote

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

In particular, this can be rewritten into the Vlasov equation with remainder terms, i.e.,

$$\begin{aligned} & \partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) \\ &= \frac{1}{(2\pi)^3} \nabla_p \cdot \int dq_2 \nabla V_N(q - q_2) \varrho_{N,t}(q_2) m_{N,t}(q, p) + \nabla_q \cdot \tilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R}, \end{aligned} \quad (4.1.6)$$

where  $\varrho_{N,t}(q) := \int dp m_{N,t}(q, p)$ ,  $\tilde{\mathcal{R}}$  and  $\mathcal{R} = \mathcal{R}_1 + \mathcal{R}_2$  are given by

$$\begin{aligned}
\tilde{\mathcal{R}} &:= \hbar \operatorname{Im} \langle \nabla_q a(f_{q,p}^h) \Psi_{N,t}, a(f_{q,p}^h) \Psi_{N,t} \rangle, \\
\mathcal{R}_1 &:= \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\
&\quad \left[ \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) - \nabla V_N(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \\
\mathcal{R}_2 &:= \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\
&\quad \nabla V_N(q - q_2) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right].
\end{aligned} \tag{4.1.7}$$

The main idea of this chapter is to rigorously prove the limit  $N \rightarrow \infty$  from (4.1.6) to the Vlasov-Poisson equation (4.1.4) in the sense of distribution.

First, from the uniform estimate of the kinetic energy shown in Lemma 4.1.1, we prove in Proposition 4.1.1 the uniform estimate for the moments of Husimi measure. Additionally, since the Husimi measure belongs to  $L^\infty([0, T]; L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3))$  (see Lemma 2.2.2), we obtain directly the weak compactness of the two linear terms on the left-hand side of (4.1.6) by the Dunford-Pettis theorem.<sup>3</sup>

For the quadratic term on the right-hand side of (4.1.6), the classical Thomas-Fermi theory gives that  $\varrho_{N,t} \in L^\infty([0, T]; L^{5/3}(\mathbb{R}^3))$ . With the *a priori* estimate obtained in Section 4.1.2, the Aubin-Lions compact embedding theorem shows the strong compactness of  $\nabla V_N * \varrho_{N,t}$ .

The estimate for the remainder term  $\tilde{\mathcal{R}}$  is provided in Proposition 3.2.4. Thus, the main work of this paper is dealing with the challenging term  $\mathcal{R}$ . Unlike the BBGKY hierarchy used in chapter 3, where the remainder term contains only the difference between the 2-particle density matrices, we write the term  $\mathcal{R}$  as a combination of the semiclassical and mean-field terms as  $\mathcal{R}_1$  and  $\mathcal{R}_2$ , respectively.<sup>4</sup> Thus, the factorization effect can be directly obtained from  $\mathcal{R}_2$  instead of using the method of the BBGKY hierarchy.

The estimates for  $\mathcal{R}_1$  and  $\mathcal{R}_2$  are shown in Proposition 4.2.2 and Proposition 4.2.3 respectively, in which we utilize the estimates of the ‘cutoff’ number operator and momentum oscillation presented in Lemma 2.3.2 and Lemma 2.3.3, to control the growth of the Lipschitz constant  $V_N$ , which is of order  $\beta_N^{-2}$ .

### 4.1.2 *A priori* estimates

Observe that due to the conservation of energy and the repulsive effect of the Coulomb force, we obtain the following estimate for the kinetic energy.

**Lemma 4.1.1.** *Assuming that  $V_N(x) \geq 0$  and the initial total energy is bounded in the sense that  $\frac{1}{N} \langle \Psi_N, \mathcal{H}_N \Psi_N \rangle \leq$*

<sup>3</sup>See Proposition 3.2.7.

<sup>4</sup>See (4.2.1) for the full structure.

$C$ , then there exists a constant  $C > 0$  independent of  $N$  such that

$$\left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle \leq C. \quad (4.1.8)$$

*Proof.* We define the operator

$$\mathcal{V}_N := \frac{1}{N} \iint dx dy V_N(x-y) a_x^* a_y^* a_y a_x.$$

Since  $V_N \geq 0$ , we have  $\langle \Psi_{N,t}, \mathcal{V}_N \Psi_{N,t} \rangle \geq 0$ . Then

$$\langle \Psi_{N,t}, \mathcal{H}_N \Psi_{N,t} \rangle = \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle + \langle \Psi_{N,t}, \mathcal{V}_N \Psi_{N,t} \rangle,$$

implies

$$0 \leq \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle \leq \langle \Psi_{N,t}, \mathcal{H}_N \Psi_{N,t} \rangle.$$

Hence,

$$\frac{1}{N} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle \leq \frac{1}{N} \langle \Psi_{N,t}, \mathcal{H}_N \Psi_{N,t} \rangle = \frac{1}{N} \langle \Psi_N, \mathcal{H}_N \Psi_N \rangle \leq C.$$

■

Consequently, the moment estimate of the Husimi measure is obtained directly from the uniform bound in Lemma 3.2.1.

**Proposition 4.1.1.** *For  $t \geq 0$ , we have the following finite moments:*

$$\iint dq dp (|q| + |p|^2) m_{N,t}(q, p) \leq C(1+t), \quad (4.1.9)$$

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

*Proof.* First, from (3.2.9), we have

$$\left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle = \frac{1}{(2\pi)^3} \iint dq dp |p|^2 m_{N,t}(q, p) + \hbar \int dq |\nabla f(q)|^2, \quad (4.1.10)$$

which implies that

$$\frac{1}{(2\pi)^3} \iint dq dp |p|^2 m_{N,t}(q, p) \leq \left\langle \Psi_{N,t}, \frac{\mathcal{K}}{N} \Psi_{N,t} \right\rangle \leq C, \quad (4.1.11)$$

where we use Lemma 4.1.1 in the last inequality.

Then, for the moment with respect to  $q$ , we obtain from (4.1.6) that

$$\begin{aligned}
& \frac{d}{dt} \iint dq dp |q| m_{N,t}(q, p) = \iint dq dp |q| \partial_t m_{N,t}(q, p) \\
&= \iint dq dp |q| \left( -p \cdot \nabla_q m_{N,t}(q, p) + \frac{1}{(2\pi)^3} \nabla_p \cdot \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \int_0^1 ds \right. \\
&\quad \left. \nabla V(su_2 + (1-s)w_1 - w_2) f_{q,p}^h(w_1) \overline{f_{q,p}^h(u_1)} f_{q_2,p_2}^h(w_2) \overline{f_{q_2,p_2}^h(u_2)} \langle a_{w_2} a_{w_1} \Psi_{N,t}, a_{u_2} a_{u_1} \Psi_{N,t} \rangle + \nabla_q \cdot \tilde{\mathcal{R}} \right). \tag{4.1.12}
\end{aligned}$$

By applying the divergence theorem first with respect to  $p$  and then with respect to  $q$  in (4.1.12), we obtain

$$\begin{aligned}
\frac{d}{dt} \iint dq dp |q| m_{N,t}(q, p) &= \iint dq dp \frac{q}{|q|} \cdot p m_{N,t}(q, p) \\
&\leq \iint dq dp (1 + |p|^2) \cdot m_{N,t}(q, p),
\end{aligned}$$

where we use Young's product inequality. Finally, taking the integral over  $t$ , we obtain the desired result. ■

### 4.1.3 Proof of Theorem 4.1.1

First, denoting  $\varrho_{N,t}(q) := \int m_{N,t}(q, p) dp$ , recall the Vlasov equation

$$\begin{aligned}
& \partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) \\
&= \frac{1}{(2\pi)^3} \nabla_p \cdot \int dq_2 \nabla V_N(q - q_2) \varrho_{N,t}(q_2) m_{N,t}(q, p) + \nabla_q \cdot \tilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R} \\
&= \frac{1}{(2\pi)^3} (\nabla V_N * \varrho_{N,t})(q) \cdot \nabla_p m_{N,t}(q, p) + \nabla_q \cdot \tilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R}, \tag{4.1.13}
\end{aligned}$$

with

$$\begin{aligned}
& \tilde{\mathcal{R}} := \hbar \operatorname{Im} \langle \nabla_q a(f_{q,p}^h) \Psi_{N,t}, a(f_{q,p}^h) \Psi_{N,t} \rangle, \\
& \mathcal{R} := (2\pi)^3 \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\
& \quad \left[ \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) \right. \\
& \quad \left. - \nabla V_N(q - q_2) \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right]. \tag{4.1.14}
\end{aligned}$$

The main task is now reduced to taking limits in (4.1.14). In fact, Section 4.2 is devoted to deriving the estimates for the residuals. As a summary, it is proven in Section 4.2 that for  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ , there exists a

positive constant  $\hat{K}$  such that

$$\begin{aligned} \left| \iint dq dp \, \varphi(q) \phi(p) \nabla_q \cdot \tilde{\mathcal{R}}(q, p) \right| &\leq \hat{K} \hbar^{\frac{1}{2}-\delta}, \\ \left| \iint dq dp \, \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}(q, p) \right| &\leq \hat{K} \left( \hbar^{\frac{1}{4}(6\alpha_1-5)-2\delta} + \hbar^{\frac{3}{2}(\alpha_2-\frac{1}{2})-2\delta} \right), \end{aligned} \quad (4.1.15)$$

where  $\frac{5}{6} < \alpha_1 < 1$ ,  $\frac{1}{2} < \alpha_2 < 1$  and  $0 < \delta \ll 1$ . The estimates in (4.1.15) show that the residual terms converge to zero in the sense of distribution.

Recall from Proposition 3.2.7, we have the following result on weak convergent in  $L^1$ :

$$\frac{1}{(2\pi)^3} \iint dq dp \, m_{N_j,t}(q, p) \Phi(q, p) \rightarrow \iint dq dp \, m_t(q, p) \Phi(q, p),$$

as  $j \rightarrow \infty$  for any  $\Phi \in C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ .

To prove the convergence of the nonlinear term  $(\nabla V_N * \rho_N) \cdot \nabla_p m_{N,t}$ , we first show the strong convergence of  $\nabla V_N * \rho_N$ .

**Lemma 4.1.2.** *Let  $V_N$  be defined as (4.0.1). Then for  $t \in [0, \infty)$  there exists constant  $C > 0$  independent on  $N$  such that*

$$\|\nabla V_N * \varrho_{N,t}\|_{L^\infty([0,\infty); W^{1,\frac{5}{3}}(\mathbb{R}^3))} \leq C, \quad (4.1.16)$$

$$\|\partial_t(\nabla V_N * \varrho_{N,t})\|_{L^\infty([0,\infty); W^{-1,\frac{15}{7}}(\mathbb{R}^3))} \leq C. \quad (4.1.17)$$

*Proof.* From Lemma 2.2.2 and Proposition 3.2.3, one finds that  $m_{N,t}$  is uniformly bounded in  $L^\infty([0, \infty); L^1(\mathbb{R}^3 \times \mathbb{R}^3)) \cap L^\infty([0, \infty); L^\infty(\mathbb{R}^3 \times \mathbb{R}^3))$  and  $|p|^2 m_{N,t}(q, p)$  uniformly in  $L^\infty([0, \infty); L^1(\mathbb{R}^3 \times \mathbb{R}^3))$  respectively. As a consequence, it holds that

$$\|\varrho_{N,t}\|_{L^\infty([0,\infty); L^{\frac{5}{3}}(\mathbb{R}^3))} \leq C.$$

Thus,  $V_N * \varrho_{N,t} = V * \mathcal{G}_{\beta_N} * \varrho_{N,t}$  is uniformly bounded in  $L^\infty([0, \infty); W^{2,\frac{5}{3}}(\mathbb{R}^3))$  due to the fact that  $V$  is the fundamental solution of the Poisson equation and

$$\|\mathcal{G}_{\beta_N} * \varrho_{N,t}\|_{L^\infty([0,\infty); L^{\frac{5}{3}}(\mathbb{R}^3))} \leq \|\mathcal{G}_{\beta_N}\|_{L^1(\mathbb{R}^3)} \cdot \|\varrho_{N,t}\|_{L^\infty([0,\infty); L^{\frac{5}{3}}(\mathbb{R}^3))}.$$

This implies the result (4.1.16).

To prove (4.1.17), recall again the transport equation for  $m_{N,t}$

$$\partial_t m_{N,t} + p \cdot \nabla_q m_{N,t} - \frac{1}{(2\pi)^3} (\nabla V_N * \varrho_{N,t}) \cdot \nabla_p m_{N,t} = \nabla_q \cdot \tilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R}, \quad (4.1.18)$$

where  $\varrho_{N,t}(q) := \int m_{N,t}(q, p) dp$ . Taking the integral with respect to  $p$ ,

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

Next, by taking the convolution with  $\nabla V_N$ , we obtain

$$\partial_t (\nabla V_N * \varrho_{N,t}) + \nabla_q \cdot (\nabla V_N \otimes_* J_{N,t}) = \nabla_q \cdot \left( \nabla V_N \otimes_* \int dp \tilde{\mathcal{R}} \right), \quad (4.1.19)$$

where  $J_{N,t}(q) := \int dp p m_{N,t}(q, p)$ ,  $(u \otimes_* v)_{ij} = u_i * v_j$  for  $u, v \in \mathbb{R}^3$ . Then, we observe that

$$\left| \int dp p m_{N,t}(q, p) \right| \leq \left[ \int dp |p|^2 m_{N,t} \right]^{\frac{1}{2}} \left[ \int dp m_{N,t} \right]^{\frac{1}{2}} = \left[ \int dp |p|^2 m_{N,t} \right]^{\frac{1}{2}} \varrho_{N,t}^{\frac{1}{2}}. \quad (4.1.20)$$

Therefore, we have

$$\int dq |J_{N,t}(q)|^{\frac{5}{4}} = \int dq \left| \int dp p m_{N,t}(q, p) \right|^{\frac{5}{4}} \leq \left[ \iint dq dp |p|^2 m_{N,t} \right]^{\frac{5}{8}} \left[ \int dq \varrho_{N,t}^{\frac{5}{3}} \right]^{\frac{3}{8}} \leq C,$$

where we use Proposition 4.1.1 in the last inequality, yielding  $J_{N,t} \in L^\infty([0, \infty); L^{\frac{5}{4}}(\mathbb{R}^3))$ . Then, for any test function  $\varphi \in L^{\frac{15}{8}}(\mathbb{R}^3)$ , we obtain

$$\begin{aligned} \int dq |\varphi(q)| \left| \int dq_2 \nabla V_N(q - q_2) J_{N,t}(q_2) \right| &\leq \iint dq dq_2 |\varphi(q)| |\nabla V_N(q - q_2)| |J_{N,t}(q_2)| \\ &\leq C \left( \int dq |\varphi(q)|^{\frac{15}{8}} \right)^{\frac{8}{15}} \left( \int dq |J_{N,t}(q)|^{\frac{5}{4}} \right)^{\frac{4}{5}} \\ &\leq C, \end{aligned}$$

where we use the Hardy-Littlewood-Sobolev inequality in the second inequality. This implies that  $(\nabla V_N * J_{N,t}) \in L^\infty([0, \infty); L^{\frac{15}{7}}(\mathbb{R}^3))$ .

Therefore, we focus on the following estimate:

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



Since

$$\begin{aligned}
& \hbar^2 \iint dq dp \langle \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t}, \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t} \rangle \\
&= \hbar^{\frac{1}{2}} \iint dq dp \iint dw du \nabla_q f \left( \frac{w-q}{\sqrt{\hbar}} \right) \nabla_q f \left( \frac{u-q}{\sqrt{\hbar}} \right) e^{\frac{i}{\hbar} p \cdot (w-u)} \langle \Psi_{N,t}, a_w^* a_u \Psi_{N,t} \rangle \\
&= \hbar^{\frac{1}{2}+3} \iint dq dw \hbar^{-1} \left| \nabla f \left( \frac{w-q}{\sqrt{\hbar}} \right) \right|^2 \langle \Psi_{N,t}, a_w^* a_w \Psi_{N,t} \rangle \\
&= \hbar^4 \int d\tilde{q} |\nabla f(\tilde{q})|^2 \langle \Psi_{N,t}, \mathcal{N} \Psi_{N,t} \rangle \\
&\leq \hbar \|\nabla f\|_2^2,
\end{aligned}$$

we have

$$\int dq \left| \int dp \tilde{\mathcal{R}} \right|^{\frac{5}{4}} \leq \left[ \hbar^2 \iint dq dp \langle \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t}, \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t} \rangle \right]^{\frac{5}{8}} \left( \int dq \varrho_{N,t}^{\frac{5}{3}} \right)^{\frac{3}{8}} \leq \hbar^{\frac{5}{4}} C.$$

Repeating the calculation in (4.1.20), we have that  $(\nabla V_N * \int dp \tilde{\mathcal{R}}) \in L^\infty([0, \infty); L^{\frac{15}{7}}(\mathbb{R}^3))$ , which implies that  $(\nabla V_N * \int dp \nabla_q \cdot \tilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R}) \in L^\infty([0, \infty); L^{\frac{15}{7}}(\mathbb{R}^3))$ . Thus, from (4.1.19), we have that

$$\partial_t (\nabla V_N * \varrho_{N,t}) \in L^\infty([0, \infty); W^{-1, \frac{15}{7}}(\mathbb{R}^3)).$$

This completes the proof for Lemma 4.1.2. ■

Finally, we conclude the proof of main theorem with the following compactness argument.

