Notes of "On the Mean Field and Classical Limits of Quantum Mechanics" by François Golse, etc.

Xuda Ye

Peking University

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1 Introduction

The study of the mean-field limits of an interacting particle system has always been an appealing topic in both theoretical physics and maths. In the historical viewpoint, Kac [1] first developed the idea of chaos to describe the ensemble behavior of the particle systems. It is natural to ask, how is the chaos of a particle system preserved in the time evolution? The study of such property is referred to as the propagation of chaos, which also indicates the mean-field dynamics of a given particle system. Later in 1960s and 1990s, McKean [2] and Snitzmann [3] studied the chaos of diffusion processes and kinetic systems, and their results build up the foundation of the propagation of chaos. Their work also promoted the theoretical understanding of the McKean-Vlasov SDE and the Boltzmann equation. So far, the propagation of chaos for particle systems in *classical mechanics* has formed a mature theory.

The study of the propagation of chaos for particle systems in *quantum mechanics* encounters additional challenges. The paper [7] considers the following (scaled) N-body quantum system evolved by the Schrödinger equation

$$\begin{cases} i\partial_t \Psi_{\varepsilon,N} = -\dfrac{\varepsilon}{2}\displaystyle\sum_{k=1}^{N} \Delta_{x_k}\Psi_{\varepsilon,N} + \dfrac{1}{2N\varepsilon}\sum_{k,l=1}^{N} V(x_k - x_l)\Psi_{\varepsilon,N}, \\ \Psi_{\varepsilon,N}\big|_{t=0} = \Psi^{in}_{\varepsilon,N}. \end{cases} \tag{1.1}$$

The parameter $\varepsilon > 0$ is called the semiclassical parameter, represneting the quantum nature of the system. As $\varepsilon \to 0$, the quantum system (1.1) is expected to become a classical system, which can be verified by the Wigner transform. The quantum system (1.1) is an important model in computational physics and chemistry, and also encounters huge difficulties in practical simulation:

1. If one direct solves the wavefunction $\Psi_{\varepsilon,N}$, complexity grows exponentially with the number of particles N;
2. The solution $\Psi_{\varepsilon,N}$ has high frequency oscillation in both space and time scales, which makes it extremely difficult to characterize and store the solution.

Due to the importance of the model and the major computational difficulties, it is necessary to study the mean-field limit of the N-body Schrödinger equation (1.1).

The paper [7] studied the mean-field limit of (1.1) as $N \to \infty$ in the semiclassical regime, i.e., the parameter ε is sufficiently small. Formally, the mean-field limit of (1.1) is given by the following nonlinear Schrödinger equation

$$\begin{cases} i\partial_t = -\dfrac{\varepsilon}{2}\Delta_x\psi + \dfrac{1}{\varepsilon}\psi_\varepsilon(t,x)\displaystyle\int_{\mathbb{R}^d} V(x-z)|\psi_\varepsilon(x,z)|^2\mathrm{d}z, \\ \psi_\varepsilon\big|_{t=0} = \psi_\varepsilon^{in}. \end{cases} \tag{1.2}$$

Now our goal is to quantify the difference between the solutions of the two Schrödinger equations (1.1)(1.2), and we expect that the results remain valid in the semiclassical limit $\varepsilon \to 0$. The paper [7] used several tricks establish the propagation of chaos result for (1.1)(1.2):

1. The density matrix is used as the main variable instead of the wavefunction. This allows us to couple the two dynamics (1.1)(1.2) in the joint von Neumann equation.

2. The initial data are chosen as the Töpliz operators. For this choice, as the semiclassical parameter $\varepsilon \to 0$, the intial data shall shrink to probability distribution of classical particles in the phase space. In this way, the initial data are physically meaningful even for small ε.

3. A special Wasserstein-2 distance $\mathcal{W}_2^\varepsilon$ (MK_2^ε in [7]) is used to quantify the difference between the density matrices. Although $\mathcal{W}_2^\varepsilon$ is not a metric, its definition imitates the Wasserstein-2 distance in the phase space $\mathbb{R}^d \times \mathbb{R}^d$.

The remaining part of the paper mainly consists of computing the time derivatives of the quantities (2.13)(3.22), and the inequalities involved in the quantum and classical cases are similar.

