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Semiclassical limit of the Bogoliubov–de Gennes equation

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Abstract. In this paper, we rewrite the time-dependent Bogoliubov–de Gennes (BdG) equation in an appropriate semiclassical form and establish its semiclassical limit to a two-particle kinetic transport equation with an effective mean-field background potential satisfying the one-particle Vlasov equation. Moreover, for some semiclassical regimes, we obtain a higher-order correction to the two-particle kinetic transport equation, capturing a nontrivial two-body interaction effect. The convergence is proven for C^2 interaction potentials in terms of a semiclassical optimal transport pseudo-metric.

Furthermore, combining our current results with the results of Marcantoni et al. [Ann. Henri Poincaré (2024)], we establish a joint semiclassical and mean-field approximation of the dynamics of a system of spin-$\frac{1}{2}$ Fermions by the Vlasov equation in some weak topology.

To Thomas Kappeler, in memory of his unwavering human and professional support

1. Introduction

1.1. The time-dependent Bogoliubov–de Gennes equation

We consider the time-dependent Bogoliubov–de Gennes (BdG) equation, sometimes also referred to as the generalized Hartree–Fock equation or the Hartree–Fock–Bogoliubov equation. It describes the time evolution of generalized one-particle reduced density operators, which are self-adjoint operators Γ acting on $\mathfrak{h} \oplus \mathfrak{h}$, satisfying the operator bound $0 \leq \Gamma \leq \mathbf{1}_{\mathfrak{h}\oplus\mathfrak{h}}$, and having the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\overline{\alpha} & \mathbf{1} - \overline{\gamma} \end{pmatrix}, \tag{1.1}$$

where $\mathfrak{h} = L^2(\mathbb{R}^d, \mathbb{C})$ denotes the one-particle state space and $\overline{A}$ represents the operator whose integral kernel is the conjugate of the kernel of the operator A. Here, the bounded linear operators γ and α acting on $\mathfrak{h}$ are called, respectively, the one-particle density operator and the pairing operator. It follows from the properties of Γ that γ and α satisfy

$$0 \leq \gamma \leq \mathbf{1}, \quad \alpha^* = -\overline{\alpha}, \quad \gamma\alpha = \alpha\overline{\gamma}, \quad \text{and} \quad |\alpha^*|^2 \leq \gamma(\mathbf{1} - \gamma), \tag{1.2}$$

where $|A| = \sqrt{A^* A}$.

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The BdG equation models many-body dynamics with an interparticle interaction potential U, which we assume to satisfy, for some constant $C \geq 0$, the conditions

$$U(x) = U(-x), \quad U \in L^2_{\mathrm{loc}}(\mathbb{R}^d), \quad \text{and} \quad U^2 \leq C(\mathbf{1} - \Delta). \tag{1.3}$$

Let $\boldsymbol{p} = -i\hbar\nabla_x$ denote the momentum operator with $\hbar = h/(2\pi)$, where h is the Planck constant, and define the Hartree–Fock Hamiltonian associated with γ by the operator

$$\mathsf{H}_\gamma = \frac{|\boldsymbol{p}|^2}{2} + V_\gamma - \mathsf{X}_\gamma.$$

In the above expression, V_γ is the multiplication operator by the mean-field potential defined by

$$V_\gamma(x) = U * \operatorname{diag}(\gamma)(x) = \int_{\mathbb{R}^d} U(x-y)\gamma(y,y)\,\mathrm{d}y,$$

and X_γ is the exchange operator defined through its integral kernel

$$\mathsf{X}_\gamma(x,y) = U(x-y)\gamma(x,y).$$

Moreover, we define the generalized Hartree–Fock Hamiltonian acting on $\mathfrak{h} \oplus \mathfrak{h}$ by the matrix operator

$$\mathsf{H}_\Gamma = \begin{pmatrix} \mathsf{H}_\gamma & \mathsf{X}_\alpha \\ \mathsf{X}_\alpha^* & -\overline{\mathsf{H}}_\gamma \end{pmatrix}.$$

Then, the BdG equation reads

$$i\hbar\,\partial_t \Gamma = [\mathsf{H}_\Gamma, \Gamma], \tag{1.4}$$

where $[A,B] := AB - BA$ is the operator commutator. Equivalently, equation (1.4) can be written as the following coupled system of equations:

$$i\hbar\,\partial_t \gamma = [\mathsf{H}_\gamma, \gamma] + \mathsf{X}_\alpha \alpha^* - \alpha \mathsf{X}_\alpha^*, \tag{1.5a}$$
$$i\hbar\,\partial_t \alpha = \mathsf{H}_\gamma \alpha + \alpha \overline{\mathsf{H}}_\gamma + \mathsf{X}_\alpha(\mathbf{1} - \overline{\gamma}) - \gamma \mathsf{X}_\alpha. \tag{1.5b}$$

Notice that if $\alpha = 0$, then γ solves the Hartree–Fock equation

$$i\hbar\,\partial_t \gamma = [\mathsf{H}_\gamma, \gamma]. \tag{1.6}$$

This justifies the claim that the BdG equation is a generalization of the Hartree–Fock equation with a non-zero pairing operator. Observe also the fact that the self-adjointness of Γ and $0 \leq \Gamma \leq \mathbf{1}_{\mathfrak{h}\oplus\mathfrak{h}}$ are preserved under the BdG dynamics; in particular, the properties (1.2) remain true along the dynamics. We refer to [7] for discussions regarding the well-posedness and additional properties of the equation. In fact, conditions (1.3) are taken from [7], which guarantees the global well-posedness of solutions.

1.2. Semiclassical regimes, classical phase space dynamics, and useful notations

The purpose of this paper is to study the BdG equation (1.4) in the semiclassical regime, that is on space-time scales where the Planck constant h becomes negligible. To make connection with earlier studies on the effective approximation of many-body interacting fermionic systems (see Section 4), we set $N = \mathrm{Tr}(\gamma)$ and write

$$U(x) = \frac{1}{N} K(x),$$

where $K : \mathbb{R}^d \to \mathbb{R}$ is independent of N and $\hbar$ and satisfies conditions (1.3), and the factor N^{-1} is the mean-field coupling constant.

In the context of the semiclassical limit, it is convenient to define the scaled operator

$$\boldsymbol{\rho} := \frac{1}{N h^d} \gamma \tag{1.7}$$

so that $h^d\, \mathrm{Tr}(\boldsymbol{\rho}) = 1$. We will call positive operators verifying this trace normalization density operators and denote this class of operators by $\mathcal{P}(\mathfrak{h})$. We also define the semiclassical Schatten norms, which are quantum analogs of the Lebesgue norms on the phase space, by

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} := h^{d/p} (\mathrm{Tr}(|\boldsymbol{\rho}|^p))^{1/p}. \tag{1.8}$$

These norms are helpful in identifying the necessary scaling of quantum objects that will lead to a nontrivial semiclassical limit.

In the case of zero pairing, we see that the scaling (1.7) leads to rewriting equation (1.6) as follows:

$$i\hbar\, \partial_t \boldsymbol{\rho} = [\mathsf{H}_{\boldsymbol{\rho}}, \boldsymbol{\rho}] \quad \text{with } \mathsf{H}_{\boldsymbol{\rho}} = \frac{|\boldsymbol{p}|^2}{2} + V_{\boldsymbol{\rho}} - h^d\, \mathsf{X}_{\boldsymbol{\rho}}, \tag{1.9}$$

where $V_{\boldsymbol{\rho}} = K * \varrho(x)$ and $\varrho(x)$ is the spatial distribution of particles defined by

$$\varrho(x) = \mathrm{diag}(\boldsymbol{\rho})(x) := h^d \boldsymbol{\rho}(x, x) \tag{1.10}$$

and the exchange operator $\mathsf{X}_{\boldsymbol{\rho}}$ has the integral kernel

$$\mathsf{X}_{\boldsymbol{\rho}}(x, y) = K(x - y)\boldsymbol{\rho}(x, y). \tag{1.11}$$

Furthermore, with this scaling, it is known that in the semiclassical limit $\hbar \to 0$ one can recover classical phase space dynamics from the Hartree–Fock dynamics (see, e.g., [6, 39, 42]). More precisely, one obtains as the semiclassical approximation of equation (1.9) the Vlasov equation

$$\partial_t f + \xi \cdot \nabla_\chi f + E_f \cdot \nabla_\xi f = 0 \quad \text{with } f(0, \chi, \xi) = f^{\mathrm{in}}(\chi, \xi) \geq 0, \tag{1.12}$$

where f is a time-dependent probability density on $\mathbb{R}^{2d} = \mathbb{R}^d_\chi \times \mathbb{R}^d_\xi$ and $E_f = -\nabla V_f$ is the self-consistent force field associated to the mean-field potential $V_f(\chi) = (K * \rho_f)(t,\chi)$ with ρ_f the spatial density defined by

$$\rho_f(t,\chi) = \int_{\mathbb{R}^d} f(t,\chi,\xi)\,\mathrm{d}\xi.$$

In this work, we want to extend the above result to the case of the BdG equation (1.5), with a non-zero pairing operator α. To this end, we define the two-particle operator

$$\boldsymbol{\rho}_\alpha = \lambda\,|\alpha\rangle\langle\alpha| \tag{1.13}$$

as the orthogonal projection in $\mathfrak{h} \otimes \mathfrak{h}$ onto the function defined by $(x,y) \mapsto \alpha(x,y)$, and where $\lambda > 0$ is chosen so that $h^{2d}\,\mathrm{Tr}(\boldsymbol{\rho}_\alpha) = 1$. This allows us to rewrite the BdG equation (1.5) in the equivalent form (2.6), as shown in Section 2.1, and compare it with its classical analog

$$\partial_t f + \xi \cdot \nabla_\chi f + E_f \cdot \nabla_\xi f = 0, \tag{1.14a}$$

$$\partial_t F + \xi_{12} \cdot \nabla_{\chi_{12}} F + E_{12} \cdot \nabla_{\xi_{12}} F = \frac{1}{N} \nabla K(\chi_1 - \chi_2) \cdot (\nabla_{\xi_1} - \nabla_{\xi_2}) F, \tag{1.14b}$$

where $F(z_{12}) = F(z_1,z_2) \geq 0$ is a two-particle distribution, that is, a probability distribution defined over the two-particle phase space $\mathbb{R}^{2d} \times \mathbb{R}^{2d}$, with $(z_1,z_2) = (\chi_1,\xi_1,\chi_2,\xi_2)$ and $\chi_{12} := (\chi_1,\chi_2) \in \mathbb{R}^{2d}_\chi$, $\xi_{12} := (\xi_1,\xi_2) \in \mathbb{R}^{2d}_\xi$, and $E_{12} := (E_f(\chi_1), E_f(\chi_2))$.

Notice that system (1.14) is well posed. Indeed, being that equation (1.14a) is a Vlasov equation with smooth interaction K, it is well posed by standard techniques (see, e.g., [17]). Given f, a solution of equation (1.14a), and the corresponding vector field E_{12}, equation (1.14b) is simply a linear transport equation with smooth vector field, which is well posed by standard characteristics methods. Heuristically, for N fixed, equation (1.14b) describes the dynamics of a typical pair of particles which follow the flow created by a background f and are correlated by the interaction force $\frac{1}{N}\nabla K$. If the l.h.s. of equation (1.14b) is absent, then it is clear that the evolution of independent particles will remain independent.

1.3. Semiclassical optimal transport pseudo-metric and main result

We now introduce the tools that we will use in our main theorem to prove the semiclassical limit of the BdG equation (2.6).

Denote $z = (\chi,\xi) \in \mathbb{R}^{2d}$. Let f be a probability density function on $\mathbb{R}^{2d}$ and $\boldsymbol{\rho} \in \mathcal{P}(\mathfrak{h})$. A coupling of f and $\boldsymbol{\rho}$ is a measurable function $\boldsymbol{\gamma} : z \mapsto \boldsymbol{\gamma}(z)$ defined for almost all $z \in \mathbb{R}^{2d}$ with values in the space of bounded linear operators acting on $\mathfrak{h}$ such that, for almost all $z \in \mathbb{R}^{2d}$, we have that $\boldsymbol{\gamma}(z) \geq 0$ and it satisfies the conditions

$$h^d\,\mathrm{Tr}_{\mathfrak{h}}(\boldsymbol{\gamma}(z)) = f(z) \quad \text{and} \quad \int_{\mathbb{R}^{2d}} \boldsymbol{\gamma}(z)\,\mathrm{d}z = \boldsymbol{\rho}. \tag{1.15}$$

The set of all couplings of f and $\boldsymbol{\rho}$ is denoted by $\mathcal{C}(f, \boldsymbol{\rho})$. Next, we define the semiclassical optimal transport pseudo-metric by

$$\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho}) = \left(\inf_{\boldsymbol{\gamma} \in \mathcal{C}(f,\boldsymbol{\rho})} \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_{\mathfrak{h}}(\boldsymbol{c}(z)\boldsymbol{\gamma}(z))\, \mathrm{d}z \right)^{\frac{1}{2}} \tag{1.16}$$

with the cost function $\boldsymbol{c}(z)$ defined by the unbounded operator whose action on test functions φ gives

$$(\boldsymbol{c}(z)\varphi)(x) = |\chi - x|^2 \varphi(x) + |\xi - \boldsymbol{p}|^2 \varphi(x)$$

and $\boldsymbol{p} = -i\hbar\nabla_x$. The notation $\operatorname{Tr}_{\mathfrak{h}}(\boldsymbol{c}\boldsymbol{\gamma})$ should in general be understood as $\operatorname{Tr}_{\mathfrak{h}}(\boldsymbol{c}^{1/2}\boldsymbol{\gamma}\boldsymbol{c}^{1/2})$ if $\boldsymbol{c}\boldsymbol{\gamma}$ is not trace class. The above semiclassical optimal transport pseudo-metric between density operators and classical phase space functions was first introduced in [23]. It can be viewed as an intermediate notion between the classical Monge–Kantorovich distance (Wasserstein distance) of exponent 2 on the space of Borel probability measures and the quantum optimal transport pseudo-metric on the space of density operators defined in [22]. The properties of these pseudo-metrics can be found in [8, 23, 25, 37].

Likewise, for any two-particle probability density function $F(z_1, z_2)$ on $\mathbb{R}^{2d} \times \mathbb{R}^{2d}$ and two-particle density operator $\boldsymbol{\rho}_2 \in \mathcal{P}(\mathfrak{h} \otimes \mathfrak{h})$, we denote by $\mathrm{W}_{2,\hbar}(F, \boldsymbol{\rho}_2)$ their semiclassical optimal transport pseudo-metric, defined in the same way with $\mathfrak{h}$ replaced by $\mathfrak{h} \otimes \mathfrak{h}$ and $\mathbb{R}^{2d}$ replaced by $\mathbb{R}^{2d} \times \mathbb{R}^{2d}$.

