

SECOND-ORDER CORRECTIONS TO MEAN FIELD EVOLUTION OF WEAKLY INTERACTING BOSONS. II.

M. GRILLAKIS, M. MACHEDON, AND D. MARGETIS

ABSTRACT. We study the evolution of a N -body weakly interacting system of Bosons. Our work forms an extension of our previous paper I [13], in which we derived a second-order correction to a mean-field evolution law for coherent states in the presence of small interaction potential. Here, we remove the assumption of smallness of the interaction potential and prove global existence of solutions to the equation for the second-order correction. This implies an improved Fock-space estimate for our approximation of the N -body state.

1. INTRODUCTION

Experimental advances in the Bose-Einstein condensation (BEC) of dilute atomic gases [1, 3] have stimulated interesting questions on the quantum theory of many-body systems. For broad reviews, see, e.g., [19, 21]. In BEC, integer-spin atoms (Bosons) occupy macroscopically a quantum state (condensate). For a large number N of interacting atoms, the evolution of this system has been described fairly well by a single-particle nonlinear Schrödinger equation [15, 16, 20, 25]. The *emergence* of this *mean-field* description from the N -body Hamiltonian evolution has been the subject of extensive studies; see, e.g., [5–10, 18, 23].

In [13], henceforth referred to as paper I, we derived a new nonlinear Schrödinger equation that describes a second-order correction to a mean-field approximation for the N -body Hamiltonian evolution. Our work was inspired by: (i) *Fock-space* estimates provided by Rodnianski and Schlein [23], with regard to the rate of convergence for Hartree dynamics; and (ii) a second-order correction formulated by Wu [25, 26], who introduced a kernel for the scattering of atoms *in pairs* from the condensate to other states. In paper I, we derived a new Fock-space estimate; and showed that for small interaction potential the equation for our second-order correction can be solved locally in time.

The present paper is a continuation of paper I. The main improvement presented here is the removal of our assumption on the smallness of the interaction potential. Notably, we prove *global existence* of solutions to the equation for the second-order correction. Our approach enables us to derive an improved with respect to time Fock-space estimate for our approximation of the N -body quantum state.

In the remainder of this introduction, we review elements of the Fock space, summarize the major results of paper I, and state the contributions of the present paper. For a more extensive discussion of the background, the reader may consult, e.g., the introduction in our paper I.

Fock space and mean field. The problem at hand concerns the time evolution of N weakly interacting Bosons described by

$$i\partial_t\psi = H_N\psi ,$$

where ψ is the N -body wave function, H_N the Hamiltonian operator

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

and v is the two-body interaction potential. A few comments on these expressions are in order. Here, we use the (convenient for our purposes) formalism of second quantization, where a^* , a are annihilation and creation operators in a Fock space \mathcal{F} [2], to be defined below; ψ is a vector in \mathcal{F} ; and V is the particle interaction. Note that, in comparison to paper I, we changed the sign of the interaction term V , i.e., we replaced v with $-v$ so that having $v \geq 0$ corresponds to repulsive interaction, which leads to defocusing behavior.

At this point, it is advisable to review the basics of the Fock space \mathcal{F} over $L^2(\mathbb{R}^3)$. For Bosons, the elements of \mathcal{F} are vectors of the form $\psi = (\psi_0, \psi_1(x_1), \psi_2(x_1, x_2), \dots)$, where $\psi_0 \in \mathbb{C}$ and $\psi_n \in L_s^2(\mathbb{R}^{3n})$ are symmetric in x_1, \dots, x_n . The Hilbert space structure of \mathcal{F} is given by the inner product $(\phi, \psi) = \sum_n \int \phi_n \bar{\psi}_n dx$.

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

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

$$(a(\bar{f})\psi_{n+1})(x_1, x_2, \dots, x_n) = \sqrt{n+1} \int \psi_{n+1}(x, x_1, \dots, x_n) \bar{f}(x) \, dx .$$

The operator valued distributions a_x^* and a_x are defined by

$$\begin{aligned} a^*(f) &= \int f(x) a_x^* dx , \\ a(\bar{f}) &= \int \bar{f}(x) a_x dx . \end{aligned}$$

It follows that the operators a, a^* satisfy the commutation relations

$$[a_x, a_y^*] = \delta(x - y) , \quad [a_x, a_y] = [a_x^*, a_y^*] = 0 .$$

We are interested in the evolution of coherent states, i.e., vectors of the form $e^{-\sqrt{N}A(\phi)}\Omega$ where $\Omega = (1, 0, \dots) \in \mathcal{F}$ is the vacuum state, $\phi(t, x)$ is the one-particle wave function (to be determined later), and

$$A(\phi) := \int (\phi(x) a_x^* - \bar{\phi}(x) a_x) dx . \quad (1)$$

It is important to notice that

$$e^{-\sqrt{N}A(\phi)}\Omega = \left(\dots c_n \prod_{j=1}^n \phi(x_j) \dots \right) .$$

Thus, the n^{th} slot in the coherent state Fock vector consists of the tensor product of n functions $\phi(x)$; the relevant constant is $c_n = \left(\frac{N^n}{n!}\right)^{1/2}$.

Furthermore, the number operator, $\mathcal{N} := \int a_x^* a_x dx$, satisfies

$$\langle \Omega e^{\sqrt{N}A(\phi)} \mid \mathcal{N} \mid e^{-\sqrt{N}A(\phi)} \Omega \rangle = N \|\phi\|^2 .$$

Thus, if we normalize the wave function by setting $\|\phi\| = 1$, the average number of particles remains constant, N .

It can be claimed that a reasonable approximation for the many-body time evolution is expressed by the Fock vector

$$\psi_{appr} := e^{\sqrt{N}A(\phi(t))}\Omega ,$$

where $\phi(t, x)$ satisfies the Hartree equation (3). This ψ_{appr} encapsulates the mean field approximation for N weakly interacting Bosons. The precise meaning of this approximation as well as its rigorous justification were studied within the PDE setting by Erdős, Schlein, Yau [6–10] via Bogoliubov-Born-Green-Kirkwood-Yvon hierarchies for reduced density matrices (see also Klainerman and Machedon, [18], for a simplification of the uniqueness part of the argument). In the Fock space setting, the mean field approximation was studied by Ginibre and Velo [12] and, most recently, by Rodnianski and Schlein [23]; see also Hepp, [17].

Main results of paper I. Starting with a coherent state as initial data, in [13] we proposed a correction of the form

$$\psi_{appr} := e^{-\sqrt{N}A(\phi)} e^{-B(k)} \Omega ,$$

where

$$B(k) := \int (k(t, x, y) a_x^* a_y^* - \bar{k}(t, x, x) a_x a_y) dx dy \quad (2)$$

and the kernel $k(t, x, y)$ satisfies an appropriate nonlinear evolution equation. This k loosely corresponds to the “pair excitation function” introduced by Wu [25, 26] but our set-up and derived equation for k are different. By assuming that the interaction potential $v(x - y)$ is small, we proved that for a *finite time interval* our approximation stays close to the exact evolution in the Fock space norm. To be more precise, we proved the following general theorem.

Theorem 1.1. *Suppose that v is an even potential. Let ϕ be a smooth solution of the Hartree equation*

$$i \frac{\partial \phi}{\partial t} + \Delta \phi - (v * |\phi|^2) \phi = 0 \quad (3)$$

with initial conditions ϕ_0 . Assume all conditions (1)-(3) listed below:

- (1) *The kernel $k(t, x, y) \in L^2(dxdy)$ for all t , is symmetric, and solves the equation*

$$(iu_t + ug^T + gu - (1 + p)m) = (ip_t + [g, p] + u\bar{m})(1 + p)^{-1}u , \quad (4)$$

where all products in (4) are interpreted as spatial compositions of kernels (or operator products), “1” is the identity operator, and

$$u(t, x, y) := \text{sh}(k) := k + \frac{1}{3!} k \bar{k} k + \dots , \quad (5a)$$

$$\delta(x - y) + p(t, x, y) := \text{ch}(k) := \delta(x - y) + \frac{1}{2!} k \bar{k} + \dots , \quad (5b)$$

$$g(t, x, y) := -\Delta_x \delta(x - y) + v(x - y) \phi(t, x) \bar{\phi}(t, y) \quad (5c)$$

$$+ (v * |\phi|^2)(t, x) \delta(x - y) , \quad (5d)$$

$$m(t, x, y) := -v(x - y) \bar{\phi}(t, x) \bar{\phi}(t, y) . \quad (5e)$$

- (2) *The functions defined by*

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

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

are locally integrable; recall that V is the interaction operator, and A, B are operators defined by (1), (2).

