QUARTERLY OF APPLIED MATHEMATICS
VOLUME LXXV, NUMBER 1
MARCH 2017, PAGES 69–104
http://dx.doi.org/10.1090/qam/1455
Article electronically published on August 24, 2016

EVOLUTION OF THE BOSON GAS AT ZERO TEMPERATURE: MEAN-FIELD LIMIT AND SECOND-ORDER CORRECTION

By

MANOUSSOS GRILLAKIS (*Department of Mathematics, University of Maryland, College Park, Maryland 20742*),

MATEI MACHEDON (*Department of Mathematics, University of Maryland, College Park, Maryland 20742*),

AND

DIONISIOS MARGETIS (*Department of Mathematics, and Institute for Physical Science and Technology, and Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, Maryland 20742*)

Abstract. A large system of N integer-spin atoms, called Bosons, manifests one of the most *coherent* macroscopic quantum states known to date, the "Bose-Einstein condensate", at extremely low temperatures. As $N \to \infty$, this system is usually described by a mean-field limit: a single-particle wave function, the *condensate wave function*, that satisfies a nonlinear Schrödinger-type equation. In this expository paper, we review kinetic aspects of the mean-field Boson evolution. Furthermore, we discuss recent advances in the rigorous study of second-order corrections to this mean-field limit. These corrections originate from the quantum-kinetic mechanism of *pair excitation*, which lies at the core of pioneering works in theoretical physics including ideas of Bogoliubov, Lee, Huang, Yang and Wu. In the course of our exposition, we revisit the formalism of Fock space, which is indispensable for the analysis of pair excitation.

1. Introduction. A significant advance in physics in the last two decades has been the first experimental observation of Bose-Einstein condensation (BEC) in dilute atomic gases at extremely low temperatures [3,29]. In BEC, a large number of atoms with integer spin, called Bosons, occupy a *single* quantum state macroscopically. This behavior, predicted by Bose and Einstein for non-interacting atoms almost a century ago [13,32,33],

Received June 29, 2016.
2010 *Mathematics Subject Classification.* Primary 35Q40, 82C10; Secondary 81V45, 70F10.
Key words and phrases. Quantum dynamics, weakly interacting Bosons, mean-field limit, Bogoliubov transformation, pair excitation, non-linear Schrödinger equation.
The third author was partly supported by the National Science Foundation through Grant DMS-1517162.
E-mail address: mng@math.umd.edu
E-mail address: mxm@math.umd.edu
E-mail address: dio@math.umd.edu

is responsible for the remarkable coherence of the Boson gas. This phenomenon bears a striking resemblance to the coherence manifested by photons in laser beams [14]. The experimental advance in BEC [3, 29] has paved the way to the precise control of atomic systems, and actively permeates several areas of physics nowadays [27, 28, 52, 53, 84].

In this expository article, we review recent mathematical progress in understanding how the quantum state of the Boson gas evolves at zero temperature. Our attention focuses on aspects intimately connected to the symmetric *many-body wave function* of the system. This is a crucial variable, since by quantum mechanics all observable properties of the atomic gas can in principle be computed as appropriate inner products with this quantity. A hurdle in the direct use of this wave function for physical prediction is due to the high dimension of its spatial domain, $\mathbb{R}^{3N}$ where N is the number of atoms ($N \gg 1$).

Accordingly, the following question has attracted much attention: How can one *approximate* the N-body wave function of the interacting Boson system for large yet finite N in terms of variables that live in *low* spatial dimensions? A complete answer to this question is as yet elusive. Studies in this direction have a long history in physics. Noteworthy are early heuristic derivations of mean-field limits that involve nonlinear Schrödinger-type equations in 3+1 dimensions [49, 74, 82]. Only recently has it been fruitful to rigorously elucidate such mean-field limits; see works by Lieb, Elgart, Erdős, Rodnianski, Schlein, and Yau [34–37, 39, 65, 75]. The comprehensive review by Bao and Cai [5] provides a discussion on the macroscopic evolution laws from an applied mathematics perspective.

Our exposition touches upon aspects of the mean-field dynamics. We also address the following question: What is the description on the N-body Boson evolution *beyond* the usual mean-field limit? We adopt the view that an *appropriate* description should be based on *pair excitation*, which permeates the pioneering works of Bogoliubov, Lee, Huang, Yang and especially Wu in physics [12, 59, 82]. The main idea is that atoms are scattered in pairs from the condensate to other states. This process is modeled by a *collision kernel* entering the many-body wave function [82].

In our view, pair excitation in the quantum setting is distinct from cases of classical physics, e.g., the classical Boltzmann gas. The main difference is that in the former case the collision kernel is *not* a-priori known; it must be determined via the many-body dynamics. A different approach in the quantum setting has been taken up in [7, 11].

Recently, we placed the formalism of pair excitation on firm mathematical grounds via Fock space estimates [44–48]. Part of our goal with the present expository paper is to review this advance and also point to related, open directions of research.

In our exposition, we place emphasis on time-dependent aspects. We assume that the reader is reasonably familiar with the fundamentals of quantum mechanics. For broad introductions to this subject, see, e.g., the texts by Dirac and von Neumann [30, 81].

1.1. *Physical setting and Hamiltonian model.* Before we discuss particularities of approximations to the many-Boson evolution, we outline prominent features of the physical setting. Our purpose with this excursion is to indicate how the experiments with dilute gases, which partly motivate recent studies in BEC, might be related to mathematical models. We believe that this connection is still incomplete; bridging laboratory observations with mathematical understanding is an ongoing endeavor open to scrutiny [5].

From a physical standpoint, one can single out the following features of experiments:
(i) the atoms in the gas are often characterized by *weak* mutual interactions;
(iii) the temperatures maintained in the experiments are finite yet extremely low; and
(iii) there is a *trapping* potential that keeps the atoms together.

Feature (i) underlies many rigorous theoretical studies of the Boson gas. The starting point is a Hamiltonian description. The assumption of weak atomic interactions may allow one to analyze the Hamiltonian evolution by methods akin to perturbation theory. However, a notable exception to this assumption renders the analysis more challenging, as we will try to explain in this paper.

Let us now describe the governing model. The N-body Hamiltonian $H_N : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$, often referred to as the "PDE Hamiltonian", underlying our exposition reads:[1]

$$H_N = H_{N,\beta} := \sum_{i=1}^{N}\{-\Delta_{x_i}+V_e(x_i)\}+(2N)^{-1}\sum_{\substack{i,j=1\\ i\neq j}}^{N} N^{3\beta}v(N^{\beta}(x_i-x_j))\,, \quad x_i\in\mathbb{R}^3\,. \tag{1.1}$$

In the above, $V_e(x)$ is the external *trapping* potential, acting simultaneously on each atom; $v(x)$ is the *two-body* repulsive interaction potential, where $v > 0$; and β is a parameter expressing the strength of the interaction potential relative to kinetic energy, where $0 \le \beta \le 1$. We set Planck's constant equal to unity, $\hbar = 1$, while $2m = 1$ where m is the atom mass. Formally speaking, the potential v is such that in the limit $N \to \infty$ the term $N^{3\beta}\, v(N^{\beta}x)$ approaches $\big(\int v\big)\delta(x)$ if $\beta > 0$. For bounded v, the scaling of the atom positions, x_i, by $N^{-\beta}$ implies that the interaction is small compared to the kinetic energy term if $\beta < 1$; in this sense, the value $\beta = 1$ is deemed as special, signifying that the particle interactions cannot be considered as a small perturbation.

By Hamiltonian (1.1), the atoms have zero spin. In addition, this model only accounts for two-body interactions, leaving out higher-order interactions. However, three-body interactions may have serious consequences on error estimates, as recently pointed out by X. Chen [18]. Such interactions lie beyond our present scope.

For Bosons, Hamiltonian (1.1) acts on symmetric square integrable wave functions $\psi_N(t,\vec{x})$, which are invariant under permutations of atom coordinates ($\vec{x} = (x_1, x_2, \ldots, x_N)$). Thus, H_N operates in the Bosonic Hilbert space, $L^2_s(\mathbb{R}^{3N})$ (see section 2).

Feature (ii) listed above suggests that the Bose-Einstein condensate observed in experiments actually co-exists with thermally excited states. This consideration almost begs for studying by first principles the effect on evolution of finite but small temperatures [4]. In our exposition, we assume that atoms of thermally excited states form a negligible fraction of the system. Hence, we adhere to the idealized regime of *zero temperature*.

Accordingly, the system properties are fully determined by the N-body wave function, $\psi_N(t,\vec{x})$, that satisfies the N-body Schrödinger equation, viz.,

$$i\partial_t\psi_N(t,\vec{x}) = H_N\psi_N(t,\vec{x})\ , \tag{1.2}$$

under given initial data, $\psi_N(0,\cdot) \in L^2_s(\mathbb{R}^{3N})$. A physically appealing case concerns initial data forming a *tensor product* of the same one-particle state, in the spirit of BEC (see

[1]We alert the reader that in sections 2 and 5 we utilize a negative-definite Hamiltonian, denoted $\acute{H}_N := -H_N$, for the sake of algebraic convenience; cf. (2.7).

section 3) [82, 83]. Although the solution to (1.2) can be abstractly expressed as

$$e^{-itH_N}\psi_N(0)\ , \tag{1.3}$$

this last expression is known to be unwieldy for large N. Approximations are needed.

In regard to feature (iii) above, the system lacks translation invariance because of V_e; thus, the total particle momentum is not conserved. A related complication, not fully resolved to this date, is how to account for a reasonably general trapping potential, V_e, in the analysis. To circumvent this issue, in our present exposition we sometimes set $V_e \equiv 0$, restricting attention to evolution at times *after* the trap is switched off. Notably, the effect of quadratic traps has been analyzed by X. Chen [19, 20].

1.2. *Flavor of mean-field limit.* We return to our discussion of approximations to many-Boson Hamiltonian evolution (1.3). This evolution has been replaced by a mean-field limit; see the classic works by Gross [49], Pitaevskii [74] and Wu [82] who heuristically derive a version of this limit in the non-translation-invariant setting.

The notion of the mean-field limit can roughly be outlined as follows. Suppose that ψ_N has the form of a tensor product of a one-particle state at $t = 0$. If the evolving ψ_N at $t > 0$ is replaced by a tensor product involving a one-particle state, this approximation is *best* provided the one-particle wave function, called condensate wave function, obeys a certain non-linear Schrödinger-type equation in $\mathbb{R}^3$. The precise criterion of what "best" means relies on error estimates in an appropriate metric (see section 3). In this mean-field picture, heuristically speaking, each atom sees an effective potential controlled by the gas density and the atomic interactions.

This mean-field evolution is of course not in strict agreement with (1.2) under (1.1). For many years, the mean-field description has led to successful predictions for laboratory experiments in the physics community [28, 53] but lacked a rigorous justification.

The nature of the mean-field limit for different values of the parameter β has only recently been understood [5]; see sections 2 and 3. In this connection, we should mention works by: Lieb and collaborators in the stationary case via a variational principle [65]; and by Elgart, Erdős, Schlein and Yau [34–37, 39] in the time-dependent case via the formalism of the quantum kinetic hierarchies [79]. In the time-dependent case [34–37, 39], the convergence of the exact dynamics to the mean-field limit is asserted in the trace norm as $N \to \infty$ by use of marginal densities; see also the work by Rodnianski and Schlein [75]. These breakthroughs have inspired further investigations in the many-Boson evolution.

1.3. *On pair excitation.* Despite the success of mean-field theories in explaining equilibrium and non-equilibrium phenomena in the Boson gas, the strict validity of such limits can be questioned on physical and mathematical grounds. There is evidence suggesting that these limits form a fundamentally incomplete description of the Boson gas.

First, from a physical standpoint, such mean-field limits may *not* account for the *depletion* of the condensate, i.e., the experimentally observed phenomenon in which a small fraction of Bosons escape from the macroscopic state in order to occupy other states of higher energies [84]. By using somewhat loose language, we are tempted to state that this effect is synonymous to *quantum fluctuations*, which originate from complicated two-body spatial correlations. This observed effect may not be described by the one-particle wave function of the condensate at the above mean-field level.

Second, it has been rigorously shown by Rodnianski and Schlein [75] via Fock space techniques that in Hartree dynamics, where $\beta = 0$ by (1.1), for fixed yet large N the error associated with the mean-field limit grows *exponentially* with time in the trace norm for marginal densities; see section 2. Thus, by this result the mean-field limit, in the sense of marginal densities, appears to be an accurate description up to times logarithmic in N. In regard to the rate of convergence to the mean-field limit, we should also mention the more recent works by Pickl [72] and Kuz [57]. Also, seeds of the pair-excitation idea can be traced in the works by Hepp [50] and Ginibre and Velo [42, 43]; see section 5.

These observations have motivated the following question: How can one transcend the mean-field limit and describe *corrections* to it in a way consistent with the many-body Hamiltonian evolution? It turns out that, in physical terms, this question is intimately related to the concept of elementary excitations, or phonons; see, e.g., [63, 82].

The effect of quantum fluctuations at zero temperature was studied by Bogoliubov [12] and Lee, Huang and Yang [59] in the periodic setting. Wu [82, 83] extended the work of Lee, Huang and Yang [59] to the non-translation-invariant case by introducing a higher-order approximation for the many-body wave function, ψ_N, in terms of a collision kernel, K_0; see (1.4) below. These works [59, 82, 83] make use of techniques in Fock space that heuristically single out the scattering of pairs of atoms from the condensate (section 2).

Wu applies the following ansatz for the N-body wave function in Fock space [82, 83]:

$$C_N(t)e^{\mathfrak{P}[K_0]}\psi_{N,\mathrm{mf}}(t) \ , \tag{1.4}$$

where $\psi_{N,\mathrm{mf}}(t)$ expresses the mean-field-related tensor product of one-particle states, $C_N(t)$ is a normalization factor, and $\mathfrak{P}[K_0]$ is an operator that spatially averages out the excitation of atoms from the condensate to other states via the kernel $K_0(t, x, y)$. The operator $\mathfrak{P}[K_0]$ is explicitly described in the language of Fock space; see sections 2 and 4. The function K_0 lives in $\mathbb{R}^6$, and is not a-priori known but should be determined consistently with the many-body dynamics [82]. This description should be contrasted to the case of the classical Boltzmann gas, in which the collision kernel is given explicitly via classical mechanics.

The terms "Bogoliubov transformation" and "Bogoliubov rotation" are often used to express an effect intimately related to pair excitation. Although our set-up and derived equation for K_0 are different from Wu's [82, 83], we primarily follow his terminology, using the term pair excitation for a transformation of form (1.4). In section 5, we use the term Bogoliubov transformation interchangeably with the term pair excitation.

1.4. *Scope and outline.* In this expository paper, we review recent progress in explicitly describing an approximation to evolution (1.3) by use of a formula for the many-body wave function in the spirit of (1.4) [44, 45]. In particular, we consider a *coherent state* (defined in section 2) in Fock space as the initial many-body state. In order to discuss the germane error estimates concerning deviations of the approximate evolution from the exact N-body evolution, we invoke tools of Fock space. In the course of our exposition, we extensively review known mean-field limits in the time-dependent setting [34–37, 39, 75].