We are now ready to state our main results. In our first theorem, we will be concerned with the limit to the following classical equations corresponding to equations (1.14a)–(1.14b) with $N = \infty$:

$$\begin{aligned} \partial_t f + \xi \cdot \nabla_\chi f + E_f \cdot \nabla_\xi f &= 0, \\ \partial_t F + \xi_{12} \cdot \nabla_{\chi_{12}} F + E_{12} \cdot \nabla_{\xi_{12}} F &= 0. \end{aligned} \tag{1.17}$$

Theorem 1.1. *Let $d \geq 3$ and assume $N\hbar \geq C$, where C does not depend on N and $\hbar$, K be an even, real-valued function such that $\nabla^2 K \in L^\infty(\mathbb{R}^d, \mathbb{R}^{2d})$, $\widehat{K} \in L^1(\mathbb{R}^d)$, and $x \mapsto |x| K(x) \in L^\infty(\mathbb{R}^d)$. Let (γ, α) be a solution of the BdG equations (1.5), and let $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_\alpha$ be their scaled versions defined in (1.7) and (1.13) with initial data $(\boldsymbol{\rho}^{\mathrm{in}}, \boldsymbol{\rho}_\alpha^{\mathrm{in}}) \in \mathcal{P}(\mathfrak{h}) \times \mathcal{P}(\mathfrak{h}^{\otimes 2})$ such that*

$$h^d \operatorname{Tr}(\boldsymbol{\rho}^{\mathrm{in}} |\boldsymbol{p}|^4), \quad h^d \operatorname{Tr}(\boldsymbol{\rho}^{\mathrm{in}} |x|^4), \quad \textit{and} \quad \|\boldsymbol{\rho}^{\mathrm{in}}\|_{\mathcal{L}^d} \tag{1.18}$$

are uniformly bounded in $\hbar$. Let (f, F) be the solutions of the system (1.17) with initial conditions $(f^{\mathrm{in}}, F^{\mathrm{in}})$, which are probability density functions defined on $\mathbb{R}^{2d}$ and $\mathbb{R}^{2d} \times \mathbb{R}^{2d}$, respectively, and such that

$$\int_{\mathbb{R}^{2d}} |z|^2 f^{\mathrm{in}}(z)\, \mathrm{d}z < \infty \quad \textit{and} \quad \iint_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} (|z_1|^2 + |z_2|^2) F^{\mathrm{in}}(z_1, z_2)\, \mathrm{d}z_1\, \mathrm{d}z_2 < \infty.$$

Then, there exist a constant C dependent on $\|K\|_{C^2}$ and the semiclassical Schatten norms of $\boldsymbol{\rho}^{\mathrm{in}}$ but independent of N and $\hbar$ such that, for any $t \geq 0$,

$$\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho})^2 + \mathrm{W}_{2,\hbar}(F, \boldsymbol{\rho}_\alpha)^2 \leq \left(\mathrm{W}_{2,\hbar}(f^{\mathrm{in}}, \boldsymbol{\rho}^{\mathrm{in}})^2 + \mathrm{W}_{2,\hbar}(F^{\mathrm{in}}, \boldsymbol{\rho}_\alpha^{\mathrm{in}})^2 + \hbar \right) e^{Ce^{Ct}}. \tag{1.19}$$

Remark 1.1. The optimal transport pseudo-metrics that are used in the above theorem are not distances since $\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho}) \geq d\,\hbar$ (see [25]). However, they still imply convergence in the semiclassical regime $\hbar \to 0$. More precisely, introducing the Wigner transform

$$f_{\boldsymbol{\rho}}(\chi, \xi) = \int_{\mathbb{R}^d} e^{-i\xi\cdot y/\hbar} \boldsymbol{\rho}(\chi + \frac{y}{2}, \chi - \frac{y}{2})\, \mathrm{d}y, \tag{1.20}$$

and the Husimi transform $\tilde{f_{\boldsymbol{\rho}}} = g_h * f_{\boldsymbol{\rho}}$ with $g_h(z) = (\pi\hbar)^{-d} e^{-|z|^2/\hbar}$, it holds (see [23, Theorem 2.4])

$$\mathrm{W}_2(f, \tilde{f_{\boldsymbol{\rho}}})^2 \leq \mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho})^2 + d\,\hbar,$$

and so, convergence of $\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho})$ to 0 implies the convergence of the Husimi transform of $\boldsymbol{\rho}$ (and so, also its Wigner transform, see [42]) to f with respect to the classical Wasserstein distance W_2. On the other hand, the right-hand side of inequality (1.19) is also small initially and, if the operator $\boldsymbol{\rho}$ is sufficiently regular, $\tilde{f_{\boldsymbol{\rho}}}$ is close to f, as follows from the following inequality which follows from [37, Theorem 1.1] and [24, Theorem 3.5]:

$$\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho}) \leq \mathrm{W}_2(f, \tilde{f_{\boldsymbol{\rho}}}) + \sqrt{d\hbar} + D_{\boldsymbol{\rho}}\,\hbar,$$

where $D_{\boldsymbol{\rho}} = \|\nabla f_{\sqrt{\boldsymbol{\rho}}}\|_{L^2(\mathbb{R}^{2d})}$ is proportional to the Wigner–Yanase skew information of $\boldsymbol{\rho}$.

Remark 1.2. The double-exponential growth on the right-hand side of (1.19) is due to the propagation of the Schatten norm $\mathcal{L}^d$ for $\boldsymbol{\rho}$. We can get a better bound in terms of time dependence in the regime where Nh^d is of order 1. Indeed, in this case, $\|\boldsymbol{\rho}\|_{\mathcal{L}^d} \leq 1$ and then the $e^{Ce^{Ct}}$ can be replaced by a function of the form $e^{\Lambda(t)}$ for some polynomial function Λ.

Remark 1.3. The restriction on the dimension in Theorem 1.1 arises from the proofs presented in Section 3, which are of a purely technical nature. However, for the purposes of the application discussed in Section 4, we are primarily concerned with the case $d = 3$.

In the next theorem, we consider semiclassical regimes, which allow us to obtain a nontrivial order $1/N$ two-body interaction effect correction to the dynamics of F.

Theorem 1.2. *Under the same assumptions as in Theorem 1.1 but with $Nh \to 0$ and (f, F) solutions of the system (1.14), let $\mathrm{Tr}(|\alpha^{\mathrm{in}}|^2) \leq C(Nh)^2$. Then, there exist T and C_T, independent of $\hbar$ and N but dependent on $\|\nabla^2 K\|_{L^\infty}$ and the semiclassical Schatten norms of $\boldsymbol{\rho}^{\mathrm{in}}$, such that, for any $t \in [0, T]$,*

$$\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho})^2 + \mathrm{W}_{2,\hbar}(F, \boldsymbol{\rho}_\alpha)^2 \leq C_T\big(\mathrm{W}_{2,\hbar}(f^{\mathrm{in}}, \boldsymbol{\rho}^{\mathrm{in}})^2 + \mathrm{W}_{2,\hbar}(F^{\mathrm{in}}, \boldsymbol{\rho}_\alpha^{\mathrm{in}})^2 + \hbar\big). \tag{1.21}$$

Remark 1.4. In this paper, the regime $Nh \to 0$ is purely mathematical. This regime allows us to capture the next order $1/N$ correction as seen in system (1.14), but this requires an assumption on the size of $\mathrm{Tr}(|\alpha^{\mathrm{in}}|^2)$, which is technical and due to Proposition 2.2.

Remark 1.5. As an immediate consequence of Theorem 1.1 and the main result of Marcantoni et al. in [43, Theorem 3.3], we establish a global-in-time joint semiclassical and mean-field approximation of the dynamics of a system of spin-$\frac{1}{2}$ fermions with quasi-free initial data that are close to Slater determinant-like states by solutions of the Vlasov equation. In particular, we establish the convergence in some negative Sobolev space. See Theorem 4.2 in Section 4.

1.4. Previous known results

As the BdG equation (1.5) can be seen as a generalization of the Hartree–Fock equation, we briefly review the literature concerning the semiclassical limit from the Hartree–Fock equation to the Vlasov equation. Equation (1.12) can be seen as the semiclassical approximation of a system of many interacting quantum particles, as pointed out in the pioneering works by Narnhofer and Sewell [45] and by Spohn [49] where the Vlasov equation was obtained directly from the many-body Schrödinger equation with smooth interaction in the combined mean-field and semiclassical regime. This has been reconsidered in [27] and more recently in [10, 13], where the case of the Coulomb potential with a N dependent cut-off has been addressed. Moreover, a combined mean-field and semiclassical limit for particles interacting via the Coulomb potential has been treated in [26] for factorized initial data whose first marginal is given by a monokinetic Wigner measure (that can be seen as the Klimontovich solutions to the Vlasov equation), which leads to the pressureless Euler–Poisson system.

Most of the above-mentioned works rely on compactness methods that do not allow for an explicit bound on the rate of convergence, which is essential for applications. For this reason, the Hartree equation (1.9) has been considered as an intermediate step to decouple the problem into two separate parts, namely, to prove the convergence of the mean-field limit from the many-body Schrödinger equation towards the Hartree equation, and then the semiclassical limit from the Hartree equation to the Vlasov equation. In this paper, we are interested in the latter problem, which has been largely studied in different settings. It was first proven by Lions and Paul in [42], and later in [19,44], that the Wigner transforms of the solutions of the Hartree equation (1.9) converge in some weak sense to solutions of the Vlasov–Poisson equation. Quantitative rates of convergence were then obtained, first in the case when the Coulomb potential is replaced by a smoother potential, in Lebesgue-type norms [1–3,6] and in a quantum analogue of the Wasserstein distances [23]. The case of singular interactions was then treated in [35, 36] with the same quantum Wasserstein distances, and in [39, 46, 47] in Lebesgue-type norms. In particular, for $K = |x|^{-1}$, the explicit rate has been established in [34, 35] for the weak topology and in [39, 46] for the Schatten norms.

In a different setting, the semiclassical limit has also been studied for local perturbations of stationary states in the case of infinite gases in [41].

The BdG equation is known to offer a self-consistent field description of a system of fermionic particles (See [15]). The global well-posedness in the energy space of the time-dependent BdG equation in $\mathbb{R}^3$, with potential U including the Coulomb potential and $\hbar$ fixed, can be found in [7]. This result was subsequently improved in [18] to include positive singular potentials up to and including

$$U(x) = |x|^{-2+\varepsilon} \quad \text{for } 0 < \varepsilon \leq 2,$$

via techniques from dispersive PDE theory. In fact, well-posedness and finite-time blowup of solutions to the BdG equation in energy space with a pseudo-relativistic kinetic energy were discussed prior in [31, 40]. For completeness, let us also mention the fact that the well-posedness theory of a related system of coupled equations, also called the time-dependent Hartree–Fock–Bogoliubov equations in the "spinless bosonic" setting, was first studied locally in time in [28–30] for the pure-state case and improved to global-in-time results along with obtaining global-in-time dispersive estimates in [11, 12, 14, 33]. The equations were also studied in the mixed-state case in [4].

It is also worth mentioning that the Hartree–Fock–Bogoliubov equations were recently obtained in [43] as the mean-field approximation of a system of N interacting fermions with initial state close to quasi-free states with non-zero pairing operator. For the associated equilibrium problem, namely, the study of the Hartree–Fock–Bogoliubov functional and its connection to BCS theory of superconductivity and superfluidity, we refer to the review papers [5, 32] and references therein.

1.5. Plan of the paper

The rest of the paper is organized as follows. In Section 2, we present the outline of the proof, give a useful equivalent formulation of the BdG equation, and present some preliminary estimates. Section 3 is devoted to the proof of the main results, while Section 4 provides an application of Theorem 1.1 in the setting of the work [43] about mean-field theory for interacting fermionic systems with non-zero pairing.

2. The strategy: Semiclassical Bogoliubov–de Gennes equation

In this section, we present the strategy of the proof, which relies on an ad hoc rewriting of the BdG equation (1.5) in the form (2.6), representing the main novelty of our approach.

We first recall that the case of the zero pairing relies on Dirac's correspondence principles, which in particular tell that if two quantum observables A and B correspond to classical observables $a(\chi, \xi)$ and $b(\chi, \xi)$, then their scaled commutator $\frac{1}{i\hbar}[A, B]$ should correspond to the Poisson bracket $\{a, b\} = \nabla_x a \cdot \nabla_\xi b - \nabla_\xi a \cdot \nabla_x b$, and that one should recover the classical dynamics in the limit $h \to 0$. It is indeed easy to see that the Vlasov equation (1.12) can be written in terms of Poisson brackets as $\partial_t f = \{H_f, f\}$, where

$$H_f = \frac{|\xi|^2}{2} + V_f.$$

Hence, with the observation that the exchange term (1.11) vanishes as $h \to 0$, one expects that the Hartree–Fock evolution (1.9) converges to the Vlasov dynamics (1.12) for h small, which can be proved using the Wigner transform, as is done in the literature mentioned in Section 1.4.

In the case of non-zero pairing, the semiclassical approximation of the BdG equation is less clear. The main difficulty comes from the fact that the correspondence principle of quantum mechanics is not immediately applicable to the pairing operator. Our strategy consists in recasting the problem for γ and α in terms of the positive self-adjoint density operators $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_\alpha$ and consider their time evolution.

2.1. Rescaling the BdG equation

To study the semiclassical limit of the pairing operator, we start by noticing from conditions (1.2) that it follows

$$\theta_\alpha := \frac{1}{N} \operatorname{Tr}(|\alpha|^2) \leq 1 - N h^d \|\boldsymbol{\rho}\|_{\mathfrak{L}^2}^2 \in [0, 1). \tag{2.1}$$

To better understand α, it is more natural to consider its integral kernel and view the kernel as a two-particle wave function. Hence, assuming $\alpha \neq 0$, we define the normalized pairing wave function as

$$\Psi_\alpha(x_1, x_2) := \frac{1}{\|\alpha\|_{L^2}} \alpha(x_1, x_2).$$

Following our scaling convention of γ and identity (1.2), it is suggestive to consider the rescaled projection operator acting on $\mathfrak{h} \otimes \mathfrak{h}$ and its normalization

$$\mathsf{A}_\alpha := \frac{1}{N h^{2d}} |\alpha\rangle\langle\alpha| \quad \text{and} \quad \boldsymbol{\rho}_\alpha := h^{-2d} |\Psi_\alpha\rangle\langle\Psi_\alpha| .$$

Clearly, $\mathsf{A}_\alpha = \theta_\alpha \boldsymbol{\rho}_\alpha$ and $\boldsymbol{\rho}_\alpha$ satisfies the normalization $h^{2d} \operatorname{Tr}(\boldsymbol{\rho}_\alpha) = 1$.

To make connection with classical phase space dynamics, we need to recast the BdG equation in terms of the rescaled operators $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_\alpha$. Define X_α by expression (1.11) and notice that $\mathsf{X}_\alpha \alpha^* = N h^{2d} \theta_\alpha \operatorname{Tr}_2(K_{12} \boldsymbol{\rho}_\alpha)$, which then implies

$$\mathsf{X}_\alpha \alpha^* - \alpha \mathsf{X}_\alpha^* = N h^{2d} \theta_\alpha \operatorname{Tr}_2([K_{12}, \boldsymbol{\rho}_\alpha]) =: N h^d \theta_\alpha [K_{12}, \boldsymbol{\rho}_\alpha]_{:1}. \tag{2.2}$$

Here, $\operatorname{Tr}_2(\cdot)$ denotes the partial trace with respect to the second Hilbert space and K_{12} denotes the operator of multiplication by $K(x_1 - x_2)$ on $\mathfrak{h} \otimes \mathfrak{h}$. Hence, we see that equation (1.5a) has the form

$$i\hbar\, \partial_t \boldsymbol{\rho} = [\mathsf{H}_{\boldsymbol{\rho}}, \boldsymbol{\rho}] + \theta_\alpha \left[\frac{1}{N} K_{12}, \boldsymbol{\rho}_\alpha\right]_{:1},$$

where $\mathsf{H}_{\boldsymbol{\rho}}$ is defined as in equation (1.9).