- (3) The trace $\int d(t, x, x) dx$ is locally integrable in time, where the kernel $d(t, x, y)$ is

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

Then, there exist real functions χ_0, χ_1 such that

$$\begin{aligned} & \|e^{-\sqrt{N}A(\phi(t))}e^{-B(\phi(t))}e^{-i\int_0^t(N\chi_0(s)+\chi_1(s))ds}\Omega - e^{itH_N}\psi_0\|_{\mathcal{F}} \\ & \leq \frac{\int_0^t f(s)ds}{\sqrt{N}} + \frac{\int_0^t g(s)ds}{N} . \end{aligned} \quad (6)$$

Moreover, we showed that the hypotheses of this theorem are satisfied locally in time if v is small.

Theorem 1.2. *Let ϵ_0 be sufficiently small and $v(x) = \chi(x)\frac{\epsilon_0}{|x|}$ for $\chi \in C_0^\infty(\mathbb{R}^3)$. Assume that ϕ is a smooth solution to the Hartree equation (3), $\|\phi\|_{L^2(dx)} = 1$. Then, there exists $k \in L^\infty([0, 1])L^2(dxdy)$ that solves (4) for $0 \leq t \leq 1$ with initial condition $k(0, x, y) = 0$. In addition, we have the estimates*

$$\int_0^1 \|e^B V e^{-B} \Omega\|_{\mathcal{F}}^2 dt \leq C ,$$

and

$$\int_0^1 \|e^B [A, V] e^{-B} \Omega\|_{\mathcal{F}}^2 dt \leq C .$$

Main results of this paper. In the present paper, we remove the smallness assumption on the interaction potential, prove that the evolution equation of $k(t, x, y)$ has a global in time solution and obtain a stronger a priori estimate for the difference of the approximate and exact solution for the N -body Fock-space vector. In particular, we prove the following theorem.

Theorem 1.3. *Let the notation be as in Theorem 1.1. Consider $v(x) = \frac{\chi(x)}{|x|} \geq 0$, where $\chi \in C_0^\infty$ and $\chi(r)$ is a decreasing cut-off function. Assume ϕ_0 has sufficiently many derivatives in L^2 and $\|x\phi_0\|_{L^2} \leq C$. Further, suppose $k(0, \cdot, \cdot) \in L^2(\mathbb{R}^6)$ is prescribed. Then, the hypotheses of Theorem 1.1 are satisfied globally in time and*

$$\begin{aligned} & \|e^{-\sqrt{N}A(\phi(t))}e^{-B(\phi(t))}e^{-i\int_0^t(N\chi_0(s)+\chi_1(s))ds}\Omega - e^{itH_N}\psi_0\|_{\mathcal{F}} \\ & \leq C \frac{(1+t)^{\frac{1}{2}}}{\sqrt{N}} . \end{aligned} \quad (7)$$

Remark 1.4. It follows from our calculations that if we omit the assumption $v \geq 0$, the hypotheses of Theorem 1.1 are still satisfied globally in time, but we no longer have estimate (7).

The remainder of this paper is largely devoted to the proof of Theorem 1.3 and is organized as follows. In section 3 we derive the a priori estimate

$$\|u(T)\|_{L^2} \leq \left(\int_0^T \|m\|_{L^2} dt + \|u(0)\|_{L^2} \right) \exp \left(\int_0^T \|m\|_{L^2} dt \right) .$$

In section 2 we prove that $\int_0^\infty \|m\|_{L^2} dt \leq C$ if $v \geq 0$. In section (4) we show that (4) is locally well posed for L^2 , possibly large, initial conditions for u . This proof is much harder than the corresponding one in paper I; the latter worked for zero (or small) L^2 initial conditions. The idea here is to transform the quasilinear equation (4) into an equivalent semilinear one. Section 5 is devoted to estimating the error terms f and g entering (6). In section 6 we construct the requisite operator e^B in the case where $\|k\|_{L^2}$ is large and e^B is no longer defined as a convergent Taylor series; and elaborate on the connection of this construction with the Segal-Shale-Weil, or metaplectic, representation. Finally, the Appendix focuses on an improved computation of some error terms previously computed in section 8 of paper I. This leads to a simpler proof of our stronger estimate (7). Our notation is not uniform across sections, but is self-explanatory and convenient. When the variables are called x_1 and x_2 , ϕ_1 abbreviates $\phi(x_1)$, $v_{1-2} = v(x_1 - x_2)$, etc.

2. PSEUDOCONFORMAL TRANSFORMATION FOR HARTREE EQUATION

The goal of this section is to find an estimate for the decay rate in time of $\|\phi(t, \cdot)\|_{L^4(\mathbb{R}^3)}$, where ϕ is a solution of the Hartree equation,

$$i \frac{\partial \phi}{\partial t} + \Delta \phi - (v * |\phi|^2) \phi = 0 , \quad (8)$$

with initial condition ϕ_0 such that $\|\phi_0\|_{H^1} + \|x\phi_0\|_{L^2}$ be finite. For this purpose, we make use of the technology of dispersive estimates from [14]

We start with some preliminaries. Let

$$W = v * |\phi|^2 . \quad (9)$$

The quantities relevant for the conservation laws (to be stated below) are defined by

$$\begin{aligned}\rho &:= (1/2)|\phi|^2 ; \\ p_j &:= (1/2i) (\phi \nabla_j \bar{\phi} - \bar{\phi} \nabla_j \phi) ; \quad p_0 = (1/2i) (\phi \partial_t \bar{\phi} - \bar{\phi} \partial_t \phi) ; \\ \sigma_{jk} &:= \nabla_j \bar{\phi} \nabla_k \phi + \nabla_k \bar{\phi} \nabla_j \phi ; \quad \sigma_{0j} = \nabla_j \bar{\phi} \partial_t \phi + \partial_t \bar{\phi} \nabla_j \phi .\end{aligned}$$

Let us call $\sigma := \text{tr}(\sigma_{jk})$, the trace of the tensor σ_{jk} , and define two more quantities, namely,

$$\begin{aligned}\lambda &:= -p_0 + (1/2)\sigma + W\rho = \Delta\rho - W\rho ; \\ e &:= (1/2)\sigma + W\rho .\end{aligned}$$

With regard to λ , see (11).

The quantity e is the energy density, while λ is the Lagrangian density. Indeed, one can see that the evolution equation can be derived as a variation of the integral

$$\mathcal{L}(\phi, \bar{\phi}) := \int dx \{ \lambda \} .$$

The associated conservation laws can be stated in the forms

$$\partial_t \rho - \nabla_j p^j = 0 , \tag{10a}$$

$$\partial_t p_j - \nabla_k \{ \sigma_j^k - \delta_j^k \lambda \} + l_j = 0 , \tag{10b}$$

$$\partial_t e - \nabla_j \sigma_0^j + l_0 = 0 . \tag{10c}$$

These laws express the conservation of mass, momentum and energy, respectively,¹ where the vector (l_j, l_0) is

$$l_j := W\rho_{,j} - W_{,j}\rho , \quad l_0 := W\rho_{,t} - W_{,t}\rho .$$

We can see that the momentum and energy are indeed conserved quantities: l_0 and l_j average to zero, since $\int (v * \partial\rho)\rho = \int (v * \rho)\partial\rho$ for an even v .

One can derive one more identity (a structure equation) by multiplying the evolution equation by $\bar{\phi}$ and taking the real part:

$$\lambda + (-\Delta\rho + W\rho) = 0 . \tag{11}$$

This equation is the result of an infinitesimal transformation on the target when we regard ϕ as a map into the complex plane. Using

¹As it is well known, any Euler-Lagrange equation derived from a local Lagrangian has a conserved energy-momentum tensor; see, for instance, section 37.2 in [4]. In our case, $T_{jk} = \sigma_{jk} - \delta_{jk}\lambda$, $T_{j0} = -p_j$, $T_{0j} = \sigma_{0j}$ and $T_{00} = -e$. The vectors l_0, l_j are corrections due to the fact that our Lagrangian is nonlocal.

the structure equation, we can recast the conservation of momentum, equation (10b), into the form

$$\partial_t p_j - \nabla_k \{ \sigma_j^k + \delta_j^k (- \Delta \rho + W \rho) \} + l_j = 0 .$$

Let us return to conservation laws (10). The conformal identity can be derived by contracting the mass equation (10a) with $|x|^2/2$; the momentum equation (10b) with tx^j ; and the energy equation (10c) with t^2 ; and adding the resulting identities. The final result can be written in the abstract form

$$\partial_t e_c - \nabla_j \tau^j + r = 0 , \quad (12)$$

where the relevant quantities are

$$\begin{aligned} e_c &:= (|x|^2/2)\rho + tx^j p_j + t^2 e = t^2 \left(\left| \nabla \left(e^{i|x|^2/4t} \phi \right) \right|^2 + W \rho \right) , \\ \tau^j &:= (|x|^2/2)p^j + tx^k \sigma_k^j + tx^j (- \Delta \rho + W \rho) + t^2 \sigma_0^j , \\ r &:= t^2 l_0 + tx^j l_j - nt \Delta \rho + t(n-2)W \rho , \end{aligned}$$