### Compactness argument

As in Section 4.1.1, the weak convergence of the linear terms in the Vlasov equation is obtained from Proposition 3.2.7. The following discussion is focused on the nonlinear term. Without loss of generality, assume that  $\Phi(q, p) = \varphi(q)\phi(p)$  for any test functions  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ , and let the sphere  $B_\ell$  with radius  $\ell > 0$  be the support of  $\varphi$ . Then, from Lemma 4.1.2 and Sobolev's embedding theorem, we have

$$W^{1, \frac{5}{3}}(B_\ell) \hookrightarrow L^r(B_\ell) \hookrightarrow W^{-1, \frac{15}{7}}(B_\ell),$$

where  $\frac{5}{4} \leq r < \frac{15}{4}$  and  $\hookrightarrow$  means the compact embedding. Aubin-Lion lemma implies that there exists a subsequence denoted also by  $\{\nabla V_N * \varrho_{N,t}\}_{N \in \mathbb{N}}$ , and  $h \in L^\infty([0, T]; L^r(B_\ell))$  such that, as  $N \rightarrow \infty$ , we have

$$\nabla V_N * \varrho_{N,t} \rightarrow h \quad \text{in } L^\infty([0, T]; L^r(\mathbb{R}^3)), \tag{4.1.21}$$

where  $\frac{5}{4} \leq r < \frac{15}{4}$ .

To show the limit  $h$ , we suppose that

$$\begin{aligned} & \int dq \varphi(q) (\nabla(V_N * \varrho_{N,t})(q) - \nabla(V * \varrho_t)(q)) \\ &= \int dq \varphi(q) ((\nabla V_N - \nabla V) * \varrho_{N,t})(q) + \int dq \varphi(q) (\nabla V * (\varrho_{N,t} - \varrho_t))(q) \\ &=: \mathcal{A}_1 + \mathcal{A}_2, \end{aligned}$$

for some test-function  $\varphi \in C_0^\infty$ . Since  $\nabla V_N$  converge strongly to  $\nabla V$  in  $L^{\frac{3}{2}-\varepsilon}$ , and  $\varrho_{N,t} \in L^1 \cap L^{\frac{5}{3}}$ , then we have, for any  $\varepsilon \in (0, \frac{1}{2})$  and  $\frac{5(2\varepsilon-3)}{2(8\varepsilon-7)} =: s \in (1, \frac{5}{3})$

$$\begin{aligned} \mathcal{A}_1 &= \iint dq dy \varphi(q) (\nabla V_N - \nabla V)(q - y) \varrho_{N,t}(y) \\ &\leq \|\varphi\|_{L^{\frac{5}{2}}} \|\nabla V_N - \nabla V\|_{L^{\frac{3}{2}-\varepsilon}} \|\varrho_{N,t}\|_{L^s} \longrightarrow 0, \end{aligned}$$

as  $N \rightarrow \infty$ . On the other hand, observe that since

$$\|\varphi * \nabla V\|_{L^{\frac{5}{2}}} \leq \|\varphi\|_{L^q} \|\nabla V\|_{L^{\frac{3}{2}-\varepsilon}} \leq C,$$

where  $q = \frac{5(2\varepsilon-3)}{14\varepsilon-11}$  for any  $\varepsilon \in (0, \frac{1}{2})$  and  $C > 0$ .

On the other hand, since  $\varrho_{N,t} \rightharpoonup^* \varrho_t$  in  $L^\infty((0, T); L^{\frac{5}{3}}(\mathbb{R}^3))$ , where  $\varrho_t(q) := \int m_t(q, p) dp$ , we obtain

$$\mathcal{A}_2 = \int dy (\varphi * \nabla V)(y) (\varrho_{N,t} - \varrho_t)(y) \longrightarrow 0,$$

as  $N \rightarrow \infty$  for fixed  $t$ . Therefore, we have the limit  $h = \nabla V * \varrho_t$  for any test function  $\varphi \in L^s(\mathbb{R}^3) \cap L^q(\mathbb{R}^3)$ .

Now, to show the convergence to the Vlasov-Poisson equation, we first compute

$$\begin{aligned} & \left| \int_0^T dt \iint dq dp \varphi(q) \nabla_p \phi(p) \cdot [(\nabla V_N * \varrho_{N,t})(q) m_{N,t}(q, p) - (\nabla V * \varrho_t) m_t(q, p)] \right| \\ &= \left| \int_0^T dt \iint dq dp \varphi(q) \nabla_p \phi(p) \cdot [(\nabla V_N * \varrho_{N,t})(q) - (\nabla V * \varrho_t)(q)] m_{N,t}(q, p) \right. \\ & \quad \left. + \int_0^T dt \iint dq dp \varphi(q) \nabla_p \phi(p) \cdot (\nabla V * \varrho_t)(q) [m_{N,t}(q, p) - m_t(q, p)] \right| \\ &\leq \left| \int_0^T dt \iint dq dp \varphi(q) \nabla_p \phi(p) \cdot [(\nabla V_N * \varrho_{N,t})(q) - (\nabla V * \varrho_t)(q)] m_{N,t}(q, p) \right| \\ & \quad + \left| \int_0^T dt \iint dq dp \varphi(q) \nabla_p \phi(p) \cdot (\nabla V * \varrho_t)(q) [m_{N,t}(q, p) - m_t(q, p)] \right| =: \mathcal{B}_1 + \mathcal{B}_2. \end{aligned}$$

Let us focus on the first term.

$$\begin{aligned}
\mathcal{B}_1 &= \left| \int_0^T dt \int_{B_\ell} dq \, \varphi(q) [(\nabla V_N * \varrho_{N,t})(q) - (\nabla V * \varrho_t)(q)] \cdot \int dp \, \nabla_p \phi(p) m_{N,t}(q, p) \right| \\
&\leq T \sup_{t \in [0, T]} \|(\nabla V_N * \varrho_{N,t}) - (\nabla V * \varrho_t)\|_{L^r(B_\ell)} \left\| \varphi \int dp \, \nabla_p \phi(p) m_{N,t}(\cdot, p) \right\|_{L^{r'}(B_\ell)} \\
&\leq T \sup_{t \in [0, T]} \|(\nabla V_N * \varrho_{N,t}) - (\nabla V * \varrho_t)\|_{L^r(B_\ell)} \|\varphi\|_{L^{r'}(B_\ell)} \|\nabla_p \phi\|_{L^1(\mathbb{R}^3)} \\
&\leq C_T \|(\nabla V_N * \varrho_{N,t}) - (\nabla V * \varrho_t)\|_{L^\infty([0, T]; L^r(B_\ell))}
\end{aligned}$$

where we use the fact that  $0 \leq m_{N,t} \leq 1$  almost everywhere. Taking the limit  $N \rightarrow \infty$  on both sides, then we have

$$\lim_{N \rightarrow \infty} \mathcal{B}_1 = 0.$$

We focus now on  $\mathcal{B}_2$ . We observe that since  $\|m_{N,t}\|_{L^\infty}$  is uniformly bounded, it is implied that there is a subsequence still denoted by  $\{m_{N,t}\}_{N \in \mathbb{N}}$  such that  $m_{N,t} \rightharpoonup^* m_t$  in  $L^\infty((0, T); L^\infty(\mathbb{R}^3 \times \mathbb{R}^3))$  as  $N \rightarrow \infty$ . Since  $\varphi(q) \nabla_p \phi(p) \cdot (\nabla V * \varrho_t)(q) \in L^1((0, T); L^1(\mathbb{R}^3 \times \mathbb{R}^3))$ , we have  $\lim_{N \rightarrow \infty} \mathcal{B}_2 = 0$ . This completes the proof of Theorem 4.1.1. ■

## 4.2 Estimates of residuals

The estimate for the residual term  $\tilde{\mathcal{R}}$  given in (4.1.7) is obtained exactly as Proposition 3.2.4, i.e.,

**Proposition 4.2.1.** *Suppose that  $f \in H^1(\mathbb{R}^3)$ ,  $\|f\|_{L^2} = 1$  and has compact support; then, we have the following bound for  $\tilde{\mathcal{R}}$  in (4.1.6); i.e., for an arbitrarily small  $\delta > 0$ , there exists  $s(\delta) > 0$  such that the following estimate holds for any test function  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$*

$$\left| \iint dq dp \, \varphi(q) \phi(p) \nabla_q \cdot \tilde{\mathcal{R}}(q, p) \right| \leq c_2 \hbar^{\frac{1}{2} - \delta},$$

where the constant  $c_2$  depends on  $\|\nabla \varphi\|_{L^\infty}$  and  $\|\phi\|_{W^{s, \infty}}$ .

For the residual term  $\mathcal{R}$ , we insert the terms

$$\pm \nabla V_N(q - q_2) \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2)$$

and write into a sum  $\mathcal{R} = \mathcal{R}_1 + \mathcal{R}_2$ , where

$$\begin{aligned}\mathcal{R}_1 &:= (2\pi)^3 \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\ &\quad \left[ \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) - \nabla V_N(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \\ \mathcal{R}_2 &:= (2\pi)^3 \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \nabla V_N(q - q_2) \\ &\quad \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right].\end{aligned}\tag{4.2.1}$$

Note that in (4.2.1),  $\mathcal{R}_1$  represents the semiclassical limit part, and  $\mathcal{R}_2$  represents the mean-field limit.

As a preparation for the estimates of the residual term  $\mathcal{R}$ , we first show that the following identity for regularized Coulomb potential, i.e.

**Lemma 4.2.1.** *Let  $\mathcal{F}_z$  be  $z$ -weighted Fourier transform given in Definition 2.2.2 for  $z > 0$  and  $h := \exp(-\lambda|x|^2) \in C_0^\infty(\mathbb{R}^3)$  for  $\lambda > 0$ . Then, the following identity holds*

$$z^a \mathcal{F}_z^{-1} \left[ \frac{1}{|p|^a} \mathcal{F}_z[h](p) \right] (x) = C \int_{\mathbb{R}^3} dy \frac{1}{|x-y|^{3-a}} h(y),\tag{4.2.2}$$

for all  $0 < a < 3$ .

*Proof.* Observe that,

$$|p|^{-a} = C \int_0^\infty d\lambda e^{-p^2 \lambda} \lambda^{\frac{a}{2}-1},$$

for  $\lambda \in \mathbb{R}$ . Next, consider the Inverse-Fourier transform of Gaussian  $e^{-p^2 \lambda}$ ,

$$\begin{aligned}\mathcal{F}_z^{-1}[e^{-p^2 \lambda}](x) &= \frac{1}{(2\pi z)^{3/2}} \int dp e^{\frac{i}{z} p \cdot x} e^{-p^2 \lambda} \\ &= \frac{1}{(2\pi z)^{3/2}} \int dp e^{\frac{i}{z} p \cdot x} e^{-(\sqrt{\lambda} p)^2} \\ &= \frac{1}{(2\pi z)^{3/2}} e^{-\left(\frac{x}{2z\sqrt{\lambda}}\right)^2} \int dp e^{-(\sqrt{\lambda} p - \frac{ix}{2z\sqrt{\lambda}})^2} \\ &= C \frac{1}{z^{3/2}} e^{-\left(\frac{x}{2z\sqrt{\lambda}}\right)^2} \lambda^{-3/2} \\ &= C(z\lambda)^{-3/2} e^{-\left(\frac{x}{2z}\right)^2 \frac{1}{\lambda}},\end{aligned}$$

note there square form here takes meaning of dot-product, i.e.,  $A^2 = A^T A$ . Then, observe that

$$\begin{aligned}\mathcal{F}_z^{-1} \left[ \frac{1}{|p|^a} \mathcal{F}_z[h](p) \right] (x) &= C \frac{1}{(2\pi z)^{3/2}} \int dp e^{\frac{i}{z} p \cdot x} \int_0^\infty d\lambda \lambda^{\frac{a}{2}-1} e^{-p^2 \lambda} \mathcal{F}_z[h](p) \\ &= C \frac{1}{(2\pi z)^3} \int dp e^{\frac{i}{z} p \cdot x} \int_0^\infty d\lambda \lambda^{\frac{a}{2}-1} e^{-p^2 \lambda} \int dy e^{-\frac{i}{z} p \cdot y} h(y)\end{aligned}$$

$$\begin{aligned}
&= C \frac{1}{(2\pi z)^3} \int dy h(y) \int_0^\infty d\lambda \lambda^{\frac{a}{2}-1} \int dp e^{\frac{i}{z} p \cdot (x-y)} e^{-p^2 \lambda} \\
&= C \frac{1}{(2\pi z)^{3/2}} \int dy h(y) \int_0^\infty d\lambda \lambda^{\frac{a}{2}-1} \mathcal{F}_z^{-1}[e^{-p^2 \lambda}](x-y) \\
&= C \frac{1}{(2\pi z)^{3/2}} \int dy h(y) \int_0^\infty d\lambda \lambda^{\frac{a}{2}-1} (z\lambda)^{-3/2} e^{-\left(\frac{x-y}{2z}\right)^2 \frac{1}{\lambda}} \\
&= C z^{-3} z^2 \int dy h(y) \int_0^\infty dr (z^2 r)^{\frac{1-a}{2}} e^{-(x-y)^2 r} \\
&= C z^{-1} z^{1-a} \int dy h(y) \int_0^\infty dr e^{-(x-y)^2 r} r^{\frac{b}{2}-1} \\
&= C z^{-a} \int dy h(y) \frac{1}{|x-y|^{3-a}}
\end{aligned}$$

where we used the substitution,

$$(x-y)^2 r = \left(\frac{x-y}{2z}\right)^2 \lambda^{-1}$$

and  $b = 2(a-1)$  ■

Now take standard Gaussian

$$\mathcal{G}_{\beta_N}(x) := \frac{1}{(2\pi\beta_N^2)^{\frac{3}{2}}} e^{-\left(\frac{x}{\beta_N}\right)^2},$$

where  $0 < \beta_N \ll 1$ . Note above that  $\int dx \mathcal{G}_{\beta_N}(x) = 1$ . Then, we have the following moment estimate for the mollified Coulomb potential

**Lemma 4.2.2.** *Let  $V_N$  be the mollification of the Coulomb potential as defined in (4.0.1); then it holds*

$$\begin{aligned}
\int dp |\widehat{V_N}(p)| &\leq C \beta_N^{-1}, \\
\int dp |p| |\widehat{V_N}(p)| &\leq C \beta_N^{-2}, \\
\int dp |p|^2 |\widehat{V_N}(p)| &\leq C \beta_N^{-3}.
\end{aligned}$$

Furthermore, we have

$$\|\nabla V_N\|_{L^\infty} \leq C \beta_N^{-2}. \quad (4.2.3)$$

*Proof.* Observe we use here  $\mathcal{F}_\infty[\phi] = \widehat{\phi}$  interchangeably. Then, the Fourier transform of the Gaussian is given by

$$\begin{aligned}
\widehat{\mathcal{G}_{\beta_N}}(p) &= \frac{1}{(2\pi)^{3/2}} \int dx e^{-ip \cdot x} \frac{1}{\beta_N^3 (2\pi)^{\frac{3}{2}}} e^{-\left(\frac{x}{\beta_N}\right)^2} \\
&= \frac{1}{(2\pi)^{3/2}} \int dx e^{-\left(\frac{p\beta_N}{2}\right)^2} \frac{1}{\alpha^3 (2\pi)^{\frac{3}{2}}} e^{-\left(\frac{x}{\beta_N} + \frac{ip\beta_N}{2}\right)^2}
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{(2\pi)^{3/2}} e^{-\left(\frac{p\beta_N}{2}\right)^2} \frac{1}{\alpha^3 (2\pi)^{\frac{3}{2}}} \int dx e^{-\left(\frac{x}{\beta_N} + \frac{ip\beta_N}{2}\right)^2} \\
&= \frac{e^{-\left(\frac{p\beta_N}{2}\right)^2}}{(2\pi)^{3/2}} \int dy \frac{e^{-y^2}}{(2\pi)^{\frac{3}{2}}} \\
&= \frac{e^{-\left(\frac{p\beta_N}{2}\right)^2}}{(2\pi)^{3/2}}.
\end{aligned}$$

Then, by Lemma 4.2.1, we have

$$\begin{aligned}
V_N(x) &= \mathcal{F}_1^{-1}[\widehat{V_N}](x) \\
&= \frac{1}{(2\pi)^{3/2}} \int dp e^{ip \cdot x} \mathcal{F}_1[(V * \mathcal{G}_{\beta_N})](p) \\
&\stackrel{(4.2.1)}{=} \frac{1}{(2\pi)^{3/2}} \int dp e^{ip \cdot x} \frac{1}{|p|^2} \mathcal{F}[\mathcal{G}_{\beta_N}](p) \\
&= \frac{1}{(2\pi)^{3/2}} \int dp e^{ip \cdot x} \frac{1}{|p|^2} \frac{e^{-\left(\frac{p\beta_N}{2}\right)^2}}{(2\pi)^{3/2}} \\
&= \frac{1}{(2\pi)^3} \int dp e^{ip \cdot x} \frac{1}{|p|^2} e^{-\left(\frac{p\beta_N}{2}\right)^2}.
\end{aligned}$$

Taking the modulus on both sides yields

$$\begin{aligned}
|V_N(x)| &\leq \frac{1}{(2\pi)^{3/2}} \int dp |\widehat{V_N}(p)| \\
&\leq C \int dp \frac{1}{|p|^2} e^{-\left(\frac{p\beta_N}{2}\right)^2} \\
&= C \beta_N^{-3} \int dk \frac{1}{|k\beta_N|^2} e^{-k^2} \\
&= C \beta_N^{-3} \beta_N^2 \int dk \frac{1}{|k|^2} e^{-k^2} \\
&\leq C \beta_N^{-1},
\end{aligned}$$

where the last inequality we used the following Spherical coordination,

$$\int dk \frac{1}{|k|^2} e^{-k^2} = \int_0^{2\pi} d\Theta \int_0^\pi d\theta \sin \theta \int_0^\infty dr r^2 \frac{1}{|r|^2} e^{-r^2}.$$

Now take the gradient,

$$\begin{aligned}
|\nabla V_N(x)| &= \frac{1}{(2\pi)^{3/2}} \left| \nabla_x \int dp e^{ip \cdot x} \widehat{V_N}(p) \right| \\
&= \frac{1}{(2\pi)^{3/2}} \left| \int dp (ip) \cdot e^{ip \cdot x} \widehat{V_N}(p) \right|
\end{aligned}$$

$$\begin{aligned}
&\leq \frac{1}{(2\pi)^{3/2}} \int dp |p| |\widehat{V}_N(p)| \\
&\leq C \int dp \frac{1}{|p|} e^{-\left(\frac{p\beta_N}{2}\right)^2} \\
&= C\beta_N^{-3} \int dk \frac{1}{|k\beta_N|} e^{-k^2} \\
&= C\beta_N^{-3} \beta_N \int dk \frac{1}{|k|^2} e^{-k^2} \\
&\leq C\beta_N^{-2}.
\end{aligned}$$

Similarly, for second derivative

$$\begin{aligned}
|D^2 V_N(x)| &= \frac{1}{(2\pi)^{3/2}} \left| D_x^2 \int dp e^{ip \cdot x} \widehat{V}_N(p) \right| \\
&= \frac{1}{(2\pi)^{3/2}} \left| \int dp (ip)^2 \cdot e^{ip \cdot x} \widehat{V}_N(p) \right| \\
&\leq \frac{1}{(2\pi)^{3/2}} \int dp |p|^2 |\widehat{V}_N(p)| \\
&\leq \frac{1}{(2\pi)^{3/2}} \int dp e^{-\left(\frac{p\beta_N}{2}\right)^2} \\
&= \frac{1}{(2\pi)^{3/2}} \beta_N^{-3} \int dk e^{-k^2} \\
&= \beta_N^{-3}.
\end{aligned}$$

■

In the next subsection, we will estimate the semiclassical and mean-field residual terms, i.e.  $\mathcal{R}_1$  and  $\mathcal{R}_2$ , by using the truncated radius  $\beta_N$ , the oscillation estimate, the cutoff number operator and the kinetic operator estimates outlined in Section 4.1.2.