To rewrite equation (4.16b), we view $\alpha = \alpha(x_1, x_2)$ as a two-body wave function as opposed to it being a Hilbert–Schmidt operator. Then, the equation has the form

$$\begin{aligned} i\hbar\,\partial_t \alpha(x_1,x_2) &= \Big(-\frac{\hbar^2}{2}\Delta_{x_1} - \frac{\hbar^2}{2}\Delta_{x_2} + \frac{1}{N}K(x_1-x_2)\Big)\alpha(x_1,x_2) \\ &\quad + h^d \int_{\mathbb{R}^d} (K(x_1-y)+K(y-x_2))\boldsymbol{\rho}(y,y)\alpha(x_1,x_2)\,\mathrm{d}y \\ &\quad - h^d \int_{\mathbb{R}^d} (K(x_1-y)+K(y-x_2))\boldsymbol{\rho}(x_1,y)\alpha(y,x_2)\,\mathrm{d}y \\ &\quad - h^d \int_{\mathbb{R}^d} (K(x_1-y)+K(y-x_2))\boldsymbol{\rho}(x_2,y)\alpha(x_1,y)\,\mathrm{d}y, \end{aligned} \tag{2.3}$$

or more compactly

$$i\hbar\,\partial_t \alpha = \Big(\mathsf{H}_{12} + \frac{1}{N}K_{12}\Big)\alpha - h^d \boldsymbol{\rho}_{12} K_{12}\alpha, \tag{2.4}$$

where $\boldsymbol{\rho}_{12} := \boldsymbol{\rho} \otimes \mathbf{1} + \mathbf{1} \otimes \boldsymbol{\rho}$ and $\mathsf{H}_{12} := \mathsf{H}_{\boldsymbol{\rho}} \otimes \mathbf{1} + \mathbf{1} \otimes \mathsf{H}_{\boldsymbol{\rho}}$.

To make connection with classical mechanics, it is better to consider the two-particle operator A_α instead of α. Using equation (2.4), it follows that A_α satisfies

$$i\hbar\,\partial_t \mathsf{A}_\alpha = \Big[\mathsf{H}_{12} + \frac{1}{N}K_{12}(\mathbf{1} - Nh^d\boldsymbol{\rho}_{12}),\, \mathsf{A}_\alpha\Big] - h^d[K_{12}, \boldsymbol{\rho}_{12}]\mathsf{A}_\alpha.$$

Since $\theta_\alpha = h^{2d}\,\mathrm{Tr}(\mathsf{A}_\alpha)$, taking the trace of the above equation yields

$$i\hbar\,\frac{\mathrm{d}}{\mathrm{d}t}\theta_\alpha = -h^d \langle [K_{12}, \boldsymbol{\rho}_{12}] \rangle_{\mathsf{A}_\alpha}, \tag{2.5}$$

where $\langle B \rangle_A := h^{2d}\,\mathrm{Tr}(AB)$ if A and B are operators acting on $L^2(\mathbb{R}^{2d})$. Finally, summarizing the above discussion and using the fact that $\mathsf{A}_\alpha = \theta_\alpha \boldsymbol{\rho}_\alpha$, we obtain the equations

$$i\hbar\,\partial_t \boldsymbol{\rho} = [\mathsf{H}_{\boldsymbol{\rho}}, \boldsymbol{\rho}] + \frac{\theta_\alpha}{N}[K_{12}, \boldsymbol{\rho}_\alpha]_{:1}, \tag{2.6a}$$

$$\begin{aligned} i\hbar\,\partial_t \boldsymbol{\rho}_\alpha &= \Big[\mathsf{H}_{12} + \frac{1}{N}K_{12}(\mathbf{1} - Nh^d\boldsymbol{\rho}_{12}), \boldsymbol{\rho}_\alpha\Big] \\ &\quad + h^d\big([K_{12}, \boldsymbol{\rho}_{12}] - \langle [K_{12}, \boldsymbol{\rho}_{12}] \rangle_{\boldsymbol{\rho}_\alpha}\big)\boldsymbol{\rho}_\alpha. \end{aligned} \tag{2.6b}$$

In particular, the traces of $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_\alpha$ are conserved.

Now, by the correspondence principle, one can expect, at least in the case when K is a sufficiently regular potential, that $F(z_{12}) = F(z_1, z_2) := F_{\boldsymbol{\rho}_\alpha}(z_1, z_2)$ defined on $\mathbb{R}^{2d} \times \mathbb{R}^{2d}$ solves in the limit $\hbar \to 0$ and $N \to \infty$

$$\partial_t F + \xi_{12} \cdot \nabla_{\chi_{12}} F + E_{12} \cdot \nabla_{\xi_{12}} F = 0,$$

where $\xi_{12} = (\xi_1, \xi_2)$ and $E_{12} := (E_f(\chi_1), E_f(\chi_2))$ with

$$E_f(\chi) := -\nabla V_f \quad \text{and} \quad V_f(\chi) = \iint_{\mathbb{R}^{2d}} K(\chi - \chi_1) f(z_1)\, \mathrm{d}z_1.$$

In fact, if $Nh^d \ll 1$, then, to the order $1/N$, we expect to have

$$\begin{aligned} i\hbar\, \partial_t \boldsymbol{\rho} &= [\mathsf{H}_{\boldsymbol{\rho}}, \boldsymbol{\rho}] + \frac{\theta_\alpha}{N} [K_{12}, \boldsymbol{\rho}_\alpha]_{:1}, \\ i\hbar\, \partial_t \boldsymbol{\rho}_\alpha &= \left[\mathsf{H}_{12} + \frac{1}{N} K_{12}, \boldsymbol{\rho}_\alpha\right] \end{aligned}$$

as the leading order dynamics; that is, formally, when $\hbar \to 0$, we have that

$$\partial_t f + \xi \cdot \nabla_\chi f + E_f \cdot \nabla_\xi f = \frac{\theta_\alpha}{N} \int_{\mathbb{R}^{2d}} \nabla K(\chi - \chi_2) \cdot \nabla_\xi F(z, z_2)\, \mathrm{d}z_2, \tag{2.7a}$$

$$\partial_t F + \xi_{12} \cdot \nabla_{\chi_{12}} F + E_{12} \cdot \nabla_{\xi_{12}} F = \frac{1}{N} \nabla K(\chi_1 - \chi_2) \cdot (\nabla_{\xi_1} - \nabla_{\xi_2}) F. \tag{2.7b}$$

Remark 2.1. As already pointed out in Remark 1.1, estimates in the semiclassical optimal transport distance give accuracy up to $\hbar$ since $\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho})^2 \geq d\hbar$. In particular, the terms on the right-hand side of equations (2.7) with the $1/N$ in front are meaningful only if $h \ll 1/N$, which is allowed from some semiclassical regime but does not include, for instance, the regime $Nh^d = 1$.

2.2. Conservation laws and a priori estimates

As indicated in the previous discussion, if $(\boldsymbol{\rho}, \boldsymbol{\rho}_\alpha)$ solves system (2.6), then it follows that

$$h^d\, \mathrm{Tr}_{\mathfrak{h}}(\boldsymbol{\rho}) = 1 \quad \text{and} \quad h^{2d}\, \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}(\boldsymbol{\rho}_\alpha) = 1 \tag{2.8}$$

hold for all $t \geq 0$ provided the identities hold at initial time. Define the one-particle density operator (first marginal) associated to $\boldsymbol{\rho}_\alpha$ by

$$\boldsymbol{\rho}_{\alpha:1} := h^d\, \mathrm{Tr}_2(\boldsymbol{\rho}_\alpha) = \frac{1}{Nh^d\theta_\alpha} |\alpha^*|^2 \geq 0. \tag{2.9}$$

In light of the semiclassical scaling, the last inequality in formula (1.2) gives

$$Nh^d \boldsymbol{\rho}^2 + \theta_\alpha \boldsymbol{\rho}_{\alpha:1} \leq \boldsymbol{\rho}, \tag{2.10}$$

which is preserved by the BdG dynamics. As an immediate consequence, we have

$$0 \leq \theta_\alpha \boldsymbol{\rho}_{\alpha:1} \leq \boldsymbol{\rho} \leq \frac{1}{Nh^d} \mathbf{1}. \tag{2.11}$$

Moreover, since $\boldsymbol{\rho}_\alpha = h^{-2d}\, |\Psi_\alpha\rangle\langle\Psi_\alpha|$ is a rank one operator, it verifies $0 \leq \boldsymbol{\rho}_\alpha \leq h^{-2d}\mathbf{1}$. The right-hand side inequality is sharp, and more generally, $\|\boldsymbol{\rho}_\alpha\|_{\mathfrak{L}^p} = h^{-2d/p'}$.

As proved, for instance, in [7], the following energy functional is conserved:

$$\mathcal{E} := h^d \operatorname{Tr}(|\boldsymbol{p}|^2\boldsymbol{\rho}) + \frac{1}{2}\int_{\mathbb{R}^d} V_{\boldsymbol{\rho}}\, \rho - \frac{h^{2d}}{2}\operatorname{Tr}(\mathsf{X}_{\boldsymbol{\rho}}\boldsymbol{\rho}) + \frac{\theta_\alpha}{N} h^{2d}\operatorname{Tr}(K_{12}\boldsymbol{\rho}_\alpha). \tag{2.12}$$

In particular, if $K \in L^\infty$ and the energy is initially bounded uniformly in $\hbar$, then the kinetic energy of $\boldsymbol{\rho}$ is bounded uniformly in $\hbar$ and time, and more precisely,

$$h^d \operatorname{Tr}(|\boldsymbol{p}|^2\boldsymbol{\rho}) \le \mathcal{E} + \left(1 + \frac{\theta_\alpha}{N}\right)\|K\|_{L^\infty} \le \mathcal{E} + 2\|K\|_{L^\infty} =: C_{\mathcal{E},K}. \tag{2.13}$$

Moments of order 2 of $\boldsymbol{\rho}_{\alpha:1}$ are also bounded uniformly in $\hbar$ and time by the energy since by formula (2.11)

$$\theta_\alpha h^d \operatorname{Tr}(\boldsymbol{\rho}_{\alpha:1}|\boldsymbol{p}|^2) \le h^d \operatorname{Tr}(\boldsymbol{\rho}|\boldsymbol{p}|^2) \le C_{\mathcal{E},K}.$$

For the two-particle density operator $\boldsymbol{\rho}_\alpha$, this can be written as $h^{2d}\operatorname{Tr}(\boldsymbol{\rho}_\alpha|\boldsymbol{p}_1|^2) \le C_{\mathcal{E},K}$, where $\boldsymbol{p}_1$ is the momentum operator acting on the first variable. By symmetry, the same is true by replacing $\boldsymbol{p}_1$ by $\boldsymbol{p}_2$, and so, we deduce that

$$\theta_\alpha h^{2d}\operatorname{Tr}\big(\boldsymbol{\rho}_\alpha(|\boldsymbol{p}_1|^2 + |\boldsymbol{p}_2|^2)\big) \le C_{\mathcal{E},K}.$$

We can propagate higher-order moments. In our case, it will be sufficient to propagate order 4 moments, as shown in the following proposition.

Proposition 2.1. *Let $(\boldsymbol{\rho}, \boldsymbol{\rho}_\alpha)$ be a solution of the BdG equation (2.6), and*

$$M_n := h^d \operatorname{Tr}(\boldsymbol{\rho}|\boldsymbol{p}|^n) \quad \text{and} \quad N_n := h^d \operatorname{Tr}(\boldsymbol{\rho}|x|^n)$$

denote the velocity and position moments of order $n \in \mathbb{N}$ of the operator $\boldsymbol{\rho}$. Then, for any $t \ge 0$,

$$\begin{aligned} M_2(t) &\le C_{\mathcal{E},K}, & M_4(t)^{1/2} &\le M_4(0)^{1/2} + C_K t, \\ N_2(t)^{1/2} &\le N_2(0)^{1/2} + C_{\mathcal{E},K}^{1/2} t, & N_4(t)^{1/4} &\le 1 + N_4(0)^{1/4} + C\,\hbar^3 t + C\big(M_4(0)^{1/2} + t\big)^{3/2}, \end{aligned}$$

where $C_K = 3(\hbar\|\Delta K\|_{L^\infty} + 2\|\nabla K\|_{L^\infty}\sqrt{C_{\mathcal{E},K}})$ and C only depends on d and C_K.

Proof. To simplify the computations, we write the evolution equation for $\boldsymbol{\rho}$ given by equation (2.6a) in the form

$$i\hbar\,\partial_t\boldsymbol{\rho} = \frac{1}{2}[|\boldsymbol{p}|^2, \boldsymbol{\rho}] + [K_{12}, \boldsymbol{\mu}]_{:1} \quad \text{with } \boldsymbol{\mu} = \boldsymbol{\rho}^{\otimes 2}(\mathbf{1} - \mathsf{X}_{12}) + \frac{\theta_\alpha}{N}\boldsymbol{\rho}_\alpha,$$

where X_{12} is the operator that exchanges the first and second coordinate; that is, for any $\varphi \in \mathfrak{h}\otimes\mathfrak{h}$, $\mathsf{X}_{12}\varphi(x_1, x_2) = \varphi(x_2, x_1)$. Observe that $\boldsymbol{\mu}$ is self-adjoint. Then, it follows from the cyclicity of the trace that

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}M_4 = h^{2d}\operatorname{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big([K_{12}, \boldsymbol{\mu}]|\boldsymbol{p}_1|^4\big) = h^{2d}\operatorname{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big(\boldsymbol{\mu}[|\boldsymbol{p}_1|^4, K_{12}]\big).$$

By Leibniz formula for commutators, $[|\boldsymbol{p}_1|^4, K_{12}] = |\boldsymbol{p}|^2[|\boldsymbol{p}_1|^2, K_{12}] + [|\boldsymbol{p}_1|^2, K_{12}]|\boldsymbol{p}|^2$, and so, since $\boldsymbol{\mu}$ is self-adjoint, it gives

$$\hbar \frac{\mathrm{d}}{\mathrm{d}t} M_4 = 2h^{2d} \operatorname{Im} \operatorname{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big(\boldsymbol{\mu}|\boldsymbol{p}_1|^2[|\boldsymbol{p}_1|^2, K_{12}]\big).$$

Since $[\boldsymbol{p}_1, K_{12}] = -i\hbar\nabla K_{12}$, where ∇K_{12} denotes the operator of multiplication by $\nabla K(x_1 - x_2)$, it follows that

$$[|\boldsymbol{p}_1|^2, K_{12}] = -i\hbar(\boldsymbol{p}_1 \cdot \nabla K_{12} + \nabla K_{12} \cdot \boldsymbol{p}_1) = -\hbar^2 \Delta K_{12} - 2i\hbar\nabla K_{12} \cdot \boldsymbol{p}_1,$$

and so, it follows from the cyclicity and Hölder's inequality for the trace that

$$\frac{\mathrm{d}}{\mathrm{d}t} M_4 \leq 2\hbar\|\Delta K\|_{L^\infty}\|\boldsymbol{\mu}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})} + 4\|\nabla K\|_{L^\infty}\|\boldsymbol{p}_1\boldsymbol{\mu}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})}. \tag{2.14}$$

