SECOND ORDER CORRECTIONS TO MEAN FIELD EVOLUTION FOR WEAKLY INTERACTING BOSONS, I

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Abstract. Inspired by the works of Rodnianski and Schlein [31] and Wu [34, 35], we derive a new nonlinear Schrödinger equation that describes a second-order correction to the usual tensor product (mean-field) approximation for the Hamiltonian evolution of a many-particle system in Bose-Einstein condensation. We show that our new equation, if it has solutions with appropriate smoothness and decay properties, implies a new Fock space estimate. We also show that for an interaction potential $v(x) = \epsilon\chi(x)|x|^{-1}$, where ϵ is sufficiently small and $\chi \in C_0^\infty$ even, our program can be easily implemented locally in time. We leave global in time issues, more singular potentials and sophisticated estimates for a subsequent part (part II) of this paper.

1. Introduction

An advance in physics in 1995 was the first experimental observation of atoms with integer spin (Bosons) occupying a macroscopic quantum state (condensate) in a dilute gas at very low temperatures [1, 4]. This phenomenon of Bose-Einstein condensation has been observed in many similar experiments since. These observations have rekindled interest in the quantum theory of large Boson systems. For recent reviews, see e.g. [23, 29].

A system of N interacting Bosons at zero temperature is described by a symmetric wave function satisfying the N-body Schrödinger equation. For large N, this description is impractical. It is thus desirable to replace the many-body evolution by effective (in an appropriate sense) partial differential equations for wave functions in much lower space dimensions. This approach has led to "mean-field" approximations

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in which the single particle wave function for the condensate satisfies nonlinear Schrödinger equations (in 3 + 1 dimensions). Under this approximation, the N-body wave function is viewed simply as a tensor product of one-particle states. For early related works, see the papers by Gross [15, 16], Pitaevskii [28] and Wu [34, 35]. In particular, Wu [34, 35] introduced a *second-order approximation* for the Boson many-body wave function in terms of the *pair-excitation* function, a suitable kernel that describes the scattering of atom *pairs* from the condensate to other states. Wu's formulation forms a nontrivial extension of works by Lee, Huang and Yang [21] for the periodic Boson system. Approximations carried out for pair excitations [21, 34, 35] make use of quantized fields in the Fock space. (The Fock space formalism and Wu's formulation are reviewed in sections 1.1 and 1.3, respectively.)

Connecting mean-field approaches to the actual many-particle Hamiltonian evolution raises fundamental questions. One question is the rigorous derivation and interpretation of the mean field limit. Elgart, Erdős, Schlein and Yau [6, 7, 8, 9, 10, 11] showed rigorously how mean-field limits for Bosons can be extracted in the limit $N \to \infty$ by using Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchies for reduced density matrices. Another issue concerns the convergence of the microscopic evolution towards the mean field dynamics. Recently, Rodnianski and Schlein [31] provided estimates for the rate of convergence in the case with Hartree dynamics by invoking the formalism of Fock space.

In this paper, inspired by the works of Rodnianski and Schlein [31] and Wu [34, 35], we derive a new nonlinear Schrödinger equation describing an improved approximation for the evolution of the Boson system. This approximation offers a second-order correction to the usual tensor product (mean field limit) for the many-body wave function. Our equation yields a corresponding new estimate in Fock space, which complements nicely the previous estimate [31].

The static version of the many-body problem is not studied here. The energy spectrum was addressed by Dyson [5] and by Lee, Huang and Yang [21]. A mathematical proof of the Bose-Einstein condensation for the time-independent case was provided recently by Lieb, Seiringer, Solovej and Yngvanson [22, 23, 24, 25].

1.1. **Fock space formalism.** Next, we review the Fock space $\mathcal{F}$ over $L^2(\mathbb{R}^3)$, following Rodnianski and Schlein [31]. The elements of $\mathcal{F}$ are vectors of the form $\boldsymbol{\psi} = (\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \cdots)$, where $\psi_0 \in \mathbb{C}$ and $\psi_n \in L^2_s(\mathbb{R}^{3n})$ are symmetric in $x_1, \ldots, x_n$. The Hilbert space structure of $\mathcal{F}$ is given by $(\boldsymbol{\phi}, \boldsymbol{\psi}) = \sum_n \int \phi_n \overline{\psi_n} dx$.

For $f \in L^2(\mathbb{R}^3)$ the (unbounded, closed, densely defined) creation operator $a^*(f) : \mathcal{F} \to \mathcal{F}$ and annihilation operator $a(\bar{f}) : \mathcal{F} \to \mathcal{F}$ are defined by

$$\left(a^*(f)\psi_{n-1}\right)(x_1, x_2, \cdots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\psi_{n-1}(x_1, \cdots, x_{j-1}, x_{j+1}, \cdots x_n) \ ,$$

$$\left(a(\overline{f})\psi_{n+1}\right)(x_1, x_2, \cdots, x_n) = \sqrt{n+1} \int \psi_{(n+1)}(x, x_1, \cdots, x_n)\overline{f}(x) \, dx \ .$$

The operator valued distributions a_x^* and a_x defined by

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

These distributions satisfy the canonical commutation relations

$$[a_x, a_y^*] = \delta(x - y) \ , \tag{1}$$
$$[a_x, a_y] = [a_x^*, a_y^*] = 0 \ .$$

Let N be a fixed integer (the total number of particles), and $v(x)$ be an even potential. Consider the Fock space Hamiltonian $H_N : \mathcal{F} \to \mathcal{F}$ defined by

$$\begin{aligned} H_N &= \int a_x^* \Delta a_x dx + \frac{1}{2N} \int v(x-y) a_x^* a_y^* a_x a_y \, dx \, dy \qquad (2) \\ &=: H_0 + \frac{1}{N} V \ . \end{aligned}$$

This H_N is a diagonal operator which acts on each ψ_n in correspondence to the Hamiltonian

$$H_{N,n} = \sum_{j=1}^{n} \Delta_{x_j} + \frac{1}{2N} \sum_{i \neq j} v(x_i - x_j) \ .$$

In the particular case $n = N$, this is the mean field Hamiltonian. Except for the introduction, this paper deals only with the Fock space Hamiltonian. The reader is alerted that "PDE" Hamiltonians such as $H_{N,n}$ will always have two subscripts. The sign of v will not play a role in our analysis. However, the reader is alerted that due to our sign convention, $v \leq 0$ is the "good" sign. The time evolution in the coordinate space for Bose-Einstein condensation deals with the function

$$e^{itH_{n,n}}\psi_0 \tag{3}$$

for tensor product initial data, i.e., if

$$\psi_0(x_1, x_2, \cdots, x_n) = \phi_0(x_1)\phi_0(x_2)\cdots\phi_0(x_n) \ ,$$

where $\|\phi_0\|_{L^2(\mathbb{R}^3)} = 1$. This approach has been highly successful, even for very singular potentials, in the work of Elgart, Erdős, Schlein and Yau [6, 7, 8, 9, 10, 11]. In this context, the convergence of evolution to the appropriate mean field limit (tensor product) as $N \to \infty$ is established at the level of marginal density matrices $\gamma_i^{(N)}$ in the trace norm topology. The density matrices are defined as

$$\gamma_i^{(N)}(t, x_1, \cdots, x_i; x_1', \cdots x_i') = \int \psi(t, x_1, \cdots, x_N)\overline{\psi}(t, x_1', \cdots, x_N')dx_{i+1}\cdots dx_N$$

1.2. **Coherent states.** There are alternative approaches, due to Hepp [17], Ginibre and Velo [13], and, most recently, Rodnianski and Schlein [31] which can treat Coulomb potentials v. These approaches rely on studying the Fock space evolution $e^{itH_N}\boldsymbol{\psi}_0$ where the initial data $\boldsymbol{\psi}_0$ is a coherent state,

$$\boldsymbol{\psi}_0 = (c_0, c_1\phi_0(x_1), c_2\phi_0(x_1)\phi_0(x_2), \cdots) \ ;$$

see (4) below. The evolution (3) can then be extracted as a "Fourier coefficient" from the Fock space evolution; see [31]. Under the assumption that v is a Coulomb potential, this approach leads to strong L^2-convergence, still at the level of the density matrices $\gamma_i^{(N)}$, as we will briefly explain below.

To clarify the issues involved, let us consider the one-particle wave function $\phi(t, x)$ (to be determined later as the solution of a Hartree equation), satisfying the initial condition $\phi(0, x) = \phi_0(x)$. Define the skew-Hermitian unbounded operator

$$A(\phi) = a(\overline{\phi}) - a^*(\phi)$$

and the vacuum state $\Omega = (1, 0, 0, \cdots) \in \mathcal{F}$. Accordingly, consider the operator

$$W(\phi) = e^{-\sqrt{N}A(\phi)} \ ,$$

which is the Weyl operator used by Rodnianski and Schlein [31]. The coherent state for the initial data ϕ_0 is

$$\begin{aligned} \boldsymbol{\psi}_0 &= W(\phi_0)\Omega = e^{-\sqrt{N}A(\phi_0)}\Omega \\ &= e^{-N\|\phi\|^2/2}\left(1, \cdots, \left(\frac{N^n}{n!}\right)^{1/2}\phi_0(x_1)\cdots\phi_0(x_n), \cdots\right) \ . \end{aligned} \tag{4}$$

Hence, the top candidate approximation for $e^{itH_N}\boldsymbol{\psi}_0$ reads

$$\boldsymbol{\psi}_{\text{tensor}}(t) = e^{-\sqrt{N}A(\phi(t,\cdot))}\Omega \ . \tag{5}$$

Rodnianski and Schlein [31] showed that this approximation works (under suitable assumptions on v), in the sense that

$$\frac{1}{N}\| \left(e^{itH_N}\boldsymbol{\psi}_0,\, a_y^* a_x e^{itH_N}\boldsymbol{\psi}_0\right) - \left(e^{-\sqrt{N}A(\phi(t,\cdot))}\Omega,\, a_y^* a_x e^{-\sqrt{N}A(\phi(t,\cdot))}\Omega\right) \|_{\text{Tr}}$$
$$= O(\frac{e^{Ct}}{N}) \qquad N \to \infty \ ;$$

the symbol Tr here stands for the trace norm in $x \in \mathbb{R}^3$ and $y \in \mathbb{R}^3$. The first term in the last relation, including $\frac{1}{N}$, is essentially the density matrix $\gamma_1^{(N)}(t,x,y)$. For the precise statement of the problem and details of the proof, see Theorem 3.1 of Rodnianski and Schlein [31].

Our goal here is to find an explicit approximation for the evolution in the Fock space. For this purpose, we adopt an idea germane to Wu's second-order approximation for the N-body wave function in Fock space [34, 35].

1.3. **Wu's approach.**

We first comment on the case with periodic boundary conditions, when the condensate is the zero-momentum state. For this setting, Lee, Huang and Yang [21] studied systematically the scattering of atoms from the condensate to states of opposite momenta. By diagonalizing an approximation for the Hamiltonian in Fock space, these authors derived a formula for the N-particle wave function that deviates from the usual tensor product, as it expresses excitation of particles from zero monentum to *pairs* of opposite momenta.