In my personal opinion, the most elegant part of the paper is the introduction of the quantum Wasserstein-2 distance $\mathcal{W}_2^\varepsilon$, which imitates the traditional definition of $\mathcal{W}_2$ and maintains the quantum nature of the particle system. Although $\mathcal{W}_2^\varepsilon(\rho,\rho) \geqslant 2d\varepsilon$ due to the uncertainty principle, $\mathcal{W}_2^\varepsilon$ does match $\mathcal{W}_2$ in the semiclassical limit $\varepsilon \to 0$. The proof of the quatum version of the propagation of chaos is quite nostalgic, especially the estimation of the consistency error (3.24), which also appeared in McKean's proof [2].

Nevertheless, their results provide convincing evidence of the mean-field limit of the quantum interacting particle system. In particular, their results remain valid in the semiclassical limit $\varepsilon \to 0$, which corresponds to the propagation of chaos in classical mechanics. Also, their results encourage us to design approximate numerical methods to solve the N-body Schrödinger equation (1.1) rather than the nonlinear Schrödinger equation (1.2) itself.

This note is organized as follows. Section 2 proves the propagation of chaos in classical mechanics. Section 3 defines the quantum Wasserstein-2 distance $\mathcal{W}_2^\varepsilon$ and the associated quantities and proves the propagation of chaos in quantum mechanics.

2 Propagation of chaos in classical mechanics

Consider the interacting particle system $\{(x_k,\xi_k)\}_{k=1}^N$ in $(\mathbb{R}^d\times\mathbb{R}^d)^N$ evolved by the Hamiltonian

$$H_N(x_1,\cdots,x_N) = \frac{1}{2}\sum_{k=1}^N |x_k|^2 + \frac{1}{2N}\sum_{k,l=1}^N V(x_k-x_l), \tag{2.1}$$

then the Liouville equation corresponding to this system is

$$\begin{cases} \partial_t F_N + \sum_{k=1}^{N} \xi_k \cdot \nabla_{x_k} F_N - \frac{1}{N} \sum_{k=1}^{N} \nabla V(x_k - x_l) \cdot \nabla_{\xi_k} F_N = 0, \\ F_N\big|_{t=0} = F_N^{in} \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^N), \end{cases} \tag{2.2}$$

where $F_N(t, x_1, \cdots, x_N, \xi_1, \cdots, \xi_N)$ is the probability density of the particle system at time t, and F_N^{in} is the initial distribution. A typical example of the initial distribution is given by

$$F_N^{in} = (f^{in})^{\otimes N} \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^N), \tag{2.3}$$

where $f^{in} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ is a probability distribution in the phase space. That is, the initial states of the N particles are sampled from μ indepedently. As a consequence, all the N particles in (2.2) are indistinguishable.

Remark 2.1 There is no external potential in the Hamiltonian (2.1), hence the N particles are driven by pairwise interactions. Since there is no diffusion in the Liouville equation (2.2), the initial distribution $f^{in} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ should not be a Dirac distribution.

As the number of particles N tends to infinity, if we focus on the dynamics of a single particle (denoted by $(\bar{x}, \bar{\xi}) \in \mathbb{R}^d \times \mathbb{R}^d$) in (2.1), then the mean-field limit of the Liouville equation (2.2) is the following Vlasov equation:

$$\begin{cases} \partial_t \bar{f} + \bar{\xi} \cdot \nabla_{\bar{x}} \bar{f} - \int_{\mathbb{R}^d \times \mathbb{R}^d} \Big(\nabla V(\bar{x} - \bar{y}) \bar{f}(t, \bar{y}, \bar{\eta}) \mathrm{d}\bar{y} \mathrm{d}\bar{\eta} \Big) \cdot \nabla_{\bar{\xi}} \bar{f} = 0, \\ \bar{f}\big|_{t=0} = f^{in} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d), \end{cases} \tag{2.4}$$

where $\bar{f}(t, \bar{x}, \bar{\xi})$ is the probability density of the particle at time t, and f^{in} is the initial distribution and coincides with f^{in} in (2.2). For convenience, we also write