#### 4.2.1 Estimate for the semiclassical residual term $\mathcal{R}_1$

In this subsection, we present in full detail the estimate for the semiclassical residue.

**Proposition 4.2.2.** *Let  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ . Then, for  $\frac{5}{6} < \alpha_1 < 1$ ,  $0 < \delta < \frac{1}{8}(6\alpha_1 - 5)$ , and  $s = \left\lceil \frac{3(2\alpha_1 + 1)}{4(1 - \alpha_1)} \right\rceil$ , we have*

$$\left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_1(q, p) \right| \leq \tilde{C} \hbar^{\frac{1}{4}(6\alpha_1 - 5) - 2\delta}, \quad (4.2.4)$$

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

*Proof.* Recall from (4.2.1) that we have

$$\begin{aligned} \mathcal{R}_1 := & (2\pi)^3 \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\ & \left[ \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) - \nabla V_N(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2). \end{aligned} \quad (4.2.5)$$

For  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ , we have

$$\begin{aligned} & \left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_1(q, p) \right| \\ &= (2\pi)^3 \left| \int \dots \int (dq dp)^{\otimes 2} \varphi(q) \nabla_p \phi(p) \cdot \iint dw_1 du_1 \iint dw_2 du_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \right. \\ & \quad \left. \left[ \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) - \nabla V_N(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) \right| \\ &= (2\pi)^6 \left| \iint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{h}}\right) f\left(\frac{u_1 - q}{\sqrt{h}}\right) \right. \\ & \quad \left. e^{\frac{i}{h}p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{h}}\right) \right|^2 \left[ \int_0^1 ds \nabla V_N(su_1 + (1-s)w_1 - w_2) - \nabla V_N(q - q_2) \right] \right. \\ & \quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right|, \end{aligned}$$

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

$$\begin{aligned} & \leq (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{h}}\right) f\left(\frac{u_1 - q}{\sqrt{h}}\right) \right. \\ & \quad \left. e^{\frac{i}{h}p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{h}}\right) \right|^2 \left[ \nabla_{w_2} \int_0^1 ds V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2) \right] \right. \\ & \quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\ & + (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{h}}\right) f\left(\frac{u_1 - q}{\sqrt{h}}\right) \right. \\ & \quad \left. e^{\frac{i}{h}p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{h}}\right) \right|^2 \nabla_q [V_N(q - w_2) - V_N(q - q_2)] \right. \\ & \quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\ & = (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{h}}\right) f\left(\frac{u_1 - q}{\sqrt{h}}\right) \right. \\ & \quad \left. e^{\frac{i}{h}p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{h}}\right) \right|^2 \left[ \int_0^1 ds V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2) \right] \right. \\ & \quad \left. \nabla_{w_2} \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \end{aligned}$$



$$\begin{aligned}
& + (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
& \quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \nabla_{w_2} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 \left[ \int_0^1 ds V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2) \right] \right. \\
& \quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
& + (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \nabla \phi(p) \cdot \nabla_q \left( \varphi(q) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right) \right. \\
& \quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 [V_N(q - w_2) - V_N(q - q_2)] \right. \\
& \quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right|, \\
& =: I_1 + J_1 + K_1
\end{aligned}$$

where we use integration by parts in the second to last equality.

Before advancing, we observe that by splitting the integral with respect to momentum space  $\Omega_{\hbar}$  and  $\Omega_{\hbar}^c$  as defined in (2.3.3), for constant  $C_1$  depending on  $\|\nabla \phi\|_{L^1 \cap W^{s,\infty}}$  and  $\text{supp } \phi$ , we have

$$\begin{aligned}
\left| \int dp \nabla \phi(p) e^{\frac{i}{\hbar} p \cdot (w - u)} \right| &= \left| \int dp (\chi_{(w_1 - u_1) \in \Omega_{\hbar}} + \chi_{(w_1 - u_1) \in \Omega_{\hbar}^c}) \phi(p) e^{\frac{i}{\hbar} p \cdot (w - u)} \right| \\
&\leq C_1 \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} + \hbar^{(1-\alpha_1)s} \right),
\end{aligned} \tag{4.2.6}$$

where we use (2.3.4) in the last inequality.

Now, we want to separately estimate the terms  $I_1$  and  $J_1$ . We begin by estimating  $I_1$ . Recall that

$$\begin{aligned}
I_1 &= (2\pi)^6 \hbar^{\frac{3}{2}} \left| \iint dq dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(p) \cdot f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \\
& \quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left( \int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \right) \left[ \int ds V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2) \right] \right. \\
& \quad \left. \nabla_{w_2} \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right|.
\end{aligned}$$

By using (4.2.6) we have,

$$\begin{aligned}
I_1 &\leq \|\nabla V_N\|_{L^\infty} C_1 \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \iiint dw_1 du_1 dw_2 \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} + \hbar^{(1-\alpha_1)s} \right) \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \\
& \quad (|u_1 - q| + |w_1 - q|) |\nabla_{w_2} \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2)| \\
&\leq \|\nabla V_N\|_{L^\infty} C_1 \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \iiint dw_1 du_1 \left( \chi_{(w_1 - u_1) \in \Omega_{\hbar}} + \hbar^{(1-\alpha_1)s} \right) \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \\
& \quad (|u_1 - q| + |w_1 - q|) \int dw_2 |\nabla_{w_2} \gamma_{N,t}^{(2)}(w_1, w_2; u_1, w_2)|
\end{aligned}$$

$$\begin{aligned}
&= \|\nabla V_N\|_{L^\infty} C_1 \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \iint dw_1 du_1 \left( \chi_{(w_1-u_1) \in \Omega_{\hbar}} + \hbar^{(1-\alpha_1)s} \right) \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\
&\quad (|u_1-q| + |w_1-q|) \int dw_2 |\nabla_{w_2} \langle a_{w_2} a_{w_1} \Psi_{N,t}, a_{w_2} a_{u_1} \Psi_{N,t} \rangle| \\
&\leq \|\nabla V_N\|_{L^\infty} C_1 \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \iint dw_1 du_1 \left( \chi_{(w_1-u_1) \in \Omega_{\hbar}} + \hbar^{(1-\alpha_1)s} \right) \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\
&\quad (|u_1-q| + |w_1-q|) \int dw_2 \left[ \|\nabla_{w_2} a_{w_2} a_{w_1} \Psi_{N,t}\| \|a_{w_2} a_{u_1} \Psi_{N,t}\| + \|a_{w_2} a_{w_1} \Psi_{N,t}\| \|\nabla_{w_2} a_{w_2} a_{u_1} \Psi_{N,t}\| \right] \\
&\leq \|\nabla V_N\|_{L^\infty} C_1 \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \iint dw_1 du_1 \left( \chi_{(w_1-u_1) \in \Omega_{\hbar}} + \hbar^{(1-\alpha_1)s} \right) \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\
&\quad (|u_1-q| + |w_1-q|) \left[ \left( \int dw_2 \|\nabla_{w_2} a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}^2\| \right)^{\frac{1}{2}} \right. \\
&\quad \left. + \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|\nabla_{w_2} a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \right] \\
&=: C_1 \|\nabla V_N\|_{L^\infty} \left[ i_{1,1} + i_{1,2} \right],
\end{aligned}$$

Before we continue, we observe that from the definition of the kinetic energy operator  $\mathcal{K}$  and number operator  $\mathcal{N}$ , we have

$$\begin{aligned}
&\int dq |\varphi(q)| \left[ \iint dw_1 du_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|\nabla_{w_2} a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right) \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right) \right]^{\frac{1}{2}} \\
&= 2\hbar^{-1} \int dq |\varphi(q)| \left[ \iint dw_1 du_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, a_{w_1}^* \mathcal{K} a_{w_1} \Psi_{N,t} \rangle \langle \Psi_{N,t}, a_{u_1}^* \mathcal{N} a_{u_1} \Psi_{N,t} \rangle \right]^{\frac{1}{2}} \\
&= 2\hbar^{-1} \int dq |\varphi(q)| \left[ \int dw_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, \mathcal{K} (a_{w_1}^* a_{w_1} - 1) \Psi_{N,t} \rangle \right. \\
&\quad \left. \int du_1 \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, (\mathcal{N} - 1) a_{u_1}^* a_{u_1} \Psi_{N,t} \rangle \right]^{\frac{1}{2}} \\
&\leq 2\hbar^{-1} \left( \iint dq dw_1 |\varphi(q)| \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, \mathcal{K} a_{w_1}^* a_{w_1} \Psi_{N,t} \rangle \right)^{\frac{1}{2}} \\
&\quad \left( \iint dq du_1 |\varphi(q)| \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, \mathcal{N} a_{u_1}^* a_{u_1} \Psi_{N,t} \rangle \right)^{\frac{1}{2}} \\
&\leq C_2 \hbar^{-4-\frac{3}{2}},
\end{aligned} \tag{4.2.7}$$

where in the last step we use a direct outcome of (2.3.2) and (3.2.1), i.e.

$$\begin{aligned}
& \iint dq dx \chi_{|x-q| \leq R_1 \sqrt{\hbar}} |\varphi(q)| \langle \Psi_{N,t}, a_x^* \mathcal{K} a_x \Psi_{N,t} \rangle \\
&= \iint dq dx \chi_{|x-q| \leq R_1 \sqrt{\hbar}} |\varphi(q)| \langle \Psi_{N,t}, \mathcal{K}(a_x^* a_x - 1) \Psi_{N,t} \rangle \\
&\leq \iint dq dx \chi_{|x-q| \leq R_1 \sqrt{\hbar}} |\varphi(q)| \langle \Psi_{N,t}, \mathcal{K} a_x^* a_x \Psi_{N,t} \rangle \\
&= \left\langle \Psi_{N,t}, \mathcal{K} \iint dq dx \chi_{|x-q| \leq R_1 \sqrt{\hbar}} |\varphi(q)| a_x^* a_x \Psi_{N,t} \right\rangle \\
&\leq C_2 \hbar^{-\frac{3}{2}} \langle \Psi_{N,t}, \mathcal{K} \Psi_{N,t} \rangle \\
&\leq C_2 \hbar^{-\frac{3}{2}-3}.
\end{aligned} \tag{4.2.8}$$

In the above estimate,  $C_2$  is a constant depends on  $\|\varphi\|_{L^\infty}$  and  $\text{supp } f$ .

To continue, we apply the Hölder inequality to  $i_{1,1}$  with respect to the terms  $w_1$  and  $u_1$ ,

$$\begin{aligned}
i_{1,1} &\leq \hbar^{\frac{3}{2}} \int dq |\varphi(q)| \left[ \iint dw_1 du_1 \chi_{(w_1-u_1) \in \Omega_{\hbar}} \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right|^2 (|u_1-q| + |w_1-q|)^2 \right]^{\frac{1}{2}} \\
&\quad \left[ \iint dw_1 du_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|\nabla_{w_2} a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right) \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right) \right. \\
&\quad \left. + \iint dw_1 du_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right) \left( \int dw_2 \|\nabla_{w_2} a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right) \right]^{\frac{1}{2}} \\
&= \hbar^{\frac{3}{2}} \left[ \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1-\tilde{u}_1| \leq \hbar^{\alpha_1+\frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u})|^2 \hbar (|\tilde{u}_1| + |\tilde{w}_1|)^2 \right]^{\frac{1}{2}} \\
&\quad \int dq |\varphi(q)| \left[ 2 \iint dw_1 du_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \right. \\
&\quad \left. \left( \int dw_2 \|\nabla_{w_2} a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right) \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right) \right]^{\frac{1}{2}}.
\end{aligned}$$

Then by using (4.2.7), the estimate goes further

$$\begin{aligned}
&\leq C_2 \hbar^{3-4-\frac{3}{2}+\frac{1}{2}} \left[ \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1-\tilde{u}_1| \leq R_1 \hbar^{\alpha_1+\frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u})|^2 (|\tilde{u}_1| + |\tilde{w}_1|)^2 \right]^{\frac{1}{2}} \\
&\leq C_2 \hbar^{-2} \left[ \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1-\tilde{u}_1| \leq R_1 \hbar^{\alpha_1+\frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u})|^2 |\tilde{u}_1 + \tilde{w}_1|^2 \right]^{\frac{1}{2}} \\
&\leq C_3 \hbar^{-2+\frac{3}{2}(\alpha_1+\frac{1}{2})} = C_3 \hbar^{\frac{6\alpha_1-5}{4}},
\end{aligned}$$

where  $C_3$  depends on  $\|\varphi\|_{L^\infty}$ ,  $\|f\|_{L^\infty \cap L^2}$ ,  $\text{supp } f$  and we use the following estimate in the last inequality

above:

$$\begin{aligned}
& \int dw |f(w)|^2 \int du \chi_{|w-u| \leq R_1 \hbar^{\alpha_1 + \frac{1}{2}}} |f(u)|^2 \\
& \leq \sup_u |f(u)|^2 \int dw |f(w)|^2 \int du \chi_{|w-u| \leq R_1 \hbar^{\alpha_1 + \frac{1}{2}}} \\
& \leq \|f\|_{L^\infty} \|f\|_{L^2} \hbar^{3(\alpha_1 + \frac{1}{2})},
\end{aligned} \tag{4.2.9}$$

where the fixed radius  $R_1$  arises from the compactness assumption of  $f$ .