Now, we decompose $\boldsymbol{\mu}$ into the three terms that define it and use the triangle inequality for the trace norm. Notice indeed that for the first term we get

$$\begin{aligned}
&\|\boldsymbol{\rho}^{\otimes 2}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})} = \|\boldsymbol{\rho}|\boldsymbol{p}|^2\|_{\mathfrak{L}^1} \leq \|\sqrt{\boldsymbol{\rho}}\|_{\mathfrak{L}^2}\|\sqrt{\boldsymbol{\rho}}|\boldsymbol{p}|^2\|_{\mathfrak{L}^2} = M_4^{1/2},\\
&\|\boldsymbol{\rho}^{\otimes 2}\mathsf{X}_{12}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})} = \|\boldsymbol{\rho}^{\otimes 2}|\boldsymbol{p}_2|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})} = \|\boldsymbol{\rho}|\boldsymbol{p}|^2\|_{\mathfrak{L}^1} \leq M_4^{1/2},\\
&\|\boldsymbol{\rho}_\alpha|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})} \leq \|\sqrt{\boldsymbol{\rho}_\alpha}\|_{\mathfrak{L}^2}\|\sqrt{\boldsymbol{\rho}_\alpha}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^2} = h^d\big(\operatorname{Tr}_{\mathfrak{h}^{\otimes 2}}\big(\boldsymbol{\rho}_\alpha|\boldsymbol{p}_1|^4\big)\big)^{\frac{1}{2}} \leq \theta_\alpha^{-1/2} M_4^{1/2},
\end{aligned}$$

where the last inequality follows from inequality (2.11). Similarly, for the second term on the right-hand side of inequality (2.14), use the fact that, for $\boldsymbol{\nu} = \boldsymbol{\rho}^{\otimes 2}$, $\boldsymbol{\nu} = \boldsymbol{\rho}^{\otimes 2}\mathsf{X}_{12}$, or $\boldsymbol{\nu} = \theta_\alpha\boldsymbol{\rho}_\alpha$,

$$\|\boldsymbol{p}_1\boldsymbol{\nu}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^1(\mathfrak{h}^{\otimes 2})} \leq \|\boldsymbol{p}_1\boldsymbol{\nu}\|_{\mathfrak{L}^2(\mathfrak{h}^{\otimes 2})}\|\boldsymbol{\nu}|\boldsymbol{p}_1|^2\|_{\mathfrak{L}^2(\mathfrak{h}^{\otimes 2})} \leq M_2^{1/2} M_4^{1/2},$$

and this gives finally, since $N \geq 1$, $\theta_\alpha \leq 1$ and $M_2 \leq C_{\mathcal{E},K}$,

$$\frac{\mathrm{d}}{\mathrm{d}t} M_4 \leq 6\big(\hbar\|\Delta K\|_{L^\infty} + 2\|\nabla K\|_{L^\infty}\sqrt{C_{\mathcal{E},K}}\big)\sqrt{M_4},$$

from which the result follows by Grönwall's lemma.

The propagation of position moments follows just by writing for $n = 2$ or $n = 4$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t} N_n = \frac{1}{2}\operatorname{Tr}([|\boldsymbol{p}|^2, \boldsymbol{\rho}]|x|^n) = \frac{1}{2}\operatorname{Tr}(\boldsymbol{\rho}[|x|^n, |\boldsymbol{p}|^2]).$$

Therefore, since $\frac{1}{i\hbar}[|x|^2, |\boldsymbol{p}|^2] = 2(x \cdot \boldsymbol{p} + \boldsymbol{p} \cdot x)$, it follows from Hölder's inequality for Schatten norms that

$$\frac{\mathrm{d}}{\mathrm{d}t} N_2 = 2 \operatorname{Re}\operatorname{Tr}(\boldsymbol{\rho} x \cdot \boldsymbol{p}) \leq 2M_2^{1/2} N_2^{1/2},$$

which yields the inequality for N_2 by Grönwall's lemma. On the other hand, it follows from [36, Lemma 3.2] that

$$\frac{\mathrm{d}}{\mathrm{d}t}(1 + N_4) = 2 \operatorname{Re}\operatorname{Tr}(\boldsymbol{\rho}|x|^2(x \cdot \boldsymbol{p} + \boldsymbol{p} \cdot x)) \leq C\big(M_4^{1/4} N_4^{3/4} + \hbar N_2\big).$$

By Hölder's inequality for Schatten norm, the fact that $N_0 = 1$, and Young's inequality for the product, $\hbar N_2 \leq \hbar N_4^{1/2} \leq \hbar^3 + N_4^{3/4}$, it gives a differential inequality for $y(t) = 1 + N_4(t)$ of the form

$$y' \leq C\big(M_4^{1/4} + \hbar^3\big) y^{3/4},$$

which again leads to the result by Grönwall's lemma. ∎

In the remainder of the section, we obtain uniform-in-$\hbar$ estimate for the semiclassical Schatten norms for $\boldsymbol{\rho}$ along the BdG dynamics in the case of bounded potential K for different semiclassical scaling regimes.

Proposition 2.2. *Let $\widehat{K} \in L^1$. Suppose that $\boldsymbol{\rho} = \boldsymbol{\rho}(t)$ is a solution to equation (2.6a) with $\boldsymbol{\rho}(0) = \boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^p$. We have the following.*

(i) *In a regime where $N\hbar \geq C$ holds for some fixed $C > 0$, independent of N and $\hbar$, then there exists $C_K > 0$, dependent only on K, such that we have the estimate*

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \|\boldsymbol{\rho}^{\mathrm{in}}\|_{\mathcal{L}^p} e^{C_K t}.$$

(ii) *If $\theta_\alpha^{\mathrm{in}} \leq C N h^{2d/p}$ for some constant C independent of $\hbar$, then there exists $C > 0$ independent of $\hbar$ such that, for any $t \in [0, T]$ with $T = C h^{1-d/p}$,*

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} \leq C \quad \textit{and} \quad \theta_\alpha \leq C N h^{2d/p}. \tag{2.15}$$

Proof. By equation (2.6a), we have

$$\frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\rho}\|_{\mathcal{L}^p}^p = \frac{h^d}{p}\frac{\mathrm{d}}{\mathrm{d}t}\operatorname{Tr}(\boldsymbol{\rho}^p) = \frac{2}{N^2\hbar}\operatorname{Im}\operatorname{Tr}(\boldsymbol{\rho}^{p-1}\mathsf{X}_\alpha\alpha^*). \tag{2.16}$$

Therefore, by Hölder's inequality, we obtain the bound

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \frac{4\pi}{N^2 h^{d+1}}\|\mathsf{X}_\alpha\|_{\mathcal{L}^{2p}}\|\alpha^*\|_{\mathcal{L}^{2p}}.$$

Now, it follows from the formula

$$\mathsf{X}_\alpha = \int_{\mathbb{R}^d} \widehat{K}(\omega) e_\omega \alpha e_{-\omega}\,\mathrm{d}\omega,$$

where e_ω is the operator of multiplication by the function $e_\omega(x) = e^{-2i\pi\omega\cdot x}$ that

$$\|\mathsf{X}_\alpha\|_{\mathcal{L}^{2p}} \leq C_K\|\alpha\|_{\mathcal{L}^{2p}}, \tag{2.17}$$

where $C_K = \|\widehat{K}\|_{L^1}$. Therefore, by definition (2.9) and inequality (2.11), we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \frac{2C_K}{N\hbar}\|\theta_\alpha\boldsymbol{\rho}_{\alpha:1}\|_{\mathcal{L}^p} \leq \frac{2C_K}{N\hbar}\|\boldsymbol{\rho}\|_{\mathcal{L}^p}, \tag{2.18}$$

and Part (i) follows from Grönwall's lemma.

To prove Part (ii), we will also need to study the size of θ_α along the BdG dynamics. By equation (2.5), cyclicity of the trace, symmetry of $\boldsymbol{\rho}_\alpha$ and K_{12}, and equation (2.2), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta_\alpha = \frac{8\pi h^{d-1}}{N}\operatorname{Im}\operatorname{Tr}(\boldsymbol{\rho}\mathsf{X}_\alpha\alpha^*).$$

Again, using Hölder's inequality and inequality (2.17), we get that

$$\frac{\mathrm{d}}{\mathrm{d}t}\theta_\alpha \leq \frac{4C_K}{N\hbar}\|\boldsymbol{\rho}\|_{\mathfrak{L}^p}\|\alpha\|^2_{\mathfrak{L}^{2p'}} \leq 8\pi C_K h^{d-1}\theta_\alpha\|\boldsymbol{\rho}\|_{\mathfrak{L}^p}\|\boldsymbol{\rho}_{\alpha:1}\|_{\mathfrak{L}^{p'}}. \tag{2.19}$$

Applying the Schatten space embedding inequality

$$\|\boldsymbol{\rho}_{\alpha:1}\|_{\mathfrak{L}^p} \leq h^{-d/p}\|\boldsymbol{\rho}_{\alpha:1}\|_{\mathfrak{L}^1} = h^{-d/p},$$

to the first inequality in formula (2.18) and to inequality (2.19) yields the following system of differential inequalities:

$$\begin{cases} u' \leq Av, \\ v' \leq auv, \end{cases}$$

where $u(t) = \|\boldsymbol{\rho}(t)\|_{\mathfrak{L}^p}$ and $v(t) = \theta_\alpha(t)$ with $A = \frac{4\pi C_K}{Nh^{1+d/p}}$ large and $a = 8\pi C_K h^{d/p-1}$ small. Setting $U(t) = u(t/a)$ and $V(t) = \frac{A}{a}v(t/a)$, it can be written as

$$\begin{cases} U' \leq V, \\ V' \leq UV. \end{cases}$$

It implies, for instance, that

$$(U^2+V)' = 3UV \leq U^3 + 2V^{3/2} \leq 2(U^2+V)^{3/2}.$$

Hence,

$$(U(t)^2+V(t))^{-1/2} \geq (U(0)^2+V(0))^{-1/2} - t;$$

that is,

$$\|\boldsymbol{\rho}\|^2_{\mathfrak{L}^p} + A\theta_\alpha/a \leq \frac{\|\boldsymbol{\rho}^{\mathrm{in}}\|^2_{\mathfrak{L}^p} + A\theta^{\mathrm{in}}_\alpha/a}{\big(1-\big(\|\boldsymbol{\rho}^{\mathrm{in}}\|^2_{\mathfrak{L}^p} + A\theta^{\mathrm{in}}_\alpha/a\big)^{1/2}at\big)^2},$$

and formula (2.15) follows from the fact that

$$\frac{a}{A} = 2Nh^{2d/p}. \qquad \blacksquare$$

3. Proof of the main results

In this section, we prove Theorems 1.1 and 1.2, and so, we will estimate the semiclassical optimal transport pseudo-metric between solutions of the BdG equation (2.6) and the corresponding proposed classical coupled equations (1.17) or (1.14).

3.1. A dynamics for the couplings

A coupling associated to F and $\boldsymbol{\rho}_\alpha$ is a measurable function

$$\boldsymbol{\Upsilon} : (z_1, z_2) \mapsto \boldsymbol{\Upsilon}(z_1, z_2)$$

defined for almost all $(z_1, z_2) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d}$ with values in the space of bounded linear operators acting on $\mathfrak{h} \otimes \mathfrak{h}$ such that, for almost all $(z_1, z_2) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d}$, $\boldsymbol{\Upsilon}(z_1, z_2) \geq 0$ and

$$h^{2d} \operatorname{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}(\boldsymbol{\Upsilon}(z_1, z_2)) = F(z_1, z_2) \quad \text{and} \quad \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} \boldsymbol{\Upsilon}(z_1, z_2)\, \mathrm{d}z_1\, \mathrm{d}z_2 = \boldsymbol{\rho}_\alpha.$$

Then, the semiclassical optimal transport pseudo-metric between F and $\boldsymbol{\rho}_\alpha$ is

$$\mathrm{W}_{2,\hbar}(F, \boldsymbol{\rho}_\alpha) := \left(\inf_{\boldsymbol{\gamma}\in\mathcal{C}(F,\boldsymbol{\rho}_\alpha)} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}(\boldsymbol{C}(z_1, z_2)\boldsymbol{\Upsilon}(z_1, z_2))\, \mathrm{d}z_1\, \mathrm{d}z_2 \right)^{\frac{1}{2}}, \tag{3.1}$$

where $\boldsymbol{C}(z_1, z_2) := \boldsymbol{c}(z_1) \otimes \mathbf{1} + \mathbf{1} \otimes \boldsymbol{c}(z_2)$, that is,

$$\begin{aligned} \boldsymbol{C}(z_1, z_2)\Psi(x_1, x_2) = {} & \left(|\chi_1 - x_1|^2 + |\xi_1 - \boldsymbol{p}_1|^2\right)\Psi(x_1, x_2) \\ & + \left(|\chi_2 - x_2|^2 + |\xi_2 - \boldsymbol{p}_2|^2\right)\Psi(x_1, x_2). \end{aligned}$$

For all $\boldsymbol{\gamma}^{\mathrm{in}} \in \mathcal{C}(f^{\mathrm{in}}, \boldsymbol{\rho}^{\mathrm{in}})$ and $\boldsymbol{\Upsilon}^{\mathrm{in}} \in \mathcal{C}(F^{\mathrm{in}}, \boldsymbol{\rho}_\alpha^{\mathrm{in}})$, let $(\boldsymbol{\gamma}, \boldsymbol{\Upsilon})$ be the solution to the Cauchy problem

$$\partial_t \boldsymbol{\gamma} = \{H_f, \boldsymbol{\gamma}\} + \frac{1}{i\hbar}[\mathsf{H}_{\boldsymbol{\rho}}, \boldsymbol{\gamma}] + \frac{1}{i\hbar}\frac{\theta_\alpha}{N} \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_2([K_{12}, \boldsymbol{\Upsilon}(z_1, z_2)])\, \mathrm{d}z_2 \tag{3.2a}$$

and

$$\begin{aligned} \partial_t \boldsymbol{\Upsilon} = {} & \{H_{f_{12}}, \boldsymbol{\Upsilon}\} + \frac{\eta}{N}\nabla K(\chi_1 - \chi_2)\cdot(\nabla_{\xi_1} - \nabla_{\xi_2})\boldsymbol{\Upsilon} \\ & + \frac{1}{i\hbar}\left[\mathsf{H}_{\boldsymbol{\rho}_{12}} + K_{12}\left(\frac{1}{N} - h^d\boldsymbol{\rho}_{12}\right), \boldsymbol{\Upsilon}\right] \\ & + \frac{h^d}{i\hbar}\left([K_{12}, \boldsymbol{\rho}_{12}] - \langle [K_{12}, \boldsymbol{\rho}_{12}]\rangle_{\boldsymbol{\rho}_\alpha}\right)\boldsymbol{\Upsilon} \end{aligned} \tag{3.2b}$$

with $(\boldsymbol{\gamma}(0), \boldsymbol{\Upsilon}(0)) = (\boldsymbol{\gamma}^{\mathrm{in}}, \boldsymbol{\Upsilon}^{\mathrm{in}})$ and $\eta \in \{0, 1\}$. More precisely, we will set $\eta = 0$ to prove Theorem 1.1 and $\eta = 1$ to prove Theorem 1.2. Notice that, in complete analogy with the well-posedness theory for the system (1.14a)–(1.14b), one deduces the existence of the coupling dynamics $(\boldsymbol{\gamma}, \boldsymbol{\Upsilon})$. It is then not difficult to see that, with the above equations, the property of being a coupling is kept along the dynamics (cf. [23, Lemma 5.1]).