$$(V * \bar{f})(t, \bar{x}) = \int_{\mathbb{R}^d} V(\bar{x} - \bar{y}) \bar{f}(t, \bar{y}, \bar{\eta}) \mathrm{d}\bar{y} \mathrm{d}\bar{\eta}, \tag{2.5}$$

then it is easy to verify $\nabla_{\bar{x}}(V * \bar{f}) = (\nabla V) * \bar{f}$. Formally, the Vlasov equation corresponds to the Hamiltonian dynamics of the following Hamiltonian

$$\bar{H}^{\bar{f}}(\bar{x}, \bar{\xi}) = \frac{1}{2} |\bar{\xi}|^2 + (V * \bar{f})(\bar{x}), \tag{2.6}$$

where the potential function depends on the probability distribution $\bar{f} \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ explicitly.

Now we aim to quantify the difference between the Liouville solution F_N and the Vlasov solution f. Note that F_N is a probability density in $(\mathbb{R}^d \times \mathbb{R}^d)^{\times N}$, and f is a probability density in $\mathbb{R}^d \times \mathbb{R}^d$, hence the difference between F_N and f cannot be measured directly. The answer is to fix an integer $n \in \mathbb{N}$ and project F_N and f onto $(\mathbb{R}^d \times \mathbb{R}^d)^n$. Since F_N is symmetric in the N particles (see Definition 3.5 in [4], Part I), we may consider its n-particle marginal $F_N^n \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^n)$ and compare it with the tensor product $f^{\otimes N} \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^n)$.

- $F_N^n \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^n)$: n-marginal of Liouville solution $F_N \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^N)$;

- $f^{\otimes N} \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^n)$: n-product of Vlasov solution $f \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$.

Finally, the difference between F_N^n and $f^{\otimes N}$ is measured by the normalized Wasserstein distance.

Definition 2.1 *For probability distributions $\mu, \nu \in \mathcal{P}_p((\mathbb{R}^d \times \mathbb{R}^d)^n)$, define*

$$\mathcal{W}_p^p(\mu,\nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \int_{(\mathbb{R}^d \times \mathbb{R}^d)^n} \left(\frac{1}{n} \sum_{j=1}^n |x_j - y_j|^p + |\xi_j - \eta_j|^p \right) \gamma(\mathrm{d}x\mathrm{d}\xi\mathrm{d}y\mathrm{d}\eta), \tag{2.7}$$

where $\Pi(\mu,\nu)$ is the set of transport plans between μ, ν. That is, when $(x,\xi,y,\eta) \sim \gamma$, we have $(x,\xi) \sim \mu$ and $(y,\eta) \sim \nu$.

Remark 2.2 The metric of the normalized Wasserstein distance has been widely used to quantify the propagation of chaos [4]. The scaling factor $1/n$ ensures that $\mathcal{W}_p(\mu,\nu)$ is $O(1)$ for arbitrary large n. The normalized Wasserstein distance can also be used to quantify the geometric ergodicity of the interacting particle system [5,6]. The definition in (2.7) also involves the momentum terms, so that can be applied in the phase space $(\mathbb{R}^d \times \mathbb{R}^d)^n$.

The difference between the Liouville equation (2.2) and the Vlasov equation (2.4) can be measured in the following theorem.

Theorem 2.1 *Assume $V \in C_b^2(\mathbb{R}^d)$ is even. Let F_N be the solution to the N-body Liouville equation (2.2) with initial data $F_N^{in} = (f^{in})^{\otimes N}$, and f be the solution to the Vlasov equation (2.4) with initial data $f^{in} \in \mathcal{P}_p(\mathbb{R}^d \times \mathbb{R}^d)$ for some $p \geqslant 1$. Then for each integer $1 \leqslant n \leqslant N$,*

$$\mathcal{W}_p^p\big(f(t)^{\otimes n}, F_N^n(t)\big) \leqslant 2^p K_p \|\nabla V\|_{L^\infty} \frac{[p/2]+1}{N^{\min(p/2,1)}} \frac{e^{\Lambda_p t} - 1}{\Lambda_p}, \tag{2.8}$$

where $K_p := \max(1, p-1)$ and $\Lambda_p := 2K_p(1 + 2^{p-1}\mathrm{Lip}(\nabla V)^p)$.