With steps similar to those for  $i_{1,1}$ , we have

$$i_{1,2} \leq C_3 \hbar^{-2} \hbar^{(1-\alpha_1)s} \left[ \iint d\tilde{w}_1 d\tilde{u}_1 |f(\tilde{w}_1) f(\tilde{u})|^2 (|\tilde{u}_1| + |\tilde{w}_1|)^2 \right]^{\frac{1}{2}} \leq C_4 \hbar^{-2+(1-\alpha_1)s},$$

where the constant  $C_4$  depends on  $\|\varphi\|_\infty$ ,  $\|f\|_{L^\infty \cap L^2}$ , and  $\text{supp } f$ . To balance the order between  $i_{1,1}$  and  $i_{1,2}$ ,  $s$  is chosen to be

$$s = \left\lceil \frac{3(2\alpha_1 + 1)}{4(1 - \alpha_1)} \right\rceil,$$

for  $\alpha_1 \in (\frac{5}{6}, 1)$ . Therefore, we have

$$I_1 \leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{6\alpha_1 - 5}{4}}. \tag{4.2.10}$$

To estimate  $J_1$ , we compute

$$\begin{aligned}
J_1 &= (2\pi)^6 \left| \iint dq dp \iiint dw_1 du_1 dw_2 \varphi(q) \nabla \phi(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[ 2\hbar \int d\tilde{q}_2 f(\tilde{q}_2) \nabla f(\tilde{q}_2) \right] \left[ \int_0^1 ds V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2) \right] \right. \\
&\quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
&\leq (2\pi)^6 \hbar \int dq |\varphi(q)| \iiint dw_1 du_1 dw_2 \left| \int dp (\chi_{(w_1 - u_1) \in \Omega_h} + \chi_{(w_1 - u_1) \in \Omega_h^c}) \nabla \phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right| \\
&\quad \left| \int d\tilde{q}_2 |\nabla f(\tilde{q}_2)| \right| \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \left[ \int_0^1 ds V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2) \right] \right. \\
&\quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
&\leq C_1 \hbar \int dq |\varphi(q)| \iiint dw_1 du_1 dw_2 \left( \chi_{(w_1 - u_1) \in \Omega_h} + \hbar^{(1-\alpha_1)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_0^1 ds |V_N(su_1 + (1-s)w_1 - w_2) - V_N(q - w_2)| \right| \left| \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\
&\leq C_1 \|\nabla V_N\|_{L^\infty} \hbar \int dq |\varphi(q)| \iiint dw_1 du_1 \left( \chi_{(w_1 - u_1) \in \Omega_h} + \hbar^{(1-\alpha_1)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 \|a_{w_2} a_{w_1} \Psi_{N,t}\|_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|_2 \\
&\leq C_1 \|\nabla V_N\|_{L^\infty} \hbar \int dq |\varphi(q)| \iiint dw_1 du_1 \left( \chi_{(w_1 - u_1) \in \Omega_h} + \hbar^{(1-\alpha_1)s} \right) \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|
\end{aligned}$$

$$\begin{aligned}
& (|u_1 - q| + |w_1 - q|) \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|_2^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|_2^2 \right)^{\frac{1}{2}} \\
& =: C_1 \|\nabla V_N\|_{L^\infty} [j_{1,1} + j_{1,2}].
\end{aligned} \tag{4.2.11}$$

As in part  $I_1$ , we separately analyze  $j_{1,1}$  and  $j_{1,2}$ .

$$\begin{aligned}
j_{1,1} &= \hbar \int dq |\varphi(q)| \iint dw_1 du_1 \chi_{(w_1 - u_1) \in \Omega_h} \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| (|u_1 - q| + |w_1 - q|) \\
&\quad \chi_{|u_1 - q| \leq R_1 \sqrt{\hbar}} \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \langle \Psi_{N,t}, a_{w_1}^* a_{w_2}^* a_{w_2} a_{w_1} \Psi_{N,t} \rangle \right)^{\frac{1}{2}} \left( \int dw_2 \langle \Psi_{N,t}, a_{u_1}^* a_{w_2}^* a_{w_2} a_{u_1} \Psi_{N,t} \rangle \right)^{\frac{1}{2}} \\
&\leq \hbar \int dq |\varphi(q)| \left( \iint dw_1 du_1 \chi_{(w_1 - u_1) \in \Omega_h} \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|^2 (|u_1 - q| + |w_1 - q|)^2 \right)^{\frac{1}{2}} \\
&\quad \left( \iint dw_1 dw_2 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, a_{w_1}^* a_{w_2}^* a_{w_2} a_{w_1} \Psi_{N,t} \rangle \right) \\
&= \hbar \left( \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{(\tilde{w}_1 - \tilde{u}_1) \in \Omega_h} |f(\tilde{w}) f(\tilde{u})|^2 \hbar (|\tilde{u}| + |\tilde{w}|)^2 \right)^{\frac{1}{2}} \iint dq dw_1 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} |\varphi(q)| \\
&\quad \langle \Psi_{N,t}, a_{w_1}^* \mathcal{N} a_{w_1} \Psi_{N,t} \rangle \\
&\leq \|\varphi\|_{L^\infty} \hbar^{1+2-3-\frac{3}{2}} \left( \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{(\tilde{w}_1 - \tilde{u}_1) \in \Omega_h} |f(\tilde{w}) f(\tilde{u})|^2 (|\tilde{u}| + |\tilde{w}|)^2 \right)^{\frac{1}{2}} \\
&\leq C_4 \hbar^{\frac{3}{2}(\alpha_1 - \frac{1}{2})},
\end{aligned}$$

where we use (4.2.9) in the last inequality.

On the other hand, from the definition of  $j_{1,2}$  in (4.2.11), we get

$$\begin{aligned}
j_{1,2} &= \hbar \int dq |\varphi(q)| \iint dw_1 du_1 \hbar^{(1-\alpha_1)s} \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| (|u_1 - q| + |w_1 - q|) \\
&\quad \chi_{|u_1 - q| \leq R_1 \sqrt{\hbar}} \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|_2^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|_2^2 \right)^{\frac{1}{2}} \\
&\leq \hbar^{1+(1-\alpha_1)s} \left( \iint dw_1 du_1 \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|^2 (|u_1 - q| + |w_1 - q|)^2 \right)^{\frac{1}{2}} \\
&\quad \int dq |\varphi(q)| \iint dw_1 dw_2 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, a_{w_1}^* a_{w_2}^* a_{w_2} a_{w_1} \Psi_{N,t} \rangle \\
&\leq \hbar^{1+(1-\alpha_1)s-3-\frac{3}{2}} \left( \hbar^4 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_1 + \frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u})|^2 (|\tilde{u}_1| + |\tilde{w}_1|)^2 \right)^{\frac{1}{2}} \\
&\leq C_4 \hbar^{(1-\alpha_1)s-\frac{3}{2}}.
\end{aligned}$$

To obtain the same order for  $j_{1,1}$  and  $j_{1,2}$ , we can choose

$$s = \left\lceil \frac{3(2\alpha_1 + 1)}{4(1 - \alpha_1)} \right\rceil.$$

Thus, for  $\alpha_1 \in (\frac{1}{2}, 1)$ , we have

$$J_1 \leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{3}{2}(\alpha_1 - \frac{1}{2})}. \quad (4.2.12)$$

Now, we want to estimate  $K_1$ .

$$\begin{aligned} K_1 &= (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \nabla \phi(p) \cdot \nabla_q \left( \varphi(q) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right) \right. \\ &\quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 [V_N(q - w_2) - V_N(q - q_2)] \right. \\ &\quad \left. \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\ &= (2\pi)^6 \left| \iiint (dq)^{\otimes 2} dp \iiint dw_1 du_1 dw_2 \nabla \phi(p) \cdot \left[ \nabla \varphi(q) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right. \right. \\ &\quad \left. \left. - \hbar^{-\frac{1}{2}} \varphi(q) \nabla f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) - \hbar^{-\frac{1}{2}} \varphi(q) f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) \nabla f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right] \right. \\ &\quad \left. e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 [V_N(q - w_2) - V_N(q - q_2)] \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) \right| \\ &=: k_{1,1} + k_{1,2} + k_{1,3}. \end{aligned}$$

Note that, for any  $\varphi \in C_0^\infty$  and  $f \in W_0^{1,2}$ , the term  $k_{1,1}$  is  $\sqrt{\hbar}$ -order higher than  $k_{1,2}$  and  $k_{1,3}$ . Moreover, the estimate of the terms  $k_{1,2}$  and  $k_{1,3}$  are the same when doing change of variables in the final steps. Therefore, we focus only on the term  $k_{1,2}$ .

$$\begin{aligned} k_{1,2} &\leq (2\pi)^6 \hbar^{-\frac{1}{2}} \iint (dq)^{\otimes 2} \iiint dw_1 du_1 dw_2 \left| \int dp \nabla \phi(p) e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right| \left| \varphi(q) \nabla f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \\ &\quad \left| f\left(\frac{w_2 - q_2}{\sqrt{\hbar}}\right) \right|^2 |V_N(q - w_2) - V_N(q - q_2)| |\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2)| \\ &= (2\pi)^6 \hbar^{-\frac{1}{2}} \int dq \iiint dw_1 du_1 dw_2 \left| \int dp \left( \chi_{(w_1 - u_1) \in \Omega_h} + \chi_{(w_1 - u_1) \in \Omega_h^c} \right) \nabla \phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right| \\ &\quad \left| \varphi(q) \nabla f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \int \hbar^{\frac{3}{2}} d\tilde{q}_2 |f(\tilde{q}_2)|^2 |V_N(q - w_2) - V_N(q - \sqrt{\hbar}\tilde{q}_2 - w_2)| \\ &\quad |\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2)| \\ &\leq C_1 \|\nabla V_N\|_{L^\infty} \hbar^{1+\frac{1}{2}} \int dq \iiint dw_1 du_1 \left| \chi_{(w_1 - u_1) \in \Omega_h} + \hbar^{(1-\alpha_1)s} \right| \\ &\quad \left| \varphi(q) \nabla f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right| \left( \int d\tilde{q}_2 |\tilde{q}_2| |f(\tilde{q}_2)|^2 \right) \int dw_2 |\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2)| \end{aligned}$$

$$\begin{aligned}
&\leq C_1 \|\nabla V_N\|_{L^\infty} \hbar^{1+\frac{1}{2}} \int dq |\varphi(q)| \iint dw_1 du_1 \left( \chi_{(w_1-u_1) \leq \hbar^{\alpha_1}} + \hbar^{(1-\alpha_1)s} \right) \left| \nabla f \left( \frac{w_1-q}{\sqrt{\hbar}} \right) f \left( \frac{u_1-q}{\sqrt{\hbar}} \right) \right| \\
&\quad \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \\
&=: C_1 \|\nabla V_N\|_{L^\infty} [\tilde{k}_1 + \tilde{k}_2, ].
\end{aligned}$$

Using the Hölder inequality with respect to  $w_1$  and  $u_1$ , we obtain that

$$\begin{aligned}
\tilde{k}_1 &\leq \hbar^{1+\frac{1}{2}} \int dq |\varphi(q)| \left[ \iint dw_1 du_1 \chi_{(w_1-u_1) \leq \hbar^{\alpha_1}} \left| \nabla f \left( \frac{w_1-q}{\sqrt{\hbar}} \right) f \left( \frac{u_1-q}{\sqrt{\hbar}} \right) \right|^2 \right]^{\frac{1}{2}} \\
&\quad \left[ \iint dw_1 du_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right) \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right) \right]^{\frac{1}{2}} \\
&= \hbar^{\frac{3}{2}} \left[ \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{(\tilde{w}_1-\tilde{u}_1) \leq \hbar^{\alpha_1+\frac{1}{2}}} \left| \nabla f(\tilde{w}_1) f(\tilde{u}_1) \right|^2 \right]^{\frac{1}{2}} \\
&\quad \int dq |\varphi(q)| \left[ \int dw_1 \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \langle \Psi_{N,t}, a_{w_1}^* \mathcal{N} a_{w_1} \Psi_{N,t} \rangle \right] \\
&\leq C_5 \hbar^{\frac{3}{2}(\alpha_1+\frac{1}{2})-\frac{3}{2}} = C_5 \hbar^{\frac{3(2\alpha_1-1)}{4}},
\end{aligned}$$

where we use (2.3.2) in the last inequality and  $C_5$  depending on  $\|f\|_{L^\infty}$ ,  $\|\nabla f\|_{L^2}$ ,  $\text{supp } f$ , and  $\|\varphi\|_{L^\infty}$ .

Similarly, to calculate  $j_{1,2}$ ,

$$\begin{aligned}
\tilde{k}_2 &\leq \hbar^{1+\frac{1}{2}} \int dq |\varphi(q)| \iint dw_1 du_1 \hbar^{(1-\alpha_1)s} \left| \nabla f \left( \frac{w_1-q}{\sqrt{\hbar}} \right) f \left( \frac{u_1-q}{\sqrt{\hbar}} \right) \right| \\
&\quad \chi_{|w_1-q| \leq R_1 \sqrt{\hbar}} \chi_{|u_1-q| \leq R_1 \sqrt{\hbar}} \left( \int dw_2 \|a_{w_2} a_{w_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \left( \int dw_2 \|a_{w_2} a_{u_1} \Psi_{N,t}\|^2 \right)^{\frac{1}{2}} \\
&\leq C_5 \hbar^{(1-\alpha_1)s-\frac{3}{2}},
\end{aligned}$$

where  $s$  is chosen as

$$s = \left\lceil \frac{3(2\alpha_1+1)}{4(1-\alpha_1)} \right\rceil,$$

for  $\alpha_1 \in (\frac{1}{2}, 1)$ . Thus,

$$K_1 \leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{3(2\alpha_1-1)}{4}}, \quad (4.2.13)$$

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

Therefore, in summary, we have

$$\left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_1(q, p) \right| \leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{1}{4}(6\alpha_1-5)} \leq \tilde{C} \beta_N^{-2} \hbar^{\frac{1}{4}(6\alpha_1-5)},$$

where we use (4.2.3) in the second inequality.

Setting  $\beta_N = \hbar^\delta$  for  $0 < \delta < \frac{1}{8}(6\alpha_1 - 5)$ , we obtain the desired result.  $\blacksquare$

#### 4.2.2 Estimate for the mean-field residual term $\mathcal{R}_2$

**Proposition 4.2.3.** *Let  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ . Then, for  $\frac{1}{2} < \alpha_2 < 1$ ,  $0 < \delta < \frac{3}{4}(\alpha_2 - \frac{1}{2})$ , and  $s = \left\lceil \frac{3(2\alpha_2+1)}{4(1-\alpha_2)} \right\rceil$ , we have*

$$\left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2(q, p) \right| \leq \tilde{C} \hbar^{\frac{3}{2}(\alpha_2 - \frac{1}{2}) - 2\delta} \quad (4.2.14)$$

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

*Proof.* Recall that from (4.2.1), we have

$$\begin{aligned} \mathcal{R}_2 := & (2\pi)^3 \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \nabla V_N(q - q_2) \\ & \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right]. \end{aligned} \quad (4.2.15)$$

Then, we have

$$\begin{aligned} & \left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2 \right| \\ &= \left| \int \dots \int (dq dp)^{\otimes 2} (dw du)^{\otimes 2} \varphi(q) \nabla \phi(p) \cdot \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \nabla V_N(q - q_2) \right. \\ & \quad \left. \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ &= \hbar^{-3} \left| \int \dots \int (dq dp)^{\otimes 2} (dw du)^{\otimes 2} \varphi(q) \nabla \phi(p) \cdot \left( f \left( \frac{w-q}{\sqrt{\hbar}} \right) f \left( \frac{u-q}{\sqrt{\hbar}} \right) e^{\frac{i}{\hbar} p \cdot (w-u)} \right)^{\otimes 2} \nabla V_N(q - q_2) \right. \\ & \quad \left. \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ &= \hbar^{-3} \left| \int \dots \int (dq dw du)^{\otimes 2} \left( f \left( \frac{w-q}{\sqrt{\hbar}} \right) f \left( \frac{u-q}{\sqrt{\hbar}} \right) \right)^{\otimes 2} \left( \int dp \varphi(q) \nabla \phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right) \right. \\ & \quad \left. \nabla V_N(q - q_2) \left( \int dp_2 e^{\frac{i}{\hbar} p_2 \cdot (w_2 - u_2)} \right) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ &= (2\pi)^3 \left| \int \dots \int (dq)^{\otimes 2} dw_1 du_1 dw_2 f \left( \frac{w_1 - q}{\sqrt{\hbar}} \right) f \left( \frac{u_1 - q}{\sqrt{\hbar}} \right) \left| f \left( \frac{w_2 - q_2}{\sqrt{\hbar}} \right) \right|^2 \left( \int dp \varphi(q) \nabla \phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right) \right. \\ & \quad \left. \nabla V_N(q - q_2) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right|, \end{aligned}$$

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

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

Now, splitting the domains of  $w_1$  and  $u_1$  into two, namely, with the characteristic functions  $\chi_{(w_1 - u_1) \in \Omega_\hbar}$  and



$\chi_{(w_1-u_1) \in \Omega_h^c}$  as defined in (2.3.3), we have

$$\begin{aligned}
&\leq (2\pi)^3 \left| \iint (dq)^{\otimes 2} \varphi(q) \iiint dw_1 du_1 dw_2 f\left(\frac{w_1-q}{\sqrt{h}}\right) f\left(\frac{u_1-q}{\sqrt{h}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{h}}\right) \right|^2 \right. \\
&\quad \left. \left( \int dp \chi_{(w_1-u_1) \in \Omega_h^c} e^{\frac{i}{h}p \cdot (w_1-u_1)} \nabla \phi(p) \right) \cdot \nabla V_N(q-q_2) \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right| \\
&+ (2\pi)^3 \left| \iint (dq)^{\otimes 2} \varphi(q) \iiint dw_1 du_1 dw_2 f\left(\frac{w_1-q}{\sqrt{h}}\right) f\left(\frac{u_1-q}{\sqrt{h}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{h}}\right) \right|^2 \right. \\
&\quad \left. \left( \int dp \chi_{(w_1-u_1) \in \Omega_h^c} e^{\frac{i}{h}p \cdot (w_1-u_1)} \nabla \phi(p) \right) \cdot \nabla V_N(q-q_2) \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right| \\
&=: \mathbf{I}_2 + \mathbf{J}_2.
\end{aligned}$$

Without the loss of generality, we let  $\Phi(q, p) = \varphi(q)\phi(p)$ . First, considering the term  $\mathbf{J}_2$ ,

$$\begin{aligned}
\mathbf{J}_2 &= (2\pi)^3 \left| \iint dq dq_2 \varphi(q) \iiint dw_1 du_1 dw_2 f\left(\frac{w_1-q}{\sqrt{h}}\right) f\left(\frac{u_1-q}{\sqrt{h}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{h}}\right) \right|^2 \right. \\
&\quad \left. \left( \int dp \chi_{(w_1-u_1) \in \Omega_h^c} \nabla \phi(p) e^{\frac{i}{h}p \cdot (w_1-u_1)} \right) \cdot \nabla V_N(q-q_2) \left( \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right) \right|.
\end{aligned}$$

By the change of variable  $\sqrt{h}\tilde{q}_2 = w_2 - q_2$ , we obtain

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

Recall again from Lemma 2.3.3 that we have

$$\left| \int dp \chi_{(w_1-u_1) \in \Omega_h^c} e^{\frac{i}{h}p \cdot (w_1-u_1)} \nabla \phi(p) \right| \leq \|\nabla \phi\|_{W^{s,\infty}} \hbar^{(1-\alpha_2)s},$$

for  $s$  to be chosen later. Then, we obtain

$$\begin{aligned} J_2 &\leq C \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{3}{2}+(1-\alpha_2)s} \int dq |\varphi(q)| \iint dw_1 du_1 \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\ &\quad \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \chi_{|w_1-u_1| \leq 2R_1\sqrt{\hbar}}, \end{aligned}$$

