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ORIGINAL ARTICLE

# Quantitative Derivation of the Euler–Poisson Equation from Quantum Many-Body Dynamics

**Xuwen Chen**[1] · **Shunlin Shen**[2] · **Zhifei Zhang**[2]

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## Abstract

We study the three dimensional quantum many-body dynamics with repulsive Coulomb interaction in the mean-field setting. The Euler–Poisson equation is its limit as the particle number tends to infinity and Planck's constant tends to zero. By a new scheme combining the hierarchy method and the modulated energy method, we establish strong and quantitative microscopic to macroscopic convergence of mass and momentum densities as well as kinetic and potential energies before the 1st blow up time of the limiting Euler–Poisson equation.

**Keywords** Euler–Poisson equation · BBGKY hierarchy · Quantum many-body dynamics · Modulated energy

**Mathematics Subject Classification** Primary 35Q31 · 76N10 · 81V70; Secondary 35Q55 · 81Q05

## 1 Introduction

Many systems in physics and other natural sciences can be described at the microscopic and the macroscopic level. Microscopically at the particle level, the evolution is governed by Newton's theory (of classical mechanics) or Schrödinger equations (of quantum mechanics). Despite the accuracy, these microscopic equations are impossi-

✉ Xuwen Chen
xuwenmath@gmail.com

Shunlin Shen
slshen@pku.edu.cn

Zhifei Zhang
zfzhang@math.pku.edu.cn

[1] Department of Mathematics, University of Rochester, Rochester, NY 14627, USA

[2] School of Mathematical Sciences, Peking University, Beijing 100871, China

ble to solve for large interacting systems. On the other hand, the macroscopic equations which make qualitative and quantitative predictions about the behaviors of physically interesting systems, make up an important part of many areas of pure and applied mathematics, science, and engineering. These macroscopic continuum equations are usually phenomenological or based on ideal assumptions and need to be modified or adapted in some experimental or engineering situations. But, they should and do have origins in the Newtonian or Schrödinger microscopic equations. Finding these origins is a key goal in physics.

In the setting of classical mechanics, a strategy of the derivation of fluid equations from particle systems is to 1st pass to some mesoscopic Boltzmann equation, then derive the desired fluid equation from the Boltzmann equation. (See, for example, the standard monographs [8, 38, 62] and references within.) From microscopic quantum dynamics, many macroscopic equations based on Newton's law have been formally derived in the mean-field and classical limit as the particle number tends to infinity and the Planck's constant tends to zero. With a great deal of progress on the qualitative part, we naturally turn to a quantitative description including the rate of convergence, since real systems have a large but, of course, finite number of particles. Bounds on the rate of convergence are therefore crucial to establish whether the limiting dynamics are a good approximation for the microscopic systems.

In this paper, we start from the quantum many-body dynamics with a repulsive Coulomb interaction and establish the strong and quantitative microscopic to macroscopic convergence of mass and momentum densities as well as kinetic and potential energies. The evolution of $N$ particles in quantum mechanics is governed by the 3D linear $N$-body Schrödinger equation:

$$\begin{cases} i\hbar\partial_t\psi_{N,\hbar} = H_{N,\hbar}\psi_{N,\hbar}, \\ \psi_{N,\hbar}(0) = \psi_{N,\hbar}^{\text{in}} \end{cases} \tag{1.1}$$

with the Hamiltonian $H_{N,\hbar}$ given by

$$H_{N,\hbar} = \sum_{j=1}^{N} -\frac{1}{2}\hbar^2\Delta_{x_j} + \frac{1}{N}\sum_{1\leq j<k\leq N} V(x_j - x_k), \tag{1.2}$$

where $\hbar$ denotes the Planck's constant and the repulsive Coulomb interaction

$$V(x) = \frac{1}{|x|}. \tag{1.3}$$

The marginal densities $\gamma_{N,\hbar}^{(k)}(t)$ associated with $\psi_{N,\hbar}(t)$ in kernel form are given by

$$\gamma_{N,\hbar}^{(k)}(t, \mathbf{x}_k, \mathbf{x}_k') = \int \psi_{N,\hbar}(t, \mathbf{x}_k, \mathbf{x}_{N-k})\overline{\psi_{N,\hbar}}(t, \mathbf{x}_k', \mathbf{x}_{N-k})d\mathbf{x}_{N-k}, \tag{1.4}$$

where $\mathbf{x}_k = (x_1, \ldots, x_k) \in \mathbb{R}^{3k}$ and $\mathbf{x}_{N-k} = (x_{k+1}, \ldots, x_N) \in \mathbb{R}^{3(N-k)}$. Notably, one can derive the Hartree equation[1] as $N \to \infty$ limit of (1.1) with Planck's constant $\hbar$ fixed, then the well-known Madelung transform [55] relates a Schrödinger type equation and the macroscopic Euler type equations in a formal limit process as $\hbar$ tends to zero. That is, the macroscopic equations could formally emerge from (1.1) as an iterated limit: $\lim_{\hbar \to 0} \lim_{N \to \infty}$. Such an iterated limit is far from satisfactory in either mathematics or physics. Not only an iterated limit could lose information in any one limit, it kills the fine interplay between $\hbar$ and $N$ and hence cannot show the $(N, \hbar)$ threshold at which classical behavior starts to dominate. Therefore, for a more complete and deeper understanding, we deal with the $(N, \hbar)$ double limit which is also a more challenging problem.

Our limiting macroscopic equation is the 3D Euler–Poisson equation, which is,

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho u) = 0, \\ \partial_t u + (u \cdot \nabla) u + \nabla_x V * \rho = 0, \\ (\rho, u)|_{t=0} = (\rho^{\text{in}}, u^{\text{in}}). \end{cases} \tag{1.5}$$

Here, as usual, $\rho(t, x) : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{R}$ is the mass density, $u(t, x) = (u^1(t, x), u^2(t, x), u^3(t, x)) : \mathbb{R} \times \mathbb{R}^3 \to \mathbb{R}^3$ denotes the velocity of the fluid,

$$J(t, x) = (\rho u)(t, x) \tag{1.6}$$

denotes the momentum of the fluid. Specifically, we consider the initial data satisfying the condition

$$\begin{cases} \rho^{\text{in}} \in H^{s-1}(\mathbb{R}^3), \quad u^{\text{in}} \in H^s(\mathbb{R}^3), \\ \rho^{\text{in}}(x) \geq 0, \quad \int_{\mathbb{R}^3} \rho^{\text{in}}(x) dx = 1, \end{cases} \tag{1.7}$$

where $s > \frac{9}{2}$ and $s \in \mathbb{N}$. Then,[2] there exists a positive time $T_0$ such that the Euler–Poisson system (1.5) has a unique solution $(\rho, u)$ satisfying

$$\begin{cases} \rho \in C([0, T_0]; H^{s-1}(\mathbb{R}^3)), \quad u \in C([0, T_0]; H^s(\mathbb{R}^3)), \\ \rho(t, x) \geq 0, \quad \int_{\mathbb{R}^3} \rho(t, x) dx = 1. \end{cases} \tag{1.8}$$

**Theorem 1.1** *Let the marginal densities $\Gamma_{N,\hbar}(t) = \{\gamma^{(k)}_{N,\hbar}(t)\}$ associated with $\psi_{N,\hbar}(t)$ be the solution to the $N$-body dynamics with Coulomb interaction. The $N$-body initial data satisfy the following conditions:*

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[1] For the approximation to Hartree dynamics, see, for example [12, 31, 40, 41, 51, 60].

[2] The local well-posedness of the Euler–Poisson equation is known by the standard theory on hyperbolic systems (see [56]). Here, for example, see [33, Proposition 2.1] and [70, Lemma 2.2] for the result of local well-posedness.

*Assumption (a): $\Gamma_{N,\hbar}(0)$ is normalized and factorized in the sense that*

$$\psi^{\text{in}}_{N,\hbar} = \prod_{j=1}^{N} \phi^{\text{in}}_{\hbar}(x_j) \tag{1.9}$$

*with* $\|\phi^{\text{in}}_{\hbar}\|_{L^2} = 1$.

*Assumption (b): $\phi^{\text{in}}_{\hbar}$ satisfies the Hamiltonian energy bound and the $H^2$ energy bound:*

$$\langle \phi^{\text{in}}_{\hbar}, \langle \hbar\nabla\rangle^2 \phi^{\text{in}}_{\hbar}\rangle + \langle V * |\phi^{\text{in}}_{\hbar}|^2, |\phi^{\text{in}}_{\hbar}|^2\rangle \leq E_0, \tag{1.10}$$

$$\|\langle \hbar\nabla\rangle^2 \phi^{\text{in}}_{\hbar}\|_{L^2} \leq E_0. \tag{1.11}$$

*Assumption (c): The initial data $(\rho^{\text{in}}, u^{\text{in}})$ to (1.5) satisfy condition (1.7) with $s = 5$. The modulated/renormalized energy[3] at initial time tends to zero:*

$$\begin{aligned}&\int_{\mathbb{R}^3} |(i\hbar\nabla - u^{\text{in}})\phi^{\text{in}}_{\hbar}|^2 dx + \int_{\mathbb{R}^3} V(x-y)\\ &\times \left(|\phi^{\text{in}}_{\hbar}|^2(x) - \rho^{\text{in}}(x)\right)\left(|\phi^{\text{in}}_{\hbar}|^2(y) - \rho^{\text{in}}(y)\right) dxdy \leq C\hbar^2.\end{aligned} \tag{1.12}$$

*Then under the restriction that*[4]

$$N \geq e^{(3)}\left([E_0\hbar^{-4}T_0]^2\right), \tag{1.13}$$

*for $N \geq N_0$, $(\rho, u)$ satisfying (1.5), and $T_0$ which is any time before the blowup time of the Euler–Poisson equation, we have the following quantitative estimates.*

*On the convergence of the mass density*[5] *for $s_1 \in (\frac{1}{4}, 1]$*

$$\|\gamma^{(1)}_{N,\hbar}(t,x;x) - \rho(t,x)\|_{L^\infty_t[0,T_0]\dot{H}^{-s_1}(\mathbb{R}^3)} \lesssim \frac{1}{\ln\ln N} + \hbar^{\frac{4s_1-1}{3}}. \tag{1.14}$$

*On the convergence of the momentum density for $s_2 \in (\frac{1}{2}, 1]$*

$$\begin{aligned}&\left\| \operatorname{Im}\left(\hbar\nabla_{x_1}\gamma^{(1)}_{N,\hbar}\right)(t,x;x) - (\rho u)(t,x)\right\|_{L^\infty_t[0,T_0]\dot{H}^{-s_2}(\mathbb{R}^3)}\\ &\lesssim \left(\frac{1}{\ln\ln N}\right)^{2s_2-1} + \hbar^{2s_2-1}.\end{aligned} \tag{1.15}$$

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[3] (1.12) is but one version of many possible renormalized/modulated energy. The second term of (1.12) could be explained via the Wick ordering as the referee has pointed out.

[4] The composite function $e^{(n)}(x) := e^{(e^{(n-1)}(x))}$.

[5] Here, we use $X \lesssim Y$ to denote the statement $X \leq CY$ for some constant $C > 0$ which could depend on the usual Sobolev constants and the fixed parameters such as the time $T_0$, the energy bound $E_0$, and the Sobolev norms of $(\rho, u)$ but is independent of $(N, \hbar)$.

*On the convergence of the kinetic energy and the potential energy*

$$\sup_{t\in[0,T_0]}\left|\langle\psi_{N,\hbar}(t),-\hbar^2\Delta_{x_1}\psi_{N,\hbar}(t)\rangle-\int\rho(t)|u|^2(t)dx\right|\lesssim\frac{1}{\ln\ln N}+\hbar, \tag{1.16}$$

$$\sup_{t\in[0,T_0]}\left|\langle\psi_{N,\hbar}(t),V(x_1-x_2)\psi_{N,\hbar}(t)\rangle-\langle\rho(t),V*\rho(t)\rangle\right|\lesssim\frac{1}{\ln\ln N}+\hbar. \tag{1.17}$$

**Theorem 1.2** *Theorem 1.1 also holds for more general initial data with condition* $(a)$ *replaced by the following conditions* $(a_1)$, $(a_2)$ *and* $(a_3)$ :

$(a_1)$ $\psi^{\text{in}}_{N,\hbar}$ *is symmetric and normalized in the sense that* $\|\psi^{\text{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}=1$ *and has finite Hamiltonian energy*

$$\langle\psi^{\text{in}}_{N,\hbar},N^{-1}(H_{N,\hbar}+N)\psi^{\text{in}}_{N,\hbar}\rangle\le E_0. \tag{1.18}$$

$(a_2)$ *The N-body energy bounds hold:*

$$\langle\psi^{\text{in}}_{N,\hbar},\langle\hbar\nabla_{x_1}\rangle^2\cdots\langle\hbar\nabla_{x_k}\rangle^2\psi^{\text{in}}_{N,\hbar}\rangle\le(E_0)^k, \tag{1.19}$$

$$\langle\psi^{\text{in}}_{N,\hbar},\langle\hbar\nabla_{x_1}\rangle^4\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_k}\rangle^2\psi^{\text{in}}_{N,\hbar}\rangle\le(E_0)^{k+1}, \tag{1.20}$$

*for* $k\le(\ln\ln N)^{10}$.

$(a_3)$ $\Gamma_{N,\hbar}(0)$ *is asymptotically factorized in the sense that*

$$\operatorname{Tr}\left|\prod_{j=1}^{k}\langle\hbar\nabla_{x_j}\rangle\langle\hbar\nabla_{x_j'}\rangle\left[\gamma^{(k)}_{N,\hbar}(0)-|\phi^{\text{in}}_{\hbar}\rangle\langle\phi^{\text{in}}_{\hbar}|^{\otimes k}\right]\right|\le\frac{(E_0)^k}{\ln N} \tag{1.21}$$

*for* $k\le(\ln\ln N)^{10}$.

Compared to the work [33] in which Golse and Paul justified the weak convergence to Euler–Poisson of the joint mean-field and classical limit of the quantum $N$-body dynamics, Theorem 1.1 establishes strong and quantitative microscopic to macroscopic convergence of mass and momentum densities as a regional double limit of $(N,\hbar)$. The limit is taken within the region (1.13) which implies the dominance of classical behaviors when $N\gg\hbar$. This requirement is physical as they indeed differ by a lot in reality but we believe (1.13) is not optimal and searching for the sharp threshold (may not exist, some mesoscopic behaviors might happen) between classical and quantum behaviors is certainly of interest. It is possible to have totally independent $N$ and $\hbar$ in weak/weak* limits as the Riemann–Lebesgue lemma shows that a weakly convergent sequence can be uniformly bounded away from its weak limit.

The proof of Theorems 1.1 and 1.2 involves the up-to-date techniques in the hierarchy method as well as the well-developed modulated energy approach and we can see it from the assumptions. Notice that condition $(a)$ is only a special case of conditions $(a_1)$–$(a_3)$. The $N$-body energy condition in $(a_2)$ is inspired by purely factorized or statistically independent data. Here, we assume $(\ln N)^{-1}$ rate in (1.21) as we will prove this rate at the first step of bootstrapping argument. The convergence rate (1.12) which we assume to be $\hbar^2$ should be optimal, since the smallness factor in the modulated kinetic part is at most $\hbar^2$. Besides, the $\hbar^2$ rate can be achieved with WKB type initial data.

The hierarchy method in general was first suggested by Kac [47] and proved to be successful in Lanford's work [52] regarding the Boltzmann equation. The hierarchy method with Coulomb potential we use in the paper is actually more related from the work [30] by Erdős–Yau and [2] by Bardos–Erdős–Golse–Mauser–Yau on deriving Hartree equation from quantum many-body dynamics. Inspired by [30], Elgart and Schlein [26] derived the relativistic Hartree equation by the hierarchy method. At that time, the difficulty to derive NLS lies in the uniqueness of the infinite Gross–Pitaevskii hierarchy. With a sophisticated Feynman graph analysis in [27], Erdős, Schlein, and Yau proved the $H^1$-type unconditional uniqueness of the $\mathbb{R}^3$ cubic GP hierarchy and derived the 3D cubic defocusing NLS from quantum many-body dynamics in the fundamental papers [27–29].[6] The first series of ground breaking papers have motivated a large amount of work.

Subsequently in 2007, Klainerman and Machedon [50], inspired by [27, 49], gave another uniqueness criterion of the GP hierarchy in a Strichartz-type space. They provided a different combinatorial argument, the now so-called Klainerman–Machedon board game, to combine the inhomogeneous terms effectively reducing their numbers and established a collapsing-type estimate to control these terms. At that time, it was unknown how to prove that the limits coming from the $N$-body dynamics satisfy the now so called KM space-time bound required for uniqueness. Nonetheless, [50] has made the delicate analysis of the GP hierarchy approachable from the perspective of PDE. Later, Kirkpatrick, Schlein, and Staffilani [48] discovered that the KM space-time bound can be obtained via a simple trace theorem in both $\mathbb{R}^2$ and $\mathbb{T}^2$ and hence derived the 2D cubic defocusing NLS from the 2D quantum many-body dynamic. Such a scheme also motivated many works [10, 12, 15, 17, 18, 37, 42, 66–68] for the uniqueness of GP hierarchies. However, how to verify the KM bound in the 3D cubic case remained fully open at that time.

Then in 2011, T. Chen and Pavlović proved that the 3D cubic KM space-time bound held for the defocusing $\beta < 1/4$ case in [11]. The result was quickly improved to $\beta < 2/7$ by X. Chen in [13] and then extended to the almost optimal case, $\beta < 1$, by X. Chen and Holmer in [14, 16], by lifting the $X_{1,b}$ space techniques from NLS theory into the field. Apart from being the first work to prove the 3D KM bound, the work [11] hinted two unforeseen directions of the hierarchy method: one direction is to prove new NLS results via the more complicated hierarchies, while the other is that it is possible to derive NLS without a compactness or uniqueness argument.

In 2013, by introducing the quantum de Finetti theorem from [53] to the field, T. Chen, Hainzl, Pavlović and Seiringer [9] provided a simplified proof of the $L_t^\infty H_x^1$-type 3D cubic uniqueness theorem as stated in [27]. This method motivated many works [24, 44, 45, 65] and [19, 21, 23, 43] on the unconditional uniqueness of NLS.

On the basis of [11, 13, 14, 16], X. Chen and Holmer in [20] reformatted the hierarchy method with KM space-time estimates and proved a bi-scattering theorem for the NLS to obtain almost optimal local in time convergence rate estimates under $H^1$

[6] See also [1] for the derivation of 1D defocusing cubic NLS around the same time.

regularity. They integrated the idea from the Fock space approach (see, for example [3, 4, 6, 38, 39] and references within[7]), that, using H-NLS as an intermediate dynamic, into the hierarchy method.

The asymptotic behavior of the wave function of NLS and Hartree equations as the Planck's constant goes to zero is studied by many authors using various approaches. See, for example [36, 46, 54, 70]. For a more detailed survey related to semiclassical limits, see [7, 71] and references within.

It is highly nontrivial to derive Euler-type equations from nonlinear Schrödinger type equations, let alone from quantum $N$-body dynamics. Golse and Paul [33], with the help of Serfaty's inequality [64, Corollary 3.4], used the modulated energy method in the quantum $N$-body setting to justify the validity of the joint mean-field and classical limit of the quantum $N$-body dynamics leading to the pressureless Euler–Poisson with repulsive Coulomb potential.[8] Subsequently, Rosenzweig complemented [33] in [61] by combining mean-field, semiclassical and quasi-neutral limits to reach a derivation of an incompressible Euler equation on $\mathbb{T}^d$ with binary Coulomb interactions.[9] In [22], Chen–Shen–Wu–Zhang created a new scheme which can combine the accuracy of the hierarchy method and the flexibility of the modulated energy method to derive the compressible Euler equations with strong and quantitative convergence rate from quantum many-body dynamics for the more singular delta-type interactions.

Here, we adopt the scheme in [22] for the Coulomb potential problem and prove the strong and quantitative convergence rate from quantum many-body dynamics to the Euler–Poisson equation.

## 1.1 Outline of the Proof

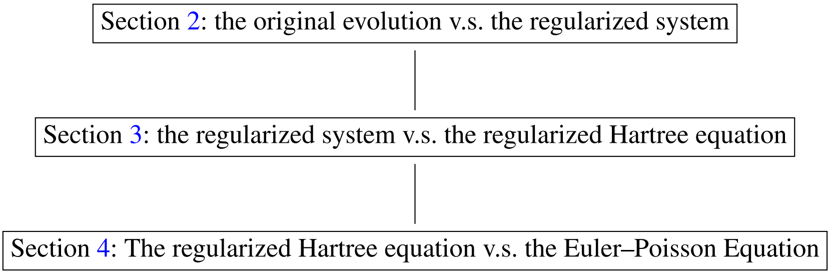
Compared to the $\delta$-type interaction considered in [22], the Coulomb interaction here has its own properties. On the one hand, the singularity near the origin makes it difficult to prove energy estimates for the BBGKY hierarchy, which is usually viewed as the first step in the hierarchy method. Due to this, we use a regularized system (2.4) similar to the one in [30]. With technical modifications and improvement, the hierarchy part of [22] works for the regularized system and gives the $k$-$H^1$ type difference estimate which should be the optimal in the sense that it matches the a priori energy bound. However, even for the one-body wave function, the modulated energy method in [22] only provides the $\dot{H}^{-1}$ convergence for the mass density because of the Coulomb potential, whose usage is limited in proving the convergence of momentum density. To circumvent it, we introduce a feedback argument to obtain the uniform in $\hbar$ bounds for densities, which improves the convergence of densities. Furthermore, this feedback argument can also improve [22] if we use it there.

[7] The Fock space approach is also a vast and deep subject right now. There are certainly more references available. But this paper is not directly related to that.

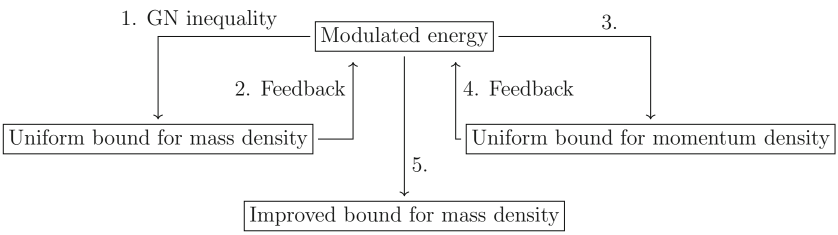
[8] For the joint mean-field and classical limit with an non-singular potential, see, for example [32, 34, 35, 59].

[9] The modulated energy method has been successful in different settings. See, for example [5, 25, 54, 63, 64, 70] and the relative entropy method in [69].

We need only prove Theorem 1.2 as Theorem 1.1 is a special case of Theorem 1.2. We divide the proof of Theorem 1.2 into three parts in Sects. 2–4 respectively. The first part is to control the difference between the original evolution and the regularized system in $H^1$ norm.[10] The second part is the quantitative estimate between the regularized BBGKY hierarchy (3.30) and the regularized Hartree equation (3.2), which we insert as an intermediate dynamics by using the hierarchy method. The third part is comparing the regularized Hartree equation with the Euler–Poisson equation (1.5) via our feedback modulated energy argument. Here, we illustrate the idea of the whole process by the following diagram.




In Sect. 4, the stronger convergence calls for stronger uniform bounds. Regarding the defining feature of the Coulomb interaction that $-\Delta V = c_0\delta$, we observe a structure compatible with a specific usage of the Gagliardo–Nirenberg inequality so that we obtain a uniform bound (4.60) for the mass density as a starting point. By feeding (4.60) back to the quantitative convergence of the kinetic energy part, we obtain a uniform bound (4.68) for momentum density. We can then feedback again to improve the uniform bound for mass density. We illustrate the idea by the following diagram.




## 2 The Regularized Hamiltonian and Initial Data

The original evolution is given by

$$\psi_{N,\hbar}(t) = e^{itH_{N,\hbar}/\hbar}\psi_{N,\hbar}^{\text{in}}. \tag{2.1}$$

[10] The $L^2$ estimate for this difference established in [30] is not enough for our goal as we need the $H^1$ approximation. It is a sharp bound in the sense that the original evolution only enjoys the $H^1$ energy bound regardless of the smoothness of initial data due to the singularity of the Coulomb interaction.

By the energy conservation and finite Hamiltonian energy (1.18) at the initial time, we have

$$\langle \psi_{N,\hbar}(t), N^{-1}(H_{N,\hbar}+N)\psi_{N,\hbar}(t)\rangle = \langle \psi_{N,\hbar}^{\mathrm{in}}, N^{-1}(H_{N,\hbar}+N)\psi_{N,\hbar}^{\mathrm{in}}\rangle \le E_0, \tag{2.2}$$

which gives the $H^1$ energy bound

$$\sup_{t\in[0,T_0]} \langle \langle \hbar\nabla_{x_1}\rangle \psi_{N,\hbar}(t), \langle \hbar\nabla_{x_1}\rangle \psi_{N,\hbar}(t)\rangle \le E_0 \tag{2.3}$$

because of the positivity of the interaction. However, due to the singularity of the Coulomb interaction, we do not expect the product energy estimates like multiple particles. Nevertheless, they are attractable for regularized Coulomb systems with regularized initial data. Therefore, we regularize the Hamiltonian by

$$H_{N,\hbar,\lambda} = -\frac{\hbar^2}{2}\sum_{j=1}^{N}\Delta_{x_j} + \frac{1}{N}\sum_{1\le i<j\le N} V_\lambda(x_i-x_j), \tag{2.4}$$

where

$$V_\lambda(x) = \theta(\lambda x)V(x) \tag{2.5}$$

and the smooth radial cutoff function $0 \le \theta(x) \le 1$ with $\theta(x)\equiv 1$ for $|x|\ge 2$ and $\theta(x)\equiv 0$ for $|x|\le 1$, and we regularize initial data by

$$\psi_{N,\hbar}^{M,\mathrm{in}} = \frac{P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}}{\|P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}, \tag{2.6}$$

where $P_{\le M}^{(1,N)}$ denotes the Littlewood–Paley projection onto the low frequency corresponding to the variable $\mathbf{x}_N$. We denote the solution to the regularized system by

$$\psi_{N,\hbar,\lambda}^{M}(t) = e^{itH_{N,\hbar,\lambda}/\hbar}\psi_{N,\hbar}^{M,\mathrm{in}} \tag{2.7}$$

and write regularized marginal densities $\Gamma_{N,\hbar,\lambda}^{M} = \{\gamma_{N,\hbar,\lambda}^{M,(k)}(t)\}_{k=1}^{N}$ associated with $\psi_{N,\hbar,\lambda}^{M}(t)$.

Before getting into the analysis of controlling the difference between the original evolution and the regularized system, we first set up an $H^1$ estimate as following.

**Lemma 2.1** *Let $M = N^{1/2}(\ln\ln N)^{10}$ and $\lambda = N^{1/2}(\ln\ln N)^{10}$. Under the same conditions $(a_1)$–$(a_3)$, $(b)$ and the restriction (1.13) of Theorem 1.1, we have*

$$\sup_{t\in[0,T_0]} \|\langle \hbar\nabla_{x_1}\rangle(\psi_{N,\hbar}(t) - \psi_{N,\hbar,\lambda}^{M}(t))\|_{L^2_{\mathbf{x}_N}} \lesssim \frac{1}{(\ln\ln N)^4}. \tag{2.8}$$

***Proof*** Due to the positivity of the potential $V$ and the symmetry of wave functions, it suffices to estimate

$$\langle \psi_{N,\hbar}(t) - \psi^M_{N,\hbar,\lambda}(t), N^{-1}(H_{N,\hbar} + N)(\psi_{N,\hbar}(t) - \psi^M_{N,\hbar,\lambda}(t))\rangle. \tag{2.9}$$

By triangle inequality, we have

$$\begin{aligned}
&\langle \psi_{N,\hbar}(t) - \psi^M_{N,\hbar,\lambda}(t), N^{-1}(H_{N,\hbar} + N)(\psi_{N,\hbar}(t) - \psi^M_{N,\hbar,\lambda}(t))\rangle^{\frac{1}{2}} \\
&\quad \le \langle \psi_{N,\hbar}(t) - \psi^M_{N,\hbar}(t), N^{-1}(H_{N,\hbar} + N)(\psi_{N,\hbar}(t) - \psi^M_{N,\hbar}(t))\rangle^{\frac{1}{2}} \\
&\qquad + \langle \psi^M_{N,\hbar}(t) - \psi^M_{N,\hbar,\lambda}(t), N^{-1}(H_{N,\hbar} + N)(\psi^M_{N,\hbar}(t) - \psi^M_{N,\hbar,\lambda}(t))\rangle^{\frac{1}{2}} \\
&\quad =: \mathrm{I} + \mathrm{II},
\end{aligned} \tag{2.10}$$

where $\psi^M_{N,\hbar}(t) = e^{itH_{N,\hbar}/\hbar}\psi^{M,\mathrm{in}}_{N,\hbar}$ is the solution corresponding to the original Hamiltonian $H_{N,\hbar}$ and the regularized initial data.