3.2. Estimating the semiclassical optimal transport pseudo-metrics

Let us now define the quantities

$$\mathcal{E}_{\boldsymbol{\gamma}}(t) := \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1(\boldsymbol{c}(z_1)\boldsymbol{\gamma}(z_1))\, \mathrm{d}z_1, \tag{3.3}$$

$$\mathcal{E}_{\boldsymbol{\Upsilon}}(t) := \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}(\boldsymbol{C}(z_1,z_2)\boldsymbol{\Upsilon}(z_1,z_2))\, \mathrm{d}z_1\, \mathrm{d}z_2, \tag{3.4}$$

where $\operatorname{Tr}_1 = \operatorname{Tr}_{\mathfrak{h}}$ and $\operatorname{Tr}_{12} = \operatorname{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}$. Since $(\boldsymbol{\gamma}, \boldsymbol{\Upsilon})$ is a solution to the coupling Cauchy problem (3.2), one obtains the following equations:

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{E}_{\boldsymbol{\gamma}}(t)}{\mathrm{d}t} &= \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1\big(\{\boldsymbol{c}(z_1), H_f\}\boldsymbol{\gamma}(z_1)\big)\, \mathrm{d}z_1 && (3.5\text{a})\\
&\quad + \frac{1}{i\hbar}\int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1\Big([\boldsymbol{c}(z_1), \tfrac{1}{2}|\boldsymbol{p}|^2 + V_{\boldsymbol{\rho}}]\boldsymbol{\gamma}(z_1)\Big)\, \mathrm{d}z_1 && (3.5\text{b})\\
&\quad - \frac{h^d}{i\hbar}\int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1\big([\boldsymbol{c}(z_1), \mathsf{X}_{\boldsymbol{\rho}}]\boldsymbol{\gamma}(z_1)\big)\, \mathrm{d}z_1 && (3.5\text{c})\\
&\quad + \frac{1}{i\hbar}\frac{\theta_\alpha}{N}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big([\boldsymbol{c}(z_1)\otimes\mathbf{1}, K_{12}]\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2, && (3.5\text{d})
\end{aligned}$$

and using the fact that

$$\boldsymbol{C}(z_1,z_2)[K_{12},\boldsymbol{\rho}_{12}] - [\boldsymbol{C}(z_1,z_2), K_{12}\boldsymbol{\rho}_{12}] = \boldsymbol{C}(z_1,z_2)\boldsymbol{\rho}_{12}K_{12} - K_{12}\boldsymbol{\rho}_{12}\boldsymbol{C}(z_1,z_2),$$

we can write

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{E}_{\boldsymbol{\Upsilon}}(t)}{\mathrm{d}t} &= \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(\{\boldsymbol{C}(z_1,z_2), H_{f_{12}}\}\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 && (3.6\text{a})\\
&\quad + \frac{1}{i\hbar}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big([\boldsymbol{C}(z_1,z_2), \mathsf{H}_{\boldsymbol{\rho}_{12}}]\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 && (3.6\text{b})\\
&\quad - \frac{\eta}{N}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(\nabla_{\xi_{12}}\boldsymbol{C}(z_1,z_2)\cdot\nabla K_{\chi_{12}}\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 && (3.6\text{c})\\
&\quad + \frac{1}{i\hbar N}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big([\boldsymbol{C}(z_1,z_2), K_{12}]\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 && (3.6\text{d})\\
&\quad - \frac{2h^d}{\hbar}\operatorname{Im}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_{12}\boldsymbol{C}(z_1,z_2)\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 && (3.6\text{e})\\
&\quad - \frac{h^d}{i\hbar}\langle[K_{12},\boldsymbol{\rho}_{12}]\rangle_{\boldsymbol{\rho}_\alpha}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(\boldsymbol{C}(z_1,z_2)\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2. && (3.6\text{f})
\end{aligned}$$

3.2.1. Estimates for $\mathcal{E}_{\boldsymbol{\gamma}}$. To estimate the right-hand side of identity (3.5), let us focus on term (3.5c) since the first two terms are already handled in [23, Theorem 2.5]. For term (3.5c), we notice that

$$[|\chi - x|^2, \mathsf{X}_{\boldsymbol{\rho}}](x,y) = \frac{1}{2} K(x-y)((x-y) - 2(\chi - y)) \cdot (x-y) \boldsymbol{\rho}(x,y),$$

which yields the estimate

$$\begin{aligned} &\left| \frac{h^d}{i\hbar} \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1\big([|\chi_1 - x|^2, \mathsf{X}_{\boldsymbol{\rho}}] \boldsymbol{\gamma}(z_1)\big) \, \mathrm{d}z_1 \right| \\ &\qquad \leq C h^{d-1} \| |\cdot| K(\cdot) \|_{L^\infty} \| [x, \boldsymbol{\rho}] \|_{\mathfrak{L}^\infty} + C h^{d-1} \| K \|_{L^\infty} \| [x, \boldsymbol{\rho}] \|_{\mathfrak{L}^\infty} \mathcal{E}_{\boldsymbol{\gamma}}. \end{aligned} \tag{3.7}$$

Next, to estimate the part involving $[|\xi - \boldsymbol{p}|^2, \mathsf{X}_{\boldsymbol{\rho}}]$, recall the identity

$$\begin{aligned} [|\boldsymbol{p} - \xi|^2, \mathsf{X}_{\boldsymbol{\rho}}] &= (\boldsymbol{p} - \xi) \cdot [\boldsymbol{p}, \mathsf{X}_{\boldsymbol{\rho}}] + [\boldsymbol{p}, \mathsf{X}_{\boldsymbol{\rho}}] \cdot (\boldsymbol{p} - \xi) \\ &= (\boldsymbol{p} - \xi) \cdot \mathsf{X}_{[\boldsymbol{p}, \boldsymbol{\rho}]} + \mathsf{X}_{[\boldsymbol{p}, \boldsymbol{\rho}]} \cdot (\boldsymbol{p} - \xi), \end{aligned}$$

and the fact that, for any $\boldsymbol{\rho} \in \mathcal{P}(\mathfrak{h})$ and A, B are self-adjoint possibly unbounded operators, we have that

$$\operatorname{Tr}((AB + BA)\boldsymbol{\rho}) \leq \operatorname{Tr}((A^2 + B^2)\boldsymbol{\rho}).$$

Then, it follows that

$$\left| \frac{h^d}{i\hbar} \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1\big([|\xi_1 - \boldsymbol{p}|^2, \mathsf{X}_{\boldsymbol{\rho}}] \boldsymbol{\gamma}(z_1)\big) \, \mathrm{d}z_1 \right| \leq C h^{2d-2} \| \mathsf{X}_{[\boldsymbol{p}, \boldsymbol{\rho}]} \|_{\mathfrak{L}^\infty}^2 + C \mathcal{E}_{\boldsymbol{\gamma}}. \tag{3.8}$$

By inequality (2.17), Hölder's inequality, and the continuous embedding of Schatten spaces into Schatten spaces of higher exponent, taking into account the dependence of the norm with respect to $\hbar$, we have that

$$\begin{aligned} \text{RHS (3.8)} &\leq C h^{2d-2} \| \widehat{K} \|_{L^1}^2 \| [\boldsymbol{p}, \boldsymbol{\rho}] \|_{\mathfrak{L}^\infty}^2 + C \mathcal{E}_{\boldsymbol{\gamma}} \\ &\leq 2 C_K' h^{2d-2} \| \boldsymbol{p} \sqrt{\boldsymbol{\rho}} \|_{\mathfrak{L}^\infty}^2 \| \boldsymbol{\rho} \|_{\mathfrak{L}^\infty} + C \mathcal{E}_{\boldsymbol{\gamma}} \\ &\leq 2 C_K' h^{3d/2-3} \| \boldsymbol{p} \sqrt{\boldsymbol{\rho}} \|_{\mathfrak{L}^4}^2 \| \boldsymbol{\rho} \|_{\mathfrak{L}^d} + C \mathcal{E}_{\boldsymbol{\gamma}} \\ &\leq 2 C_K' h^{(3d-7)/2} \big(h^d \operatorname{Tr}(|\boldsymbol{p}|^2 \boldsymbol{\rho} |\boldsymbol{p}|^2) \big)^{\frac{1}{2}} \| \boldsymbol{\rho} \|_{\mathfrak{L}^d}^{3/2} + C \mathcal{E}_{\boldsymbol{\gamma}}. \end{aligned} \tag{3.9}$$

We proceed similarly to estimate $\| [x, \boldsymbol{\rho}] \|_{\mathfrak{L}^\infty}$ in inequality (3.7); that is, we write

$$h^{d-1} \| [x, \boldsymbol{\rho}] \|_{\mathfrak{L}^\infty} \leq C h^{(3d-7)/2} \big(h^d \operatorname{Tr}(|x|^2 \boldsymbol{\rho} |x|^2) \big)^{1/2} \| \boldsymbol{\rho} \|_{\mathfrak{L}^d}^{3/2}. \tag{3.10}$$

Now, combining inequalities (3.7) and (3.9), we obtain the following bound:

$$\begin{aligned} |(3.5\text{c})| &\leq C_K h^{(3d-7)/2} (M_4 + N_4)^{1/2} \| \boldsymbol{\rho} \|_{\mathfrak{L}^d}^{3/2} \\ &\quad + C_K \big(1 + h^{(3d-7)/2} (M_4 + N_4)^{1/2} \| \boldsymbol{\rho} \|_{\mathfrak{L}^d}^{3/2} \big) \mathcal{E}_{\boldsymbol{\gamma}}, \end{aligned}$$

where $M_4 = \operatorname{Tr}(\boldsymbol{\rho} |\boldsymbol{p}|^4)$ and $N_4 = \operatorname{Tr}(\boldsymbol{\rho} |x|^4)$.

Next, notice that

$$\frac{1}{i\hbar}[\boldsymbol{c}(z_1)\otimes\mathbf{1}, K_{12}] = (\xi_1-\boldsymbol{p}_1)\cdot\nabla K_{12} + \nabla K_{12}\cdot(\xi_1-\boldsymbol{p}_1), \tag{3.11}$$

where x_2 is viewed as a constant; then, we can rewrite term (3.5d) as follows:

$$\begin{aligned}|(3.5\mathrm{d})| &= \frac{2\theta_\alpha}{N}\operatorname{Re}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\,\mathrm{Tr}_{12}\big((\xi_1-\boldsymbol{p}_1)\cdot\nabla K_{12}\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &\leq \frac{\theta_\alpha}{N}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\,\mathrm{Tr}_{12}\big(|\xi_1-\boldsymbol{p}_1|^2\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2 \qquad (3.12\mathrm{a})\\ &\quad+\frac{\theta_\alpha}{N}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\,\mathrm{Tr}_{12}\big(|\nabla K_{12}|^2\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2. \qquad (3.12\mathrm{b})\end{aligned}$$

It is clear that term (3.12a) is bounded by $\frac{\theta_\alpha}{N}\mathcal{E}_{\boldsymbol{\Upsilon}}$. For term (3.12b), we use the fact that ∇K_{12} is a bounded multiplication operator of norm $\|\nabla K_{12}\|_{L^\infty}$, Hölder's inequality, and the fact that $h^{2d}\,\mathrm{Tr}_{12}(\boldsymbol{\Upsilon}(z_1,z_2)) = F(z_1,z_2)$ has integral one on $\mathbb{R}^{2d}\times\mathbb{R}^{2d}$ to deduce that term (3.12b) is bounded by $\|\nabla K\|_{L^\infty}^2\frac{\theta_\alpha}{N}$. Hence, combining our calculations with the result in [23], we obtain the bound

$$\begin{aligned}\frac{\mathrm{d}\mathcal{E}_{\boldsymbol{\gamma}}}{\mathrm{d}t} &\leq \big(C_K' + C_K h^{(3d-7)/2}(M_4+N_4)^{1/2}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/2}\big)\mathcal{E}_{\boldsymbol{\gamma}} + \frac{\theta_\alpha}{N}\mathcal{E}_{\boldsymbol{\Upsilon}}\\ &\quad+\frac{\theta_\alpha}{N}\|\nabla K\|_{L^\infty}^2 + C_K h^{(3d-7)/2}(M_4+N_4)^{1/2}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/2}, \qquad (3.13)\end{aligned}$$

where C_K' depends on the uniform bound of $\nabla^2 K$.

3.2.2. Estimates for $\mathcal{E}_{\boldsymbol{\Upsilon}}$. To estimate the right-hand side of equation (3.6), we need the following identities:

$$\begin{aligned}\{\boldsymbol{C}(z_1,z_2), H_{f_{12}}\} &= \{\boldsymbol{c}(z_1), H_f(z_1)\}\otimes\mathbf{1} + \mathbf{1}\otimes\{\boldsymbol{c}(z_2), H_f(z_2)\},\\ [\boldsymbol{C}(z_1,z_2), \mathsf{H}_{\boldsymbol{\rho}_{12}}] &= [\boldsymbol{c}(z_1), \mathsf{H}_{\boldsymbol{\rho}}]\otimes\mathbf{1} + \mathbf{1}\otimes[\boldsymbol{c}(z_2), \mathsf{H}_{\boldsymbol{\rho}}],\end{aligned}$$

and

$$\begin{aligned}[\boldsymbol{C}(z_1,z_2), K_{12}\boldsymbol{\rho}_{12}] &= [\boldsymbol{c}(z_1)\otimes\mathbf{1}, K_{12}]\boldsymbol{\rho}_{12} + [\mathbf{1}\otimes\boldsymbol{c}(z_2), K_{12}]\boldsymbol{\rho}_{12}\\ &\quad+K_{12}([\boldsymbol{c}(z_1),\boldsymbol{\rho}]\otimes\mathbf{1} + \mathbf{1}\otimes[\boldsymbol{c}(z_2),\boldsymbol{\rho}]). \qquad (3.14)\end{aligned}$$

For the first term, we see that

$$\begin{aligned}|(3.6\mathrm{a})| &= \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\,\mathrm{Tr}_{12}\big((\{\boldsymbol{c}(z_1), H_f(z_1)\}\otimes\mathbf{1})\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &\quad+\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\,\mathrm{Tr}_{12}\big((\mathbf{1}\otimes\{\boldsymbol{c}(z_2), H_f(z_2)\})\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &= 2\int_{\mathbb{R}^{2d}} h^d\,\mathrm{Tr}_1\big(\{\boldsymbol{c}(z), H_f(z)\}\boldsymbol{\Upsilon}_{:1}(z)\big)\,\mathrm{d}z,\end{aligned}$$

where

$$\boldsymbol{\Upsilon}_{:1}(z_1) := \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_2(\boldsymbol{\Upsilon}(z_1, z_2))\, \mathrm{d}z_2.$$

Then, using the same argument as in [23], we obtain the bound

$$\begin{aligned}
|(3.6a)| &\leq 2\big(1 + \max\big(4\|\nabla^2 K\|_{L^\infty}^2, 1\big)\big) \int_{\mathbb{R}^{2d}} h^d \operatorname{Tr}_1(\boldsymbol{c}(z)\boldsymbol{\Upsilon}_{:1}(z))\, \mathrm{d}z \\
&= 2\big(1 + \max\big(4\|\nabla^2 K\|_{L^\infty}^2, 1\big)\big)\mathcal{E}_{\boldsymbol{\Upsilon}}(t).
\end{aligned}$$

A similar argument holds for term (3.6b) with minor modification for the term $h^d \chi_{\boldsymbol{\rho}}$ as seen in the above estimate for term (3.5c).