The organization of the remainder of our paper is summarized as follows. Section 2 introduces the formalism of Fock space and some of the related techniques. In section 3, we review the derivations of mean-field limits in terms of particle marginal densities and

their kinetic hierarchies for a closed particle system [34–37, 39]. Section 4 outlines aspects of modeling pair excitation [69, 83]. In section 5, we review a rigorous approach to the approximation of the many-body evolution via the formalism of pair excitation. Finally, section 6 concludes our paper with a short discussion of open challenging problems at the interface of quantum kinetic theory and mathematical physics.

2. Background: Bosonic Fock space. In this section, we review notions of the Fock space and explain the meaning of Hamiltonian evolution in this space. For an introduction to Fock space, see also [78]. In physics, the underlying formalism is often called the *second quantization* [9]. The Fock space is needed for the formulation of pair excitation (sections 4 and 5). We also introduce the useful notion of the Weyl or coherent state and explain how one can derive the mean-field limit in this setting.[2]

2.1. *Generalities.* The Fock space is an infinite direct sum of Hilbert spaces, e.g., [78]

$$\mathbb{F} = \bigoplus_{n=0}^{\infty} \mathbb{F}_n \qquad \text{where} \qquad \mathbb{F}_n = L^2(\mathbb{R}^{3n}) \ .$$

The Hilbert space $\mathbb{F}_n$ is the n-particle Fock fiber or sector; this is the space of n-particle wave functions. In accord with physics, one usually considers separately the Fermionic and Bosonic Fock spaces, viz.,

$$\mathbb{F}^{\text{fermi}} = \bigoplus_{n=0}^{\infty} \mathbb{F}_n^{\text{fermi}} \qquad \text{where} \qquad \mathbb{F}_n^{\text{fermi}} = L^2_{\text{a}}(\mathbb{R}^{3n}) \ ;$$

$$\mathbb{F}^{\text{bose}} = \bigoplus_{n=0}^{\infty} \mathbb{F}_n^{\text{bose}} \qquad \text{where} \qquad \mathbb{F}_n^{\text{bose}} = L^2_{\text{s}}(\mathbb{R}^{3n}) \ ;$$

where $L^2_a(\mathbb{R}^{3n})$ and $L^2_s(\mathbb{R}^{3n})$ are the L^2-spaces of antisymmetric and symmetric functions for n particles, respectively. Thus, $L^2_a(\mathbb{R}^{3n})$ and $L^2_s(\mathbb{R}^{3n})$ consist of square integrable functions $\psi_n(x_1 \dots x_n)$ with $x_j \in \mathbb{R}^3$ and $j = 1, \dots, n$ that for any permutation, $\pi : (1, 2, \dots, N) \mapsto (1, 2, \dots, N)$, respectively obey the relations

$$\psi_n(x_{\pi(1)}, x_{\pi(2)} \dots x_{\pi(n)}) = \text{sgn}(\pi)\psi_n(x_1, x_2 \dots x_n) \quad \text{if } \psi_n \in L^2_a(\mathbb{R}^{3n}) \text{ (Fermions) ;}$$
$$\psi_n(x_{\pi(1)}, x_{\pi(2)} \dots x_{\pi(n)}) = \psi_n(x_1, x_2 \dots x_n) \qquad \text{if } \psi_n \in L^2_s(\mathbb{R}^{3n}) \text{ (Bosons).}$$

Each of these properties is preserved by the many-body evolution.

Thus, any vector (or state) in Fock space has the form $\psi = (\psi_0, \psi_1, \dots \psi_n, \dots)$. Here, ψ_0 is a constant complex-valued function which can be identified with a complex number; thus, $\mathbb{F}_0 = \mathbb{C}$ and we set $\psi_0 = c_0 \in \mathbb{C}$. Hence, the Fock space describes an *open* system in which the number of particles is not specified. The element ψ_0 is the vacuum state, or simply "vacuum", with no particles. Since vacuum plays a special role, we denote it by

$$\Omega := (1, 0, \dots, 0, \dots) \ . \tag{2.1}$$

[2]The exposition for the mean-field limit in this section should be compared to section 3 where we discuss the mean-field for a (closed) system with a fixed number, N, of particles.

Of course, the Fock space is a Hilbert space equipped with an inner product and norm:

$$\langle \phi, \psi \rangle_{\mathbb{F}} := \overline{\phi}_0 c_0 + \sum_{n=1}^{\infty} \int_{\mathbb{R}^{3n}} dx_1 \dots dx_n \left\{ \overline{\phi}_n(x_1 \dots x_n) \psi_n(x_1 \dots x_n) \right\} \ ; \quad \|\psi\|_{\mathbb{F}}^2 := \langle \psi, \psi \rangle_{\mathbb{F}} \ .$$

The Fock space vectors are normalized to unity, $\|\psi\|_{\mathbb{F}} = 1$, unless we state otherwise.[3]

2.2. *Bosonic Fock space.* We henceforth consider n-particle wave functions, $\psi_n(x_1, \dots, x_n)$, that are symmetric, the focus of this paper. In the Bosonic Fock space, we define the distribution-valued creation and annihilation operators, a_x^* and a_x, respectively. These operate on wave functions in Fock fibers, i.e., $\psi_{n-1} \in \mathbb{F}_{n-1}$ and $\psi_{n+1} \in \mathbb{F}_{n+1}$, as follows:

$$a_x^*(\psi_{n-1}) := \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \delta(x - x_j) \psi_{n-1}(x_1 \dots x_{j-1}, x_{j+1} \dots x_{n+1}) \ , \tag{2.2}$$

$$a_x(\psi_{n+1}) := \sqrt{n+1} \psi_{n+1}([x], x_1 \dots x_{n-1}) \ ; \tag{2.3}$$

where the symbol $[x]$ denotes "freezing" of the indicated coordinate, x. Loosely speaking, a_x^* (a_x) creates (annihilates) a particle at position x. The operators a_x^* and a_x are time independent.[4] An important convention is that

$$a_x \Omega = 0 \ . \tag{2.4}$$

The right-hand sides of (2.2) and (2.3) are not L^2-functions but are rather understood as distributions. We leave it to the reader to verify the canonical commutation relation

$$[a_x, a_y^*] := a_x a_y^* - a_y^* a_x = \delta(x - y) \ . \tag{2.5}$$

As mentioned above, a_x^* and a_x are distribution valued. In order to introduce useful operators with values in the Fock space, pick an arbitrary $\phi \in L^2(\mathbb{R}^3)$ and define

$$a_\phi^* := \int_{\mathbb{R}^3} dx \left\{ \phi(x) a_x^* \right\} \qquad \text{and} \qquad a_{\overline{\phi}} := \int_{\mathbb{R}^3} dx \left\{ \overline{\phi}(x) a_x \right\} \ . \tag{2.6}$$

By (2.2) and (2.3), operators a_ϕ^* and $a_{\overline{\phi}}$ act on Fock fibers as follows:

$$a_\phi^*(\psi_{n-1}) = \int dx \left\{ \phi(x) a_x^*(\psi_{n-1}) \right\} \in \mathbb{F}_n \ ,$$

$$a_{\overline{\phi}}(\psi_{n+1}) \ = \int dx \left\{ \overline{\phi}(x) a_x(\psi_{n+1}) \right\} \in \mathbb{F}_n \ ,$$

which imply that a_ϕ^* ($a_{\overline{\phi}}$) creates (annihilates) a particle at state ϕ. The norms of these operators, restricted on the appropriate fiber, read

$$\|a_\phi^*\|_{\mathbb{F}_{n-1}} = \sqrt{n} \, \|\phi\|_{L^2(\mathbb{R}^3)} \ , \quad \|a_{\overline{\phi}}\|_{\mathbb{F}_{n+1}} = \sqrt{n+1} \, \|\phi\|_{L^2(\mathbb{R}^3)} \ .$$

Clearly, a_ϕ^* and $a_{\overline{\phi}}$ are not bounded in $\mathbb{F}$. By (2.5), the commutator of $a_{\overline{\phi}}$ and a_g^* is

$$\left[a_{\overline{\phi}}, a_g^* \right] = \langle \phi, g \rangle_{L^2(\mathbb{R}^3)} \ .$$

[3]Throughout the paper, $\langle \cdot, \cdot \rangle_{\mathbb{F}}$ denotes the Fock space inner product. On the other hand, the use of $\langle \cdot, \cdot \rangle$ without a subscript or with a subscript different from $\mathbb{F}$ indicates an inner product in a suitable space with a finite number of particles; ditto for the induced norms. The meaning of such symbols for inner products and corresponding norms should be self-explanatory in the main text.

[4]In the language of physics, we can state that we use a_x^* and a_x in the "Schrödinger picture" [30].

2.3. *Evolution in Bosonic Fock space.* Next, we discuss how the Fock space formalism can be used in the study of the N-Boson evolution. Recall Hamiltonian (1.1). By reversing the sign, consider the "negative" Hamiltonian

$$\acute{H}_N := \sum_{j=1}^{N} \acute{\mathfrak{H}}_{x_j} - \frac{1}{2N} \sum_{j \neq k}^{N} N^{3\beta} v\big(N^{\beta}(x_j - x_k)\big) \ , \quad 0 \leq \beta \leq 1 \ , \tag{2.7}$$

where $\acute{\mathfrak{H}}_x = \Delta_x - V_e(x)$ is the negative one-body Hamiltonian. This $\acute{H}_N$ acts on symmetric wave functions $\psi_N(t, x_1, \ldots, x_N)$. Evolution equation (1.2) reads

$$\frac{1}{i}\partial_t \psi_N - \acute{H}_N \psi_N = 0 \ , \tag{2.8}$$

which may be solved for given initial data, say, $\psi_N(0, x_1, \ldots, x_N) =: \psi_{N,0}(x_1, \ldots, x_N)$.

In the Fock space, the negative Hamiltonian, $\acute{\mathcal{H}}_N : \mathbb{F} \to \mathbb{F}$, reads[5]

$$\acute{\mathcal{H}}_N = \int_{\mathbb{R}^3} dx \ \left\{ a_x^* \acute{\mathfrak{H}}_x a_x \right\} - \frac{1}{2N} \int_{\mathbb{R}^3 \times \mathbb{R}^3} dxdy \ \left\{ N^{3\beta} v\big(N^{\beta}(x-y)\big) a_x^* a_y^* a_x a_y \right\} \ . \tag{2.9}$$

If $\psi(t)$ denotes a vector in Fock space, consider the following evolution equation on $\mathbb{F}$:

$$\frac{1}{i}\partial_t \psi - \acute{\mathcal{H}}_N \psi = 0 \ , \tag{2.10}$$

which agrees with the PDE N-body evolution problem, expressed by (2.8), on sector $\mathbb{F}_N$. The reader may verify that the restriction, ψ_N, of $\psi(t)$ on $\mathbb{F}_N$ obeys $\left\{\acute{\mathcal{H}}_N \psi\right\}\big|_{\mathbb{F}_N} = \acute{H}_N \psi_N$.

Thus, in order to describe time evolution in Fock space, we prescribe some initial data, $\psi(0)$, and subsequently write an abstract formula, the Fock space counterpart of (1.3), for the time-evolved $\psi(t)$, viz., $\psi(t) = e^{it\acute{\mathcal{H}}_N}\psi(0)$. An issue is to understand the evolution of special initial data $\psi(0)$, called the *coherent or Weyl state*, which is central in rigorous treatments of mean-field approximations. In fact, the projection of a coherent state onto $\mathbb{F}_n$ is a tensor product of n one-particle states, a state intimately related to BEC; see sections 2.3.1 and 3.1.

It is worthwhile noting that any Fock space operator commuting with $\acute{\mathcal{H}}_N$ gives rise to a conservation law. The number operator, $\mathcal{N}$, is particularly useful; it is defined by

$$\mathcal{N} := \int_{\mathbb{R}^3} dx \, \{a_x^* a_x\} \ . \tag{2.11}$$

The expectation of this $\mathcal{N}$ over any given state, $\psi \in \mathbb{F}$, equals

$$\langle \psi, \mathcal{N}\psi \rangle_{\mathbb{F}} = \sum_{n=0}^{\infty} n \|\psi_n\|^2 \ .$$

This result can be derived by use of (2.2) and (2.3). If we interpret ψ as the Fock state of an open system (with $\|\psi\|_{\mathbb{F}} = 1$), then $\|\psi_n\|^2$ are the probabilities of finding n particles, and $\langle \psi, \mathcal{N}\psi \rangle_{\mathbb{F}}$ is the average number of particles in state ψ. Thus, setting $N = \langle \psi, \mathcal{N}\psi \rangle_{\mathbb{F}}$ fixes the expectation of the number of particles to N. Because $\left[\acute{\mathcal{H}}_N, \mathcal{N}\right] = 0$, as the reader may readily verify, the above expectation is indeed preserved by evolution.

[5]We use calligraphic letters for Fock space operators, with the exception of a and a^* as well as $\mathfrak{H}$.

Next, we discuss: the notion of coherent states (section 2.3.1), which will be invoked in section 5; and a formal derivation of the mean-field limit via Fock space techniques (section 2.3.2), as a prelude to the rigorous theory outlined in section 3.

2.3.1. *Coherent state.* The definition of the coherent state relies on the *Weyl operator*, $\mathcal{W}$. This operator is introduced in terms of the skew-symmetric operator $\mathcal{A}$, viz.,

$$\mathcal{W}(\phi) := e^{-\sqrt{N}\mathcal{A}(\phi)} \qquad \text{where} \quad \mathcal{A}(\phi) := a_{\overline{\phi}} - a^*_{\phi} \ . \tag{2.12}$$

The coherent state, W, is produced by applying the Weyl operator to the vacuum, viz.,

$$W(\phi) := \mathcal{W}(\phi)\Omega = e^{-\sqrt{N}\mathcal{A}(\phi)}\Omega \ . \tag{2.13}$$

To better understand (2.13), we use the following known lemma.

Lemma 2.1. Suppose $\mathcal{A}$ and $\mathcal{B}$ are two operators such that their commutator, $[\mathcal{A},\mathcal{B}]$, commutes with both $\mathcal{A}$ and $\mathcal{B}$, i.e., $\big[\mathcal{A},[\mathcal{A},\mathcal{B}]\big] = \big[\mathcal{B},[\mathcal{A},\mathcal{B}]\big] = 0$. Then,

$$e^{\mathcal{A}+\mathcal{B}} = e^{-(1/2)[\mathcal{A},\mathcal{B}]}e^{\mathcal{A}}e^{\mathcal{B}} = e^{-(1/2)[\mathcal{B},\mathcal{A}]}e^{\mathcal{B}}e^{\mathcal{A}} \ . \tag{2.14}$$

For the present case of computing state W according to (2.13), we set (abusing notation) $\mathcal{A} := \sqrt{N}a^*_{\phi}$ and $\mathcal{B} := -\sqrt{N}a_{\overline{\phi}}$ in (2.14). Thus, we compute

$$\begin{aligned} W(\phi) &= e^{\{\sqrt{N}a^*_{\phi} - \sqrt{N}a_{\overline{\phi}}\}}\Omega = e^{-N\|\phi\|^2/2}e^{\sqrt{N}a^*_{\phi}}e^{-\sqrt{N}a_{\overline{\phi}}}\Omega = e^{-N\|\phi\|^2/2}e^{\sqrt{N}a^*_{\phi}}\Omega \\ &= e^{-N\|\phi\|^2/2}\left\{\sum_{n=0}^{\infty}\frac{N^{n/2}}{n!}\big(a^*_{\phi}\big)^n\Omega\right\} = e^{-N\|\phi\|^2/2}\left\{\sum_{n=0}^{\infty}\frac{N^{n/2}}{\sqrt{n!}}\prod_{j=1}^{n}\phi(x_j)\right\} \ . \end{aligned}$$

By $\|\phi\| = 1$ (for simplicity), the last formula entails

$$W(\phi) = \sum_{n=0}^{\infty} c_{N,n}\prod_{j=1}^{n}\phi(x_j) \ ; \quad c_{N,n} := e^{-N/2}\frac{N^{n/2}}{\sqrt{n!}} \ . \tag{2.15}$$

Equation (2.15) expresses a direct sum of entries in Fock space fibers; $\prod_{j=1}^{n}\phi(x_j) \in \mathbb{F}_n$. This expansion signifies that the Weyl operator, $\mathcal{W}(\phi)$, applied to the vacuum, Ω, creates a tensor product involving a single-particle wave-function, $\phi(x)$, in each sector $\mathbb{F}_n$. By (2.15), the average number of particles at state $W(\phi)$ is

$$\sum_{n=0}^{\infty} n\big(c_{N,n}\big)^2 = N \ .$$

Another appealing property of coherent states should be mentioned. By Lemma 2.1, the following "approximate orthogonality relation" holds:

$$\big\langle W(\phi_1), W(\phi_2)\big\rangle = e^{-(N/2)\|\phi_1-\phi_2\|^2}e^{(N/2)(\langle\phi_1,\phi_2\rangle - \langle\phi_2,\phi_1\rangle)} \ ,$$

for one-particle wave functions ϕ_1, ϕ_2; in particular, if $\langle\phi_1,\phi_2\rangle = 0$ with $\|\phi_1\| = \|\phi_2\| = 1$, then $\langle W(\phi_1), W(\phi_2)\rangle = e^{-N}$, which is exponentially small for $N \gg 1$.