For I, by the energy conservation and the symmetry of wave function, we have

$$\begin{aligned}
\mathrm{I} &= \langle (\psi_{N,\hbar}(t) - \psi^M_{N,\hbar}(t)), N^{-1}(H_{N,\hbar} + N)(\psi_{N,\hbar}(t) - \psi^M_{N,\hbar}(t))\rangle^{\frac{1}{2}} \\
&= \langle \psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar}, N^{-1}(H_{N,\hbar} + N)(\psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar})\rangle^{\frac{1}{2}} \\
&= \langle \psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar}, (1 - \hbar^2\Delta_{x_1} + V(x_1 - x_2))(\psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar})\rangle^{\frac{1}{2}}.
\end{aligned}$$

By Hardy's inequality that $V(x_1 - x_2) \le \langle \nabla_{x_1} \rangle$ and $-\hbar^2\Delta_{x_1} \le -\Delta_{x_1}$, we obtain

$$\mathrm{I} \le \langle \psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar}, (1 - \Delta_{x_1})(\psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar})\rangle^{\frac{1}{2}}.$$

Note that

$$\psi^{\mathrm{in}}_{N,\hbar} - \psi^{M,\mathrm{in}}_{N,\hbar} = \frac{(\|P^{(1,N)}_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} - 1)\psi^{\mathrm{in}}_{N,\hbar}}{\|P^{(1,N)}_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}} + \frac{(1 - P^{(1,N)}_{\le M})\psi^{\mathrm{in}}_{N,\hbar}}{\|P^{(1,N)}_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}}.$$

By the triangle inequality that $1 - \|P^{(1,N)}_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} \le \|(1 - P^{(1,N)}_{\le M})\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}$, we get

$$\begin{aligned}
\mathrm{I} &\le \frac{\|(1 - P^{(1,N)}_{\le M})\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} \|\langle \nabla_{x_1} \rangle \psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} + \|\langle \nabla_{x_1} \rangle (1 - P^{(1,N)}_{\le M})\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}}{\|P^{(1,N)}_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}} \\
&\le \frac{\hbar^{-1}\|(1 - P^{(1,N)}_{\le M})\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} \|\langle \hbar\nabla_{x_1} \rangle \psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} + \|\langle \nabla_{x_1} \rangle (1 - P^{(1,N)}_{\le M})\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}}{\|P^{(1,N)}_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}}.
\end{aligned}$$

By the energy bound (1.19) for $\psi_{N,\hbar}^{\text{in}}$

$$\mathrm{I} \lesssim \frac{(E_0)^{\frac{1}{2}}\hbar^{-1}\|\langle\nabla_{x_1}\rangle(1-P_{\leq M}^{(1,N)})\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}}{\|P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}}. \tag{2.11}$$

We are left to estimate $\|\langle\nabla_{x_1}\rangle(1-P_{\leq M}^{(1,N)})\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}$ and $\|P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}$. Notice that

$$1-P_{\leq M}^{(1,N)} = P_{>M}^{1} + \sum_{j=2}^{N} P_{\leq M}^{(1,j-1)} P_{>M}^{j},$$

where $P_{\leq M}^{(1,j-1)}$ denotes the Littlewood–Paley projection onto the low frequency corresponding to variables $(x_1,\ldots,x_{j-1})$ and $P_{>M}^{j} = 1-P_{\leq M}^{j}$ denotes the high frequency corresponding to variable $x_j$. Then we use triangle inequality and Bernstein's inequality to get

$$\begin{aligned}
&\|\langle\nabla_{x_1}\rangle(1-P_{\leq M}^{(1,N)})\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}\\
&\leq \|\langle\nabla_{x_1}\rangle P_{>M}^{1}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}} + \sum_{j=2}^{N}\|\langle\nabla_{x_1}\rangle P_{\leq M}^{(1,j-1)} P_{>M}^{j}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}\\
&\leq \frac{1}{M}\|\langle\nabla_{x_1}\rangle^2 P_{>M}^{1}\psi_{N,\hbar}\|_{L^2_{\mathbf{x}_N}} + \frac{1}{M^2}\sum_{j=2}^{N}\|\langle\nabla_{x_1}\rangle\langle\nabla_{x_j}\rangle^2 P_{\leq M}^{(1,j-1)} P_{>M}^{j}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}.
\end{aligned}$$

By the energy bounds (1.19) and (1.20) for $\psi_{N,\hbar}^{\text{in}}$, the above

$$\leq \frac{E_0}{M\hbar^2} + \frac{N(E_0)^{\frac{3}{2}}}{M^2\hbar^3}.$$

Inserting in $M = N^{1/2}(\ln\ln N)^{10}$, the above

$$= \frac{E_0}{N(\ln\ln N)^{10}\hbar^2} + \frac{(E_0)^{\frac{3}{2}}}{(\ln\ln N)^{20}\hbar^3}.$$

Therefore, we can use the restriction (1.13) to obtain

$$(E_0)^{\frac{1}{2}}\hbar^{-1}\|\langle\nabla_{x_1}\rangle(1-P_{\leq M}^{(1,N)})\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}} \lesssim \frac{1}{(\ln\ln N)^{10}}. \tag{2.12}$$

By the triangle inequality that $\|P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}} \geq 1-\|(1-P_{\leq M}^{(1,N)})\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}}$ and estimate (2.12), we also have

$$\|P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}} \geq 1-\|(1-P_{\leq M}^{(1,N)})\psi_{N,\hbar}^{\text{in}}\|_{L^2_{\mathbf{x}_N}} \geq \frac{1}{2}. \tag{2.13}$$

Combining estimates (2.11), (2.12) and (2.13), we arrive at

$$\mathrm{I} \lesssim \frac{1}{(\ln\ln N)^{10}}. \tag{2.14}$$

For II, we set

$$\widetilde{\psi}(t) = \psi_{N,\hbar}^{M}(t) - \psi_{N,\hbar,\lambda}^{M}(t) \tag{2.15}$$

and then have

$$i\partial_t\widetilde{\psi} = H_{N,\hbar}\psi_{N,\hbar}^{M} - H_{N,\hbar,\lambda}\psi_{N,\hbar,\lambda}^{M} = H_{N,\hbar}\widetilde{\psi} + H_W\psi_{N,\hbar,\lambda}^{M}, \tag{2.16}$$

where

$$H_W = \frac{1}{N}\sum_{1\leq i<j\leq N} W_\lambda(x_i - x_j)$$

with $W_\lambda = V - V_\lambda$. To estimate II, it suffices to bound its time derivative. Hence, we compute

$$\begin{aligned}
&\frac{d}{dt}\langle\widetilde{\psi}, N^{-1}(H_{N,\hbar}+N)\widetilde{\psi}\rangle \\
&\quad= \frac{d}{dt}\langle\widetilde{\psi},\widetilde{\psi}\rangle + \frac{d}{dt}\langle\widetilde{\psi},(H_{N,\hbar}/N)\widetilde{\psi}\rangle \\
&\quad= 2\,\mathrm{Re}\langle\partial_t\widetilde{\psi},\widetilde{\psi}\rangle + 2\,\mathrm{Re}\langle\partial_t\widetilde{\psi},(H_{N,\hbar}/N)\widetilde{\psi}\rangle.
\end{aligned} \tag{2.17}$$

By Eq. (2.16), the above

$$= -2\,\mathrm{Re}\langle\widetilde{\psi}, iH_W\psi_{N,\hbar,\lambda}^{M}\rangle - 2\,\mathrm{Re}\langle N^{-1}\partial_t\widetilde{\psi}, H_W\psi_{N,\hbar,\lambda}^{M}\rangle.$$

By Cauchy–Schwarz inequality, the above

$$\leq 2(\|\widetilde{\psi}\|_{L^2_{\mathbf{x}_N}} + N^{-1}\|\partial_t\widetilde{\psi}\|_{L^2_{\mathbf{x}_N}})\|H_W\psi_{N,\hbar,\lambda}^{M}\|_{L^2_{\mathbf{x}_N}}.$$

By Eq. (2.16) and $\|\widetilde{\psi}\|_{L^2_{\mathbf{x}_N}} \leq 2$, the above

$$\leq 2(2+N^{-1}\|H_{N,\hbar}\psi_{N,\hbar}^{M}(t)\|_{L^2_{\mathbf{x}_N}} + N^{-1}\|H_{N,\hbar,\lambda}\psi_{N,\hbar,\lambda}^{M}(t)\|_{L^2_{\mathbf{x}_N}})\|H_W\psi_{N,\hbar,\lambda}^{M}(t)\|_{L^2_{\mathbf{x}_N}}.$$

We are left to bound the above terms. First, by the energy conservation and the symmetry of wave function, we have

$$\begin{aligned}\|(H_{N,\hbar}/N)\psi_{N,\hbar}^{M}(t)\|_{L^2_{\mathbf{x}_N}} &= \|(H_{N,\hbar}/N)\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}\\ &\leq \|\hbar^2\Delta_{x_1}\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}} + \|V(x_1-x_2)\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}\\ &\lesssim \|\hbar^2\Delta_{x_1}\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}} + \|\langle\nabla_{x_1}\rangle\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}},\end{aligned}$$

where in the last inequality we used the Hardy's inequality that $|V(x_1-x_2)|^2 \lesssim -\Delta_{x_1}$. By estimate (2.13) which gives that

$$\|P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}} \geq \frac{1}{2}, \tag{2.18}$$

we arrive at

$$\begin{aligned}\|(H_{N,\hbar}/N)\psi_{N,\hbar}^{M}(t)\|_{L^2_{\mathbf{x}_N}} &\lesssim \|\hbar^2\Delta_{x_1}\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}} + \|\langle\nabla_{x_1}\rangle\psi_{N,\hbar}^{M,\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}\\ &= \frac{\|\hbar^2\Delta_{x_1}P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}} + \|\langle\nabla_{x_1}\rangle P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}{\|P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}\\ &\lesssim \|\langle\hbar\nabla_{x_1}\rangle^2 P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}} + \hbar^{-1}\|\langle\hbar\nabla_{x_1}\rangle P_{\leq M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}\\ &\lesssim \hbar^{-1},\end{aligned} \tag{2.19}$$

where in the last inequality we used the energy bounds (1.19) and (1.20) for $\psi_{N,\hbar}^{\mathrm{in}}$.

In the same way, we also have

$$\|(H_{N,\hbar,\lambda}/N)\psi_{N,\hbar,\lambda}^{M}(t)\|_{L^2_{\mathbf{x}_N}} \lesssim \hbar^{-1}. \tag{2.20}$$

Next, we deal with the term $\|H_W\psi_{N,\hbar,\lambda}^{M}(t)\|_{L^2_{\mathbf{x}_N}}$. By the symmetry of wave function, we obtain

$$\|H_W\psi_{N,\hbar,\lambda}^{M}(t)\|_{L^2_{\mathbf{x}_N}}^2 \lesssim A_1 + NA_2 + N^2A_3, \tag{2.21}$$

where

$$\begin{aligned}A_1 &= \int |W_\lambda(x_1-x_2)|^2|\psi_{N,\hbar,\lambda}^{M}(t,\mathbf{x}_N)|^2 d\mathbf{x}_N,\\ A_2 &= \int |W_\lambda(x_1-x_2)||W_\lambda(x_1-x_3)||\psi_{N,\hbar,\lambda}^{M}(t,\mathbf{x}_N)|^2 d\mathbf{x}_N,\\ A_3 &= \int |W_\lambda(x_1-x_2)||W_\lambda(x_3-x_4)||\psi_{N,\hbar,\lambda}^{M}(t,\mathbf{x}_N)|^2 d\mathbf{x}_N.\end{aligned}$$

For $A_1$, by Lemma A.3, we have

$$A_1 \lesssim \frac{1}{\lambda}\langle \psi^M_{N,\hbar,\lambda}(t), \langle \nabla_{x_1}\rangle^2 \langle \nabla_{x_2}\rangle^2 \psi^M_{N,\hbar,\lambda}(t)\rangle. \tag{2.22}$$

For $A_2$, we first use the Hardy's inequality that $|W_\lambda(x_1-x_2)| \le |x_1-x_2|^{-1} \lesssim \langle \nabla_{x_2}\rangle$ and then Lemma A.3 to obtain

$$\begin{aligned} A_2 &\lesssim \langle \psi^M_{N,\hbar,\lambda}(t), \langle \nabla_{x_2}\rangle^2 |W_\lambda(x_1-x_3)| \psi^M_{N,\hbar,\lambda}(t)\rangle \\ &\lesssim \frac{1}{\lambda^2}\langle \psi^M_{N,\hbar,\lambda}(t), \langle \nabla_{x_2}\rangle^2 \langle \nabla_{x_1}\rangle^2 \langle \nabla_{x_3}\rangle^2 \psi^M_{N,\hbar,\lambda}(t)\rangle. \end{aligned} \tag{2.23}$$

For $A_3$, by Lemma A.3, we have

$$A_3 \lesssim \frac{1}{\lambda^4}\langle \psi^M_{N,\hbar,\lambda}(t), \langle \nabla_{x_1}\rangle^2 \langle \nabla_{x_2}\rangle^2 \langle \nabla_{x_3}\rangle^2 \langle \nabla_{x_4}\rangle^2 \psi^M_{N,\hbar,\lambda}(t)\rangle. \tag{2.24}$$

By the energy estimate bound for $\psi^M_{N,\hbar,\lambda}(t)$ in Proposition 3.3 which we postpone to Sect. 3.1, we arrive at

$$\|H_W \psi^M_{N,\hbar,\lambda}(t)\|^2_{L^2_{\mathbf{x}_N}} \lesssim \frac{1}{\lambda\hbar^4} + \frac{N}{\lambda^2\hbar^6} + \frac{N^2}{\lambda^4\hbar^8}. \tag{2.25}$$

Combining estimates (2.17), (2.19), (2.20) and (2.25), we reach

$$\begin{aligned} (\mathrm{II})^2 &= \langle \widetilde{\psi}, N^{-1}(H_{N,\hbar}+N)\widetilde{\psi}\rangle = \int_0^t \frac{d}{ds}\langle \widetilde{\psi}, N^{-1}(H_{N,\hbar}+N)\widetilde{\psi}\rangle(s)ds \\ &\lesssim T_0\hbar^{-1}\left(\frac{1}{\lambda\hbar^4} + \frac{N}{\lambda^2\hbar^6} + \frac{N^2}{\lambda^4\hbar^8}\right)^{\frac{1}{2}}. \end{aligned}$$

Then, we insert in $\lambda = N^{1/2}(\ln\ln N)^{10}$ to get

$$\mathrm{II} \lesssim (T_0\hbar^{-1})^{\frac{1}{2}}\left(\frac{1}{N^{1/2}(\ln\ln N)^{10}\hbar^4} + \frac{1}{(\ln\ln N)^{20}\hbar^6} + \frac{1}{(\ln\ln N)^{80}\hbar^8}\right)^{\frac{1}{4}}. \tag{2.26}$$

As the factor $\hbar^{-1}$ can be absorbed into $\ln\ln N$ under the restriction (1.13), we arrive at

$$\mathrm{II} \lesssim \frac{1}{(\ln\ln N)^4}. \tag{2.27}$$

Combining estimates (2.10), (2.14) and (2.27), we complete the proof of estimate (2.8). $\square$

Based on the $H^1$ estimate in Lemma 2.1, we can control the difference between the original evolution and the regularized system in the following proposition.

**Proposition 2.2** *Let $M = N^{1/2}(\ln\ln N)^{10}$ and $\lambda = N^{1/2}(\ln\ln N)^{10}$. Under the same conditions $(a_1)$–$(a_3)$, $(b)$ and the restriction* (1.13) *of Theorem* 1.1*, we have the quantitative estimates*

$$\sup_{t\in[0,T_0]} \operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\big(\gamma^{(1)}_{N,\hbar}(t)-\gamma^{M,(1)}_{N,\hbar,\lambda}(t)\big)\langle\hbar\nabla_{x_1}\rangle\right| \le \left(\frac{1}{\ln\ln N}\right)^3, \tag{2.28}$$

$$\sup_{t\in[0,T_0]} \operatorname{Tr}_1\left|\operatorname{Tr}_2\big[V(x_1-x_2)\big(\gamma^{(2)}_{N,\hbar}(t)-\gamma^{M,(2)}_{N,\hbar,\lambda}(t)\big)\big]\right| \lesssim \frac{1}{\ln\ln N}. \tag{2.29}$$

***Proof*** For $H^1$ estimate (2.28), we compute

$$\begin{aligned}
&\operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\big(\gamma^{(1)}_{N,\hbar}(t)-\gamma^{M,(1)}_{N,\hbar,\lambda}(t)\big)\langle\hbar\nabla_{x_1}\rangle\right| \\
&\quad= \operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\operatorname{Tr}_{2,N}\big(|\psi_{N,\hbar}\rangle\langle\psi_{N,\hbar}| - |\psi^M_{N,\hbar,\lambda}\rangle\langle\psi^M_{N,\hbar,\lambda}|\big)\langle\hbar\nabla_{x_1}\rangle\right|.
\end{aligned}$$

By triangle inequality, the above

$$\begin{aligned}
&\le \operatorname{Tr}\left|\operatorname{Tr}_{2,N}\big(|\langle\hbar\nabla_{x_1}\rangle(\psi_{N,\hbar}-\psi^M_{N,\hbar,\lambda})\rangle\langle\langle\hbar\nabla_{x_1}\rangle\psi_{N,\hbar}|\big)\right| \\
&\quad+ \operatorname{Tr}\left|\operatorname{Tr}_{2,N}\big(|\langle\hbar\nabla_{x_1}\rangle\psi^M_{N,\hbar,\lambda}\rangle\langle\langle\hbar\nabla_{x_1}\rangle(\psi_{N,\hbar}-\psi^M_{N,\hbar,\lambda})|\big)\right|.
\end{aligned}$$

By $\operatorname{Tr}_1|\operatorname{Tr}_2 A| \le \operatorname{Tr}_{1,2}|A|$ in Lemma A.5 and $\operatorname{Tr}\big||f\rangle\langle g|\big| \le \|f\|_{L^2}\|g\|_{L^2}$, the above

$$\begin{aligned}
&\le \|\langle\hbar\nabla_{x_1}\rangle(\psi_{N,\hbar}-\psi^M_{N,\hbar,\lambda})\|_{L^2}\|\langle\hbar\nabla_{x_1}\rangle\psi_{N,\hbar}\|_{L^2} \\
&\quad+ \|\langle\hbar\nabla_{x_1}\rangle\psi^M_{N,\hbar,\lambda}\|_{L^2}\|\langle\hbar\nabla_{x_1}\rangle(\psi_{N,\hbar}-\psi^M_{N,\hbar,\lambda})\|_{L^2}.
\end{aligned}$$

As shown in estimate (2.3), we have

$$\|\langle\hbar\nabla_{x_1}\rangle\psi_{N,\hbar}(t)\|^2_{L^2_{\mathbf{x}_N}} \le E_0. \tag{2.30}$$

In the same way, we also have

$$\begin{aligned}
\|\langle\hbar\nabla_{x_1}\rangle\psi^M_{N,\hbar,\lambda}(t)\|^2_{L^2_{\mathbf{x}_N}} &\le \langle\psi^{M,\mathrm{in}}_{N,\hbar}, N^{-1}(H_{N,\hbar,\lambda}+N)\psi^{M,\mathrm{in}}_{N,\hbar}\rangle \\
&= \langle\psi^{M,\mathrm{in}}_{N,\hbar}, (\langle\hbar\nabla_{x_1}\rangle^2 + V_\lambda(x_1-x_2))\psi^{M,\mathrm{in}}_{N,\hbar}\rangle.
\end{aligned}$$

By Hardy's inequality that $V_\lambda(x_1-x_2) \le V(x_1-x_2) \le \langle\nabla_{x_1}\rangle$ and $-\hbar^2\Delta_{x_1} \le -\Delta_{x_1}$, we obtain

$$\|\langle\hbar\nabla_{x_1}\rangle\psi^M_{N,\hbar,\lambda}(t)\|^2_{L^2_{\mathbf{x}_N}} \le \|\langle\nabla_{x_1}\rangle\psi^{M,\mathrm{in}}_{N,\hbar}\|^2_{L^2_{\mathbf{x}_N}} = \left(\frac{\|\langle\nabla_{x_1}\rangle\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}}{\|P_{\le M}\psi^{\mathrm{in}}_{N,\hbar}\|_{L^2_{\mathbf{x}_N}}}\right)^2 \le 4E_0\hbar^{-2},$$

where in the last inequality we used estimates (2.3) and (2.13).

Then by estimate (2.8) in Lemma 2.1, we obtain

$$\mathrm{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\big(\gamma_{N,\hbar}^{(1)}(t)-\gamma_{N,\hbar,\lambda}^{M,(1)}(t)\big)\langle\hbar\nabla_{x_1}\rangle\right|\leq\frac{4(E_0\hbar^{-2})^{\frac{1}{2}}}{(\ln\ln N)^4}\lesssim\frac{1}{(\ln\ln N)^3},$$

where in the last inequality we used the restriction (1.13) to absorb the term $E_0\hbar^{-2}$. This completes the proof of estimate (2.28).

For the potential part (2.29), by partial trace inequality in Lemma A.5 we have

$$\begin{aligned}&\mathrm{Tr}_1\left|\mathrm{Tr}_2\big[V(x_1-x_2)\big(\gamma_{N,\hbar}^{(2)}(t)-\gamma_{N,\hbar,\lambda}^{M,(2)}(t)\big)\big]\right|\\&\quad\leq\mathrm{Tr}\left|V(x_1-x_2)\big(\gamma_{N,\hbar}^{(2)}(t)-\gamma_{N,\hbar,\lambda}^{M,(2)}(t)\big)\right|.\end{aligned}\tag{2.31}$$

By Hardy's inequality that $|V(x_1-x_2)|^2\lesssim-\Delta_{x_1}$ and the operator inequality in Lemma A.6, the above

$$\lesssim\mathrm{Tr}\left|\langle\nabla_{x_1}\rangle\big(\gamma_{N,\hbar}^{(2)}(t)-\gamma_{N,\hbar,\lambda}^{M,(2)}(t)\big)\right|\leq\hbar^{-1}\mathrm{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\big(\gamma_{N,\hbar}^{(2)}(t)-\gamma_{N,\hbar,\lambda}^{M,(2)}(t)\big)\right|.$$

Then by repeating the proof of estimate (2.8), we arrive at

$$\mathrm{Tr}_1\left|\mathrm{Tr}_2\big[V(x_1-x_2)\big(\gamma_{N,\hbar}^{(2)}(t)-\gamma_{N,\hbar,\lambda}^{M,(2)}(t)\big)\big]\right|\lesssim\frac{\hbar^{-1}}{(\ln\ln N)^4}\lesssim\frac{1}{\ln\ln N},\tag{2.32}$$

where in the last inequality we used the restriction (1.13) to absorb the term $\hbar^{-1}$. Hence, we complete the proof of estimate (2.29). □

## 3 Comparing the Regularized BBGKY Hierarchy and the Regularized Hartree Equation

In Sects. 3.1–3.4, the main goal is to establish a long-time estimate for the difference

$$\gamma_{N,\hbar,\lambda}^{M,(k)}-|\phi_{\hbar,\lambda}^M\rangle\langle\phi_{\hbar,\lambda}^M|^{\otimes k},\tag{3.1}$$

where $\phi_{\hbar,\lambda}^M(t)$ is the solution to the regularized Hartree equation

$$i\hbar\partial_t\phi_{\hbar,\lambda}^M=-\frac{1}{2}\hbar^2\Delta\phi_{\hbar,\lambda}^M+\big(V_\lambda*|\phi_{\hbar,\lambda}^M|^2\big)\phi_{\hbar,\lambda}^M\tag{3.2}$$

with the regularized initial data

$$\phi_{\hbar,\lambda}^M(0)=\frac{P_{\leq M}\phi_h^{\mathrm{in}}}{\|P_{\leq M}\phi_h^{\mathrm{in}}\|_{L_x^2}}.\tag{3.3}$$

In Sect. 3.1, we first provide a $k$-$H^1$ type a priori energy bound for the regularized marginal densities $\gamma_{N,\hbar,\lambda}^{M,(k)}$, which lays the foundation of the hierarchy method. Then in Sect. 3.2, we consider the difference (3.1) between regularized BBGKY hierarchy and regularized Hartree hierarchy and establish a preliminary estimate by means of Klainerman–Machedon board game argument. In Sect. 3.3, we are able to give the local-in-time quantitative estimate for the difference. Finally in Sect. 3.4, we sacrifice some decays in $N$ to bootstrap the quantitative estimate to every finite time.

As stated in Proposition 3.8 which we postpone to Sect. 3.4, we have

$$\sup_{t\in[0,T_0]} \operatorname{Tr}\Big|\langle\hbar\nabla_{x_1}\rangle\big(\gamma_{N,\hbar,\lambda}^{M,(1)}(t)-|\phi_{\hbar,\lambda}^M\rangle\langle\phi_{\hbar,\lambda}^M|(t)\big)\langle\hbar\nabla_{x_1}\rangle\Big| \lesssim \left(\frac{1}{\ln\ln N}\right)^{10}, \tag{3.4}$$

$$\sup_{t\in[0,T_0]} \operatorname{Tr}_1\Big|\operatorname{Tr}_2\big[V(x_1-x_2)\big(\gamma_{N,\hbar,\lambda}^{M,(2)}(t)-|\phi_{\hbar,\lambda}^M\rangle\langle\phi_{\hbar,\lambda}^M|^{\otimes 2}(t)\big)\big]\Big| \lesssim \frac{1}{\ln\ln N}. \tag{3.5}$$

Here, we combine estimates (2.28)–(2.29) in Proposition 2.2 and estimates (3.4)–(3.5) in Proposition 3.8 to control the difference between the original evolution and the regularized Hartree equation. For convenience, we define the quantum $N$-body mass density and momentum density

$$\gamma_{N,\hbar}^{(1)}(t,x;x),\quad J_{N,h}^{(1)}(t,x;x)=\operatorname{Im}\big(\hbar\nabla_{x_1}\gamma_{N,\hbar}^{(1)}\big)(t,x;x)$$

as well as the intermediate quantum mass density and momentum density

$$\rho_{\hbar,\lambda}^M(t,x)=|\phi_{\hbar,\lambda}^M(t,x)|^2,\quad J_{\hbar,\lambda}^M(t,x)=\operatorname{Im}\big(\overline{\phi_{\hbar,\lambda}^M}(t,x)\hbar\nabla\phi_{\hbar,\lambda}^M(t,x)\big)$$

with respect to the regularized Hartree equation (3.2).

Now, we sum up the results of Sect. 2 and Sects. 3.1–3.4 to give the following theorem.