To prove Theorem (2.1), one has to define the coupling between the two dynamics (2.2)(2.4). We duplicate the Vlasov equation (2.4) by N times, where the k-th equation is denoted by $f(t, \bar{x}_k, \bar{\xi}_k)$. In this case the total Hamiltonian of the N-particle Vlasov equation (2.4) can be written as

$$\bar{H}^{\bar{f}}(\bar{x}_1, \cdots, \bar{x}_N, \bar{\xi}_1, \cdots, \bar{\xi}_N) = \sum_{k=1}^N \left(\frac{1}{2}|\bar{\xi}_k|^2 + (V * \bar{f})(\bar{x}_k) \right). \tag{2.9}$$

In the following, we use the shorthand $\boldsymbol{x} = (x_1, \cdots, x_N)$, $\boldsymbol{\xi} = (\xi_1, \cdots, \xi_N)$ and $\bar{\boldsymbol{x}} = (\bar{x}_1, \cdots, \bar{x}_N)$, $\bar{\boldsymbol{\xi}} = (\bar{\xi}_1, \cdots, \bar{\xi}_N)$ to denote the particle systems in (2.2)(2.4). Then the probability density

$$\pi_N(t, \boldsymbol{x}, \boldsymbol{\xi}, \bar{\boldsymbol{x}}, \bar{\boldsymbol{\xi}}) = \pi_N(t, x_1, \cdots, x_N, \xi_1, \cdots, \xi_N, \bar{x}_1, \cdots, \bar{x}_N, \bar{\xi}_1, \cdots, \bar{\xi}_N) \tag{2.10}$$

in $(\mathbb{R}^d \times \mathbb{R}^d)^N$ describes the coupling of the Liouville equation (2.2) and the Vlasov equation (2.4).

- The initial distribution $\pi_N^{in} \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^N)$ is given by

$$\pi_N^{in} = \prod_{k=1}^N f^{in}(x_k, \xi_k) \delta(x_k - \bar{x}_k) \delta(\xi_k - \bar{\xi}_k). \tag{2.11}$$

  That is, the initial values should satisfy $x_k = \bar{x}_k$ and $\xi_k = \bar{\xi}_k$.

- π_N evolves with time according to the following joint Liouville equation

$$\partial_t \pi_N + \{H_N(\boldsymbol{x}, \boldsymbol{\xi}) + \bar{H}^{\bar{f}}(\bar{\boldsymbol{x}}, \bar{\boldsymbol{\xi}}), \pi_N\}_{2N} = 0, \tag{2.12}$$

  where $\{\cdot,\cdot\}_{2N}$ is the Poisson bracket in $(\mathbb{R}^d \times \mathbb{R}^d)^N$.

Remark 2.3 An alternative way to describe the coupling is to write (2.2)(2.4) in the SDE forms and use the synchronous coupling, i.e., the initial values of the SDEs are synchronized. The benefit of using the joint Liouville equation (2.12) rather than the SDEs is that (2.12) motivates the coupling in the quantum mechanics case.

Under the joint Liouville equation (2.12), introduce the following normalized L^p distance by

$$D_N^p(t) = \int \frac{1}{N} \sum_{k=1}^N \big(|x_k - \bar{x}_k|^p + |\xi_k - \bar{\xi}_k|^p\big) \pi_N(t, \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{\xi}\mathrm{d}\bar{\boldsymbol{x}}\mathrm{d}\bar{\boldsymbol{\xi}}). \tag{2.13}$$

Then by direct (but tedious) calculations, one obtains

$$\frac{\mathrm{d}D_N^p}{\mathrm{d}t} \leqslant \Lambda_p D_N + \frac{2^{p-1}K_p}{N} \int \left|(\nabla V * \bar{f})(\bar{x}_k) - \frac{1}{N}\sum_{j=1}^N \nabla V(\bar{x}_k - \bar{x}_j)\right|^p \mathrm{d}\pi_N(t), \tag{2.14}$$

where the dependence on $\bar{f}(t, \bar{x}, \bar{\xi})$ is maintained. Note that in the probability distribution π_N, each $(\bar{x}_k, \bar{\xi}_k) \sim f(t, \bar{x}, \bar{\xi})$, hence we can derive the estimate