Coherent states play a central role in the derivation of the mean-field limit, as well as in the rigorous analysis of pair excitation, as we explain in sections 2.3.2 and 5.

2.3.2. *Mean-field limit via Fock space techniques.* The use of Fock space techniques has been the primary method of tackling many-body problems in the physics community. In mathematics, this approach was pioneered by Hepp [50] and by Ginibre and Velo [42,43]; see also the fundamental work by Shale [76]. In this section, we outline this approach.

The notion of a coherent state, introduced in section 2.3.1, can be invoked to extract the mean-field dynamics: Start with factorized initial data, i.e., $\psi(0) = e^{-\sqrt{N}\mathcal{A}(\phi_0)}\Omega$ where $\phi_0(x)$ is some initial datum. The key idea is to compare the exact evolution

$$\psi_{\text{exact}}(t) = e^{it\acute{\mathcal{H}}_N}\psi(0) = e^{it\acute{\mathcal{H}}_N}e^{-\sqrt{N}\mathcal{A}(\phi_0)}\Omega$$

to the approximate evolution

$$\psi_{\text{app}}(t) := e^{-\sqrt{N}\mathcal{A}(\phi(t))}\Omega \ . \tag{2.16}$$

An issue in this comparison is to *determine* an evolution for $\phi(t,x)$ that *best* approximates, in a certain sense, the exact evolution. The criterion for what "best" means will be explained later. The Fock space formalism gives a *relatively simple recipe to this end.*

A way to proceed is to follow the exact evolution up to time $t > 0$ and then go back in time by following the approximate evolution [42,43,50]. Thus, consider the state

$$\psi_{\text{red}}(t) := e^{\sqrt{N}\mathcal{A}(\phi(t))}e^{it\acute{\mathcal{H}}_N}e^{-\sqrt{N}\mathcal{A}(\phi_0)}\Omega \ . \tag{2.17}$$

To describe the evolution of this *reduced* dynamics, we compute

$$\frac{1}{i}\partial_t\psi_{\text{red}} = \left\{\frac{1}{i}\Big(\partial_t e^{\sqrt{N}\mathcal{A}(\phi(t))}\Big)e^{-\sqrt{N}\mathcal{A}(\phi(t))} + e^{\sqrt{N}\mathcal{A}(\phi(t))}\acute{\mathcal{H}}_N e^{-\sqrt{N}\mathcal{A}(\phi(t))}\right\}\psi_{\text{red}} \ .$$

Accordingly, we set

$$\mathcal{H}_{\text{red}} := \frac{1}{i}\big(\partial_t e^{\sqrt{N}\mathcal{A}(\phi(t))}\big)e^{-\sqrt{N}\mathcal{A}(\phi(t))} + e^{\sqrt{N}\mathcal{A}(\phi(t))}\acute{\mathcal{H}}_N e^{-\sqrt{N}\mathcal{A}(\phi(t))} \ . \tag{2.18}$$

Then, the evolution of the reduced dynamics reads

$$\frac{1}{i}\partial_t\psi_{\text{red}} = \mathcal{H}_{\text{red}}\psi_{\text{red}} \qquad \text{with} \qquad \psi_{\text{red}}(0) = \Omega \ .$$

Next, we need to calculate $\mathcal{H}_{\text{red}}$. For this purpose, we invoke the following lemma.

LEMMA 2.2. Any two operators, $\mathcal{A}$ and $\mathcal{B}$, in Fock space satisfy the identity

$$e^{\mathcal{A}}\mathcal{B}e^{-\mathcal{A}} = e^{ad(\mathcal{A})}\mathcal{B} = \sum_{n=0}^{\infty}\frac{ad(\mathcal{A})^n(\mathcal{B})}{n!} \ , \tag{2.19}$$

where $ad(\mathcal{A})^0(\mathcal{B}) = \mathcal{B}$ and

$$ad(\mathcal{A})^n(\mathcal{B}) = \big[\mathcal{A}, ad(\mathcal{A})^{n-1}(\mathcal{B})\big] \qquad n \geq 1 \ . \tag{2.20}$$

We now discuss the computation of $\mathcal{H}_{\text{red}}$ by (2.18). In this case, series (2.19) is finite and computable. This conclusion is drawn by the observation that if $\mathcal{P}_n$ is an n-th degree polynomial in a, a^*, then its commutator with $\mathcal{A}(\phi)$ is an $(n-1)$-th degree polynomial.

Thus, the recipe for computations is to write the Hamiltonian, $\acute{\mathcal{H}}_N$, as the sum of a quadratic and a quartic term, $\acute{\mathcal{H}}_N = \acute{\mathcal{H}}_{(2)} + N^{-1}\acute{\mathcal{H}}_{(4)}$, and apply Lemma 2.2, viz.,

$$e^{\sqrt{N}\mathcal{A}(\phi)}\acute{\mathcal{H}}_{(2)}e^{-\sqrt{N}\mathcal{A}(\phi)} = \acute{\mathcal{H}}_{(2)} + N^{1/2}ad(\mathcal{A}(\phi))(\acute{\mathcal{H}}_{(2)}) + \frac{1}{2!}N\,ad(\mathcal{A}(\phi))^2(\acute{\mathcal{H}}_{(2)}) \ ,$$

$$\begin{aligned} e^{\sqrt{N}\mathcal{A}(\phi)}\Big(N^{-1}\acute{\mathcal{H}}_{(4)}\Big)e^{-\sqrt{N}\mathcal{A}(\phi)} &= N^{-1}\acute{\mathcal{H}}_{(4)} + N^{-1/2}ad(\mathcal{A}(\phi))(\acute{\mathcal{H}}_{(4)}) + \frac{1}{2!}ad(\mathcal{A}(\phi))^2(\acute{\mathcal{H}}_{(4)}) \\ &\quad + \frac{1}{3!}N^{1/2}ad(\mathcal{A}(\phi))^3(\acute{\mathcal{H}}_{(4)}) + \frac{N}{4!}ad(\mathcal{A}(\phi))^4(\acute{\mathcal{H}}_{(4)}) \ . \end{aligned}$$

By (2.18), it remains to compute the time derivative of $e^{\sqrt{N}\mathcal{A}(\phi(t))}$. The relation

$$\partial_t\mathcal{A}^n = n\big(\partial_t\mathcal{A}\big)\mathcal{A}^{n-1} + \frac{n(n-1)}{2}\big[\mathcal{A},\partial_t\mathcal{A}\big]\mathcal{A}^{n-2} \ ,$$

for which use was made of $\big[\mathcal{A},\big[\mathcal{A},\partial_t\mathcal{A}\big]\big] = 0$, yields

$$\Big(\partial_t e^{\sqrt{N}\mathcal{A}(\phi)}\Big)e^{-\sqrt{N}\mathcal{A}(\phi)} = N^{1/2}\mathcal{A}(\partial_t\phi) + \frac{N}{2}\big[\mathcal{A}(\phi),\mathcal{A}(\partial_t\phi)\big] \ .$$

By collecting and rearranging all the above terms according to (2.18), we find

$$\mathcal{H}_{\rm red} = N\mu + N^{1/2}\mathcal{P}_1 + \mathcal{P}_2 - N^{-1/2}\mathcal{P}_3 - N^{-1}\mathcal{P}_4 \ , \tag{2.21}$$

where $\mathcal{P}_\ell$ is an ℓ-th degree polynomial in a, a^*. The first term, $N\mu$, is simply a real "constant" (times the identity operator) and, thus, only contributes an overall phase to the many-body evolution. In regard to the second term, $\mathcal{P}_1$, of (2.21), a direct (but tedious) computation gives the formula

$$\mathcal{P}_1 = a_{\overline{h}} + a_h^* \qquad \text{where} \qquad h := -\frac{1}{i}\partial_t\phi + \{\Delta - V_e\}\,\phi - \big(v_{N,\beta} * |\phi|^2\big)\phi \ ,$$

where we introduce the shorthand notation $v_{N,\beta} := N^{3\beta}v(N^\beta\cdot)$. At this point, we do not need to discuss any specifics for the remaining terms, $\mathcal{P}_\ell$ with $\ell \geq 2$; see section 5.

The mean-field limit emerges formally if one sets $h \equiv 0$, which eliminates the term $\mathcal{P}_1$ in expansion (2.21). This choice entails the following equation for $\phi(t,x)$:

$$\frac{1}{i}\partial_t\phi + \{-\Delta + V_e\}\,\phi + \big(v_{N,\beta} * |\phi|^2\big)\phi = 0 \ . \tag{2.22}$$

In the limit $N \to \infty$ with $\beta \in (0,1]$, (2.22) reduces to the (cubic) non-linear Schrödinger equation (NLS),

$$(1/i)\partial_t\phi - \Delta\phi + V_e\phi + b|\phi|^2\phi = 0 \quad \text{with} \quad b := \int dx\,\{v(x)\} \ . \tag{2.23}$$

This finding is false, i.e., inconsistent with the exact dynamics, for $\beta = 1$. In this case, an important effect of many-body dynamics, not captured by the above mean-field approximation, is the development of short-range particle correlations, at a distance between atoms of the order of $1/N$. As $N \to \infty$, these correlations give rise to the Gross-Pitaevskii evolution [49, 74]. Specifically, in the absence of the trap ($V_e \equiv 0$), the correct mean-field equation is [49, 74, 82]

$$\frac{1}{i}\partial_t\phi - \Delta\phi + 8\pi a|\phi|^2\phi = 0 \qquad \text{(Gross-Pitaevskii evolution)} \tag{2.24}$$

where a is the scattering length, which comes from the two-body scattering problem [10]; see section 3.3. To incorporate this length a into the many-body evolution, an idea is to replace the interaction potential $N^3 v(N\cdot)$ by $8\pi a \delta_F$ where δ_F is the Fermi pseudo-potential [51, 59, 82, 83]. A rigorous justification for the emergence of the scattering length as $N \to \infty$ was given recently by Erdős, Schlein and Yau [36, 37, 39] by a different approach.

Recently, Fock space techniques were invoked by Rodnianski and Schlein [75] in their study of the rate of convergence to the mean-field approximation in Hartree dynamics, i.e., the case with $\beta = 0$ in Hamiltonian (2.9). Their work has partly inspired our studies in pair excitation (section 5). The remainder of this section is devoted to their result.

Rodnianski and Schlein [75] consider the one-particle marginal density

$$\gamma_N^{(1)}(t,x,y) := \frac{1}{N}\langle \psi, a_x^* a_y \psi \rangle \ ,$$

and compare it to the corresponding marginal for a coherent state, $W(\phi)$, viz.,

$$\gamma_{\text{coh}}^{(1)}(t,x,y) := \frac{1}{N}\langle W(\phi), a_x^* a_y W(\phi)\rangle = \overline{\phi}(t,x)\phi(t,y) \ .$$

The reader who wishes to derive the above formula for $\gamma_{\text{coh}}^{(1)}$ may recall definition (2.13) for the coherent state, and then compute $\gamma_{\text{coh}}^{(1)}$ by use of Lemma 2.2.

The main result of Rodnianski and Schlein [75] can be stated as follows.

THEOREM 2.3. Suppose that for some constant $D > 0$ the potential $v(x)$ satisfies the operator bound $v^2(x) \le D\{-\Delta_x + 1\}$. Moreover, assume that ϕ obeys

$$\frac{1}{i}\partial_t \phi - \Delta\phi + \big(v * |\phi|^2\big)\phi = 0 \qquad \text{(Hartree evolution, for } \beta = 0) \ , \tag{2.25}$$

with initial data $\phi_0 \in H^1(\mathbb{R}^3)$ and normalization $\|\phi_0\|_{L^2} = 1$. Then, for some constants C_1 and C_2 that depend only on D and $\|\phi\|_{H^1}$, the following estimate holds:

$$\text{Tr}\Big|\gamma_N^{(1)}(t,x,y) - \gamma_{\text{coh}}^{(1)}(t,x,y)\Big| \le C_1 \frac{e^{C_2 t}}{N} \ .$$

Note that the marginal density $\gamma_N^{(1)}$ for the exact N-body evolution is the average

$$\gamma_N^{(1)}(t,x,y) = \int_{\mathbb{R}^{3(N-1)}} dz_1 \dots dz_{N-1} \left\{\overline{\psi_N}(t,x,z_1 \dots z_{N-1})\psi_N(t,y,z_1 \dots z_{N-1})\right\} \ , \tag{2.26}$$

where in this formulation ψ_N satisfies $(1/i)\partial_t \psi_N + H_N \psi_N = 0$ with $\|\psi_N\|_{L^2(\mathbb{R}^{3N})} = 1$ and factorized initial data, $\psi_N(0, x_1 \dots x_N) = \prod_{j=1}^N \phi_0(x_j)$ [75]. We add a few remarks as a sample of the Fock space techniques (and algebra) involved in these computations [75]. Use of the number operator, $\mathcal{N}$, and computation of commutators with $\mathcal{A}(\phi)$ yield

$$ad(\mathcal{N})(\mathcal{A}(\phi)) = -a_{\overline{\phi}} - a_\phi^* \ , \qquad ad(\mathcal{N})^2(\mathcal{A}(\phi)) = \mathcal{A}(\phi) \ ,$$

which reveals a 2-periodicity. Subsequently, for real θ, one can compute

$$e^{i\theta\mathcal{N}}\mathcal{A}(\phi)e^{-i\theta\mathcal{N}} = \mathcal{A}(e^{i\theta}\phi) \ , \qquad e^{i\theta\mathcal{N}}e^{-\sqrt{N}\mathcal{A}(\phi)}e^{-i\theta\mathcal{N}} = e^{-\sqrt{N}\mathcal{A}(e^{i\theta}\phi)} \ .$$

By $e^{-i\theta\mathcal{N}}\Omega = \Omega$, one may recover the N-th entry in Fock space via the formula

$$\int_0^{2\pi} \frac{d\theta}{2\pi} \left\{ e^{i\theta(\mathcal{N}-N)} e^{-\sqrt{N}\mathcal{A}(\phi)}\Omega \right\} = (0, \ldots 0, c_{N,N} \prod_{j=1}^{N} \phi(x_j), 0 \ldots) \ .$$

More recently, there is further work that uses the Fock space approach. Section 5 provides related developments and bibliography.