**Theorem 3.1** *Let $M=N^{1/2}(\ln\ln N)^{10}$ and $\lambda=N^{1/2}(\ln\ln N)^{10}$. Under the same conditions $(a_1)$–$(a_3)$, $(b)$ and the restriction (1.13) of Theorem 1.1, we have quantitative estimates for the mass density and the momentum density*

$$\|\gamma_{N,\hbar}^{(1)}(t,x;x)-\rho_{\hbar,\lambda}^M(t,x)\|_{L_t^\infty[0,T_0]L^p(\mathbb{R}^3)} \lesssim \left(\frac{1}{\ln\ln N}\right)^{\frac{6-2p}{p}},\quad p\in[1,3), \tag{3.6}$$

$$\|J_{N,\hbar}^{(1)}(t,x;x)-J_{\hbar,\lambda}^M(t,x)\|_{L_t^\infty[0,T_0]L^q(\mathbb{R}^3)} \lesssim \left(\frac{1}{\ln\ln N}\right)^{\frac{6-4q}{q}},\quad q\in\left[1,\frac{3}{2}\right), \tag{3.7}$$

*as well as quantitative estimates for the kinetic energy density and the potential density*

$$\sup_{t\in[0,T_0]}\left\|\left(\hbar\nabla_{x_1}\gamma^{(1)}_{N,\hbar}\hbar\nabla_{x_1}-|\hbar\nabla_{x_1}\phi^M_{\hbar,\lambda}\rangle\langle\hbar\nabla_{x_1}\phi^M_{\hbar,\lambda}|\right)(t,x;x)\right\|_{L^1(\mathbb{R}^3)}\lesssim\frac{1}{\ln\ln N},\tag{3.8}$$

$$\sup_{t\in[0,T_0]}\left\|\int V(x_1-x_2)\gamma^{(2)}_{N,\hbar}(t,x_1,x_2;x_1,x_2)dx_2-\left(\rho^M_{\hbar,\lambda}V*\rho^M_{\hbar,\lambda}\right)(t,x_1)\right\|_{L^1(\mathbb{R}^3)}\lesssim\frac{1}{\ln\ln N}.\tag{3.9}$$

***Remark 3.2*** To match the homogeneous Sobolev norm as stated in Theorem 1.1, we use the Sobolev embedding that $L^p(\mathbb{R}^3)\subset\dot{H}^{-s}(\mathbb{R}^3)$ where $1<p\le 2$ and $s=\frac{3}{p}-\frac{3}{2}$ to obtain

$$\|\gamma^{(1)}_{N,\hbar}(t,x;x)-\rho^M_{\hbar,\lambda}(t,x)\|_{L^\infty_t[0,T_0]\dot{H}^{-s_1}(\mathbb{R}^3)}\lesssim\frac{1}{\ln\ln N},\quad s_1\in[0,1],\tag{3.10}$$

$$\|J^{(1)}_{N,\hbar}(t,x;x)-J^M_{\hbar,\lambda}(t,x)\|_{L^\infty_t[0,T_0]\dot{H}^{-s_2}(\mathbb{R}^3)}\lesssim\left(\frac{1}{\ln\ln N}\right)^{2s_2-1},\quad s_2\in\left(\frac{1}{2},1\right].\tag{3.11}$$

***Proof of Theorem 3.1*** By estimates (2.28)–(2.29) in Proposition 2.2 and estimates (3.4)–(3.5) in Proposition 3.8, we use the triangle inequality to obtain

$$\sup_{t\in[0,T_0]}\operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\left(\gamma^{(1)}_{N,\hbar}(t)-|\phi^M_{\hbar,\lambda}\rangle\langle\phi^M_{\hbar,\lambda}|(t)\right)\langle\hbar\nabla_{x_1}\rangle\right|\lesssim\left(\frac{1}{\ln\ln N}\right)^3,\tag{3.12}$$

$$\sup_{t\in[0,T_0]}\operatorname{Tr}_1\left|\operatorname{Tr}_2\left[V(x_1-x_2)\left(\gamma^{(2)}_{N,\hbar}(t)-|\phi^M_{\hbar,\lambda}\rangle\langle\phi^M_{\hbar,\lambda}|^{\otimes 2}(t)\right)\right]\right|\lesssim\frac{1}{\ln\ln N}.\tag{3.13}$$

For the mass density estimate (3.6) with $p=1$, we have

$$\begin{aligned}\|\gamma^{(1)}_{N,\hbar}(t,x;x)-\rho^M_{\hbar,\lambda}(t,x)\|_{L^1}&=\sup_{\|f\|_{L^\infty}=1}\left|\int_{\mathbb{R}^3}f(x)\left(\gamma^{(1)}_{N,\hbar}(t,x;x)-\rho^M_{\hbar,\lambda}(t,x)\right)dx\right|\\&\le\sup_{\|f\|_{L^\infty}=1}\|f\|_{\mathrm{op}}\operatorname{Tr}\left|\gamma^{(1)}_{N,\hbar}(t)-|\phi^M_{\hbar,\lambda}\rangle\langle\phi^M_{\hbar,\lambda}|(t)\right|\\&\lesssim\left(\frac{1}{\ln\ln N}\right)^3,\end{aligned}\tag{3.14}$$

where in the last inequality we used $\|f\|_{\mathrm{op}}\le\|f\|_{L^\infty}$ and estimate (3.12). This completes the proof for the case $p=1$. For the case $p\in(1,3)$, by interpolation inequality, we have

$$\begin{aligned}&\|\gamma^{(1)}_{N,\hbar}(t,x;x)-\rho^M_{\hbar,\lambda}(t,x)\|_{L^p}\\&\le\|\gamma^{(1)}_{N,\hbar}(t,x;x)-\rho^M_{\hbar,\lambda}(t,x)\|_{L^1}^{\frac{3-p}{2p}}\|\gamma^{(1)}_{N,\hbar}(t,x;x)-\rho^M_{\hbar,\lambda}(t,x)\|_{L^3}^{\frac{3(p-1)}{2p}}.\end{aligned}\tag{3.15}$$

Therefore, to obtain estimate (3.6), it suffices to bound the $L^3$ norm. Here, we only deal with $\gamma_{N,\hbar}^{(1)}(t,x;x)$ as we can estimate $\rho_{\hbar,\lambda}^{M}(t,x)$ in the same way. By the definition of $\gamma_{N,\hbar}^{(1)}$, we have

$$\|\gamma_{N,\hbar}^{(1)}(t,x;x)\|_{L_x^3} = \left[\int_{\mathbb{R}^3}\left|\int \psi_{N,\hbar}(t,x,\mathbf{x}_{2,N})\overline{\psi_{N,\hbar}}(t,x,\mathbf{x}_{2,N})d\mathbf{x}_{2,N}\right|^3 dx\right]^{\frac{1}{3}}. \tag{3.16}$$

By Hölder, Minkowski, Sobolev, and the $H^1$ energy bound (2.3), we get that the above

$$\begin{aligned}&\leq \|\psi_{N,\hbar}\|_{L^2_{\mathbf{x}_{2,N}}L^6_{x_1}}\|\psi_{N,\hbar}\|_{L^2_{\mathbf{x}_{2,N}}L^6_{x_1}}\\ &\lesssim \|\langle\nabla_{x_1}\rangle\psi_{N,\hbar}\|_{L^2}^2 \lesssim E_0\hbar^{-2}.\end{aligned}$$

Combining estimates (3.14), (3.15) and (3.16), we obtain

$$\begin{aligned}\|\gamma_{N,\hbar}^{(1)}(t,x;x)-\rho_{\hbar,\lambda}^{M}(t,x)\|_{L^p} &\leq \left(\frac{1}{\ln\ln N}\right)^{\frac{3(3-p)}{2p}}\left(E_0\hbar^{-2}\right)^{\frac{3(p-1)}{2p}}\\ &= \left(\frac{1}{\ln\ln N}\right)^{\frac{6-2p}{2p}}\left(\frac{1}{\ln\ln N}\right)^{\frac{3-p}{2p}}\left(E_0\hbar^{-2}\right)^{\frac{3(p-1)}{2p}}\\ &\leq \left(\frac{1}{\ln\ln N}\right)^{\frac{6-2p}{2p}},\end{aligned}$$

where in the last inequality we used the restriction (1.13) to absorb the term $E_0\hbar^{-2}$. Hence, we complete the proof of estimate (3.6).

For the momentum estimate (3.7) with $q=1$, we have

$$\begin{aligned}&\|J_{N,\hbar}^{(1)}(t,x;x)-J_{\hbar,\lambda}^{M}(t,x)\|_{L^1}\\ &\quad\leq \left\|(\hbar\nabla_{x_1}(\gamma_{N,\hbar}^{(1)}-|\phi_{\hbar,\lambda}^{M}\rangle\langle\phi_{\hbar,\lambda}^{M}|))(t,x;x)\right\|_{L^1}\\ &\quad= \sup_{\|f\|_{L^\infty}=1}\left|\int_{\mathbb{R}^3} f(x)\big(\hbar\nabla_{x_1}\gamma_{N,\hbar}^{(1)}(t,x;x)-\hbar\nabla_x\phi_{\hbar,\lambda}^{M}(t,x)\overline{\phi_{\hbar,\lambda}^{M}}(t,x)\big)dx\right|\\ &\quad\leq \operatorname{Tr}\left|\hbar\nabla_{x_1}(\gamma_{N,\hbar}^{(1)}-|\phi_{\hbar,\lambda}^{M}\rangle\langle\phi_{\hbar,\lambda}^{M}|)\right|.\end{aligned}\tag{3.17}$$

By the operator inequality in Lemma A.6 and estimate (3.12), the above

$$\begin{aligned}&\leq \operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle(\gamma_{N,\hbar}^{(1)}(t)-|\phi_{\hbar,\lambda}^{M}\rangle\langle\phi_{\hbar,\lambda}^{M}|(t))\langle\hbar\nabla_{x_1}\rangle\right|\\ &\lesssim \left(\frac{1}{\ln\ln N}\right)^3,\end{aligned}$$

which completes the proof for $q = 1$. For the case $q \in (1, \frac{3}{2})$, by interpolation inequality, we have

$$\begin{aligned}&\|J^{(1)}_{N,\hbar}(t,x;x) - J^{M}_{\hbar,\lambda}(t,x)\|_{L^q}\\ &\le \|J^{(1)}_{N,\hbar}(t,x;x) - J^{M}_{\hbar,\lambda}(t,x)\|_{L^1}^{\frac{3-2q}{q}} \|J^{(1)}_{N,\hbar}(t,x;x) - J^{M}_{\hbar,\lambda}(t,x)\|_{L^{\frac{3}{2}}}^{\frac{4q-3}{q}}. \qquad (3.18)\end{aligned}$$

Therefore, we are left to bound the $L^{\frac{3}{2}}$ norm. Here, we deal with $J^{(1)}_{N,\hbar}(t,x;x)$ as we can estimate $J^{M}_{\hbar,\lambda}(t,x)$ in the same way. By the definition of $J^{(1)}_{N,\hbar}(t,x;x)$, we have

$$\begin{aligned}\|J^{(1)}_{N,\hbar}(t,x;x)\|_{L^{\frac{3}{2}}} &\le \left\| \left(\hbar\nabla_{x_1}\gamma^{(1)}_{N,\hbar}\right)(t,x;x)\right\|_{L^{\frac{3}{2}}}\\ &= \left[\int \left| \int \hbar\nabla_{x_1}\psi_{N,\hbar}(t,x,\mathbf{x}_{2,N})\overline{\psi_{N,\hbar}}(t,x,\mathbf{x}_{2,N})d\mathbf{x}_{2,N}\right|^{\frac{3}{2}} dx\right]^{\frac{2}{3}}. \qquad (3.19)\end{aligned}$$

By Hölder, Minkowski, Sobolev, and the $H^1$ energy bound (2.3), we get that the above

$$\begin{aligned}&\le \|\hbar\nabla_{x_1}\psi_{N,\hbar}\|_{L^2_{x_1}L^2_{\mathbf{x}_{2,N}}} \|\psi_{N,\hbar}\|_{L^6_{x_1}L^2_{\mathbf{x}_{2,N}}}\\ &\le \|\hbar\nabla_{x_1}\psi_{N,\hbar}\|_{L^2_{x_1}L^2_{\mathbf{x}_{2,N}}} \|\psi_{N,\hbar}\|_{L^2_{\mathbf{x}_{2,N}}L^6_{x_1}}\\ &\lesssim \|\hbar\nabla_{x_1}\psi_{N,\hbar}\|_{L^2_{x_1}L^2_{\mathbf{x}_{2,N}}} \|\langle\nabla_{x_1}\rangle\psi_{N,\hbar}\|_{L^2_{\mathbf{x}_{2,N}}L^2_{x_1}}\\ &\le E_0\hbar^{-1}.\end{aligned}$$

Combining estimates (3.17), (3.18) and (3.19), we obtain

$$\begin{aligned}\|J^{(1)}_{N,\hbar}(t,x;x) - J^{M}_{\hbar,\lambda}(t,x)\|_{L^q} &\le \left(\frac{1}{\ln\ln N}\right)^{\frac{3(3-2q)}{q}} (E_0\hbar^{-1})^{\frac{4q-3}{q}}\\ &= \left(\frac{1}{\ln\ln N}\right)^{\frac{6-4q}{q}} \left(\frac{1}{\ln\ln N}\right)^{\frac{3-2q}{q}} (E_0\hbar^{-1})^{\frac{4q-3}{q}}\\ &\le \left(\frac{1}{\ln\ln N}\right)^{\frac{6-4q}{q}},\end{aligned}$$

where in the last inequality we used the restriction (1.13) to absorb the term $E_0\hbar^{-1}$. Hence, we arrive at estimate (3.7) as long as $N \ge N_0$ where $N_0$ can depend on the index $q$.

For the kinetic energy (3.8), we have

$$
\begin{aligned}
&\left\| \left(\hbar\nabla_{x_1}\gamma_{N,\hbar}^{(1)}\hbar\nabla_{x_1} - |\hbar\nabla_{x_1}\phi_{\hbar,\lambda}^{M}\rangle\langle\hbar\nabla_{x_1}\phi_{\hbar,\lambda}^{M}|\right)(t,x;x)\right\|_{L_x^1(\mathbb{R}^3)} \\
&= \sup_{\|f\|_{L^\infty}=1}\left|\int_{\mathbb{R}^3} f(x)\left(\hbar\nabla_{x_1}\gamma_{N,\hbar}^{(1)}\hbar\nabla_{x_1} - |\hbar\nabla_{x_1}\phi_{\hbar,\lambda}^{M}\rangle\langle\hbar\nabla_{x_1}\phi_{\hbar,\lambda}^{M}|\right)(t,x;x)dx\right| \\
&\le \operatorname{Tr}\left|\hbar\nabla_{x_1}\left(\gamma_{N,\hbar}^{(1)} - |\phi_{\hbar,\lambda}^{M}\rangle\langle\phi_{\hbar,\lambda}^{M}|\right)\hbar\nabla_{x_1}\right| \\
&\lesssim \|\hbar\nabla\langle\hbar\nabla\rangle^{-1}\|_{\mathrm{op}}\operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\left(\gamma_{N,\hbar}^{(1)}(t) - |\phi_{\hbar,\lambda}^{M}\rangle\langle\phi_{\hbar,\lambda}^{M}|(t)\right)\langle\hbar\nabla_{x_1}\rangle\right|\|\langle\hbar\nabla\rangle^{-1}\hbar\nabla\|_{\mathrm{op}} \\
&\lesssim \frac{1}{\ln\ln N},
\end{aligned}
$$

where in the last inequality we used estimate (3.12) and $\|\hbar\nabla\langle\hbar\nabla\rangle^{-1}\|_{\mathrm{op}} \lesssim 1$.

For the potential energy (3.9), we have

$$
\begin{aligned}
&\left\|\int V(x_1-x_2)\gamma_{N,\hbar}^{(2)}(t,x_1,x_2;x_1,x_2)dx_2 - \left(\rho_{\hbar,\lambda}^{M} V * \rho_{\hbar,\lambda}^{M}\right)(t,x_1)\right\|_{L_{x_1}^1(\mathbb{R}^3)} \\
&= \sup_{\|f\|_{L^\infty}=1}\left|\int_{\mathbb{R}^3} f(x_1)\left[\int V(x_1-x_2)\gamma_{N,\hbar}^{(2)}(t,x_1,x_2;x_1,x_2)dx_2 - \left(\rho_{\hbar,\lambda}^{M} V * \rho_{\hbar,\lambda}^{M}\right)(t,x_1)\right]dx_1\right| \\
&\le \operatorname{Tr}_1\left|\operatorname{Tr}_2\left[V(x_1-x_2)\left(\gamma_{N,\hbar}^{(2)}(t) - |\phi_{\hbar,\lambda}^{M}\rangle\langle\phi_{\hbar,\lambda}^{M}|^{\otimes 2}(t)\right)\right]\right| \\
&\le \frac{1}{\ln\ln N},
\end{aligned}
$$

where we used estimate (3.13) in the last line. This completes the proof of estimate (3.9). □

Next, we will get into the analysis of Sects. 3.1–3.4 and eventually arrive at the desired result in Proposition 3.8.

### 3.1 A Priori Energy Bound

In this section, we establish a priori energy bound for the regularized marginal densities $\gamma_{N,\hbar,\lambda}^{M,(k)}$, which is usually the first step of the hierarchy method. For convenience, we adopt the notation

$$
S_{\hbar}^{(1,k)} = \prod_{j=1}^{k}\langle\hbar\nabla_{x_j}\rangle\langle\hbar\nabla_{x_j'}\rangle. \tag{3.20}
$$

**Proposition 3.3** *Let $M = N^{1/2}(\ln\ln N)^{10}$, $\lambda = N^{1/2}(\ln\ln N)^{10}$, and $k \le (\ln\ln N)^{10}$. We have the $N$-body energy bounds*

$$
\sup_{t\in[0,T_0]}\operatorname{Tr}\left|S_{\hbar}^{(1,k)}\gamma_{N,\hbar,\lambda}^{M,(k)}(t)\right| \le \left(E_{0,\hbar}\right)^k, \tag{3.21}
$$

*where* $E_{0,\hbar}=128E_0\hbar^{-2}$.

***Proof*** By the lower bound of energy estimates (B.1) in Lemma B.1, we have

$$\begin{aligned}\operatorname{Tr}\left|S_\hbar^{(1,k)}\gamma_{N,\hbar,\lambda}^{M,(k)}(t)\right| &= \langle\psi_{N,\hbar,\lambda}^M(t),\langle\hbar\nabla_{x_1}\rangle^2\cdots\langle\hbar\nabla_{x_k}\rangle^2\psi_{N,\hbar,\lambda}^M(t)\rangle\\ &\le 2^kN^{-k}\langle\psi_{N,\hbar,\lambda}^M(t),(H_{N,\hbar,\lambda}+N)^k\psi_{N,\hbar,\lambda}^M(t)\rangle.\end{aligned}\tag{3.22}$$

By the energy conservation, the above

$$=2^kN^{-k}\langle\psi_{N,\hbar}^{M,\mathrm{in}},(H_{N,\hbar,\lambda}+N)^k\psi_{N,\hbar}^{M,\mathrm{in}}\rangle.$$

By the upper bound of energy estimates (B.4) in Lemma B.2, the above

$$\le 16^kN^{-k}\left\langle\psi_{N,\hbar}^{M,\mathrm{in}},\left(\sum_{i=1}^N\langle\nabla_{x_i}\rangle^2\right)^k\psi_{N,\hbar}^{M,\mathrm{in}}\right\rangle.\tag{3.23}$$

Let $\vec{n}=(n_1,n_2,\ldots,n_l)$ be a sequence of positive integers. Define

$$\operatorname{sum}(\vec{n})=n_1+\cdots+n_l,\quad \operatorname{length}(\vec{n})=l.$$

By the symmetry of $\psi_{N,\hbar}^{M,\mathrm{in}}$, we have

$$\begin{aligned}&\left\langle\psi_{N,\hbar}^{M,\mathrm{in}},\left(\sum_{i=1}^N\langle\nabla_{x_i}\rangle^2\right)^k\psi_{N,\hbar}^{M,\mathrm{in}}\right\rangle\\ &\quad\le N^k\langle\psi_{N,\hbar}^{M,\mathrm{in}},\langle\nabla_{x_1}\rangle^2\cdots\langle\nabla_{x_k}\rangle^2\psi_{N,\hbar}^{M,\mathrm{in}}\rangle\\ &\qquad+(k-1)!\sum_{l=1}^{k-1}\sum_{\operatorname{length}(\vec{n})=l,\operatorname{sum}(\vec{n})=k}N^l\langle\psi_{N,\hbar}^{M,\mathrm{in}},\langle\nabla_{x_1}\rangle^{2n_1}\cdots\langle\nabla_{x_l}\rangle^{2n_l}\psi_{N,\hbar}^{M,\mathrm{in}}\rangle\\ &\quad=:\mathrm{I}+\mathrm{II}.\end{aligned}\tag{3.24}$$

For I, we have

$$\begin{aligned}\mathrm{I}&\le N^k\left(\frac{\|\langle\nabla_{x_1}\rangle\cdots\langle\nabla_{x_k}\rangle P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}{\|P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}\right)^2\\ &\le N^k\hbar^{-2k}\left(\frac{\|\langle\hbar\nabla_{x_1}\rangle\cdots\langle\hbar\nabla_{x_k}\rangle P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}{\|P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}}\right)^2\le 4N^k(E_0\hbar^{-2})^k,\end{aligned}\tag{3.25}$$

where in the last inequality we used the energy bound condition (1.19) for $\psi_{N,\hbar}^{\mathrm{in}}$ and the estimate (2.13) which gives that $\|P_{\le M}^{(1,N)}\psi_{N,\hbar}^{\mathrm{in}}\|_{L^2_{\mathbf{x}_N}}\ge\frac{1}{2}$.

For II, we note that

$$\langle \psi^{M,\mathrm{in}}_{N,\hbar}, \langle \nabla_{x_1} \rangle^{2n_1} \cdots \langle \nabla_{x_l} \rangle^{2n_l} \psi^{M,\mathrm{in}}_{N,\hbar} \rangle = \left( \frac{\| \langle \nabla_{x_1} \rangle^{n_1} \cdots \langle \nabla_{x_l} \rangle^{n_l} P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}}{\| P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}} \right)^2,$$

where $n_1 + \cdots + n_l = k$. Due to the fact that $l \leq k-1$, there exists $n_i$ such that $n_i \geq 2$. By the symmetry, we might as well assume that $n_1 \geq 2$. Then, we use Bernstein's inequality to obtain

$$\begin{aligned}
&\frac{\| \langle \nabla_{x_1} \rangle^{n_1} \cdots \langle \nabla_{x_l} \rangle^{n_l} P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}}{\| P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}} \\
&\leq \frac{M^{n_1-2} M^{n_2-1} \cdots M^{n_l-1} \| \langle \nabla_{x_1} \rangle^{2} \langle \nabla_{x_2} \rangle \cdots \langle \nabla_{x_l} \rangle P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}}{\| P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}} \\
&\leq \frac{M^{n_1-2} M^{n_2-1} \cdots M^{n_l-1} \hbar^{-l-1} \| \langle \hbar\nabla_{x_1} \rangle^{2} \langle \hbar\nabla_{x_2} \rangle \cdots \langle \hbar\nabla_{x_l} \rangle P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}}{\| P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}}} \\
&\leq 2 M^{k-l-1} (E_0 \hbar^{-2})^{\frac{l+1}{2}},
\end{aligned} \tag{3.26}$$

where in the last inequality we used the energy bound condition (1.20) for $\psi^{\mathrm{in}}_{N,\hbar}$ and the estimate (2.13) which gives that $\| P^{(1,N)}_{\leq M} \psi^{\mathrm{in}}_{N,\hbar} \|_{L^2_{\mathbf{x}_N}} \geq \frac{1}{2}$. Therefore, we get

$$\begin{aligned}
\mathrm{II} &= (k-1)! \sum_{l=1}^{k-1} \sum_{\mathrm{length}(\vec{n})=l, \mathrm{sum}(\vec{n})=k} N^l \langle \psi^{M,\mathrm{in}}_{N,\hbar}, \langle \nabla_{x_1} \rangle^{2n_1} \cdots \langle \nabla_{x_l} \rangle^{2n_l} \psi^{M,\mathrm{in}}_{N,\hbar} \rangle \\
&\leq (k-1)! \sum_{l=1}^{k-1} \sum_{\mathrm{length}(\vec{n})=l, \mathrm{sum}(\vec{n})=k} 4 N^l M^{2(k-l-1)} (E_0 \hbar^{-2})^{l+1}.
\end{aligned}$$

Inserting in $M = N^{1/2} (\ln \ln N)^{10}$, the above

$$= (k-1)! \sum_{l=1}^{k-1} \sum_{\mathrm{length}(\vec{n})=l, \mathrm{sum}(\vec{n})=k} 4 N^{k-1} (\ln \ln N)^{20(k-l-1)} (E_0 \hbar^{-2})^k.$$

As the combinatorics number $\sum_{l=1}^{k-1} \sum_{\mathrm{length}(\vec{n})=l, \mathrm{sum}(\vec{n})=k}$ can be bounded by $2^k$, we have

$$\mathrm{II} \leq \frac{4 k! 2^k (\ln \ln N)^{20k}}{N} N^k (E_0 \hbar^{-2})^k. \tag{3.27}$$

By the condition that $k \leq (\ln \ln N)^{10}$, it holds that

$$\frac{4k!2^k(\ln \ln N)^{2k}}{N} \leq 1$$

as long as $N \geq N_0$. Hence, we arrive at

$$\mathrm{II} \leq N^k (E_0 \hbar^{-2})^k. \tag{3.28}$$

Now, combining estimates (3.22), (3.23), (3.25) and (3.27), we arrive at

$$\operatorname{Tr}\left|S_{\hbar}^{(1,k)} \gamma_{N,\hbar,\lambda}^{M,(k)}(t)\right| \leq 16^k N^{-k} \left\langle \psi_{N,\hbar}^{M,\mathrm{in}}, \left(\sum_{i=1}^{N} \langle \nabla_{x_i} \rangle^2\right)^k \psi_{N,\hbar}^{M,\mathrm{in}} \right\rangle \leq (128 E_0 \hbar^{-2})^k, \tag{3.29}$$

which completes the proof. □

### 3.2 Preliminary Part

In this section, we make preparations for comparing the regularized BBGKY hierarchy and regularized Hartree hierarchy. It is well-known that $\Gamma_{N,\hbar,\lambda}^{M}(t) = \{\gamma_{N,\hbar,\lambda}^{M,(k)}\}$ satisfies the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy

$$\begin{aligned} i\hbar \partial_t \gamma_{N,\hbar,\lambda}^{M,(k)} &= \sum_{j=1}^{k} \left[ -\frac{\hbar^2}{2} \Delta_{x_j}, \gamma_{N,\hbar,\lambda}^{(k)} \right] + \frac{1}{N} \sum_{1 \leq i < j \leq k} \left[ V_\lambda(x_i - x_j), \gamma_{N,\hbar,\lambda}^{(k)} \right] \\ &\quad + \frac{N-k}{N} \sum_{j=1}^{k} \operatorname{Tr}_{k+1} \left[ V_\lambda(x_j - x_{k+1}), \gamma_{N,\hbar,\lambda}^{(k+1)} \right]. \end{aligned} \tag{3.30}$$

In addition to (3.30), we will use the regularized Hartree hierarchy which takes the form

$$i\hbar \partial_t \gamma_{H,\hbar,\lambda}^{M,(k)} = \sum_{j=1}^{k} \left[ -\frac{\hbar^2}{2} \Delta_{x_j}, \gamma_{H,\hbar,\lambda}^{M,(k)} \right] + \sum_{j=1}^{k} \operatorname{Tr}_{k+1} \left[ V_\lambda(x_j - x_{k+1}), \gamma_{H,\hbar,\lambda}^{M,(k+1)} \right], \tag{3.31}$$

generated by

$$\left\{ \gamma_{H,\hbar,\lambda}^{M,(k)}(t, \mathbf{x}_k; \mathbf{x}_k') = |\phi_{\hbar,\lambda}^{M}\rangle \langle \phi_{\hbar,\lambda}^{M}|^{\otimes k} \right\},$$

the tensor products[11] of solutions to the regularized Hartree equation (3.2).