For non-periodic settings, Wu [34, 35] invokes the splitting $a_x = a_0(t)\phi(t,x) + a_{x,1}(t)$ where a_0 corresponds to the condensate, $[a_0, a_0^*] = 1$, and $a_{x,1}$ corresponds to states orthogonal to the condensate, $[a_0, a_{x,1}] = 0 = [a_0, a_{x,1}^*]$. Wu applies the following ansatz for the N-body wave function in Fock space:

$$\mathcal{N}(t)\, e^{\mathcal{P}[K_0]}\psi_N^0(t) \ , \tag{6}$$

where $\psi_N^0(t)$ describes the tensor product, $\mathcal{N}(t)$ is a normalization factor, and $\mathcal{P}[K_0]$ is an operator that averages out in space the excitation of particles from the condensate ϕ to other states with the effective kernel (pair excitation function) K_0. An explicit formula for $\mathcal{P}[K_0]$ is

$$\mathcal{P}[K_0] = [2N_0(t)]^{-1} \int a_{x,1}^* a_{y,1}^*\, K_0(t,x,y)\, a_0(t)^2 \ , \tag{7}$$

where N_0 is the expectation value of particle number at the condensate. This K_0 is not a-priori known (in contrast to the case of the classical Boltzmann gas) but is determined by means consistent with the many-body dynamics. In the periodic case, (6) reduces to the many-body wave function of Lee, Huang and Yang [21].

Wu derives a coupled system of dispersive hyperbolic partial differential equations for (ϕ, K_0) via an approximation for the N-body Hamiltonian that is consistent with ansatz (6). A feature of this system is the *spatially nonlocal* couplings induced by K_0. Observable quantities such that the depletion of the condensate can be computed directly from solutions of this PDE system. This system has been solved only in a limited number of cases [35, 26, 27].

1.4. **Scope and outline.** Our objective in this work is to find an explicit approximation for the evolution

$$e^{itH_N}\boldsymbol{\psi}_0$$

in the Fock space norm, where $\boldsymbol{\psi}_0$ is the coherent state (4). This would imply an approximation for the evolution

$$e^{itH_{N,N}}\psi_0$$

in $L^2(\mathbb{R}^{3N})$ as $N \to \infty$. To the best of our knowledge, no such approximation is available in the mathematics or physics literature. In particular, the tensor product type approximation (5) for ϕ satisfying a Hartree equation, as in [31], is not known to be such a Fock space approximation (nor do we expect it to be).

To accomplish our goal, we propose to modify (5) in two ways. One minor correction is the multiplication by an oscillatory term. A second correction is a composition with a second-order "Weyl operator". Both corrections are inspired by the work of Wu [34, 35]; see also [26, 27]. However, our set-up and derived equation is essentially different from these works.

We proceed to describe the second order correction. Let $k(t, x, y) = k(t, y, x)$ be a function (or kernel) to be determined later, with $k(0, x, y) = 0$. The minimum regularity expected of k is $k \in L^2(dx\, dy)$ for a.e. t.

We define the operator

$$B = \frac{1}{2}\int \left(k(t,x,y)a_x a_y - \overline{k}(t,x,y)a_x^* a_y^*\right)\, dx\, dy\ . \tag{8}$$

Notice that B is skew-Hermitian, i.e., iB is self-adjoint. The operator e^B could be defined by the spectral theorem; see [30]. However, we prefer the more direct approach of defining it first on the dense subset of vectors with finitely many non-zero components, where it can be defined by a convergent Taylor series if $\|k\|_{L^2(dxdy)}$ is sufficiently small. Indeed, B restricted to the subspace of vectors with all entries past the first N identically zero has norm $\leq CN\|k\|_{L^2}$. Then e^B is extended to $\mathcal{F}$ as a unitary operator.

Now we have described all ingredients needed to state our results and derivations. The remainder of the paper is organized as follows. In section 2 we state our main result and outline its proof. In section 3 we study implications of the Hartree equation satisfied by the one-particle wave function $\phi(t,x)$. In section 4 we develop bookkeeping tools of Lie algebra for computing requisite operators containing B. In section 5 we study the evolution equation for a matrix K that involves the kernel k. In section 6 we develop an argument for the existence of solution to the equation for the kernel k. In section 7 we find conditions under which terms involved in the error term $e^B V e^{-B}$ are bounded. In section 8 we study similarly the error term $e^B[A,V]e^{-B}$. In section 9 we show that we can control traces needed in derivations.

2. Statement of main result and outline of proof

In this section we state our strategy for general potentials satisfying certain properties. Later in the paper we show that all assumptions of the related theorem are satisfied locally in time for $v(x) = \chi(x)\frac{\epsilon}{|x|}$, ϵ: sufficiently small, and $\chi \in C_0^\infty$: even.

Theorem 2.1. *Suppose that v is an even potential. Let ϕ be a smooth solution of the Hartree equation*

$$i\frac{\partial\phi}{\partial t} + \Delta\phi + (v * |\phi|^2)\phi = 0 \tag{9}$$

with initial conditions ϕ_0, and assume the three conditions listed below:

(1) *Assume that we have $k(t,x,y) \in L^2(dxdy)$ for a.e. t, where k is symmetric, and solves*

$$(iu_t + ug^T + gu - (1+p)m) = (ip_t + [g,p] + u\overline{m})(1+p)^{-1}u \ , \tag{10}$$

where all products in (10) are interpreted as spatial compositions of kernels, "1" is the identity operator, and

$$u(t,x,y) := \mathrm{sh}(k) := k + \frac{1}{3!}k\overline{k}k + \dots \ , \tag{11}$$

$$\delta(x-y) + p(t,x,y) := \mathrm{ch}(k) := \delta(x-y) + \frac{1}{2!}k\overline{k} + \dots \ ,$$

$$g(t,x,y) := -\Delta_x\delta(x-y) - v(x-y)\phi(t,x)\overline{\phi}(t,y) - (v*|\phi|^2)(t,x)\delta(x-y) \ ,$$

$$m(t,x,y) := v(x-y)\overline{\phi}(t,x)\overline{\phi}(t,y) \ .$$

(2) *Also, assume that the functions*

$$f(t) := \|e^{B}[A, V]e^{-B}\Omega\|_{\mathcal{F}}$$

and

$$g(t) := \|e^{B}Ve^{-B}\Omega\|_{\mathcal{F}}$$

are locally integrable (V is defined in (2)).

(3) *Finally, assume that $\int d(t, x, x)\, dx$ is locally integrable in time, where*

$$\begin{aligned} d(t, x, y) = &\big(i\mathrm{sh}(k)_t + \mathrm{sh}(k)g^T + g\mathrm{sh}(k)\big)\,\overline{\mathrm{sh}(k)} \\ &- \left(i\mathrm{ch}(k)_t + [g, \mathrm{ch}(k)]\right)\mathrm{ch}(k) \\ &-\mathrm{sh}(k)\overline{m}\mathrm{ch}(k) - \mathrm{ch}(k)m\overline{\mathrm{sh}(k)}\ . \end{aligned}$$

Then, there exist real functions χ_0, χ_1 such that

$$\begin{aligned} &\|e^{-\sqrt{N}A(t)}e^{-B(t)}e^{-i\int_0^t (N\chi_0(s)+\chi_1(s))ds}\Omega - e^{itH_N}\boldsymbol{\psi}_0\|_{\mathcal{F}} \\ &\le \frac{\int_0^t f(s)ds}{\sqrt{N}} + \frac{\int_0^t g(s)ds}{N}\ . \end{aligned} \tag{12}$$

Recall that we defined (see section 1)

$$\begin{aligned} &\boldsymbol{\psi}_0 = e^{-\sqrt{N}A(0)}\Omega \quad \textit{an arbitrary coherent state (initial data)}\ , \\ &A(t) = a(\overline{\phi}(t,\cdot)) - a^*(\phi(t,\cdot))\ , \\ &B(t) = \frac{1}{2}\int \left(k(t,x,y)a_xa_y - \overline{k}(t,x,y)a^*_xa^*_y\right)\ dx\,dy\ . \end{aligned}$$

A few remarks on Theorem 2.1 are in order.

Remark 2.2. Written explicitly, the left-hand side of (10) equals

$$\begin{aligned} &iu_t + ug^T + gu - (1+p)m = \left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right)u(t,x,y) \\ &- \phi(t,x)\int v(x-z)\overline{\phi}(t,z)u(t,z,y)\ dz - \phi(t,y)\int u(t,x,z)v(z-y)\overline{\phi}(t,z)\ dz \\ &- (v * |\phi|^2)(t,x)u(t,x,y) - (v*|\phi|)^2(t,y)u(t,x,y) \\ &- v(x-y)\overline{\phi}(t,x)\overline{\phi}(t,y) \\ &- \overline{\phi}(t,y)\int (1+p)(t,x,z)v(z-y)\overline{\phi}(t,z)\ dz\ . \end{aligned}$$

The main term in the right-hand side equals

$$
\begin{aligned}
&ip_t + [g,p] + u\overline{m} = i\frac{\partial}{\partial t}p(t,x,y) + \left(-\Delta_x + \Delta_y\right)p(t,x,y)\\
&- \phi(t,x)\int v(x-z)\overline{\phi}(t,z)p(t,z,y)\ dz\\
&+ \phi(t,y)\int p(t,x,z)v(z-y)\overline{\phi}(t,z)\ dz\\
&- (v*|\phi|^2)(t,x)p(t,x,y) + (v*|\phi|)^2(t,y)p(t,x,y)\\
&+ \int u(t,x,z)v(z-y)\phi(t,z)\phi(t,x)\ dz\ .
\end{aligned}
$$

Remark 2.3. The algebra, as well as the local analysis presented in this paper do not depend on the sign of v. However, the global in time analysis of our equations would require v to be non-positive.

Remark 2.4. Our techniques would allow us to consider more general initial data of the form $\boldsymbol{\psi}_0 = e^{-\sqrt{N}A(0)}e^{-B(0)}\Omega$. For convenience, we only consider the case of tensor products ($B(0)=0$) in this paper.