3. Anatomy of mean-field limit of many-Boson evolution. In this section, we consider a closed system of N particles and derive the mean-field limit, mainly via Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchies, paying a tribute to the work by Elgart, Erdős, Schlein and Yau [34–37, 39]. We start with a heuristic derivation and proceed to the more elaborate formulation with marginal densities and their hierarchy.

Consider Hamiltonian (1.1) with a two-body interaction potential, v, that is symmetric $[v(-x) = v(x)]$, positive and integrable ($\int_{\mathbb{R}^3} dx\{v(x)\} < \infty$). The Hamiltonian reads[6]

$$H_{N,\beta} := \sum_{j=1}^{N} \mathfrak{H}_{x_j} + \frac{1}{N} \sum_{j<k}^{N} v_{N,\beta}(x_j - x_k) \ , \quad x_j \in \mathbb{R}^3 \ , \ \beta \in [0,1] \ , \tag{3.1}$$

where $\mathfrak{H}_x := -\Delta_x + V_e(x)$ is the positive one-body Hamiltonian. Recall that $v_{N,\beta}(x) := N^{3\beta} v(N^\beta x)$, as defined in section 2. A remark on the role of parameter β is in order.

Remark 3.1. As mentioned in section 1, the case $\beta = 1$ is special. In fact, it corresponds to a *critical scaling*, and influences the mean-field evolution in a non-trivial way. A way to justify this distinction is to consider the two-body Hamiltonian (with $\beta = 1$)

$$H_{1,2} = -\Delta_{x_1} - \Delta_{x_2} + N^2 v\big(N(x_1 - x_2)\big) \ .$$

In the center-of-mass coordinates, $x := (x_1 + x_2)/2$ and $y := x_1 - x_2$, this $H_{1,2}$ becomes

$$H_{1,2} = -\Delta_x + 2\left\{ -\Delta_y + \frac{N^2}{2} v(Ny) \right\} \ .$$

Let us write down the quadratic form of $-\Delta_y + (N^2/2)v(Ny)$, which is

$$\int dy \left\{ \left|\nabla_y \varphi\right|^2 + \frac{N^2}{2} v(Ny) |\varphi|^2 \right\} \ .$$

In this form, the interaction term is bounded. By use of Hölder and Sobolev inequalities,

$$\begin{aligned} \int dy \left\{ \frac{N^2}{2} v(Ny)|\varphi|^2 \right\} &\leq C \left(\int dy \left\{ N^3 |v(Ny)|^{3/2} \right\} \right)^{2/3} \left(\int dy \left\{ |\varphi|^6 \right\} \right)^{1/3} \\ &\leq \|v\|_{L^{3/2}} \|\varphi\|_{\dot{H}^1}^2 \ . \end{aligned}$$

This estimate suggests that the interaction term can be "as strong as" the kinetic-energy term. In contrast, if $\beta < 1$ the interaction term tends to zero as $N \to \infty$.

[6]In this section, we use a positive Hamiltonian, whereas in section 2 we used a negative Hamiltonian.

The Boson evolution problem is expressed by the statements

$$\frac{1}{i}\partial_t\psi + H_{N,\beta}\psi_N = 0 \ ; \tag{3.2a}$$

$$\psi_N(0, x_1 \dots x_N) := \psi_0(x_1 \dots x_N) \ , \tag{3.2b}$$

where $N \gg 1$ and the N-body wave function, $\psi_N(t, x_1, \dots, x_N)$, is symmetric. We are interested in describing the evolution of factorized initial data, ψ_0.

3.1. *Static problem and Bose-Einstein condensation.* To explain why factorized initial data is appealing, let us first review the notion of BEC. For the ground state of N-body Hamiltonian (3.1), one must consider the minimization problem

$$E_{N,0} := \min_{\|\psi_N\|^2=1} \left\langle \psi_N, H_N\psi_N \right\rangle \ .$$

The task at hand is to compute the ground state energy, $E_{N,0}$, and describe the ground state wave function, $\psi_N = \psi_{N,0}$. For non-interacting particles [13, 32, 33], the energy minimum occurs at $\psi_{N,0} = \prod_{j=1}^N \phi_0(x_j)$ where $\phi_0(x)$ minimizes $\langle \phi, \mathfrak{H}\phi \rangle$ subject to the normalization $\|\phi\| = 1$; thus, ϕ_0 is the ground state of the one-particle Hamiltonian, $\mathfrak{H}$.

For interacting particles the problem is challenging. Early results are due to Bogoliubov [12] and Lee, Huang and Yang [59]. On the other hand, Dyson [31] ingeniously proposed an approximate wave function that gives the correct energy upper bound for $E_{N,0}$ but fails to provide a sharp lower bound. Notably, Lieb and Seiringer [64] and Lieb, Seiringer and Yngvanson [66] obtained the correct lower bound for $E_{N,0}$. A comprehensive review of these results can be found in [65].

Next, we state a result that is relevant to problem (3.2). Compare the ground state energy per particle, $E_{N,0}/N$, to the minimum of the "Gross-Pitaevskii energy functional"

$$E_{GP}[\phi] = \int_{\mathbb{R}^3} dx \left\{ \left|\nabla\phi\right|^2 + V_e(x)|\phi|^2 + 4\pi a|\phi|^4 \right\} \ , \qquad \|\phi\| = 1 \ ,$$

where a is the scattering length for potential $v(x)$. The following limit has been proved [65]:

$$\lim_{N\to\infty} \frac{E_{N,0}}{N} = \min_{\|\phi\|=1} \{E_{GP}[\phi]\} =: E_{GP}[\phi_0] \ .$$

The minimizer ϕ_0 satisfies the Gross-Pitaevskii equation, viz.,

$$-\Delta\phi_0 + V_e(x)\phi_0 + 8\pi a|\phi_0|^2\phi_0 = \mu\phi_0 \ ,$$

where μ is a Lagrange multiplier, the chemical potential per particle [49, 65, 74, 82]. The meaning of the scattering length, a, is discussed in section 3.3.

A subtlety in the concept of BEC for interacting particles should be spelled out. Mathematically, the idea of condensation cannot be expressed by the naive statement "all particles occupy the same state", since this does not have a clear meaning for interacting particles. An alternate definition of condensation by Penrose and Onsager [71] is that the static version of one-particle marginal density (2.26) for the minimizer ϕ_0 is approximately a projection of the form $\phi_0(x)\overline{\phi_0}(y)$. In fact, Lieb and Seiringer [64] have proved that

$$\mathrm{Tr}\left|\gamma_N^{(1)}(x,y) - \phi_0(x)\overline{\phi_0}(y)\right| \to 0 \qquad \text{as} \quad N \to \infty \ ,$$

thus demonstrating "complete condensation" in the limit $N \to \infty$. This suggests that the ground state is approximately factorized, if N is large yet finite.

3.2. *Heuristic derivation of mean-field limit.* We now turn our attention to evolution problem (3.2). The heuristic idea of mean-field dynamics is rather simple but leads to an absurd approximation: One expects that the N-body wave function is factorized as

$$\psi_{\mathrm{mf}}(t, x_1 \dots x_N) = \prod_{j=1}^{N} \phi(t, x_j) \ , \tag{3.3}$$

for a state ϕ that needs to be determined. However, this ψ_{mf} cannot solve (3.3). To show this, let $\phi_j := \phi(t, x_j)$. By inserting (3.3) into (3.2a), we end up with the statement

$$\sum_j \left\{ \frac{1}{i}\partial_t \phi_j + \mathfrak{H}_{x_j}\phi_j \right\} \prod_{l \neq j} \phi_l + \frac{1}{N} \sum_{j<l} v_{N,\beta}(x_j - x_l)\phi_j\phi_l \prod_{m \neq j,l} \phi_m = 0 \quad (?) \ ,$$

where the question mark above indicates that the right-hand side cannot be zero. By picking the criterion that the expression is orthogonal to all products of the form

$$\Phi_l := \prod_{j \neq l} \phi_j \ ,$$

we arrive at the Hartree-type equation

$$\left\{ \frac{1}{i}\partial_t + \mathfrak{H}_x \right\} \phi(t,x) + \frac{N-1}{N} \big(v_{N,\beta} * |\phi|^2 \big)(t,x)\phi(t,x) = 0 \ . \tag{3.4}$$

For $\beta = 0$ the formal limit of (3.4) as $N \to \infty$ is (2.25), the Hartree equation. For $\beta \in (0,1]$ the formal limit of (3.4) is evolution law (2.23), the cubic NLS.

As we note in section 2.3.2, mean-field law (3.4) is correct for $0 < \beta < 1$ but it is false for the critical scaling, $\beta = 1$. In this case, the correct mean-field equation is (2.24), which involves the scattering length, a.

3.3. *On the scattering length.* The notion of the scattering length, a, deserves our attention. This a is defined via the solution, $f(x)$, of the scattering problem

$$-\Delta f + \frac{1}{2} v f = 0 \qquad \text{with} \qquad \lim_{|x| \to \infty} f(x) = 1 \ . \tag{3.5}$$

If the interaction potential, $v(x)$, decays sufficiently fast at infinity, say, in case $v(x)$ has compact support, then $f(x)$ has the asymptotic behavior

$$f(x) \sim 1 - \frac{a}{|x|} \quad \text{as} \quad |x| \to \infty \ , \tag{3.6}$$

which defines the scattering length [10]. The formal idea for correcting mean-field equation (3.4) for $\beta = 1$ is that $v_{N,1}(x) = N^3 v(Nx)$ should be replaced by $(vf)_{N,1}(x) = N^3 v(Nx) f(Nx)$. The modified mean-field evolution law, in place of (3.4), reads

$$\left\{ \frac{1}{i}\partial_t + \mathfrak{H}_x \right\} \phi(t,x) + \frac{N-1}{N} \big((vf)_{N,1} * |\phi|^2 \big)(t,x)\phi(t,x) = 0 \ ; \tag{3.7}$$

cf. (2.24) as $N \to \infty$.

A few comments on mean-field equations (3.4) and (3.7), or their respective counterparts (2.23) and (2.24), are in order. From a mathematical viewpoint, there is little

difference between (2.23) and (2.24) since they are both NLS-type equations with a cubic defocusing non-linearity. In comparing the two equations, it suffices to state that $8\pi a < b$. This can be seen by the following argument. For $v \geq 0$, the maximum principle implies that $0 < f < 1$; hence, set $f = 1 - w$, $0 < w < 1$, where $w \to 0$ as $|x| \to \infty$. Thus, scattering equation (3.5) becomes $\Delta w - \frac{1}{2}vw + \frac{1}{2}v = 0$. By integration of (3.5), we obtain

$$\int_{\mathbb{R}^3} dx \, \{v(x)f(x)\} = 8\pi a \ ,$$

which justifies the claim that modified Hartree equation (3.7) yields evolution law (2.24) as $N \to \infty$. By multiplying the equation for w with w and integrating, we find

$$\int_{\mathbb{R}^3} dx \, \{v(x)\} - 8\pi a = b - 8\pi a = \int_{\mathbb{R}^3} dx \, \left\{2|\nabla w|^2 + v|w|^2\right\} > 0 \ .$$

3.4. *Marginals and their kinetic hierarchy.* We now review aspects of a kinetic theory that places the mean-field limit on firm mathematical grounds [34–37, 39]. The idea is to consider the l-particle marginals, $\gamma_N^{(l)}$ $(l = 1, \ldots, N)$, and study their BBGKY hierarchy [79]. These marginals are defined by

$$\begin{aligned} &\gamma_N^{(l)}(t, x_1 \ldots x_l; x_1' \ldots x_l') \\ &:= \int\limits_{\mathbb{R}^{3(N-l)}} dy_{l+1} \ldots dy_N \left\{\overline{\psi}_N(t, x_1' \ldots x_l', y_{l+1} \ldots y_N)\psi_N(t, x_1 \ldots x_l, y_{l+1} \ldots y_N)\right\} \ . \end{aligned} \tag{3.8}$$

To simplify the notation, set $\mathbf{r}_l := (x_1 \ldots x_l)$. The marginals $\gamma_N^{(l)}$ obey the symmetries

$$\begin{aligned} &\overline{\gamma_N^{(l)}}(t, \mathbf{r}_l'; \mathbf{r}_l) = \gamma_N^{(l)}(t, \mathbf{r}_l; \mathbf{r}_l') \ , \quad \gamma_N^{(l)}(t, \mathbf{r}_{\pi(l)}; \mathbf{r}_l') = \gamma_N^{(l)}(t, \mathbf{r}_l; \mathbf{r}_l') \ ; \\ &\mathbf{r}_{\pi(l)} := (x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(l)}) \ . \end{aligned}$$

Note that $\gamma_N^{(N)} = \overline{\psi}(t, x_1' \ldots x_N')\psi(t, x_1 \ldots x_N)$, which satisfies the Wigner equation [79]. Our goal is to describe the evolution of every $\gamma_N^{(l)}$ $(l = 1, \ldots, N)$.