Denote the difference between the BBGKY hierarchy and the regularized Hartree hierarchy by

$$w_{N,\hbar,\lambda}^{M,(k)} = \gamma_{N,\hbar,\lambda}^{M,(k)} - \gamma_{H,\hbar,\lambda}^{M,(k)}. \tag{3.32}$$

For convenience, we first set up some notations. Recall

$$S_{\hbar}^{(1,k)} = \prod_{j=1}^{k} \langle \hbar \nabla_{x_j} \rangle \langle \hbar \nabla_{x_j'} \rangle \tag{3.33}$$

and define the collision operator

$$\begin{aligned} B_{\lambda,j,k+1} f^{(k+1)} &= B_{\lambda,j,k+1}^{+} f^{(k+1)} - B_{\lambda,j,k+1}^{-} f^{(k+1)} \\ &= \int V_\lambda(x_j - x_{k+1}) f^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}_k', x_{k+1}) dx_{k+1} \\ &\quad - \int V_\lambda(x_j' - x_{k+1}) f^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}_k', x_{k+1}) dx_{k+1}, \end{aligned} \tag{3.34}$$

and

$$B_{\hbar,\lambda,j,k+1} = \frac{1}{\hbar} B_{\lambda,j,k+1}, \quad B_{\hbar,\lambda,j,k+1}^{\pm} = \frac{1}{\hbar} B_{\lambda,j,k+1}^{\pm}. \tag{3.35}$$

Rewrite $\gamma_{N,\hbar,\lambda}^{M,(k)}(t_k)$ in integral form

$$\begin{aligned} \gamma_{N,\hbar,\lambda}^{M,(k)}(t_k) &= U_{\hbar}^{(k)}(t_k) \gamma_{N,\hbar,\lambda}^{M,(k)}(0) + \int_0^{t_k} U_{\hbar}^{(k)}(t_k - t_{k+1}) V_{N,\hbar,\lambda}^{(k)} \gamma_{N,\hbar,\lambda}^{M,(k)}(t_{k+1}) dt_{k+1} \\ &\quad + \frac{N-k}{N} \int_0^{t_k} U_{\hbar}^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)} \gamma_{N,\hbar,\lambda}^{M,(k+1)}(t_{k+1}) dt_{k+1}, \end{aligned} \tag{3.36}$$

[11] As it is indeed a tensor product, with the $H^1$ energy bound (4.35) for the one-body wave function $\phi_{\hbar,\lambda}^{M}(t)$ which is independently set up in Sect. 4.2, the energy bound (3.21) also holds for $\gamma_{H,\hbar,\lambda}^{M,(k)}$ with $E_{0,\hbar}$ replaced by $E_0$.

where we have adopted the shorthands[12]

$$U_{\hbar}^{(k)}(t)=\prod_{j=1}^{k}e^{it\hbar\Delta_{x_j}/2}e^{-it\hbar\Delta_{x_j'}/2}, \tag{3.37}$$

$$V_{N,\hbar,\lambda}^{(k)}\gamma_{N,\hbar,\lambda}^{M,(k)}=\frac{1}{N}\sum_{1\le i<j\le k}\left[V_{\hbar,\lambda}(x_i-x_j),\gamma_{N,\hbar,\lambda}^{M,(k)}\right], \tag{3.38}$$

$$V_{\hbar,\lambda}(x)=\frac{1}{\hbar}V_{\lambda}(x), \tag{3.39}$$

$$B_{\hbar,\lambda}^{(k+1)}\gamma_{N,\hbar,\lambda}^{M,(k+1)}=\sum_{j=1}^{k}B_{\hbar,\lambda,j,k+1}\gamma_{N,\hbar,\lambda}^{(k+1)}=\sum_{j=1}^{k}\mathrm{Tr}_{k+1}\left[V_{\hbar,\lambda}(x_j-x_{k+1}),\gamma_{N,\hbar,\lambda}^{M,(k+1)}\right], \tag{3.40}$$

and we have omitted the $(-i)$ in front of the second and third terms in the right hand side of (3.36) as it serves as 1 in our estimates. In addition to (3.36), we write (3.31) in integral form

$$\gamma_{H,\hbar,\lambda}^{M,(k)}(t_k)=U_{\hbar}^{(k)}(t_k)\gamma_{H,\hbar,\lambda}^{M,(k)}(0)+\int_0^{t_k}U_{\hbar}^{(k)}(t_k-t_{k+1})B_{\hbar,\lambda}^{(k+1)}\gamma_{H,\hbar,\lambda}^{M,(k+1)}(t_{k+1})dt_{k+1}. \tag{3.41}$$

The difference $w_{N,\hbar,\lambda}^{M,(k)}=\gamma_{N,\hbar,\lambda}^{M,(k)}-\gamma_{H,\hbar,\lambda}^{M,(k)}$ solves the hierarchy

$$\begin{aligned}w_{N,\hbar,\lambda}^{M,(k)}(t_k)&=U_{\hbar}^{(k)}(t_k)w_{N,\hbar,\lambda}^{M,(k)}(0)+\int_0^{t_k}U_{\hbar}^{(k)}(t_k-t_{k+1})V_{N,\hbar,\lambda}^{(k)}\gamma_{N,\hbar,\lambda}^{M,(k)}(t_{k+1})dt_{k+1}\\&\quad-\frac{k}{N}\int_0^{t_k}U_{\hbar}^{(k)}(t_k-t_{k+1})B_{\hbar,\lambda}^{(k+1)}\gamma_{N,\hbar,\lambda}^{M,(k+1)}(t_{k+1})dt_{k+1}\\&\quad+\int_0^{t_k}U_{\hbar}^{(k)}(t_k-t_{k+1})B_{\hbar,\lambda}^{(k+1)}w_{N,\hbar,\lambda}^{M,(k+1)}(t_{k+1})dt_{k+1}.\end{aligned} \tag{3.42}$$

Iterating hierarchy (3.42) $l_c$ times[13] at the last term of (3.42), we have

$$w_{N,\hbar,\lambda}^{M,(k)}(t_k)=\mathrm{FP}^{(k,l_c)}(t_k)+\mathrm{DP}^{(k,l_c)}(t_k)+\mathrm{EP}^{(k,l_c)}(t_k)+\mathrm{IP}^{(k,l_c)}(t_k), \tag{3.43}$$

where we have grouped the terms in $w_{N,\hbar,\lambda}^{M,(k)}(t_k)$ into four parts: the free/ driving/ error/ interaction parts. We remark that (3.43) holds for all $l_c\ge 1$ and we will select $l_c$ depending on what aspect of $w_{N,\hbar,\lambda}^{M,(k)}$ we need in Sects. 3.3–3.4. To write out the four

[12] Please notice that we have divided by $\hbar$ to use (3.37).

[13] $l_c$ means "coupling level".

parts of $w_{N,\hbar,\lambda}^{M,(k)}$, we define the notation that, for $j \geq 1$,

$$\begin{aligned} &J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)})(f^{(k+j)}(t_{k+j})) \\ &\quad = \big(U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)}\big) \cdots \big(U_\hbar^{(k+j-1)}(t_{k+j-1} - t_{k+j}) B_{\hbar,\lambda}^{(k+j)}\big) f^{(k+j)}(t_{k+j}), \end{aligned} \tag{3.44}$$

and $J_{\hbar,\lambda}^{(k,0)}(t_k, \underline{t}_{(k,0)}) = f^{(k)}(t_k)$, where $\underline{t}_{(k,j)} = (t_{k+1}, \ldots, t_{k+j})$ for $j \geq 1$. In this notation, the free part of $w_{N,\hbar,\lambda}^{M,(k)}$ at $l_c$ coupling level is

$$\begin{aligned} \mathrm{FP}^{(k,l_c)}(t_k) &= U_\hbar^{(k)}(t_k) w_{N,\hbar,\lambda}^{M,(k)}(0) \\ &\quad + \sum_{j=1}^{l_c} \int_0^{t_k} \cdots \int_0^{t_{k+j-1}} U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)} \cdots \\ &\quad \times U_\hbar^{(k+j-1)}(t_{k+j-1} - t_{k+j}) B_{\hbar,\lambda}^{(k+j)} \big(U_\hbar^{(k+j)}(t_{k+j}) w_{N,\hbar}^{(k+j)}(0)\big) d\underline{t}_{(k,j)} \\ &= \sum_{j=0}^{l_c} \int_0^{t_k} \cdots \int_0^{t_{k+j-1}} J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)}) \big(f_{\mathrm{FP}}^{(k,j)}(t_{k+j})\big) d\underline{t}_{(k,j)}, \end{aligned} \tag{3.45}$$

where in the $j = 0$ case, it is meant that there are no time integrals and $J_{\hbar,\lambda}^{(k,0)}$ is the identity operator, and

$$f_{\mathrm{FP}}^{(k,j)}(t_{k+j}) = U_\hbar^{(k+j)}(t_{k+j}) w_{N,\hbar,\lambda}^{M,(k+j)}(0). \tag{3.46}$$

The driving part is given by

$$\begin{aligned} \mathrm{DP}^{(k,l_c)}(t_k) &= \int_0^{t_k} U_\hbar^{(k)}(t_k - t_{k+1}) V_{N,\hbar,\lambda}^{(k)} \gamma_{N,\hbar,\lambda}^{M,(k)}(t_{k+1}) dt_{k+1} \\ &\quad + \sum_{j=1}^{l_c} \int_0^{t_k} \cdots \int_0^{t_{k+j-1}} U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)} \cdots U_\hbar^{(k+j-1)}(t_{k+j-1} - t_{k+j}) B_{\hbar,\lambda}^{(k+j)} \\ &\quad \times \left( \int_0^{t_{k+j}} U_\hbar^{(k+j)}(t_{k+j} - t_{k+j+1}) V_{\hbar,\lambda}^{(k+j)} \gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j+1}) dt_{k+j+1} \right) d\underline{t}_{(k,j)} \\ &= \sum_{j=0}^{l_c} \int_0^{t_k} \cdots \int_0^{t_{k+j-1}} J_{\hbar,\lambda}^{(k,j)}(\underline{t}_{(k,j)}) \big(f_{\mathrm{DP}}^{(k,j)}(t_{k+j})\big) d\underline{t}_{(k,j)}, \end{aligned} \tag{3.47}$$

where in the $j = 0$ case, it is meant that there are no time integrals and $J_{\hbar,\lambda}^{(k,0)}$ is the identity operator, and

$$f_{\mathrm{DP}}^{(k,j)}(t_{k+j}) = \int_0^{t_{k+j}} U_\hbar^{(k+j)}(t_{k+j} - t_{k+j+1}) V_{\hbar,\lambda}^{(k+j)} \gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j+1}) dt_{k+j+1}. \tag{3.48}$$

The error part is given by

$$
\begin{aligned}
&\mathrm{EP}^{(k,l_c)}(t_k)\\
&= -\frac{k}{N}\int_0^{t_k} U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)} \gamma_{N,\hbar,\lambda}^{M,(k+1)}(t_{k+1}) dt_{k+1}\\
&\quad - \sum_{j=1}^{l_c} \frac{k+j}{N} \int_0^{t_k} \cdots \int_0^{t_{k+j-1}} U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)} \cdots U_\hbar^{(k+j-1)}(t_{k+j-1} - t_{k+j}) B_{\hbar,\lambda}^{(k+j)}\\
&\quad \times \left( \int_0^{t_{k+j}} U_\hbar^{(k+j)}(t_{k+j} - t_{k+j+1}) B_{\hbar,\lambda}^{(k+j+1)} \gamma_{N,\hbar,\lambda}^{M,(k+j+1)}(t_{k+j+1}) dt_{k+j+1} \right) d\underline{t}_{(k,j)}\\
&= \sum_{j=1}^{l_c+1} \int_0^{t_k} \cdots \int_0^{t_{k+j-1}} J_{\hbar,\lambda}^{(k,j)}(\underline{t}_{(k,j)}) \big(f_{\mathrm{EP}}^{(k,j)}(t_{k+j})\big) d\underline{t}_{(k,j)},
\end{aligned}
\tag{3.49}
$$

where in the $j = 0$ case, it is meant that there are no time integrals and $J_{\hbar,\lambda}^{(k,0)}$ is the identity operator, and

$$
f_{\mathrm{IP}}^{(k,j)}(t_{k+j}) = -\frac{k+j-1}{N} \gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j}). \tag{3.50}
$$

The interaction part is given by

$$
\begin{aligned}
\mathrm{IP}^{(k,l_c)}(t_k) &= \int_0^{t_k} \cdots \int_0^{t_{k+l_c}} U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda}^{(k+1)} \cdots\\
&\quad \cdot U^{(k+l_c)}(t_{k+l_c} - t_{k+l_c+1}) B_{\hbar,\lambda}^{(k+l_c+1)} \big(w_{N,\hbar,\lambda}^{M,(k+l_c+1)}(t_{k+l_c+1})\big) dt_{k+1} \cdots dt_{k+l_c+1}\\
&= \int_0^{t_k} \cdots \int_0^{t_{k+l_c}} J_{\hbar,\lambda}^{(k,l_c+1)}(t_k, \underline{t}_{(k,l_c+1)}) \big(f_{\mathrm{IP}}^{(k,l_c+1)}(t_{k+l_c+1})\big) d\underline{t}_{(k,l_c+1)},
\end{aligned}
\tag{3.51}
$$

where

$$
f_{\mathrm{IP}}^{(k,l_c+1)}(t_{k+l_c+1}) = w_{N,\hbar,\lambda}^{M,(k+l_c+1)}(t_{k+l_c+1}). \tag{3.52}
$$

There are around $\frac{(k+l_c)!}{k!}$ many summands in each part. They can be grouped together by using the KM board game argument [50], which is below.

**Lemma 3.4** ([50, Lemma 2.1])[14] *For $j \geq 1$, one can express*

$$
\begin{aligned}
&\int_0^{t_k} \cdots \int_0^{t_{k+j-1}} J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)}) (f^{(k+j)}) d\underline{t}_{(k,j)}\\
&\quad = \sum_m \int_D J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)}, \mu_m) (f^{(k+j)}) d\underline{t}_{(k,j)}.
\end{aligned}
\tag{3.53}
$$

[14] More advanced version of this combinatoric is now available, see [21, 23].

*Here* $D \subset [0, t_k]^j$, $\mu_m$ *are a set of maps from* $\{k+1, \ldots, k+j\}$ *to* $\{1, \ldots, k+j-1\}$ *and* $\mu_m(l) < l$ *for all* $l$, *and*

$$J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)}, \mu_m)(f^{(k+j)}) = \left(U_\hbar^{(k)}(t_k - t_{k+1}) B_{\hbar,\lambda,\mu_m(k+1),k+1}\right) \cdots \\ \cdot \left(U_\hbar^{(k+j-1)}(t_{k+j-1} - t_{k+j}) B_{\hbar,\lambda,\mu_m(k+j),k+j}\right) f^{(k+j)}(t_{k+j}). \tag{3.54}$$

*The summing number can be controlled by* $2^{k+2j-2}$, *see, for example* [20, Lemma 2.5].

Then we are able to estimate $J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)})(f^{(k+j)})$ via collapsing estimates in Lemma A.1.

**Lemma 3.5** *For* $j \geq 1$, *we have*

$$\begin{aligned} &\mathrm{Tr}\left|\int_0^{t_k} \cdots \int_0^{t_{k+j-1}} S_\hbar^{(1,k)} J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)})(f^{(k+j)}(t_{k+j}))d\underline{t}_{(k,j)}\right| \\ &\quad \leq 2^k (C\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k+j)} f^{(k+j)}(t_{k+j})\right|. \end{aligned} \tag{3.55}$$

***Proof*** We start by using Lemma 3.4,

$$\begin{aligned} &\mathrm{Tr}\left|\int_0^{t_k} \cdots \int_0^{t_{k+j-1}} S_\hbar^{(1,k)} J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)})(f^{(k+j)}(t_{k+j}))d\underline{t}_{(k,j)}\right| \\ &\leq 2^{k+2j} \mathrm{Tr}\left|\int_D S_\hbar^{(1,k)} J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)}, \mu_m)(f^{(k+j)}(t_{k+j}))d\underline{t}_{(k,j)}\right| \\ &\leq 2^{k+2j} \int_0^T \cdots \int_0^T \mathrm{Tr}\left|S_\hbar^{(1,k)} J_{\hbar,\lambda}^{(k,j)}(t_k, \underline{t}_{(k,j)}, \mu_m)(f^{(k+j)}(t_{k+j}))\right| d\underline{t}_{(k,j)}. \end{aligned}$$

By $S_\hbar^{(1,k)} U_\hbar^{(k)}(t) = U_\hbar^{(k)}(t) S_\hbar^{(1,k)}$ and $\mathrm{Tr}|AB| \leq \mathrm{Tr}|A| \|B\|_{\mathrm{op}}$, the above

$$\leq 2^{k+2j} \int_0^T \cdots \int_0^T \mathrm{Tr}\left|S_\hbar^{(1,k)} B_{\hbar,\lambda,\mu_m(k+1),k+1} \cdots f^{(k+j)}(t_{k+j})\right| d\underline{t}_{(k,j)}.$$

Applying Lemma A.1, the above

$$\leq 2^{k+2j} \widetilde{C} \hbar^{-2} \int_0^T \cdots \int_0^T \mathrm{Tr}\left|S_\hbar^{(1,k+1)} U_\hbar^{(k+1)}(t_{k+1} - t_{k+2}) \cdots (f^{(k+j)}(t_{k+j}))\right| d\underline{t}_{(k,j)}.$$

Repeating such a process gives that the above

$$\begin{aligned} &\leq 2^{k+2j} (\widetilde{C}\hbar^{-2})^j \int_0^T \cdots \int_0^T \mathrm{Tr}\left|S_\hbar^{(1,k+j)} f^{(k+j)}(t_{k+j})\right| d\underline{t}_{(k,j)} \\ &\leq 2^k (4\widetilde{C}\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k+j)} f^{(k+j)}(t_{k+j})\right|, \end{aligned}$$

which completes the proof with $C = 4\widetilde{C}$. □

### 3.3 Local-in-Time Estimate

In the section, we first estimate the four parts contained in the difference hierarchy (3.43). Then combining estimates for the four parts, we arrive at a local-in-time $k$-$H^1$ type estimate as shown in Proposition 3.7.

**Lemma 3.6** *For $k \le (\ln\ln N)^2$ and $l_c \le \ln\ln N$, we have the following estimates for the four parts.*

*For the free part,*

$$\sup_{t_k\in[t_0,t_0+T]} \mathrm{Tr}\left|S_\hbar^{(1,k)}\mathrm{FP}^{(k,l_c)}(t_k)\right| \le 2^k \sum_{j=0}^{l_c}(C\hbar^{-2}T)^j\,\mathrm{Tr}\left|S_\hbar^{(1,k+j)}w_{N,\hbar,\lambda}^{M,(k+j)}(t_0)\right|. \tag{3.56}$$

*For the driving part,*

$$\sup_{t_k\in[t_0,t_0+T]} \mathrm{Tr}\left|S_\hbar^{(1,k)}\mathrm{DP}^{(k,l_c)}(t_k)\right| \le N^{-\frac{1}{10}}(4E_{0,\hbar})^k \sum_{j=0}^{l_c}(16E_{0,\hbar}C\hbar^{-2}T)^{j+1}. \tag{3.57}$$

*For the error part,*

$$\sup_{t_k\in[t_0,t_0+T]} \mathrm{Tr}\left|S_\hbar^{(1,k)}\mathrm{EP}^{(k,l_c)}(t_k)\right| \le N^{-1}(4E_{0,\hbar})^k \sum_{j=0}^{l_c}(16E_{0,\hbar}C\hbar^{-2}T)^{j+1}. \tag{3.58}$$

*For the interaction part,*

$$\sup_{t_k\in[t_0,t_0+T]} \mathrm{Tr}\left|S_\hbar^{(1,k)}\mathrm{IP}^{(k,l_c)}(t_k)\right| \le (4E_{0,\hbar})^k(4E_{0,\hbar}C\hbar^{-2}T)^{l_c+1}. \tag{3.59}$$

***Proof*** For convenience, we might as well take $t_0 = 0$ as the proof works the same for general case by time translation.

For the free part, applying estimate (3.55) in Lemma 3.5, we arrive at

$$\begin{aligned}&\sup_{t_k\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k)}\mathrm{FP}^{(k,l_c)}(t_k)\right|\\ &\quad\le \sup_{t_k\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k)}f_{\mathrm{FP}}^{(k,0)}(t_k)\right| + \sum_{j=1}^{l_c}2^k(C\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k+j)}f_{\mathrm{FP}}^{(k,j)}(t_{k+j})\right|.\end{aligned}$$

Plugging in $f_{\mathrm{FP}}^{(k,j)}(t_{k+j}) = U_\hbar^{(k+j)}(t_{k+j}) w_{N,\hbar,\lambda}^{M,(k+j)}(0)$, the above

$$\leq \sup_{t_k\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k)} U_\hbar^{(k)}(t_k) w_{N,\hbar,\lambda}^{M,(k)}(0)\right| \\ + \sum_{j=1}^{l_c} 2^k (C\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k+j)} U_\hbar^{(k+j)}(t_{k+j}) w_{N,\hbar,\lambda}^{M,(k+j)}(0)\right|.$$

By $S_\hbar^{(1,k)} U_\hbar^{(k)}(t) = U_\hbar^{(k)}(t) S_\hbar^{(1,k)}$ and $\operatorname{Tr}|AB| \leq \operatorname{Tr}|A| \|B\|_{\mathrm{op}}$, the above

$$\leq \sum_{j=0}^{l_c} 2^k (C\hbar^{-2}T)^j \operatorname{Tr}\left|S_\hbar^{(1,k+j)} w_{N,\hbar,\lambda}^{M,(k+j)}(0)\right|. \tag{3.60}$$

We have (3.56) as claimed.

For the driving part, the same process yields

$$\sup_{t_k\in[0,T]} \left|S_\hbar^{(1,k)} \mathrm{DP}^{(k,l_c)}(t_k)\right| \\ \leq \sup_{t_k\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k)} f_{\mathrm{DP}}^{(k,0)}(t_k)\right| + \sum_{j=1}^{l_c} 2^k (C\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k+j)} f_{\mathrm{DP}}^{(k,j)}(t_{k+j})\right|.$$

Plugging in $f_{\mathrm{DP}}^{(k,j)}(t_{k+j}) = \int_0^{t_{k+j}} U_\hbar^{(k+j)}(t_{k+j} - t_{k+j+1}) V_{\hbar,\lambda}^{(k+j)} \gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j+1}) \cdot dt_{k+j+1}$, the above

$$\leq T \sup_{t_{k+1}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k)} V_{N,\hbar,\lambda}^{(k)} \gamma_{N,\hbar,\lambda}^{M,(k)}(t_{k+1})\right| \\ + \sum_{j=1}^{l_c} 2^k (C\hbar^{-2}T)^j T \sup_{t_{k+j+1}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k+j)} V_{N,\hbar,\lambda}^{(k+j)} \gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j+1})\right|.$$

Expanding $V_{N,\hbar,\lambda}^{(k+j)}$ defined in (3.38) and using estimate (A.9) in Lemma A.2 give that the above

$$\leq \frac{C\lambda^{7/4} k^2 \hbar^{-1} T}{N} \sup_{t_{k+1}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k)} \gamma_{N,\hbar,\lambda}^{M,(k)}(t_{k+1})\right| \\ + \sum_{j=1}^{l_c} 2^k (C\hbar^{-2}T)^j \frac{C\lambda^{7/4}(k+j)^2 \hbar^{-1} T}{N} \sup_{t_{k+j+1}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k+j)} \gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j+1})\right|.$$

Since $k+l_c \leq (\ln\ln N)^{10}$, we can appeal to the $N$-body energy bounds (3.21) to yield that the above

$$\leq \frac{C\lambda^{7/4}k^2\hbar^{-1}T}{N}(E_{0,\hbar})^k + \sum_{j=1}^{l_c} 2^k (C\hbar^{-2}T)^j \frac{C\lambda^{7/4}(k+j)^2\hbar^{-1}T}{N}(E_{0,\hbar})^{k+j}.$$

Inserting in $\lambda = N^{1/2}(\ln\ln N)^{10}$ gives that the above

$$\begin{aligned}
&\leq \frac{Ck^2\hbar^{-1}T}{N^{\frac{1}{10}}}(E_{0,\hbar})^k + \sum_{j=1}^{l_c} 2^k (C\hbar^{-2}T)^j \frac{C(k+j)^2\hbar^{-1}T}{N^{\frac{1}{10}}}(E_{0,\hbar})^{k+j} \\
&\leq N^{-\frac{1}{10}}(4E_{0,\hbar})^k C\hbar^{-1}T + N^{-\frac{1}{10}}(4E_{0,\hbar})^k \sum_{j=1}^{l_c}\left(C\hbar^{-2}T\right)^{j+1}(4E_{0,\hbar})^j \\
&\leq N^{-\frac{1}{10}}(4E_{0,\hbar})^k \sum_{j=0}^{l_c}(4E_{0,\hbar}C\hbar^{-2}T)^{j+1},
\end{aligned}$$

which completes the proof for the driving part.

For the error part, it reads

$$\sup_{t_k\in[0,T]}\left|S_\hbar^{(1,k)}\mathrm{EP}^{(k,l_c)}(t_k)\right| \leq \sum_{j=1}^{l_c+1} 2^k (C\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k+j)} f_{\mathrm{EP}}^{(k,j)}(t_{k+j})\right|.$$

Plugging in $f_{\mathrm{EP}}^{(k,j)}(t_{k+j}) = -\frac{k+j-1}{N}\gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j})$, the above

$$\leq \frac{1}{N}\sum_{j=1}^{l_c+1}(k+j)2^k(C\hbar^{-2}T)^j \sup_{t_{k+j}\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k+j)}\gamma_{N,\hbar,\lambda}^{M,(k+j)}(t_{k+j})\right|.$$

Since $k+l_c \leq (\ln\ln N)^{10}$, we can appeal to the $N$-body energy bounds (3.21) to yield that the above

$$\begin{aligned}
&\leq \frac{1}{N}\sum_{j=1}^{l_c+1}(k+j)2^k(C\hbar^{-2}T)^j(E_{0,\hbar})^{k+j} \\
&\leq N^{-1}(4E_{0,\hbar})^k \sum_{j=1}^{l_c+1}(4E_{0,\hbar}C\hbar^{-2}T)^j,
\end{aligned}$$

which completes the proof for the error part.

For the interaction part, we have similarly

$$\sup_{t_k\in[0,T]}\left|S_\hbar^{(1,k)}\mathrm{IP}^{(k,l_c)}(t_k)\right| \leq 2^k(C\hbar^{-2}T)^{l_c+1} \sup_{t_{k+l_c+1}\in[0,T]} \mathrm{Tr}\left|S_\hbar^{(1,k+l_c+1)} f_{\mathrm{IP}}^{(k,l_c+1)}(t_{k+l_c+1})\right|.$$

Plugging in $f_{\mathrm{IP}}^{(k,l_c+1)}(t_{k+l_c+1}) = w_{N,\hbar,\lambda}^{M,(k+l_c+1)}(t_{k+l_c+1})$, the above

$$\leq 2^k (C\hbar^{-2}T)^{l_c+1} \sup_{t_{k+l_c+1}\in[0,T]} \operatorname{Tr}\left|S_\hbar^{(1,k+l_c+1)} w_{N,\hbar,\lambda}^{M,(k+l_c+1)}(t_{k+l_c+1})\right|.$$

Since $k + l_c + 1 \leq (\ln\ln N)^{10}$, we can appeal to the $N$-body energy bounds (3.21) to yield that the above

$$\leq 2^k (C\hbar^{-2}T)^{l_c+1} (2E_{0,\hbar})^{k+l_c+1},$$

which is (3.59). □

Now, we could use Lemma 3.6 to set up the $k$-$H^1$ type estimate for the difference $w_{N,\hbar,\lambda}^{M,(k)}$ as following.

**Proposition 3.7** *Let* $T \leq \frac{\hbar^2}{4E_{0,\hbar}Ce}$. *For* $k \leq (\ln\ln N)^2$, $l_c \leq \ln\ln N$, *we have*

$$\begin{aligned}
&\sup_{t\in[t_0,t_0+T]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \\
&\quad\leq 2^k \sum_{j=0}^{l_c} (C\hbar^{-2}T)^j \operatorname{Tr}\left|S_\hbar^{(1,k+j)} w_{N,\hbar,\lambda}^{M,(k+j)}(t_0)\right| \\
&\qquad + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.
\end{aligned} \tag{3.61}$$

***Proof*** The conclusion of Lemma 3.6 reads

$$\begin{aligned}
&\sup_{t\in[t_0,t_0+T]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \\
&\quad\leq 2^k \sum_{j=0}^{l_c} (C\hbar^{-2}T)^j \operatorname{Tr}\left|S_\hbar^{(1,k+j)} w_{N,\hbar,\lambda}^{M,(k+j)}(t_0)\right| \\
&\qquad + 2N^{-\frac{1}{10}} (4E_{0,\hbar})^k \sum_{j=0}^{l_c} (16E_{0,\hbar}C\hbar^{-2}T)^{j+1} \\
&\qquad + (4E_{0,\hbar})^k (4E_{0,\hbar}C\hbar^{-2}T)^{l_c+1}.
\end{aligned} \tag{3.62}$$

Plugging in $T \leq \frac{\hbar^2}{4E_{0,\hbar}Ce}$, we obtain (3.61). □

### 3.4 Bootstrapping to Long-Time Estimate

In the section, we will iteratively use Proposition 3.7 to obtain the convergence rate for every finite time at the price of weakening the convergence rate.

**Proposition 3.8** *Let $T_0 < +\infty$. For $k \le (\ln\ln N)^2 - \sum_{j=0}^{n(T_0,\hbar)} \frac{\ln\ln N}{2^j j!}$, we have*

$$\sup_{t\in[0,T_0]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \le (e^{n(T_0,\hbar)} 4E_{0,\hbar})^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2^{n(T_0,\hbar)} n(T_0,\hbar)!}}, \tag{3.63}$$

*where $n(T_0,\hbar) = 4eCE_{0,\hbar}\hbar^{-2}T_0$. Moreover, under the restriction (1.13) that*

$$N \ge e^{(3)}\left([E_{0,\hbar}\hbar^{-2}T_0]^2\right),$$

*for $N \ge N_0$ we have (3.4) and (3.5) which we restate here*

$$\sup_{t\in[0,T_0]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \le \left(\frac{1}{\ln\ln N}\right)^{10},$$
$$\sup_{t\in[0,T_0]} \operatorname{Tr}_1\left|\operatorname{Tr}_2\left[V(x_1-x_2)\left(\gamma_{N,\hbar}^{(2)}(t) - |\phi_{\hbar,\lambda}^M\rangle\langle\phi_{\hbar,\lambda}^M|^{\otimes 2}(t)\right)\right]\right| \le \frac{1}{\ln\ln N}.$$

***Proof*** Step 0. Set $\tau = \frac{\hbar^2}{4E_{0,\hbar}Ce}$. Then for

$$k \le (\ln\ln N)^2 - \ln\ln N, \quad l_c \le \ln\ln N,$$

by estimate (3.61) in Proposition 3.7, we have

$$\begin{aligned}&\sup_{t\in[0,\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \\ &\le 2^k \sum_{j=0}^{l_c} (C\hbar^{-2}\tau)^j \operatorname{Tr}\left|S_\hbar^{(1,k+j)} w_{N,\hbar,\lambda}^{M,(k+j)}(0)\right| + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.\end{aligned}$$

By the initial condition (1.21), the above

$$\le \frac{(2E_0)^k}{\ln N} \sum_{j=0}^{l_c} (CE_0\hbar^{-2}\tau)^j + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.$$

Plugging in $\tau = \frac{\hbar^2}{4E_{0,\hbar}Ce}$, the above

$$\le \frac{(2E_0)^k}{\ln N} \sum_{j=0}^{l_c} \left(\frac{1}{2}\right)^j + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.$$

By taking $l_c + 1 = \ln\ln N$, we arrive at

$$\sup_{t\in[0,\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \le \frac{2(4E_{0,\hbar})^k}{\ln N} \tag{3.64}$$

for every $k \le (\ln\ln N)^2 - \ln\ln N$.