$$\int \left|(\nabla V * \bar{f})(\bar{x}_k) - \frac{1}{N}\sum_{j=1}^N \nabla V(\bar{x}_k - \bar{x}_j)\right|^p \leqslant \frac{2[p/2]+2}{N^{\min(p/2,1)}} (2\|\nabla V\|_{L^\infty})^p, \tag{2.15}$$

and so that we obtain the Gronwall type inequality

$$\frac{\mathrm{d}D_N^p}{\mathrm{d}t} \leqslant \Lambda_p D_N^p + 2^{2p} K_p \frac{[p/2]+1}{N^{\min(p/2,1)}} \|\nabla V\|_{L^\infty}^p. \tag{2.16}$$

Under the synchronous coupling, $D_N^p(0) = 0$ and thus Theorem 2.1 holds true.

3 Propagation of chaos in quantum mechanics

The major contribution of [7] is to extend the propagation of chaos to the semiclassical Schrödinger equation of interacting particle systems. Let $\mathfrak{H} = L^2(\mathbb{R}^d)$ be the Hilber space of the single particle wavefunction, and $\mathfrak{H}_N = \mathfrak{H}^{\otimes N} \simeq L^2((\mathbb{R}^d)^N)$ be its product space. The *probability distribution* of the interacting particle system can be interpreted as the density matrix. Let $\mathcal{D}(\mathfrak{H}_N)$ be the set of operators A on $\mathfrak{H}_N$ such that

$$A = A^*, \qquad \mathrm{tr}(A) = 1, \tag{3.1}$$

then the elements $A \in \mathcal{D}(\mathfrak{H}_N)$ corresponds to the density matrix of a quantum state in $L^2((\mathbb{R}^d)^N)$.

In terms of the density matrix, we can write the N-body Schrödinger equation as the following von Neumann equation.

$$\begin{cases} i\partial_t \rho_{\varepsilon,N} = \Big[-\dfrac{\varepsilon}{2}\displaystyle\sum_{k=1}^N \Delta_k + \frac{1}{2N\varepsilon}\sum_{k,l=1}^N V_{kl}, \rho_{\varepsilon,N}\Big], \\ \rho_{\varepsilon,N}\big|_{t=0} = \rho_{\varepsilon,N}^{in}, \end{cases} \tag{3.2}$$

where V_{kl} is a linear operator on $\mathfrak{H}_N$ defined by

$$(V_{kj}\psi)(x_1,\cdots,x_N) := V(x_k - x_l)\psi(x_1,\cdots,x_N), \quad \forall \psi \in \mathfrak{H}_N, \tag{3.3}$$

and $[\cdot,\cdot]$ denotes the commutator of operators. As the number of particles $N \to \infty$, the von Neumann equation (3.2) formally becomes the Hatree equation

$$\begin{cases} i\partial_t \rho_\varepsilon = \Big[-\dfrac{\varepsilon}{2}\Delta + \dfrac{1}{2\varepsilon} V_{\rho_\varepsilon}, \rho_\varepsilon \Big], \\ \rho_\varepsilon\big|_{t=0} = \rho_\varepsilon^{in}, \end{cases} \tag{3.4}$$

where $\rho_\varepsilon \in D(\mathfrak{H})$ is the density matrix of a single particle, and V_{ρ_ε} is an operator on $\mathfrak{H}$ defined by

$$V_{\rho_\varepsilon}(t,x) := \langle V(x-\cdot)\rangle_{\rho_\varepsilon} = \int_{\mathbb{R}^d} V(x-y)\langle y|\rho_\varepsilon(t)|y\rangle \mathrm{d}y. \tag{3.5}$$

To measure the difference between the von Neumann equation (3.2) and the Hatree equation (3.4), we have to clarify the following notions:

1. How do we define the coupling between two elements of $\mathcal{D}(\mathfrak{H}_N)$?
2. How do we define the projection of elements of $\mathcal{D}(\mathfrak{H}_N)$?
3. How do we define the *Wasserstein distance* in $\mathcal{D}(\mathfrak{H}_N)$?
4. How do we choose the initial data of (3.2)(3.4)?

Answers to these questions are inspired from the classical mechanics case.