To this end, let us define the partial, l-particle, Hamiltonian as

$$H_{N,\beta}^{(l)} := \sum_{j=1}^{l} \mathfrak{H}_{x_j} + \frac{1}{N} \sum_{1 \leq j_1 < j_2 \leq l} v_{N,\beta}(x_{j_1} - x_{j_2}) \ . \tag{3.9}$$

It can now be directly shown that the marginals $\{\gamma_N^{(l)}\}_{l=1}^N$ satisfy the BBGKY hierarchy

$$\frac{1}{i}\partial_t \gamma_N^{(l)} + \left[H_{N,\beta}^{(l)}, \gamma_N^{(l)}\right] + \frac{N-l}{N}\left[B_v^{(l)}, \gamma_N^{(l+1)}\right] = 0 \ , \qquad l = 1, 2, \ldots, N \ , \tag{3.10}$$

where $[\,\cdot,\cdot\,]$ denotes the commutator and $B_v^{(l)}$ is a linear operator that acts on $\gamma_N^{(l+1)}$. This $B_v^{(l)}$ can be described in the following manner. First, write it as

$$B_v^{(l)} = \sum_{j=1}^{l} B_v^{l,j} \quad \text{where}$$

$$B_v^{l,j}\gamma_N^{(l+1)} := \int_{\mathbb{R}^3} dy \left\{ v_{N,\beta}(x_j - y)\gamma_N^{(l+1)}(t, x_1 \dots x_j \dots x_l, y; x_1' \dots x_j' \dots x_l', y) \right\} \ ,$$

$$\gamma_N^{(l+1)} B_v^{l,j} := \int_{\mathbb{R}^3} dy \left\{ \gamma_N^{(l+1)}(t, x_1 \dots x_j \dots x_l, y; x_1' \dots x_j' \dots x_l', y) v_{N,\beta}(x_j' - y) \right\} \ .$$

For example, consider the case of $B_v^{(1)}$, in which we have

$$\big[B_v^{(1)}, \gamma_N^{(2)}\big](t, x_1; x_1') := \int_{\mathbb{R}^3} dy \left\{ \big(v_{N,\beta}(x_1 - y) - v_{N,\beta}(x_1' - y)\big)\gamma_N^{(2)}(t, x_1, y; x_1', y) \right\} \ .$$

The limit of the above operator as $N \to \infty$ is a useful collapsing mechanism. By assuming that $\gamma_N^{(l)} \to \gamma^{(l)}$ and denoting the limit operator by $B^{(1)}$, we express this mechanism by

$$\big[B^{(1)}, \gamma^{(2)}\big] = b\big(\gamma^{(2)}(t, x_1, x_1; x_1', x_1) - \gamma^{(2)}(t, x_1, x_1'; x_1', x_1')\big) \ ; \ b = \int_{\mathbb{R}^3} dy \, \{v(y)\} \ .$$

In this vein, the formal limit as $N \to \infty$ of $B_v^{l,j}$ is written as $B^{l,j}$ where

$$B^{l,j}\gamma^{(l+1)} = b \int_{\mathbb{R}^3} dy \left\{ \delta(x_j - y)\gamma^{(l+1)}(t, x_1 \dots x_j \dots x_l, y \ ; \ x_1' \dots x_j' \dots x_l', y) \right\}, \quad (3.11)$$

$$\gamma^{(l+1)} B^{l,j} = b \int_{\mathbb{R}^3} dy \left\{ \gamma^{(l+1)}(t, x_1 \dots x_j \dots x_l, y \ ; \ x_1' \dots x_j' \dots x_l', y)\delta(x_j' - y) \right\}; \quad (3.12)$$

$$B^{(l)} = \sum_{j=1}^{l} B^{l,j} \ , \quad \big[B^{(l)}, \gamma^{(l+1)}\big] = \sum_{j=1}^{l} \left\{ B^{l,j}\gamma^{(l+1)} - \gamma^{(l+1)} B^{l,j} \right\} \ . \quad (3.13)$$

Remark 3.2. Let us now discuss a scenario relevant to mean-field dynamics. Assume that $\gamma_N^{(1)}$ and $\gamma_N^{(2)}$ in the BBGKY hierarchy are projections, i.e., they have the forms

$$\gamma_N^{(1)}(t, x_1; x_1') = \overline{\phi}(t, x_1')\phi(t, x_1) \ ,$$
$$\gamma_N^{(2)}(t, x_1, x_2; x_1', x_2') = \overline{\phi}(t, x_1')\overline{\phi}(t, x_2')\phi(t, x_1\phi(t, x_2) \ .$$

By the evolution of $\gamma_N^{(1)}$, $\frac{1}{i}\partial_t\gamma_N^{(1)} + \big[H_{N,\beta}^{(1)}, \gamma_N^{(1)}\big] + \frac{N-1}{N}\big[B_v^1, \gamma_N^{(2)}\big] = 0$, we conclude that ϕ should satisfy Hartree-type equation (3.4). The assumption that $\gamma_N^{(l)}$, $l \geq 2$, has the above particular form fails for the next equation of the BBGKY hierarchy, which involves

$$H_{N,\beta}^{(2)} = -\Delta_{x_1} + V_e(x_1) - \Delta_{x_2} + V_e(x_2) + (1/N)v_{N,\beta}(x_1 - x_2) \ .$$

This failure is due to the interaction term, $(1/N)v_{N,\beta}(x_1 - x_2)$; however, this term presumably approaches zero as $N \to \infty$. More generally, for fixed l one would expect that

$$H_{N,\beta}^{(l)} \to H^{(l)} := \sum_{j=1}^{l} \mathfrak{H}_{x_j} \qquad \text{as} \quad N \to \infty \ .$$

If this formal limit is applied to (3.10), it leads to an infinite BBGKY hierarchy, called the "Gross-Pitaevskii (GP) hierarchy" (probably for historical reasons). Equation (3.10) yields

$$\frac{1}{i}\partial_t\gamma^{(l)} + \left[H^{(l)}, \gamma^{(l)}\right] + \left[B^{(l)}, \gamma^{(l+1)}\right] = 0 \ , \quad l = 1, 2, \dots \quad \text{(GP hierarchy)} \ . \tag{3.14}$$

It is important to notice that the GP hierarchy has a solution of the form

$$\gamma^{(l)} = \prod_{j=1}^{l} \overline{\phi}(t, x_j') \prod_{j=1}^{l} \phi(t, x_j) \tag{3.15}$$

provided that $\phi(t, x)$ satisfies (2.23), the cubic NLS. This is the correct limit if $0 < \beta < 1$.

3.4.1. *On the rigorous derivation of mean-field limit.* The above discussion suggests a rigorous derivation of the mean-field approximation. This approach was originally proposed by Spohn [79]; see also the works of Adami, Bardos, Golse and Teta [1], and Adami, Golse and Teta [2]. The full program was carried out in a series of papers by Elgart, Erdős, Schlein and Yau (e.g., [34, 36, 39]). Their main steps can be outlined as follows.

STEP 1. Consider the family of marginals $\left\{\gamma_N^{(l)}(t, \mathbf{r}_l; \mathbf{r}_l')\right\}_{N=1}^{\infty}$, $t \in [0, T]$, which satisfy hierarchy (3.10). Assume that the initial data is factorized. Prove that, for fixed l, the sequence $\{\gamma_N^{(l)}\}$ is compact and therefore converges, up to some subsequence in a weak* topology, to a limit. Denote this limit by $\gamma^{(l)}$ for $l = 1, 2, \dots$.

STEP 2. Show that any weak* limit from the previous step satisfies the infinite GP hierarchy, equation (3.14), with factorized initial data.

STEP 3. Prove that the infinite GP hierachy with factorized initial data has a unique solution in a fixed time interval $[0, T]$ for any $T > 0$.

These steps prove that as $N \to \infty$ the time evolution is governed by the NLS. This follows from Remark 3.2 by which the infinite GP hierarchy admits a factorized solution involving $\phi(t, x)$, the one-particle wave function, provided this $\phi(t, x)$ satisfies (2.23).

Let us now elaborate on the general ideas and techniques used to carry out the above program, especially steps 1 and 3, paying attention to some of their subtle aspects.

Step 1 requires energy-type estimates in order to take a limit (as $N \to \infty$). The germane norm is the trace of $|\gamma_N^{(l)}|$; see (3.16) below. The following theorem illustrates the main ingredients of this step.

THEOREM 3.3. Let $\psi_N \in L_s^2(\mathbb{R}^{3N})$ and assume that $0 \le \beta < 3/5$ and the interaction potential, v, is positive and integrable. Then, there exists some $N_0(l)$ such that for $N > N_0(l)$ the following estimate holds:

$$\langle \psi_N, \prod_{j=1}^{l}(-\Delta_{x_j} + 1)\psi_N\rangle \le \frac{2^l}{N^l}\langle \psi_N, (H_{N,\beta} + N)^l \psi_N\rangle \ .$$

Step 3 requires an existence and uniqueness theorem for the GP hierarchy. Set $S_j := (-\Delta_{x_j} + 1)^{1/2}$ as a notion of derivative in the x_j variable. The norm associated with this derivative is

$$\|\gamma^{(l)}\|_{\mathcal{H}_l} = \mathrm{Tr}\big|S_1 \dots S_l \gamma^{(l)} S_1' \dots S_l'\big| \ . \tag{3.16}$$

The following theorem is one of the main results by Erdős, Schlein and Yau [36, 39].

THEOREM 3.4. Fix $T > 0$ and consider the (infinite) GP hierarchy, equation (3.14), in $[0,T] \times \mathbb{R}^{3l} \times \mathbb{R}^{3l}$ for $l = 1, 2, \ldots$. Suppose the initial data, $\gamma_0^{(l)}$, satisfies the bound $\|\gamma_0^{(l)}\|_{\mathcal{H}_l} \leq C^l$ for all $l \geq 1$ and for some constant C. Then, the GP hierarchy has at most one solution $\gamma^{(l)}(t, \mathbf{r}_l; \mathbf{r}_l')$ that satisfies the bound $\|\gamma^{(l)}(t)\|_{\mathcal{H}_l} \leq C^l$ for all l and $t \in [0,T]$.

The proof of this theorem involves an expansion in Duhamel-type series and a rearrangement of the resulting integrals using techniques of Feynman diagrams [36, 39]. On the other hand, Klainerman and Machedon [55] proposed a different approach to the uniqueness of the GP hierarchy; their methodology is based on a different norm and, most importantly, on a new coordinate-collapse estimate over space-time. In addition, in this paper [55] the authors reworked the critical argument based on Feynman diagrams [36, 39], which they reformulate as a board game.

The approach in [55] is summarized as follows. Define $R_j = \big(-\Delta_{x_j}\big)^{1/2}$ and the norm

$$\|\gamma^{(l)}\| := \big\|R_1 \ldots R_l \gamma^{(l)} R_1' \ldots R_l'\big\|_{L^2(\mathbb{R}^{3l} \times \mathbb{R}^{3l})} \ .$$

One may compare this norm with $\|\cdot\|_{\mathcal{H}_l}$. The collapse estimate is stated in the following theorem, whoce proof relies on techniques of harmonic analysis that lie beyond our scope.

THEOREM 3.5. Let $H^l := \sum_{j=1}^{l} \big(-\Delta_{x_j}\big)$ and consider the evolution problem

$$\begin{aligned} &\frac{1}{i}\partial_t \gamma^{(l+1)} + \big[H^{l+1}, \gamma^{(l+1)}\big] = 0 \ , \\ &\gamma^{(l+1)}(0, \mathbf{r}_{l+1}; \mathbf{r}_{l+1}') := \gamma_0(\mathbf{r}_{l+1}; \mathbf{r}_{l+1}') \ . \end{aligned}$$

Then, there exists a constant C independent of the data and j, l such that

$$\begin{aligned} &\big\|R_1 \ldots R_l B^{j,l} \gamma^{(l+1)} R_1' \ldots R_l'\big\|_{L^2(\mathbb{R} \times \mathbb{R}^{3l} \times \mathbb{R}^{3l})} \\ &\leq C \big\|R_1 \ldots R_{l+1} \gamma_0^{(l+1)} R_1' \ldots R_{l+1}'\big\|_{L^2(\mathbb{R}^{3(l+1)} \times \mathbb{R}^{3(l+1)})} \ , \end{aligned}$$

where $B^{l,j}$ is the collapsing mechanism described in (3.11) and (3.12).

The question arises naturally as to what happens at the critical scaling, $\beta = 1$. The estimate of Theorem 3.3 does not hold in this case. The idea is to replace it with an estimate of the form (for $l = 2$)

$$\int dx_1 dx_2 \left\{ \big|\nabla_1 \cdot \nabla_2 W_{1,2}^* \psi\big|^2 \right\} \leq C N^{-2} \langle \psi, \big(H_{N,1} + N\big)^2 \psi \rangle \ ,$$

where $W_{1,2}$ is the wave operator $-\Delta + (1/2)N^2 v(N\cdot)$ acting on $x_1 - x_2$.

3.4.2. *Further works.* There are subsequent developments in the rigorous understanding of mean-field dynamics, which we comment on briefly in the remainder of this section. Our list of related works is non-exhaustive, aiming to provide an initial motivation and guide for further study of the relevant bibliography.

Notably, Pickl [73] derived the mean-field equation by an approach different from the one outlined above; see also [56]. Note the important work by Kirkpatrick, Schlein and Staffilani [54] who used the approach of Klainerman and Machedon [55] in order

to derive the two-dimensional (2-d) cubic defocusing NLS from the 2-d time-dependent many-body system. On the other hand, X. Chen [19, 20] analyzed the significant case of the condensate evolution in the presence of a quadratic trap, V_e. Furthermore, X. Chen and Holmer [22] developed the a-priori energy-type estimates needed for the uniqueness in the program of Klainerman and Machedon [55] for $\beta = 1$; see also [26]. We should also mention work by the same authors [21, 23] investigating the case of dimensional reduction, i.e., the derivation of the mean-field equation under strong confinement due to the trap of the condensate in one direction. X. Chen and Holmer [23–25] also developed methods in dimension $n = 1, 2$ that treat *negative* interaction potentials; in this case, the resulting mean-field equation is the focusing NLS. In this respect, see also the earlier work by Pickl [72]. This case of negative potentials required new ideas since the corresponding energy estimates are challenging; see also the work by Sohinger [77] on the derivation of the defocusing cubic NLS on a torus. There is substantial work by T. Chen and Pavlović [16] on the existence and uniqueness of solutions to the (infinite) GP hierarchy; see also the significant a-priori estimates established by T. Chen, Pavlović and Tzirakis [17]. The reader should be aware of the general unconditional uniqueness techniques for the GP hierarchy developed by T. Chen, Hainzl, Pavlović and Seiringer [15]. The interested reader may consult the aforementioned papers for further details and bibliography.

4. Pair excitation: Physical modeling and heuristics. In this section, we review aspects of the Fock space formalism of pair excitation introduced by Wu [82, 83] for the non-translation invariant setting; cf. (1.4). This formalism enables a systematic yet heuristic description of a correction to mean-field dynamics [69]. We will also see that the corresponding pair-excitation operator, denoted $e^{\mathfrak{P}[K_0]}$ in ansatz (1.4), acting on the tensor product involving a one-particle state, lacks unitarity. This may be the chief reason why this approach has not yet been placed into a rigorous framework.

A goal of this section is to indicate some of the concepts and the algebra involved in Wu's formalism as well as its recent application to a spatially varying scattering length [69]. For an alternate formulation of pair excitation that respects unitarity, exploits an ensuing isomorphism to a class of matrices and has enabled some rigorous results [44, 45], the reader may consult section 5.

Wu's approach is a non-trivial extension of the work by Lee, Huang and Yang [59] who systematically tackled the static problem, namely, the ground state energy and phonon spectrum, of the interacting Boson gas under periodic boundary conditions by use of the Fermi pseudo-potential. In particular, these authors [59] were able to derive a second-order correction to the mean-field ground state energy of the Boson gas; see the recent rigorous work by Erdős, Schlein and Yau [38].

4.1. *Formalism.* Recall ansatz (1.4) for the many-body wave function. Next, we describe the related exponent, $\mathfrak{P}[K_0] : \mathbb{F} \to \mathbb{F}$, by using tools of Fock space. First, for a *given* one-particle wave function ϕ, consider the following splitting of the distribution-valued operators a_x^* and a_x (see (2.2) and (2.3)):

$$a_x^* = a_\phi^*(t)\,\overline{\phi}(t,x) + a_{x,\perp}^*(t)\ , \quad a_x = a_{\overline{\phi}}(t)\,\phi(t,x) + a_{x,\perp}(t)\ ,$$

where $a_{x,\perp}$ denotes the Boson field operator in the space orthogonal to ϕ and $a^*_{x,\perp}$ is its adjoint; $\int dx\, \overline{\phi}(t,x)\, a_{x,\perp}(t) = 0$ and $[a_{\overline{\phi}}(t), a_{x,\perp}(t)] = [a_{\overline{\phi}}(t), a^*_{x,\perp}(t)] = 0$. Accordingly, $\mathfrak{P}[K_0]$ is defined by [82]

$$\mathfrak{P}[K_0] := [2N_0(t)]^{-1} \int dx\, dy\; a^*_{x,\perp}(t) a^*_{y,\perp}(t) K_0(t,x,y) a_{\overline{\phi}}(t)^2 \;, \tag{4.1}$$

where $K_0(t,x,y)$ is the pair-excitation kernel ($(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3$), $N_0(t)$ is the expected number of particles in state $\phi(t,x)$,

$$N_0(t) = \langle \psi(t), a^*_{\phi}(t) a_{\overline{\phi}}(t) \psi(t) \rangle_{\mathbb{F}} \;,$$

and $\psi(t)$ represents the many-body state vector in Fock space. In addition, Wu assumes that K_0 satisfies the following properties [82]:

$$K_0(t,x,y) = K_0(t,y,x) \;, \qquad \int dx\, \overline{\phi}(t,x)\, K_0(t,x,y) = 0 \;.$$

By (4.1), the operator $\mathfrak{P}$ annihilates two particles from state ϕ and at the same time creates two particles at states orthogonal to ϕ. This $\mathfrak{P}[K_0]$ is considered as an elaborate extension of the transformation of the tensor product involving the zero-momentum one-particle state, for the periodic case, which was investigated by Lee, Huang and Yang [59]. Notice that in $\mathfrak{P}[K_0]$ the operators $a^*_{q,\perp}$ can be replaced by a^*_q ($q = x,\, y$).