Proof. Since $e^{\sqrt{N}A}$ and e^B are unitary, the left-hand side of (12) equals

$$
\|e^{i\int_0^t(N\chi_0(s)+\chi_1(s))ds}e^{B(t)}e^{\sqrt{N}A(t)}e^{itH_N}e^{-\sqrt{N}A(0)}\Omega - \Omega\|_{\mathcal{F}}\ .
$$

Define

$$
\Psi(t) = e^{B(t)}e^{\sqrt{N}A(t)}e^{itH}e^{-\sqrt{N}A(0)}\Omega\ .
$$

In Corollary 5.2 of section 5 we show that our equations for ϕ, k insure that

$$
\frac{1}{i}\frac{\partial}{\partial t}\Psi = L\Psi\ ,
$$

where $L = \widetilde{L} - N\chi_0 - \chi_1$ for some $\widetilde{L}$: Hermitian, i.e. $\widetilde{L} = \widetilde{L}^*$, where $\widetilde{L}$ commutes with functions of time, χ_0, χ_1 are real functions of time, and, most importantly (see corollary 5.2 of section 5 and the remark following it),

$$
\|\widetilde{L}\Omega\|_{\mathcal{F}} \le N^{-1/2}\|e^B[A,V]e^{-B}\Omega\|_{\mathcal{F}} + N^{-1}\|e^BVe^{-B}\Omega\|_{\mathcal{F}}\ . \tag{13}
$$

We apply energy estimates to

$$
\left(\frac{1}{i}\frac{\partial}{\partial t} - \widetilde{L}\right)\left(e^{i\int_0^t(N\chi_0(s)+\chi_1(s))ds}\Psi - \Omega\right) = \widetilde{L}\Omega\ .
$$

Explicitly,

$$\frac{\partial}{\partial t}\left(\|(e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega)\|_{\mathcal{F}}^2\right)$$
$$=2\Re\left(\frac{\partial}{\partial t}(e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega),\ e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega\right)$$
$$=2\Re\left(\left(\frac{\partial}{\partial t}-i\widetilde{L}\right)(e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega),\ e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega\right)$$
$$=2\Re\left(i\widetilde{L}\Omega,\ e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega\right)$$
$$\leq 2\left(N^{-1/2}\|e^B[A,V]e^{-B}\Omega\|_{\mathcal{F}}+N^{-1}\|e^BVe^{-B}\Omega\|_{\mathcal{F}}\right)\|(e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega)\|_{\mathcal{F}}\ .$$

Thus

$$\frac{\partial}{\partial t}\|(e^{i\int_0^t (N\chi_0(s)+\chi_1)ds}\Psi-\Omega)\|\leq N^{-1/2}\|e^B[A,V]e^{-B}\Omega\|_{\mathcal{F}}+N^{-1}\|e^BVe^{-B}\Omega\|_{\mathcal{F}}\ .$$

and (12) holds. This concludes the proof. □

□

3. The Hartree equation

In this section we see how far we can go by using only the Hartree equation for the one-particle wave function ϕ.

Lemma 3.1. *The following commutation relations hold (where the t dependence is suppressed, A denotes $A(\phi)$ and V is defined by formula* (2)*):*

$$[A,V]=\int v(x-y)\left(\overline{\phi}(y)a_x^*a_xa_y+\phi(y)a_x^*a_y^*a_x\right)\,dx\,dy$$
$$\big[A,[A,V]\big] \tag{14}$$
$$=\int v(x-y)\left(\overline{\phi}(y)\overline{\phi}(x)a_xa_y+\phi(y)\phi(x)a_x^*a_y^*+2\overline{\phi}(y)\phi(x)a_x^*a_y\right)\,dx\,dy$$
$$+2\int\left(v*|\phi^2|\right)(x)a_x^*a_x\,dx$$
$$\Big[A,\big[A,[A,V]\big]\Big]$$
$$=6\int\left(v*|\phi^2|\right)(x)\left(\phi(x)a_x^*+\overline{\phi}(x)a_x\right)\,dx$$
$$\Bigg[A,\Big[A,\big[A,[A,V]\big]\Big]\Bigg]$$
$$=12\int\left(v*|\phi^2|\right)(x)|\phi(x)|^2\,dx\ .$$

Proof. This is an elementary calculation and is left to the interested reader. □

Now, we consider $\Psi_1(t) = e^{\sqrt{N}A(t)}e^{itH}e^{-\sqrt{N}A(0)}\Omega$ for which we have the basic calculation in the spirit of Hepp [17], Ginibre-Velo [13], and Rodnianski-Schlein [31]; see equation (3.7) in [31].

Proposition 3.2. *If ϕ satisfies the Hartree equation*

$$i\frac{\partial \phi}{\partial t} + \Delta\phi + (v * |\phi|^2)\phi = 0$$

while

$$\Psi_1(t) = e^{\sqrt{N}A(t)}e^{itH}e^{-\sqrt{N}A(0)}\Omega \ ,$$

then $\Psi_1(t)$ satisfies

$$\frac{1}{i}\frac{\partial}{\partial t}\Psi_1(t) = \Bigg(H_0 + \frac{1}{2}[A,[A,V]]$$
$$+N^{-1/2}[A,V] + N^{-1}V - \frac{N}{2}\int v(x-y)|\phi(t,x)|^2|\phi(t,y)|^2 dx\, dy\Bigg)\Psi_1(t) \ .$$

Proof. Recall the formulas

$$\left(\frac{\partial}{\partial t}e^{C(t)}\right)\left(e^{-C(t)}\right) = \dot{C} + \frac{1}{2!}[C,\dot{C}] + \frac{1}{3!}\big[C,[C,\dot{C}]\big] + \dots$$

and

$$e^C H e^{-C} = H + [C,H] + \frac{1}{2!}\big[C,[C,H]\big] + \dots \ .$$

Applying these relations to $C = \sqrt{N}A$ we get

$$\frac{1}{i}\frac{\partial}{\partial t}\psi_1(t) = L_1\psi_1 \ , \tag{15}$$

where

$$L_1 = \frac{1}{i}\left(\frac{\partial}{\partial t}e^{\sqrt{N}A(t)}\right)e^{-\sqrt{N}A(t)} + e^{\sqrt{N}A(t)}He^{-\sqrt{N}A(t)}$$
$$=\frac{1}{i}\left(N^{1/2}\dot{A} + \frac{N}{2}[A,\dot{A}]\right) + H + N^{1/2}[A,H_0]$$
$$+ N^{-1/2}[A,V] + \frac{N}{2}\big[A,[A,H_0]\big]$$
$$\frac{1}{2}\big[A,[A,V]\big] + \frac{N^{1/2}}{3!}\Big[A,\big[A,[A,V]\big]\Big] + \frac{N}{4!}\Big[A,\Big[A,\big[A,[A,V]\big]\Big]\Big] \ .$$

Eliminating the terms with a weight of $\sqrt{N}$, or setting

$$\frac{1}{i}\dot{A} + [A, H_0] + \frac{1}{3!}\Big[A, \big[A, [A, V]\big]\Big] = 0 \ , \tag{16}$$

is exactly equivalent to the Hartree equation (9). By taking an additional bracket with A in (16), we have

$$\frac{1}{i}[A, \dot{A}] + \big[A, [A, H_0]\big] + \frac{1}{3!}\Bigg[A, \Big[A, \big[A, [A, V]\big]\Big]\Bigg] = 0 \ ,$$

and thus simplify (15) to

$$\frac{1}{i}\frac{\partial}{\partial t}\psi_1(t) = \Bigg(H_0 + \frac{1}{2}[A, [A, V]]$$

$$+N^{-1/2}[A, V] + N^{-1}V - N\frac{1}{4!}\Bigg[A, \Big[A, \big[A, [A, V]\big]\Big]\Bigg]\Bigg)\psi_1 \ .$$

This concludes the proof. □

□

The first two terms on the right-hand side are the main ones. The next two terms are $O\left(\frac{1}{\sqrt{N}}\right)$ and $O\left(\frac{1}{N}\right)$. The last term equals

$$-\frac{N}{2}\int v(x-y)|\phi(t,x)|^2|\phi(t,y)|^2 dx\, dy := -N\chi_0 \ .$$

Notice that $\|L_1(\Omega)\|$ is not small because of the presence of $a^*_x a^*_y$ in $\big[A, [A, V]\big]$. In order to eliminate these terms, we introduce B (see (8)) and take

$$\psi = e^B \psi_1 \ .$$

Accordingly, we compute

$$\frac{1}{i}\frac{\partial}{\partial t}\psi = L\psi \ ,$$

where

$$L = \frac{1}{i}\left(\frac{\partial}{\partial t}e^B\right)e^{-B} + e^B L_1 e^{-B}$$

$$= L_Q + N^{-1/2}e^B[A, V]e^{-B} + N^{-1}e^B V e^{-B} - N\chi_0 \ ,$$

and

$$L_Q = \frac{1}{i}\left(\frac{\partial}{\partial t}e^B\right)e^{-B} + e^B\left(H_0 + \frac{1}{2}\big[A, [A, V]\big]\right)e^{-B} \tag{17}$$

contains all quadratics in the operators a, a^*.

Equation (10) for k turns out to be equivalent to the requirement that L has no terms of the form a^*a^* . Terms of the form aa^* will occur, and will be converted to a^*a at the expense of χ_1.

In other words, we require that L_Q have no terms of the form a^*a^*. For a similar argument (but for a different set-up), see Wu [35].

4. The Lie algebra of "symplectic matrices"

In this section we describe the bookkeeping tools needed to compute L_Q of (17) in closed form. The results of this section are essentially standard, but they are included here for the sake of completeness.

We start with the remark that

$$[a(f_1) + a^*(g_1), a(f_2) + a^*(g_2)] = \int f_1 g_2 - f_2 g_1 \tag{18}$$
$$= -\begin{pmatrix} f_1 & g_1 \end{pmatrix} J \begin{pmatrix} f_2 \\ g_2 \end{pmatrix}$$

where

$$J = \begin{pmatrix} 0 & -\delta(x-y) \\ \delta(x-y) & 0 \end{pmatrix}.$$

This observation explains why we have to invoke symplectic linear algebra. We thus consider the infinite-dimensional Lie algebra sp of "matrices" of the form

$$S(d,k,l) = \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix}$$

for symmetric kernels $k = k(t,x,y)$ and $l = l(t,x,y)$, and arbitrary kernel $d(t,x,y)$. (The dependence on t will be suppressed when not needed.) This situation is analogous to the Lie algebra of the finite-dimensional complex symplectic group, with x, y playing the role of i and j. We also consider the Lie algebra $Quad$ of quadratics of the form

$$Q(d,k,l) := \frac{1}{2}\begin{pmatrix} a_x & a_x^* \end{pmatrix} \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} \begin{pmatrix} -a_y^* \\ a_y \end{pmatrix} \tag{19}$$
$$= -\int d(x,y)\frac{a_x a_y^* + a_y^* a_x}{2}\, dx\, dy + \frac{1}{2}\int k(x,y) a_x a_y\, dx\, dy$$
$$- \frac{1}{2}\int l(x,y) a_x^* a_y^*\, dx\, dy$$

(k, l and d as before). Furthermore, we agree to identify operators which differ (formally) by a scalar operator. Thus, $\int d(x,y) a_x a_y^*$ is considered equivalent to $\int d(x,y) a_y^* a_x$. We recall the following result related to the metaplectic representation (see, e.g. [12]).