The terms (3.6c) and (3.6d) follow the same argument as in the case of the term (3.5d), that is,

$$\begin{aligned}
|(3.6c) + (3.6d)| \leq \frac{1}{N} &\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(|\xi_1 - \boldsymbol{p}_1|^2 \boldsymbol{\Upsilon}(z_1, z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&+ \frac{1}{N} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(|\xi_2 - \boldsymbol{p}_2|^2 \boldsymbol{\Upsilon}(z_1, z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&+ \frac{1}{N} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(|\nabla K_{12} - \eta \nabla K_{\chi_{12}}|^2 \boldsymbol{\Upsilon}(z_1, z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2.
\end{aligned}$$

If $\eta = 1$, then we use the fact that

$$|\nabla K(x_1 - x_2) - \nabla K(\chi_1 - \chi_2)|^2 \leq 2\|\nabla^2 K\|_{L^\infty}^2 \big(|x_1 - \chi_1|^2 + |x_2 - \chi_2|^2\big)$$

to obtain

$$|(3.6c) + (3.6d)| \leq \frac{2\max(\|\nabla^2 K\|_{L^\infty}^2, 1)}{N} \mathcal{E}_{\boldsymbol{\Upsilon}}(t).$$

If $\eta = 0$, then we use instead the fact that ∇K_{12} is a bounded multiplication operator to get

$$|(3.6c) + (3.6d)| \leq \frac{1}{N}(\mathcal{E}_{\boldsymbol{\Upsilon}}(t) + \|\nabla K\|_{L^\infty}).$$

For the term (3.6f), we notice that

$$|\langle [K_{12}, \boldsymbol{\rho}_{12}]\rangle_{\boldsymbol{\rho}_\alpha}| = |h^{2d} \operatorname{Tr}_{12}([K_{12}, \boldsymbol{\rho}_{12}]\boldsymbol{\rho}_\alpha)| \leq C\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty};$$

then, this yields the bound

$$|(3.6f)| \leq C h^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}(t).$$

Finally, to handle the term (3.6e), we start by expanding the expression

$$K_{12}\boldsymbol{\rho}_{12}\boldsymbol{C}(z_1, z_2) = K_{12}(\boldsymbol{\rho}_1\boldsymbol{c}(z_1) + \boldsymbol{c}(z_1)\boldsymbol{\rho}_2 + \boldsymbol{\rho}_1\boldsymbol{c}(z_2) + \boldsymbol{\rho}_2\boldsymbol{c}(z_2)),$$

where $\boldsymbol{\rho}_1 = \boldsymbol{\rho} \otimes \mathbf{1}$ and $\boldsymbol{\rho}_2 = \mathbf{1} \otimes \boldsymbol{\rho}$. It suffices to consider the first two terms in the above expansion since the others are handled in the exact same manner; i.e., we estimate

$$\frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}(K_{12}\boldsymbol{\rho}_1 \boldsymbol{c}(z_1)\boldsymbol{\Upsilon}(z_1,z_2))\, \mathrm{d}z_1\, \mathrm{d}z_2, \tag{3.15a}$$

$$\frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}(K_{12}\boldsymbol{c}(z_1)\boldsymbol{\rho}_2\boldsymbol{\Upsilon}(z_1,z_2))\, \mathrm{d}z_1\, \mathrm{d}z_2. \tag{3.15b}$$

In the first case, notice that

$$\begin{aligned}
&\frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_1|\chi_1 - x_1|^2\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&= \frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}[x_1,\boldsymbol{\rho}_1]\cdot(\chi_1 - x_1)\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&\quad + \frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_1(\chi_1 - x_1)\boldsymbol{\Upsilon}(z_1,z_2)\cdot(\chi_1 - x_1)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2,
\end{aligned} \tag{3.16a}$$

from which it follows

$$\begin{aligned}
|(3.16a)| &\le C h^{d-1}\|K\|_{L^\infty}\|[x,\boldsymbol{\rho}]\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}^{1/2} + C h^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}} \\
&\le C_K h^{(3d-7)/2} N_4^{1/2}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/2} + C\big(1 + h^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\big)\mathcal{E}_{\boldsymbol{\Upsilon}},
\end{aligned}$$

where the second inequality follows the same argument as in (3.9). Similarly, we see that

$$\begin{aligned}
&\frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_1|\xi_1 - \boldsymbol{p}_1|^2\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&= \frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}[\boldsymbol{p}_1,\boldsymbol{\rho}_1]\cdot(\xi_1 - \boldsymbol{p}_1)\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&\quad - h^d \operatorname{Re} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(\nabla K_{12}\boldsymbol{\rho}_1\cdot(\xi_1 - \boldsymbol{p}_1)\boldsymbol{\Upsilon}(z_1,z_2)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2 \\
&\quad + \frac{h^d}{\hbar} \operatorname{Im} \iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d} \operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_1(\xi_1 - \boldsymbol{p}_1)\boldsymbol{\Upsilon}(z_1,z_2)\cdot(\xi_1 - \boldsymbol{p}_1)\big)\, \mathrm{d}z_1\, \mathrm{d}z_2;
\end{aligned} \tag{3.16b}$$

then, by the same argument as for inequality (3.9), we have that

$$\begin{aligned}
|(3.16b)| &\le C h^{(3d-7)/4}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/4} M_4^{1/4}\mathcal{E}_{\boldsymbol{\Upsilon}}^{1/2} \\
&\quad + C h^d\|\nabla K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}^{1/2} + C h^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}.
\end{aligned}$$

This completes the estimate for the term (3.15a).

To estimate term (3.15b), we follow a similar idea as above. We write

$$\begin{aligned}&\frac{h^d}{\hbar}\operatorname{Im}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\operatorname{Tr}_{12}\big(K_{12}|\chi_1-x_1|^2\boldsymbol{\rho}_2\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &=\frac{h^d}{\hbar}\operatorname{Im}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_2(\chi_1-x_1)\boldsymbol{\Upsilon}(z_1,z_2)\cdot(\chi_1-x_1)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2,\end{aligned}\tag{3.17a}$$

from which it follows that

$$|(3.17\text{a})|\le Ch^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}.$$

Next, we have

$$\begin{aligned}&\frac{h^d}{\hbar}\operatorname{Im}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\operatorname{Tr}_{12}\big(K_{12}|\xi_1-\boldsymbol{p}_1|^2\boldsymbol{\rho}_2\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &=\frac{h^d}{\hbar}\operatorname{Im}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\operatorname{Tr}_{12}\big(K_{12}\boldsymbol{\rho}_2(\xi_1-\boldsymbol{p}_1)\boldsymbol{\Upsilon}(z_1,z_2)\cdot(\xi_1-\boldsymbol{p}_1)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &\quad-h^d\operatorname{Re}\iint_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} h^{2d}\operatorname{Tr}_{12}\big(\nabla K_{12}\boldsymbol{\rho}_2\cdot(\xi_1-\boldsymbol{p}_1)\boldsymbol{\Upsilon}(z_1,z_2)\big)\,\mathrm{d}z_1\,\mathrm{d}z_2,\end{aligned}\tag{3.17b}$$

which yields

$$|(3.17\text{b})|\le Ch^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}+Ch^d\|\nabla K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\mathcal{E}_{\boldsymbol{\Upsilon}}^{1/2}.$$

Hence, we obtain the following bound:

$$\begin{aligned}|(3.6\text{e})|\le{}&C\big(1+h^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}+h^d\|\nabla K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\big)\mathcal{E}_{\boldsymbol{\Upsilon}}\\ &+C_K\big(h^d\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}+h^{(3d-7)/2}(N_4+M_4)^{1/2}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/2}\big).\end{aligned}$$

Finally, combining the above estimates, we see that there exists a constant C, dependent on K, such that we have the following inequality:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_{\boldsymbol{\Upsilon}}(t)\le{}&C_K'\big(1+h^{(3d-7)/2}(M_4+N_4)^{1/2}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/2}+h^{d-1}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\big)\mathcal{E}_{\boldsymbol{\Upsilon}}(t)\\ &+C_K\bigg(\frac{1-\eta}{N}+h^d\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}+h^{(3d-7)/2}(N_4+M_4)^{1/2}\|\boldsymbol{\rho}\|_{\mathcal{L}^d}^{3/2}\bigg).\end{aligned}\tag{3.18}$$

In the case when Nh is bounded from below by a constant independent of N and $\hbar$, then it follows from the last inequality in formula (2.11) that

$$h^{d-1}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}\le\frac{1}{Nh}\tag{3.19}$$

is bounded uniformly in $\hbar$ and N. Moreover, by Proposition 2.1 and Proposition 2.2 (ii), we see that $\|\boldsymbol{\rho}\|_{\mathcal{L}^d}$, M_4, and N_4 are propagated uniformly in N and $\hbar$. Then, by inequalities (3.13) and (3.18), we see there exists a constant $C_{K,\boldsymbol{\rho}}$, dependent on K and $\boldsymbol{\rho}$, such that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{E}_{\boldsymbol{\gamma}}(t) + \mathcal{E}_{\boldsymbol{\Upsilon}}(t)) &\le C_{K,\boldsymbol{\rho}}\big(1 + h^{(3d-7)/2}(M_4 + N_4)^{1/2}\big)(\mathcal{E}_{\boldsymbol{\gamma}}(t) + \mathcal{E}_{\boldsymbol{\Upsilon}}(t)) \\ &\quad + C_{K,\boldsymbol{\rho}} h\Big(\frac{\theta_\alpha + 1}{Nh} + h^{(3d-9)/2}(N_4 + M_4)^{1/2}\Big) \\ &\le C_{K,\boldsymbol{\rho}} g_1(t)(\mathcal{E}_{\boldsymbol{\gamma}}(t) + \mathcal{E}_{\boldsymbol{\Upsilon}}(t)) + C_{K,\boldsymbol{\rho}} h g_0(t),\end{aligned}$$

where $g_i(t) \ge 1 + h^{i+(3d-9)/2}(N_4 + M_4)^{1/2}$. Recalling the definition (1.16) and (3.1), we conclude the proof of Theorem 1.1 by Grönwall's lemma.

In the case when $Nh \ll 1$, $\theta_\alpha^{\mathrm{in}} \le CNh^{2d/p}$, and $\|\boldsymbol{\rho}^{\mathrm{in}}\|_{\mathcal{L}^p} \le C$ for some constant C independent of $\hbar$, then it follows from Proposition 2.2 that there exists $C > 0$ independent of $\hbar$ such that, for any $t \in [0, T]$ with $T = Ch^{1-d/p}$,

$$h^{d-1}\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} \le h^{\frac{d}{p'}-1}\|\boldsymbol{\rho}\|_{\mathcal{L}^p} \le C.$$

The moments also remain propagated uniformly in $\hbar$ and N in this case. Then, by inequalities (3.13) and (3.18), we see there exists $C_{K,\boldsymbol{\rho}}$, depending on K and $\|\boldsymbol{\rho}\|_{\mathcal{L}^d}$, such that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{E}_{\boldsymbol{\gamma}}(t) + \mathcal{E}_{\boldsymbol{\Upsilon}}(t)) &\le C_{K,\boldsymbol{\rho}}\big(1 + h^{(3d-7)/2}(M_4 + N_4)^{1/2}\big)(\mathcal{E}_{\boldsymbol{\gamma}}(t) + \mathcal{E}_{\boldsymbol{\Upsilon}}(t)) \\ &\quad + C_{K,\boldsymbol{\rho}} h\Big(\frac{\theta_\alpha}{Nh} + h^{(3d-9)/2}(N_4 + M_4)^{1/2}\Big) \\ &\le C'_{K,\boldsymbol{\rho}} g_1(t)(\mathcal{E}_{\boldsymbol{\gamma}}(t) + \mathcal{E}_{\boldsymbol{\Upsilon}}(t)) + C'_{K,\boldsymbol{\rho}} h g_0(t),\end{aligned}$$

where $g_i(t) \ge 1 + h^{i+(3d-9)/2}(N_4 + M_4)^{1/2}$ for $i \in \{0, 1\}$. Notice that the last inequality is possible since $\theta_\alpha/(Nh) \le Ch$ on $[0, T]$. Again, we conclude the proof of Theorem 1.2 by Grönwall's lemma.

4. Application to the effective approximation of quantum systems

In this section, we combine the result from the previous section and the result in [43]. To avoid a substantial detour from the goal of the paper, we will provide a concise introduction on the method of second quantization, covering only the essential definitions necessary for stating the main result of [43, Theorem 3.3]. Also, in this section, we assume the scaling $Nh^d = 1$ with $d = 3$.

4.1. Quasi-free approximation of interacting spin-$\frac{1}{2}$ fermions

Let $\mathfrak{H}$ denote the complex Hilbert space $L^2(X)$, where $X = \mathbb{R}^d \times \{\uparrow, \downarrow\}$. The elements of X are expressed as ordered pairs $\mathbf{x} = (x, \tau)$, where $x \in \mathbb{R}^d$ is the spatial variable and $\tau \in \{\uparrow, \downarrow\}$ is called the spin label. Notice that we have the identification $\mathfrak{H} \cong L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$.

Let $\mathfrak{H}^{\wedge n} := \mathfrak{H} \wedge \cdots \wedge \mathfrak{H}$ denote the n-fold anti-symmetric tensor product. We define the fermionic Fock space $\mathcal{F}$ over $\mathfrak{H}$ to be the closure of algebraic direct sum

$$\mathcal{F}^{\mathrm{alg}}(\mathfrak{H}) := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathfrak{H}^{\wedge n}$$

with respect to the norm $\|\cdot\|_{\mathcal{F}}$ induced by the endowed inner product

$$\langle \Psi \mid \Phi \rangle = \overline{\psi^{(0)}}\varphi^{(0)} + \sum_{n \geq 1} \left\langle \psi^{(n)} \,\middle|\, \varphi^{(n)} \right\rangle_{\mathfrak{H}^{\otimes n}}$$

for any pair of vectors $\Psi = (\psi^{(0)}, \psi^{(1)}, \ldots)$ and $\Phi = (\varphi^{(0)}, \varphi^{(1)}, \ldots)$ in $\mathcal{F}^{\mathrm{alg}}(\mathfrak{H})$. A normalized vector Ψ in $\mathcal{F}$ is called a Fock state or a pure state. The vacuum, defined by the vector $\Omega_{\mathcal{F}} = (1, 0, 0, \ldots) \in \mathcal{F}$, describes the state with no particles.