Definition 3.1 *Suppose $\rho_1, \rho_2 \in \mathcal{D}(\mathfrak{H}_N)$ are two density matrices, then $R \in \mathcal{D}(\mathfrak{H}_{2N})$ is called a coupling of ρ_1, ρ_2 if for any lineae operator A on $\mathfrak{H}_N$, we have*

$$\begin{cases} \mathrm{tr}_{\mathfrak{H}_{2N}}\big((A \otimes I_{\mathfrak{H}_N})R\big) = \mathrm{tr}_{\mathfrak{H}_N}(A\rho_1), \\ \mathrm{tr}_{\mathfrak{H}_{2N}}\big((I_{\mathfrak{H}_N} \otimes A)R\big) = \mathrm{tr}_{\mathfrak{H}_N}(A\rho_2). \end{cases} \tag{3.6}$$

The set of all couplings of ρ_1, ρ_2 is denoted by $\mathcal{Q}(\rho_1, \rho_2)$, which is a subset of $\mathcal{D}(\mathfrak{H}_{2N})$.

Definition 3.1 makes sense because both sides compute the quantum average corresponding to the observable A. Also we note that the tensor product $\rho_1 \otimes \rho_2 \in \mathcal{D}(\mathfrak{H}_{2N})$ is an element of $\mathcal{Q}(\rho_1, \rho_2)$, which corresponds to the independent coupling of two probability distributions.

Definition 3.2 *For a density matrix $\rho_N \in \mathcal{D}(\mathfrak{H}_N)$, its n-marginal $\rho_N^n \in \mathcal{D}(\mathfrak{H}_n)$ is defined by*

$$\mathrm{tr}_{\mathfrak{H}_n}(A\rho_N^n) = \mathrm{tr}_{\mathfrak{H}_N}((A \otimes I_{\mathfrak{H}_{N-n}})\rho_N) \tag{3.7}$$

for any linear operator A on $\mathfrak{H}_n$.

The definition of the Wasserstein distance in the quantum mechanics is tricky work. The notions of positions and momenta are presented as operators, thus one should replace the statistical averages by the corresponding quantum averages.

Definition 3.3 *Let $\psi(x_1, x_2)$ be a wavefunction in $\mathfrak{H}_2 \simeq L^2(\mathbb{R}^d \times \mathbb{R}^d)$, define the position and momentum difference operators Q, P on $\mathfrak{H}_2$ by*

$$\begin{cases} (Q\psi)(x_1, x_2) := (x_1 - x_2)\psi(x_1, x_2), \\ (P\psi)(x_1, x_2) := -i\varepsilon(\nabla_{x_1} - \nabla_{x_2})\psi(x_1, x_2). \end{cases} \tag{3.8}$$

For a wavefunction $\psi(\boldsymbol{x}_1, \boldsymbol{x}_2)$ in $\mathfrak{H}_{2N}$, let Q_k, P_k denote the position and momentum operators corresponding to $\boldsymbol{x}_{1,k}, \boldsymbol{x}_{2,k}$.

Now we define the normalized Wasserstein distance between two density matrices $\rho_1, \rho_2 \in \mathcal{D}(\mathfrak{H}_N)$.

Definition 3.4 *For two density matrices $\rho_1, \rho_2 \in \mathcal{D}(\mathfrak{H})$, the Wasserstein-2 distance is defined by*

$$\mathcal{W}_2^{\varepsilon}(\rho_1, \rho_2) = \left(\inf_{R \in \mathcal{Q}(\rho_1, \rho_2)} \mathrm{tr}_{\mathfrak{H}_{2N}} \left((Q^*Q + P^*P)R \right) \right)^{\frac{1}{2}}. \tag{3.9}$$

If $\rho_1, \rho_2 \in \mathcal{D}(\mathfrak{H}_N)$, then the normalized Wasserstein-2 distance is defined by

$$\mathcal{W}_2^{\varepsilon}(\rho_1, \rho_2) = \left(\inf_{R \in \mathcal{Q}(\rho_1, \rho_2)} \mathrm{tr}_{\mathfrak{H}_{2N}} \left(\frac{1}{N} \sum_{k=1}^{N} (Q_k^*Q_k + P_k^*P_k) R \right) \right)^{\frac{1}{2}}. \tag{3.10}$$