Theorem 4.1. *Let $S = S(d,k,l)$, $Q = Q(d,k,l)$ related as above. Let f, g be functions (or distributions). Denote*

$$(a_x, a_x^*) \begin{pmatrix} f \\ g \end{pmatrix} := \int \left(f(x) a_x + g(x) a_x^* \right) dx \ .$$

We have the following commutation relation:

$$[Q, (a_x, a_x^*) \begin{pmatrix} f \\ g \end{pmatrix}] = (a_x, a_x^*) S \begin{pmatrix} f \\ g \end{pmatrix} \tag{20}$$

where products are interpreted as compositions. We also have

$$e^Q (a_x, a_x^*) \begin{pmatrix} f \\ g \end{pmatrix} e^{-Q} = (a_x, a_x^*) e^S \begin{pmatrix} f \\ g \end{pmatrix} \ , \tag{21}$$

provided that e^Q makes sense as a unitary operator (Q: skew-Hermitian).

Proof. The commutation relation (20) can be easily checked directly, but we point out that it follows from (18). In fact, using (18), for any rank one quadratic we have

$$\begin{aligned} &[(a(f_1) + a^*(g_1))\,(a(f_2) + a^*(g_2))\,, a(f) + a^*(g)] \\ &= -\begin{pmatrix} a_x & a_x^* \end{pmatrix} \left(\begin{pmatrix} f_2 \\ g_2 \end{pmatrix} \begin{pmatrix} f_1 & g_1 \end{pmatrix} + \begin{pmatrix} f_1 \\ g_1 \end{pmatrix} \begin{pmatrix} f_2 & g_2 \end{pmatrix} \right) J \begin{pmatrix} f \\ g \end{pmatrix} \ . \end{aligned}$$

Thus, for any R we have

$$[\begin{pmatrix} a_x & a_x^* \end{pmatrix} R \begin{pmatrix} a_y \\ a_y^* \end{pmatrix}, a(f) + a^*(g)] = -\begin{pmatrix} a_x & a_x^* \end{pmatrix} \left(R + R^T \right) J \begin{pmatrix} f \\ g \end{pmatrix} \ .$$

Now specialize to $R = \frac{1}{2} SJ$, $S \in sp$, and use $S^T = JSJ$ to complete the proof.

The second part, equation (21), follows from the identity

$$e^Q C e^{-Q} = C + [Q, C] + \frac{1}{2!} \left[Q, [Q, C] \right] + \dots \ ,$$

or, in the language of adjoint representations, $\mathrm{Ad}(e^Q)(C) = e^{\mathrm{ad}(Q)}(C)$, which is applied to $C = a(f) + a^*(g)$. □

□

A closely related result is provided by the following theorem.

Theorem 4.2. (1) *The linear map $\mathcal{I} : sp \to Quad$ defined by*

$$S(d,k,l) \to Q(d,k,l)$$

is a Lie algebra isomorphism.

(2) *Moreover, if $S = S(t)$, $Q = Q(t)$ and $\mathcal{I}(S(t)) = Q(t)$ is skew-Hermitian, so that e^Q is well defined, we have*

$$\mathcal{I}\left(\left(\frac{\partial}{\partial t}e^S\right)e^{-S}\right) = \left(\frac{\partial}{\partial t}e^Q\right)e^{-Q} \ . \tag{22}$$

(3) *Also, if $R \in sp$, we have*

$$\mathcal{I}\left(e^S R e^{-S}\right) = e^Q \mathcal{I}(R) e^{-Q} \ . \tag{23}$$

Remark 4.3. In the finite-dimensional case, this is (closely related to) the "infinitesimal metaplectic representation"; see p. 186 in [12] . In the infinite dimensional case, we must be careful, as some of our operators are not of trace class. For instance, $\int a_x a_x^*$ does not make sense.

Proof. First, we point out that (21) implies (23), at least in the case where R is the "rank one" matrix

$$R = \begin{pmatrix} f \\ g \end{pmatrix} \begin{pmatrix} h & i \end{pmatrix} \ .$$

Notice that (21) can also be written as

$$e^Q \begin{pmatrix} f & g \end{pmatrix} \begin{pmatrix} a_x \\ a_x^* \end{pmatrix} e^{-Q} = \begin{pmatrix} f & g \end{pmatrix} e^{S^T} \begin{pmatrix} a_x \\ a_x^* \end{pmatrix} \ .$$

In conclusion, we find

$$\begin{aligned}
&e^Q \begin{pmatrix} a_x & a_x^* \end{pmatrix} R \begin{pmatrix} -a_y^* \\ a_y \end{pmatrix} e^{-Q} \\
&= e^Q \begin{pmatrix} a_x & a_x^* \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \begin{pmatrix} h & i \end{pmatrix} J \begin{pmatrix} a_y \\ a_y^* \end{pmatrix} e^{-Q} \\
&= e^Q \begin{pmatrix} a_x & a_x^* \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} e^{-Q} e^Q \begin{pmatrix} h & i \end{pmatrix} J \begin{pmatrix} a_y \\ a_y^* \end{pmatrix} e^{-Q} \\
&= \begin{pmatrix} a_x & a_x^* \end{pmatrix} e^S \begin{pmatrix} f \\ g \end{pmatrix} \begin{pmatrix} h & i \end{pmatrix} J e^{JSJ} \begin{pmatrix} a_y \\ a_y^* \end{pmatrix} \\
&= \begin{pmatrix} a_x & a_x^* \end{pmatrix} e^S R e^{-S} \begin{pmatrix} -a_y^* \\ a_y \end{pmatrix}
\end{aligned}$$

since $S^T = JSJ$ if $S \in sp$, and $Je^{JSJ} = e^{-S}J$.

We now give a direct proof that (19) preserves Lie brackets. Denote the quadratic building blocks by $Q_{xy} = a_x a_y$, $Q^*_{xy} = a^*_x a^*_y$, $N_{xy} = \frac{1}{2}\left(a_x a_y^* + a_y^* a_x\right)$. One can verify the following commutation relations, which will be also needed below:

$$\left[Q_{xy}, Q^*_{zw}\right] = \delta(x-z)N_{yw} + \delta(x-w)N_{yz} + \delta(y-z)N_{xw} + \delta(y-w)N_{xz} \ , \tag{24}$$

$$\left[Q_{xy}, N_{zw}\right] = \delta(x-w)Q_{yz} + \delta(y-w)Q_{xz} \ , \tag{25}$$

$$\left[N_{xy}, Q^*_{zw}\right] = \delta(x-z)Q^*_{yw} + \delta(x-w)Q_{yz} \ , \tag{26}$$

$$\left[N_{xy}, N_{zw}\right] = \delta(x-w)N_{zy} - \delta(y-z)N_{xw} \ . \tag{27}$$

Using (24) we compute

$$\left[\frac{1}{2}\int k(x,y)a_x a_y dxdy, -\frac{1}{2}\int l(x,y)a^*_x a^*_y dxdy\right] = -\int (kl)(x,y)N_{xy}\ dx\,dy \ ,$$

which corresponds to the relation

$$\left[\begin{pmatrix} 0 & k \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ l & 0 \end{pmatrix}\right]$$
$$= \begin{pmatrix} kl & 0 \\ 0 & -lk \end{pmatrix}.$$

The other three cases are similar.

To prove (22), expand both the left-hand side and the right-hand side as

$$\mathcal{I}\left(\left(\frac{\partial}{\partial t}e^S\right)e^{-S}\right)$$
$$= \mathcal{I}\left(\dot{S} + \frac{1}{2}[S,\dot{S}] + \cdots\right)$$
$$= \dot{Q} + \frac{1}{2}[Q,\dot{Q}] + \cdots$$
$$= \left(\frac{\partial}{\partial t}e^Q\right)e^{-Q} \ .$$

The proof of (23) is along the same lines. □

□

Remark 4.4. Note on rigor: All the Lie algebra results that we have used are standard in the finite-dimensional case. In our applications, S will be K where K is a matrix of the form (29), see below, and Q will be $B = \mathcal{I}(K)$. The unbounded operator B is skew-Hermitian and $e^B\psi$ is defined by a convergent Taylor series if $\psi \in \mathcal{F}$ has only finitely many non-zero components, provided $\|k(t,\cdot,\cdot)\|_{L^2(dx\,dy)}$ is small . We then extend e^B to all $\mathcal{F}$ as a unitary operator. The norm $\|k(t,\cdot,\cdot)\|_{L^2(dx\,dy)}$

iterates under compositions; thus, the kernel e^K is well defined by its convergent Taylor expansion. In the expression

$$e^B P e^{-B} = P + [B, P] + \dots \tag{28}$$

for P, a first- or second-order polynomial in a, a^*, we point out that the right-hand side stays a polynomial of the same degree, and converges when applied to a Fock space vector with finitely many non-zero components. For our application, we need to know (28) is true when applied to Ω. The same comment applies to the series

$$\left(\frac{\partial}{\partial t} e^B\right) e^{-B} = \dot{B} + \frac{1}{2}[B, \dot{B}] + \dots \ .$$

5. Equation for kernel k

Now apply the isomorphism of the previous section to the operator

$$B = \mathcal{I}(K)$$

for

$$K = \begin{pmatrix} 0 & k(t,x,y) \\ \overline{k}(t,x,y) & 0 \end{pmatrix} \ . \tag{29}$$

This agrees to the letter with the isomorphism (19). The next two isomorphisms, (30) and (31), require special treatment because aa^* terms mirroring the a^*a terms are missing in (2), (14). However, the discrepancy only happens on the diagonal. Once the relevant terms are commuted with B, they fit the pattern exactly. It isn't quite true that

$$\begin{aligned} H_0 =& \mathcal{I}\left(\begin{pmatrix} -(\Delta\delta)(x-y) & 0 \\ 0 & (\Delta\delta)(x-y) \end{pmatrix}\right) \\ =& \mathcal{I}\left(\begin{pmatrix} -\Delta & 0 \\ 0 & \Delta \end{pmatrix}\right) \end{aligned} \tag{30}$$

since, strictly speaking,

$$\mathcal{I}\left(\begin{pmatrix} -(\Delta\delta)(x-y) & 0 \\ 0 & (\Delta\delta)(x-y) \end{pmatrix}\right) = \int \frac{a_x^* \Delta a_x + a_x \Delta a_x^*}{2} dx$$

is undefined. However, one can compute directly that $[\Delta_x a_x, a_y^*] = (\Delta\delta)(x-y)$. Using that, we compute

$$[B, H_0] = \frac{1}{2} \int \left((\Delta_x + \Delta_y) k(x,y) a_x a_y + (\Delta_x + \Delta_y)\overline{k}(x,y) a_x^* a_y^*\right) \ dx\, dy \ .$$

This commutator is in agreement with (29), (30), and the result can be represented in accordance with (19), namely

$$[B, H_0] = \mathcal{I}\left(\left[\begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix}, \begin{pmatrix} -(\Delta\delta)(x-y) & 0 \\ 0 & (\Delta\delta)(x-y) \end{pmatrix}\right]\right) .$$

We also have

$$e^B H_0 e^{-B} - H_0$$
$$= \mathcal{I}\left(e^K \begin{pmatrix} -(\Delta\delta)(x-y) & 0 \\ 0 & (\Delta\delta)(x-y) \end{pmatrix} e^{-K} - \begin{pmatrix} -(\Delta\delta)(x-y) & 0 \\ 0 & (\Delta\delta)(x-y) \end{pmatrix}\right)$$

since $e^B H_0 e^{-B} - H_0 = [B, H_0] + \frac{1}{2}\big[B, [B, H_0]\big] + \cdots$ The same comment applies to the diagonal part of

$$\frac{1}{2}\big[A, [A, V]\big] =$$
$$\mathcal{I}\begin{pmatrix} -v_{12}\overline{\phi}_1\phi_2 - (v * |\phi|^2)\,\delta_{12} & v_{12}\overline{\phi}_1\overline{\phi}_2 \\ -v_{12}\phi_1\phi_2 & v_{12}\phi_1\overline{\phi}_2 + (v * |\phi|^2)\,\delta_{12} \end{pmatrix}, \tag{31}$$

where $v_{12}\phi_1\phi_2$ is an abbreviation for the product $v(x-y)\phi(x)\phi(y)$, etc. Formula (31) isn't quite true either, but becomes true after commuting with B.