By integrating (12) in space, we obtain the ODE

$$\dot{E}_c + R_c = 0 ,$$

where

$$E_c := \int dx \{ e_c \} , \quad (13)$$

$$R_c := \int dx \{ (n-2)tW\rho + tx^j l_j \} ; \quad (14)$$

note that E_c is the pseudoconformal energy. Next, we recast R_c into a convenient form. By inspection of (14), it remains to compute

$$\begin{aligned} & \int x^j l_j dx \\ &= \int dx \{ W x^j \rho_{,j} - x^j W_{,j} \rho \} = 2 \int dx_1 dx_2 \{ v_{1-2} (x_1 \cdot \nabla_{1-2} (\rho_1 \rho_2)) \} \\ &= \int dx_1 dx_2 \left\{ v_{1-2} \left((x_1 + x_2) \cdot \nabla_{1-2} + (x_1 - x_2) \cdot \nabla_{1-2} \right) (\rho_1 \rho_2) \right\} \\ &= \int dx_1 dx_2 \left\{ \left(-2n v_{1-2} - 2(x_1 - x_2) \cdot \nabla v_{1-2} \right) (\rho_1 \rho_2) \right\} . \end{aligned}$$

In the above calculation, we used the fact that v_{1-2} is symmetric with respect to the $1 \rightarrow 2$ and $2 \rightarrow 1$ transposition, while ∇_{1-2} is antisymmetric. Moreover, we have

$$\nabla_{1-2} \cdot (x_1 - x_2) = 2n ; \quad (x_1 - x_2) \cdot \nabla_{1-2} v_{1-2} = 2(x_1 - x_2) \cdot \nabla v_{1-2} .$$

Finally, regarding (14), notice that

$$\int dx \{(n-2)W\rho\} = \int dx_1 dx_2 \{2(n-2)v_{1-2}\rho_1\rho_2\} .$$

Substituting back into (14), we wind up with the integral

$$R_c = t \int dx_1 dx_2 \{ [(-4)v_{1-2} - 2r_{1-2}v'_{1-2}] (\rho_1\rho_2) \} . \quad (15)$$

This integral is used as an alternate expression for R_c .

Thus, we have proved the following lemma.

Lemma 2.1. *Let ϕ be a solution of the Hartree equation (8), and let E_c , R_c be defined by (13), (15). Then, the following equation holds:*

$$\dot{E}_c + R_c = 0 . \quad (16)$$

Remark 2.2. In order to obtain a *decreasing* pseudoconformal energy, we need $R_c \geq 0$, which is unfortunately *not true* for the Coulomb potential. Instead, we proceed to show that R_c is integrable in time.

We first state another consequence of our previous calculations.

Lemma 2.3. *Define*

$$E_{cc} := \frac{E_c}{t} = \int dx \left\{ t \left(\left| \nabla \left(e^{i|x|^2/4t} \phi \right) \right|^2 + W\rho \right) \right\} .$$

Then, E_{cc} satisfies

$$\dot{E}_{cc} + R_{cc} = 0 ,$$

where R_{cc} is defined by

$$R_{cc} := \left| \nabla \left(e^{i|x|^2/4t} \phi \right) \right|^2 - 2 \int (v + r_{1-2}v'_{1-2}) \rho_1 \rho_2 .$$

Remark 2.4. Notice that for $v(x) = \chi(|x|)\frac{1}{|x|}$, R_{cc} is *positive* if $\chi(r)$ is decreasing for $r > 0$; thus, E_{cc} is decreasing.

In conclusion, using the Sobolev embedding and interpolation we have the following corollary.

Corollary 2.5. *Let ϕ be a solution of the Hartree equation (8). Then, the following estimates hold for all $t \geq 1$:*

$$\begin{aligned} \|\phi(t, \cdot)\|_{L^6(\mathbb{R}^3)} &\leq \frac{C}{\sqrt{t}} E_{cc}(1) , \\ \|\phi(t, \cdot)\|_{L^4(\mathbb{R}^3)} &\leq \frac{C}{t^{3/8}} E_{cc}(1) . \end{aligned} \quad (17)$$

Using Lemma (2.1), the result of Corollary 2.5 can be improved:

Theorem 2.6. *Let ϕ be a global smooth solution of the Hartree equation*

$$i\frac{\partial\phi}{\partial t} + \Delta\phi - (v * |\phi|^2)\phi = 0 \quad (18)$$

with initial condition ϕ_0 such that $E_c(1)$ is finite. Then,

$$\begin{aligned} \|\phi(t, \cdot)\|_{L^6} &\leq Ct^{-3/4} , \\ \|\phi(t, \cdot)\|_{L^4} &\leq Ct^{-9/16} , \end{aligned}$$

and, thus,

$$\begin{aligned} \int_1^\infty \|\phi(t, \cdot)\|_{L^6(\mathbb{R}^3)}^2 dt &\leq C , \\ \int_1^\infty \|\phi(t, \cdot)\|_{L^4(\mathbb{R}^3)}^2 dt &\leq C . \end{aligned}$$

Proof. Using the fact that $-4v - 2rv' \in L^1$ together with (17), we see that

$$R_c(t) \leq Ct\|\phi(t, \cdot)\|_{L^4}^4 \leq Ct^{-1/2} .$$

By integrating (16), we conclude that

$$E_c(t) \leq Ct^{1/2}$$

for $t \geq 1$. Using the Sobolev inequality and the definition of E_c (see (13)) we conclude that

$$\|\phi(t, \cdot)\|_{L^6} \leq C \|\nabla (e^{i|x|^2/4t}\phi)\|_{L^2} \leq Ct^{-3/4} .$$

Interpolation with energy conservation gives

$$\|\phi(t, \cdot)\|_{L^4} \leq Ct^{-9/16} .$$

□

3. A PRIORI ESTIMATES

In this section, by using Theorem 2.6 we derive a priori estimates for the solution u of (4). We recall definitions (5) of Theorem 1.1, suitably

abbreviated, and add a few new ones:

$$\begin{aligned}
m_{12} &:= -v_{1-2}\bar{\phi}_1\bar{\phi}_2 = (-v(x-y)\bar{\phi}(x)\bar{\phi}(y)) \ , \\
g_{12} &:= -\Delta_1\delta_{12} + w_{12} \ , \\
w_{12} &:= -v_{1-2}\phi_1\bar{\phi}_2 \ , \\
\text{sh}(k) &:= u \ , \\
\text{ch}(k) &:= 1 + p := \delta_{12} + p \ , \\
r &:= (1 + p)^{-1} \ , \\
q &:= u\bar{u} \ .
\end{aligned}$$

These are all operators kernels, and their products are interpreted as compositions. Notice that w and m have the symmetries $w_{21} = \bar{w}_{12}$, i.e., $w^* = w$; and $m_{21} = m_{12}$, i.e., $m^T = m$. The evolution equation for $u = \text{sh}(k)$, given by (4), is abbreviated to

$$S(u) - (1 + p)m = (W(p) + u\bar{m})ru \ , \quad (19)$$

where

$$\begin{aligned}
S(u) &:= iu_t + gu + ug^T \ , \\
W(p) &:= ip_t + [g, p] \ ,
\end{aligned}$$

and u_{12} is symmetric, $u_{21} = u_{12}$, i.e., $u^T = u$, while p_{12} is self-adjoint, $p_{21} = \bar{p}_{12}$, i.e., $p^* = p$.

Notice that q is related to p by

$$q = 2p + p^2 \ . \quad (20)$$

Trigonometric identities such as (20) follow from $e^K e^{-K} = I$ for

$$K = \begin{pmatrix} 0 & k \\ \bar{k} & 0 \end{pmatrix} \ .$$

The key observation in this section is the following lemma.

Lemma 3.1. *The following identities hold:*

$$(W(p) + u\bar{m})r + r(W(p) - m\bar{u}) = 0 \ , \quad (21)$$

$$F := W(q) = m\bar{u}(1 + p) - (1 + p)u\bar{m} \ . \quad (22)$$

These equations are equivalent for any positive semi-definite kernel p , $q = p^2 + 2p$, and $r = (1 + p)^{-1}$.