Step 1. Let $t_1 = \tau$. For

$$k \le (\ln\ln N)^2 - \left(\ln\ln N + \frac{\ln\ln N}{2}\right), \quad l_c \le \frac{\ln\ln N}{2},$$

we make use of estimate (3.61) in Proposition 3.7 again to obtain

$$\begin{aligned}
&\sup_{t\in[t_1,t_1+\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \\
&\quad\le 2^k \sum_{j=0}^{l_c} (C\hbar^{-2}\tau)^j \operatorname{Tr}\left|S_\hbar^{(1,k+j)} w_{N,\hbar,\lambda}^{M,(k+j)}(t_1)\right| \\
&\qquad + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.
\end{aligned}$$

Since $k + l_c \le (\ln\ln N)^2 - \ln\ln N$, one can adopt estimate (3.64) in Step 0 to make the above reach

$$\le \frac{2(4E_{0,\hbar})^k}{\ln N} \sum_{j=0}^{l_c} (C\hbar^{-2}\tau)^j (4E_{0,\hbar})^j + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.$$

Recalling $\tau = \frac{\hbar^2}{4E_{0,\hbar}Ce}$, the above

$$\begin{aligned}
&\le \frac{2(4E_{0,\hbar})^k}{\ln N} \sum_{j=0}^{l_c} \left(\frac{1}{2}\right)^j + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1} \\
&\le \frac{2(4E_{0,\hbar})^k}{\ln N} + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.
\end{aligned}$$

By taking $l_c + 1 = (\ln\ln N)/2$, we arrive at

$$\sup_{t\in[t_1,t_1+\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \le e^k (4E_{0,\hbar})^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2}} \tag{3.65}$$

for every $k \le (\ln\ln N)^2 - \left(\ln\ln N + \frac{\ln\ln N}{2}\right)$.

Step $m$. Let $t_m = m\tau$. Now we assume that (3.65) is true for the case $n = m$, that is,

$$\sup_{t\in[t_m,t_m+\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \le e^{mk} (4E_{0,\hbar})^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2^m m!}} \tag{3.66}$$

for every $k \le (\ln\ln N)^2 - \sum_{j=0}^{m} \frac{\ln\ln N}{2^j j!}$. Then we will prove it for $n = m + 1$.

For

$$k \leq (\ln \ln N)^2 - \sum_{j=0}^{m+1} \frac{\ln \ln N}{2^j j!}, \quad l_c \leq \frac{\ln \ln N}{2^{m+1}(m+1)!},$$

one can employ estimate (3.61) in Proposition 3.7 to reach to

$$\begin{aligned}
&\sup_{t \in [t_{m+1}, t_{m+1}+\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \\
&\leq 2^k \sum_{j=0}^{l_c} (C\hbar^{-2}\tau)^j \operatorname{Tr}\left|S_\hbar^{(1,k+j)} w_{N,\hbar,\lambda}^{M,(k+j)}(t_{m+1})\right| \\
&\quad + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.
\end{aligned}$$

Since $k + l_c \leq (\ln \ln N)^2 - \sum_{j=0}^{m} \frac{\ln \ln N}{2^j j!}$, one can use estimate (3.66) in the case $n = m$ to get that the above

$$\begin{aligned}
&\leq \left(\frac{1}{\ln N}\right)^{\frac{1}{2^m m!}} (2e^m)^k (4E_{0,\hbar})^k \sum_{j=0}^{l_c} (e^m 4E_{0,\hbar} C\hbar^{-2}\tau)^j \\
&\quad + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.
\end{aligned}$$

Recalling $\tau = \frac{\hbar^2}{4E_{0,\hbar}Ce}$, the above

$$\leq (2e^m)^k (4E_{0,\hbar})^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2^m m!}} (e^m)^{l_c+1} + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{e}\right)^{l_c+1}.$$

By taking $l_c + 1 = \frac{\ln \ln N}{2^{m+1}(m+1)!}$, we arrive at

$$\begin{aligned}
&\sup_{t \in [t_{m+1}, t_{m+1}+\tau]} \operatorname{Tr}\left|S_\hbar^{(1,k)} w_{N,\hbar,\lambda}^{M,(k)}(t)\right| \\
&\leq (4E_{0,\hbar})^k (2e^m)^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2^m m!}} (\ln N)^{\frac{1}{2^{m+1} m!}} \\
&\quad + (4E_{0,\hbar})^k 2N^{-\frac{1}{10}} + (4E_{0,\hbar})^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2^{m+1}(m+1)!}} \\
&\leq e^{(m+1)k} \left(4E_{0,\hbar}\right)^k \left(\frac{1}{\ln N}\right)^{\frac{1}{2^{m+1}(m+1)!}}.
\end{aligned}$$

This proves (3.66) and completes the proof of (3.63) as we can take

$$m = n(T_0, \hbar) = 4eCE_{0,\hbar}\hbar^{-2}T_0.$$

For estimates (3.4), under the restriction (1.13) that

$$N \geq e^{(3)}\big([E_{0,\hbar}^{-2}T_0]^2\big), \tag{3.67}$$

which implies that $n(T_0,\hbar) \leq C_1\sqrt{\ln\ln\ln N}$ with an absolute constant $C_1 = 4eC$, we have

$$2^{n(T_0,\hbar)}n(T_0,\hbar)! \leq n(T_0,\hbar)^{n(T_0,\hbar)} \leq (C_1\sqrt{\ln\ln\ln N})^{C_1\sqrt{\ln\ln\ln N}} \leq \sqrt{\ln\ln N}.$$

Hence, we obtain

$$\begin{aligned}\sup_{t\in[0,T_0]} \operatorname{Tr}\left|S_\hbar^{(1,1)} w_{N,\hbar,\lambda}^{M,(1)}(t)\right| &\leq (e^{n(T_0,\hbar)}4E_{0,\hbar})\left(\frac{1}{\ln N}\right)^{\frac{1}{2^{n(T_0,\hbar)}n(T_0,\hbar)!}}\\ &\leq \frac{\sqrt{\ln\ln N}}{(\ln N)^{\frac{1}{\sqrt{\ln\ln N}}}} \leq \left(\frac{1}{\ln\ln N}\right)^{10}\end{aligned} \tag{3.68}$$

as long as $N$ is large enough. This completes the proof of estimate (3.4).

For (3.5), by partial trace inequality in Lemma A.5 we have

$$\operatorname{Tr}_1\Big|\operatorname{Tr}_2\big[V(x_1-x_2)w_{N,\hbar,\lambda}^{M,(2)}(t)\big]\Big| \leq \operatorname{Tr}\Big|V(x_1-x_2)w_{N,\hbar,\lambda}^{M,(2)}(t)\Big|. \tag{3.69}$$

By Hardy's inequality that $|V(x_1-x_2)|^2 \lesssim -\Delta_{x_1}$ and the operator inequality in Lemma A.6, the above

$$\begin{aligned}&\lesssim \operatorname{Tr}\Big|\langle\nabla_{x_1}\rangle w_{N,\hbar,\lambda}^{M,(2)}(t)\Big|\\ &\leq \hbar^{-1}\operatorname{Tr}\Big|\langle\hbar\nabla_{x_1}\rangle w_{N,\hbar,\lambda}^{M,(2)}(t)\Big|\\ &\leq \hbar^{-1}\operatorname{Tr}\Big|S_\hbar^{(1,2)} w_{N,\hbar,\lambda}^{M,(2)}(t)\Big|.\end{aligned}$$

Then repeating the proof of estimate (3.68) for $k=2$, we arrive at

$$\operatorname{Tr}_1\Big|\operatorname{Tr}_2\big[V(x_1-x_2)w_{N,\hbar,\lambda}^{M,(2)}(t)\big]\Big| \lesssim \frac{1}{\ln\ln N}.$$

This completes the proof of estimates (3.5). □

## 4 Regularized Hartree Equation vs. the Euler–Poisson Equation: A Modulated Energy Approach

We will compare the regularized Hartree equation (3.2) and the Euler–Poisson equation (1.5) before its blowup time by the method of modulated energy. Specifically, in Sect. 4.1, we derive the evolution of modulated energy. Subsequently in Sect. 4.2, we control the error term originating from the evolution of modulated energy to obtain a

Gronwall type estimate. Because of the Coulomb interaction, the modulated energy method only provides $\dot{H}^{-1}$ convergence for the mass density. In Sect. 4.3, to strengthen the convergence, we prove the uniform bounds for mass and momentum densities by a feedback argument. The interpolation inequality can then raise the regularity index of the convergence norm.

Recall the regularized Hartree equation (3.2)

$$i\hbar\partial_t\phi^M_{\hbar,\lambda} = -\frac{1}{2}\hbar^2\Delta\phi^M_{\hbar,\lambda} + \big(V_\lambda * |\phi^M_{\hbar,\lambda}|^2\big)\phi^M_{\hbar,\lambda}$$

with the regularized initial data

$$\phi^M_{\hbar,\lambda}(0) = \frac{P_{\le M}\phi^{\mathrm{in}}_\hbar}{\|P_{\le M}\phi^{\mathrm{in}}_\hbar\|_{L^2}}, \tag{4.1}$$

the mass density and momentum density

$$\rho^M_{\hbar,\lambda}(t,x) = |\phi^M_{\hbar,\lambda}(t,x)|^2, \quad J^M_{\hbar,\lambda}(t,x) = \mathrm{Im}\big(\overline{\phi^M_{\hbar,\lambda}}(t,x)\hbar\nabla\phi^M_{\hbar,\lambda}(t,x)\big),$$

and the Euler–Poisson equation (1.5)

$$\begin{cases} \partial_t\rho + \nabla\cdot(\rho u) = 0, \\ \partial_t u + (u\cdot\nabla)u + \nabla_x V * \rho = 0, \\ (\rho,u)|_{t=0} = (\rho^{\mathrm{in}}, u^{\mathrm{in}}). \end{cases}$$

Here is the main theorem of the section.

**Theorem 4.1** *Let $M = N^{1/2}(\ln\ln N)^{10}$, $\lambda = N^{1/2}(\ln\ln N)^{10}$. Let $\phi^M_{\hbar,\lambda}(t)$ be the solution to the regularized Hartree equation with the regularized initial data $\phi^M_{h,\lambda}(0)$. Under the same conditions of Theorem 1.1, we have*

$$\|\rho^M_{\hbar,\lambda} - \rho\|_{L^\infty([0,T_0];\dot{H}^{-s_1}(\mathbb{R}^3))} \lesssim \hbar^{\frac{4s_1-1}{3}}, \quad s_1 \in \left(\frac{1}{4}, 1\right], \tag{4.2}$$

$$\|J^M_{\hbar,\lambda} - \rho u\|_{L^\infty([0,T_0];\dot{H}^{-s_2}(\mathbb{R}^3))} \lesssim \hbar^{2s_2-1}, \quad s_2 \in \left(\frac{1}{2}, 1\right], \tag{4.3}$$

*and*

$$\sup_{t\in[0,T_0]}\left|\langle\phi^M_{\hbar,\lambda}(t), -\hbar^2\Delta_{x_1}\phi^M_{\hbar,\lambda}(t)\rangle - \int\rho(t)|u|^2(t)dx\right| \lesssim \hbar, \tag{4.4}$$

$$\sup_{t\in[0,T_0]}\left|\langle\rho^M_{\hbar,\lambda}(t), V * \rho^M_{\hbar,\lambda}(t)\rangle - \langle\rho(t), V*\rho(t)\rangle\right| \lesssim \hbar. \tag{4.5}$$

***Proof of Theorem 4.1*** To prove estimates (4.2)–(4.5), we need the following estimates as stated in Proposition 4.5

$$\|\rho^M_{\hbar,\lambda} - \rho\|_{L^\infty([0,T_0];\dot{H}^{-1}(\mathbb{R}^3))} \lesssim \hbar, \tag{4.6}$$

$$\|(i\hbar\nabla - u)\phi^M_{\hbar,\lambda}\|_{L^\infty([0,T_0];L^2(\mathbb{R}^3))} \lesssim \hbar \tag{4.7}$$

as well as the uniform in $\hbar$ bounds for densities as stated in Proposition 4.7

$$\sup_{t\in[0,T_0]} \left\|\phi^M_{\hbar,\lambda}\hbar\nabla\phi^M_{\hbar,\lambda}(t)\right\|_{L^{\frac{3}{2}}} \leq C, \tag{4.8}$$

$$\sup_{t\in[0,T_0]} \|\rho^M_{\hbar,\lambda}(t)\|_{L^{\frac{12}{7}}} \leq C. \tag{4.9}$$

We postpone the proof of Propositions 4.5 and 4.7 to Sects. 4.2 and 4.3. Here, we use estimates (4.6)–(4.9) to prove the desired estimates (4.2)–(4.5).

For (4.2), we use the interpolation and Sobolev inequalities to get

$$\begin{aligned}\|\rho^M_{\hbar,\lambda} - \rho\|_{\dot{H}^{-s_1}} &\leq \|\rho^M_{\hbar,\lambda} - \rho\|^{\frac{4s-1}{3}}_{\dot{H}^{-1}} \|\rho^M_{\hbar,\lambda} - \rho\|^{\frac{4-4s}{3}}_{\dot{H}^{-\frac{1}{4}}} \\ &\lesssim \|\rho^M_{\hbar,\lambda} - \rho\|^{\frac{4s-1}{3}}_{\dot{H}^{-1}} \|\rho^M_{\hbar,\lambda} - \rho\|^{\frac{4-4s}{3}}_{L^{\frac{12}{7}}}.\end{aligned} \tag{4.10}$$

By estimate (4.6) and the $L^{\frac{12}{7}}$ bound (4.9), we arrive at estimate (4.2).

For (4.3), by the triangle, Sobolev and Hölder's inequalities, we have

$$\begin{aligned}\|J^M_{\hbar,\lambda} - \rho u\|_{\dot{H}^{-1}} &\leq \|J^M_{\hbar,\lambda} - \rho^M_{\hbar,\lambda}u\|_{\dot{H}^{-1}} + \|\rho^M_{\hbar,\lambda}u - \rho u\|_{\dot{H}^{-1}} \\ &= \left\|\mathrm{Im}\Big(\overline{\phi^M_{\hbar,\lambda}}(\hbar\nabla - iu)\phi^M_{\hbar,\lambda}\Big)\right\|_{\dot{H}^{-1}} + \|\rho^M_{\hbar,\lambda}u - \rho u\|_{\dot{H}^{-1}} \\ &\leq \left\|\mathrm{Im}\Big(\overline{\phi^M_{\hbar,\lambda}}(\hbar\nabla - iu)\phi^M_{\hbar,\lambda}\Big)\right\|_{L^{\frac{6}{5}}} + \|\rho^M_{\hbar,\lambda}u - \rho u\|_{\dot{H}^{-1}} \\ &\leq \|\phi^M_{\hbar,\lambda}\|_{L^3}\|(i\hbar\nabla - u)\phi^M_{\hbar,\lambda}\|_{L^2} + \|\rho^M_{\hbar,\lambda}u - \rho u\|_{\dot{H}^{-1}}.\end{aligned} \tag{4.11}$$

On the one hand, by the uniform bound (4.9) and estimate (4.7), we have

$$\|\phi^M_{\hbar,\lambda}\|_{L^3}\|(i\hbar\nabla - u)\phi^M_{\hbar,\lambda}\|_{L^2} \lesssim \hbar. \tag{4.12}$$

On the other hand, by the dual argument, we get

$$\begin{aligned}\|\rho^M_{\hbar,\lambda}u - \rho u\|_{\dot{H}^{-1}} &= \sup_{\|\nabla f\|_{L^2}=1} \langle\rho^M_{\hbar,\lambda} - \rho, uf\rangle \\ &\leq \sup_{\|\nabla f\|_{L^2}=1} \|\rho^M_{\hbar,\lambda} - \rho\|_{\dot{H}^{-1}}\|uf\|_{\dot{H}^1}.\end{aligned} \tag{4.13}$$

By estimate (4.6), Leibniz rule and Sobolev inequality, the above

$$\lesssim \hbar \sup_{\|\nabla f\|_{L^2}=1} \left(\|\nabla u\|_{L^3}\|f\|_{L^6} + \|u\|_{L^\infty}\|\nabla f\|_{L^2}\right) \lesssim \hbar\|u\|_{H^2}.$$

Hence, combining estimates (4.11), (4.12) and (4.13), we arrive at

$$\|J^M_{\hbar,\lambda} - \rho u\|_{\dot{H}^{-1}} \lesssim \hbar. \tag{4.14}$$

Next, we use the interpolation and Sobolev inequalities to obtain

$$\begin{aligned}\|J^M_{\hbar,\lambda} - \rho u\|_{\dot{H}^{-s}} &\le \|J^M_{\hbar,\lambda} - \rho u\|^{2s-1}_{\dot{H}^{-1}}\|J^M_{\hbar,\lambda} - \rho u\|^{2-2s}_{\dot{H}^{-\frac{1}{2}}}\\ &\lesssim \|J^M_{\hbar,\lambda} - \rho u\|^{2s-1}_{\dot{H}^{-1}}\|J^M_{\hbar,\lambda} - \rho u\|^{2-2s}_{L^{\frac{3}{2}}}.\end{aligned} \tag{4.15}$$

Then by the $L^{\frac{3}{2}}$ bound (4.8) for the momentum density, we arrive at the desired estimate (4.3).

For (4.4), we have

$$\begin{aligned}&\langle \phi^M_{\hbar,\lambda}(t), -\hbar^2\Delta_{x_1}\phi^M_{\hbar,\lambda}(t)\rangle - \int \rho(t)|u|^2(t)dx\\ &= \langle \hbar\nabla_{x_1}\phi^M_{\hbar,\lambda}(t), \hbar\nabla_{x_1}\phi^M_{\hbar,\lambda}(t)\rangle - \langle \phi^M_{\hbar,\lambda}u, \phi^M_{\hbar,\lambda}u\rangle + \int (\rho^M_{\hbar,\lambda}(t) - \rho(t))|u(t)|^2 dx.\end{aligned} \tag{4.16}$$

By triangle and dual inequalities, the above

$$\le 2\|(i\hbar\nabla - u)\phi^M_{\hbar,\lambda}\|^2_{L^2_x} + \|\rho^M_{\hbar,\lambda}(t) - \rho(t)\|_{\dot{H}^{-1}}\||u|^2\|_{\dot{H}^1}.$$

By estimates (4.6) and (4.7), we arrive at

$$\left|\langle \phi^M_{\hbar,\lambda}(t), -\hbar^2\Delta_{x_1}\phi^M_{\hbar,\lambda}(t)\rangle - \int \rho(t)|u|^2(t)dx\right| \lesssim \hbar^2 + \hbar\|u\|^2_{H^2} \lesssim \hbar.$$

For (4.5), since $\rho^M_{\hbar,\lambda} \in L^{\frac{6}{5}}$ and $\rho \in L^{\frac{6}{5}}$, we can rewrite

$$\begin{aligned}\langle \rho^M_{\hbar,\lambda}(t), V * \rho^M_{\hbar,\lambda}(t)\rangle - \langle \rho(t), V * \rho(t)\rangle &= \|\rho^M_{\hbar,\lambda}(t)\|^2_{\dot{H}^{-1}} - \|\rho(t)\|^2_{\dot{H}^{-1}}\\ &\le (\|\rho^M_{\hbar,\lambda} - \rho\|_{\dot{H}^{-1}})(\|\rho^M_{\hbar,\lambda}\|_{\dot{H}^{-1}} + \|\rho\|_{\dot{H}^{-1}}).\end{aligned}$$

By estimate (4.6), we arrive at estimate (4.5). □

### 4.1 The Evolution of the Modulated Energy

We consider the following modulated energy

$$\begin{aligned}\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)=\frac{1}{2}\int_{\mathbb{R}^3}|(i\hbar\nabla-u)\phi^M_{\hbar,\lambda}(t)|^2dx\\+\frac{1}{2}\langle V_\lambda*\rho^M_{\hbar,\lambda},\rho^M_{\hbar,\lambda}\rangle+\frac{1}{2}\langle V*\rho,\rho-2\rho^M_{\hbar,\lambda}\rangle.\end{aligned}\tag{4.17}$$

We need to derive a time evolution equation for $\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)$. The related quantities for $\phi^M_{\hbar,\lambda}$ are given as the following.

**Lemma 4.2** *We have the following estimates regarding* $\phi^M_{\hbar,\lambda}$*:*

$$\partial_t\rho^M_{\hbar,\lambda}+\operatorname{div}J^M_{\hbar,\lambda}=0,\tag{4.18}$$

$$\partial_t J^{M,j}_{\hbar,\lambda}+\sum_{k=1}^3\partial_k\left[\hbar^2\mathrm{Re}\big(\partial_j\overline{\phi^M_{\hbar,\lambda}}\partial_k\phi^M_{\hbar,\lambda}\big)-\frac{\hbar^2}{4}\partial_{jk}\rho^M_{\hbar,\lambda}\right]+(\partial_j(V_\lambda*\rho^M_{\hbar,\lambda}))\rho^M_{\hbar,\lambda}=0,\tag{4.19}$$

*where* $J^M_{\hbar,\lambda}=(J^{M,1}_{\hbar,\lambda},J^{M,2}_{\hbar,\lambda},J^{M,3}_{\hbar,\lambda})$.

*Moreover, we have energy conservation law as follows*

$$E^M_{\hbar,\lambda}(t)\equiv E^M_{\hbar,\lambda}(0),\tag{4.20}$$

*where the energy* $E^M_{\hbar,\lambda}(t)$ *is defined by*

$$E^M_{\hbar,\lambda}(t)=\frac{1}{2}\|\hbar\nabla\phi^M_{\hbar,\lambda}(t)\|^2_{L^2}+\frac{1}{2}\langle V_\lambda*\rho^M_{\hbar,\lambda},\rho^M_{\hbar,\lambda}\rangle(t).\tag{4.21}$$

We omit the proof of Lemma 4.2 as it is a direct computation and is well-known in $H^1$ wellposedness theory. Next let us derive the time derivative of $\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)$.

**Proposition 4.3** *There holds*

$$\begin{aligned}&\frac{d}{dt}\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)\\&=-\sum_{j,k}\int_{\mathbb{R}^3}\partial_k u^j\mathrm{Re}\Big((\hbar\partial_k-iu^k)\phi^M_{\hbar,\lambda}\overline{(\hbar\partial_j-iu^j)\phi^M_{\hbar,\lambda}}\Big)dx\\&\quad-\frac{\hbar^2}{4}\int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}(\Delta\operatorname{div}u)dx+c_0\sum_{j,k}\int_{\mathbb{R}^3}\partial_k u^j\big[\partial_j V*(\rho-\rho^M_{\hbar,\lambda})\partial_k V*(\rho-\rho^M_{\hbar,\lambda})\big]dx\\&\quad-\frac{c_0}{2}\int_{\mathbb{R}^3}\operatorname{div}u|\nabla V*(\rho-\rho^M_{\hbar,\lambda})|^2dx+\mathrm{Er},\end{aligned}\tag{4.22}$$

*where $c_0$ is the normalization constant s.t. $-\Delta V = c_0\delta$ and the error term is given by*

$$\mathrm{Er} = \sum_{j=1}^{3} \int_{\mathbb{R}^3} \rho^M_{\hbar,\lambda} u^j \partial_j (V_\lambda - V) * \rho^M_{\hbar,\lambda} dx. \tag{4.23}$$

***Proof*** By energy conservation law (4.20) in Lemma (4.2), we obtain

$$\begin{aligned}
\frac{d}{dt}\mathcal{M}[\phi^M_{\hbar,\lambda}, \rho, u](t) &= \frac{1}{2}\frac{d}{dt}\|\hbar\nabla\phi^M_{\hbar,\lambda}(t)\|^2_{L^2} + \frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} |u|^2\rho^M_{\hbar,\lambda} dx - \frac{d}{dt}\int_{\mathbb{R}^3} J^M_{\hbar,\lambda}\cdot u dx \\
&\quad + \frac{1}{2}\frac{d}{dt}\langle V_\lambda * \rho^M_{\hbar,\lambda}, \rho^M_{\hbar,\lambda}\rangle + \langle V * \partial_t\rho, \rho - 2\rho^M_{\hbar,\lambda}\rangle + \langle V * \rho, \partial_t\rho - 2\partial_t\rho^M_{\hbar,\lambda}\rangle \\
&= \frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} |u|^2\rho^M_{\hbar,\lambda} dx - \frac{d}{dt}\int_{\mathbb{R}^3} J^M_{\hbar,\lambda}\cdot u dx + \frac{1}{2}\frac{d}{dt}\langle V * \rho, \rho\rangle - \frac{d}{dt}\langle V * \rho, \rho^M_{\hbar,\lambda}\rangle.
\end{aligned}$$

Next, we calculate the above four terms separately. For the first term, by (1.5) and (4.18) we find

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} |u|^2\rho^M_{\hbar,\lambda} dx &= \int_{\mathbb{R}^3}\left(u\partial_t u\rho^M_{\hbar,\lambda} + \frac{1}{2}|u|^2\partial_t\rho^M_{\hbar,\lambda}\right)dx \\
&= \int_{\mathbb{R}^3}\left(\rho^M_{\hbar,\lambda}u^j\partial_t u^j - \frac{1}{2}|u|^2 \mathrm{div} J^M_{\hbar,\lambda}\right)dx \\
&= \sum_{j,k}\int_{\mathbb{R}^3}\big(-\rho^M_{\hbar,\lambda}u^j u^k\partial_k u^j + J^{M,j}_{\hbar,\lambda}u^k\partial_j u^k\big)dx \\
&\quad - \int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}u\cdot\nabla(V * \rho)dx,
\end{aligned} \tag{4.24}$$

where we have used integration by parts in the last equality.