To apply our isomorphism, we quarantine the "bad" terms in (30) and the diagonal part of (31). Define

$$G = \begin{pmatrix} g & 0 \\ 0 & -g^T \end{pmatrix} \qquad \text{and} \qquad M = \begin{pmatrix} 0 & m \\ -\overline{m} & 0 \end{pmatrix}$$

where

$$g = -\Delta\delta_{12} - v_{12}\overline{\phi}_1\phi_2 - (v * |\phi|^2)\delta_{12} ,$$
$$m = v_{12}\overline{\phi}_1\overline{\phi}_2 ,$$

and split

$$H_0 + \frac{1}{2}\big[A, [A, V]\big] = H_G + \mathcal{I}(M)$$

where

$$H_G = H_0 + \int v(x-y)\overline{\phi}(y)\phi(x)a_x^* a_y \, dx\, dy$$
$$+ \int \big(v * |\phi^2|\big)(x) a_x^* a_x \, dx . \tag{32}$$

By the above discussion we have

$$[B, H_G] = \mathcal{I}([K, G]) \qquad \text{and}$$
$$[e^B, H_G]e^{-B} = \mathcal{I}([e^K, G]e^{-K}) .$$

Write

$$
\begin{aligned}
L_Q =& \frac{1}{i}\left(\frac{\partial}{\partial t}e^B\right)e^{-B}\\
&+e^B\left(H_0+\frac{1}{2}\big[A,[A,V]\big]\right)e^{-B}\\
=&\frac{1}{i}\left(\frac{\partial}{\partial t}e^B\right)e^{-B}\\
&+H_G+[e^B,H_G]e^{-B}+e^B\mathcal{I}(M)e^{-B}\\
=&H_G+\mathcal{I}\left(\left(\frac{1}{i}\frac{\partial}{\partial t}e^K\right)e^{-K}+[e^K,G]e^{-K}+e^KMe^{-K}\right)\\
&= H_G+\mathcal{I}(\mathcal{M}_1+\mathcal{M}_2+\mathcal{M}_3)\ .
\end{aligned} \tag{33}
$$

Notice that if K is given by (29), then

$$e^K=\begin{pmatrix}\mathrm{ch}(k) & \mathrm{sh}(k)\\ \overline{\mathrm{sh}(k)} & \overline{\mathrm{ch}(k)}\end{pmatrix},$$

where

$$\mathrm{ch}(k)=I+\frac{1}{2}k\overline{k}+\frac{1}{4!}k\overline{k}k\overline{k}+\dots\ , \tag{34}$$

and similarly for $\mathrm{sh}(k)$. Products are interpreted, of course, as compositions of operators.

We compute

$$
\begin{aligned}
\mathcal{M}_1 =& \frac{1}{i}\begin{pmatrix}\mathrm{ch}(k)_t & \mathrm{sh}(k)_t\\ \overline{\mathrm{sh}(k)}_t & \overline{\mathrm{ch}(k)}_t\end{pmatrix}\begin{pmatrix}\overline{\mathrm{ch}(k)} & -\mathrm{sh}(k)\\ -\overline{\mathrm{sh}(k)} & \mathrm{ch}(k)\end{pmatrix}\\
=&\frac{1}{i}\begin{pmatrix}\mathrm{ch}(k)_t\mathrm{ch}(k)-\mathrm{sh}(k)_t\overline{\mathrm{sh}(k)} & -\mathrm{ch}(k)_t\mathrm{sh}(k)+\mathrm{sh}(k)_t\overline{\mathrm{ch}(k)}\\ * & *\end{pmatrix}
\end{aligned}
$$

$$[e^K,G]=\begin{pmatrix}[\mathrm{ch}(k),g] & -\mathrm{sh}(k)g^T-g\mathrm{sh}(k)\\ * & *\end{pmatrix}$$

and

$$
\begin{aligned}
&\mathcal{M}_2=[e^K,G]e^{-K}=\\
&\begin{pmatrix}[\ \mathrm{ch},g]\ \mathrm{ch}+(\mathrm{sh}g^T+g\mathrm{sh})\overline{\mathrm{sh}} & -[\ \mathrm{ch},g]\mathrm{sh}-(\mathrm{sh}g^T+g\mathrm{sh})\overline{\mathrm{ch}}\\ * & *\end{pmatrix}\ ,
\end{aligned}
$$

where sh is an abbreviation for $\mathrm{sh}(k)$, etc, and

$$\mathcal{M}_3=e^KMe^{-K}=\begin{pmatrix}-\mathrm{sh}\overline{m}\ \mathrm{ch}-\ \mathrm{ch}m\overline{\mathrm{sh}} & \mathrm{sh}\overline{m}\mathrm{sh}+\ \mathrm{ch}m\overline{\mathrm{ch}}\\ * & *\end{pmatrix}\ .$$

Now define

$$\mathcal{M} = \mathcal{M}_1 + \mathcal{M}_2 + \mathcal{M}_3 \ .$$

We have proved the following theorem.

Theorem 5.1. *Recall the isomorphism* (19) *of Theorem 4.2.*

(1) *If* L_Q *is given by* (17)*, then*

$$\begin{aligned} L_Q =& H_0 + \int v(x-y)\overline{\phi}(y)\phi(x)a_x^* a_y \, dx\, dy \\ &+ \int \left(v * |\phi^2|\right)(x) a_x^* a_x \, dx + \mathcal{I}\left(\mathcal{M}\right) \ . \end{aligned} \tag{35}$$

(2) *The coefficient of* $a_x a_y$ *in* $\mathcal{I}(\mathcal{M})$ *is* $-\mathcal{M}_{12}$ *or*

$$\begin{aligned} &(i\mathrm{sh}(k)_t + \mathrm{sh}(k)g^T + g\mathrm{sh}(k))\overline{\mathrm{ch}(k)} - (i\mathrm{ch}(k)_t - [\mathrm{ch}(k), g])\mathrm{sh}(k) \\ &- \mathrm{sh}(k)\overline{m}\mathrm{sh}(k) - \mathrm{ch}(k)m\overline{\mathrm{ch}(k)} \ . \end{aligned}$$

(3) *The coefficient of* $a_x^* a_y^*$ *equals minus the complex conjugate of the coefficient of* $a_x a_y$*.*

(4) *The coefficient of* $-\frac{a_x a_y^* + a_y^* a_x}{2}$ *is* $\mathcal{M}_{11}$*, or*

$$\begin{aligned} d(t,x,y) = &\left(i\mathrm{sh}(k)_t + \mathrm{sh}(k)g^T + g\mathrm{sh}(k)\right)\overline{\mathrm{sh}(k)} \\ &- \left(i\mathrm{ch}(k)_t + [g, \mathrm{ch}(k)]\right)\mathrm{ch}(k) \\ &-\mathrm{sh}(k)\overline{m}\mathrm{ch}(k) - \mathrm{ch}(k)m\overline{\mathrm{sh}(k)} \ . \end{aligned} \tag{36}$$

Corollary 5.2. *If* ϕ *and* k *satisfy* (9) *and* (10) *of theorem* (2.1)*, then the coefficients of* $a_x a_y$ *and* $a_x^* a_y^*$ *drop out and* L_Q *becomes*

$$\begin{aligned} L_Q =& H_0 + \int v(x-y)\overline{\phi}(t,y)\phi(t,x)a_x^* a_y \, dx\, dy + \int \left(v * |\phi^2|\right)(x) a_x^* a_x \, dx \\ &- \int d(t,x,y)\frac{a_x a_y^* + a_y^* a_x}{2} \, dx\, dy \ , \end{aligned}$$

where d *is given by* (36) *and the full operator reads*

$$\begin{aligned} L =& H_0 + \int v(x-y)\overline{\phi}(y)\phi(t,x)a_x^* a_y dx dy + \int \left(v * |\phi^2|\right)(x) a_x^* a_x dx \\ &- \int d(t,x,y)a_y^* a_x dx + N^{-1/2}e^B[A,V]e^{-B} + N^{-1}e^B V e^{-B} - N\chi_0 - \chi_1 \\ &:= \widetilde{L} - N\chi_0 - \chi_1 \ , \end{aligned}$$

and

$$\chi_0 = \frac{1}{2}\int v(x-y)|\phi(t,x)|^2|\phi(t,y)|^2 dx\, dy \ ,$$

$$\chi_1(t) = -\frac{1}{2}\int d(t,x,x)dx \ .$$

Remark 5.3. Notice that

$$\widetilde{L}\Omega = \left(N^{-1/2}e^B[A,V]e^{-B} + N^{-1}e^BVe^{-B}\right)\Omega \ ,$$

and therefore we can derive the bound

$$\|\widetilde{L}\Omega\| \le N^{-1/2}\|e^B[A,V]e^{-B}\Omega\| + N^{-1}\|e^BVe^{-B}\Omega\| \ .$$

Also, L is (formally) self-adjoint by construction. The kernel $d(t,x,y)$, being the sum of the (1,1) entry of the self-adjoint matrices $\left(\frac{1}{i}\frac{\partial}{\partial t}e^K\right)e^{-K}$, $[e^K, G]e^{-K} = e^KGe^{-K} - G$ and the visibly self-adjoint term $-\mathrm{sh}(k)\overline{m}\mathrm{ch}(k) - \mathrm{ch}(k)m\overline{\mathrm{sh}(k)}$, is self-adjoint; thus, it has a real trace. Hence, $\widetilde{L}$ is also self-adjoint.

In the remainder of this paper, we check that the hypotheses of our main theorem are satisfied, locally in time, for the potential $v(x) = \chi(x)\frac{\epsilon}{|x|}$.