Proof. To prove (21), multiply (19) on the right by \bar{u} , take the adjoint of (19), namely,

$$\bar{S}(\bar{u}) - \bar{m}(1 + p) = \bar{u}r(-W(p) + m\bar{u})$$

,

multiply it on the left by u , and then subtract. The resulting equation reads

$$\begin{aligned} W(q) &= W(p)r q + q r W(p) + u \bar{m} r q - q r m \bar{u} \\ &\quad + (1+p)m \bar{u} - u \bar{m}(1+p) . \end{aligned}$$

Now we can combine two terms as follows, using the fact that $r = (1+p)^{-1}$ and $q = (1+p)^2 - 1$:

$$u \bar{m} r q - u \bar{m}(1+p) = u \bar{m} \left((1+p)^{-1} [(1+p)^2 - 1] - (1+p) \right) = -u \bar{m} r .$$

Using the equation $q = 2p + p^2$, we obtain

$$W(2p + p^2) + u \bar{m} r - r m \bar{u} = W(p)r(2p + p^2) + (2p + p^2)r W(p) ;$$

hence,

$$\begin{aligned} 2W(p) + pW(p) + W(p)p + u \bar{m} r - r m \bar{u} \\ = W(p)(1+p)^{-1} [1 + (1+p)] p + p [1 + (1+p)] (1+p)^{-1} W(p) . \end{aligned}$$

Thus, we have

$$2W(p) + u \bar{m} r - r m \bar{u} = W(p) r p + p r W(p) .$$

Now observe that $1 - r p = r$ to conclude the proof of (21). To prove (22), multiply (21) on the right and left by $(1+p)$ and recall $q = 2p + p^2$. \square

We are ready to state and prove our main a priori estimate:

Theorem 3.2. *Let $u = \text{sh}(k)$ be a solution of (4) on some interval $[0, T]$. Then, the following estimate holds:*

$$\|u(T)\|_{L^2} \leq \left(\int_0^T \|m\|_{L^2} dt + \|u(0)\|_{L^2} \right) \exp \left(\int_0^T \|m\|_{L^2} dt \right) . \quad (23)$$

Proof. Taking the trace in (22) we obtain

$$\frac{d}{dt} \|u\|_{L^2}^2 = \text{tr} \left[(1/i) (m \bar{u} (1+p) - (1+p) u \bar{m}) \right] . \quad (24)$$

Thus, we have

$$\begin{aligned} \frac{d}{dt} \|u\|_{L^2}^2 &\leq 2 (\|m\|_{L^2} \|u\|_{L^2} + \|m\|_{L^2} \|u\|_{L^2} \|p\|_{L^2}) \\ &\leq 2 (\|m\|_{L^2} \|u\|_{L^2} + \|m\|_{L^2} \|u\|_{L^2}^2) . \end{aligned}$$

The inequality $\|p\| \leq \|u\|$ follows by taking the trace of (20) together with the observation that $\text{tr}(p) \geq 0$. Now we can employ a Gronwall type inequality to deduce (23). \square

Summarizing the results of the previous two sections, we draw our main conclusion.

Corollary 3.3. *Let ϕ be a solution of the Hartree equation satisfying the assumptions of Theorem 2.6 and let $u = \text{sh}(k)$ be a solution of equation (4) on $[0, T]$, as in Theorem 3.2. Assume the potential v is in $L^2(\mathbb{R}^3)$. Then the following estimate holds:*

$$\|u(T)\|_{L^2} \leq C(1 + \|u(0)\|_{L^2}) . \quad (25)$$

Proof. By Theorem 3.2, it suffices to control $\|m\|_{L^1(dt)L^2(dx dy)}$. Notice that $\|m\|_{L^2(\mathbb{R}^6)}^2 = \int (v^2 * |\phi|^2) |\phi|^2 dx \leq C\|v^2\|_{L^1(\mathbb{R}^3)}\|\phi\|_{L^4(\mathbb{R}^3)}^4$. Using the estimates of Theorem 2.6, we conclude that $\|m\|_{L^1(dt)L^2(dx dy)} \leq C$. \square

4. THE LOCAL EXISTENCE THEOREM FOR EQUATION (4)

In paper I, we showed that (4) has local solutions provided $u(0) = 0$ and $v(x) = \epsilon \frac{\chi(x)}{|x|}$ for $\chi \in C_0^\infty$. In this section we relax the assumptions to $u(0) \in L^2(\mathbb{R}^6)$ and $v(x) = \frac{\chi(x)}{|x|}$ and prove local existence in an interval where $\|\phi\|_{L^2([0,T])L^4(dx dy)}$ is small. Notice that by Theorem 2.6, $[0, \infty)$ can be divided into finitely many such intervals. This implies global existence for equation (4).

In this setting, we can no longer assume that $\|u\|_{L^\infty L^2}$ is small, and terms such as $W(p)ru$ are no longer small compared to $S(k)$ (see (19) for the notation). Our equation seems quasilinear, but can be transformed into a semilinear one. In order to prove local existence, we must solve for $u = \text{sh}(k)$ rather than k , and express $p = \sqrt{1 + u\bar{u}}$ in the operator sense. Thus we have to prove the following proposition:

Proposition 4.1. *The map*

$$k \mapsto \text{sh}(k) = u$$

is one to one, onto, continuous, with a continuous inverse, from symmetric Hilbert-Schmidt kernels k onto symmetric Hilbert-Schmidt kernels u .

Proof. The appropriate context for this proof is set by noticing that the equation $u = \text{sh}(k)$ is equivalent to

$$\exp \begin{pmatrix} 0 & k \\ \bar{k} & 0 \end{pmatrix} = \begin{pmatrix} \sqrt{1 + u\bar{u}} & u \\ \bar{u} & \sqrt{1 + \bar{u}u} \end{pmatrix}$$

By the spectral theorem, the exponential map is a continuous bijection from self-adjoint Hilbert-Schmidt "matrices" to positive definite

"matrices" P for which $\|I - P\|_{L^2}$ is finite. Our target matrix is

$$P = \begin{pmatrix} \sqrt{1 + u\bar{u}} & u \\ \bar{u} & \sqrt{1 + \bar{u}u} \end{pmatrix}.$$

Besides being positive definite, this matrix is symplectic; thus, it satisfies $P^T J P = J$ where

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

and also satisfies $L P L = P^{-1}$ where

$$L = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Thus, we have $P = e^p$ where p is self-adjoint. Since $e^{p^T} J e^p = J$, we conclude that p is symplectic, or $p^T J + J p = 0$. (Proof: $e^{JpJ} J = J e^{-p} J$ is always true; thus, by easy algebra $e^{p^T} = e^{JpJ}$. Since both p^T and JpJ are self-adjoint, the exponential is one-to-one, and we conclude that $p^T J + J p = 0$.) Similarly, from $L e^p L = e^{-p}$ we infer $L p L = -p$. The first two conditions force p to be of the form

$$p = \begin{pmatrix} a & b \\ c & -a^T \end{pmatrix},$$

where $a = a^*$, $b = b^T$, $c = b^*$. The third condition entails $a = 0$. Thus, p can be re-written as

$$p = \begin{pmatrix} 0 & k \\ \bar{k} & 0 \end{pmatrix}.$$

□

The main *new* ingredient of this section is the following theorem.

Theorem 4.2. *The following equations are equivalent for a symmetric, Hilbert-Schmidt u :*

$$S(u) = (1 + p)m + (W(p) + u\bar{m})ru; \quad (26)$$

$$S(u) = (1 + p)m + \frac{1}{2}[W(p), r]u + \frac{1}{2}(rm\bar{u} + u\bar{m}r)u; \quad (27)$$

$$S(u) = (1 + p)m + \frac{1}{2}[W, r]u + \frac{1}{2}(rm\bar{u} + u\bar{m}r)u; \quad (28)$$

where we set

$$\begin{aligned} F &:= m\bar{u}(1+p) - (1+p)u\bar{m} , \\ W &:= \frac{1}{2\pi i} \int_{\Gamma} (q-z)^{-1} F(q-z)^{-1} \sqrt{1+z} dz , \\ q &:= u\bar{u} , \\ 1+p &:= \sqrt{1+u\bar{u}} , \\ r &:= (1+u\bar{u})^{-1} . \end{aligned}$$

Here, Γ is a contour enclosing the spectrum of the non-negative Hilbert-Schmidt operator $u\bar{u}$. Equation (26) is the same as (4), suitably re-written. Note that F corresponds to $W(q)$ and W corresponds to $W(p)$.

Proof. Assume u satisfies (26). Recalling the estimate (21) we conclude u satisfies

$$\begin{aligned} S(u) &= \frac{1}{2} (W(p)r + rW(p)) u + \frac{1}{2} (W(p)r - rW(p)) u \\ &\quad + (1+p)m + u\bar{m}ru \\ &= \frac{1}{2} (rm\bar{u} - u\bar{m}r) u + \frac{1}{2} [W(p), r] u + (1+p)m + u\bar{m}ru \\ &= \frac{1}{2} [W(p), r] u + \frac{1}{2} (rm\bar{u} + u\bar{m}r) u + (1+p)m . \end{aligned}$$

Thus, u satisfies (27). Notice that both (27) and (28) are of the form

$$S(u) = Xu + (1+p)m , \quad (29)$$

where X is self-adjoint. To see that X is self-adjoint, notice that both $W(p)$ and W are skew-Hermitian. Then, the procedure can be reversed to show that if u satisfies (29) then the identity (22), and thus (21), holds.