For the second term, via (4.19) and (1.5) we have

$$\begin{aligned}
&-\frac{d}{dt}\int_{\mathbb{R}^3} J^M_{\hbar,\lambda}\cdot u dx \\
&= \int_{\mathbb{R}^3}\big(-\partial_t J^M_{\hbar,\lambda}\cdot u - J^M_{\hbar,\lambda}\cdot\partial_t u\big)dx \\
&= \sum_j\int_{\mathbb{R}^3}\left(\sum_k \partial_k\left(\hbar^2\mathrm{Re}(\partial_j\overline{\phi^M_{\hbar,\lambda}}\partial_k\phi^M_{\hbar,\lambda}) - \frac{\hbar^2}{4}\partial^2_{jk}\rho^M_{\hbar,\lambda}\right) + \big(\partial_j(V_\lambda * \rho^M_{\hbar,\lambda})\big)\rho^M_{\hbar,\lambda}\right)u^j dx \\
&\quad + \sum_{j,k}\int_{\mathbb{R}^3} J^{M,j}_{\hbar,\lambda}u^k\partial_k u^j dx + \int_{\mathbb{R}^3} J^M_{\hbar,\lambda}\cdot\nabla(V * \rho)dx.
\end{aligned} \tag{4.25}$$

Integrating by parts and using (4.23), the above

$$\begin{aligned}
&= \sum_{j,k}\int_{\mathbb{R}^3} -\hbar^2\partial_k u^j\Big[\mathrm{Re}\big(\partial_j\overline{\phi^M_{\hbar,\lambda}}\partial_k\phi^M_{\hbar,\lambda}\big)\Big]dx - \frac{\hbar^2}{4}\int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}(\mathrm{div}\Delta u)dx \\
&\quad + \int\rho^M_{\hbar,\lambda}u\cdot\nabla(V * \rho^M_{\hbar,\lambda})dx + \mathrm{Er} + \sum_{j,k}\int_{\mathbb{R}^3} J^{M,j}_{\hbar,\lambda}u^k\partial_k u^j dx - \int_{\mathbb{R}^3}(V * \rho)\mathrm{div} J^M_{\hbar,\lambda}dx.
\end{aligned}$$

For the third term, using (1.5) and integration by parts, we obtain

$$\frac{1}{2}\frac{d}{dt}\langle V*\rho,\rho\rangle = \langle V*\rho,\partial_t\rho\rangle = -\langle V*\rho,\operatorname{div}(\rho u)\rangle \\ = \int_{\mathbb{R}^3}\rho u\cdot\nabla(V*\rho)dx. \tag{4.26}$$

For the fourth term, plugging in (1.5) and (4.18), we integrate by parts to get

$$\begin{aligned}-\frac{d}{dt}\langle V*\rho,\rho^M_{\hbar,\lambda}\rangle &= -\langle\partial_t\rho, V*\rho^M_{\hbar,\lambda}\rangle - \langle V*\rho,\partial_t\rho^M_{\hbar,\lambda}\rangle\\ &= \langle\operatorname{div}(\rho u), V*\rho^M_{\hbar,\lambda}\rangle + \langle V*\rho,\operatorname{div}J^M_{\hbar,\lambda}\rangle\\ &= -\int_{\mathbb{R}^3}\rho u\cdot\nabla(V*\rho^M_{\hbar,\lambda})dx + \int_{\mathbb{R}^3}(V*\rho)\operatorname{div}J^M_{\hbar,\lambda}dx.\end{aligned} \tag{4.27}$$

Summing up (4.24)–(4.27), we conclude

$$\begin{aligned}&\frac{d}{dt}\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)\\ &=\sum_{j,k}\int_{\mathbb{R}^3}\big[-\rho^M_{\hbar,\lambda}u^ju^k\partial_ku^j + J^{M,j}_{\hbar,\lambda}u^k\partial_ju^k\big]dx - \int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}u\cdot\nabla(V*\rho)dx\\ &\quad+\sum_{j,k}\int_{\mathbb{R}^3}-\hbar^2\partial_ku^j\Big[\operatorname{Re}\big(\partial_j\overline{\phi^M_{\hbar,\lambda}}\partial_k\phi^M_{\hbar,\lambda}\big)\Big]dx - \frac{\hbar^2}{4}\int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}(\operatorname{div}\Delta u)dx\\ &\quad+\int\rho^M_{\hbar,\lambda}u\cdot\nabla(V*\rho^M_{\hbar,\lambda})dx + \mathrm{Er} + \sum_{j,k}\int_{\mathbb{R}^3}J^{M,j}_{\hbar,\lambda}u^k\partial_ku^jdx - \int_{\mathbb{R}^3}(V*\rho)\operatorname{div}J^M_{\hbar,\lambda}dx\\ &\quad+\int_{\mathbb{R}^3}\rho u\cdot\nabla(V*\rho)dx - \int_{\mathbb{R}^3}\rho u\cdot\nabla(V*\rho^M_{\hbar,\lambda})dx + \int_{\mathbb{R}^3}(V*\rho)\operatorname{div}J^M_{\hbar,\lambda}dx\\ &=-\sum_{j,k}\int_{\mathbb{R}^3}\partial_ku^j\Big\{\rho^M_{\hbar,\lambda}u^ju^k + \hbar^2\Big[\operatorname{Re}\big(\partial_j\overline{\phi^M_{\hbar,\lambda}}\partial_k\phi^M_{\hbar,\lambda}\big)\Big] - J^{M,j}_{\hbar,\lambda}u^k - J^{M,k}_{\hbar,\lambda}u^j\Big\}dx\\ &\quad-\frac{\hbar^2}{4}\int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}(\Delta\operatorname{div}u)dx + \int_{\mathbb{R}^3}(\rho-\rho^M_{\hbar,\lambda})u\cdot\nabla V*(\rho-\rho^M_{\hbar,\lambda})dx + \mathrm{Er}.\end{aligned} \tag{4.28}$$

On the one hand, we have

$$\begin{aligned}&\sum_{j,k}\int_{\mathbb{R}^3}\partial_ku^j\operatorname{Re}\Big((\hbar\partial_k - iu^k)\phi^M_{\hbar,\lambda}\overline{(\hbar\partial_j - iu^j)\phi^M_{\hbar,\lambda}}\Big)dx\\ &=\sum_{j,k}\int_{\mathbb{R}^3}\partial_ku^j\Big\{\rho^M_{\hbar,\lambda}u^ju^k + \hbar^2\Big[\operatorname{Re}\big(\partial_j\overline{\phi^M_{\hbar,\lambda}}\partial_k\phi^M_{\hbar,\lambda}\big)\Big] - J^{M,j}_{\hbar,\lambda}u^k - J^{M,k}_{\hbar,\lambda}u^j\Big\}dx.\end{aligned} \tag{4.29}$$

On the other hand, notice that there holds

$$\partial_k(\partial_kf\partial_jf) = \partial^2_{kk}f\partial_jf + \frac{1}{2}\partial_j(\partial_kf\partial_kf)$$

for $f \in C^2(\mathbb{R}^3)$. By $-\Delta V = c_0\delta$, we can rewrite

$$
\begin{aligned}
&(\rho - \rho^M_{\hbar,\lambda})\partial_j\big(V * (\rho - \rho^M_{\hbar,\lambda})\big) \\
&\quad = c_0 \sum_{k=1}^{3} \big( - \partial^2_{kk} V * (\rho - \rho^M_{\hbar,\lambda})\big)\partial_j\big(V * (\rho - \rho^M_{\hbar,\lambda})\big) \\
&\quad = \frac{c_0}{2} \sum_{k=1}^{3} \partial_j\big[\partial_k V * (\rho - \rho^M_{\hbar,\lambda})\partial_k V * (\rho - \rho^M_{\hbar,\lambda})\big] \\
&\qquad - c_0 \sum_{k=1}^{3} \partial_k\big[\partial_j V * (\rho - \rho^M_{\hbar,\lambda})\partial_k V * (\rho - \rho^M_{\hbar,\lambda})\big].
\end{aligned}
$$

By integration by parts, we obtain

$$
\begin{aligned}
&\int_{\mathbb{R}^3} (\rho - \rho^M_{\hbar,\lambda})u \cdot \nabla V * (\rho - \rho^M_{\hbar,\lambda})dx \\
&\quad = c_0 \sum_{j,k} \int_{\mathbb{R}^3} \partial_k u^j \big[\partial_j V * (\rho - \rho^M_{\hbar,\lambda})\partial_k V * (\rho - \rho^M_{\hbar,\lambda})\big]dx \\
&\qquad - \frac{c_0}{2} \int_{\mathbb{R}^3} \operatorname{div} u |\nabla V * (\rho - \rho^M_{\hbar,\lambda})|^2 dx. 
\end{aligned}
\tag{4.30}
$$

Combining estimates (4.28), (4.29) and (4.30), we arrive at estimate (4.22). This completes the proof. □

### 4.2 Modulated Energy Estimate

We rewrite the modulated energy defined by (4.17) as follows,

$$
\begin{aligned}
\mathcal{M}[\phi^M_{\hbar,\lambda}, \rho, u](t) = &\frac{1}{2} \int_{\mathbb{R}^3} |(i\hbar\nabla - u)\phi^M_{\hbar,\lambda}(t)|^2 dx + \frac{1}{2}\langle V * (\rho - \rho^M_{\hbar,\lambda})(t), (\rho - \rho^M_{\hbar,\lambda})(t)\rangle \\
&+ \frac{1}{2}\langle W_\lambda * \rho^M_{\hbar,\lambda}(t), \rho^M_{\hbar,\lambda}(t)\rangle,
\end{aligned}
\tag{4.31}
$$

where $W_\lambda = V_\lambda - V$. We first estimate the error part $\langle W_\lambda * \rho^M_{\hbar,\lambda}, \rho^M_{\hbar,\lambda}\rangle$ and the error term Er in (4.23) as shown in the evolution of the modulated energy, and then establish Gronwall's inequality for the modulated energy $\mathcal{M}[\phi^M_{\hbar,\lambda}, \rho, u](t)$.

**Lemma 4.4** *Let $M \geq \hbar^{-3}$ and $\lambda \geq \hbar^{-3}$. For the error terms, we have the following estimates*

$$
\sup_{t\in[0,T_0]} |\langle W_\lambda * \rho^M_{\hbar,\lambda}(t), \rho^M_{\hbar,\lambda}(t)\rangle| \lesssim \frac{1}{\hbar^4\lambda^2} \leq \hbar^2, \tag{4.32}
$$

$$
|\mathrm{Er}| \lesssim \frac{1}{\hbar^4\lambda^2} \leq \hbar^2. \tag{4.33}
$$

***Proof*** As we need the $H^1$ energy bound for $\phi_{\hbar,\lambda}^M(t)$, we first check that $\phi_{\hbar,\lambda}^M(0)$ has finite Hamiltonian energy. Indeed, for the kinetic energy, we have

$$\|\langle\hbar\nabla\rangle\phi_{\hbar,\lambda}^M(0)\|_{L^2} = \frac{\|\langle\hbar\nabla\rangle P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2}}{\|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2}} \le \frac{\|\langle\hbar\nabla\rangle\phi_\hbar^{\text{in}}\|_{L^2}}{\|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2}}.$$

For the lower bound of $\|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2}$, we use the triangle inequality and Bernstein's inequality to obtain

$$\begin{aligned}\|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2} &\ge 1 - \|P_{>M}\phi_\hbar^{\text{in}}\|_{L^2} \\ &\ge 1 - \frac{\|\langle\hbar\nabla\rangle P_{>M}\phi_\hbar^{\text{in}}\|_{L^2}}{\hbar M} \ge 1 - \frac{\|\langle\hbar\nabla\rangle\phi_\hbar^{\text{in}}\|_{L^2}}{\hbar M} \ge \frac{1}{2},\end{aligned} \tag{4.34}$$

where in the last inequality we have used the energy bound for $\phi_\hbar^{\text{in}}$ and the restriction that $M \ge \hbar^{-3}$.

For the potential energy, we use that $V_\lambda \le V$ and estimate (4.34) to obtain

$$\begin{aligned}\langle V_\lambda * |\phi_{\hbar,\lambda}^M(0)|^2, |\phi_{\hbar,\lambda}^M(0)|^2\rangle &\le \frac{\langle V * |P_{\le M}\phi_\hbar^{\text{in}}|^2, |P_{\le M}\phi_\hbar^{\text{in}}|^2\rangle}{\|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2}^4} \\ &\le 8\langle V * |P_{\le M}\phi_\hbar^{\text{in}}|^2, |P_{\le M}\phi_\hbar^{\text{in}}|^2\rangle.\end{aligned}$$

In addition, we take a difference to get

$$\begin{aligned}\langle V_\lambda * |\phi_{\hbar,\lambda}^M(0)|^2, |\phi_{\hbar,\lambda}^M(0)|^2\rangle &\le \frac{\langle V * |P_{\le M}\phi_\hbar^{\text{in}}|^2, |P_{\le M}\phi_\hbar^{\text{in}}|^2\rangle}{\|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^2}^4} \\ &\le 8\langle V * |P_{\le M}\phi_\hbar^{\text{in}}|^2, |P_{\le M}\phi_\hbar^{\text{in}}|^2\rangle.\end{aligned}$$

By Hardy–Littlewood–Sobolev inequality, the above

$$\lesssim \left\| |P_{\le M}\phi_\hbar^{\text{in}}|^2 - |\phi_\hbar^{\text{in}}|^2 \right\|_{L^{\frac{6}{5}}} \left( \left\| |P_{\le M}\phi_\hbar^{\text{in}}|^2 \right\|_{L^{\frac{6}{5}}} + \left\| |\phi_\hbar^{\text{in}}|^2 \right\|_{L^{\frac{6}{5}}} \right).$$

By Hölder inequality, the above

$$\lesssim \|P_{\le M}\phi_\hbar^{\text{in}} - \phi_\hbar^{\text{in}}\|_{L^2} \left( \|P_{\le M}\phi_\hbar^{\text{in}}\|_{L^3} + \|\phi_\hbar^{\text{in}}\|_{L^3} \right) \|\phi_\hbar^{\text{in}}\|_{L^{\frac{12}{5}}}^2.$$

By Bernstein's inequality and interpolation inequality, the above

$$\lesssim \frac{1}{\hbar M} \|\langle\hbar\nabla\rangle P_{>M}\phi_\hbar^{\text{in}}\|_{L^2} \left( \|\phi_\hbar^{\text{in}}\|_{L^2}^{\frac{1}{2}} \|\phi_\hbar^{\text{in}}\|_{L^6}^{\frac{1}{2}} \right) \left( \|\phi_\hbar^{\text{in}}\|_{L^2}^{\frac{3}{4}} \|\phi_\hbar^{\text{in}}\|_{L^6}^{\frac{1}{4}} \right)^2.$$

By Sobolev inequality, the energy bound condition (1.10) and normalized condition for $\phi_\hbar^{\text{in}}$, the above

$$\lesssim \frac{1}{\hbar M}\|\langle \hbar\nabla\rangle P_{>M}\phi_\hbar^{\text{in}}\|_{L^2}\left(\|\phi_\hbar^{\text{in}}\|_{L^2}^{\frac{1}{2}}\|\phi_\hbar^{\text{in}}\|_{L^6}^{\frac{1}{2}}\right)\left(\|\phi_\hbar^{\text{in}}\|_{L^2}^{\frac{3}{4}}\|\phi_\hbar^{\text{in}}\|_{L^6}^{\frac{1}{4}}\right)^2,$$

where in the last inequality we used the condition that $M \geq \hbar^{-3}$. With the finite Hamiltonian energy bound condition (1.10) for $\phi_\hbar^{\text{in}}$, we obtain

$$\begin{aligned}
&\langle V_\lambda * |\phi_{\hbar,\lambda}^M(0)|^2, |\phi_{\hbar,\lambda}^M(0)|^2\rangle \\
&\quad \lesssim \langle V * |P_{\leq M}\phi_\hbar^{\text{in}}|^2, |P_{\leq M}\phi_\hbar^{\text{in}}|^2\rangle \\
&\quad = \langle V * |P_{\leq M}\phi_\hbar^{\text{in}}|^2, |P_{\leq M}\phi_\hbar^{\text{in}}|^2\rangle - \langle V * |\phi_\hbar^{\text{in}}|^2, |\phi_\hbar^{\text{in}}|^2\rangle + \langle V * |\phi_\hbar^{\text{in}}|^2, |\phi_\hbar^{\text{in}}|^2\rangle \\
&\quad \lesssim \hbar + E_0.
\end{aligned}$$

Then, with the energy conservation (4.20), we have

$$\begin{aligned}
&\frac{1}{2}\|\hbar\nabla\phi_{\hbar,\lambda}^M(t)\|_{L^2}^2 + \frac{1}{2}\langle V_\lambda * \rho_{\hbar,\lambda}^M, \rho_{\hbar,\lambda}^M\rangle(t) \\
&\quad = \frac{1}{2}\|\hbar\nabla\phi_{\hbar,\lambda}^M(0)\|_{L^2}^2 + \frac{1}{2}\langle V_\lambda * \rho_{\hbar,\lambda}^M, \rho_{\hbar,\lambda}^M\rangle(0) \lesssim E_0,
\end{aligned}$$

which together with the mass conservation gives the $H^1$ energy bound for $\phi_{\hbar,\lambda}^M(t)$, that is,

$$\sup_{t\in[0,T_0]} \|\langle\hbar\nabla\rangle\phi_{\hbar,\lambda}^M(t)\|_{L^2}^2 \lesssim E_0. \tag{4.35}$$

Next, we get into the analysis of error estimates. For (4.32), we use Young's inequality to get

$$|\langle W_\lambda * \rho_{\hbar,\lambda}^M(t), \rho_{\hbar,\lambda}^M(t)\rangle| \lesssim \|W_\lambda\|_{L^1}\|\rho_{\hbar,\lambda}^M(t)\|_{L^2}\|\rho_{\hbar,\lambda}^M(t)\|_{L^2}.$$

By interpolation inequality, Sobolev inequality, and $\|W_\lambda\|_{L^1} \lesssim \lambda^{-2}$, the above

$$\lesssim \lambda^{-2}\|\phi_{\hbar,\lambda}^M(t)\|_{L^2}\|\nabla\phi_{\hbar,\lambda}^M(t)\|_{L^2}^3.$$

By the energy bound (4.35) for $\phi_{\hbar,\lambda}^M(t)$, the above

$$\lesssim \frac{E_0}{\hbar^3\lambda^2},$$

which completes the proof of (4.32).

For (4.33), we rewrite

$$\mathrm{Er} = \sum_{j=1}^{3} \int_{\mathbb{R}^3} \rho_{\hbar,\lambda}^M u^j W_\lambda * \partial_j \rho_{\hbar,\lambda}^M dx. \tag{4.36}$$

By Young's inequality,

$$|\mathrm{Er}| \le \sum_{j=1}^{3} \|u^j\|_{L^\infty} \|W_\lambda\|_{L^1} \|\partial_j \rho_{\hbar,\lambda}^M\|_{L^{\frac{3}{2}}} \|\rho_{\hbar,\lambda}^M\|_{L^3}.$$

By Hölder and Sobolev inequalities, the above

$$\begin{aligned} &\le 2\sum_{j=1}^{3} \|u^j\|_{L^\infty} \|W_\lambda\|_{L^1} \|\partial_j \phi_{\hbar,\lambda}^M\|_{L^2} \|\phi_{\hbar,\lambda}^M\|_{L^6} \|\phi_{\hbar,\lambda}^M\|_{L^6}^2 \\ &\lesssim \|u\|_{L^\infty} \|W_\lambda\|_{L^1} \|\nabla \phi_{\hbar,\lambda}^M\|_{L^2}^4. \end{aligned}$$

By $\|W_\lambda\|_{L^1} \lesssim \lambda^{-2}$ and the energy bound (4.35) for $\phi_{\hbar,\lambda}^M$, we obtain

$$|\mathrm{Er}| \lesssim \frac{1}{\hbar^4 \lambda^2},$$

which completes the proof of (4.33). □

We can now provide a closed estimate for the modulated energy.

**Proposition 4.5** *Let $M \ge \hbar^{-3}$, $\lambda \ge \hbar^{-3}$ and $\mathcal{M}[\phi_{\hbar,\lambda}^M, \rho, u](t)$ be defined as in (4.17). We have the lower bound estimate*

$$\mathcal{M}[\phi_{\hbar,\lambda}^M, \rho, u](t) + \frac{C}{\hbar^4 \lambda^2} \ge 0 \tag{4.37}$$

*and the following Gronwall's inequality*

$$\frac{d}{dt} \mathcal{M}[\phi_{\hbar,\lambda}^M, \rho, u](t) \lesssim \mathcal{M}[\phi_{\hbar,\lambda}^M, \rho, u](t) + \frac{1}{\hbar^4 \lambda^2} + \hbar^2, \tag{4.38}$$

*which implies that*

$$\mathcal{M}[\phi_{\hbar,\lambda}^M, \rho, u](t) + \frac{C}{\hbar^4 \lambda^2} \le \exp(CT_0)\Big(\mathcal{M}[\phi_{\hbar,\lambda}^M, \rho, u](0) + \frac{C}{\hbar^4 \lambda^2} + C\hbar^2 t\Big). \tag{4.39}$$

*Moreover, we have*

$$\|\rho_{\hbar,\lambda}^M - \rho\|_{L^\infty([0,T_0]; \dot{H}^{-1}(\mathbb{R}^3))} \lesssim \hbar, \tag{4.40}$$

$$\|(i\hbar\nabla - u)\phi_{\hbar,\lambda}^M\|_{L^\infty([0,T_0]; L^2(\mathbb{R}^3))} \lesssim \hbar. \tag{4.41}$$

***Proof*** For (4.37), we recall

$$\begin{aligned}\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t) &= \frac{1}{2}\int_{\mathbb{R}^3}|(i\hbar\nabla-u)\phi^M_{\hbar,\lambda}(t)|^2dx+\frac{1}{2}\langle V*(\rho-\rho^M_{\hbar,\lambda}),(\rho-\rho^M_{\hbar,\lambda})\rangle\\ &\quad+\frac{1}{2}\langle W_\lambda*\rho^M_{\hbar,\lambda},\rho^M_{\hbar,\lambda}\rangle.\end{aligned}\tag{4.42}$$

Since $\rho-\rho^M_{\hbar,\lambda}\in L^{\frac{6}{5}}$, we can rewrite

$$\langle V*(\rho-\rho^M_{\hbar,\lambda}),(\rho-\rho^M_{\hbar,\lambda})\rangle=\int_{\mathbb{R}^3}|\xi|^{-2}|\widehat{\rho}(\xi)-\widehat{\rho^M_{\hbar,\lambda}}(\xi)|^2d\xi=\|\rho-\rho^M_{\hbar,\lambda}\|^2_{\dot{H}^{-1}}\geq 0.\tag{4.43}$$

Hence, by estimate (4.32), we arrive at

$$\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)\gtrsim-\frac{1}{\hbar^4\lambda^2},\tag{4.44}$$

which completes the proof of (4.37).

For (4.38), we make use of Proposition 4.3 to obtain[15]

$$\begin{aligned}&\frac{d}{dt}\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)\\ &\quad=-\sum_{j,k}\int_{\mathbb{R}^3}\partial_k u^j\,\mathrm{Re}\Big((\hbar\partial_k-iu^k)\phi^M_{\hbar,\lambda}\overline{(\hbar\partial_j-iu^j)\phi^M_{\hbar,\lambda}}\Big)dx\\ &\qquad-\frac{\hbar^2}{4}\int_{\mathbb{R}^3}\rho^M_{\hbar,\lambda}(\Delta\mathrm{div}\,u)dx\\ &\qquad+c_0\sum_{j,k}\int_{\mathbb{R}^3}\partial_k u^j\big[\partial_j V*(\rho-\rho^M_{\hbar,\lambda})\partial_k V*(\rho-\rho^M_{\hbar,\lambda})\big]dx\\ &\qquad-\frac{c_0}{2}\int_{\mathbb{R}^3}\mathrm{div}\,u|\nabla V*(\rho-\rho^M_{\hbar,\lambda})|^2dx+\mathrm{Er}\\ &\quad\lesssim\|\nabla u\|_{L^\infty}\left(\int_{\mathbb{R}^3}|(i\hbar\nabla-u)\phi^M_{\hbar,\lambda}(t)|^2dx+\|\rho-\rho^M_{\hbar,\lambda}\|^2_{\dot{H}^{-1}}\right)\\ &\qquad+\hbar^2\|\rho^M_{\hbar,\lambda}\|_{L^1}\|\Delta\mathrm{div}\,u\|_{L^\infty}+|\mathrm{Er}|.\end{aligned}\tag{4.45}$$

By the error term estimate (4.33), we reach

$$\frac{d}{dt}\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)\lesssim\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)+\hbar^2+\frac{1}{\hbar^4\lambda^2},\tag{4.46}$$

which completes the proof of (4.38).

[15] The regularity requirement that $s>\frac{d}{2}+3$ comes from $\|\Delta\mathrm{div}\,u\|_{L^\infty}$, the second term on the right side of (4.45).

Combining (4.37) and (4.38), we have

$$\begin{aligned}
&\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)+\frac{C}{\hbar^4\lambda^2}\\
&\quad=\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](0)+\frac{C}{\hbar^4\lambda^2}+\int_0^t\frac{d}{d\tau}\left(\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](\tau)+\frac{C}{\hbar^4\lambda^2}\right)d\tau\\
&\quad\le\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](0)+\frac{C}{\hbar^4\lambda^2}+C\int_0^t\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](\tau)+\frac{C}{\hbar^4\lambda^2}+\hbar^2d\tau\\
&\quad=\left(\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](0)+\frac{C}{\hbar^4\lambda^2}+C\hbar^2t\right)+C\int_0^t\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](\tau)+\frac{C}{\hbar^4\lambda^2}d\tau.
\end{aligned}\tag{4.47}$$

Then by Gronwall's inequality, we obtain estimate (4.39).

Finally, we deal with (4.40) and (4.41). By error estimate (4.32), we note that

$$\int_{\mathbb{R}^3}|(i\hbar\nabla-u)\phi^M_{\hbar,\lambda}(t)|^2dx+\|\rho(t)-\rho^M_{\hbar,\lambda}(t)\|^2_{\dot{H}^{-1}}\lesssim\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](t)+\frac{1}{\hbar^4\lambda^2},\tag{4.48}$$

$$\mathcal{M}[\phi^M_{\hbar,\lambda},\rho,u](0)\lesssim\int_{\mathbb{R}^3}|(i\hbar\nabla-u^{\mathrm{in}})\phi^M_{\hbar,\lambda}(0)|^2dx+\|\rho^{\mathrm{in}}-\rho^M_{\hbar,\lambda}(0)\|^2_{\dot{H}^{-1}}+\frac{1}{\hbar^4\lambda^2}.\tag{4.49}$$

It needs to control the modulated energy at the initial time. For the kinetic energy part, we use the triangle inequality to obtain

$$\begin{aligned}
&\|(i\hbar\nabla-u^{\mathrm{in}})\phi^M_{\hbar,\lambda}(0)\|_{L^2}\\
&\quad\le\|(i\hbar\nabla-u^{\mathrm{in}})(\phi^M_{\hbar,\lambda}(0)-\phi^{\mathrm{in}}_\hbar)\|_{L^2}+\|(i\hbar\nabla-u^{\mathrm{in}})\phi^{\mathrm{in}}_\hbar\|_{L^2}\\
&\quad\le\|\hbar\nabla(\phi^M_{\hbar,\lambda}(0)-\phi^{\mathrm{in}}_\hbar)\|_{L^2}+\|u^{\mathrm{in}}\|_{L^\infty}\|\phi^M_{\hbar,\lambda}(0)-\phi^{\mathrm{in}}_\hbar\|_{L^2}+\|(i\hbar\nabla-u^{\mathrm{in}})\phi^{\mathrm{in}}_\hbar\|_{L^2}.
\end{aligned}\tag{4.50}$$

We recall

$$\phi^M_{\hbar,\lambda}(0)=\frac{P_{\le M}\phi^{\mathrm{in}}_\hbar}{\|P_{\le M}\phi^{\mathrm{in}}_\hbar\|_{L^2}}$$

and insert in $P_{\le M}\phi^{\mathrm{in}}_\hbar$ to get

$$\hbar\nabla(\phi^M_{\hbar,\lambda}(0)-\phi^{\mathrm{in}}_\hbar)\le\frac{\hbar\nabla P_{\le M}\phi^{\mathrm{in}}_\hbar}{\|P_{\le M}\phi^{\mathrm{in}}_\hbar\|_{L^2}}(1-\|P_{\le M}\phi^{\mathrm{in}}_\hbar\|_{L^2})+\hbar\nabla P_{>M}\phi^{\mathrm{in}}_\hbar,$$

where $P_{>M}=1-P_{\le M}$. Together with estimate (4.34) that $\|P_{\le M}\phi^{\mathrm{in}}_\hbar\|\ge\frac{1}{2}$, we use triangle inequality to obtain

$$\|\hbar\nabla(\phi^M_{\hbar,\lambda}(0)-\phi^{\mathrm{in}}_\hbar)\|_{L^2}\le2\|P_{>M}\phi^{\mathrm{in}}_\hbar\|\|\hbar\nabla P_{\le M}\phi^{\mathrm{in}}_\hbar\|_{L^2}+\|\hbar\nabla P_{>M}\phi^{\mathrm{in}}_\hbar\|_{L^2}.$$

By Bernstein inequality, the above

$$\lesssim \frac{1}{\hbar M}\|\hbar\nabla P_{>M}\phi_\hbar^{\mathrm{in}}\|\|\hbar\nabla P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}+\frac{1}{\hbar M}\|(\hbar\nabla)^2P_{>M}\phi_\hbar^{\mathrm{in}}\|_{L^2}.$$

By the uniform $H^2$ energy bound (1.11) for $\phi_\hbar^{\mathrm{in}}$, we arrive at

$$\|\hbar\nabla(\phi_{\hbar,\lambda}^M(0)-\phi_\hbar^{\mathrm{in}})\|_{L^2}\lesssim\frac{E_0}{\hbar M}. \tag{4.51}$$

In the same way, we also have

$$\|u^{\mathrm{in}}\|_{L^\infty}\|\phi_{\hbar,\lambda}^M(0)-\phi_\hbar^{\mathrm{in}}\|_{L^2}\lesssim\frac{E_0}{\hbar M}. \tag{4.52}$$

Combining estimates (4.50), (4.51) and (4.52), we use the initial condition (1.12) to reach

$$\|(i\hbar\nabla-u^{\mathrm{in}})\phi_{\hbar,\lambda}^M(0)\|_{L^2}\lesssim\frac{1}{\hbar M}+\hbar. \tag{4.53}$$

For the potential energy part, we insert in $\rho_\hbar^{\mathrm{in}}=|\phi_\hbar^{\mathrm{in}}|^2$ to obtain

$$\|\rho^{\mathrm{in}}-\rho_{\hbar,\lambda}^M(0)\|_{\dot H^{-1}}\leq\|\rho^{\mathrm{in}}-\rho_\hbar^{\mathrm{in}}\|_{\dot H^{-1}}+\|\rho_\hbar^{\mathrm{in}}-\rho_{\hbar,\lambda}^M(0)\|_{\dot H^{-1}}. \tag{4.54}$$

By triangle inequality, we have

$$\begin{aligned}&\|\rho_{\hbar,\lambda}^M(0)-\rho_\hbar^{\mathrm{in}}\|_{\dot H^{-1}}\\&\leq\left\|\left(\frac{P_{\leq M}\phi_\hbar^{\mathrm{in}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}-\phi_\hbar^{\mathrm{in}}\right)\frac{\overline{P_{\leq M}\phi_\hbar^{\mathrm{in}}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}\right\|_{\dot H^{-1}}+\left\|\left(\frac{\overline{P_{\leq M}\phi_\hbar^{\mathrm{in}}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}-\overline{\phi_\hbar^{\mathrm{in}}}\right)\phi_\hbar^{\mathrm{in}}\right\|_{\dot H^{-1}}.\end{aligned}$$