For every $\mathbf{x} \in X$, we define the corresponding creation and annihilation operator-valued distributions, denoted by $a^*_{\mathbf{x}}$ and $a_{\mathbf{x}}$, acting on $\mathcal{F}$ by their actions on the n-sector of $\mathcal{F}$ as follows:

$$\begin{aligned}
(a^*_{\mathbf{x}}\Psi)^{(n)}(\underline{\mathbf{x}}_n) &:= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1} \delta(x - x_j) \delta_{\tau,\tau_j} \psi^{(n-1)}(\underline{\mathbf{x}}_{n\setminus j}),\\
(a_{\mathbf{x}}\Psi)^{(n)}(\underline{\mathbf{x}}_n) &:= \sqrt{n+1}\,\psi^{(n+1)}(\mathbf{x}, \underline{\mathbf{x}}_n),
\end{aligned}$$

where $\underline{\mathbf{x}}_n := (\mathbf{x}_1, \ldots, \mathbf{x}_n)$, $\underline{\mathbf{x}}_{n\setminus j} := (\mathbf{x}_1, \ldots, \cancel{\mathbf{x}_j}, \ldots, \mathbf{x}_n)$, and $\delta_{\tau,\tau'}$ is the Kronecker delta. Moreover, the action of the annihilation operator on the vacuum of $\mathcal{F}$ is defined to be $a_{\mathbf{x}}\Omega_{\mathcal{F}} = 0$. Then, we extend the operators linearly to the whole $\mathcal{F}$. It can easily be checked that the collection of creation and annihilation operators on $\mathcal{F}$ satisfies the canonical anti-commutation relations

$$[a_{\mathbf{x}}, a^*_{\mathbf{x}'}]_+ = \delta(x - x')\delta_{\tau,\tau'}, \quad [a_{\mathbf{x}}, a_{\mathbf{x}'}]_+ = [a^*_{\mathbf{x}}, a^*_{\mathbf{x}'}]_+ = 0 \tag{4.1}$$

for all $\mathbf{x}, \mathbf{x}' \in X$, where $[A, B]_+ = AB + BA$ is the anti-commutator of the operators A and B. Another useful operator is given by the number operator

$$\mathcal{N} = \bigoplus_{n=1}^{\infty} n \mathbf{1}_{\mathfrak{H}^{\wedge n}},$$

which counts the number of particles in each sector.

Consider the fermionic Fock state $\Psi \in \mathcal{F}$ with an expected number of particles equal to N, i.e., $\langle \Psi \mid \mathcal{N}\Psi \rangle_{\mathcal{F}} = N$. We define its one-particle reduced density operator $\boldsymbol{\rho}$ and its pairing operator α to be the operators with integral kernels

$$\boldsymbol{\rho}(\mathbf{x}; \mathbf{y}) := \left\langle \Psi \,\middle|\, a^*_{\mathbf{y}} a_{\mathbf{x}} \Psi \right\rangle, \tag{4.2a}$$

$$\alpha(\mathbf{x}, \mathbf{y}) := \left\langle \Psi \,\middle|\, a_{\mathbf{y}} a_{\mathbf{x}} \Psi \right\rangle, \quad \boldsymbol{\rho}_{\alpha,\Psi}(\mathbf{x}_{12}; \mathbf{y}_{12}) := \frac{1}{h^d \theta_\Psi} \alpha(\mathbf{x}_1; \mathbf{x}_2)\alpha(\mathbf{y}_1; \mathbf{y}_2), \tag{4.2b}$$

where $\theta_\Psi = \frac{1}{N}\|\alpha_\Psi\|_2^2 = \|\alpha_\Psi\|_{\mathcal{L}^2}^2 \in [0,1]$ is such that $h^{2d}\operatorname{Tr}(\boldsymbol{\rho}_{\alpha,\Psi}) = 1$. Notice that we have that $h^d \operatorname{Tr}_{\mathfrak{H}}(\boldsymbol{\rho}) = 1$ while $\operatorname{Tr}_{\mathfrak{H}}(\alpha) = 0$. Moreover, since we are in the case of fermions, it follows from properties (4.1) that $0 \le \boldsymbol{\rho} \le \mathbf{1}$ and α is anti-symmetric. More compactly, we introduce the generalized one-particle density operator acting on $\mathfrak{H} \oplus \mathfrak{H}$ by

$$\Gamma_\Psi := \begin{pmatrix} \boldsymbol{\rho} & \alpha \\ \alpha^* & \mathbf{1} - \overline{\boldsymbol{\rho}} \end{pmatrix}, \tag{4.3}$$

which satisfies $0 \le \Gamma \le \mathbf{1}_{\mathfrak{H}\oplus\mathfrak{H}}$.

We say that Ψ is a quasi-free pure state if

$$\left\langle \Psi \,\middle|\, a_{\mathbf{x}_1}^{\sharp_1} a_{\mathbf{x}_2}^{\sharp_2} \cdots a_{\mathbf{x}_{2\ell-1}}^{\sharp_{2\ell-1}} \Psi \right\rangle = 0$$

and

$$\left\langle \Psi \,\middle|\, a_{\mathbf{x}_1}^{\sharp_1} a_{\mathbf{x}_2}^{\sharp_2} \cdots a_{\mathbf{x}_{2\ell}}^{\sharp_{2\ell}} \Psi \right\rangle = \sum_{\pi \in \mathbb{P}_{2\ell}} \operatorname{sgn}(\pi) \prod_{\mathrm{j}=1}^{\ell} \left\langle \Psi \,\middle|\, a_{\mathbf{x}_{\pi(2\mathrm{j}-1)}}^{\sharp_{\pi(2\mathrm{j}-1)}} a_{\mathbf{x}_{\pi(2\mathrm{j})}}^{\sharp_{\pi(2\mathrm{j})}} \Psi \right\rangle$$

for all $\ell \in \mathbb{N}$, where $a^\sharp$ denotes either a^* or a and $\mathbb{P}_{2\ell}$ is the set of pairings, that is, the subset of permutations of 2ℓ elements satisfying

$$\pi(2\mathrm{j}-1) < \pi(2\mathrm{j}) \quad \forall \mathrm{j} = 1,\ldots,\ell \quad \text{and} \quad \pi(2\mathrm{j}-1) < \pi(2\mathrm{j}+1) \quad \forall \mathrm{j} = 1,\ldots,\ell-1.$$

In other words, observables associated with product of creation and annihilation operators of a quasi-free state are completely characterized by $\boldsymbol{\rho}$ and α. Moreover, if Ψ is quasi-free, then Γ_Ψ is a projection operator, or more precisely,

$$0 \le \boldsymbol{\rho} \le \mathbf{1}, \quad \alpha^* = -\overline{\alpha}, \quad \boldsymbol{\rho}\alpha = \alpha\overline{\boldsymbol{\rho}}, \quad \text{and} \quad |\alpha^*|^2 = \boldsymbol{\rho}(\mathbf{1} - \boldsymbol{\rho}). \tag{4.4}$$

Conversely, if Γ is of the form (1.1) satisfying conditions (4.4) and γ is a trace class operator, then there exists a quasi-free pure state Ψ such that $\Gamma_\Psi = \Gamma$ (cf. Chapter 10 or Appendix G in [48]). Furthermore, if Ψ is a quasi-free pure state with finite expected number of particles, then there exists a unitary transformation R, parameterized by $\boldsymbol{\rho}$ and α, such that $\Psi = \mathsf{R}\Omega_{\mathcal{F}}$. R is a Bogoliubov transformation (cf. [48]).

Let $K(x)$ be a spin-independent radial function. Define the Hamiltonian in the Fock space by

$$\mathcal{H}_N = \int_X a_{\mathbf{x}}^* \left(-\frac{\hbar^2}{2}\Delta_x \right) a_{\mathbf{x}}\, \mu(\mathrm{d}\mathbf{x}) + \frac{1}{2N} \int_{X\times X} K(x-y) a_{\mathbf{x}}^* a_{\mathbf{y}}^* a_{\mathbf{y}} a_{\mathbf{x}}\, \mu(\mathrm{d}\mathbf{x})\mu(\mathrm{d}\mathbf{y}),$$

where μ is the tensor product of the Lebesgue measure on $\mathbb{R}^d$ and the counting measure, and consider the time-dependent Fock state $\Psi(t) = \Psi$ given by

$$\Psi = e^{-i\mathcal{H}_N t/\hbar}\Psi^{\mathrm{in}} = e^{-i\mathcal{H}_N t/\hbar}\mathsf{R}^{\mathrm{in}}\Omega_{\mathcal{F}}, \tag{4.5}$$

where Ψ^{in} is some quasi-free state such that $\boldsymbol{\rho}^{\mathrm{in}} := \boldsymbol{\rho}_{\Psi^{\mathrm{in}}}$ and $\alpha^{\mathrm{in}} := \alpha_{\Psi^{\mathrm{in}}}$ satisfy the following conditions:

$$h^d \operatorname{Tr}_{\mathfrak{H}}(\boldsymbol{\rho}^{\mathrm{in}}) = 1 \quad \text{and} \quad \theta_{\alpha^{\mathrm{in}}} \le CN^{-1/3}. \tag{4.6}$$

Then, it was proved that the quadratic in creation and annihilation operators observables of the state Ψ_t are well approximated by the BdG dynamics (1.5) (with spins) in norms. More precisely, the main result in [43] states the following.

Theorem 4.1 ([43, Theorem 3.3]). *Assume $K \in L^1(\mathbb{R}^d)$ and $\widehat{K}(\xi)(1+|\xi|^2) \in L^1(\mathbb{R}^d)$. Assume that the initial data Ψ^{in} is a quasi-free state, with $\boldsymbol{\rho}^{\mathrm{in}} = \boldsymbol{\rho}_{\Psi^{\mathrm{in}}}$ and $\alpha^{\mathrm{in}} = \alpha_{\Psi^{\mathrm{in}}}$, satisfying conditions (4.6). Furthermore, assume that $\boldsymbol{\rho}^{\mathrm{in}}$ and α^{in} satisfy the following commutator bounds: there exists $C > 0$ independent of $\hbar$ such that*

$$\sup_{\xi\in\mathbb{R}^d} \frac{1}{1+|\xi|} \|[e^{i\xi\cdot x}, \boldsymbol{\rho}^{\mathrm{in}}]\|_{\mathcal{L}^2} \leq C\sqrt{\hbar}, \quad \|[\nabla, \boldsymbol{\rho}^{\mathrm{in}}]\|_{\mathcal{L}^2} \leq \frac{C}{\sqrt{\hbar}}, \quad \|[\nabla, \alpha^{\mathrm{in}}]\|_{\mathcal{L}^2} \leq \frac{C}{\hbar^{\frac{5}{2}}}. \tag{4.7}$$

Suppose that Ψ is given by expression (4.5) and let $(\boldsymbol{\rho}, \alpha)$ be a solution of the BdG dynamics (1.5) with initial data $(\boldsymbol{\rho}^{\mathrm{in}}, \alpha^{\mathrm{in}})$. Then, there exists $\kappa_1, \kappa_2 > 0$, independent of N, such that we have the estimates for any $t \geq 0$,

$$\|\boldsymbol{\rho}_\Psi - \boldsymbol{\rho}\|_{\mathcal{L}^2(\mathfrak{H})} \leq \frac{1}{\sqrt{N}} \exp(\kappa_1 \exp(\kappa_2 t)), \tag{4.8}$$

$$\|\alpha_\Psi - \alpha\|_{\mathcal{L}^2(\mathfrak{H})} \leq \frac{1}{\sqrt{N}} \exp(\kappa_1 \exp(\kappa_2 t)), \tag{4.9}$$

where $\mathcal{L}^2(\mathfrak{H})$ denotes the scaled Hilbert–Schmidt norm for operators on $\mathfrak{H}$, also given in terms of the integral kernel by $\|\boldsymbol{\rho}\|^2_{\mathcal{L}^2(\mathfrak{H})} = h^d \int_{X\times X} |\boldsymbol{\rho}(\mathbf{x},\mathbf{y})|^2 \mu(\mathrm{d}\mathbf{x})\mu(\mathrm{d}\mathbf{y})$.

Remark 4.1. In the case of zero pairing, that is, when $\alpha = 0$, the commutator bounds (4.7) are proven to be satisfied by the ground states of noninteracting Fermi gases in [9, 16, 20]. In the case of $\alpha \neq 0$, these bounds are expected to hold at least when α is sufficiently small (cf. [43, Appendix A]).

The $\mathcal{L}^2(\mathfrak{H})$ estimates on α in the above theorem imply $\mathcal{L}^1(\mathfrak{H})$ estimates for $\boldsymbol{\rho}_{\alpha:1}$.

Corollary 4.1. *For any $t \geq 0$, we have the estimate*

$$\|\boldsymbol{\rho}_{\alpha,\Psi:1} - \boldsymbol{\rho}_{\alpha:1}\|_{\mathcal{L}^1(\mathfrak{H})} \leq \frac{2e^{2C_K h^{d-1} t}}{\theta_{\alpha^{\mathrm{in}}} N} C_t^2 + \frac{4e^{C_K h^{d-1} t}}{\sqrt{\theta_{\alpha^{\mathrm{in}}} N}} C_t,$$

where $C_t/\sqrt{N}$ is the constant appearing on the right-hand side of inequality (4.9) and $C_K = \|K\|_{L^\infty}$. Similarly, we also have

$$\|\boldsymbol{\rho}_{\alpha,\Psi} - \boldsymbol{\rho}_\alpha\|_{\mathcal{L}^1(\mathfrak{H}^{\otimes 2})} := h^{2d}\,\mathrm{Tr}|\boldsymbol{\rho}_{\alpha,\Psi} - \boldsymbol{\rho}_\alpha| \leq \frac{e^{2C_K h^{d-1} t} C_t}{\sqrt{\theta_{\alpha^{\mathrm{in}}} N}}. \tag{4.10}$$

Hence, if $\theta_{\alpha^{\mathrm{in}}} \geq N^{-c}$ with $c \in [1/3, 1]$, then

$$\|\boldsymbol{\rho}_{\alpha,\Psi:1} - \boldsymbol{\rho}_{\alpha:1}\|_{\mathcal{L}^1(\mathfrak{H})} \leq \frac{4e^{2C_K h^{d-1} t} C_t}{N^{(1-c)/2}}. \tag{4.11}$$

Proof. Since $Nh^d = 1$, it holds $\theta_\alpha \boldsymbol{\rho}_{\alpha:1} = |\alpha^*|^2$. Hence,

$$\begin{aligned}\|\boldsymbol{\rho}_{\alpha,\Psi:1} - \boldsymbol{\rho}_{\alpha:1}\|_{\mathfrak{L}^1(\mathfrak{H})} &\le \left\| \frac{\theta_\Psi \boldsymbol{\rho}_{\alpha,\Psi:1} - \theta_\alpha \boldsymbol{\rho}_{\alpha:1}}{\theta_\alpha} \right\|_{\mathfrak{L}^1(\mathfrak{H})} + \frac{|\theta_\alpha - \theta_\Psi|}{\theta_\alpha} \|\boldsymbol{\rho}_{\alpha,\Psi:1}\|_{\mathfrak{L}^1(\mathfrak{H})} \\ &\le \frac{1}{\theta_\alpha}\big(\||\alpha_\Psi^*|^2 - |\alpha^*|^2\|_{\mathfrak{L}^1(\mathfrak{H})} + |\theta_\alpha - \theta_\Psi|\big) \\ &\le \frac{1}{\theta_\alpha}\big(\|\alpha_\Psi^* - \alpha^*\|_{\mathfrak{L}^2}^2 + 2\|\alpha_\Psi^* - \alpha^*\|_{\mathfrak{L}^2}\|\alpha^*\|_{\mathfrak{L}^2} + |\theta_\alpha - \theta_\Psi|\big).\end{aligned}$$