6. Solutions to equation (10)

Theorem 6.1. *Let ϵ_0 be sufficiently small and assume that $v(x) = \frac{\epsilon_0}{|x|}$, or $v(x) = \chi(x)\frac{\epsilon_0}{|x|}$ for $\chi \in C_0^\infty(\mathbb{R}^3)$. Assume that ϕ is a smooth solution to the Hartree equation (16), $\|\phi\|_{L^2(dx)} = 1$. Then there exists $k \in L^\infty([0,1])L^2(dxdy)$ solving (10) with initial conditions $k(0,x,y) = 0$ for $0 \le t \le 1$. The solution k satisfies the following additional properties.*

(1)
$$\|\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right)k\|_{L^\infty[0,1]L^2(dxdy)} \le C \ .$$

(2)
$$\|\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right)\mathrm{sh}(k)\|_{L^\infty[0,1]L^2(dxdy)} \le C \ .$$

(3)
$$\|\left(i\frac{\partial}{\partial t} - \Delta_x + \Delta_y\right)p\|_{L^\infty[0,1]L^2(dxdy)} \le C \ .$$

(4) *The kernel k agrees on $[0,1]$ with a kernel $\widetilde{k}$ for which*

$$\|\widetilde{k}\|_{X^{\frac{1}{2},\frac{1}{2}+}} \le C \ ;$$

see (38) for the definition of the space $X^{s,\delta}$ and, of course, $\frac{1}{2}+$ denotes a fixed number slightly bigger than $\frac{1}{2}$.

Proof. We first establish some notation. Let S denote the Schrödinger operator

$$S = i\frac{\partial}{\partial t} - \Delta_x - \Delta_y$$

and let T be the transport operator

$$T = i\frac{\partial}{\partial t} - \Delta_x + \Delta_y \ .$$

Let $\epsilon : L^2(dxdy) \to L^2(dxdy)$ denote schematically any linear operator of operator norm $\leq C\epsilon_0$, where C is a "universal constant". In practice, ϵ will be (composition with) a kernel of the type $\phi(t,x)\phi(t,y)v(x-y)$, or multiplication by $v * |\phi|^2$. Also, recall the inhomogeneous term

$$m(t,x,y) = v(x-y)\overline{\phi}(t,x)\overline{\phi}(t,y) \ .$$

Then, equation (10), written explicitly, becomes

$$Sk = m + S(k-u) + \epsilon(u) + \epsilon(p) + (Tp + \epsilon(p) + \epsilon(u))(1+p)^{-1}u \ . \quad (37)$$

Note that $\mathrm{ch}(k)^2 - \mathrm{sh}(k)\overline{\mathrm{sh}(k)} = 1$; thus, $1 + p = \mathrm{ch}(k) \geq 1$ as an operator and $(1+p)^{-1}$ is bounded from L^2 to L^2. We plan to iterate in the norm $N(k) = \|k\|_{L^\infty[0,1]L^2(dxdy)} + \|Sk\|_{L^\infty[0,1]L^2(dxdy)}$. Notice that $\|m\|_{L^2(dxdy)} \leq C\epsilon_0$.

Now solve

$$Sk_0 = m$$

with initial conditions $k_0(0,\cdot,\cdot) = 0$, where $N(k_0) \leq C\epsilon_0$. Define u_0, p_0 corresponding to k_0.

For the next iterate, solve

$$Sk_1 = m + S(k_0 - u_0) + \epsilon(u_0) + \epsilon(p_0) + (Tp_0 + \epsilon(p_0) + \epsilon(u_0))(1+p_0)^{-1}u_0 \ ;$$

the non-linear terms satisfy

$$\begin{aligned} &\|S(u_0 - k_0)\|_{L^\infty[0,1]L^2(dxdy)} = \\ &\|\frac{1}{3!}\left((Sk_0)\overline{k}_0 k_0 - k_0\overline{(Sk_0)}k_0 + k_0\overline{k}_0 Sk_0\right) + \cdots \|_{L^\infty[0,1]L^2(dxdy)} \\ &= O(N(k_0)^3) \ . \end{aligned}$$

Also, recalling that $p_0 = \mathrm{ch}(k_0) - 1$, we have

$$\begin{aligned} \|T(p_0)\|_{L^\infty[0,1]L^2(dxdy)} &= \|\frac{1}{2}\left((Sk_0)\overline{k}_0 - k_0\overline{(Sk_0)}\right) + \cdots \|_{L^\infty[0,1]L^2(dxdy)} \\ &= O\left(N(k_0)^2\right) \ . \end{aligned}$$

Thus, $N(k_1) \leq C\epsilon_0 + C\epsilon_0^2$. Continuing this way, we obtain a fixed point solution in this space which satisfies the first three requirements of theorem 6.1.

In fact, we can apply the same argument to $\left(\frac{\partial}{\partial t}\right)^N D^a k$, since $\left(\frac{\partial}{\partial t}\right)^N D^a m \in L^\infty[0,1]L^2(dx\,dy)$ for $0 \le a < \frac{1}{2}$. However, we cannot repeat the argument for $D^{1/2}k$.

We would like to have $\|SD^{1/2}k\|_{L^\infty[0,1]L^2(dx\,dy)}$ finite. Unfortunately, this misses "logarithmically" because of the singularity of v.

Fortunately, we can use the well-known $X^{s,\delta}$ spaces (see [2, 18, 20]) to show that $\||S|^s D^{1/2}u\|_{L^2(dt)L^2(dx\,dy)}$ is finite locally in time for (all) $1 > s > \frac{1}{2}$. This assertion will be sufficient for our purposes. Recall the definition of $X^{s,\delta}$:

$$\||\xi|^s\big(|\tau - |\xi|^2| + 1\big)^\delta \widehat{u}\|_{L^2(d\tau d\xi)} := \|u\|_{X^{s,\delta}} \ . \tag{38}$$

Going back to (37), we write

$$S(k) = m + F$$

where we define the expression

$$F(k) := S(k-u) - \epsilon(u) + pm + (T(p) + \epsilon(p) + u\overline{m})\,(1+p)^{-1}u \ .$$

The idea is to localize in time on the right-hand side:

$$S(\widetilde{k}) = \chi(t)\,(m+F) \ ,$$

where $\chi \in C_0^\infty(\mathbb{R})$, $\chi = 1$ on $[0,1]$. Then, $\widetilde{k} = k$ on $[0,1]$.

As we already pointed out, we can estimate $\|S\left(\frac{\partial}{\partial t}\right)^N D^a k\|_{L^2[0,1]L^2(dx\,dy)} \le C$ for $0 \le a < \frac{1}{2}$. We can further localize $\widetilde{k}$ in time to insure that these relations hold globally in time. By using the triangle inequality $|\tau - |\xi|^2| + |\tau| \ge |\xi|^2$, we immediately conclude that

$$\||\xi|^{\frac{3}{2}-}\big(|\tau - |\xi|^2| + 1\big)^{\frac{1}{2}+}\widehat{k_\chi}\|_{L^2(d\tau d\xi)} \le C \ .$$

□

□

7. Error term $e^B V e^{-B}$

The goal of this section is to list explicitly all terms in $e^B V e^{-B}$ and to find conditions under which these terms are bounded. Recall that V is defined by $V = \int v(x_0 - y_0) Q^*_{x_0 y_0} Q_{x_0 y_0}\, dx_0\, dy_0$. For simplicity, $\mathrm{shb}(k)$ denotes either $\mathrm{sh}(k)$ or $\overline{\mathrm{sh}(k)}$, and $\mathrm{chb}(k)$ denotes either $\mathrm{ch}(k)$ or $\overline{\mathrm{ch}(k)}$.

Let $x_0 \ne y_0$; we obtain

$$e^B Q^*_{x_0 y_0} Q_{x_0 y_0} e^{-B} = e^B Q^*_{x_0 y_0} e^{-B} e^B Q_{x_0 y_0} e^{-B} \ .$$

According to the isomorphism (19), we have

$$Q^*_{x_0y_0} = \mathcal{I}\begin{pmatrix} 0 & 0 \\ -2\delta(x-x_0)\delta(y-y_0) & 0 \end{pmatrix}$$

where the operator

$$e^B Q^*_{x_0y_0} e^{-B}$$
$$= \mathcal{I}\left(\begin{pmatrix} \overline{\mathrm{ch}(k)} & \overline{\mathrm{sh}(k)} \\ \mathrm{sh}(k) & \mathrm{ch}(k) \end{pmatrix}\begin{pmatrix} 0 & 0 \\ -2\delta(x-x_0)\delta(y-y_0) & 0 \end{pmatrix}\begin{pmatrix} \mathrm{ch}(k) & -\overline{\mathrm{sh}(k)} \\ -\mathrm{sh}(k) & \overline{\mathrm{ch}(k)} \end{pmatrix}\right)$$

is a linear combination of the terms

$$\int \mathrm{chb}(k)(x,x_0)\mathrm{chb}(k)(y_0,y)Q^*_{xy}dx\,dy\ , \tag{39}$$
$$\int \mathrm{shb}(k)(x,x_0)\mathrm{chb}(k)(y_0,y)N_{xy}dx\,dy\ ,$$
$$\int \mathrm{shb}(k)(x,x_0)\mathrm{shb}(k)(y_0,y)Q_{xy}dx\,dy\ .$$

A similar calculation shows that $e^B Q_{x_0y_0} e^{-B}$ is a linear combination of

$$\int \mathrm{chb}(k)(x,x_0)\mathrm{chb}(k)(y_0,y)Q_{xy}dx\,dy\ , \tag{40}$$
$$\int \mathrm{shb}(k)(x,x_0)\mathrm{chb}(k)(y_0,y)N_{xy}dx\,dy\ ,$$
$$\int \mathrm{shb}(k)(x,x_0)\mathrm{shb}(k)(y_0,y)Q^*_{xy}dx\,dy\ .$$

Thus, $e^B Q^*_{x_0y_0}Q_{x_0y_0}e^{-B}$ is a linear combination of the nine possible terms obtained by combining the above.

Now we list all terms in $e^B V e^{-B}\Omega$. Terms in $e^B V e^{-B}$ ending in Q_{xy} are automatically discarded because they contribute nothing when applied to Ω. The remaining six terms are listed below.

$$\int \mathrm{chb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{chb}(k)(y_0,y_2)$$
$$v(x_0-y_0)Q^*_{x_1y_1}N_{x_2y_2}\Omega dx_1\,dy_1\,dx_2\,dy_2\,dx_0\,dy_0\ , \tag{41}$$

$$\int \mathrm{chb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{shb}(k)(y_0,y_2)$$
$$v(x_0-y_0)Q^*_{x_1y_1}Q^*_{x_2y_2}\Omega dx_1\,dy_1\,dx_2\,dy_2\,dx_0\,dy_0\ , \tag{42}$$

$$\int \mathrm{shb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{chb}(k)(y_0,y_2)$$
$$v(x_0-y_0)N_{x_1y_1}N_{x_2y_2}\Omega dx_1\,dy_1\,dx_2\,dy_2\,dx_0\,dy_0\ , \tag{43}$$

$$\int \mathrm{shb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{shb}(k)(y_0,y_2) \tag{44}$$
$$v(x_0-y_0)N_{x_1y_1}Q^*_{x_2y_2}\Omega dx_1\,dy_1\,dx_2\,dy_2\,dx_0\,dy_0\ ,$$

$$\int \mathrm{shb}(k)(x_1,x_0)\mathrm{shb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{chb}(k)(y_0,y_2)$$
$$v(x_0-y_0)Q_{x_1y_1}N_{x_2y_2}\Omega dx_1\,dy_1\,dx_2\,dy_2\,dx_0\,dy_0\ , \tag{45}$$

$$\int \mathrm{shb}(k)(x_1,x_0)\mathrm{shb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{shb}(k)(y_0,y_2)$$
$$v(x_0-y_0)Q_{x_1y_1}Q^*_{x_2y_2}\Omega dx_1\,dy_1\,dx_2\,dy_2\,dx_0\,dy_0\ . \tag{46}$$

To compute the above six terms, recall (24) through (27) as well as (1). In general, $N_{xy}\Omega = 1/2\delta(x-y)\Omega$, while $\int f(x,y)Q^*_{xy}dxdy\Omega = (0,0,f(x,y),0,\cdots)$ up to symmetrization and normalization.