The Hölder inequality yields

$$\begin{aligned} J_2 &\leq C \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{3}{2}+(1-\alpha_2)s} \int dq |\varphi(q)| \left( \iint dw_1 du_1 \chi_{|w_1-u_1| \leq 2R_1\sqrt{\hbar}} \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right|^2 \right)^{\frac{1}{2}} \\ &\quad \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \\ &= C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{3}{2}+(1-\alpha_2)s} \left( \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1-\tilde{u}_1| \leq 2R_1} |f(\tilde{w}) f(\tilde{u})|^2 \right)^{\frac{1}{2}} \\ &\quad \int dq \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \chi_{|w_1-q| \leq R_1\sqrt{\hbar}} \right)^{\frac{1}{2}} \\ &\leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V_N\|_{L^\infty} \hbar^{3+(1-\alpha_2)s} \left( \iint d\tilde{w}_1 d\tilde{u}_1 |f(\tilde{w}) f(\tilde{u})|^2 \right)^{\frac{1}{2}} \\ &\quad \hbar^{\frac{3}{2}} \int d\tilde{q}_1 \chi_{|\tilde{q}_1| \leq R_1} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \\ &\leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{3+(1-\alpha_2)s+\frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}, \end{aligned}$$

where we denote

$$\text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) = \int dw_2 |\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2)|.$$

Thus, we have

$$J_2 \leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{3+(1-\alpha_2)s+\frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}.$$

Now, we focus on  $I_{2,1}$

$$\begin{aligned} I_{2,1} &= (2\pi)^3 \left| \iint (dq)^{\otimes 2} \varphi(q) \iiint dw_1 du_1 dw_2 f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\ &\quad \left( \int dp \chi_{(w_1-u_1) \in \Omega_\hbar} e^{\frac{1}{\hbar} p \cdot (w_1-u_1)} \nabla \phi(p) \right) \cdot \nabla V_N(q-q_2) \\ &\quad \left. \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right|. \end{aligned}$$

We observe that

$$\left| \int dp e^{\frac{1}{\hbar} p \cdot (w_1 - u_1)} \nabla \phi(p) \right| \leq \|\nabla \phi\|_{L^1}.$$

Then, we obtain the following estimate:

$$\begin{aligned} I_2 &\leq C \|\nabla \phi\|_{L^1} \|\nabla V_N\|_{L^\infty} \int dq |\varphi(q)| \left( \iint dw_1 du_1 \chi_{|w_1 - u_1| \leq \hbar^{\alpha_2}} \chi_{|w_1 - u_1| \leq 2R_1 \sqrt{\hbar}} \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|^2 \right)^{\frac{1}{2}} \\ &\quad \hbar^{\frac{3}{2}} \int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \right)^{\frac{1}{2}} \\ &\leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V_N\|_{L^\infty} \hbar^{\frac{3}{2}} \left( \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_2 + \frac{1}{2}}} \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq 2R_1} |f(\tilde{w}_1) f(\tilde{u}_1)|^2 \right)^{\frac{1}{2}} \\ &\quad \int dq \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \right)^{\frac{1}{2}} \\ &\leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^3 \left( \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_2 + \frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u}_1)|^2 \right)^{\frac{1}{2}} \\ &\quad \hbar^{\frac{3}{2}} \int d\tilde{q}_1 \chi_{|\tilde{q}_1| \leq R_1} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}. \end{aligned}$$

From (4.2.9), we have

$$I_2 \leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{3 + \frac{3}{2}(\alpha_2 + \frac{1}{2}) + \frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}.$$

To balance the order between  $I_2$  and  $J_2$ ,  $s$  is chosen to be

$$s = \left\lceil \frac{3(2\alpha_2 + 1)}{4(1 - \alpha_2)} \right\rceil,$$

for  $\alpha_2 \in [0, 1)$ . Therefore, we have

$$\begin{aligned} \left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2 \right| &\leq I_2 + J_2 \\ &\leq \tilde{C} \|\nabla V_N\|_{L^\infty} \hbar^{3 + \frac{3}{2}(\alpha_2 + \frac{1}{2}) + \frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \\ &\leq \tilde{C} \beta_N^{-2} \hbar^{3 + \frac{3}{2}(\alpha_2 + \frac{1}{2}) + \frac{3}{2}} N^2. \end{aligned}$$

Setting  $\beta_N = \hbar^\delta$  for  $0 < \delta < \frac{1}{8}(6\alpha_1 - 5)$ , we have the desired inequality. ■

## Chapter 5

# Vlasov equation with Bogoliubov transformation

In chapter 3, we obtained the convergence by the use of BBGKY hierarchy method. It is, however, possible to obtain the result for the regular potential with the use of the Bogoliubov Transformation instead, the latter which will give us more insight on the structure on the convergence. In this chapter, we obtain the convergence from Schrödinger to Vlasov equation by following closely the Bogoliubov structure introduced in Benedikter, Porta, Schlein in [BPS14a]. In fact, we assume the interaction potential as follows.

**Assumption H4.** For any  $x \in \mathbb{R}^3$ , we assume  $V(x) = V(-x)$  and

$$\int dp (1 + |p|)^2 |\widehat{V}(p)| \leq C,$$

where  $C$  is a positive constant.

*Remark 5.0.1.* Observe that by Fourier transformation and Young's product inequality, it holds

$$\begin{aligned} |\nabla V(x)| &= \left| \nabla_x \int dp e^{ip \cdot x} \widehat{V}(p) \right| \\ &\leq \int dp |p| |\widehat{V}(p)| \\ &\leq \frac{1}{2} \int dp (1 + |p|^2) |\widehat{V}(p)|. \end{aligned} \tag{5.0.1}$$

### 5.1 Main theorem

In this section, we will present the main proof as well as the proof strategy.

**Theorem 5.1.1.** *Let Assumptions H1 and H4 hold. Moreover, we assume*

$$\begin{aligned} \sup_{p \in \mathbb{R}^3} \frac{1}{1 + |p|} \|[e^{ip \cdot x}, \omega_N]\|_{\text{Tr}} &\leq CN\hbar, \\ \|[\hbar \nabla, \omega_N]\|_{\text{Tr}} &\leq CN\hbar, \end{aligned} \quad (5.1.1)$$

where  $\omega_N$  be a sequence of projection given in (1.1.13). For  $t \in [0, \infty)$ , let  $m_{N,t}$  be the 1-particle Husimi measure defined in (2.2.3), where  $f$  is a compact supported positive-valued function in  $H^1(\mathbb{R}^3)$  with  $\|f\|_{L^2} = 1$ . Furthermore, let  $m_N^{\text{Slater}}$  be the initial 1-particle Husimi measure as defined in (2.2.7) with its  $L^1$ -weak limit  $m_0$  and satisfy

$$\iint dq dp (|p|^2 + |q|) m_N(q, p) < \infty. \quad (5.1.2)$$

Then,  $m_{N,t}$  has a weak- $\star$  convergent subsequence in  $L^\infty((0, T]; L^1(\mathbb{R}^3 \times \mathbb{R}^3))$  with limit  $m_t$ , where  $m_t$  is, in the sense of distribution, the solution of the following Vlasov equation.

$$\partial_t m_t(q, p) + p \cdot \nabla_q m_t(q, p) = \frac{1}{(2\pi)^3} (\nabla V * \varrho_t)(q) \cdot \nabla_q m_t(q, p), \quad (5.1.3)$$

where  $\varrho_t(q) := \int dp m_t(q, p)$ .

*Remark 5.1.1.* Similar to Theorem 3.1.1, the result in Theorem (5.1.1) also implies convergence in terms 1-Wasserstein pseudo-distance.

## Proof strategy

Recall from Proposition 3.2.1, we obtain the following reformulation of Schrödinger equation given (2.1.10), i.e.,

$$\begin{aligned} &\partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) - \nabla_q \cdot (\hbar \text{Im} \langle \nabla_q a(f_{q,p}^\hbar) \Psi_{N,t}, a(f_{q,p}^\hbar) \Psi_{N,t} \rangle) \\ &= \frac{1}{(2\pi)^3} \nabla_p \cdot \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \\ &\quad \int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \end{aligned} \quad (5.1.4)$$

where we denote

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

In particular, this can be rewritten into the Vlasov equation with remainder terms, i.e.,

$$\begin{aligned} &\partial_t m_{N,t}(q, p) + p \cdot \nabla_q m_{N,t}(q, p) \\ &= \frac{1}{(2\pi)^3} \nabla_p \cdot \int dq_2 \nabla V(q - q_2) \varrho_{N,t}(q_2) m_{N,t}(q, p) + \nabla_q \cdot \tilde{\mathcal{R}} + \nabla_p \cdot \mathcal{R}, \end{aligned} \quad (5.1.5)$$

where  $\varrho_{N,t}(q) := \int dp m_{N,t}(q, p)$ ,  $\tilde{\mathcal{R}}$  and  $\mathcal{R} = \mathcal{R}_1 + \mathcal{R}_2$  are given by

$$\begin{aligned}\tilde{\mathcal{R}} &:= \hbar \operatorname{Im} \langle \nabla_q a(f_{q,p}^{\hbar}) \Psi_{N,t}, a(f_{q,p}^{\hbar}) \Psi_{N,t} \rangle, \\ \mathcal{R}_1 &:= \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes 2} \\ &\quad \left[ \int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \\ \mathcal{R}_2 &:= \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^{\hbar}(w) \overline{f_{q,p}^{\hbar}(u)} \right)^{\otimes 2} \\ &\quad \nabla V(q - q_2) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right].\end{aligned}\tag{5.1.6}$$

The main idea of this chapter is to rigorously prove the limit  $N \rightarrow \infty$  from (4.1.6) to the Vlasov-Poisson equation (4.1.4) in the sense of distribution.

Under the assumptions of Theorem 5.1.1, the estimate for the residual term  $\tilde{\mathcal{R}}$  and the mean-field residue given in (4.1.7) can be inferred from Proposition 3.2.4 and Proposition 3.2.5 respectively. In particular, for an arbitrarily small  $\delta > 0$ , there exists  $s(\delta) > 0$  such that the following estimates holds for any test function  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ ,

$$\begin{aligned}\left| \iint dq dp \varphi(q) \phi(p) \nabla_q \cdot \tilde{\mathcal{R}}(q, p) \right| &\leq c \hbar^{\frac{1}{2}-\delta}, \\ \left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_1(q, p) \right| &\leq c \hbar^{\frac{1}{2}-\delta},\end{aligned}\tag{5.1.7}$$

where the constant  $c$  depends on  $\|\nabla \varphi\|_{L^\infty}$  and  $\|\phi\|_{W^{s,\infty}}$ .

However, more effort is needed in estimate the residue for the semiclassical term. In particular, we insert the intermediate terms in  $\mathcal{R}_2$  as follows:

$$\begin{aligned}&\gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \\ &= \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \omega_{N,t}(u_1; w_1) \omega_{N,t}(u_2; w_2) \\ &\quad + [\omega_{N,t}(u_1; w_1) - \gamma_{N,t}^{(1)}(u_1; w_1)] \omega_{N,t}(u_2; w_2) \\ &\quad + \gamma_{N,t}^{(1)}(u_1; w_1) [\omega_{N,t}(u_2; w_2) - \gamma_{N,t}^{(1)}(u_2; w_2)] \\ &=: T_1 + T_2 + T_3.\end{aligned}\tag{5.1.8}$$

We observe that  $T_2$  and  $T_3$  can be estimated by the trace norm and Hilbert-Schmidt norm of  $\gamma_{N,t}^{(1)} - \omega_{N,t}$ , respectively. As shown in Lemma 5.2.1, the estimate for residue term involving  $T_1$  requires estimates of the following quantity due to the fast oscillation effect from the coherent state of the second particle:

$$\left( \iint dw_1 du_1 \left[ \int dw_2 \left| \gamma_{N,t}^{(2)}(w_1, w_2; u_1, w_2) - \omega_{N,t}(w_1; u_1) \omega_{N,t}(w_2; w_2) \right| \right]^2 \right)^{\frac{1}{2}}.\tag{5.1.9}$$

In [BPS14a], 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, we do not directly use Wick's theorem to compute (5.1.9) as extra effort is needed to estimate the residue term involving  $T_1$ . This is a different approach for the 2-particle reduced density matrix given in [BPS14a]. In particular, we trace the strategies given in [BPS14a] to obtain the rate of convergence estimate in the mean-field limit. After the Bogoliubov transformation, the main estimates are reduced to the expectation of the number operator  $\mathcal{N}$  along the quantum fluctuation which will be bounded under the assumption of Theorem 5.1.1.

From the assumption of Theorem 5.1.1, the moment estimate is the same as in chapter 3 which implies that the 1-particle Husimi measure is tight. Finally, we conclude the convergence by making the standard compactness argument as in chapter 4.

## 5.2 Estimate of mean field residue

Recall that the residue of the mean-field term is given by

$$\begin{aligned} \mathcal{R}_2 := & \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\ & \nabla V(q - q_2) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right]. \end{aligned}$$

Then, we obtain the following estimate.

**Proposition 5.2.1.** *Let  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ . Then, for  $\frac{1}{2} < \alpha < 1$ ,  $0 < \delta < \frac{3}{8}(\alpha - \frac{1}{2})$ , and  $s = \left\lceil \frac{3(2\alpha+1)}{4(1-\alpha)} \right\rceil$ , we have*

$$\left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2(q, p) \right| \leq \hat{C} h^{\frac{3}{2}(\alpha - \frac{1}{2})} \quad (5.2.1)$$

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

### 5.2.1 Proof of Proposition 5.2.1

To proof Proposition 5.2.1, we will first show some important estimates as preparation. In particular, denoting

$$\text{Tr}^{(1)} |\gamma^{(2)} - \gamma^{(1)} \otimes \gamma^{(1)}| := \int dy |\gamma^{(2)}(x, y; z, y) - \gamma^{(1)}(x; y) \gamma^{(1)}(z; y)|,$$

we have the following estimate,

**Lemma 5.2.1.** *Let  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ . Then, for  $\frac{1}{2} < \alpha_2 < 1$ ,  $0 < \delta < \frac{3}{4}(\alpha - \frac{1}{2})$ , and  $s = \left\lceil \frac{3(2\alpha+1)}{4(1-\alpha)} \right\rceil$ , we have*

$$\left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2(q, p) \right| \leq \hat{C} \|\nabla V\|_{L^\infty} \hbar^{3+\frac{3}{2}(\alpha_2+\frac{1}{2})+\frac{3}{2}} \cdot \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}, \quad (5.2.2)$$

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

*Proof.* Recall that from (4.2.1), we have

$$\begin{aligned} \mathcal{R}_2 := & (2\pi)^3 \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \nabla V(q - q_2) \\ & \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right]. \end{aligned} \quad (5.2.3)$$

Then, we have

$$\begin{aligned} & \left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2 \right| \\ &= \left| \int \dots \int (dq dp)^{\otimes 2} (dw du)^{\otimes 2} \varphi(q) \nabla \phi(p) \cdot \left( f_{q,p}^\hbar(w) \overline{f_{q,p}^\hbar(u)} \right)^{\otimes 2} \nabla V(q - q_2) \right. \\ & \quad \left. \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ &= \hbar^{-3} \left| \int \dots \int (dq dp)^{\otimes 2} (dw du)^{\otimes 2} \varphi(q) \nabla \phi(p) \cdot \left( f \left( \frac{w-q}{\sqrt{\hbar}} \right) f \left( \frac{u-q}{\sqrt{\hbar}} \right) e^{\frac{i}{\hbar} p \cdot (w-u)} \right)^{\otimes 2} \nabla V(q - q_2) \right. \\ & \quad \left. \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ &= \hbar^{-3} \left| \int \dots \int (dq dw du)^{\otimes 2} \left( f \left( \frac{w-q}{\sqrt{\hbar}} \right) f \left( \frac{u-q}{\sqrt{\hbar}} \right) \right)^{\otimes 2} \left( \int dp \varphi(q) \nabla \phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right) \right. \\ & \quad \left. \nabla V(q - q_2) \left( \int dp_2 e^{\frac{i}{\hbar} p_2 \cdot (w_2 - u_2)} \right) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right] \right| \\ &= (2\pi)^3 \left| \int \dots \int (dq)^{\otimes 2} dw_1 du_1 dw_2 f \left( \frac{w_1 - q}{\sqrt{\hbar}} \right) f \left( \frac{u_1 - q}{\sqrt{\hbar}} \right) \left| f \left( \frac{w_2 - q_2}{\sqrt{\hbar}} \right) \right|^2 \left( \int dp \varphi(q) \nabla \phi(p) \cdot e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \right) \right. \\ & \quad \left. \nabla V(q - q_2) \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right|, \end{aligned}$$

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

$$\frac{1}{(2\pi\hbar)^3} \int dp_2 e^{\frac{i}{\hbar} p_2 \cdot (w_2 - u_2)} = \delta_{w_2}(u_2). \quad (5.2.4)$$