The principal idea in this approach is to identify ϕ with the wave function of the condensate (macroscopic state), treat $a_{x,\perp}$ and its adjoint as "small" in a heuristic fashion, and carry out an expansion of the Fock space (positive) Hamiltonian, $\mathcal{H}_N$, in $a^*_\perp$ and $a_\perp$. The task is to derive evolution laws for ϕ and K_0 consistent with many-body dynamics (1.2). In this prescription, the scattering length is introduced as an *ad hoc* parameter in the microscopic Hamiltonian, $\mathcal{H}_N$, which is written as [82, 83]

$$\mathcal{H}_N = \int dx\; \{a^*_x \mathfrak{H}_x a_x\} + 4\pi a^0 \int dx\, (a^*_x)^2 a^2_x \;, \tag{4.2}$$

where $\mathfrak{H}_x = -\Delta_x + V_e(x)$ and a^0 plays the role of the scattering length, $a^0 = a/N$;[7] cf. (2.9) and (3.6). According to the proposed splitting of a^*_x and a_x, all terms in $\mathcal{H}_N$ are classified according to how many times the operators $a^*_{x,\perp}$ and $a_{x,\perp}$ appear. Thus, $\mathcal{H}_N$ is written as $\mathcal{H}_N = \mathcal{H}_{(0)} + \mathcal{H}_{(1)} + \mathcal{H}_{(2)} + \mathcal{H}_{(3)} + \mathcal{H}_{(4)}$ where $a^*_{x,\perp}$ and $a_{x,\perp}$ appear ℓ times in $\mathcal{H}_{(\ell)}$.

The first-order theory, which amounts to mean-field dynamics, results from the replacement of $\mathcal{H}_N$ by $\mathcal{H}_{(0)} + \mathcal{H}_{(1)}$ and use of state vector (3.3) with unknown ϕ in the corresponding many-body Schrödinger equation. This procedure is actually not different from that outlined in section 3.2. Consequently, the condensate wave function, ϕ, is found to satisfy [82, 83]

$$i\partial_t \phi(t,x) = \{\mathfrak{H}_x + 8\pi a |\phi|^2 - 4\pi a \zeta(t)\} \phi(t,x) \;; \quad \zeta(t) := \int dx\, |\phi(t,x)|^4 \quad (\|\phi\| = 1) \;. \tag{4.3}$$

Clearly, the term $-4\pi a \zeta(t) \phi(t,x)$ can be absorbed into a phase function.

[7] This a^0 might be interpreted as a microscopic scattering length. We note in passing that in Wu's approach this a^0 is kept fixed; whereas in the recent rigorous work by Erdős, Schlein and Yau, $a = a^0 N$ enters the Gross-Pitaevskii evolution law as a fixed parameter [39]. In our exposition, we choose to invoke the latter parameter, a, in the evolution laws for ϕ and K_0.

The next order of approximation, in which ansatz (1.4) with (4.1) is used, deserves some attention. By assuming that ϕ obeys (4.3), $\mathcal{H}_N$ is now replaced by [83]

$$\mathcal{H}_{N,2} = \mathcal{H}_{(0)} + \mathcal{H}_{(1)} + \mathcal{H}_{(2)} \ .$$

After some commutator-related algebra, at this level of approximation one finds

$$\begin{aligned}
&\mathcal{H}_{(0)} + \mathcal{H}_{(1)} = \zeta_\triangle(t) + \zeta_e(t) + 4\pi a \zeta(t) \ , \\
&\mathcal{H}_{(2)} = \int dx\, a^*_{x,\perp} \{ -\Delta_x + V_e(x) - \zeta_\triangle(t) - \zeta_e(t) - 8\pi a \zeta(t) + 16\pi a |\phi(t,x)|^2 \} a_{x,\perp} \\
&\qquad + 4\pi a \int dx \, \{ a^2_{\overline{\phi}} \overline{\phi}(t,x)^2 \, (a^*_{x,\perp})^2 + (a^*_\phi)^2 \, \phi(t,x)^2 \, a^2_{x,\perp} \} \ ,
\end{aligned}$$

with

$$\zeta_\triangle(t) := \int dx \, |\nabla \phi(t,x)|^2 \ , \quad \zeta_e(t) := \int dx \, V_e(x) |\phi(t,x)|^2 \ .$$

The second line in the above expression for $\mathcal{H}_{(2)}$ is responsible for pair excitation, and is dealt with by the transformation involving the operator $\mathfrak{P}[K_0]$, as indicated below.

In this higher-order theory, the enforcement of ansatz (1.4) along with the many-body Schrödinger equation, with $\mathcal{H}_N$ replaced by $\mathcal{H}_{N,2}$ in Fock space, leads to the following statement:

$$C_N(t)^{-1} e^{-\mathfrak{P}[K_0]} (i\partial_t) \left\{ C_N(t) e^{\mathfrak{P}[K_0]} (a^*_\phi(t))^N \Omega \right\} = \left\{ e^{-\mathfrak{P}[K_0]} \mathcal{H}_{N,2} e^{\mathfrak{P}[K_0]} \right\} (a^*_\phi(t))^N \Omega \ .$$

Roughly, the objective is to extract an evolution law for K_0 by balancing out the two sides of this equation. The right-hand side of this relation can be conveniently simplified by use of Lemma 2.2 since the corresponding expansion of commutators reduces to a *finite sum*. However, the explicit computation of the left-hand side is remarkably cumbersome, mainly because of the specific construction of the operator $\mathfrak{P}[K_0]$ in this model. The details of this computation lie beyond our present scope.[8]

REMARK 4.1. To sketch the main idea in the heuristic derivation of an equation for K_0 here, it suffices to state that one picks this kernel so that the $a^*_\perp a^*_\perp$ term is eliminated in $e^{-\mathfrak{P}} \mathcal{H}_{N,2} e^{\mathfrak{P}}$. This program is illustrated more easily in the static case, in which $i\partial_t$ can be replaced by a constant. This idea of picking K_0 so as to eliminate "bad" terms in the quadratic part of the Fock space Hamiltonian is also invoked in the different set-up of the rigorous analysis in [44]; see section 5.

[8]The reader is encouraged to compare the algebra involved in this model to the pair-excitation formalism of section 5, in which the respective operator, denoted $\mathcal{B}(k)$ where k is the pair-excitation kernel introduced in [44], is skew-symmetric; cf. (5.7).

In [82], Wu organizes an analogous computation by use of a variational principle. The ensuing evolution equation for K_0 turns out to be [83]

$$\begin{aligned}\{i\partial_t - 2E(t)\}\, K_0(t,x,y) &= \{\mathfrak{H}_x + \mathfrak{H}_y + 16\pi a(|\phi(t,x)|^2 + |\phi(t,y)|^2) - 2\zeta_\triangle(t) - 2\zeta_e(t)\\ &\quad - 16\pi a\zeta(t)\}K_0 + 8\pi a\phi(t,x)^2\delta(x-y) + 8\pi a\int dz\,\overline{\phi}(t,z)^2\, K_0(t,x,z)K_0(t,y,z)\\ &\quad - 8\pi a\Big\{\phi(t,x)\phi(t,y)\big(|\phi(t,x)|^2+|\phi(t,y)|^2-\zeta(t)\big)+\phi(t,x)\int dz\, K_0(t,y,z)|\phi(t,z)|^2\overline{\phi}(t,z)\\ &\quad + \phi(t,y)\int dz\, K_0(t,x,z)|\phi(t,z)|^2\overline{\phi}(t,z)\Big\}\ ; \quad E(t) := \int dx\,\{i\partial_t\phi(t,x)\}\overline{\phi}(t,x)\ . \quad (4.4)\end{aligned}$$

It should be borne in mind that ϕ satisfies mean-field evolution (4.3).

At this level of description, the mean-field evolution for ϕ remains intact, uncoupled from K_0. A refinement of this procedure leads to a fully coupled system of equations for ϕ and K_0, in which K_0 affects the equation for ϕ [82].

We should point out that (4.4) has not yet been studied rigorously. In particular, the issue of existence of solution remains unresolved to date. A particular solution to this equation under certain assumptions for the behavior of ϕ is heuristically studied in [68].

Recently, Wu's model was slightly modified to include a spatially dependent scattering length, as an *ad hoc* parameter $a(x)$ in the microscopic Hamiltonian; see [69]. The resulting mean-field evolution law for ϕ can be written down through the replacement of $a|\phi(t,x)|^2$ by $a(x)|\phi(t,x)|^2$ in (4.3); thus, $4\pi a\zeta(t) = 4\pi a\int dx\,|\phi(t,x)|^2$ becomes $4\pi\int dx\, a(x)|\phi(t,x)|^2$. In a similar vein, evolution law (4.4) for K_0 must be modified, e.g., by replacement of $8\pi a\phi(t,x)^2\delta(x-y)$ by $8\pi a(x)\phi(t,x)^2\delta(x-y)$ and of

$$a\int dz\,\overline{\phi}(t,z)^2\, K_0(t,x,z)\, K_0(t,y,z) \quad \text{by} \quad \int dz\, a(z)\overline{\phi}(t,z)^2\, K_0(t,x,z)\, K_0(t,y,z)\ .$$

This model may be relevant to the setting of "Feshbach resonance" [27], in which the scattering length can be controlled externally by use of a magnetic or laser field. However, predictions of this model have not yet been connected to experiments.

4.2. *An application via classical homogenization.* In the remainder of this section, we provide a sample of an application of pair excitation in the static case [69] by focusing on the evolution laws for ϕ and K_0. The objective is to describe these variables in the hypothetical case where the scattering length, $a(x)$, has a periodic microstructure [69]. In particular, we set [40, 69]

$$a(x) = a_0\big[1 + A(x/\epsilon)\big]\ ,$$

where a_0 is a constant and $A(\cdot)$ is a smooth and periodic function of zero average, $\langle A\rangle_{\mathbb{T}} := \int_{\mathbb{T}} dy\, A(y) = 0$; $\mathbb{T}$ is the unit torus. A simplification in formulating this problem is that the external potential, $V_e(x)$, is assumed to be an ϵ-independent trapping potential [69]. The formulation for $a(x)$ bears similarities to the model of Fibich, Sivan and Weinstein who use the focusing NLS [40].

This problem is amenable to periodic homogenization [8]. In the (static) case with the lowest bound state [69], set $\phi(t,x) = e^{-iEt}\varphi(x)$ and $K_0(t,x,y) = e^{-i2Et}k_0(x,y)$, and consider φ to be real. By use of Wu's many-body formalism as a starting point,

the evolution equations for ϕ and K_0 (and, thus, for φ and k_0) can be written down as outlined at the end of section 4.1.

The homogenization program relies on the formal two-scale expansions

$$\varphi(x) = \sum_{l=0}^{\infty} \epsilon^l \, \varphi^{(l)}(\tilde{x}, x) \ , \quad k_0(x,y) = \sum_{l=0}^{\infty} \epsilon^l k_0^{(l)}(\tilde{x}, \tilde{y}, x, y) \ ; \quad (\tilde{x}, \tilde{y}) := (x/\epsilon, y/\epsilon) \ ,$$

where $\tilde{x}$ is the fast variable. The substitution of these expansions into the PDEs for φ and k_0 yields a cascade of equations for $\varphi^{(l)}$ and $k_0^{(l)}$. The extraction of homogenized equations relies on the following known lemma, related to the Fredholm altrernative.

LEMMA 4.2. Equation $-\Delta u = S(\cdot, x)$, where $S(\cdot, x)$ is periodic, admits a periodic solution $u(\cdot, x)$ only if $\langle S(\cdot, x)\rangle_{\mathbb{T}} = 0$. Then, $u(\cdot, x) = -\Delta^{-1} S(\cdot, x) + \breve{C}(x)$ where $\breve{C}(x)$ is reasonably arbitrary.

In [69], use is also made of asymptotics for oscillatory integrals in order to simplify a non-local term that is present in the evolution law for k_0. This program yields leading-order coefficients, $\varphi^{(0)}$ and $k_0^{(0)}$, that (not surprisingly) do not depend on the fast variables and satisfy the static versions of (4.3) and (4.4) with the scattering length a replaced by a_0. For a description of higher-order coefficients, see [69]. Under certain assumptions on the functions A and V_e, it was shown that [69]

$$\begin{aligned}
&\varphi^{(1)} = 0 \ , \qquad \varphi^{(2)}(\tilde{x}, x) = 8\pi a_0 \varphi^{(0)}(x)^3 \{\Delta_{\tilde{x}}^{-1} A(\tilde{x})\} + f_2(x) \ , \\
&k_0^{(1)} = 0 \ , \\
&k_0^{(2)} = 8\pi a_0 \{(\Delta_{\tilde{x}}^{-1} A)\varphi^{(0)}(x)^2 \delta(x-y) + 2[(\Delta_{\tilde{x}}^{-1} A)\varphi^{(0)}(x)^2 + (\Delta_{\tilde{y}}^{-1} A)\varphi^{(0)}(y)^2]\} k_0^{(0)}(x,y) \\
&\qquad\qquad + k_{0,2}(x,y) \ ,
\end{aligned}$$

where $f_2(x)$ and $k_{0,2}(x,y)$ are consequences of Lemma 4.2, playing the role of $\breve{C}(x)$, and obey linear PDEs which have forcing terms depending on $\varphi^{(0)}(x)$ and $k_0^{(0)}(x,y)$. For more details, see [69]. The above results can be further simplified if the external potential, $V_e(x)$, is an independently slowly-varying function of x. This assumption leads to explicit, closed-form asymptotic expressions for $\varphi^{(0)}$, f_2, $k_0^{(0)}$ and $k_{0,2}$ [69].

An open problem is to apply this framework to the case in which both the scattering length and the external potential have the same periodic microstructure [27]. A more fundamental question is how the spatially varying scattering length can possibly emerge from a limit of the exact many-body dynamics. This issue deserves further study.

5. Second-order correction to mean-field limit: Rigorous framework. In this section, we rigorously describe pair excitation via techniques of the Fock space, $\mathbb{F}$. Our purpose is to illustrate concepts and tools in deriving second-order corrections to the mean-field evolution of interacting Bosons in a non-translation invariant setting. Bearing this in mind, we start from the mean-field approximation in Fock space, which was heuristically discussed in section 2; and then review main aspects of our recent work on the rigorous analysis of the second-order correction [44–48]. The underlying formalism of vectors and operators in the Fock space is outlined in section 2.