As indicated in [7], $\mathcal{W}_2^{\varepsilon}$ is not a distance on $\mathcal{D}(\mathfrak{H}_N)$. In particular, the position and momentum operators Q, P satisfy

$$Q^*Q + P^*P = (Q + iP)^*(Q + iP) + i(P^*Q - Q^*P) \geqslant i(P^*Q - Q^*P) = 2d\varepsilon I_{\mathfrak{H}_2}, \tag{3.11}$$

hence the Wasserstein-2 distance satisfies $\mathcal{W}_2(\rho, \rho) \geqslant 2\mathrm{d}\varepsilon$. The relation (3.11) can be viewed as the uncertainty principle, while the parameter ε characterizes the quantum nature.

Finally we specify the initial data of the quantum systems.

Definition 3.5 *Given the positon q and momentum p in $\mathbb{R}^d$, the wavefunction at (q, p) is*

$$|q, p, \varepsilon\rangle = (\pi\varepsilon)^{-d/4} e^{-(x-q)^2/2\varepsilon} e^{ip\cdot x/\varepsilon}. \tag{3.12}$$

Given the Borel measure μ on $\mathbb{R}^d \times \mathbb{R}^d$, the Töpliz operator with symbol μ is defined by

$$\mathrm{OP}_{\varepsilon}^{T}(\mu) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} |q, p, \varepsilon\rangle \langle q, p, \varepsilon| \, \mu(\mathrm{d}q\mathrm{d}p). \tag{3.13}$$

The Töpliz operator satisfies

$$\mathrm{tr}\big(\mathrm{OP}_{\varepsilon}^{T}(\mu)\big) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \mu(\mathrm{d}q\mathrm{d}p). \tag{3.14}$$

Therefore, if $\mu \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ is a probability distribution, then the Töpliz operator with symbol $(2\pi\varepsilon)^d$ is a density matrix.

Remark 3.1 As $\varepsilon \to \infty$, the quantum state $|q, p, \varepsilon\rangle$ shrinks to the classical phase (q, p). Therefore, the quantum corresponding object of a probability distribution $\mu \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ is the Töpliz operator with symbol $(2\pi\varepsilon)^d\mu$, which is a density matrix in $\mathcal{D}(\mathfrak{H})$. In the particle system case, the probability distribution $\mu_N \in \mathcal{P}((\mathbb{R}^d \times \mathbb{R}^d)^N)$ corresponds to the Töpliz operator with symbol $(2\pi\varepsilon)^{dN}\mu_N$, which is a density matrix in $\mathcal{D}(\mathfrak{H}_N)$.

Now we are ready to measure the difference between the von Neumann equation (3.2) and the Hatree equation (3.4). The main result is as follows.

Theorem 3.1 *Given $\varepsilon > 0$ and $N \in \mathbb{N}$, let $\rho_{\varepsilon,N}(t)$ be the solution to the von Neumann equation (3.2) with initial data $\rho^{in}_{\varepsilon,N} \in \mathcal{D}(\mathfrak{H}_N)$, and $\rho_\varepsilon(t)$ be the solution to the Hatree equation (3.4) with initial data $\rho^{in}_\varepsilon \in \mathcal{D}(\mathfrak{H})$. Then for each integer $n \leqslant N$ and all $t \geqslant 0$, one has*

$$\mathcal{W}_2^\varepsilon(\rho_\varepsilon(t)^{\otimes n}, \rho^n_{\varepsilon,N}(t))^2 \leqslant \frac{8}{N}\|\nabla V\|^2_{L^\infty}\frac{e^{\Lambda t}-1}{\Lambda} + e^{\Lambda t}\mathcal{W}_2^\varepsilon((\rho^{in}_\varepsilon)^{\otimes N}, \rho^{in}_{\varepsilon,N})^2, \tag{3.15}$$

where $\Lambda := 3 + 4\mathrm{Lip}(\nabla V)^2$. In particular, if for some probability distribution $\mu \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$, one chooses ρ^{in}_ε to be the Töpliz operator with symbol $(2\pi\varepsilon)^d\mu$, and $\rho^{in}_{\varepsilon,N}$ to be the Töpliz operator with symbol $(2\pi\varepsilon)^{Nd}\mu^{\otimes N}$, then

$$\mathcal{W}_2^\varepsilon(\rho_\varepsilon(t)^{\otimes n}, \rho^n_{\varepsilon,N}(t))^2 \leqslant \left(2d\varepsilon + \frac{8}{N}\|\nabla V\|^2_{L^\infty}\frac{1-e^{-\Lambda t}}{\Lambda}\right)e^{\Lambda t}. \tag{3.16}$$