Now, splitting the domains of  $w_1$  and  $u_1$  into two, namely, with the characteristic functions  $\chi_{(w_1 - u_1) \in \Omega_h}$  and  $\chi_{(w_1 - u_1) \in \Omega_h^c}$  as defined in (2.3.3), we have



$$\begin{aligned}
&\leq (2\pi)^3 \left| \iint (\mathrm{d}q)^{\otimes 2} \varphi(q) \iiint \mathrm{d}w_1 \mathrm{d}u_1 \mathrm{d}w_2 f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\
&\quad \left. \left( \int \mathrm{d}p \chi_{(w_1-u_1) \in \Omega_{\hbar}^c} e^{\frac{i}{\hbar} p \cdot (w_1-u_1)} \nabla \phi(p) \right) \cdot \nabla V(q-q_2) \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right| \\
&+ (2\pi)^3 \left| \iint (\mathrm{d}q)^{\otimes 2} \varphi(q) \iiint \mathrm{d}w_1 \mathrm{d}u_1 \mathrm{d}w_2 f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\
&\quad \left. \left( \int \mathrm{d}p \chi_{(w_1-u_1) \in \Omega_{\hbar}^c} e^{\frac{i}{\hbar} p \cdot (w_1-u_1)} \nabla \phi(p) \right) \cdot \nabla V(q-q_2) \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right| \\
&=: \mathbf{I}_2 + \mathbf{J}_2.
\end{aligned}$$

Without the loss of generality, we let  $\Phi(q, p) = \varphi(q)\phi(p)$ . First, considering the term  $\mathbf{J}_{2,1}$ ,

$$\begin{aligned}
\mathbf{J}_2 &= (2\pi)^3 \left| \iint \mathrm{d}q \mathrm{d}q_2 \varphi(q) \iiint \mathrm{d}w_1 \mathrm{d}u_1 \mathrm{d}w_2 f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\
&\quad \left. \left( \int \mathrm{d}p \chi_{(w_1-u_1) \in \Omega_{\hbar}^c} \nabla \phi(p) e^{\frac{i}{\hbar} p \cdot (w_1-u_1)} \right) \cdot \nabla V(q-q_2) \left( \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right) \right|.
\end{aligned}$$

By the change of variable  $\sqrt{\hbar} \tilde{q}_2 = w_2 - q_2$ , we obtain

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

Recall again from Lemma 2.3.3 that we have

$$\left| \int \mathrm{d}p \chi_{(w_1-u_1) \in \Omega_{\hbar}^c} e^{\frac{i}{\hbar} p \cdot (w_1-u_1)} \nabla \phi(p) \right| \leq \|\nabla \phi\|_{W^{s,\infty}} \hbar^{(1-\alpha_2)s}, \quad (5.2.5)$$

for  $s$  to be chosen later. Then, continuing from  $J_{2,1}$ ,

$$J_2 \leq C \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2}+(1-\alpha_2)s} \int dq |\varphi(q)| \iint dw_1 du_1 \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right| \\ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \chi_{|w_1-u_1| \leq 2R_1\sqrt{\hbar}},$$

The Hölder inequality yields

$$J_2 \leq C \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2}+(1-\alpha_2)s} \int dq |\varphi(q)| \left( \iint dw_1 du_1 \chi_{|w_1-u_1| \leq 2R_1\sqrt{\hbar}} \left| f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \right|^2 \right)^{\frac{1}{2}} \\ \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \\ = C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2}+(1-\alpha_2)s} \left( \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1-\tilde{u}_1| \leq 2R_1} |f(\tilde{w}) f(\tilde{u})|^2 \right)^{\frac{1}{2}} \\ \int dq \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \chi_{|w_1-q| \leq R_1\sqrt{\hbar}} \right)^{\frac{1}{2}} \\ \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3+(1-\alpha_2)s} \left( \iint d\tilde{w}_1 d\tilde{u}_1 |f(\tilde{w}) f(\tilde{u})|^2 \right)^{\frac{1}{2}} \\ \hbar^{\frac{3}{2}} \int d\tilde{q}_1 \chi_{|\tilde{q}_1| \leq R_1} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \\ \leq C \|f\|_{L^2}^2 \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3+(1-\alpha_2)s+\frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}},$$

where we denote

$$\text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) = \int dw_2 |\gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2)|.$$

Thus, we have

$$J_2 \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3+(1-\alpha_2)s+\frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}. \quad (5.2.6)$$

Now, we focus on  $I_{2,1}$

$$I_{2,1} = (2\pi)^3 \left| \iint (dq)^{\otimes 2} \varphi(q) \iiint dw_1 du_1 dw_2 f\left(\frac{w_1-q}{\sqrt{\hbar}}\right) f\left(\frac{u_1-q}{\sqrt{\hbar}}\right) \left| f\left(\frac{w_2-q_2}{\sqrt{\hbar}}\right) \right|^2 \right. \\ \left. \left( \int dp \chi_{(w_1-u_1) \in \Omega_{\hbar}} e^{\frac{i}{\hbar} p \cdot (w_1-u_1)} \nabla \phi(p) \right) \cdot \nabla V(q-q_2) \right. \\ \left. \left[ \gamma_{N,t}^{(2)}(u_1, w_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(w_2; w_2) \right] \right|.$$

We observe that

$$\left| \int dp e^{\frac{i}{\hbar} p \cdot (w_1 - u_1)} \nabla \phi(p) \right| \leq \|\nabla \phi\|_{L^1}.$$

Then, we obtain the following estimate:

$$\begin{aligned} I_2 &\leq C \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \int dq |\varphi(q)| \left( \iint dw_1 du_1 \chi_{|w_1 - u_1| \leq \hbar^{\alpha_2}} \chi_{|w_1 - u_1| \leq 2R_1 \sqrt{\hbar}} \left| f\left(\frac{w_1 - q}{\sqrt{\hbar}}\right) f\left(\frac{u_1 - q}{\sqrt{\hbar}}\right) \right|^2 \right)^{\frac{1}{2}} \\ &\quad \hbar^{\frac{3}{2}} \int d\tilde{q}_2 |f(\tilde{q}_2)|^2 \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \right)^{\frac{1}{2}} \\ &\leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \hbar^{\frac{3}{2}} \left( \hbar^3 \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_2 + \frac{1}{2}}} \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq 2R_1} |f(\tilde{w}_1) f(\tilde{u}_1)|^2 \right)^{\frac{1}{2}} \\ &\quad \int dq \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \chi_{|w_1 - q| \leq R_1 \sqrt{\hbar}} \right)^{\frac{1}{2}} \\ &\leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \hbar^3 \left( \iint d\tilde{w}_1 d\tilde{u}_1 \chi_{|\tilde{w}_1 - \tilde{u}_1| \leq \hbar^{\alpha_2 + \frac{1}{2}}} |f(\tilde{w}_1) f(\tilde{u}_1)|^2 \right)^{\frac{1}{2}} \\ &\quad \hbar^{\frac{3}{2}} \int d\tilde{q}_1 \chi_{|\tilde{q}_1| \leq R_1} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}. \end{aligned}$$

From (4.2.9), we have

$$I_2 \leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{L^1} \|\nabla V\|_{L^\infty} \hbar^{3 + \frac{3}{2}(\alpha_2 + \frac{1}{2}) + \frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}.$$

To balance the order between  $I_2$  and  $J_2$ ,  $s$  is chosen to be

$$s = \left\lceil \frac{3(2\alpha_2 + 1)}{4(1 - \alpha_2)} \right\rceil,$$

for  $\alpha_2 \in [0, 1)$ . Therefore, setting  $\beta_N = \hbar^\delta$ , we have

$$\begin{aligned} &\left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}_2 \right| \leq I_2 + J_2 \\ &\leq C \|\varphi\|_{L^\infty} \|\nabla \phi\|_{W^{s,\infty}} \|\nabla V\|_{L^\infty} \hbar^{3 + \frac{3}{2}(\alpha_2 + \frac{1}{2}) + \frac{3}{2}} \left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}}, \end{aligned}$$

and we obtained the desired result. ■

We estimate the equations above by the following proposition.

**Proposition 5.2.2.** *Let  $\gamma_{N,t}^{(k)}$  be  $k$ -particle reduced density associated with the evolved states  $\Psi_{N,t} = e^{-\frac{i}{\hbar} \mathcal{H}_N t} \Psi_N$ . Moreover, let  $\omega_N$  be sequence of projection as in (1.1.13) and  $\omega_{N,t}$  be the solution of the Hartree-Fock equa-*

tion in (1.1.15). Then, if  $\int dp (1 + |p|)^2 |\widehat{V}(p)| \leq C$ , it holds for all  $t \in \mathbb{R}$  that

$$\left\| \gamma_{N,t}^{(1)} - \omega_{N,t} \right\|_{HS} \leq C e^{c|t|}, \quad (5.2.7)$$

and

$$\left\| \gamma_{N,t}^{(1)} - \omega_{N,t} \right\|_{Tr} \leq C \sqrt{N} e^{c|t|}. \quad (5.2.8)$$

Furthermore, it holds that

$$\left( \iint dw_1 du_1 \left[ \text{Tr}_2^{(1)} \left| \gamma_{N,t}^{(2)} - \omega_{N,t} \otimes \omega_{N,t} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \leq C N e^{c|t|}, \quad (5.2.9)$$

where we denote the partial trace  $\text{Tr}_2^{(1)} |\omega_{N,t}(x_1, \cdot; y_1, \cdot)| := \int dx_2 |\omega_{N,t}(x_1, x_2; y_1, x_2)|$  and the constant  $c$  depends on potential  $V$ .

The prove of Proposition 5.2.2 is postponed to chapter 5.2.2.

More importantly, from Proposition 5.2.2, one may obtain the estimate for the factorization of 2-reduced particle density as follows.

**Corollary 5.2.1.** *Suppose the assumptions given in Proposition 5.2.2 hold. Then, we have the following estimate*

$$\left( \iint dw_1 du_1 \left[ \text{Tr}^{(1)} \left| \gamma_{N,t}^{(2)} - \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)} \right| (u_1; w_1) \right]^2 \right)^{\frac{1}{2}} \leq C_t N, \quad (5.2.10)$$

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

*Proof.* Inserting the intermediate terms as discussed in (5.1.8), we will arrive the sum of the following terms.

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

Then, the estimate in (5.2.10) is obtained directly from the fact that  $\left\| \omega_{N,t} \right\|_{Tr} \leq N$  and Proposition 5.2.2. ■

## 5.2.2 Proof of Proposition 5.2.2.

The proof for proposition 5.2.2 requires the following important results from [BPS14a].

**Lemma 5.2.2** (Lemma 3.1 of [BPS14a]). *Let  $d\Gamma(O)$  be the second quaziation of any bounded operator  $O$  on  $L^2(\mathbb{R}^3)$  as defined in (2.1.4) and  $\Psi \in \mathcal{F}_a$ . Then, the following inequalities hold*

$$\|d\Gamma(O)\Psi\| \leq \|O\| \|\mathcal{N}\Psi\|. \quad (5.2.11)$$

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

$$\|d\Gamma(O)\Psi\| \leq \|O\|_{HS} \|\mathcal{N}^{1/2}\Psi\|, \quad (5.2.12)$$

$$\left\| \int dx dy O(x; y) a_x a_y \Psi \right\| \leq \|O\|_{HS} \|\mathcal{N}^{1/2}\Psi\|, \quad (5.2.13)$$

$$\left\| \int dx dy O(x; y) a_x^* a_y^* \Psi \right\| \leq 2\|O\|_{HS} \|(\mathcal{N} + 1)^{1/2}\Psi\|. \quad (5.2.14)$$

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

$$\|d\Gamma(O)\Psi\| \leq 2\|O\|_{\text{Tr}}, \quad (5.2.15)$$

$$\left\| \int dx dy O(x; y) a_x a_y \Psi \right\| \leq 2\|O\|_{\text{Tr}}, \quad (5.2.16)$$

$$\left\| \int dx dy O(x; y) a_x^* a_y^* \Psi \right\| \leq 2\|O\|_{\text{Tr}}, \quad (5.2.17)$$

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

**Proposition 5.2.3** (Proposition 3.4 of [BPS14a]). *Let Assumption H4 holds and  $\omega_N$  be a non-negative trace class operator on  $L^2(\mathbb{R}^3)$  with  $\text{Tr} \omega_N = N$ ,  $\|\omega_N\|_{op} \leq 1$  and satisfies (5.1.1). Then, there exists a constants  $K, c > 0$  depending only on potential  $V$  such that*

$$\begin{aligned} \sup_{p \in \mathbb{R}^3} \frac{1}{1 + |p|} \text{Tr} |[\omega_{N,t}, e^{ip \cdot x}]| &\leq KN\hbar e^{c|t|} \\ \text{Tr} |[\omega_{N,t}, \hbar \nabla]| &\leq KN\hbar e^{c|t|} \end{aligned}$$

for all  $p \in \mathbb{R}^3$  and  $t \in \mathbb{R}$ .

Next, we modified the Theorem 3.2 of [BPS14a] to rid one of the two exponentials by using Ou-Iang's inequality. Namely,

**Proposition 5.2.4.** *Let  $\mathcal{U}_N(t; s)$  be the quantum fluctuation dynamics defined in (2.1.25) and  $\mathcal{N}$  be the number operator. If the assumptions in Proposition 5.2.3 and  $\langle \xi, \mathcal{N}^k \xi \rangle \leq C$  hold for any  $k \geq 1$ , then we have the following inequality:*

$$\|(\mathcal{N} + 1)^k \mathcal{U}_N(t; 0) \xi_N\| \leq C_t, \quad (5.2.18)$$

where  $C_t := K e^{c|t|}$  is a positive constant depending on  $t \in \mathbb{R}$ ,  $k$  and potential  $V$ .

*Proof.* Following equations (3.17) and (3.20) in [BPS14a, Lemma 3.5] we have

$$\left| i\hbar \frac{d}{dt} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \leq \hbar C_t |\langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle|. \quad (5.2.19)$$

Observe that since  $\|\omega_{N,t}\|_{\text{Tr}} = N$  and  $\|\Psi_{N,t}\| = 1$ , we have

$$\|(\mathcal{N} + 1)\mathcal{U}_N(t; 0)\xi_N\| \leq CN. \quad (5.2.20)$$

Then, from (5.2.19), we obtain

$$\hbar \frac{d}{dt} \|(\mathcal{N} + 1)\mathcal{U}_N(t; 0)\xi_N\|^2 \leq \hbar C_t N \|(\mathcal{N} + 1)\mathcal{U}_N(t; 0)\xi_N\|.$$

Dividing both side by  $\hbar$  and applying the Ou-Iang inequality [OY57], we obtain

$$\|(\mathcal{N} + 1)\mathcal{U}_N(t; 0)\xi_N\| \leq C_t N \|(\mathcal{N} + 1)\xi_N\|. \quad (5.2.21)$$

■

We are ready to prove Proposition 5.2.2.

*Proposition 5.2.2.* The proof of the inequalities (5.2.7) and (5.2.8) follows by modifying Theorem 2.1 of [BPS14a]. In particular, from equation (4.3) in [BPS14a], we obtain

$$\begin{aligned} \left\| \gamma_{N,t}^{(1)} - \omega_{N,t} \right\|_{\text{HS}} &\leq C \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0)\xi_N \right\|, \\ \left\| \gamma_{N,t}^{(1)} - \omega_{N,t} \right\|_{\text{Tr}} &\leq C \sqrt{N} \left\| \mathcal{N} \mathcal{U}_N(t; 0)\xi_N \right\|, \end{aligned}$$

by choosing the appropriate operator  $O$  as discussed in [BPS14a]. Our results for (5.2.7) and (5.2.8) are obtained by applying Proposition 5.2.4 and taking the assumption that  $\|(\mathcal{N} + 1)\xi_N\| \leq C$ .

Therefore, it remains to prove for (5.2.9). 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 [BPS14a]. For our term, however, we do not directly use Wick's theorem to compute (5.2.9) as each terms requires similar but still unique method when taking the estimation.