Indeed, composing the complex conjugate of (27) on the left with u , we obtain

$$u\overline{S(u)} = u\overline{Xu} + u\overline{(1+p)m} .$$

The adjoint of this operator is

$$S(u)\bar{u} = u\overline{Xu} + m\overline{(1+p)u}$$

Subtracting the first equation from the second one gives

$$W(u\bar{u}) = m\overline{(1+p)u} - u\overline{(1+p)m} ,$$

which is the same as (22), using $\overline{(1+p)u} = \bar{u}(1+p)$ and $u\overline{(1+p)} = (1+p)u$. Thus, (26) and (27) are equivalent, and all three equations – (26), (27) and (28) – imply the equivalent formulas (21), (22).

Next, assume (27) holds. Then, we have [22]

$$q = \frac{1}{2\pi i} \int_{\Gamma} (z - q)^{-1} dz \quad \text{and}$$

$$\sqrt{1 + q} = -\frac{1}{2\pi i} \int_{\Gamma} (q - z)^{-1} \sqrt{1 + z} dz ,$$

and

$$W((q - z)^{-1}) = -(q - z)^{-1} W(q) (q - z)^{-1} ,$$

$$W(\sqrt{1 + q}) = \frac{1}{2\pi i} \int_{\Gamma} (q - z)^{-1} W(q) (q - z)^{-1} \sqrt{1 + z} dz . \quad (30)$$

So, (28) follows, since $W(p) = W(\sqrt{1 + q})$ and $W(q) = F$.

Conversely, assume (28) holds. Then, $W(q) = F$ as before; and $W(p)$ is given by (30), thus (27) holds. \square

Theorem 4.3. *Using the same notation as in Theorem 4.2, let $u_0 \in L^2(\mathbb{R}^6)$ be symmetric, given. There exists ϵ_0 such that if $\|m\|_{L^1([0,T])L^2(dx dy)} \leq \epsilon_0$ then there exists $u \in L^\infty([0,T])L^2(dx dy)$ solving (28) with prescribed initial condition $u(0, x, y) = u_0(x, y) \in L^2(\mathbb{R}^6)$. The solution u satisfies the following additional properties:*

(1)

$$\left\| \left(i \frac{\partial}{\partial t} - \Delta_x - \Delta_y \right) u \right\|_{L^1([0,T])L^2(dx dy)} \leq C ; \quad (31)$$

(2)

$$\left\| \left(i \frac{\partial}{\partial t} - \Delta_x + \Delta_y \right) p \right\|_{L^1([0,T])L^2(dx dy)} \leq C . \quad (32)$$

In this context, p is defined as $\sqrt{1 + u\bar{u}} - 1$.

Proof. The equation (28) is of the form

$$S(u) = m + N(u) , \quad (33)$$

where $N(u)$ involves no derivatives of u . Recall the fixed time estimate $\|kl\|_{L^2} \leq \|k\|_{op}\|l\|_{L^2}$, where op stands for the operator norm, and L^2 stands for the Hilbert-Schmidt norm. Since r and $(q - z)^{-1}$ have uniformly bounded operator norms and $\|p\|_{L^2} \leq \|u\|_{L^2}$, and also

$|z| \leq C\|u\|_{L^2}^2$ on Γ , we have

$$\begin{aligned} \|N(u)\|_{L^1 L^2} &\leq C(1 + \|u\|_{L^\infty L^2}^5) \|m\|_{L^1 L^2} , \\ \|N(u) - N(v)\|_{L^1 L^2} &\leq C \max\{1, \|u\|_{L^\infty L^2}^4, \|v\|_{L^\infty L^2}^4\} \|m\|_{L^1 L^2} , \\ &\times \|u - v\|_{L^\infty L^2} \end{aligned}$$

where $L^1 L^2$ stands for $L^1([0, T])L^2(\mathbb{R}^6)$ and $L^\infty L^2 = L^\infty([0, T])L^2(\mathbb{R}^6)$. Recalling the energy estimate

$$\|u\|_{L^\infty L^2} \leq \|u(0, \cdot)\|_{L^2} + \|Su\|_{L^1 L^2} ,$$

we see that, for any given C there exists an ϵ_0 such that (33) has a fixed point solution in the set $\|u\|_{L^\infty L^2} \leq C$ provided $\|m\|_{L^1 L^2} \leq \epsilon_0$.

To prove (31), we already know that $\|Su\|_{L^1 L^2} \leq C$, so we must only account for the lower order terms in g , namely $v_{12}\phi_1\overline{\phi_2}u$ (composition of kernels) and $(v*|\phi|^2)u$ (multiplication). These are both easy because we know $\|u\|_{L^\infty L^2} \leq C$ and Theorem 2.6 implies $\|v_{12}\phi_1\overline{\phi_2}\|_{L^1 L^2} \leq C$ as well as $\|v*|\phi|^2\|_{L^1 L^\infty} \leq C$, since $v \in L^2$.

A similar proof applies in order to show that (32) follows from estimate (22). □

5. ESTIMATES FOR ERROR TERMS

In this section we obtain estimates for the error terms $\int_0^T \|e^B V e^{-B} \Omega\|_{\mathcal{F}} dt$ (quartic term) and $\int_0^T \|e^B [A, V] e^{-B} \Omega\|_{\mathcal{F}} dt$ (cubic term). These terms were encountered in paper I.

We start by recalling the following result (Proposition 2, section 7 of paper I):

Proposition 5.1. *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 in paper I. In addition, if*

$$\left\| \left(i \frac{\partial}{\partial t} - \Delta_x - \Delta_y \right) u \right\|_{L^1[0, T] L^2(dx dy)} \leq C_1 ,$$

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

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

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

where C only depends on C_1 and C_2 .

Based on this result, estimates (31) and (32) and Cauchy-Schwarz in time we conclude:

Proposition 5.2. *The following estimate holds:*

$$\int_0^T \|e^B V e^{-B} \Omega\|_{\mathcal{F}} dt \leq C T^{1/2} . \quad (34)$$

Now we turn attention to $\int_0^T \|e^B[A, V]e^{-B}\Omega\|_{\mathcal{F}} dt$, seizing the opportunity of improving on results in section 8 of paper I. There, we had to estimate a certain trace; see equations (61) and (62) of paper I. This task can be avoided by commuting a_{x_2} and $a_{y_2}^*$ in equation (60) of paper I. Thus, terms involving $\text{sh}(k)(x, x)$, as in (62) of paper I, can in fact be avoided. To illustrate this point, we include the calculations here in the Appendix, which in effect replaces section 8 of paper I, incorporating the above remark. Our result is now simpler and stronger.

Proposition 5.3. *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 $\psi_I - \psi_{III}$ and $\psi_{I'} - \psi_{III'}$ given in the Appendix. In addition, if*

$$\begin{aligned} & \left\| \left(i \frac{\partial}{\partial t} - \Delta_x - \Delta_y \right) u \right\|_{L^1[0, T] L^2(dx dy)} \leq C_1, \\ & \left\| \left(i \frac{\partial}{\partial t} - \Delta_x + \Delta_y \right) p \right\|_{L^1[0, T] L^2(dx dy)} \leq C_2 , \\ & \left\| \left(i \frac{\partial}{\partial t} + \Delta_x \right) \phi \right\|_{L^1[0, T] L^2(dx dy)} \leq C_3 , \end{aligned} \quad (35)$$

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

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

where C only depends on C_1 , C_2 and C_3 . Thus, the following estimate holds:

$$\int_0^T \|e^B[A, V]e^{-B}\Omega\|_{\mathcal{F}} dt \leq C T^{1/2} . \quad (36)$$

Remark 5.4. Notice that (35) is satisfied by Theorem (2.6).

Estimates (34) and (36) form the basis of Theorem 1.3, which is the main result of this paper.

6. THE OPERATOR e^B

In paper I, we used the definition

$$B(t) := \frac{1}{2} \int (k(t, x, y) a_x a_y - \bar{k}(t, x, y) a_x^* a_y^*) \, dx \, dy \quad (37)$$

with $\|k\|_{L^2(dx \, dy)}$ small; e^B was defined as a convergent Taylor series on the dense subset of vectors in \mathcal{F} with finitely many nonzero components, and then it was extended to \mathcal{F} as a unitary operator. Consider the Lie algebra $sp(\mathbb{R})$, or $sp(\mathbb{C})$ of symplectic matrices with real (or complex), bounded operator coefficients. These satisfy $JS + S^T J = 0$ and have the form

$$S = \begin{pmatrix} a & b \\ c & -a^t \end{pmatrix}$$

where $b = b^T$, $c = c^T$. Further, consider the corresponding groups $Sp(\mathbb{R})$, $Sp(\mathbb{C})$ of bounded operators G which satisfy $G^T J G = J$. In applications, $G = e^S \in Sp$ is defined by a convergent Taylor series. By definition, G acts on $\phi = f + ig$ by acting on the vector $\begin{pmatrix} f \\ g \end{pmatrix}$ and, of course, preserves the symplectic form $\Im \int \phi \bar{\psi}$.