The proof of Theorem 3.1 is directly inspired from Theorem 2.1. Denote the N-body quantum Hamiltonian by

$$H_{\varepsilon,N} = -\frac{\varepsilon}{2}\sum_{k=1}^N \Delta_k + \frac{1}{2N}\sum_{j,k=1}^N V_{jk}, \tag{3.17}$$

then the von Neumann equation (3.2) can be written as

$$i\varepsilon\partial_t\rho_{\varepsilon,N} = [H_{\varepsilon,N}, \rho_{\varepsilon,N}], \quad \rho_{\varepsilon,N}\big|_{t=0} = \rho^{in}_{\varepsilon,N} \in \mathcal{D}(\mathfrak{H}_N). \tag{3.18}$$

Denote the mean-field quantum Hamiltonian by

$$H^\rho_\varepsilon = -\frac{\varepsilon^2}{2}\Delta + V_\rho, \tag{3.19}$$

then the Hatree equation (3.4) can be written as

$$i\varepsilon\partial_t\rho_\varepsilon = [H^{\rho_\varepsilon}_\varepsilon, \rho_\varepsilon], \quad \rho_\varepsilon\big|_{t=0} = \rho^{in}_\varepsilon. \tag{3.20}$$

We duplicate the mean-field quantum systems by defining $H^\rho_{\varepsilon,N} = (H^\rho_\varepsilon)^{\otimes N}$ to be the tensor product of H^ρ_ε. Then the coupling of (3.2)(3.4) can be defined by

- The initial data $R^{in}_{\varepsilon,N} \in \mathcal{Q}((\rho^{in}_\varepsilon)^{\otimes N}, \rho^{in}_{\varepsilon,N})$ is a coupling of the initial data of (3.2)(3.4);
- $R_{\varepsilon,N}(t)$ solves the joint von Neumann equation

$$i\varepsilon\partial_t R_{\varepsilon,N} = [H^{\rho_\varepsilon}_{\varepsilon,N}\otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N}\otimes H_{\varepsilon,N}], \quad R_{\varepsilon,N}\big|_{t=0} = R^{in}_{\varepsilon,N}. \tag{3.21}$$

Similar to (2.13), we define the L^2 distance in the quantum mechanics by

$$D_{\varepsilon,N}(t) = \mathrm{tr}\left(\frac{1}{N}\sum_{k=1}^N (Q_k^*Q_k + P_k^*P_k)R_{\varepsilon,N}(t)\right). \tag{3.22}$$

By direct (but still tedious) calculations, similar to (2.14) we have

$$\frac{\mathrm{d}D_{\varepsilon,N}}{\mathrm{d}t} \leqslant (3+4\mathrm{Lip}(\nabla V)^2)D_{\varepsilon,N} + \frac{1}{N}\sum_{k=1}^{N} \mathrm{tr}\left(\left|\nabla V_{\rho_\varepsilon}(x_k) - \frac{1}{N}\sum_{j=1}^{N}\nabla V(x_k-x_j)\right|^2 \rho_\varepsilon^{\otimes N}\right). \tag{3.23}$$

For the mean-field density $\rho_\varepsilon \in \mathcal{D}(\mathfrak{H})$, the corresponding probability density in the position space is $f_\varepsilon(t,x) = \rho_\varepsilon(t,x,x)$, hence we can again use (2.15) to deduce

$$\mathrm{tr}\left(\left|\nabla V_{\rho_\varepsilon}(x_k) - \frac{1}{N}\sum_{j=1}^{N}\nabla V(x_k-x_j)\right|^2 \rho_\varepsilon^{\otimes N}\right) \leqslant \frac{8}{N}\|V\|_{L^\infty}^2. \tag{3.24}$$

The remaining part is the same with Theorem 2.1.

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