Since $\|\alpha^*\|_{\mathfrak{L}^2}^2 = \|\alpha\|_{\mathfrak{L}^2}^2 = \theta_\alpha$ and

$$|\theta_\Psi - \theta_\alpha| = h^d \operatorname{Tr}(|\alpha_\Psi|^2 - |\alpha|^2) \le \|\alpha_\Psi - \alpha\|_{\mathfrak{L}^2}^2 + 2\|\alpha_\Psi - \alpha\|_{\mathfrak{L}^2}\sqrt{\theta_\alpha},$$

it yields

$$\|\boldsymbol{\rho}_{\alpha,\Psi:1} - \boldsymbol{\rho}_{\alpha:1}\|_{\mathfrak{L}^1(\mathfrak{H})} \le \frac{2}{\theta_\alpha}\|\alpha_\Psi - \alpha\|_{\mathfrak{L}^2}^2 + \frac{4}{\sqrt{\theta_\alpha}}\|\alpha_\Psi - \alpha\|_{\mathfrak{L}^2}.$$

To finish the proof, notice first that by equation (2.5)

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\theta_\alpha\right| \le 2h^{d-1}\|K\|_{L^\infty}\|\boldsymbol{\rho}\|_{\mathfrak{L}^\infty}\theta_\alpha \le 2C_K h^{d-1}\theta_\alpha, \tag{4.12}$$

hence $e^{-2C_K h^{d-1} t}\theta_{\alpha^{\text{in}}} \le \theta_\alpha$, and use the previous theorem. The proof of inequality (4.10) is similar. ∎

4.2. SU(2) invariance

The presence of spin labels in the BdG equation complicates our studies of its semiclassical limit. To overcome this difficulty, we need to isolate out the spin labels from the BdG equation (cf. [5]). We start by noting the isomorphism $L^2(\mathbb{R}^d \times \{\uparrow,\downarrow\}) \cong L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$. In particular, we have the identification between the two spaces of bounded operators

$$\mathcal{B}(L^2(\mathbb{R}^d \times \{\uparrow,\downarrow\})) \cong \mathcal{B}(L^2(\mathbb{R}^d)) \otimes M_{2\times 2}(\mathbb{C}),$$

i.e., a bounded operator T acting on $L^2(\mathbb{R}^d \times \{\uparrow,\downarrow\})$ is identified with the matrix

$$T = \begin{pmatrix} T_{\uparrow\uparrow} & T_{\uparrow\downarrow} \\ T_{\downarrow\uparrow} & T_{\downarrow\downarrow} \end{pmatrix}, \tag{4.13}$$

where $T_{\sigma\tau}$ are bounded operators acting on $L^2(\mathbb{R}^d)$. To factor out the spins, we further restrict ourselves to the class of Γ operators satisfying the following SU(2) invariance condition in the spin space: for every $S \in \mathrm{SU}(2)$, we have that

$$\mathsf{S}^*\Gamma\mathsf{S} = \Gamma, \quad \text{where } \mathsf{S} = \begin{pmatrix} S & 0 \\ 0 & \overline{S} \end{pmatrix}.$$

In terms of $\boldsymbol{\rho}$ and α, the SU(2) invariance reads

$$S^*\boldsymbol{\rho}S = \boldsymbol{\rho} \quad \text{and} \quad S^*\alpha\overline{S} = \alpha.$$

By means of elementary linear algebra, we have that $\boldsymbol{\rho}$ is a scalar multiple of the identity matrix and α is a scalar multiple of the second Pauli matrix

$$\sigma^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

or, equivalently, we have that

$$\boldsymbol{\rho}(x,\tau;x',\tau') = \boldsymbol{\rho}_s(x,x')\delta_{\tau\tau'} \quad \text{and} \quad \alpha(x,\tau,x',\tau') = \alpha_s(x,x')\sigma^{(2)}_{\tau\tau'}. \tag{4.14}$$

By the Pauli exclusion principle, we must have that α_s is symmetric, that is,

$$\alpha_s(x,x') = \alpha_s(x',x).$$

We also write $\boldsymbol{\rho} = \boldsymbol{\rho}_s \otimes I$, where I is the 2×2 identity matrix and $\alpha = \alpha_s \otimes \sigma^{(2)}$. Also, notice, by expressions (4.14), the last identity of conditions (4.4) now reads

$$|\alpha_s^*|^2 = \boldsymbol{\rho}_s(\mathbf{1} - \boldsymbol{\rho}_s). \tag{4.15}$$

The physical meaning of the SU(2) invariance is discussed in [32].

By expressions (4.14), we write

$$\mathsf{H}_{\boldsymbol{\rho}} = \left(\frac{|\boldsymbol{p}|^2}{2} + 2K * \varrho_s(x) - h^d\mathsf{X}_{\boldsymbol{\rho}_s}\right) \otimes I =: \mathsf{H}_{\boldsymbol{\rho}_s} \otimes I \quad \text{and} \quad \mathsf{X}_\alpha\alpha^* = (\mathsf{X}_{\alpha_s}\alpha_s^*) \otimes I.$$

Then, this yields the spinless equations

$$i\hbar\,\partial_t\boldsymbol{\rho}_s = [\mathsf{H}_{\boldsymbol{\rho}_s}, \boldsymbol{\rho}_s] + \mathsf{X}_{\alpha_s}\overline{\alpha}_s - \alpha_s\mathsf{X}_{\overline{\alpha}_s}, \tag{4.16a}$$
$$i\hbar\,\partial_t\alpha_s = \mathsf{H}_{\boldsymbol{\rho}_s}\alpha_s + \alpha_s\overline{\mathsf{H}}_{\boldsymbol{\rho}_s} + h^d(\mathsf{X}_{\alpha_s}(\mathbf{1} - \overline{\boldsymbol{\rho}}_s) - \boldsymbol{\rho}_s\mathsf{X}_{\alpha_s}), \tag{4.16b}$$

or, equivalently, in matrix form

$$i\hbar\,\partial_t\Gamma_s = [\mathsf{H}_{\Gamma_s}, \Gamma_s], \tag{4.17}$$

where

$$\Gamma_s = \begin{pmatrix} \boldsymbol{\rho}_s & \alpha_s \\ \overline{\alpha}_s & \mathbf{1} - \overline{\boldsymbol{\rho}}_s \end{pmatrix} \quad \text{and} \quad \mathsf{H}_{\Gamma_s} = \begin{pmatrix} \mathsf{H}_{\boldsymbol{\rho}_s} & h^d\mathsf{X}_{\alpha_s} \\ h^d\mathsf{X}_{\overline{\alpha}_s} & -\overline{\mathsf{H}}_{\boldsymbol{\rho}_s} \end{pmatrix}.$$

Notice $0 \leq \Gamma_s \leq \mathbf{1}$ is self-adjoint and $\Gamma_s^2 = \Gamma_s$.

Notice that the form of the system (4.16) is almost identical to that of the system (1.5), except for the fact that α_s is symmetric and that there is a 2 in front of $K * \varrho_s$. In particular, we could reuse the argument in Section 2 to obtain a semiclassical limit for equations (4.16) since the discussion in Section 2 is independent of the fact whether α is a symmetric or an anti-symmetric function. In short, Theorem 1.1 remains true for $\boldsymbol{\rho}_s$ and α_s. Moreover, inequalities (4.8) and (4.11) now read

$$\|\boldsymbol{\rho}_\Psi - \boldsymbol{\rho}_s \otimes I\|_{\mathfrak{L}^2(\mathfrak{H})} \le \frac{C}{\sqrt{N}} \exp(\kappa_1 \exp(\kappa_2 t)),$$

$$\|\boldsymbol{\rho}_{\alpha,\Psi} - \boldsymbol{\rho}_{\alpha,s} \otimes I\|_{\mathfrak{L}^1(\mathfrak{H}^{\otimes 2})} \le \frac{C \exp(\kappa_1 \exp(\kappa_2 t))}{N^{(1-c)/2}},$$

if the initial state is SU(2) invariant.

4.3. The joint mean-field and semiclassical limit

It follows from Theorem 4.1 and our main result, Theorem 1.1, that one can obtain a joint limit from the many-body model described above to the Vlasov equation. Indeed, we start by defining the (matrix-valued) Wigner transform for an operator T of the form (4.13) by

$$\mathbf{f}_T(\chi,\xi) = \int_{\mathbb{R}^d} e^{-i\xi\cdot y/\hbar}\, T\Big(\chi + \frac{y}{2}, \chi - \frac{y}{2}\Big)\,\mathrm{d}y,$$

i.e., take the Wigner transform of each entry of T (as, for instance, in [21]). Then, it follows from [37, Corollary 1.1] that

$$\begin{aligned}\|f \otimes I - \mathbf{f}_{\boldsymbol{\rho}_s \otimes I}\|_{H^{-1}(\mathbb{R}^{2d})\otimes \mathbb{C}^{2\times 2}} &= 2\|f - f_{\boldsymbol{\rho}_s}\|_{H^{-1}(\mathbb{R}^{2d})} \\ &\le 2\,\mathrm{W}_{2,\hbar}(f, \boldsymbol{\rho}_s) + 2(1+\sqrt{d})\sqrt{\hbar},\end{aligned}$$

where $f_{\boldsymbol{\rho}_s}$ is the Wigner transform of $\boldsymbol{\rho}_s$ and f is the solution of the Vlasov equation. If $\mathbf{F}_{\boldsymbol{\rho}_{\alpha,s}\otimes I}$ denotes the Wigner transform of $\boldsymbol{\rho}_{\alpha,s} \otimes I$, i.e., $\mathbf{F}_{\boldsymbol{\rho}_{\alpha,s}\otimes I}$ is a 2×2 matrix with entries being functions of $4d$ variables, then it also follows that

$$\begin{aligned}\|F \otimes I - \mathbf{F}_{\boldsymbol{\rho}_{\alpha,s} \otimes I}\|_{H^{-1}(\mathbb{R}^{2d}\times\mathbb{R}^{2d})\otimes \mathbb{C}^{2\times 2}} &= 2\|F - F_{\boldsymbol{\rho}_{\alpha,s}}\|_{H^{-1}(\mathbb{R}^{2d}\times\mathbb{R}^{2d})} \\ &\le 2\,\mathrm{W}_{2,\hbar}(F, \boldsymbol{\rho}_{\alpha,s}) + 2(1+\sqrt{2d})\sqrt{\hbar}.\end{aligned}$$

On the other hand, Theorem 4.1 implies an estimate in H^{-1} for the Wigner transforms since the Wigner transform is an isometry from $\mathfrak{L}^2$ to L^2, and then by the continuous embedding $L^2 \subset H^{-1}$, we have that

$$\|\mathbf{f}_{\boldsymbol{\rho}_\Psi} - \mathbf{f}_{\boldsymbol{\rho}_s\otimes I}\|_{H^{-1}(\mathbb{R}^{2d})\otimes\mathbb{C}^{2\times 2}} \le C\|\mathbf{f}_{\boldsymbol{\rho}_\Psi} - \mathbf{f}_{\boldsymbol{\rho}_s\otimes I}\|_{L^2(X)} = C\|\boldsymbol{\rho}_\Psi - \boldsymbol{\rho}_s \otimes I\|_{\mathfrak{L}^2(\mathfrak{H})}.$$

Similarly, by the isometry property of the Wigner transform and the quantum Sobolev inequality (see [38, Theorem 1]), we have that

$$\|\mathbf{F}_{\boldsymbol{\rho}_{\alpha,\Psi}} - \mathbf{F}_{\boldsymbol{\rho}_{\alpha,s}\otimes I}\|_{H^{-6}(\mathbb{R}^{2d}\times\mathbb{R}^{2d})\otimes\mathbb{C}^{2\times 2}} \le C\|\boldsymbol{\rho}_{\alpha,\Psi} - \boldsymbol{\rho}_{\alpha,s} \otimes I\|_{\mathfrak{L}^1(\mathfrak{H}\otimes\mathfrak{H})}.$$

Let us summarize the result in the following theorem.

Theorem 4.2. *Let K satisfy the conditions of Theorem 1.1 and Theorem 4.1. Assume that the initial data have the forms $\boldsymbol{\rho}^{\mathrm{in}} = \boldsymbol{\rho}_s^{\mathrm{in}} \otimes I$ and $\alpha^{\mathrm{in}} = \alpha_s^{\mathrm{in}} \otimes \sigma^{(2)}$ satisfying conditions (4.6). Furthermore, assume that $\boldsymbol{\rho}_s^{\mathrm{in}}$ and α_s^{in} satisfy the following commutator bounds: there exists $C > 0$ independent of $\hbar$ such that*

$$\sup_{\xi \in \mathbb{R}^d} \frac{1}{1+|\xi|} \| [e^{i\xi\cdot x}, \boldsymbol{\rho}^{\mathrm{in}}] \|_{\mathcal{L}^2} \leq C\sqrt{\hbar}, \quad \| [\nabla, \boldsymbol{\rho}^{\mathrm{in}}] \|_{\mathcal{L}^2} \leq \frac{C}{\sqrt{\hbar}}, \tag{4.18}$$

and $\theta_{\alpha^{\mathrm{in}}} \geq N^{-c}$ with $c \in [1/3, 1]$. Let (f, F) be the solutions of the system (1.17) with initial conditions $(f^{\mathrm{in}}, F^{\mathrm{in}})$ satisfying the conditions of Theorem 1.1. Then, there exist constants $C, \kappa_1, \kappa_2 > 0$ and a polynomial function $\Lambda(t)$, independent of N, such that we have the following estimates:

$$\begin{aligned}
\| \mathbf{f}_{\boldsymbol{\rho}_\Psi} - f \otimes I \|_{H^{-1}(\mathbb{R}^{2d}) \otimes \mathbb{C}^{2\times 2}} &\leq C \frac{\exp(\kappa_1 \exp(\kappa_2 t))}{N^{1/2}} \\
&\quad + \big(\mathrm{W}_{2,\hbar}(f^{\mathrm{in}}, \boldsymbol{\rho}^{\mathrm{in}}) + \mathrm{W}_{2,\hbar}(F^{\mathrm{in}}, \boldsymbol{\rho}_\alpha^{\mathrm{in}}) + \sqrt{\hbar} \big) e^{\Lambda(t)}, \\
\| \mathbf{F}_{\boldsymbol{\rho}_{\alpha,\Psi}} - F \otimes I \|_{H^{-6}(\mathbb{R}^{2d} \times \mathbb{R}^{2d}) \otimes \mathbb{C}^{2\times 2}} &\leq C \frac{\exp(\kappa_1 \exp(\kappa_2 t))}{N^{(1-c)/2}} \\
&\quad + \big(\mathrm{W}_{2,\hbar}(f^{\mathrm{in}}, \boldsymbol{\rho}^{\mathrm{in}}) + \mathrm{W}_{2,\hbar}(F^{\mathrm{in}}, \boldsymbol{\rho}_\alpha^{\mathrm{in}}) + \sqrt{\hbar} \big) e^{\Lambda(t)}.
\end{aligned}$$

Remark 4.2. In this case, the conditions in (4.18) together with the uniform-in-$\hbar$ bound of the total energy imply the conditions (4.7). The fact that the energy is bounded in our case indeed follows from hypothesis (1.18).

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