The resulting contributions (neglecting symmetrization and normalization) follow.

From (41):

$$\psi(x_1,y_1) = \tag{47}$$
$$\int \mathrm{chb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{chb}(k)(y_0,x_2)v(x_0-y_0)$$
$$\times\, dx_2\,dx_0\,dy_0\ .$$

From (42):

$$\psi(x_1,y_1,x_2,y_2) = \tag{48}$$
$$\int \mathrm{chb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,y_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{shb}(k)(y_0,y_2)v(x_0-y_0)$$
$$\times\, dx_0\,dy_0\ .$$

From (43):

$$\psi = \tag{49}$$
$$\int \mathrm{shb}(k)(x_1,x_0)\mathrm{chb}(k)(y_0,x_1)\mathrm{shb}(k)(x_2,x_0)\mathrm{chb}(k)(y_0,x_2)v(x_0-y_0)$$
$$\times\, dx_1\,dx_2\,dx_0\,dy_0\ .$$

From (44), with the N and Q^* reversed, we get

$$\psi(x_2, y_2) = \tag{50}$$
$$\int \mathrm{shb}(k)(x_1, x_0)\mathrm{chb}(k)(y_0, x_1)\mathrm{shb}(k)(x_2, x_0)\mathrm{shb}(k)(y_0, y_2)v(x_0 - y_0)$$
$$\times\, dx_1\, dx_0\, dy_0 \ ,$$

as well as the contribution from $[N, Q^*]$, i.e.

$$\psi(y_1, y_2) = \tag{51}$$
$$\int \mathrm{shb}(k)(x_1, x_0)\mathrm{chb}(k)(y_0, y_1)\mathrm{shb}(k)(x_1, x_0)\mathrm{shb}(k)(y_0, y_2)v(x_0 - y_0)$$
$$\times\, dx_1\, dx_0\, dy_0 \ .$$

The contribution of (45) is zero, and, finally, the contribution of (46), using (24), consists of four numbers, which can be represented by the two formulas

$$\psi = \int \mathrm{shb}(k)(x_1, x_0)\mathrm{shb}(k)(y_0, x_1)\mathrm{shb}(k)(x_2, x_0)\mathrm{shb}(k)(y_0, x_2)v(x_0 - y_0) \tag{52}$$
$$\times\, dx_1\, dx_2\, dx_0\, dy_0$$

and

$$\psi = \int |\mathrm{shb}(k)|^2(x_1, x_0)|\mathrm{shb}(k)|^2(y_0, y_1)v(x_0 - y_0) dx_1\, dy_1\, dx_0\, dy_0 \ . \tag{53}$$

We can now state the following proposition.

Proposition 7.1. *The state $e^B V e^{-B}\Omega$ has entries on the zeroth, second and fourth slot of a Fock space vector of the form given above. In addition, if*

$$\| \left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y \right) \mathrm{sh}(k) \|_{L^1[0,T]L^2(dxdy)} \le C_1,$$

$$\| \left(i\frac{\partial}{\partial t} - \Delta_x + \Delta_y \right) p \|_{L^1[0,T]L^2(dxdy)} \le C_2$$

and $v(x) = \frac{1}{|x|}$, or $v(x) = \chi(x)\frac{1}{|x|}$, then

$$\int_0^T \|e^B V e^{-B}\Omega\|_{\mathcal{F}}^2 \, dt \le C \ ,$$

where C only depends on C_1 and C_2.

Proof. This follows by writing $\mathrm{ch}(k) = \delta(x-y) + p$ and applying Cauchy-Schwartz and local smoothing estimates as in the work of Sjölin [32], Vega [33]; see also Constantin and Saut [3]. In fact, we need the following slight generalization (see Lemma 7.2 below): If

$$\| \left(i\frac{\partial}{\partial t} - \Delta_{x_1} - \Delta_{x_2} \pm \Delta_{x_3} \cdots \pm \Delta_{x_n} \right) f(t, x_1, \cdots x_n) \|_{L^1[0,T]L^2(dtdx)} \leq C \ ,$$

with initial conditions 0, then

$$\| \frac{f(t, x_1, x_2, \cdots)}{|x_1 - x_2|} \|_{L^2[0,T]L^2(dxdy)} \leq C \ . \tag{54}$$

We will check a typical term, (48). This amounts to proving the following three terms are in L^2.

(1)

$$\psi_{pp}(t, x_1, y_1, x_2, y_2) =$$
$$\int p(t, x_1, x_0) p(t, y_0, y_1) \mathrm{shb}(k)(t, x_2, x_0) \mathrm{shb}(k)(t, y_0, y_2) v(x_0 - y_0) \ dx_0 \, dy_0 \ .$$

We use Cauchy-Schwartz in x_0, y_0 to get

$$\int_0^T \int |\psi_{pp}|^2 dt \, dx_1 \, dx_2 \, dy_1 \, dy_2$$
$$\leq \sup_t \int |p(t, x_1, x_0) p(t, y_0, y_1)|^2 dx_1 \, dx_0 \, dy_1 \, dy_0$$
$$\times \int_0^T \int |\mathrm{shb}(k)(t, x_2, x_0) \mathrm{shb}(k)(t, y_0, y_2) v(x_0 - y_0)|^2 dt \, dx_2 \, dx_0 \, dy_2 \, dy_0 \leq C \ .$$

The first term is estimated by energy, and the second one is an application of (54) with $f = \mathrm{shb}(k)\mathrm{shb}(k)$. Notice that, because of the absolute value, we can choose either $\mathrm{sh}(k)$ or $\overline{\mathrm{sh}(k)}$ to insure that the Laplacians in x_0, y_0 have the same signs.

(2)

$$\psi_{p\delta}(t, x_1, y_1, x_2, y_2) =$$
$$\int p(t, x_1, x_0) \mathrm{shb}(k)(t, x_2, x_0) \mathrm{shb}(k)(t, y_1, y_2) v(x_0 - y_1) \ dx_0 \ .$$

Here, we use Cauchy-Schwartz in x_0 to estimate, in a similar fashion,

$$\int_0^T \int |\psi_{p\delta}|^2 dt\, dx_1\, dx_2\, dy_1\, dy_2$$
$$\leq \sup_t \int |p(t, x_1, x_0)|^2 dx_1\, dx_0$$
$$\times \int_0^T \int |\mathrm{shb}(k)(t, x_2, x_0)\mathrm{shb}(k)(t, y_1, y_2) v(x_0 - y_1)|^2 dt\, dx_2\, dx_0\, dy_2\, dy_0 \leq C \ .$$

(3)

$$\psi_{\delta\delta}(x_1, y_1, x_2, y_2) = \mathrm{shb}(k)(t, x_2, x_1)\mathrm{shb}(k)(t, y_1, y_2) v(x_1 - y_1) \ ,$$

which is just a direct application of (54).

All other terms are similar. □

□

We have to sketch the proof of the local smoothing estimate that we used above.

Lemma 7.2. *If* $f : \mathbb{R}^{3n+1} \to \mathbb{C}$ *satisfies*

$$\| \left(i\frac{\partial}{\partial t} - \Delta_{x_1} - \Delta_{x_2} \pm \Delta_{x_3} \cdots \pm \Delta_{x_n} \right) f(t, x_1, \cdots x_n) \|_{L^1[0,T] L^2(dx dy)} \leq C$$

with initial conditions $f(0, \cdots) = 0$*, then*

$$\| \frac{f(t, x_1, x_2, \cdots)}{|x_1 - x_2|} \|_{L^2[0,T] L^2(dx)} \leq C \ .$$

Proof. We follow the general outline of Sjolin, [32]. Using Duhamel's principle, it suffices to assume that

$$\left(i\frac{\partial}{\partial t} - \Delta_{x_1} - \Delta_{x_2} \pm \Delta_{x_3} \cdots \pm \Delta_{x_n} \right) f(t, x_1, \cdots x_n) = 0 \qquad (55)$$

with initial conditions $f(0, \cdots) = f_0 \in L^2$. Furthermore, after the change of variables $x_1 \to \frac{x_1 + x_2}{\sqrt{2}}$, $x_2 \to \frac{x_2 - x_1}{\sqrt{2}}$, it suffices to prove that

$$\| \frac{f(t, x_1, x_2, \cdots)}{|x_1|} \|_{L^2[0,T] L^2(dx)} \leq C \ ,$$

where f satisfies the same equation (55). Changing notation, denote $x = (x_2, x_3, \cdots)$ and let $< \xi >^2$ be the relevant expression $\pm |\xi_2|^2 \pm |\xi_3|^2 \ldots$. Write

$$f(t, x_1, x) = \int e^{it(|\xi_1|^2 + <\xi>^2)} e^{ix_1 \cdot \xi_1 + ix \cdot \xi} \widehat{f_0}(\xi_1, \xi)\ d\xi_1\, d\xi \ .$$

Thus, we obtain

$$\int \frac{|f(t,x_1,x)|^2}{|x_1|^2} dt dx_1 dx$$

$$= \int\int e^{it(|\xi_1|^2-|\eta_1|^2+<\xi>^2-<\eta>^2)} \frac{e^{ix_1\cdot(\xi_1-\eta_1)+ix\cdot(\xi-\eta)}}{|x_1|^2} \widehat{f}_0(\xi_1,\xi)\overline{\widehat{f}}_0(\eta_1,\eta) d\xi_1\, d\xi\, d\eta_1\, d\eta$$

$$\times\, dt\, dx\, dx_1$$

$$= c\int \delta(|\xi_1|^2-|\eta_1|^2)\frac{1}{|\xi_1-\eta_1|}\widehat{f}_0(\xi_1,\xi)\overline{\widehat{f}}_0(\eta_1,\xi)d\xi_1 d\eta_1 d\xi$$

$$\le \int |\widehat{f}_0(\xi_1,\xi)|^2 dx_1\, d\xi \ ,$$

because one can easily check that

$$\sup_{\xi_1}\int \delta(|\xi_1|^2-|\eta_1|^2)\frac{1}{|\xi_1-\eta_1|}d\eta_1 \le C \ .$$