Simplifying the notation  $\mathcal{R}_t := \mathcal{R}_{\mathcal{V}_{N,t}}$ , we have, from the definition of a 2-particle reduced density matrix

and (2.1.19). that

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

where we use (2.1.19) in the third equality. Note that since  $\langle \bar{v}_{t,x}, \bar{v}_{t,y} \rangle = \omega_{N,t}(y; x)$ , it holds that

$$\begin{aligned}
& a(\bar{v}_{t,y_1}) a(\bar{v}_{t,y_2}) a^*(\bar{v}_{t,x_2}) a^*(\bar{v}_{t,x_1}) \\
&= a^*(\bar{v}_{t,x_1}) a(\bar{v}_{t,y_1}) a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_2}) + \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle a(\bar{v}_{t,y_1}) a^*(\bar{v}_{t,x_1}) \\
&\quad - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a(\bar{v}_{t,y_1}) a^*(\bar{v}_{t,x_2}) - \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_2}) \\
&= a^*(\bar{v}_{t,x_1}) a(\bar{v}_{t,y_1}) a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_2}) \\
&\quad - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle a^*(\bar{v}_{t,x_1}) a(\bar{v}_{t,y_1}) + \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle \\
&\quad + \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_1}) - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_2} \rangle \\
&\quad - \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_2}) \\
&= a^*(\bar{v}_{t,x_1}) a(\bar{v}_{t,y_1}) a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_2}) \\
&\quad - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle a^*(\bar{v}_{t,x_1}) a(\bar{v}_{t,y_1}) + \omega_{N,t}(x_1; y_1) \omega_{N,t}(x_2; y_2) \\
&\quad + \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_1}) - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_2} \rangle \\
&\quad - \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2}) a(\bar{v}_{t,y_2}).
\end{aligned}$$

Therefore, we obtain

$$\begin{aligned}
& \gamma_{N,t}^{(2)}(x_1, x_2; y_1, y_2) - \omega_{N,t}(x_1; y_1)\omega_{N,t}(x_2; y_2) \\
&= \left\langle \xi_N, \mathcal{U}_N^*(t; 0) \left[ a(\bar{v}_{t,y_1})a(u_{t,x_1})a(\bar{v}_{t,y_2})a(u_{t,x_2}) \right. \right. \\
&\quad + a(\bar{v}_{t,y_1})a(u_{t,x_1})a^*(u_{t,y_2})a(u_{t,x_2}) + a(\bar{v}_{t,y_1})a(u_{t,x_1})a^*(u_{t,y_2})a^*(\bar{v}_{t,x_2}) + a^*(\bar{v}_{t,x_1})a(\bar{v}_{t,y_1})a^*(u_{t,y_2})a(u_{t,x_2}) \\
&\quad + a^*(\bar{v}_{t,x_1})a(\bar{v}_{t,y_1})a^*(\bar{v}_{t,x_2})a^*(u_{t,y_2}) - a^*(u_{t,y_1})a(u_{t,x_1})a(\bar{v}_{t,y_2})a(u_{t,x_2}) + a^*(u_{t,y_1})a(u_{t,x_1})a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_2}) \\
&\quad + a^*(u_{t,y_1})a^*(\bar{v}_{t,x_1})a(\bar{v}_{t,y_2})a(u_{t,x_2}) + a^*(\bar{v}_{t,x_1})a^*(u_{t,y_1})a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_2}) + a^*(u_{t,y_1})a(u_{t,x_1})a^*(u_{t,y_2})a(u_{t,x_2}) \\
&\quad + a^*(u_{t,y_1})a(u_{t,x_1})a^*(u_{t,y_2})a^*(\bar{v}_{t,x_2}) + a^*(u_{t,y_1})a^*(\bar{v}_{t,x_1})a^*(u_{t,y_2})a^*(\bar{v}_{t,x_2}) + a^*(\bar{v}_{t,x_1})a(\bar{v}_{t,y_1})a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_2}) \\
&\quad - a^*(\bar{v}_{t,x_1})a(\bar{v}_{t,y_1})a(u_{t,x_2})a(\bar{v}_{t,y_2}) + a^*(u_{t,y_1})a^*(\bar{v}_{t,x_1})a^*(u_{t,y_2})a(u_{t,x_2}) - a(u_{t,x_1})a(\bar{v}_{t,y_1})a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_2}) \\
&\quad - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a(\bar{v}_{t,y_1})a(u_{t,x_2}) + \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a(\bar{v}_{t,y_2})a(u_{t,x_2}) \\
&\quad - \langle u_{t,x_1}, u_{t,y_2} \rangle a(\bar{v}_{t,y_1})a(u_{t,x_2}) + \langle u_{t,x_1}, u_{t,y_2} \rangle a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_1}) - \langle u_{t,x_1}, u_{t,y_2} \rangle \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_2} \rangle \\
&\quad + \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a^*(u_{t,y_2})a(u_{t,x_2}) + \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a^*(u_{t,y_2})a^*(\bar{v}_{t,x_2}) \\
&\quad - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a^*(u_{t,y_1})a(u_{t,x_2}) - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a^*(u_{t,y_1})a^*(\bar{v}_{t,x_2}) \\
&\quad - \langle u_{t,x_1}, u_{t,y_2} \rangle a^*(u_{t,y_1})a(u_{t,x_2}) - \langle u_{t,x_1}, u_{t,y_2} \rangle a^*(u_{t,y_1})a^*(\bar{v}_{t,x_2}) \\
&\quad - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle a^*(\bar{v}_{t,x_1})a(\bar{v}_{t,y_1}) + \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_1}) \\
&\quad + \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle a^*(u_{t,y_1})a(u_{t,x_1}) - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_2} \rangle a^*(\bar{v}_{t,x_1})a^*(u_{t,y_1}) \\
&\quad \left. \left. - \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_1} \rangle a^*(\bar{v}_{t,x_2})a(\bar{v}_{t,y_2}) - \langle \bar{v}_{t,y_2}, \bar{v}_{t,x_1} \rangle \langle \bar{v}_{t,y_1}, \bar{v}_{t,x_2} \rangle \right] \mathcal{U}_N(t; 0)\xi_N \right\rangle,
\end{aligned}$$

where we used the fact that  $\langle \bar{v}_{t,x}, u_{t,y} \rangle = 0$ ,  $\langle u_{t,x}, \bar{v}_{t,y} \rangle = 0$  and CAR.

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



$$\begin{aligned}
& + \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_1} \rangle a^*(u_{t,x_2})a(u_{t,z_2}) + \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_1} \rangle a^*(u_{t,x_2})a^*(\bar{v}_{t,z_2}) \\
& - \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_1} \rangle a^*(u_{t,x_1})a(u_{t,z_2}) - \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_1} \rangle a^*(u_{t,x_1})a^*(\bar{v}_{t,z_2}) \\
& - \langle u_{t,z_1}, u_{t,x_2} \rangle a^*(u_{t,x_1})a(u_{t,z_2}) - \langle u_{t,z_1}, u_{t,x_2} \rangle a^*(u_{t,x_1})a^*(\bar{v}_{t,z_2}) \\
& - \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_2} \rangle a^*(\bar{v}_{t,z_1})a(\bar{v}_{t,x_1}) + \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_1} \rangle a^*(\bar{v}_{t,z_2})a(\bar{v}_{t,x_1}) \\
& + \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_2} \rangle a^*(u_{t,x_1})a(u_{t,z_1}) - \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_2} \rangle a^*(\bar{v}_{t,z_1})a^*(u_{t,x_1}) \\
& - \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_1} \rangle a^*(\bar{v}_{t,z_2})a(\bar{v}_{t,x_2}) - \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_1} \rangle \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_2} \rangle \mathcal{U}_N(t;0)\xi_N \Big\rangle \\
& =: \sum_{i=1}^{16} A_i + \sum_{j=1}^{16} B_j + \mathcal{C}.
\end{aligned}$$

Using the fact that  $\|u_t\|_{\text{op}}, \|v_t\|_{\text{op}} \leq 1$ ,  $\|v_t\|_{\text{HS}} \leq \sqrt{N}$ ,  $\|\omega_{N,t}\|_{\text{Tr}} = N$ , inequality in (5.2.20) and the assumption  $\|\xi_N\| \leq 1$ , we compute the first two estimates each from  $\{A_i\}_{i=1}^{16}$  and  $\{B_i\}_{i=1}^{16}$ . The estimates for the rest of the terms can be done with similar steps.

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

$$\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| (\mathcal{N} + 1)^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\|.$$

$$\begin{aligned}
& |A_2| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a(\bar{v}_{t, x_1}) a(u_{t, z_1}) a^*(u_{t, x_2}) a(u_{t, z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 \langle \xi_N, U_N^*(t; 0) O_1(x_1; z_1) O_2(x_2; z_2) \iint d\eta_1 d\eta'_1 a_{\eta_1} a_{\eta'_1} v_t(\eta_1; x_1) \overline{u_t(\eta'_1; z_1)} \right. \\
&\quad \left. \iint d\eta_2 d\eta'_2 a_{\eta_2}^* a_{\eta'_2} u_t(\eta_2; x_2) \overline{u_t(\eta'_2; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 \langle \xi_N, U_N^*(t; 0) \iint 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. \iint d\eta_2 d\eta'_2 a_{\eta_2}^* a_{\eta'_2} u_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| \langle \xi_N, U_N^*(t; 0) \iint d\eta_1 d\eta'_1 a_{\eta_1} a_{\eta'_1} (v_t O_1 u_t)(\eta_1; \eta'_1) \iint d\eta_2 d\eta'_2 a_{\eta_2}^* a_{\eta'_2} (u_t O_2 u_t)(\eta_2; \eta'_2) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \int d\eta_1 \langle a^*(\bar{v}_t O_1 u_t)(\eta_1; \eta'_1) a_{\eta_1}^* \mathcal{U}_N(t; 0) \xi_N, d\Gamma(u_t O_2 u_t) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \int d\eta_1 \|v_t O_1 u_t\|_2 \|a_{\eta_1}^* \mathcal{U}_N(t; 0) \xi_N\| \|d\Gamma(u_t O_2 u_t) \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq \|v_t O_1 u_t\|_{\text{HS}} \left( \int d\eta_1 \langle \xi_N, \mathcal{U}_N^*(t; 0) a_{\eta_1} a_{\eta_1}^* \mathcal{U}_N(t; 0) \xi_N \rangle \right)^{\frac{1}{2}} \|u_t O_2 u_t\|_{\text{op}} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq \|v_t\|_{\text{op}} \|O_1\|_{\text{HS}} \|u_t\|_{\text{op}} \|u_t\|_{\text{op}} \|O_2\|_{\text{op}} \|u_t\|_{\text{op}} \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\| \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\|.
\end{aligned}$$

$$\begin{aligned}
& |A_3| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a(\bar{v}_{t, x_1}) a(u_{t, z_1}) a^*(u_{t, x_2}) a^*(\bar{v}_{t, z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|v_t O_1 u_t\|_{\text{HS}} \|u_t O_2 \bar{v}_t\|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|(\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N\|.
\end{aligned}$$

$$|A_4|$$

$$\begin{aligned}
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\bar{v}_{t,z_1}) a(\bar{v}_{t,x_1}) a^*(u_{t,x_2}) a(u_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \bar{v}_t \overline{O_1^*} v_t \|_{\text{op}} \| u_t O_2 u_t \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

$$\begin{aligned}
&|A_5| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\bar{v}_{t,z_1}) a(\bar{v}_{t,x_1}) a^*(\bar{v}_{t,z_2}) a^*(u_{t,x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \bar{v}_t \overline{O_1^*} v_t \|_{\text{HS}} \| \bar{v}_t \overline{O_2^*} \bar{u}_t \|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

$$\begin{aligned}
&|A_6| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(u_{t,x_1}) a(u_{t,z_1}) a(\bar{v}_{t,x_2}) a(u_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| u_t O_1 u_t \|_{\text{op}} \| v_t O_2 u_t \|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

$$\begin{aligned}
&|A_7| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(u_{t,x_1}) a(u_{t,z_1}) a^*(\bar{v}_{t,z_2}) a(\bar{v}_{t,x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| u_t O_1 u_t \|_{\text{op}} \| v_t \overline{O_2^*} v_t \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

$$|A_8|$$

$$\begin{aligned}
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_1}) a(\bar{\mathbf{v}}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \mathbf{u}_t O_1 \bar{\mathbf{v}}_t \|_{\text{HS}} \| \mathbf{v}_t O_2 \mathbf{u}_t \|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq \sqrt{N} \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
&|A_9| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\bar{\mathbf{v}}_{t,z_1}) a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) a(\bar{\mathbf{v}}_{t,x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \bar{\mathbf{v}}_t \overline{O_1^*} \bar{\mathbf{u}}_t \|_{\text{HS}} \| \bar{\mathbf{v}}_t \overline{O_2^*} \bar{\mathbf{v}}_t \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \\
&\leq \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

$$\begin{aligned}
&|A_{10}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a(\mathbf{u}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \mathbf{u}_t O_1 \mathbf{u}_t \|_{\text{op}} \| \mathbf{u}_t O_2 \mathbf{u}_t \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

$$\begin{aligned}
&|A_{11}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\mathbf{u}_{t,x_1}) a(\bar{\mathbf{v}}_{t,z_1}) a^*(\mathbf{u}_{t,x_2}) a^*(\bar{\mathbf{v}}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \mathbf{u}_t O_1 \mathbf{u}_t \|_{\text{HS}} \| \mathbf{u}_t O_2 \bar{\mathbf{v}}_t \|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \\
&\leq \sqrt{N} \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \left\| (\mathcal{N} + 1)^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
& |A_{12}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(u_{t,x_1}) a^*(\bar{v}_{t,z_1}) a^*(u_{t,x_2}) a^*(\bar{v}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|u_t O_1 v_t\|_{\text{HS}} \|u_t O_2 \bar{v}_t\|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| (\mathcal{N} + 1)^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
& |A_{13}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\bar{v}_{t,z_1}) a(\bar{v}_{t,x_1}) a^*(\bar{v}_{t,z_2}) a(\bar{v}_{t,x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|\bar{v}_t \bar{O}_1^* v_t\|_{\text{op}} \|\bar{v}_t \bar{O}_2^* v_t\|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\|.
\end{aligned}$$

$$\begin{aligned}
& |A_{14}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(\bar{v}_{t,z_1}) a(\bar{v}_{t,x_1}) a(u_{t,z_2}) a(\bar{v}_{t,x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|\bar{v}_t \bar{O}_1^* v_t\|_{\text{HS}} \|\bar{u}_t \bar{O}_2^* v_t\|_{\text{HS}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \\
&\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
& |A_{15}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a^*(u_{t,x_1}) a^*(\bar{v}_{t,z_1}) a^*(u_{t,x_2}) a(u_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|u_t O_1 \bar{v}_t\|_{\text{HS}} \|u_t O_2 u_t\|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\|.
\end{aligned}$$

$$\begin{aligned}
& |A_{16}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0) a(\mathbf{u}_{t, z_1}) a(\bar{\mathbf{v}}_{t, x_1}) a^*(\bar{\mathbf{v}}_{t, z_2}) a(\bar{\mathbf{v}}_{t, x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \bar{\mathbf{u}}_t \bar{O}_1^* \bar{\mathbf{v}}_t \|_{\text{HS}} \| \bar{\mathbf{v}}_t \bar{O}_1^* \mathbf{v}_t \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) \mathcal{N}^2 \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1) \mathcal{U}_N(t; 0) \xi_N \rangle^{\frac{1}{2}} \\
&\leq \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \langle \xi_N, \mathcal{U}_N^*(t; 0) (\mathcal{N} + 1)^2 \mathcal{U}_N(t; 0) \xi_N \rangle \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

Additionally, we have

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

$$\begin{aligned}
& |B_2| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{\mathbf{v}}_{t, x_1}, \bar{\mathbf{v}}_{t, z_1} \rangle a(\bar{\mathbf{v}}_{t, x_2}) a(\mathbf{u}_{t, z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \overline{\omega_{N, t}(x_1; z_1)} \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta a_{\eta'} \mathbf{v}_t(\eta; x_2) \overline{\mathbf{u}_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right|
\end{aligned}$$

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

where we use the fact that

$$|\text{Tr } O_1 \omega_{N,t}| \leq \|O_1 \omega_{N,t}\|_{\text{Tr}} \leq \|O_1\|_{\text{HS}} \|\omega_{N,t}\|_{\text{HS}} \leq \sqrt{N} \|O_1\|_{\text{HS}}.$$

$$\begin{aligned}
&|B_3| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle u_{t,z_1}, u_{t,x_2} \rangle a(\bar{v}_{t,x_1}) a(u_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), u_t(z_1; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta a_{\eta'} v_t(\eta; x_1) \overline{u_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 \iint d\eta d\eta' \langle \xi_N, \mathcal{U}_N^*(t; 0), a_\eta a_{\eta'} \right. \\
&\quad \left. v_t(\eta; x_1) O_1(x_1; z_1) u_t(z_1; x_2) O_2(x_2; z_2) u_t(z_2; \eta') \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint d\eta d\eta' \langle \xi_N, \mathcal{U}_N^*(t; 0), a_\eta a_{\eta'} (v_t O_1 u_t O_2 u_t)(\eta; \eta') \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|v_t O_1 u_t O_2 u_t\|_{\text{HS}} \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
&|B_4| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle u_{t,z_1}, u_{t,x_2} \rangle a^*(\bar{v}_{t,z_2}) a(\bar{v}_{t,x_1}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|v_t O_1 u_t O_2 \bar{v}_t\|_{\text{HS}} \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\|
\end{aligned}$$

$$\leq \|O_1\|_{\text{HS}}\|O_2\|_{\text{op}}\left\|\mathcal{N}^{1/2}\mathcal{U}_N(t;0)\xi_N\right\|.$$

$$\begin{aligned} & |B_5| \\ &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \mathbf{u}_{t, z_1}, \mathbf{u}_{t, x_2} \rangle \langle \bar{\mathbf{v}}_{t, x_1}, \bar{\mathbf{v}}_{t, z_2} \rangle \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \mathbf{u}_t(z_1; x_2) \omega_{N, t}(z_2; x_1) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \langle \xi_N, \mathcal{U}_N^*(t; 0), \iint dx_1 dx_2 (O_1 \mathbf{u}_t)(x_1; x_2) (O_2 \omega_{N, t})(x_2; x_1) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \langle \xi_N, \mathcal{U}_N^*(t; 0), \int dx_1 (O_1 \mathbf{u}_t O_2 \omega_{N, t})(x_1; x_1) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &\leq \|O_1 \mathbf{u}_t O_2\|_{\text{HS}} \|\omega_{N, t}\|_{\text{HS}} \\ &\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}}. \end{aligned}$$

$$\begin{aligned} & |B_6| \\ &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{\mathbf{v}}_{t, x_1}, \bar{\mathbf{v}}_{t, z_1} \rangle a^*(\mathbf{u}_{t, x_2}) a(\mathbf{u}_{t, z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N, t}(z_1; x_1) \right. \\ &\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} \mathbf{u}_t(\eta; x_2) \overline{\mathbf{u}_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \iint d\eta d\eta' \langle \xi_N, \mathcal{U}_N^*(t; 0), \int dx_1 (O_1 \omega_{N, t})(x_1; x_1) a_\eta^* a_{\eta'} (\mathbf{u}_t O_2 \mathbf{u}_t)(\eta; \eta') \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &\leq \|O_1\|_{\text{HS}} \|\omega_{N, t}\|_{\text{HS}} \|\mathbf{u}_t O_2 \mathbf{u}_t\|_{\text{op}} \|\xi_N\| \left\|\mathcal{N}^{1/2}\mathcal{U}_N(t;0)\xi_N\right\| \\ &\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\|\mathcal{N}^{1/2}\mathcal{U}_N(t;0)\xi_N\right\| \end{aligned}$$