By Sobolev inequality, the above

$$\lesssim\left\|\left(\frac{P_{\leq M}\phi_\hbar^{\mathrm{in}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}-\phi_\hbar^{\mathrm{in}}\right)\frac{\overline{P_{\leq M}\phi_\hbar^{\mathrm{in}}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}\right\|_{L^{\frac65}}+\left\|\left(\frac{\overline{P_{\leq M}\phi_\hbar^{\mathrm{in}}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}-\overline{\phi_\hbar^{\mathrm{in}}}\right)\phi_\hbar^{\mathrm{in}}\right\|_{L^{\frac65}}.$$

By Hölder inequality, the above

$$\begin{aligned}&\leq\left\|\frac{P_{\leq M}\phi_\hbar^{\mathrm{in}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}-\phi_\hbar^{\mathrm{in}}\right\|_{L^2}\left(\frac{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^3}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}+\|\phi_\hbar^{\mathrm{in}}\|_{L^3}\right)\\&\leq\left(\left\|\frac{P_{\leq M}\phi_\hbar^{\mathrm{in}}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}(1-\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2})\right\|_{L^2}+\|P_{>M}\phi_\hbar^{\mathrm{in}}\|_{L^2}\right)\left(\frac{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^3}}{\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^2}}+\|\phi_\hbar^{\mathrm{in}}\|_{L^3}\right).\end{aligned}$$

By estimate (4.34) that $\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|\geq\frac12$, we get

$$\|\rho_{\hbar,\lambda}^M(0)-\rho_\hbar^{\mathrm{in}}\|_{\dot H^{-1}}\lesssim\|P_{>M}\phi_\hbar^{\mathrm{in}}\|_{L^2}\big(\|P_{\leq M}\phi_\hbar^{\mathrm{in}}\|_{L^3}+\|\phi_\hbar^{\mathrm{in}}\|_{L^3}\big).$$

By Bernstein inequality and interpolation inequality, the above

$$\lesssim \frac{1}{\hbar M}\|\hbar\nabla P_{>M}\phi_\hbar^{\rm in}\|_{L^2}\|\phi_\hbar^{\rm in}\|_{L^2}^{\frac{1}{2}}\|\phi_\hbar^{\rm in}\|_{L^6}^{\frac{1}{2}}.$$

By Sobolev inequality, the energy bound, and the normalized condition for $\phi_\hbar^{\rm in}$, we arrive at

$$\|\rho_{\hbar,\lambda}^M(0)-\rho_\hbar^{\rm in}\|_{\dot H^{-1}} \lesssim \frac{1}{\hbar^{\frac{3}{2}}M}\|\hbar\nabla\phi_\hbar^{\rm in}\|_{L^2}^{\frac{3}{2}}\|\phi_\hbar^{\rm in}\|_{L^2}^{\frac{1}{2}} \lesssim \frac{1}{\hbar^{\frac{3}{2}}M}. \tag{4.55}$$

Combining estimates (4.54) and (4.55), we use the initial condition (1.12) to reach

$$\|\rho^{\rm in}-\rho_{\hbar,\lambda}^M(0)\|_{\dot H^{-1}} \lesssim \frac{1}{\hbar^{\frac{3}{2}}M}+\hbar. \tag{4.56}$$

Together estimates (4.49), (4.53) and (4.56), we obtain

$$\mathcal{M}[\phi_{\hbar,\lambda}^M,\rho,u](0) \lesssim \frac{1}{\hbar^3M^2}+\frac{1}{\hbar^4\lambda^2}+\hbar^2. \tag{4.57}$$

Now, we appeal to estimates (4.48) and (4.39) to get

$$\begin{aligned}
&\int_{\mathbb{R}^3}|(i\hbar\nabla-u)\phi_{\hbar,\lambda}^M(t)|^2dx+\|\rho(t)-\rho_{\hbar,\lambda}^M(t)\|_{\dot H^{-1}}^2\\
&\le C\Big(\mathcal{M}[\phi_{\hbar,\lambda}^M,\rho,u](t)+\frac{1}{\hbar^4\lambda^2}\Big)\\
&\le C\exp(CT_0)\Big(\mathcal{M}[\phi_{\hbar,\lambda}^M,\rho,u](0)+\frac{C}{\hbar^4\lambda^2}+C\hbar^2t\Big).
\end{aligned} \tag{4.58}$$

By estimate (4.57), the above

$$\begin{aligned}
&\le C\exp(CT_0)\Big(\frac{C}{\hbar^3M^2}+C\hbar^2+\frac{C}{\hbar^4\lambda^2}+C\hbar^2t\Big)\\
&\lesssim C(T_0)\Big(\frac{1}{\hbar^4M^2}+\frac{1}{\hbar^4\lambda^2}+\hbar^2\Big).
\end{aligned}$$

This completes the proof of estimates (4.40) and (4.41) under the restriction that $M\ge\hbar^{-3}$ and $\lambda\ge\hbar^{-3}$. □

### 4.3 Uniform Bounds for Densities

Even for the one-body wave function $\phi_{\hbar,\lambda}^M(t)$, the modulated energy only shows the $\dot H^{-1}$ convergence for the mass density due to the Coulomb interaction. Nevertheless, we point out that the convergence rate with the help of uniform bounds can make a further improvement for the convergence. The convergence rate for the modulated energy which we establish in Proposition 4.5 should be optimal in the sense that it matches the optimal $\hbar^2$ rate at the initial time. Therefore, in this section, we are devoted to setting up the uniform bounds for densities by a feedback argument.

From (4.40), we have established

$$\|\rho^M_{\hbar,\lambda} - \rho\|_{L^\infty([0,T_0];\dot{H}^{-1}(\mathbb{R}^3))} \le C(T_0)\hbar \tag{4.59}$$

as long as the parameters $M$, $\lambda$ satisfy that $M \ge \hbar^{-3}$, $\lambda \ge \hbar^{-3}$. Then, by the defining feature of Coulomb potential that $-\Delta V = c_0\delta$, we observe a structure compatible with a specific way of using Gagliardo–Nirenberg inequality, so that we obtain the $L^{\frac{3}{2}}$ uniform bound for the mass density $\rho^M_{\hbar,\lambda}$ as a starting point.

**Lemma 4.6** *Let $M \ge \hbar^{-3}$, $\lambda \ge \hbar^{-3}$. Then we have*

$$\sup_{t\in[0,T_0]} \|\rho^M_{\hbar,\lambda}(t)\|_{L^{\frac{3}{2}}} \le C \tag{4.60}$$

*where $C$ is a constant independent of these parameters $\hbar$, $M$ and $\lambda$.*

***Proof*** Let

$$f_{\hbar,i} = \partial_i(-\Delta)^{-1}(\rho^M_{\hbar,\lambda} - \rho) \tag{4.61}$$

where we omit parameters $M$ and $\lambda$. Then we have

$$(\rho - \rho^M_{\hbar,\lambda}) = \partial_1 f_{\hbar,1} + \partial_2 f_{\hbar,2} + \partial_3 f_{\hbar,3}$$

and

$$\|\rho^M_{\hbar,\lambda}\|_{L^{\frac{3}{2}}} \le \|\rho^M_{\hbar,\lambda} - \rho\|_{L^{\frac{3}{2}}} + \|\rho\|_{L^{\frac{3}{2}}} \le \sum_{i=1}^{3} \|\partial_i f_{\hbar,i}\|_{L^{\frac{3}{2}}} + \|\rho\|_{L^{\frac{3}{2}}}. \tag{4.62}$$

Since $f_{\hbar,i} \in \dot{W}^{2,\frac{6}{5}} \cap H^1$, we can use Gagliardo–Nirenberg inequality in Lemma A.4 to get

$$\|\partial_i f_{\hbar,i}\|_{L^{\frac{3}{2}}} \lesssim \|\nabla^2 f_{\hbar,i}\|^{\frac{1}{2}}_{L^{\frac{6}{5}}} \|f_{\hbar,i}\|^{\frac{1}{2}}_{L^2} \lesssim \|\Delta f_{\hbar,i}\|^{\frac{1}{2}}_{L^{\frac{6}{5}}} \|f_{\hbar,i}\|^{\frac{1}{2}}_{L^2},$$

where in the last inequality we used Calderón–Zygmund theory that the operator $\nabla^2(-\Delta)^{-1}$ is bounded for $1 < p < \infty$. Noticing that

$$-\Delta f_{\hbar,i} = \partial_i(\rho^M_{\hbar,\lambda} - \rho),$$

we use triangle inequality to obtain

$$
\begin{aligned}
\|\partial_i f_{\hbar,i}\|_{L^{\frac{3}{2}}} &\leq \|\partial_i(\rho^M_{\hbar,\lambda} - \rho)\|^{\frac{1}{2}}_{L^{\frac{6}{5}}} \|f_{\hbar,i}\|^{\frac{1}{2}}_{L^2} \\
&\leq \left(\|\partial_i \rho^M_{\hbar,\lambda}\|_{L^{\frac{6}{5}}} + \|\partial_i \rho\|_{L^{\frac{6}{5}}}\right)^{\frac{1}{2}} \|f_{\hbar,i}\|^{\frac{1}{2}}_{L^2}.
\end{aligned} \tag{4.63}
$$

By Hölder inequality and estimate (4.59), the above

$$
\leq \left(2\hbar^{-1}\|\hbar\nabla\phi^M_{\hbar,\lambda}\|_{L^2}\|\phi^M_{\hbar,\lambda}\|_{L^3} + \|\partial_i\rho\|_{L^{\frac{6}{5}}}\right)^{\frac{1}{2}} \hbar^{\frac{1}{2}}.
$$

By the energy bound (4.35) for $\phi^M_{\hbar,\lambda}$, the above

$$
\lesssim \left(\hbar^{-1} C_0 \|\rho^M_{\hbar,\lambda}\|^{\frac{1}{2}}_{L^{\frac{3}{2}}} + \|\partial_i\rho\|_{\frac{6}{5}}\right)^{\frac{1}{2}} \hbar^{\frac{1}{2}}.
$$

By $\rho \in H^3 \cap L^1$, we can use Gagliardo–Nirenberg inequality (A.23) to get

$$
\|\nabla\rho\|_{L^{\frac{6}{5}}} \leq \|\rho\|^{\frac{1}{3}}_{H^3}\|\rho\|^{\frac{2}{3}}_{L^1} \tag{4.64}
$$

and hence we obtain

$$
\|\partial_i f_{\hbar,i}\|_{L^{\frac{3}{2}}} \lesssim \left(\hbar^{-1} C_0\|\rho^M_{\hbar,\lambda}\|^{\frac{1}{2}}_{L^{\frac{3}{2}}} + \|\rho\|^{\frac{1}{3}}_{H^3}\|\rho\|^{\frac{2}{3}}_{L^1}\right)^{\frac{1}{2}} \hbar^{\frac{1}{2}}. \tag{4.65}
$$

Combining estimates (4.62) and (4.65), we arrive at

$$
\|\rho^M_{\hbar,\lambda}\|_{L^{\frac{3}{2}}} \lesssim \|\rho^M_{\hbar,\lambda}\|^{\frac{1}{4}}_{L^{\frac{3}{2}}} + 1, \tag{4.66}
$$

which implies (4.60). ◻

Now, we have set up a starting point that the mass density has the $L^{\frac{3}{2}}$ uniform bound. Then we will feed it back to the quantitative convergence for the kinetic energy part and establish the uniform bound for the momentum density. From (4.41), we have

$$
\|(i\hbar\nabla - u)\phi^M_{\hbar,\lambda}\|_{L^\infty([0,T_0];L^2(\mathbb{R}^3))} \lesssim C(T_0)\hbar \tag{4.67}
$$

as long as the parameters $M, \lambda$ satisfy $M \geq \hbar^{-3}$, $\lambda \geq \hbar^{-3}$. Together with the uniform $L^{\frac{3}{2}}$ bound (4.60) for the mass density $\rho^M_{\hbar,\lambda}$, we could provide a uniform bound for $\phi^M_{\hbar,\lambda}\hbar\nabla\phi^M_{\hbar,\lambda}$ and hence the momentum density. Subsequently, we feed them back again to further improve the $L^{\frac{3}{2}}$ bound to $L^{\frac{12}{7}}$ bound for the mass density $\rho^M_{\hbar,\lambda}$.

**Proposition 4.7** *Let $M \geq \hbar^{-3}$, $\lambda \geq \hbar^{-3}$. Then we have*

$$\sup_{t\in[0,T_0]} \left\| \phi^M_{\hbar,\lambda} \hbar \nabla \phi^M_{\hbar,\lambda}(t) \right\|_{L^{\frac{3}{2}}} \leq C, \tag{4.68}$$

$$\sup_{t\in[0,T_0]} \| \rho^M_{\hbar,\lambda}(t) \|_{L^{\frac{12}{7}}} \leq C, \tag{4.69}$$

*where $C$ is a constant independent of these parameters $\hbar$, $M$ and $\lambda$.*

***Proof*** We use triangle inequality to get

$$\left\| \phi^M_{\hbar,\lambda} \hbar \nabla \phi^M_{\hbar,\lambda}(t) \right\|_{L^{\frac{3}{2}}} \leq \left\| \phi^M_{\hbar,\lambda} (i\hbar\nabla - u) \phi^M_{\hbar,\lambda}(t) \right\|_{L^{\frac{3}{2}}} + \| u \rho^M_{\hbar,\lambda}(t) \|_{L^{\frac{3}{2}}}.$$

By Hölder inequality, the above

$$\leq \| \phi^M_{\hbar,\lambda} \|_{L^6} \| (i\hbar\nabla - u) \phi^M_{\hbar,\lambda} \|_{L^2} + \| u \|_{L^\infty} \| \rho^M_{\hbar,\lambda}(t) \|_{L^{\frac{3}{2}}}.$$

By Sobolev inequality and the energy bound for $\phi^M_{\hbar,\lambda}$, the above

$$\lesssim \hbar^{-1} E_0 \| (i\hbar\nabla - u) \phi^M_{\hbar,\lambda} \|_{L^2} + \| u \|_{L^\infty} \| \rho^M_{\hbar,\lambda}(t) \|_{L^{\frac{3}{2}}}.$$

By estimate (4.67) and the $L^{\frac{3}{2}}$ uniform bound (4.60) for density, we arrive at

$$\left\| \phi^M_{\hbar,\lambda} \hbar \nabla \phi^M_{\hbar,\lambda}(t) \right\|_{L^{\frac{3}{2}}} \leq C,$$

which completes the proof of estimate (4.68).

For the $L^{\frac{12}{7}}$ bound (4.69), we use the triangle inequality to get

$$\| \rho^M_{\hbar,\lambda} \|_{L^{\frac{12}{7}}} \leq \| \rho^M_{\hbar,\lambda} - \rho \|_{L^{\frac{12}{7}}} + \| \rho \|_{L^{\frac{12}{7}}} \leq \sum_{i=1}^{3} \| \partial_i f_{\hbar,i} \|_{L^{\frac{12}{7}}} + \| \rho \|_{L^{\frac{12}{7}}}, \tag{4.70}$$

where $f_{\hbar,i} = \partial_i (-\Delta)^{-1} (\rho^M_{\hbar,\lambda} - \rho)$. Since $f_{\hbar,i} \in \dot{W}^{2,\frac{3}{2}} \cap H^1$, we can use Gagliardo–Nirenberg inequality in Lemma A.4 to get

$$\| \partial_i f_{\hbar,i} \|_{L^{\frac{12}{7}}} \lesssim \| \nabla^2 f_{\hbar,i} \|^{\frac{1}{2}}_{L^{\frac{3}{2}}} \| f_{\hbar,i} \|^{\frac{1}{2}}_{L^2} \lesssim \| \Delta f_{\hbar,i} \|^{\frac{1}{2}}_{L^{\frac{3}{2}}} \| f_{\hbar,i} \|^{\frac{1}{2}}_{L^2},$$

where in the last inequality we used Calderón–Zygmund theory that the operator $\nabla^2 (-\Delta)^{-1}$ is bounded for $1 < p < \infty$. Noticing that $-\Delta f_{\hbar,i} = \partial_i (\rho^M_{\hbar,\lambda} - \rho)$, we use triangle inequality to obtain

$$
\begin{aligned}
\|\partial_i f_{\hbar,i}\|_{L^{\frac{12}{7}}} &\leq \|\partial_i(\rho^M_{\hbar,\lambda}-\rho)\|^{\frac{1}{2}}_{L^{\frac{3}{2}}}\|\rho^M_{\hbar,\lambda}-\rho\|^{\frac{1}{2}}_{\dot{H}^{-1}} \\
&\leq \left(\|\partial_i\rho^M_{\hbar,\lambda}\|_{L^{\frac{3}{2}}}+\|\partial_i\rho\|_{L^{\frac{3}{2}}}\right)^{\frac{1}{2}}\|\rho^M_{\hbar,\lambda}-\rho\|^{\frac{1}{2}}_{\dot{H}^{-1}} \\
&\leq \left(2\hbar^{-1}\|\phi^M_{\hbar,\lambda}\hbar\nabla\phi^M_{\hbar,\lambda}\|_{L^{\frac{3}{2}}}+\|\partial_i\rho\|_{L^{\frac{3}{2}}}\right)^{\frac{1}{2}}\|\rho^M_{\hbar,\lambda}-\rho\|^{\frac{1}{2}}_{\dot{H}^{-1}}. \qquad (4.71)
\end{aligned}
$$

As we have bounded $\|\nabla\rho\|_{L^{\frac{6}{5}}}$ in the estimate (4.64), we can use interpolation inequality to get

$$
\|\nabla\rho\|_{L^{\frac{3}{2}}} \leq \|\nabla\rho\|^{\frac{1}{2}}_{L^{\frac{6}{5}}}\|\nabla\rho\|^{\frac{1}{2}}_{L^2} \leq C. \qquad (4.72)
$$

Together with the uniform bound (4.68) and estimate (4.59), we arrive at

$$
\|\rho^M_{\hbar,\lambda}\|_{L^{\frac{12}{7}}} \lesssim \left(\hbar^{-1}\|\phi^M_{\hbar,\lambda}\hbar\nabla\phi^M_{\hbar,\lambda}\|_{L^{\frac{3}{2}}}+1\right)^{\frac{1}{2}}\|\rho^M_{\hbar,\lambda}-\rho\|^{\frac{1}{2}}_{\dot{H}^{-1}} \lesssim 1,
$$

which completes the proof of estimate (4.69). □

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## Appendix A: Miscellaneous Lemmas

### A.1 Collapsing Estimate

Recall

$$
S^{(1,k)}_{\hbar} = \prod_{j=1}^{k}\langle\hbar\nabla_{x_j}\rangle\langle\hbar\nabla_{x'_j}\rangle,
$$

and the collision operator

$$
B_{\hbar,\lambda,j,k+1}f^{(k+1)} = \frac{1}{\hbar}B_{\lambda,j,k+1}f^{(k+1)} = \frac{1}{\hbar}\mathrm{Tr}_{k+1}\big[V_\lambda(x_j-x_{k+1}),\, f^{(k+1)}\big]. \qquad (A.1)
$$

**Lemma A.1**

$$
\mathrm{Tr}\left|S^{(1,k)}_{\hbar}B_{\hbar,\lambda,j,k+1}f^{(k+1)}\right| \leq C\hbar^{-2}\,\mathrm{Tr}\left|S^{(1,k+1)}_{\hbar}f^{(k+1)}\right|. \qquad (A.2)
$$

***Proof*** For $\hbar = 1$, see [30, Lemma 7.1]. Since we have that

$$B_{\hbar,\lambda,j,k+1} = \frac{1}{\hbar} B_{\lambda,j,k} = \frac{1}{\hbar}(B^{+}_{\lambda,j,k+1} - B^{-}_{\lambda,j,k+1}),$$

it suffices to prove that

$$\operatorname{Tr}\left|S_{\hbar}^{(1,k)} B^{+}_{\lambda,j,k+1} f^{(k+1)}\right| \leq C\hbar^{-1} \operatorname{Tr}\left|S_{\hbar}^{(1,k+1)} f^{(k+1)}\right|. \tag{A.3}$$

Here, we might as well assume that $j = 1$ and compute

$$\begin{aligned} &\operatorname{Tr}\left|S_{\hbar}^{(1,k)} B^{+}_{\lambda,1,k+1} f^{(k+1)}\right| \\ &\quad\leq \operatorname{Tr}\left|S_{\hbar}^{(2,k)} B^{+}_{\lambda,1,k+1} f^{(k+1)}\right| + \operatorname{Tr}\left|\hbar\nabla_{x_1} S_{\hbar}^{(2,k)} B^{+}_{\lambda,1,k+1} f^{(k+1)} \hbar\nabla_{x_1}\right|, \end{aligned} \tag{A.4}$$

where $S_{\hbar}^{(2,k)} = \prod_{j=2}^{k} \langle \hbar\nabla_{x_j}\rangle\langle\hbar\nabla_{x'_j}\rangle$.

For the first term of (A.4), we use that $S_{\hbar}^{(2,k)}$ can commute $B^{\pm}_{\lambda,1,k+1}$ to obtain

$$\begin{aligned} &\operatorname{Tr}\left|S_{\hbar}^{(2,k)} B^{+}_{\lambda,1,k+1} f^{(k+1)}\right| \\ &\quad= \operatorname{Tr}\left|B^{+}_{\lambda,1,k+1} S_{\hbar}^{(2,k)} f^{(k+1)}\right| \\ &\quad= \operatorname{Tr}\left|\operatorname{Tr}_{k+1}\big(V_{\lambda}(x_1 - x_{k+1}) S_{\hbar}^{(2,k)} f^{(k+1)}\big)\right|. \end{aligned} \tag{A.5}$$

By the partial trace inequality in Lemma A.5, the above

$$\leq \operatorname{Tr}\left|V_{\lambda}(x_1 - x_{k+1}) S_{\hbar}^{(2,k)} f^{(k+1)}\right|.$$

By Hardy's inequality that $|V_{\lambda}(x_1 - x_{k+1})|^2 \leq |V(x_1 - x_{k+1})|^2 \lesssim -\Delta_{x_1}$ and the operator inequality in Lemma A.6, the above

$$\lesssim \operatorname{Tr}\left|\langle\nabla_{x_1}\rangle S_{\hbar}^{(2,k)} f^{(k+1)}\right| \leq \hbar^{-1} \operatorname{Tr}\left|S_{\hbar}^{(1,k)} f^{(k+1)}\right|.$$

For the second term of (A.4), we notice that

$$\begin{aligned} \nabla_{x_1} B_{\lambda,1,k+1} f^{(k+1)} &= \nabla_{x_1} \int V_{\lambda}(x_1 - x_{k+1}) f^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) dx_{k+1} \\ &= \int V_{\lambda}(x_1 - x_{k+1}) \nabla_{x_1} f^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) dx_{k+1} \\ &\quad+ \int \nabla_{x_1} V_{\lambda}(x_1 - x_{k+1}) f^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) dx_{k+1}. \end{aligned}$$

Then, we use that $\nabla_{x_1} V_\lambda(x_1 - x_{k+1}) = -\nabla_{x_{k+1}} V_\lambda(x_1 - x_{k+1})$ and integration by parts to obtain

$$\begin{aligned}\nabla_{x_1} B_{\lambda,1,k+1} f^{(k+1)} &= \int V_\lambda(x_1 - x_{k+1}) \nabla_{x_1} f^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) dx_{k+1} \\ &\quad + \int V_\lambda(x_1 - x_{k+1}) (\nabla_{x_{k+1}} f^{(k+1)})(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) dx_{k+1} \\ &\quad + \int V_\lambda(x_1 - x_{k+1}) (\nabla_{x'_{k+1}} f^{(k+1)})(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) dx_{k+1}.\end{aligned}$$

Therefore, we use the partial trace inequality in Lemma A.5 to get

$$\begin{aligned}&\mathrm{Tr}\big|\hbar\nabla_{x_1} S_\hbar^{(2,k)} B^+_{\lambda,1,k+1} f^{(k+1)} \hbar\nabla_{x_1}\big| \\ &= \mathrm{Tr}\big|\hbar\nabla_{x_1} S_\hbar^{(2,k)} \mathrm{Tr}_{k+1}(V_{\lambda,1(k+1)} f^{(k+1)}) \hbar\nabla_{x_1}\big| \\ &= \mathrm{Tr}\Big|\mathrm{Tr}_{k+1}\big(\hbar\nabla_{x_1} V_{\lambda,1(k+1)} S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1}\big)\Big| \\ &\le \mathrm{Tr}\big|\hbar\nabla_{x_1} V_{\lambda,1(k+1)} S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1}\big| \\ &\le \mathrm{I} + \mathrm{II} + \mathrm{III},\end{aligned}$$

where

$$\begin{aligned}\mathrm{I} &= \mathrm{Tr}\big|\hbar\nabla_{x_{k+1}} V_{\lambda,1(k+1)} S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1}\big|, \\ \mathrm{II} &= \mathrm{Tr}\big|V_{\lambda,1(k+1)} \hbar\nabla_{x_{k+1}} S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1}\big|, \\ \mathrm{III} &= \mathrm{Tr}\big|V_{\lambda,1(k+1)} \hbar\nabla_{x_1} S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1}\big|.\end{aligned}$$

For I, by Hardy's inequality that $|V_\lambda(x_1 - x_{k+1})|^2 \le |V(x_1 - x_{k+1})|^2 \lesssim -\Delta_{x_{k+1}}$ and the operator inequality in Lemma A.6, we have

$$\begin{aligned}\mathrm{I} &= \mathrm{Tr}\big|\hbar\nabla_{x_{k+1}} V_{\lambda,1(k+1)} S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1}\big| \\ &\lesssim \mathrm{Tr}\big|\langle\nabla_{x_{k+1}}\rangle S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1} \hbar\nabla_{x_{k+1}}\big| \\ &\le \hbar^{-1}\mathrm{Tr}\big|\langle\hbar\nabla_{x_{k+1}}\rangle S_\hbar^{(2,k)} f^{(k+1)} \hbar\nabla_{x_1} \hbar\nabla_{x_{k+1}}\big| \\ &\le \hbar^{-1}\mathrm{Tr}\big|S_\hbar^{(1,k+1)} f^{(k+1)}\big|.\end{aligned} \tag{A.6}$$

In the same way, we also have

$$\mathrm{II} \lesssim \hbar^{-1}\mathrm{Tr}\big|S_\hbar^{(1,k+1)} f^{(k+1)}\big| \tag{A.7}$$

and

$$\mathrm{III} \lesssim \hbar^{-1}\mathrm{Tr}\big|S_\hbar^{(1,k+1)} f^{(k+1)}\big|. \tag{A.8}$$

Combining estimates (A.5), (A.6), (A.7) and (A.8), we complete the proof of the desired estimate (A.3). □

### A.2 Sobolev Type Estimates

**Lemma A.2**

$$\operatorname{Tr}\left|S_{\hbar}^{(1,k)}V_{\lambda}(x_1-x_2)\gamma^{(k)}\right| \leq C\lambda^{7/4}\operatorname{Tr}\left|S_{\hbar}^{(1,k)}\gamma^{(k)}\right|. \tag{A.9}$$

***Proof*** Notice that

$$S_{\hbar}^{(1,k)} = \langle\hbar\nabla_{x_1}\rangle\langle\hbar\nabla_{x_2}\rangle S_{\hbar}^{(3,k)}\langle\hbar\nabla_{x_1'}\rangle\langle\hbar\nabla_{x_2'}\rangle$$

where $S_{\hbar}^{(3,k)} = \prod_{j=3}^{k}\langle\hbar\nabla_{x_j}\rangle\langle\hbar\nabla_{x_j'}\rangle$. We commute $V_{\lambda}(x_1-x_2)$ with $S_{\hbar}^{(3,k)}$ and obtain

$$\begin{aligned}
&\operatorname{Tr}\left|S_{\hbar}^{(1,k)}V_{\lambda}(x_1-x_2)\gamma^{(k)}\right| \\
&\quad = \operatorname{Tr}\left|\langle\hbar\nabla_{x_1}\rangle\langle\hbar\nabla_{x_2}\rangle V_{\lambda}(x_1-x_2)S_{\hbar}^{(3,k)}\gamma^{(k)}\langle\hbar\nabla_{x_1}\rangle\langle\hbar\nabla_{x_2}\rangle\right| \\
&\quad \leq 8\operatorname{Tr}\left|V_{\lambda}(x_1-x_2)S_{\hbar}^{(3,k)}\gamma^{(k)}\right| + 8\operatorname{Tr}\left|\hbar\nabla_{x_1}\hbar\nabla_{x_2}V_{\lambda}(x_1-x_2)S_{\hbar}^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\right|,
\end{aligned} \tag{A.10}$$

where in the last inequality we used the operator inequality in Lemma A.6 and the triangle inequality.