The following Lie algebra isomorphism from $sp(\mathbb{C})$ to operators (not necessarily skew-Hermitian) was a crucial ingredient in paper I:

$$\begin{aligned} \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} &\rightarrow \mathcal{I} \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} := \frac{1}{2} \begin{pmatrix} a_x & a_x^* \end{pmatrix} \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} J \begin{pmatrix} a_y \\ a_y^* \end{pmatrix} \\ &= - \int d(x, y) \frac{a_x a_y^* + a_y^* a_x}{2} \, dx \, dy + \frac{1}{2} \int k(x, y) a_x a_y \, dx \, dy \\ &\quad - \frac{1}{2} \int l(x, y) a_x^* a_y^* \, dx \, dy . \end{aligned} \quad (38)$$

To ensure that the resulting operator is skew-Hermitian we now restrict this isomorphism to the Lie subalgebra $sp_c(\mathbb{R}) := \overline{C} sp(\mathbb{R}) C^T$ for

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} .$$

This is a change of basis that will be explained below.

Lemma 6.1. *The map*

$$S \mapsto \overline{C} S C^T \quad (39)$$

is a Lie algebra isomorphism of $sp(\mathbb{C})$ to $sp(\mathbb{C})$.

Proof. The "matrix" C is unitary ($C^T = (\overline{C})^{-1}$) and also satisfies $C^T J C = C J C^T = iJ$; thus, $i^{-\frac{1}{2}}C$ and $i^{-\frac{1}{2}}C^T$ belong to the symplectic group $Sp(\mathbb{C})$ (and the choice of $i^{-\frac{1}{2}}$ does not matter). Since (39) does not change if we replace C by $i^{-\frac{1}{2}}C$, we see that (39) is just conjugation by an element of $Sp(\mathbb{C})$, and thus is a Lie algebra isomorphism. \square

Lemma 6.2. *If $S \in sp_c(\mathbb{R})$, then $\mathcal{I}(S)$ is skew-Hermitian.*

Proof. This proof will also motivate the choice of C .

Define the self-adjoint operators of "momentum"

$$P_x := D_x = \frac{a_x + a_x^*}{\sqrt{2}}$$

and "position"

$$Q_x := X_x = \frac{i(a_x - a_x^*)}{\sqrt{2}}.$$

These satisfy the canonical relations

$$[D_x, X_y] = \frac{1}{i} \delta(x - y).$$

We will rewrite (38) in terms of the self-adjoint operators D and X . The change-of-basis formula is

$$\begin{pmatrix} a_x \\ a_x^* \end{pmatrix} = C \begin{pmatrix} D_x \\ X_x \end{pmatrix} \quad (40)$$

for

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix};$$

see page 174, (4.13) of [11] for a closely related construction. Notice that $JC = i\overline{C}J$ with $\overline{C} = (C^T)^{-1}$; thus,

$$\begin{aligned} & \frac{1}{2} \begin{pmatrix} a_x & a_x^* \end{pmatrix} \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} J \begin{pmatrix} a_y \\ a_y^* \end{pmatrix} \\ &= \frac{i}{2} \begin{pmatrix} D_x & X_x \end{pmatrix} C^T \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} \overline{C} J \begin{pmatrix} D_y \\ X_y \end{pmatrix}. \end{aligned}$$

At this point it is natural to introduce the Lie algebra isomorphism $sp(\mathbb{C}) \rightarrow sp(\mathbb{C})$,

$$A = A_{a, a^*} \rightarrow A_{D, X} := C^T A_{a, a^*} \overline{C}. \quad (41)$$

Since C is unitary ($C^T = (\overline{C})^{-1}$), this is the inverse of (39). At this stage it is clear that if

$$C^T \begin{pmatrix} d & k \\ l & -d^T \end{pmatrix} \overline{C}$$

is real then the corresponding operator is skew-Hermitian. Thus, $sp_c(\mathbb{R})$ consists of those A_{a,a^*} such that the corresponding $A_{D,X} \in sp(\mathbb{R})$. \square

Remark 6.3. In particular, for our K ,

$$K = \begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix} ,$$

the corresponding decomposition in D_x and X_x is (see (40))

$$K_{D,X} = C^T K C = \begin{pmatrix} \Re k & \Im k \\ \Im k & -\Re k \end{pmatrix} ; \quad (42)$$

thus, $K \in sp_C(\mathbb{R})$.

It is easy to check that, if $S \in sp_c(\mathbb{R})$, then

$$e^S \begin{pmatrix} \overline{\phi} \\ -\phi \end{pmatrix} \text{ is of the form } \begin{pmatrix} \overline{\psi} \\ -\psi \end{pmatrix} .$$

Thus, it is legitimate to parametrize the vector $\begin{pmatrix} \overline{\phi} \\ -\phi \end{pmatrix}$ by ϕ and denote

$$e^S(\phi) := e^S \begin{pmatrix} \overline{\phi} \\ -\phi \end{pmatrix} .$$

We also define $A \begin{pmatrix} f \\ g \end{pmatrix} = a(f) + a^*(g)$ so that $A(\phi) := A \begin{pmatrix} \overline{\phi} \\ -\phi \end{pmatrix}$.

We now recall the results of section 4 in paper I:

Theorem 6.4. *Let $\phi \in L^2$ and $R, S \in sp(\mathbb{C})$ with L^2 (or Hilbert-Schmidt) coefficients. Then*

$$[\mathcal{I}(S), A \begin{pmatrix} f \\ g \end{pmatrix}] = A(S \begin{pmatrix} f \\ g \end{pmatrix}) , \quad (43)$$

and therefore

$$[\mathcal{I}(S), A(\phi)] = A(S(\phi)) , \quad (44)$$

$$[\mathcal{I}(S), \mathcal{I}(R)] = \mathcal{I}[S, R] . \quad (45)$$

In addition, if $S \in sp_C(\mathbb{R})$ and $\|S\|_{L^2}$ is small, then

$$e^{\mathcal{I}(S)} A \begin{pmatrix} f \\ g \end{pmatrix} e^{-\mathcal{I}(S)} = A(e^S \begin{pmatrix} f \\ g \end{pmatrix}) , \quad (46)$$

$$e^{\mathcal{I}(S)} A(\phi) e^{-\mathcal{I}(S)} = A(e^S(\phi)) , \quad (47)$$

$$e^{\mathcal{I}(S)} I(R) e^{-\mathcal{I}(S)} = \mathcal{I}(e^S R e^{-S}) , \quad (48)$$

$$\left(\frac{\partial}{\partial t} e^{\mathcal{I}(S)} \right) e^{-\mathcal{I}(S)} = \mathcal{I} \left(\left(\frac{\partial}{\partial t} e^S \right) e^{-S} \right) . \quad (49)$$

Proof. The formulas (43)–(45) are elementary calculations. Formulas (46)–(49) follow by analyticity (power series) since $e^{\mathcal{I}(S)}$ is given by a convergent Taylor series on the dense subset of Fock space vectors with finitely many non-zero components. Replace S by tS ($t \in \mathbb{C}$, small) and check that all derivatives of the left-hand side agree with all derivatives of the right-hand side at $t = 0$. \square

For $\|S\|_{L^2(dx dy)}$ large, $S \in sp_c(\mathbb{R})$, the series defining $e^{\mathcal{I}(S)}$ may not converge on a dense subset. So, we define

$$e^{\mathcal{I}(S)} = \left(e^{\mathcal{I}(S)/n} \right)^n ,$$

where n is so large that $e^{\mathcal{I}(S)/n}$ is defined by a convergent series on vectors with finitely many components, and is then extended as a unitary operator to \mathcal{F} . This definition is clearly independent of n and still satisfies the crucial properties (46)–(49).

For the rest of this section, we discuss connections with well-known results and explain the change-of-basis formula.