$$\begin{aligned} & |B_7| \\ &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{\mathbf{v}}_{t, x_1}, \bar{\mathbf{v}}_{t, z_1} \rangle a^*(\mathbf{u}_{t, x_2}) a^*(\bar{\mathbf{v}}_{t, z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\ &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N, t}(z_1; x_1) \right. \\ &\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'}^* \mathbf{u}_t(\eta; x_2) \overline{\mathbf{v}_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \end{aligned}$$



$$\begin{aligned}
&\leq \|O_1\|_{\text{HS}}\|\omega_{N,t}\|_{\text{HS}}\|\mathbf{u}_t O_2 \bar{\mathbf{v}}_t\|_{\text{HS}}\|\xi\|\left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t;0)\xi_N\right\| \\
&\leq \sqrt{N}\|O_1\|_{\text{HS}}\|\mathbf{u}_t\|_{\text{op}}\|O_2\|_{\text{op}}\|\mathbf{v}_t\|_{\text{HS}}\|\xi_N\|\left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t;0)\xi_N\right\| \\
&\leq N\|O_1\|_{\text{HS}}\|O_2\|_{\text{op}}\left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t;0)\xi_N\right\|.
\end{aligned}$$

$$\begin{aligned}
&|B_8| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N,t}(z_1; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} \mathbf{u}_t(\eta; x_1) \overline{\mathbf{u}_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|\mathbf{u}_1 O_1 \omega_{N,t} O_2 \mathbf{u}_t\|_{\text{op}} \|\xi\| \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq \|O_1\|_{\text{op}} \|O_2\|_{\text{op}} \|\omega_{N,t}\|_{\text{op}} \|\xi_N\| \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\xi\| \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\|.
\end{aligned}$$

$$\begin{aligned}
&|B_9| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{\mathbf{v}}_{t,x_2}, \bar{\mathbf{v}}_{t,z_1} \rangle a^*(\mathbf{u}_{t,x_1}) a^*(\bar{\mathbf{v}}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N,t}(z_1; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} \mathbf{u}_t(\eta; x_1) \overline{\mathbf{v}_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|\mathbf{u}_t O_1 \bar{\omega}_{N,t} O_2 \bar{\mathbf{v}}_t\|_{\text{HS}} \|\xi_N\| \left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t;0)\xi_N\right\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t;0)\xi_N\right\|.
\end{aligned}$$

$$\begin{aligned}
&|B_{10}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \mathbf{u}_{t,z_1}, \mathbf{u}_{t,x_2} \rangle a^*(\mathbf{u}_{t,x_1}) a(\mathbf{u}_{t,z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \mathbf{u}_t(z_1; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} \mathbf{u}_t(\eta; x_1) \overline{\mathbf{u}_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right|
\end{aligned}$$

$$\begin{aligned}
&\leq \|u_t O_1 u_t O_2 u_t\|_{\text{HS}} \|\xi_N\| \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
&|B_{11}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle u_{t, z_1}, u_{t, x_2} \rangle a^*(u_{t, x_1}) a^*(\bar{v}_{t, z_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), u_t(z_1; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'}^* u_t(\eta; x_1) \overline{v_t(\eta'; z_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|u_t O_1 u_t O_2 \bar{v}_t\|_{\text{HS}} \|\xi_N\| \left\| (\mathcal{N} + 1)^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| (\mathcal{N} + 1)^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
&|B_{12}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{v}_{t, x_2}, \bar{v}_{t, z_1} \rangle a^*(\bar{v}_{t, z_1}) a(\bar{v}_{t, x_1}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N, t}(z_2; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'}^* \overline{v_t(\eta; z_1)} v_t(\eta'; x_1) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|O_2\|_{\text{op}} \|\omega_{N, t}\|_{\text{Tr}} \|\bar{v}_t \bar{O}_1^* v_t\|_{\text{op}} \|\xi_N\| \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\| \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\mathcal{N} \mathcal{U}_N(t; 0) \xi_N\|.
\end{aligned}$$

$$\begin{aligned}
&|B_{13}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{v}_{t, x_2}, \bar{v}_{t, z_1} \rangle a^*(\bar{v}_{t, z_2}) a(\bar{v}_{t, x_1}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N, t}(z_1; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'}^* \overline{v_t(\eta; z_2)} v_t(\eta'; x_1) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \|\bar{v}_t \bar{O}_2^* \bar{\omega}_{N, t} \bar{O}_1^* v_t\|_{\text{HS}} \|\xi_N\| \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
& |B_{14}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_2} \rangle a^*(u_{t,x_1}) a(u_{t,z_1}) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N,t}(z_2; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} u_t(\eta; x_1) \overline{u_t(\eta)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| \bar{v}_t \overline{O_2^*} \omega_{N,t} \overline{O_1^*} v_t \|_{\text{HS}} \| \xi_N \| \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \left\| \mathcal{N}^{1/2} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
& |B_{15}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_2} \rangle a^*(\bar{v}_{t,z_1}) a^*(u_{t,x_1}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N,t}(z_2; x_2) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} \overline{v_t(\eta; z_1) u_t(x_1; \eta')} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| O_2 \omega_{N,t} \|_{\text{Tr}} \| \bar{v}_t \overline{O_1^*} \bar{u}_t \|_{\text{HS}} \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq \| O_1 \|_{\text{HS}} \| \omega_{N,t} \|_{\text{HS}} \| v_t \|_{\text{HS}} \| O_2 \|_{\text{op}} \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\| \\
&\leq N \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \left\| \mathcal{N}^{\frac{1}{2}} \mathcal{U}_N(t; 0) \xi_N \right\|.
\end{aligned}$$

$$\begin{aligned}
& |B_{16}| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_1} \rangle a^*(\bar{v}_{t,z_2}) a(\bar{v}_{t,x_2}) \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t; 0), \omega_{N,t}(z_1; x_1) \right. \\
&\quad \left. \iint d\eta d\eta' a_\eta^* a_{\eta'} \overline{v_t(\eta; z_2) v_t(\eta'; x_2)} \mathcal{U}_N(t; 0) \xi_N \rangle \right| \\
&\leq \| O_1 \|_{\text{HS}} \| \omega_{N,t} \|_{\text{HS}} \| \bar{v}_t \overline{O_2^*} v_t \|_{\text{op}} \| \xi_N \| \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \| \\
&\leq \sqrt{N} \| O_1 \|_{\text{HS}} \| O_2 \|_{\text{op}} \| \mathcal{N} \mathcal{U}_N(t; 0) \xi_N \|.
\end{aligned}$$

In summary, we have so far the following estimates

$$\begin{aligned}
\left| \sum_{i=1}^{16} A_i \right| &\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|\mathcal{N}\mathcal{U}_N(t;0)\xi_N\|, \\
\left| \sum_{j=1}^{16} B_j \right| &\leq \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \left( N \left\| (\mathcal{N}+1)^{1/2} \mathcal{U}_N(t;0)\xi_N \right\| + \sqrt{N} \|(\mathcal{N}+1)\mathcal{U}_N(t;0)\xi_N\| \right) \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|(\mathcal{N}+1)\mathcal{U}_N(t;0)\xi_N\|.
\end{aligned} \tag{5.2.22}$$

Lastly, we compute for the final term.

$$\begin{aligned}
|C| &= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t;0) \langle \bar{v}_{t,x_2}, \bar{v}_{t,z_1} \rangle \langle \bar{v}_{t,x_1}, \bar{v}_{t,z_2} \rangle \mathcal{U}_N(t;0)\xi_N \rangle \right| \\
&= \left| \iint dx_1 dx_2 \iint dz_1 dz_2 O_1(x_1; z_1) O_2(x_2; z_2) \langle \xi_N, \mathcal{U}_N^*(t;0) \omega_{N,t}(z_1; x_2) \omega_{N,t}(z_2; x_1) \mathcal{U}_N(t;0)\xi_N \rangle \right| \\
&= \left| \int dx_2 \langle \xi_N, \mathcal{U}_N^*(t;0) (O_1 \omega_{N,t} O_2 \omega_{N,t})(x_2; x_2) \mathcal{U}_N(t;0)\xi_N \rangle \right| \\
&= \left| \left\langle \xi_N, \mathcal{U}_N^*(t;0) \left( \int dx_2 (\bar{\omega}_{N,t} \bar{O}_1^* \bar{\omega}_{N,t} \bar{O}_2^*)(x_2; x_2) \right) \mathcal{U}_N(t;0)\xi_N \right\rangle \right| \\
&\leq \|O_1 \omega_{N,t} O_2 \omega_{N,t}\|_{\text{Tr}} |\langle \xi_N, \mathcal{U}_N^*(t;0) \mathcal{U}_N(t;0)\xi_N \rangle| \\
&\leq \|O_1 \omega_{N,t}\|_{\text{HS}} \|O_2 \omega_{N,t}\|_{\text{HS}} \\
&\leq \|O_1\|_{\text{HS}} \|\omega_{N,t}\|_{\text{op}} \|O_2\|_{\text{op}} \|\omega_{N,t}\|_{\text{HS}} \\
&\leq \sqrt{N} \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\left| \text{Tr } O(\gamma_{N,t}^{(2)} - \omega_{N,t} \otimes \omega_{N,t}) \right| &\leq \left| \sum_{i=1}^{16} A_i \right| + \left| \sum_{j=1}^{16} B_j \right| + |C| \\
&\leq N \|O_1\|_{\text{HS}} \|O_2\|_{\text{op}} \|(\mathcal{N}+1)\mathcal{U}_N(t;0)\xi_N\|,
\end{aligned} \tag{5.2.23}$$

which implies that, for  $O_1$  and  $O_2$  be Hilbert-Schmidt and trace class operator, we get

$$\begin{aligned}
&\left( \iint dx_1 dy_1 \left[ \int dx_2 \left| \gamma_{N,t}^{(2)}(x_1, x_2; y_1, x_2) - \omega_{N,t}(x_1; y_1) \omega_{N,t}(x_2; x_2) \right| \right]^2 \right)^{\frac{1}{2}} \\
&\leq N \|(\mathcal{N}+1)\mathcal{U}_N(t;0)\xi_N\|.
\end{aligned} \tag{5.2.24}$$

Applying Proposition 5.2.4, we obtain the inequalities in Proposition 5.2.2 as desired. ■

Finally, combining the estimates from Lemma 5.2.1 and Proposition 5.2.2, we conclude the proof of Proposition 5.2.1.  $\blacksquare$

### 5.3 Proof of main theorem 5.1.1

Now we complete the proof for the main theorem. Recall the Vlasov equation with remainder terms is given as,

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

where  $\varrho_{N,t}(q) := \int dp m_{N,t}(q, p)$ ,  $\tilde{\mathcal{R}}$  and  $\mathcal{R} := \mathcal{R}_1 + \mathcal{R}_2$  are given by

$$\begin{aligned} \tilde{\mathcal{R}} &:= \hbar \operatorname{Im} \langle \nabla_q a(f_{q,p}^h) \Psi_{N,t}, a(f_{q,p}^h) \Psi_{N,t} \rangle, \\ \mathcal{R}_1 &:= \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\ &\quad \left[ \int_0^1 ds \nabla V(su_1 + (1-s)w_1 - w_2) - \nabla V(q - q_2) \right] \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2), \\ \mathcal{R}_2 &:= \frac{1}{(2\pi)^3} \iint dw_1 du_1 \iint dw_2 du_2 \iint dq_2 dp_2 \left( f_{q,p}^h(w) \overline{f_{q,p}^h(u)} \right)^{\otimes 2} \\ &\quad \nabla V(q - q_2) \left[ \gamma_{N,t}^{(2)}(u_1, u_2; w_1, w_2) - \gamma_{N,t}^{(1)}(u_1; w_1) \gamma_{N,t}^{(1)}(u_2; w_2) \right]. \end{aligned}$$

Then, from Proposition 3.2.4, Proposition 3.2.5 and Proposition 5.2.1, there exists  $s(\delta) > 0$  such that, for an arbitrarily small  $\delta > 0$ , the following estimates holds for any test function  $\varphi, \phi \in C_0^\infty(\mathbb{R}^3)$ ,

$$\begin{aligned} \left| \iint dq dp \varphi(q) \phi(p) \nabla_q \cdot \tilde{\mathcal{R}}(q, p) \right| &\leq c \hbar^{\frac{1}{2}-\delta}, \\ \left| \iint dq dp \varphi(q) \phi(p) \nabla_p \cdot \mathcal{R}(q, p) \right| &\leq c \hbar^{\frac{1}{2}-\delta}, \end{aligned} \tag{5.3.1}$$

where the constant  $c$  depends on  $\|\nabla \varphi\|_{L^\infty}$ ,  $\|\phi\|_{W^{s,\infty}}$ ,  $V$ , and  $t$ .

Furthermore, since from (5.0.1) and Assumption H4, we have  $\|\nabla V\|_\infty \leq \int (1+|p|)^2 |\hat{V}(p)| dp < \infty$ . Then, we obtain the same moment estimates from Proposition 3.2.3. Namely,

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

where  $C$  is a constant dependent on  $\iint dq dp (|q| + |p|^2) m_N(q_1, p_1)$ , and  $V$ . Therefore, by the similar compactness argument made in chapter 4.1.3, we obtain the desired convergence result in Theorem 5.1.1.  $\blacksquare$

# Chapter 6

## Summary & future research

### 6.1 Summary

The study of deriving the effective equation for many-particle systems at quantum scale is very crucial due to limitations of computational power. As the existing literature on this topic for large fermionic system often centers around the use of the Wigner measure, a pseudo-probability measure, this thesis set out to study the macroscopic dynamics with respect of Husimi measure instead. In this regard, we have derived in chapter 3 the full structure of the Vlasov hierarchy from the time-dependent Schrödinger equation with respect to the Husimi measure for  $N$ -fermionic system. Then, by estimating the residual terms arose from the aforementioned hierarchy structure, we prove that the Husimi measure converges to Vlasov equation in terms of 1-Wasserstein distance with a regularized interaction potential. In chapter 4, we extend our convergence result to the Vlasov-Poisson equation by assuming the interaction potential to be a truncated Coulomb potential for repulsive case. Finally, with the help of preceding results, we prove in chapter 5 the convergence from Schrödinger equation to Vlasov equation by using the Bogoliubov transformation instead of BBGKY hierarchy, giving us a different method compared to the preceding chapters.

Furthermore, the distinguishing features of our research in comparison to the existing literature can be summarized as follows:

1. Derivation of Vlasov hierarchy from many-fermionic Schrödinger equation with respect to Husimi measure.
2. In contrast to [Spo81] where BBGKY hierarchy method is applied directly at  $k$ -reduced density matrices, we used the Husimi measure with combination of second quantization and the BBGKY hierarchy method

3. Compared to [Spo81], the assumption on the interaction potential is slightly relaxed from  $C^2(\mathbb{R}^3)$  to  $W^{2,\infty}(\mathbb{R}^3)$ .
4. The assumption of interaction potential is further relaxed to truncated Coulomb potential (repulsive), yielding the convergence result from  $N$ -fermionic Schrödinger equation to the Vlasov-Poisson equation in the sense of distribution.
5. For the result of convergence from  $N$ -fermionic Schrödinger equation to Vlasov-Poisson equation, the assumption on moments is more relaxed compared to [PRSS17, Saf20b].
6. Convergence from the large fermionic system to Vlasov equation with help of Bogoliubov transformation in the sense of distribution.
7. Estimation of the 2-reduced density matrices with respect to mixed norm as shown in 5.2.9, an extension to result in [BPS14a].
8. The convergence results hold in terms of 1-Wasserstein distance.

## 6.2 Research prospective

In [GP17, GP19, GP21], the convergence rate in terms of 2-Wasserstein pseudometric was obtained from the many-fermionic Schrödinger equation to Vlasov equation under higher moment assumption. In this thesis, we have shown our convergence results for Vlasov and Vlasov-Poisson equation can be extended to 1-Wasserstein distance due to the moment results we obtained in Proposition 3.2.3 and in Proposition 4.1.1 for the repulsive case respectively. It is therefore possible to obtain the convergence rate in terms of 1-Wasserstein distance by first reformulating the Vlasov equation into a transport equation and obtain the convergence rate by making use of the Drobrushin's estimate similar to the steps given in [GP17, GP19, GP21].

One may also consider other Schrödinger equations such as the relativistic or magnetic field case. In [DRS18], the mean-field convergence from Hartree to relativistic Vlasov has been obtained for bosonic particles where they make use of Taylor's expansion on the relativistic term. It is therefore possible to following similar steps to obtain the case for fermionic system.

Recently in [CLS21], it has been remarked that  $\hbar$  can be allowed in a certain range instead of just setting it at  $N^{-1/3}$  (see Figure 1 in [CLS21]). This opens up a new research opportunity for our framework. Namely, by choosing an appropriate  $\hbar$ , the moment estimates for the 1-particle Husimi measure remains finite. Although the Husimi measure will be less than one, its convergence has been explored in [FLS18] for such an unconfined probability density, i.e. that there is possibility where fermions can escape. With a more flexible choice of  $\hbar$ , one may get the convergence in terms of a certain operator norm. For convergence to the Vlasov-Poisson equation, it is likely that this allows us to start from Schrödinger equation with Coulomb

potential instead of its truncation. However, more work is need to understand its physical background since, for a different  $\hbar$ , the order of kinetic and potential energy would be different than what we have discussed in chapter 1.



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