In our approach, we are partly inspired by the pioneering work of Wu [82] who introduces pair excitation via a kernel; cf. (1.4) and section 4. We also recognize that important seeds of this concept can be found in the works of Hepp [50] and Ginibre and Velo [42, 43]. At the risk of redundancy, we repeat that, in our view, the pair-excitation kernel is not a-priori known but must be determined by the many-body quantum dynamics; hence, this approach should be contrasted to analogous methodologies applied in classical kinetic theory, e.g., in the context of the Boltzmann gas. For a different approach, see [7, 11].

Despite our inspiration by Wu's formulation, our set-up and derived evolution equations are different from his, as explained below. In fact, we use an approximation for the many-body wave function that involves a *unitary* operator for pairs acting on a coherent state. This approximation makes it possible to utilize a certain isomorphism between operators in Fock space and a class of matrices; this in turn facilitates the algebra and enables the rigorous derivation of error estimates in Fock space.

In our formalism, we make use of (negative) Hamiltonian $\acute{\mathcal{H}}_N$ in Fock space; recall (2.9). For ease of notation, we remove the subscript, N, and write $\acute{\mathcal{H}}$ in the place of $\acute{\mathcal{H}}_N$. Set

$$\acute{\mathcal{H}} =: \acute{\mathcal{H}}^0 - \frac{1}{N}\mathcal{V} \ ,$$

where $\acute{\mathcal{H}}^0 = \int dx \ \{a_x^* \Delta a_x\}$ corresponds to the kinetic-energy operator and $\mathcal{V}$ amounts to the atomic interactions, assuming that the trapping potential is switched off, $V_e \equiv 0$. It will be useful to recall that $v_{N,\beta}(x) := N^{3\beta} v(N^\beta x)$, which, if $\beta > 0$, approaches $\big(\int v\big)\delta(x)$ as $N \to \infty$.

In the mathematics literature, the origins of a rigorous description of corrections to mean-field limits can be traced in the works of Hepp [50] and Ginibre and Velo [42, 43]. These authors recognize the importance of the *fluctuation dynamics* unitary operator

$$\mathcal{U}_{\rm red}(t) = e^{\sqrt{N}\mathcal{A}(\phi(t,\cdot))} e^{it\acute{\mathcal{H}}} e^{-\sqrt{N}\mathcal{A}(\phi(0,\cdot))} \ , \tag{5.1}$$

where the skew-symmetric operator $\mathcal{A}(\phi)$ is defined in (2.12). The operator $\mathcal{U}_{\rm red}$ is key to understanding if one can (or, more precisely, cannot) approximate, in Fock space norm, the evolution of an *initial* coherent state, namely, the vector

$$\psi_{\rm exact} = e^{it\acute{\mathcal{H}}} e^{-\sqrt{N}\mathcal{A}(\phi(0,\cdot))}\Omega \ , \tag{5.2}$$

by a coherent state of form (2.16), which we write here again for the convenience of the reader:

$$\psi_{\rm app} = e^{-\sqrt{N}\mathcal{A}(\phi(t,\cdot))}\Omega \ .$$

Recall that this approximation is heuristically discussed in section 2.

5.1. *Some recent results on pair excitation.* We now proceed to the description of rigorous aspects of the above approximation, which naturally lead to the concept of pair excitation. To start with, note the equality

$$\|e^{it\acute{\mathcal{H}}} e^{-\sqrt{N}\mathcal{A}(\phi(0,\cdot))} - e^{-\sqrt{N}\mathcal{A}(\phi(t,\cdot))}\Omega\|_{\mathbb{F}} = \|\mathcal{U}_{\rm red}(t)\Omega - \Omega\|_{\mathbb{F}} \ .$$

As we explain below, the above crucial quantity is *not* small. This observation leads to the introduction of a second-order correction in terms of a Bogoliubov transformation,

expressing pair excitation, which modifies the above coherent state, $\psi_{\rm app}$ [44]; see (5.6) below.[9] This correction is motivated and analyzed in due course in this section.

The fluctuation dynamics operator, $\mathcal{U}_{\rm red}(t)$, satisfies the evolution equation

$$\frac{1}{i}\frac{\partial}{\partial t}\mathcal{U}_{\rm red}(t) = \mathcal{H}_{\rm red}\mathcal{U}_{\rm red}(t),\ \ \mathcal{U}_{\rm red}(0) = I\ ,$$

with a generator given by the reduced Hamiltonian

$$\mathcal{H}_{\rm red} = \frac{1}{i}\left(\frac{\partial}{\partial t}e^{\sqrt{N}\mathcal{A}(t)}\right)e^{-\sqrt{N}\mathcal{A}(t)} + e^{\sqrt{N}\mathcal{A}(t)}\acute{\mathcal{H}}e^{-\sqrt{N}\mathcal{A}(t)}\ ; \tag{5.3}$$

see (2.18) for an earlier discussion on this operator. We also refer the reader to (2.21) for the explicit form of $\mathcal{H}_{\rm red}$ involving the polynomial terms $\mathcal{P}_\ell$, which we invoke below.

At face value, this $\mathcal{H}_{\rm red}$ is a sum of terms of zeroth up to fourth order in the Fock space operators a, a^*. The zeroth-order term, $N\mu$, is harmless for our purposes, because it contributes only a phase function. However, this term has an interesting conceptual meaning: the quantity μ can be identified with the Lagrangian of the Hartree equation:

$$\mu = \int \Im\left(\phi\overline{\partial_t\phi}\right)dx - \int \left|\nabla\phi\right|^2 dx - \frac{1}{2}\int v_{N,\beta}(x-y)|\phi(x)\phi(y)|^2 dxdy\ , \tag{5.4}$$

where we suppress the time dependence of ϕ for notational ease. As discussed in section 2, setting the first-order term, denoted $\mathcal{P}_1$ in (2.21), equal to zero is equivalent to imposing the Hartree equation for ϕ,

$$\frac{1}{i}\partial_t\phi - \Delta\phi + (v_{N,\beta} * |\phi|^2)\phi = 0\ .$$

We now turn our attention to the quadratic term, which is denoted $\mathcal{P}_2$ and has an N^0 prefactor in (2.21). This term reads

$$\begin{aligned}\mathcal{P}_2 &= \acute{\mathcal{H}}^0 - \tfrac{1}{2}\left[\mathcal{A},[\mathcal{A},\mathcal{V}]\right]\\ &= \acute{\mathcal{H}}^0 - \tfrac{1}{2}\int v_{N,\beta}(x-y)\left(\overline{\phi}(y)\overline{\phi}(x)a_xa_y + \phi(y)\phi(x)a_x^*a_y^* + 2\overline{\phi}(y)\phi(x)a_x^*a_y\right)\ dx\,dy\\ &\qquad - \int\left(v_{N,\beta} * |\phi^2|\right)(x)a_x^*a_x\ dx\ .\end{aligned}$$

By this formula, it becomes evident that the Fock space vector $\mathcal{P}_2\Omega$ is of the order of N^0 because of the presence of the a^*a^* terms. Therefore, we do not expect $\|\mathcal{U}_{\rm red}(t)\Omega - \Omega\|_{\mathbb{F}}$ to be small. This observation can mathematically motivate the introduction of pair excitation.

At this point, in regard to $\mathcal{H}_{\rm red}$, one wonders what happens with the remaining polynomial terms $\mathcal{P}_\ell$ (for $\ell = 3,\,4$) which have prefactors $N^{-1/2}$ and N^{-1}; cf. (2.21). One of course hopes that, under suitable assumptions on the interaction potential, $v_{N,\beta}$, these terms $\mathcal{P}_\ell$ can be treated as small error terms. This is indeed the case for sufficiently low

[9] To the best of our knowledge, this introduction of a Bogoliubov transformation, or pair excitation, is novel at least in the rigorous mathematics literature for the many-body Boson evolution. Bogoliubov transformations have been used extensively in the physics community to diagonalize quadratic Hamiltonians. However, we have not been able to find any reference appearing earlier than [44] in which Bogoliubov transformations are applied explicitly to the norm approximation problem considered here; or to related problems such as convergence of the gamma density matrices to tensor products, as in [7].

values of the parameter $\beta > 0$ [46, 58]; but refinements of the treatment are needed for higher values of β [47, 48].

We continue our discussion on the "interesting" term $\mathcal{P}_2$ contained in $\mathcal{H}_{\rm red}$. Define the unitary operator $\mathcal{U}_2(t)$ through the evolution equation

$$\frac{1}{i}\frac{\partial}{\partial t}\mathcal{U}_2(t) = \mathcal{P}_2\mathcal{U}_2(t)\ ,\ \ \mathcal{U}_2(0) = I\ . \tag{5.5}$$

An ingredient of the results by Hepp [50] and Ginibre and Velo [42, 43] should be emphasized in this context. In the case with $\beta = 0$ under suitable condition on $v_{N,0}$, i.e., this potential is smooth in [50] and more singular in [42, 43], the following property holds:

$$\mathcal{U}_{\rm red}(t) \to \mathcal{U}_2(t) \quad \text{strongly as} \quad N \to \infty\ .$$

While the above papers [42, 43, 50] make no explicit reference to a pair-excitation kernel or Bogoliubov transformation, they lead naturally to the introduction of such a notion, recently carried out in [44], in order to handle the a^*a^* terms in $\mathcal{P}_2$. More discussion on this point is provided below.

A comment on the operator $\mathcal{U}_2$ defined by (5.5) is in order. In [6], the authors state that, under suitable assumptions on the interaction potential v, the operator $\mathcal{U}_2(t)$ can be written (abstractly) as a Bogoliubov transformation. The reader is also referred to Remark 5.1 below which outlines how the operator $\mathcal{U}_2$ of Hepp [50] and Ginibre and Velo [42, 43] is related to our construction of pair excitation [44], expressed by the operator $e^{\mathcal{B}}$ as we see next.

To illustrate the nature of pair excitation rigorously, we have to revisit what mathematicians call the *metaplectic or Segal-Shale-Weil representation* [76], and physicists often call the Bogoliubov transformation. These notions are encapsulated by a (double-valued) unitary representation of the group of matrices that have the form

$$E = \begin{pmatrix} P(x,y) & Q(x,y) \\ \overline{Q}(x,y) & \overline{P}(x,y) \end{pmatrix}\ ,$$

where P and Q are distribution kernels bounded on L^2; in particular, Q satisfies the condition that Q^*Q is of trace class. The above matrices satisfy one of the following equivalent properties: E belongs to $U(\infty,\infty)$, meaning

$$E^*\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} E = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\ ;$$

or E is symplectic, i.e.,

$$E^T\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} E = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}\ .$$

Next, we elaborate on a few specifics of the rigorous program in pair excitation laid out in [44–48], with some emphasis to most recent results. The primary goal is to approximate in Fock space norm exact evolution (5.2) by a *modified* coherent state, herein called $\psi_{\rm app\,2}$, which incorporates second-order corrections, viz.,

$$\psi_{\rm app\,2}(t) = e^{-\sqrt{N}\mathcal{A}(\phi(t))}e^{-\mathcal{B}(k(t))}\Omega\ ; \tag{5.6}$$

cf. (2.16). In the above, the operator $\mathcal{B}$ in Fock space is skew-symmetric, defined by

$$\mathcal{B}(k) := \frac{1}{2}\int dxdy\left\{\bar{k}(t,x,y)a_x a_y - k(t,x,y)a_x^* a_y^*\right\} \ , \tag{5.7}$$

where $k(t,x,y)$ is the pair-excitation kernel ($(x,y)\in\mathbb{R}^3\times\mathbb{R}^3$). Thus, $e^{\mathcal{B}(k(t))}$ is unitary; and forms the metaplectic representation of the matrix

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

where

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

and

$$\mathrm{sh}(k) := k + \frac{1}{3!}k\circ\overline{k}\circ k + \dots \ ,$$
$$\mathrm{ch}(k) := \delta(x-y) + \frac{1}{2!}\overline{k}\circ k + \dots \ ,$$

and the symbol $\circ$ indicates composition. We should add that, in a language familiar to many physicists, the operator $e^{\mathcal{B}(k(t))}$ expresses the implementation of a Bogoliubov transformation (see Remark 5.1).

In the static case of the Boson gas, which concerns the ground state of the many-body Hamiltonian, the above construction of $e^{\mathcal{B}(k(t))}$ is related to the physics papers of Bogoliubov [12], and Lee, Huang and Yang [59]; and the mathematically rigorous papers of Lieb and Solovej [67] and Erdős, Schlein and Yau [38]. For a recent account of diagonalizing quadratic Hamiltonians such as $\mathcal{P}_2$, the interested reader is referred to [70].

Let us continue with our program of analyzing approximation (5.6). A central issue is to derive an evolution equation for the pair-excitation kernel, k, consistent with the many-body quantum dynamics. For an interaction potential, v, of the Coulomb type if $\beta = 0$, or a more general potential $v_{N,\beta}$ corresponding to low values of $\beta > 0$, it suffices to impose the Hartree equation for ϕ; and choose k in order to *diagonalize* the resulting evolution operator

$$\begin{aligned} &\frac{1}{i}\left(\frac{\partial}{\partial t}e^{\mathcal{B}(t)}\right)e^{-\mathcal{B}(t)} + e^{\mathcal{B}(t)}\mathcal{P}_2 e^{-\mathcal{B}(t)} \\ &= \text{diagonal operator } \mathcal{D} = \frac{1}{2}\int dxdy\left\{-d_N(t,x,y)a_x^* a_y - d_N(t,y,x)a_y^* a_x\right\} \\ &\qquad + \text{a scalar term} \ . \end{aligned} \tag{5.8}$$

Note that we write $\mathcal{B}(t)$ instead of $\mathcal{B}(k(t))$ for notational ease. In the above, d_N is a distribution kernel of the form $d_N = \Delta_x\delta(x-y)$ plus less singular terms. The evolution equation for k resulting from this diagonalization in Fock space looks highly non-linear at first. Nonetheless, as duly noticed in [46], in the right coordinates $\mathrm{sh}(2k), \mathrm{ch}(2k)$ this equation becomes in fact *linear*.

REMARK 5.1. We mention in passing that, once the diagonalization of (5.8) is accomplished, it is possible to find a matrix of the form

$$C = \begin{pmatrix} P(t,x,y) & 0 \\ 0 & \overline{P}(t,x,y) \end{pmatrix} , \qquad P : \text{ unitary } ,$$

such that, denoting its representation (implementation) by $\mathcal{C}$,

$$\frac{1}{i}\left(\frac{\partial}{\partial t}\mathcal{C}\right)\mathcal{C}^{-1} + \mathcal{C}\left(\frac{1}{i}\left(\frac{\partial}{\partial t}e^{\mathcal{B}(t)}\right)e^{-\mathcal{B}(t)} + e^{\mathcal{B}(t)}\mathcal{D}e^{-\mathcal{B}(t)}\right)\mathcal{C}^{-1} = 0 \ . \tag{5.9}$$

This amounts to the Schrödinger type PDE $\frac{1}{i}\frac{\partial}{\partial t}P + Pd_N = 0$, with $P(0) = I$, and identifies the operator $\mathcal{U}_2$ with $e^{-\mathcal{B}}\mathcal{C}^{-1}$.

The main result of [46], which involves $\beta > 0$ and is based on the methodology of the two earlier papers on pair excitation [44, 45], is encapsulated by the following theorem.