6.5. Connection to the Heisenberg group and metaplectic representation. Recall that the classical Heisenberg group \mathbf{H}_n is $\mathbb{C}^n \times \mathbb{R}$ with multiplication law $(z, t)(w, s) = (z + w, t + s - \Im z \bar{w})$; see (1.20) in [11]. In our setting, \mathbf{H} is $L^2(\mathbb{R}^3) \times \mathbb{R}$ with multiplication law $(\phi, t)(\psi, s) = (\phi + \psi, t + s - \Im \phi \bar{\psi})$. The map $(\phi, t) \rightarrow e^{-A(\phi)} e^{it}$ is a unitary representation of \mathbf{H} . Indeed, we have

$$\begin{aligned} e^{-A(\phi)} e^{it} e^{-A(\psi)} e^{is} &= e^{-A(\phi+\psi) + \frac{1}{2}[A(\phi), A(\psi)]} e^{it+is} \\ &= e^{-A(\phi+\psi) + \frac{1}{2} \int (\bar{\phi}\psi - \phi\bar{\psi})} e^{it+is} \\ &= e^{-A(\phi+\psi)} e^{i(t+s - \Im \int \phi \bar{\psi})} . \end{aligned}$$

Shale [24] extended the standard construction of the metaplectic representation (see chapter 4 in [11]) to the infinite dimensional “restricted symplectic group” $rSp(\mathbb{R}) = \{T \in Sp(\mathbb{R}), (T^*T)^{1/2} - I \text{ is Hilbert-Schmidt}\}$. We do not use his results directly; and the following comments are just

meant for completeness. His results, and those of [11], are written with respect to the basis D_x, X_x . By assuming $G \in rSp(\mathbb{R})$, Shale showed there exists a unitary transformation of \mathcal{F} , $Y(G)$, such that

$$e^{-A(G\phi)} = Y(G)e^{-A(\phi)}Y(G)^{-1} ; \quad (50)$$

also, any two such unitary transformations $Y_1(G)$, $Y_2(G)$ are related by $Y_1(G) = e^{i\theta}Y_2(G)$. The mapping $G \mapsto Y(G)$ is a projective unitary representation, meaning that $Y(G_1)Y(G_2) = e^{i\theta(G_1, G_2)}Y(G_1G_2)$. In particular, we identify our unitary operator $e^{\mathcal{I}(S)}$ (after we reconcile the bases) as $e^{\mathcal{I}(S)} = e^{i\theta}Y(e^S)$ for some $\theta = \theta(S) \in \mathbb{R}$; we skip further details.

APPENDIX A. COMPUTATION OF CUBIC ERROR TERM

With recourse to equation (56) of paper I, and because of the comments following Proposition (5.2), we now carefully compute the error term

$$e^B[A, V]e^{-B} = \int v(x-y) \left(\bar{\phi}(y)e^B a_x^* e^{-B} e^B a_x e^{-B} e^B a_y e^{-B} \right. \quad (51)$$

$$\left. + \phi(y)e^B a_x^* e^{-B} e^B a_y^* e^{-B} e^B a_x e^{-B} \right) dx dy , \quad (52)$$

which acts on the vacuum state, Ω . All terms ending in a can be ignored. After commuting all a terms to the right, we are left with a pure cubic and a pure linear term in a^* , which we proceed to compute. Recall the following formula proved in paper I:

$$e^B(a_y, a_y^*) \begin{pmatrix} f \\ g \end{pmatrix} e^{-B} = (a_y, a_y^*) e^K \begin{pmatrix} f \\ g \end{pmatrix} . \quad (53)$$

Thus, we have

$$e^B a_x e^{-B} = \int \left(\text{ch}(k)(y, x) a_y + \overline{\text{sh}(k)}(y, x) a_y^* \right) dy ,$$

and, similarly,

$$e^B a_x^* e^{-B} = \int \left(\text{sh}(k)(y, x) a_y + \overline{\text{ch}(k)}(y, x) a_y^* \right) dy .$$

We are ready to extract the pure a^* term from (51). Before any simplifications, (51) reads

$$\begin{aligned} \int v(x-y)\bar{\phi}(y) & \left(\text{sh}(k)(z_1, x)a_{z_1} + \overline{\text{ch}(k)}(z_1, x)a_{z_1}^* \right) \\ & \left(\text{ch}(k)(z_2, x)a_{z_2} + \overline{\text{sh}(k)}(z_2, x)a_{z_2}^* \right) \\ & \left(\text{ch}(k)(z_3, y)a_{z_3} + \overline{\text{sh}(k)}(z_3, y)a_{z_3}^* \right) dz_1 dz_2 dz_3 dx dy . \end{aligned}$$

Thus, (51) contributes the cubic term

$$I = \int v(x-y)\bar{\phi}(y) \left(\overline{\text{ch}(k)}(z_1, x)\overline{\text{sh}(k)}(z_2, x)\overline{\text{sh}(k)}(z_3, y) \right) a_{z_1}^* a_{z_2}^* a_{z_3}^* dz_1 dz_2 dz_3 dx dy .$$

Thus $I(\Omega)$ has entries in the third slot of Fock space equal to (after normalization and symmetrization)

$$\psi_I(z_1, z_2, z_3) = \int v(x-y)\bar{\phi}(y) \left(\overline{\text{ch}(k)}(z_1, x)\overline{\text{sh}(k)}(z_2, x)\overline{\text{sh}(k)}(z_3, y) \right) dx dy .$$

For the linear terms, keep only the a^* term from the last row, and exactly one a and one a^* s from the first and second rows, and commute the a 's to the right. Hence, we are left with two terms:

$$\begin{aligned} II &= \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{sh}(k)}(z_2, x)\overline{\text{sh}(k)}(z_3, y)a_{z_1}a_{z_2}^*a_{z_3}^*dz_1dz_2dz_3dx dy \\ &= \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{sh}(k)}(z_2, x)\overline{\text{sh}(k)}(z_3, y) \\ & \quad (\delta(z_1 - z_3)a_{z_2}^* + \delta(z_1 - z_2)a_{z_3}^*) dz_1 dz_2 dz_3 dx dy \text{ (modulo linear terms in } a) \\ &= \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{sh}(k)}(z_2, x)\overline{\text{sh}(k)}(z_1, y)a_{z_2}^* dz_1 dz_2 dx dy \\ & \quad + \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{sh}(k)}(z_1, x)\overline{\text{sh}(k)}(z_3, y)a_{z_3}^* dz_1 dz_3 dx dy , \end{aligned}$$

and

$$\begin{aligned} III &= \int v(x-y)\bar{\phi}(y)\overline{\text{ch}(k)}(z_1, x)\text{ch}(k)(z_2, x)\overline{\text{sh}(k)}(z_3, y)a_{z_1}^*a_{z_2}a_{z_3}^*dz_1dz_2dz_3dx dy \\ &= \int v(x-y)\bar{\phi}(y)\overline{\text{ch}(k)}(z_1, x)\text{ch}(k)(z_2, x)\overline{\text{sh}(k)}(z_2, y)a_{z_1}^* dz_1 dz_2 dx dy . \end{aligned}$$

These terms contribute to the first slot of Fock space entries of the form

$$\begin{aligned}\psi_{II}(z) &= \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{sh}(k)}(z, x)\overline{\text{sh}(k)}(z_1, y)dz_1dxdy \\ &\quad + \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{sh}(k)}(z_1, x)\overline{\text{sh}(k)}(z, y)dz_1dxdy\end{aligned}$$

and

$$\psi_{III}(z) = \int v(x-y)\bar{\phi}(y)\overline{\text{ch}(k)}(z, x)\text{ch}(k)(z_2, x)\overline{\text{sh}(k)}(z_2, y)dz_2dxdy .$$

Next, we concentrate on the contributions of (52).

$$\begin{aligned}(52) &= \int v(x-y)\phi(y) \left(\text{sh}(k)(z_1, x)a_{z_1} + \overline{\text{ch}(k)}(z_1, x)a_{z_1}^* \right) \\ &\quad \left(\text{sh}(k)(z_2, y)a_{z_2} + \overline{\text{ch}(k)}(z_2, y)a_{z_2}^* \right) \\ &\quad \left(\text{ch}(k)(z_3, x)a_{z_3} + \overline{\text{sh}(k)}(z_3, x)a_{z_3}^* \right) dz_1dz_2dz_3dxdy ,\end{aligned}$$

which contributes a cubic in a^* :

$$I' = \int v(x-y)\phi(y)\overline{\text{ch}(k)}(z_1, x)\overline{\text{ch}(k)}(z_2, y)\overline{\text{sh}(k)}(z_3, x)a_{z_1}^*a_{z_2}^*a_{z_3}^*dz_1dz_2dz_3dxdy .$$

Here, we have

$$\psi_{I'}(z_1, z_2, z_3) = \int v(x-y)\phi(y)\overline{\text{ch}(k)}(z_1, x)\overline{\text{ch}(k)}(z_2, y)\overline{\text{sh}(k)}(z_3, x)dxdy .$$