Thus, the kernel $\delta(|\xi_1|^2-|\eta_1|^2)\frac{1}{|\xi_1-\eta_1|}$ is bounded from $L^2(d\eta_1)$ to $L^2(d\xi_1)$. □

□

8. Error terms $e^B[A,V]e^{-B}$

We proceed to check the operator $e^B[A,V]e^{-B}$. The calculations of this section are similar to those of the preceding section with the notable exception of (61)–(64). Recall the calculations of Lemma 3.1 and write

$$e^B[A,V]e^{-B} = \int v(x-y)\Big(\overline{\phi}(y)e^B a_x^* e^{-B}e^B a_x a_y e^{-B} \tag{56}$$

$$+ \phi(y)e^B a_x^* a_y^* e^{-B} e^B a_x e^{-B}\Big)\ dx\, dy\ . \tag{57}$$

Now fix x_0. We start with the term (56). According to Theorem 4.1, we have

$$e^B a_{x_0}^* e^{-B} = \int \Big(\mathrm{sh}(k)(x,x_0)a_x + \overline{\mathrm{ch}(k)}(x,x_0)a_x^*\Big)\, dx$$

while $e^B a_{x_0}a_{y_0}e^{-B}$ has been computed in (40). The relevant terms are

$$\int \mathrm{shb}(k)(x,x_0)\mathrm{chb}(k)(y_0,y)N_{xy}dx\, dy \qquad \text{and}$$

$$\int \mathrm{shb}(k)(x,x_0)\mathrm{shb}(k)(y_0,y)Q_{xy}^* dx\, dy\ .$$

Combining these two terms, there are three non-zero terms (which will act on Ω):

(1)

$$\int v(x_0-y_0)\overline{\phi}(y_0)\mathrm{shb}(k)(x_1,x_0)\mathrm{shb}(k)(x_2,x_0)\mathrm{shb}(k)(y_0,y_2)a_{x_1}Q^*_{x_2y_2}\Omega \times dx_1 dx_2\, dy_2\, dx_0\, dy_0\ . \tag{58}$$

This term contributes terms of the form

$$\psi(t,y_2)=\int v(x_0-y_0)\overline{\phi}(t,y_0)(\mathrm{shb}(k)(t,x_1,x_0))^2\mathrm{shb}(k)(t,y_0,y_2)dx_1\, dx_0\, dy_0 \tag{59}$$

as well as the term

$$\psi(t,x_2)=\int v(x_0-y_0)\overline{\phi}(t,y_0)\mathrm{shb}(k)(t,x_1,x_0)\mathrm{shb}(k)(t,x_2,x_0)\mathrm{shb}(k)(t,y_0,x_1) \times dx_1\, dx_0\, dy_0\ , \tag{60}$$

which we know how to estimate. The second contribution is

(2)

$$\int v(x_0-y_0)\overline{\phi}(y_0)\mathrm{chb}(k)(x_1,x_0)\mathrm{shb}(k)(x_2,x_0)\mathrm{chb}(k)(y_0,y_2)a^*_{x_1}N_{x_2y_2}\Omega \times dx_1 dx_2\, dy_2\, dx_0\, dy_0\ . \tag{61}$$

Commuting $a^*_{x_1}$ with a_{x_2}, we find that (61) contributes

$$\psi(t,y_2)=\int v(x_0-y_0)\overline{\phi}(t,y_0)\mathrm{chb}(k)(t,x_1,x_0)\mathrm{shb}(k)(t,x_1,x_0)\mathrm{chb}(k)(t,y_0,y_2) \times dx_1\, dx_0\, dy_0\ . \tag{62}$$

We expand $\mathrm{chb}(k)(t,x_1,x_0)=\delta(x_1-x_0)+\mathrm{p}(k)(t,x_1-x_0)$. The contributions of p are similar to previous terms, but $\delta(x_1-x_0)$ presents a new type of term, which will be addressed in Lemma 8.2. These contributions are

$$\psi_{\delta p}(t,y_2)=\int v(x_1-y_0)\overline{\phi}(t,y_0)\mathrm{shb}(k)(t,x_1,x_1)\mathrm{p}(k)(t,y_0,y_2)\, dx_1\, dy_0 \tag{63}$$

and

$$\psi_{\delta\delta}(t,y_2)=\overline{\phi}(t,y_2)\int v(x_1-y_2)\mathrm{shb}(k)(t,x_1,x_1)dx_1\ . \tag{64}$$

The last contribution of (56) is

(3)

$$\int v(x_0-y_0)\overline{\phi}(y_0)\mathrm{chb}(k)(x_1,x_0)\mathrm{shb}(k)(x_2,x_0)\mathrm{shb}(k)(y_0,y_2)a^*_{x_1}Q^*_{x_2y_2}\Omega$$
$$\times\, dx_1dx_2\,dy_2\,dx_0\,dy_0 \sim \psi(x_1,x_2,y_2)$$

where

$$\psi(t,x_1,x_2,y_2)$$
$$=\int v(x_0-y_0)\overline{\phi}(t,y_0)\mathrm{chb}(k)(t,x_1,x_0)\mathrm{shb}(k)(t,x_2,x_0)\mathrm{shb}(k)(t,y_0,y_2)dx_0\,dy_0\ ,$$

modulo normalization and symmetrization. This term, as well as all the terms in (57), are similar to previous ones and are omitted.

We can now state the following proposition.

Proposition 8.1. *The state $e^B[A,V]e^{-B}\Omega$ has entries in the first and third slot of a Fock space vector of the form given above. In addition, if*

$$\|\left(i\frac{\partial}{\partial t}-\Delta_x-\Delta_y\right)\mathrm{sh}(k)\|_{L^1[0,T]L^2(dxdy)}\le C_1,$$

$$\|\left(i\frac{\partial}{\partial t}-\Delta_x+\Delta_y\right)p\|_{L^1[0,T]L^2(dxdy)}\le C_1$$

and

$$\|\mathrm{shb}(k)(t,x,x)\|_{L^2([0,T]L^2(dx))}\le C_3\ , \tag{65}$$

and $v(x)=\frac{\chi(x)}{|x|}$ for χ a C_0^∞ cut-off function, then

$$\int_0^T\|e^B[A,V]e^{-B}\Omega\|^2_{\mathcal{F}}\le C\ ,$$

where C only depends on C_1, C_2, C_3.

Proof. The proof is similar to that of Proposition 7.1, the only exception being the terms (63), (64). It is only for the purpose of handling these terms that the Coulomb potential has to be truncated, since the convolution of the Coulomb potential with the L^2 function $\mathrm{shb}(k)(x,x)$ does not make sense. If v is truncated to be in $L^1(dx)$, then we estimate the convolution in $L^2(dx)$, and take $\phi\in L^\infty(dydt)$. □

□

To apply this proposition, we need the following lemma.

Lemma 8.2. *Let* $u \in X^{\frac{1}{2},\frac{1}{2}+}$. *Then,*

$$\|u(t,x,x)\|_{L^2(dt\,dx)} \le C\|u\|_{X^{\frac{1}{2},\frac{1}{2}+}} \ .$$

Proof. As it is well known, it suffices to prove the result for u satisfying

$$\left(i\frac{\partial}{\partial t} - \Delta_x - \Delta_y\right) u(t,x,y) = 0$$

with initial conditions $u(0,x,y) = u_0(x,y) \in H^{\frac{1}{2}}$. This can be proved as a "Morawetz estimate", see [14], or as a space-time estimate as in [19]. Following the second approach, the space-time Fourier transform of u (evaluated at 2ξ rather than ξ for neatness) is

$$\begin{aligned}\widetilde{u}(\tau, 2\xi) &= c\int \delta(\tau - |\xi-\eta|^2 - |\xi+\eta|^2)\widetilde{u}_0(\xi-\eta, \xi+\eta)d\eta \\ &= c\int \frac{\delta(\tau - |\xi-\eta|^2 - |\xi+\eta|^2)}{(|\xi-\eta| + |\xi+\eta|)^{1/2}} F(\xi-\eta,\xi+\eta)d\eta \ ,\end{aligned}$$

where $F(\xi-\eta,\xi+\eta) = (|\xi-\eta|+|\xi+\eta|)^{1/2}\widetilde{u}_0(\xi-\eta,\xi+\eta)$. By Plancherel's theorem, it suffices to show that

$$\|\widetilde{u}\|_{L^2(d\tau d\xi)} \le C\|F\|_{L^2(d\xi d\eta)} \ .$$

This, in turn, follows from the pointwise estimate (Cauchy-Schwartz with measures)

$$\begin{aligned}&|\widetilde{u}(\tau,2\xi)|^2 \\ &\le c\int \frac{\delta(\tau - |\xi-\eta|^2 - |\xi+\eta|^2)}{|\xi-\eta| + |\xi+\eta|}d\eta \\ &\times \int \delta(\tau - |\xi-\eta|^2 - |\xi+\eta|^2)|F(\xi-\eta,\xi+\eta)|^2 d\eta\end{aligned}$$

and the remark that

$$\int \frac{\delta(\tau - |\xi-\eta|^2 - |\xi+\eta|^2)}{|\xi-\eta| + |\xi+\eta|}d\eta \le C \ .$$

□

□

9. The trace $\int d(t,x,x)dx$

This section addresses the control of traces involved in derivations. Recall that

$$\begin{aligned} d(t,x,y) = &\left(i\mathrm{sh}(k)_t + \mathrm{sh}(k)g^T + g\mathrm{sh}(k)\right)\overline{\mathrm{sh}(k)} \\ &- \left(i\mathrm{ch}(k)_t + [g, \mathrm{ch}(k)]\right)\mathrm{ch}(k) \\ &- \mathrm{sh}(k)\overline{m}\mathrm{ch}(k) - \mathrm{ch}(k)m\overline{\mathrm{sh}(k)} \ . \end{aligned}$$

Notice that if $k_1(x,y) \in L^2(dx\,dy)$ and $k_2(x,y) \in L^2(dx\,dy)$ then

$$\begin{aligned} &\int |k_1k_2|(x,x)dx \leq \int |k_1(x,y)||k_2(y,x)|dy\,dx \\ &\leq \|k_1\|_{L^2}\|k_2\|_{L^2} \ . \end{aligned}$$

Recall from Theorem 6.1 that if $v(x) = \frac{\epsilon}{|x|}$ or $v(x) = \chi(x)\frac{\epsilon}{|x|}$ then $i\mathrm{sh}(k)_t + \mathrm{sh}(k)g^T + g\mathrm{sh}(k)$, $i\mathrm{ch}(k)_t + [g, \mathrm{ch}(k)]$ and $\mathrm{sh}(k)$ are in $L^\infty([0,1])L^2(dxdy)$. This allows us to control all traces except the contribution of $\delta(x-y)$ to the second term. But, in fact, we have

$$i\mathrm{ch}(k)_t + [g, \mathrm{ch}(k)] = \left(ik_t - \Delta_x k - \Delta_y k\right)\overline{k} - k\overline{\left(ik_t - \Delta_x k - \Delta_y k\right)} + \dots \ ,$$

which has bounded trace, uniformly in $[0,1]$.

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