For the first term of (A.10), we use that $\operatorname{Tr}|AB| \leq \|A\|_{\infty}\operatorname{Tr}|B|$ and $\|V_{\lambda}(x_1 - x_2)\|_{L^{\infty}} \lesssim \lambda$ to get

$$\operatorname{Tr}\left|V_{\lambda}(x_1-x_2)S_{\hbar}^{(3,k)}\gamma^{(k)}\right| \lesssim \lambda\operatorname{Tr}\left|S_{\hbar}^{(3,k)}\gamma^{(k)}\right| \leq \lambda\operatorname{Tr}\left|S_{\hbar}^{(1,k)}\gamma^{(k)}\right|. \tag{A.11}$$

For the second term of (A.10), we use integration by parts to obtain

$$\operatorname{Tr}\left|\hbar\nabla_{x_1}\hbar\nabla_{x_2}V_{\lambda}(x_1-x_2)S_{\hbar}^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\right| \leq \mathrm{I}+\mathrm{II}+\mathrm{III}+\mathrm{IV}, \tag{A.12}$$

where

$$\begin{aligned}
\mathrm{I} &= \operatorname{Tr}\left|V_{\lambda}(x_1-x_2)\hbar\nabla_{x_1}\hbar\nabla_{x_2}S_{\hbar}^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\right|, \\
\mathrm{II} &= \operatorname{Tr}\left|(\hbar\nabla_{x_1}\hbar\nabla_{x_2}V_{\lambda}(x_1-x_2))S_{\hbar}^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\right|, \\
\mathrm{III} &= \operatorname{Tr}\left|(\hbar\nabla_{x_1}V_{\lambda}(x_1-x_2))\hbar\nabla_{x_2}S_{\hbar}^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\right|, \\
\mathrm{IV} &= \operatorname{Tr}\left|(\hbar\nabla_{x_2}V_{\lambda}(x_1-x_2))\hbar\nabla_{x_1}S_{\hbar}^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\right|.
\end{aligned}$$

For I, we use that $\operatorname{Tr}|AB| \le \|A\|_\infty \operatorname{Tr}|B|$ and $\|V_\lambda(x_1-x_2)\|_{L^\infty} \lesssim \lambda$ to get

$$\begin{aligned} \mathrm{I} &= \operatorname{Tr}\Big|V_\lambda(x_1-x_2)\hbar\nabla_{x_1}\hbar\nabla_{x_2}S_\hbar^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\Big| \\ &\lesssim \lambda \operatorname{Tr}\Big|\hbar\nabla_{x_1}\hbar\nabla_{x_2}S_\hbar^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\Big| \\ &\le \lambda \operatorname{Tr}\Big|S_\hbar^{(1,k)}\gamma^{(k)}\Big|, \end{aligned} \tag{A.13}$$

where in the last inequality we used the operator inequality in Lemma A.6.

For II, we notice that

$$|\nabla_{x_1}\nabla_{x_2}V_\lambda(x_1-x_2)|^2 \lesssim \lambda^{6-a}|x_1-x_2|^{-a}, \tag{A.14}$$

where $a \le 6$. As we can decompose $|x|^{-a} = |x|^{-a}1_{B(0,1)}(x) + |x|^{-a}1_{B(0,1)^C}(x)$, we use Lemma A.3 to treat the first part and obtain

$$|\nabla_{x_1}\nabla_{x_2}V_\lambda(x_1-x_2)|^2 \lesssim \lambda^{6-\frac{5}{2}}\langle\nabla_{x_1}\rangle^2\langle\nabla_{x_2}\rangle^2 \tag{A.15}$$

where we take $a = \frac{5}{2}$. By (A.15) and the operator inequality in Lemma A.6, we arrive at

$$\begin{aligned} \mathrm{II} &= \operatorname{Tr}\Big|(\hbar\nabla_{x_1}\hbar\nabla_{x_2}V_\lambda(x_1-x_2))S_\hbar^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\Big| \\ &\lesssim \lambda^{\frac{7}{4}} \operatorname{Tr}\Big|\hbar^2\langle\nabla_{x_1}\rangle\langle\nabla_{x_2}\rangle S_\hbar^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\Big| \\ &\lesssim \lambda^{\frac{7}{4}} \operatorname{Tr}\Big|S_\hbar^{(1,k)}\gamma^{(k)}\Big|. \end{aligned} \tag{A.16}$$

For III, we notice that

$$|\nabla_{x_2}V_\lambda(x_1-x_2)|^2 \lesssim \lambda^2|x_1-x_2|^{-2} \lesssim \lambda^2\langle\nabla_{x_1}\rangle^2, \tag{A.17}$$

where in the last inequality we used Hardy's inequality. Therefore, we use Lemma A.6 to obtain

$$\begin{aligned} \mathrm{III} &= \operatorname{Tr}\Big|(\hbar\nabla_{x_2}V_\lambda(x_1-x_2))\hbar\nabla_{x_1}S_\hbar^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\Big| \\ &\lesssim \lambda \operatorname{Tr}\Big|(\hbar\langle\nabla_{x_1}\rangle\hbar\nabla_{x_1}S_\hbar^{(3,k)}\gamma^{(k)}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\Big| \\ &\lesssim \lambda \operatorname{Tr}\Big|S_\hbar^{(1,k)}\gamma^{(k)}\Big|. \end{aligned} \tag{A.18}$$

In the same way, we also have

$$\mathrm{IV} \lesssim \lambda \operatorname{Tr}\Big|S_\hbar^{(1,k)}\gamma^{(k)}\Big|. \tag{A.19}$$

Combining estimates for I–IV and (A.11), we complete the proof. □

**Lemma A.3** ([30]) *Let $U \in L^1(\mathbb{R}^3)$ be any nonnegative potential, then*

$$U(x-y) \le C\|U\|_{L^1}(1-\Delta_x)(1-\Delta_y). \tag{A.20}$$

**Lemma A.4** ([57, Gagliardo–Nirenberg inequality]) *Let $f$ belong to $L^q(\mathbb{R}^d)$ and its derivatives of order $m$, $\nabla^m f$, belong to $L^r(\mathbb{R}^d)$, $1 \le q, r \le \infty$. For the derivatives $\nabla^j f$, $0 \le j < m$, the following inequalities hold*

$$\|\nabla^j f\|_{L^p(\mathbb{R}^d)} \le C\|\nabla^m f\|^{\alpha}_{L^r(\mathbb{R}^d)}\|f\|^{1-\alpha}_{L^q(\mathbb{R}^d)} \tag{A.21}$$

*where*

$$\frac{1}{p} = \frac{j}{d} + \alpha\left(\frac{1}{r} - \frac{m}{d}\right) + \frac{1-\alpha}{q}, \quad \frac{j}{m} \le \alpha < 1.$$

*Here, we list some cases we used with $d = 3$ as below*

$$\|\nabla f\|_{L^{\frac{3}{2}}(\mathbb{R}^3)} \le C\|\nabla^2 f\|^{\frac{1}{2}}_{L^{\frac{6}{5}}(\mathbb{R}^3)}\|f\|^{\frac{1}{2}}_{L^2(\mathbb{R}^3)}, \tag{A.22}$$

$$\|\nabla f\|_{L^{\frac{6}{5}}(\mathbb{R}^3)} \le C\|\nabla^3 f\|^{\frac{1}{3}}_{L^2(\mathbb{R}^3)}\|f\|^{\frac{2}{3}}_{L^1(\mathbb{R}^3)}, \tag{A.23}$$

$$\|\nabla f\|_{L^{\frac{12}{7}}(\mathbb{R}^3)} \le C\|\nabla^2 f\|^{\frac{1}{2}}_{L^{\frac{3}{2}}(\mathbb{R}^3)}\|f\|^{\frac{1}{2}}_{L^2(\mathbb{R}^3)}. \tag{A.24}$$

### A.3 Basic Operator Facts

**Lemma A.5** ([30, Proposition 9.4]) *The partial trace satisfies the following relation*

$$\mathrm{Tr}_1 |\mathrm{Tr}_2 A| \le \mathrm{Tr}_{1,2} |A|. \tag{A.25}$$

**Lemma A.6** *Let $A_1$ and $A_2$ be non-negative self-adjoint operators satisfying $A_1^2 \le A_2^2$. Then we have*

$$\mathrm{Tr}\,|A_1 B| \le \mathrm{Tr}\,|A_2 B|. \tag{A.26}$$

***Proof*** We compute

$$\mathrm{Tr}|A_1 B| = \mathrm{Tr}\sqrt{B^* A_1^2 B}. \tag{A.27}$$

Since $B^* A_1^2 B \le B^* A_2^2 B$, by Löwner–Heinz inequality (see for example [58]) or the fact that the square root is monotonic for operators, we have $\sqrt{B^* A_1^2 B} \le \sqrt{B^* A_2^2 B}$ and hence

$$\mathrm{Tr}\,|A_1 B| = \mathrm{Tr}\sqrt{B^* A_1^2 B} \le \mathrm{Tr}\sqrt{B^* A_2^2 B} = \mathrm{Tr}\,|A_2 B|. \tag{A.28}$$

□

# Appendix B: Energy Estimates

## B.1 Lower Bound

**Lemma B.1** *Let $\lambda \leq N^{3/4}$ and $k \leq \ln N$. There exists $N_0$ independent of $k$, $\lambda$ and $\hbar$ such that*

$$\langle \psi, (H_{N,\hbar,\lambda} + N)^k \psi \rangle \geq \frac{N^k}{2^k} \langle \psi, \langle \hbar \nabla_{x_1} \rangle^2 \langle \hbar \nabla_{x_2} \rangle^2 \cdots \langle \hbar \nabla_{x_k} \rangle^2 \psi \rangle \tag{B.1}$$

*for every $N \geq N_0$.*

***Proof*** For $\hbar = 1$, this proof has been done by many authors in many works. For completeness, we include a proof here. For $k = 0$ and $k = 1$, the claim is trivial because of the positivity of the potential. Now we assume the proposition is true for all $k \leq n$, and we prove it for $k = n + 2$.

$$\begin{aligned} \langle \psi, (H_{N,\hbar,\lambda} + N)^{n+2} \psi \rangle &= \langle \left( H_{N,\hbar,\lambda} + N \right) \psi, \left( H_{N,\hbar,\lambda} + N \right)^n \left( H_{N,\hbar,\lambda} + N \right) \psi \rangle \\ &\geq \frac{N^n}{2^n} \langle \psi, (H_{N,\hbar,\lambda} + N) \langle \hbar \nabla_{x_1} \rangle^2 \cdots \langle \hbar \nabla_{x_n} \rangle^2 (H_{N,\hbar,\lambda} + N) \psi \rangle. \end{aligned} \tag{B.2}$$

We set

$$H^{(n)}_{N,\hbar,\lambda} = \sum_{j=1}^{n} \langle \hbar \nabla_{x_j} \rangle^2 + \frac{1}{N} \sum_{j<m}^{N} V_{\lambda,jm}$$

with $V_{\lambda,jm} = V_\lambda(x_j - x_m)$. Then we have

$$\begin{aligned} &\left\langle \psi, (H_{N,\hbar,\lambda} + N) \langle \hbar \nabla_{x_1} \rangle^2 \cdots \langle \hbar \nabla_{x_n} \rangle^2 (H_{N,\hbar,\lambda} + N) \psi \right\rangle \\ &\quad = \sum_{j_1, j_2 \geq n+1} \left\langle \psi, \langle \hbar \nabla_{x_{j_1}} \rangle^2 \langle \hbar \nabla_{x_1} \rangle^2 \cdots \langle \hbar \nabla_{x_n} \rangle^2 \langle \hbar \nabla_{x_{j_2}} \rangle^2 \psi \right\rangle \\ &\qquad + \sum_{j \geq n+1} \left( \left\langle \psi, \langle \hbar \nabla_{x_j} \rangle^2 \langle \hbar \nabla_{x_1} \rangle^2 \cdots \langle \hbar \nabla_{x_n} \rangle^2 H^{(n)}_{N,\hbar,\lambda} \psi \right\rangle + \text{c.c.} \right) \\ &\qquad + \left\langle \psi, H^{(n)}_{N,\hbar,\lambda} \langle \hbar \nabla_{x_1} \rangle^2 \cdots \langle \hbar \nabla_{x_n} \rangle^2 H^{(n)}_{N,\hbar,\lambda} \psi \right\rangle, \end{aligned}$$

where c.c. denotes the complex conjugate. Since $H^{(n)}_{N,\hbar,\lambda} \langle \hbar \nabla_{x_1} \rangle^2 \cdots \langle \hbar \nabla_{x_n} \rangle^2 H^{(n)}_{N,\hbar,\lambda} \geq 0$, we have, using the symmetry with respect to permutations,

$$
\begin{aligned}
&\langle\psi, (H_{N,\hbar,\lambda}+N)\langle\hbar\nabla_{x_1}\rangle^2\cdots\langle\hbar\nabla_{x_n}\rangle^2(H_{N,\hbar,\lambda}+N)\psi\rangle\\
&\quad\geq (N-n)(N-n-1)\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^2\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+2}}\rangle^2\psi\big\rangle\\
&\qquad+(2n+1)(N-n)\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^4\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\\
&\qquad+\frac{n(n+1)(N-n)}{2N}\Big(\big\langle\psi, V_{\lambda,12}\langle\hbar\nabla_{x_1}\rangle^2\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\Big)\\
&\qquad+\frac{(n+1)(N-n)(N-n-1)}{N}\Big(\big\langle\psi, V_{\lambda,1(n+2)}\langle\hbar\nabla_{x_1}\rangle^2\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\Big).
\end{aligned}
\tag{B.3}
$$

Here we also used the fact that

$$
\big\langle\psi, V_{\lambda,jm}\langle\hbar\nabla_{x_1}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\geq 0
$$

if $j, m > n+1$, because of the positivity of the potential. Next, we will bound the last two terms on the r.h.s of (B.3) from below. Then we have

$$
\begin{aligned}
&\big\langle\psi, V_{\lambda,12}\langle\hbar\nabla_{x_1}\rangle^2\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\\
&\quad=\big\langle\psi, V_{\lambda,12}(1-\hbar^2\Delta_{x_1})(1-\hbar^2\Delta_{x_2})\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\\
&\quad\geq\big\langle\psi, \hbar\nabla V_{\lambda,12}\hbar\nabla_{x_2}\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\\
&\qquad+\big\langle\hbar\nabla_{x_2}\psi, \hbar\nabla V_{\lambda,12}\hbar\nabla_{x_1}\hbar\nabla_{x_2}\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\\
&\qquad+\big\langle\psi, \hbar\nabla V_{\lambda,12}\hbar^2\Delta_{x_1}\hbar\nabla_{x_2}\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\text{c.c.}\\
&\quad=:\mathrm{I}+\mathrm{II}+\mathrm{III}.
\end{aligned}
$$

Applying Cauchy–Schwarz, we get

$$
\begin{aligned}
\mathrm{I}&\geq -2\Big\{\alpha_1\big\langle\psi, |\hbar\nabla V_{\lambda,12}|\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\\
&\qquad+\alpha_1^{-1}\big\langle|\hbar\nabla_{x_2}|\psi, |\hbar\nabla V_{\lambda,12}|\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2|\hbar\nabla_{x_2}|\psi\big\rangle\Big\},\\
\mathrm{II}&\geq -2\Big\{\alpha_2\big\langle|\hbar\nabla_{x_2}|\psi, |\hbar\nabla V_{\lambda,12}|\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2|\hbar\nabla_{x_2}|\psi\big\rangle\\
&\qquad+\alpha_2^{-1}\big\langle|\hbar\nabla_{x_1}||\hbar\nabla_{x_2}|\psi, |\hbar\nabla V_{\lambda,12}|\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2|\hbar\nabla_{x_1}||\hbar\nabla_{x_2}|\psi\big\rangle\Big\},\\
\mathrm{III}&\geq -2\Big\{\alpha_3\big\langle\psi, |\hbar\nabla V_{\lambda,12}|\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\\
&\qquad+\alpha_3^{-1}\big\langle|\hbar\nabla_{x_1}|^2|\hbar\nabla_{x_2}|\psi, |\hbar\nabla V_{\lambda,12}|\langle\hbar\nabla_{x_3}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2|\hbar\nabla_{x_1}|^2|\hbar\nabla_{x_2}|\psi\big\rangle\Big\}.
\end{aligned}
$$

By Lemma A.3,

$$
\begin{aligned}
&\mathrm{I}\geq -C\Big\{\alpha_1\lambda\big\langle\psi, \langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\alpha_1^{-1}\lambda\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^2\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\Big\},\\
&\mathrm{II}\geq -C\Big\{\alpha_2\lambda\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\alpha_2^{-1}\lambda\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^4\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\Big\},\\
&\mathrm{III}\geq -C\Big\{\alpha_3\lambda\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle+\alpha_3^{-1}\lambda^2\big\langle\psi, \langle\hbar\nabla_{x_1}\rangle^4\langle\hbar\nabla_{x_2}\rangle^2\cdots\langle\hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\Big\}.
\end{aligned}
$$

Optimizing the choice of $\alpha_1$, $\alpha_2$ and $\alpha_3$, we find that

$$\begin{aligned}
&\big\langle \psi, V_{\lambda,12}\langle \hbar\nabla_{x_1}\rangle^2\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle + \text{c.c.}\\
&\quad \geq -CN^{-3/2}\lambda^{3/2}\Big\{N^2\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\\
&\qquad + N\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^4\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\Big\}.
\end{aligned}$$

As for the last term on the r.h.s. of (B.3), we have

$$\begin{aligned}
&\big\langle \psi, V_{\lambda,1(n+2)}\langle \hbar\nabla_{x_1}\rangle^2\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle + \text{c.c.}\\
&\quad\geq \big\langle \psi, V_{\lambda,1(n+2)}(-\hbar^2\Delta_{x_1})\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle + \text{c.c.}\\
&\quad\geq \big\langle \psi, |\hbar\nabla V_{\lambda,1(n+2)}||\hbar\nabla_{x_1}|\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle + \text{c.c.}\\
&\quad\geq -\alpha\big\langle \psi, |\hbar\nabla V_{\lambda,1(n+2)}|\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle\\
&\qquad -\alpha^{-1}\big\langle |\hbar\nabla_{x_1}|\psi, |\hbar\nabla V_{\lambda,1(n+2)}|\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2|\hbar\nabla_{x_1}|\psi\big\rangle\\
&\quad\geq -C(\alpha\lambda+\alpha^{-1}\lambda)\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_{n+2}}\rangle^2\psi\big\rangle\\
&\quad\geq -C\lambda\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_{n+2}}\rangle^2\psi\big\rangle,
\end{aligned}$$

where we optimized the choice of $\alpha$. Then we get

$$\begin{aligned}
&\langle \psi, (H_{N,\hbar}+N)\big\langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_n}\rangle^2(H_{N,\hbar}+N)\psi\big\rangle\\
&\quad\geq (N-n)(N-n-1)\left(1-\frac{C\lambda^{3/2}n^2}{N^{1/2}(N-n)}-\frac{C\lambda n}{N}\right)\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_{n+2}}\rangle^2\psi\big\rangle\\
&\qquad+(2n+1)(N-n)\left(1-\frac{C\lambda^{3/2}n}{N^{3/2}}\right)\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^4\langle \hbar\nabla_{x_2}\rangle^2\cdots\langle \hbar\nabla_{x_{n+1}}\rangle^2\psi\big\rangle.
\end{aligned}$$

As we require that $\lambda \leq N^{3/4}$ and $n \leq \ln N$, we can find $N_0(\beta)$ which is independent of $n$, $\lambda$ and $\hbar$, so that

$$\big\langle\psi, (H_{N,\hbar}+N)\langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_n}\rangle^2(H_{N,\hbar}+N)\psi\big\rangle \geq \frac{N^2}{4}\big\langle\psi, \langle \hbar\nabla_{x_1}\rangle^2\cdots\langle \hbar\nabla_{x_{n+2}}\rangle^2\psi\big\rangle$$

for every $N \geq N_0$. Together with (B.2), this completes the proof. □

## B.2 Upper Bound

**Lemma B.2** *Let* $N^{1/2} \leq \lambda \leq N^{1/2}(\ln\ln N)^{10}$ *and* $k \leq (\ln\ln N)^{10}$. *There exists* $N_0$ *independent of* $k$, $\lambda$ *and* $\hbar$ *such that*

$$H_{N,\hbar,\lambda}+N)^k \leq 8^k\left(\sum_{i=1}^N\langle\nabla_{x_i}\rangle^2\right)^k \tag{B.4}$$

*for all* $N \geq N_0$.

***Proof*** For $\hbar = 1$, see [30, Proposition 5.1] in which $N_0$ could depend on $k$. Here, as we require that $N_0$ is independent of parameters $k$, $\lambda$ and $\hbar$, we include a complete proof. For convenience, we first set up some notations. Let

$$A_{N,\hbar} = \sum_{i=1}^{N} \langle \hbar \nabla_{x_i} \rangle^2, \quad A_N = \sum_{i=1}^{N} \langle \nabla_{x_i} \rangle^2, \tag{B.5}$$

$$B_{N,\lambda} = \frac{1}{N} \sum_{1 \le i < j \le N}^{N} V_{\lambda,ij}, \tag{B.6}$$

where $V_{\lambda,ij} = V_\lambda(x_i - x_j)$. Therefore, we can rewrite

$$H_{N,\hbar,\lambda} + N = A_{N,\hbar} + B_{N,\lambda}. \tag{B.7}$$

For $k = 0$ and $k = 1$, the claim is trivial because of the positivity of the potential. Now we assume the proposition is true for all $k \le n$, and we prove it for $k = n + 2$. We compute

$$\begin{aligned}
&(H_{N,\hbar,\lambda} + N)^{k+2} \\
&\quad \le 8^k (H_{N,\hbar,\lambda} + N)(A_N)^k (H_{N,\hbar,\lambda} + N) \\
&\quad = 8^k (A_{N,\hbar} + B_{N,\lambda})(A_N)^k (A_{N,\hbar} + B_{N,\lambda}) \\
&\quad = 8^k \big(A_{N,\hbar}(A_N)^k A_{N,\hbar} + B_{N,\lambda}(A_N)^k B_{N,\lambda} + B_{N,\lambda}(A_N)^k A_{N,\hbar} + A_{N,\hbar}(A_N)^k B_{N,\lambda}\big) \\
&\quad \le 8^k \big(2A_{N,\hbar}(A_N)^k A_{N,\hbar} + 2B_{N,\lambda}(A_N)^k B_{N,\lambda}\big),
\end{aligned} \tag{B.8}$$

where in the last inequality we used the operator inequality that $A^*B + B^*A \le A^*A + B^*B$. Therefore, we are left to prove that

$$B_{N,\lambda}(A_N)^k B_{N,\lambda} \le 3(A_N)^{k+2}. \tag{B.9}$$

Expanding $B_{N,\lambda}(A_N)^k B_{N,\lambda}$ gives that

$$B_{N,\lambda}(A_N)^k B_{N,\lambda} = N^{-2} \sum_{i_1 < j_1, i_2 < j_2} V_{\lambda,i_1 j_1}(A_N)^k V_{\lambda,i_2 j_2}.$$

By the operator inequality that $A^*B + B^*A \le A^*A + B^*B$, the above

$$\begin{aligned}
&\le N^{-2} \sum_{i_1 < j_1, i_2 < j_2} \big(V_{\lambda,i_1 j_1}(A_N)^k V_{\lambda,i_1 j_1} + V_{\lambda,i_2 j_2}(A_N)^k V_{\lambda,i_2 j_2}\big) \\
&= \sum_{i<j} V_{\lambda,ij}(A_N)^k V_{\lambda,ij}.
\end{aligned}$$

By the symmetry, it suffices to prove that

$$V_{\lambda,12}(A_N)^k V_{\lambda,12} \le 6\langle\nabla_{x_1}\rangle^2\langle\nabla_{x_2}\rangle^2(A_N)^k. \tag{B.10}$$

By the weighted Minkowski inequality, we have for some constant $C$

$$(A_N)^k \le (Ck)^k\big(\langle\nabla_{x_1}\rangle^{2k} + \langle\nabla_{x_2}\rangle^{2k}\big) + \frac{5}{4}\left(\sum_{i=3}^{N}\langle\nabla_{x_i}\rangle^2\right)^k. \tag{B.11}$$

Hence, we have

$$V_{\lambda,12}(A_N)^k V_{\lambda,12} \le \mathrm{I} + \mathrm{II} + \mathrm{III},$$

where

$$\mathrm{I} = (Ck)^k V_{\lambda,12}\langle\nabla_{x_1}\rangle^{2k} V_{\lambda,12}, \tag{B.12}$$

$$\mathrm{II} = (Ck)^k V_{\lambda,12}\langle\nabla_{x_2}\rangle^{2k} V_{\lambda,12}, \tag{B.13}$$

$$\mathrm{III} = \frac{5}{4} V_{\lambda,12}\left(\sum_{i=3}^{N}\langle\nabla_{x_i}\rangle^2\right)^k V_{\lambda,12}. \tag{B.14}$$

For $I$, by Leibniz rule, we obtain

$$\begin{aligned} V_{\lambda,12}\langle\nabla_{x_1}\rangle^{2k} V_{\lambda,12} &\le 2^k V_{\lambda,12}(1 + (-\Delta_{x_1})^k) V_{\lambda,12} \\ &\le 2^k |V_{\lambda,12}|^2 + \sum_{m=0}^{k} C_k^m |\nabla_{x_1}|^{k-m} | \big(\nabla_{x_1}^m V_{\lambda,12}\big) |^2 |\nabla_{x_1}|^{k-m}. \end{aligned} \tag{B.15}$$

For $|V_{\lambda,12}|^2$, by Hardy's inequality we have

$$|V_{\lambda,12}|^2 \le 4\langle\nabla_{x_1}\rangle^2. \tag{B.16}$$

To estimate the derivative of $V_{\lambda,12}$, we notice that

$$|\nabla_{x_1}^m V_{\lambda,12}|^2 \le C^m \lambda^{2m+2-a}|x_1 - x_2|^{-a}, \tag{B.17}$$

for $a \le 2m+2$. As we can decompose $|x|^{-a} = |x|^{-a}1_{B(0,1)}(x) + |x|^{-a}1_{B(0,1)^C}(x)$, we use Lemma A.3 to treat the first part and obtain

$$|\nabla_{x_1}^m V_{\lambda,12}|^2 \le C^m \lambda^{2m+2-\frac{5}{2}}\langle\nabla_{x_1}\rangle^2\langle\nabla_{x_2}\rangle^2, \tag{B.18}$$

where $m \geq 1$ and $a = \frac{5}{2}$. Combining estimates (B.15) and (B.18), we arrive at

$$\begin{aligned} \mathrm{I} &\leq (2Ck)^k \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 + (Ck)^k \lambda^{-\frac{1}{2}} \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 \sum_{m=0}^{k} (C\lambda^2)^m C_k^m (-\Delta_{x_1})^{k-m} \\ &\leq (Ck)^k \lambda^{-\frac{1}{2}} \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (2C\lambda^2 - \Delta_{x_1})^k. \end{aligned}$$

With $N^{1/2} \leq \lambda$, we have that the above

$$\begin{aligned} &\leq (Ck)^k N^{-\frac{1}{4}} \left( \frac{2C\lambda^2}{N} \right)^k \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (N - \Delta_{x_1})^k \\ &\leq (Ck)^k N^{-\frac{1}{4}} \left( \frac{2C\lambda^2}{N} \right)^k \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (A_N)^k. \end{aligned}$$

Since we require that $\lambda \leq N^{\frac{1}{2}} (\ln \ln N)^{10}$ and $k \leq (\ln \ln N)^{10}$, we obtain

$$\mathrm{I} \leq N^{-\frac{1}{4}} (Ck)^k (2C \ln \ln N)^{10k} \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (A_N)^k \leq \frac{1}{2} \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (A_N)^k \tag{B.19}$$

as long as $N \geq N_0$. In the same way, we also have

$$\mathrm{II} \leq \frac{1}{2} \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (A_N)^k. \tag{B.20}$$

As for III, we compute

$$\mathrm{III} = 2V_{\lambda,12} \left( \sum_{i=3}^{N} \langle \nabla_{x_i} \rangle^2 \right)^k V_{\lambda,12} = \frac{5}{4} |V_{\lambda,12}|^2 \left( \sum_{i=3}^{N} \langle \nabla_{x_i} \rangle^2 \right)^k.$$

By estimate (B.16), we arrive at

$$\mathrm{III} \leq 5 \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (A_N)^k. \tag{B.21}$$

Combining these estimates for I, II and III, we reach

$$V_{\lambda,12} (A_N)^k V_{\lambda,12} \leq 6 \langle \nabla_{x_1} \rangle^2 \langle \nabla_{x_2} \rangle^2 (A_N)^k, \tag{B.22}$$

which completes the proof of the desired estimate (B.10). □

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