The linear terms in a^* (modulo a) are

$$\begin{aligned}II' &= \int v(x-y)\phi(y)\text{sh}(k)(z_1, x)a_{z_1}\overline{\text{ch}(k)}(z_2, y)a_{z_2}^*\overline{\text{sh}(k)}(z_3, x)a_{z_3}^*dz_1dz_2dz_3dxdy \\ &= \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{ch}(k)}(z_2, y)\overline{\text{sh}(k)}(z_1, x)a_{z_2}^*dz_1dz_2dxdy \\ &\quad + \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{ch}(k)}(z_1, y)\overline{\text{sh}(k)}(z_3, x)a_{z_3}^*dz_1dz_3dxdy\end{aligned}$$

and

$$\begin{aligned}III' &= \int v(x-y)\bar{\phi}(y)\overline{\text{ch}(k)}(z_1, x)\text{sh}(k)(z_2, y)\overline{\text{sh}(k)}(z_3, x)a_{z_1}^*a_{z_2}a_{z_3}^*dz_1dz_2dz_3dxdy \\ &= \int v(x-y)\bar{\phi}(y)\overline{\text{ch}(k)}(z_1, x)\text{sh}(k)(z_2, y)\overline{\text{sh}(k)}(z_2, x)a_{z_1}^*dz_1dz_2dxdy .\end{aligned}$$

The Fock space entries read

$$\begin{aligned}\psi_{II'}(z) &= \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{ch}(k)}(z, y)\overline{\text{sh}(k)}(z_1, x) dz_1 dx dy \\ &\quad + \int v(x-y)\bar{\phi}(y)\text{sh}(k)(z_1, x)\overline{\text{ch}(k)}(z_1, y)\overline{\text{sh}(k)}(z, x) dz_1 dx dy\end{aligned}$$

and

$$\psi_{III'}(z) = \int v(x-y)\bar{\phi}(y)\overline{\text{ch}(k)}(z, x)\text{sh}(k)(z_2, y)\overline{\text{sh}(k)}(z_2, x) dz_2 dx dy .$$

All the resulting ψ can be estimated in $L^2(dtdz)$ by the method of section 7 of paper I, without using $X_{s,\delta}$ spaces. We remind the reader how to estimate these terms. Take, for instance, $\psi_{III'}(t, z)$. Write $\text{ch}(k)(t, z, x) = \delta(z - x) + p(t, z, x)$ to express $\psi_{III'} = \psi_\delta + \psi_p$. We estimate the first of these terms:

$$\begin{aligned}|\psi_\delta(z)| &= \left| \int v(z-y)\bar{\phi}(y)\text{sh}(k)(z_2, y)\overline{\text{sh}(k)}(z_2, z) dz_2 dy \right| \\ &\leq \|v(z-y)\bar{\phi}(y)\overline{\text{sh}(k)}(z_2, z)\|_{L^2(dz_2 dy)} \|\text{sh}(k)(z_2, y)\|_{L^2(dz_2 dy)} .\end{aligned}$$

The second term is uniformly bounded in time; thus,

$$\begin{aligned}&\int_0^\infty \int_{\mathbb{R}^3} |\psi_\delta(t, z)|^2 dt dz \\ &\leq C \int_0^\infty \int |v(z-y)\phi(y)\overline{\text{sh}(k)}(z_2, z)|^2 dz dz_2 dy dt \leq C\end{aligned}$$

by a local smoothing type result (see Lemma 2, section 7 of paper I). All other terms can be estimated by the same method.

REFERENCES

- [1] Anderson, M. H., Ensher, J. R., Matthews, M. R., Wieman, C. E., Cornell, E.A.: Observation of Bose-Einstein condensation in a dilute atomic vapor. *Science* **269**, 198–201 (1995)
- [2] Berezin, F. A.: *The Method of Second Quantization*. New York: Academic Press, 1966
- [3] Davis, K. B., Mewes, M.-O., Andrews, M. R., van Druten, N. J., Durfee, D. S., Kurn, D. M., Ketterle, W.: Bose-Einstein condensation in a gas of sodium atoms. *Phys. Rev. Lett.* **75**, 3969–3973 (1995)
- [4] Dubrovin, B. A., Fomenko, A. T., Novikov, S. P.: *Modern Geometry- Methods and Applications, Part I*. New York: Springer-Verlag, 1992
- [5] Elgart, A., Erdős, L., Schlein, B., Yau, H. T.: Gross-Pitaevskii equation as the mean field limit of weakly coupled bosons. *Arch. Rat. Mech. Anal.* **179**, 265–283 (2006)

- [6] Erdős, L., Yau, H. T.: Derivation of the non-linear Schrödinger equation from a many-body Coulomb system. *Adv. Theor. Math. Phys.* **5**, 1169–1205 (2001)
- [7] Erdős, L., Schlein, B., Yau, H. T.: Derivation of the Gross-Pitaevskii hierarchy for the dynamics of Bose-Einstein condensate. *Comm. Pure Appl. Math.* **59**, 1659–1741 (2006)
- [8] Erdős, L., Schlein, B., Yau, H. T.: Derivation of the cubic non-linear Schrödinger equation from quantum dynamics of many-body systems. *Invent. Math.* **167**, 515–614 (2007)
- [9] Erdős, L., Schlein, B., Yau, H. T.: Rigorous derivation of the Gross-Pitaevskii equation. *Phys. Rev. Lett.* **98**, 040404 (2007)
- [10] Erdős, L., Schlein, B., Yau, H. T.: Derivation of the Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensate. To appear in *Annals Math.*
- [11] Folland, G. B.: *Harmonic analysis in phase space*. *Annals of Math. Studies*, Vol. **122**. Princeton, NJ: Princeton University Press, 1989
- [12] Ginibre, J., Velo, G.: The classical field limit of scattering theory for non-relativistic many-boson systems, I and II. *Comm. Math. Phys.* **66**, 37–76 (1979) and **68**, 45–68 (1979)
- [13] Grillakis, M., Machedon, M., Margetis, D.: Second-order corrections to mean field evolution of weakly interacting Bosons. I. *Comm. Math. Phys.* **294**, 273–301 (2010)
- [14] Grillakis, M. G., Margetis, D.: A priori estimates for many-body Hamiltonian evolution of interacting Boson system. *J. Hyperb. Differential Eqs.* **5**, 857–883 (2008)
- [15] Gross, E. P.: Structure of a quantized vortex in boson systems. *Nuovo Cim.* **20**, 454–477 (1961)
- [16] Gross, E. P.: Hydrodynamics of a superfluid condensate. *J. Math. Phys.* **4**, 195–207 (1963)
- [17] Hepp, K.: The classical limit for quantum mechanical correlation functions. *Comm. Math. Phys.* **35**, 265–277 (1974)
Comm. Pure Appl. Math. **46**, 1221–1268 (1993)
Duke Math. J. **81**, 99–103 (1995)
- [18] Klainerman, S., Machedon, M.: On the uniqueness of solutions to the Gross-Pitaevskii hierarchy, *Communications in Mathematical Physics* **279**, 169–185, 2008
- [19] Lieb, E. H., Seiringer, R., Solovej, J. P., Yngvanson, J.: *The mathematics of the Bose gas and its condensation*. Basel, Switzerland: Birkhäuser Verlag, 2005
- [20] Pitaevskii, L. P.: Vortex lines in an imperfect Bose gas. *Soviet Phys. JETP* **13**, 451–454 (1961)
- [21] Pitaevskii, L. P., Stringari, S.: *Bose-Einstein condensation*. Oxford, UK: Oxford University Press, 2003
- [22] Riesz, F., Nagy, B.: *Functional analysis*. New York: Frederick Ungar Publishing, 1955
- [23] Rodnianski, I., Schlein, B.: Quantum fluctuations and rate of convergence towards mean field dynamics. *Comm. Math. Phys.* **291**(2), 31–61 (2009)
- [24] Shale, D.: Linear symmetries of free Boson fields, *Trans. Amer. Math. Soc.* **103**(1), 149–167 (1962)

- [25] Wu, T. T.: Some nonequilibrium properties of a Bose system of hard spheres at extremely low temperatures. J. Math. Phys. **2**, 105–123 (1961)
- [26] Wu, T. T.: Bose-Einstein condensation in an external potential at zero temperature: General Theory. Phys. Rev. A **58**, 1465–1474 (1998)

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF MARYLAND, COLLEGE PARK,
MD 20742

E-mail address: mng@math.umd.edu

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF MARYLAND, COLLEGE PARK,
MD 20742

E-mail address: mxm@math.umd.edu

DEPARTMENT OF MATHEMATICS, AND INSTITUTE FOR PHYSICAL SCIENCE AND
TECHNOLOGY, AND CENTER FOR SCIENTIFIC COMPUTATION AND MATHEMATI-
CAL MODELING, UNIVERSITY OF MARYLAND, COLLEGE PARK, MD 20742

E-mail address: dio@math.umd.edu