THEOREM 5.2. Let ϕ and k satisfy

$$\frac{1}{i}\partial_t\phi - \Delta\phi + \left(v_{N,\beta} * |\phi|^2\right)\phi = 0 \ ,$$

and

$$\mathbf{S}\left(\mathrm{sh}(2k)\right) = m_N \circ \mathrm{ch}(2k) + \overline{\mathrm{ch}(2k)} \circ m_N \ ,$$
$$\mathbf{W}\left(\overline{\mathrm{ch}(2k)}\right) = m_N \circ \overline{\mathrm{sh}(2k)} - \mathrm{sh}(2k) \circ \overline{m}_N \ ,$$

with prescribed initial conditions $\phi(0,\cdot) = \phi_0$, $k(0,\cdot,\cdot) = 0$, where

$$\mathbf{S} = \frac{1}{i}\frac{\partial}{\partial t} - \Delta_{x_1} - \Delta_{x_2} + \text{potential terms of Hartree type} \ ,$$
$$\mathbf{W} = \frac{1}{i}\frac{\partial}{\partial t} - \Delta_{x_1} + \Delta_{x_2} + \text{potential terms of Hartree type} \ ,$$
$$m_N(t,x,y) = -v_{N,\beta}\phi(t,x)\phi(t,y) = -N^{3\beta}v(N^\beta|x-y|)\phi(t,x)\phi(t,y) \ .$$

Then, there exists a real phase function χ such that, with respect to the Fock space norm, the following estimate holds:

$$\|\psi_{\text{exact}}(t) - e^{iN\chi(t)}\psi_{\text{app}\,2}(t)\|_{\mathbb{F}} \le \frac{C(1+t)\log^4(1+t)}{N^{(1-3\beta)/2}} \tag{5.10}$$

provided $0 < \beta < \frac{1}{3}$.

The Hartree case, $\beta = 0$, in which a similar error estimate is satisfied in Fock space norm, was treated in the earlier works [44, 45]. The type of result stated in Theorem 5.2 was extended to the case of three-body interactions by X. Chen [18]; and to the range $0 < \beta < \frac{1}{2}$ by Kuz [58], where it is also argued that the exponent $\beta = \frac{1}{2}$ is as far as one can go with these equations.

We now elaborate on an important point, namely, that the value $\beta = 1/2$ signifies some sort of a threshold for results such as the one stated in Theorem 5.2. In order to get past $\beta = \frac{1}{2}$ with the pair-excitation construction involving $e^{\mathcal{B}}$, one must impose different types of equations on ϕ and k.

Let us briefly explain the germane idea, introduced in [47]. One should *not* impose the Hartree equation for ϕ or truncate $\mathcal{H}_{\rm red}$ up to the quadratic term $\mathcal{P}_2$; but instead introduce the (alternate) operator

$$\mathcal{U}_{\rm red\,2}(t) := e^{\mathcal{B}(k(t))} e^{\sqrt{N}\mathcal{A}(\phi(t))} e^{it\acute{\mathcal{H}}} e^{-\sqrt{N}\mathcal{A}(\phi_0)} e^{-\mathcal{B}(k(0))} \ ,$$

and the "doubly reduced Hamiltonian", $\mathcal{H}_{\rm red\,2}$, given by the formula

$$\begin{aligned}\mathcal{H}_{\rm red\,2} := & \frac{1}{i}\big(\partial_t e^{\mathcal{B}}\big)e^{-\mathcal{B}} \\ & + e^{\mathcal{B}}\left(\frac{1}{i}\big(\partial_t e^{\sqrt{N}\mathcal{A}}\big)e^{-\sqrt{N}\mathcal{A}} + e^{\sqrt{N}\mathcal{A}}\acute{\mathcal{H}}e^{-\sqrt{N}\mathcal{A}}\right)e^{-\mathcal{B}} \ ;\end{aligned}$$

compare to (5.3). The operators $\mathcal{U}_{\rm red\,2}$ and $\mathcal{H}_{\rm red\,2}$ satisfy

$$\frac{1}{i}\frac{\partial}{\partial t}\mathcal{U}_{\rm red\,2}(t) = \mathcal{H}_{\rm red\,2}\mathcal{U}_{\rm red\,2}(t) \ .$$

The operator $\mathcal{H}_{\rm red\,2}$ is of fourth-order in a and a^*. Hence, the Fock space vector $\mathcal{H}_{\rm red\,2}\Omega$ can be written in terms of n-particle states X_n as

$$\mathcal{H}_{\rm red\,2}\Omega = (X_0, X_1, X_2, X_3, X_4, 0, 0, \ldots) \ . \tag{5.11}$$

The new, coupled equations for ϕ and k introduced in [47] can be written abstractly as

$$X_1 = 0 \ \text{ and } X_2 = 0 \ . \tag{5.12}$$

These equations are refinements of the earlier equations [46] and take into account Wick ordering.[10] In [47], it is shown that the solutions to (5.12) are Euler-Lagrange equations for the Lagrangian $\int X_0$ and conserve the number of particles and the energy.[11] These equations can be written down, but their analysis is much more difficult. In their most elegant form, these equations are expressed in terms of the matrix [48]

$$\begin{aligned}\mathcal{L}_{m,n}(t, y_1, \ldots, y_m; x_1, \ldots, x_n) : &= \frac{1}{N^{(m+n)/2}}\big\langle a_{y_1}\cdots a_{y_m}\mathcal{M}\Omega,\ a_{x_1}\cdots a_{x_n}\mathcal{M}\Omega\big\rangle \\ &= \frac{1}{N^{(m+n)/2}}\big\langle \mathcal{M}\Omega,\ \mathcal{P}_{m,n}\mathcal{M}\Omega\big\rangle \ ,\end{aligned}$$

where $\mathcal{P}_{m,n} = a^*_{y_1}a^*_{y_2}\ldots a^*_{y_m}a_{x_1}a_{x_2}\ldots a_{x_n}$ and $\mathcal{M} = e^{-\sqrt{N}\mathcal{A}}e^{-\mathcal{B}}$. We should add that the following relation always holds:

$$\frac{1}{i}\partial_t\big\langle \mathcal{M}\Omega, \mathcal{P}\mathcal{M}\Omega\big\rangle = \big\langle \Omega, \big[\mathcal{H}_{\rm red\,2}, \mathcal{M}^*\mathcal{P}\mathcal{M}\big]\Omega\big\rangle + \big\langle \Omega, \mathcal{M}^*\big[\mathcal{P}, \mathcal{H}\big]\mathcal{M}\Omega\big\rangle \ . \tag{5.13}$$

In [48], it is shown that if $\mathcal{H}_{\rm red\,2}\Omega = \big(X_0, 0, 0, X_3, X_4, 0, 0, \ldots\big)$ and $\mathcal{P}$ is a first- or second-order Wick-ordered monomial, then

$$\big\langle \Omega, \big[\mathcal{H}_{\rm red\,2}, \mathcal{M}^*\mathcal{P}\mathcal{M}\big]\Omega\big\rangle = 0 \ ;$$

[10] In the theory of quantized fields, a product of creation and annihilation operators obeys Wick, or normal, ordering if all creation operators are to the left of all annihilation operators in the product.

[11] This formulation is natural, since the corresponding term, μ, after the first reduction is a Lagrangian for the Hartree equation, as pointed out in (5.4).

thus,

$$\frac{1}{i}\partial_t\langle \mathcal{M}\Omega, \mathcal{P}\mathcal{M}\Omega\rangle = \langle \Omega, \mathcal{M}^*\big[\mathcal{P},\mathcal{H}\big]\mathcal{M}\Omega\rangle \ . \tag{5.14}$$

This last equation would be satisfied by the exact evolution, and it only works for the approximate evolution if $\mathcal{P}$ is of degree ≤ 2. Furthermore, it turns out that

$$\mathcal{L}_{0,1}(t,x) = \phi(t,x) \ , \quad \mathcal{L}_{1,1}(t,x,y) = \overline{\phi}(t,x)\phi(t,y) + \frac{1}{N}(\overline{\mathrm{sh}(k)} \circ \mathrm{sh}(k))(t,x,y) \ ,$$
$$\mathcal{L}_{0,2}(t,x,y) = \phi(t,x)\phi(t,y) + \frac{1}{2N}\mathrm{sh}(2k)(t,x,y) \ ;$$

and all the higher $\mathcal{L}$-matrices can be expressed in terms of the above three.

Remark 5.3. As previously mentioned, the conservation of the number of particles and the energy for $\mathcal{M}\Omega$ is proved in [47]. The proof is based on the invariance properties of the underlying Lagrangian. However, this conservation can also be seen from the above formulation in the following way. Take $\mathcal{P} = \mathcal{N} = \int a_x^* a_x dx$, which commutes with $\acute{\mathcal{H}}$ in (5.14), in order to obtain conservation of the number of particles, $\langle \mathcal{M}\Omega, \mathcal{N}\mathcal{M}\Omega\rangle$. Furthermore, set $\mathcal{P} = \acute{\mathcal{H}}$ in (5.13). Then, the second term on the right-hand side of this equation drops out. For the first term, write

$$\mathcal{H}_{\mathrm{red}\,2} = \frac{1}{i}\big(\partial_t e^{\mathcal{B}}\big)e^{-\mathcal{B}} + e^{\mathcal{B}}\frac{1}{i}\big(\partial_t e^{\sqrt{N}\mathcal{A}}\big)e^{-\sqrt{N}\mathcal{A}}e^{-\mathcal{B}} + \mathcal{M}^*\acute{\mathcal{H}}\mathcal{M} \ ,$$

which reduces the problem to commuting $\mathcal{H}_{\mathrm{red}\,2}$ with terms of degree ≤ 2, so that the first term in (5.13) is also zero. Consequently, one obtains conservation of the energy, $\langle \mathcal{M}\Omega, \mathcal{H}\mathcal{M}\Omega\rangle$.

We now elaborate on (5.14). This relation can be written explicitly as

$$\begin{aligned}
&\left(\frac{1}{i}\frac{\partial}{\partial t} - \Delta_{x_1}\right)\mathcal{L}_{0,1}(t,x_1) \\
&= -\int v_{N,\beta}(x_1-x_2)\,\mathcal{L}_{1,2}(t,x_2;x_1,x_2)\,dx_2 \ , \qquad (5.15a)\\
&\left(\frac{1}{i}\frac{\partial}{\partial t} + \Delta_{x_1} - \Delta_{y_1}\right)\mathcal{L}_{1,1}(t,x_1;y_1) \\
&= \int v_{N,\beta}(x_1-x_2)\,\mathcal{L}_{2,2}(t,x_1,x_2;y_1,x_2)\,dx_2 - \int v_{N,\beta}(y_1-y_2)\mathcal{L}_{2,2}(t,x_1,y_2;y_1,y_2)\,dy_2 \ , \qquad (5.15b)\\
&\left(\frac{1}{i}\frac{\partial}{\partial t} - \Delta_{x_1} - \Delta_{x_2} + \frac{1}{N}v_{N,\beta}(x_1-x_2)\right)\mathcal{L}_{0,2}(x_1,x_2) \\
&= -\int v_{N,\beta}(x_1-y)\mathcal{L}_{1,3}(y;x_1,x_2,y)\,dy - \int v_{N,\beta}(x_2-y)\mathcal{L}_{1,3}(y;x_1,x_2,y)\,dy \ . \qquad (5.15c)
\end{aligned}$$

The matrices $\mathcal{L}_{i,j}$ on the right-hand side can be expressed in a straightforward way in terms of $\mathcal{L}_{0,1}(t,x)$, $\mathcal{L}_{1,1}(t,x,y)$ and $\mathcal{L}_{0,2}(t,x,y)$; see [48] for details.

The main result proved in [48] can be sketchily summarized as follows.

Theorem 5.4. Let $\frac{1}{3} < \beta < \frac{2}{3}$ and the interaction potential $v \in \mathcal{S}$ (with some additional technical assumptions). In addition, suppose that ϕ and k are solutions to (5.15) with

suitable initial conditions $\phi(0,\cdot)$, $k(0,\cdot)$. Then, for some real function $\chi(t) = \chi_N(t)$ and for every $\epsilon > 0$, there exist constants $T_0 > 0$ and C such that

$$\|e^{it\acute{\mathcal{H}}} e^{-\sqrt{N}\mathcal{A}(\phi_0)} e^{-\mathcal{B}(k(0))}\Omega - e^{i\chi(t)} e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))}\Omega\|_{\mathbb{F}} \to 0$$

as $N \to \infty$, uniformly for $0 \le t \le T_0$.

Although this theorem appears to involve a restricted range of values for β, its validity might be more general.

5.2. *Recent related works.* We conclude this section by commenting on a few related works in the existing mathematics literature. Most recently, we became aware that Bach, Breteaux, T. Chen, Fröhlich and Sigal [4], independently and in a different setting, derived equations that are closely related to the equations derived in [47, 48]. Their equations [4] become equivalent to those in [47, 48] in the case of pure states.

We should also mention the recent related result by Benedikter, de Oliveira and Schlein [7] in regard to applications of a construction similar to $e^{\mathcal{B}}$ (with an explicit choice of k) to estimates for the γ density matrices in the case with $\beta = 1$. In a similar vein, Boccato, Cenatiempo and Schlein [11] analyzed quantum fluctuations by use of a quadratic generator. Specifically, in [11] the authors prove an estimate globally in time in the full range $\beta < 1$. In this work, it is proved that the exact evolution of the system state is approximated, in Fock space, by $e^{i\chi(t)} e^{-\sqrt{N}\mathcal{A}(\phi(t))} e^{-\mathcal{B}(k(t))} \tilde{U}_{2,N}(t)\Omega$, where $k(t) = k(t,x,y)$ is explicit (and related to but different from our $k(t)$) and $\tilde{U}_{2,N}(t)$ is an evolution in Fock space with a quadratic generator [11]. In the list of related results, we also add an important direction: a construction by Lewin, Nam, and Schlein [62] that allows direct approximations of a pure Hartree state, as opposed to a coherent state.

6. Conclusion and outlook. In this expository paper, we reviewed recent advances in understanding how large systems of interacting Bosons evolve in non-translation invariant settings at extremely low temperatures. Studies in this direction have partly been motivated by the wealth of experimental observations on atomic gases, characterized by precise controls of atomic features. In this kinetic regime, the Boson evolution is reasonably governed by the many-body Schrödinger equation. However, this description is usually deemed as impractical for a large number of particles. In our review, we described approximations to this evolution, particularly mean-field limits and second-order corrections to these limits, by focusing on the many-body wave function of the Boson system. The analysis of these approximations is pregnant with novel mathematical problems. A guide in the construction of second-order corrections to the mean-field dynamics has been offered by pair excitation, a physical process by which atoms are scattered in pairs from the macroscopic quantum state [12, 59, 82]. Mathematically, this concept is intimately related to the metaplectic or Segal-Shale-Weil representation, which has been recently invoked in the rigorous derivation of error estimates for second-order corrections [44, 45].

Despite the growing body of work in this research direction, there are pending issues. Therefore, it is worthwhile concluding this paper by highlighting open challenging questions. In our review, we focused on the Boson dynamics at zero temperature. As the temperature increases, it is intuitively expected that pair excitation may significantly be

coupled with thermally excited states; see the renowned work by Lee and Yang [60, 61] in physics, as well as more rigorous studies, e.g., [4, 41, 65]. We believe that the rigorous description of the quantum many-particle evolution at finite temperatures below the phase transition for the Boson gas deserves additional attention. More broadly speaking, the derivation of macroscopic descriptions in the quantum setting is a rich area for mathematical research. Some kinetic models, e.g., the quantum Boltzmann equation [80], that are often invoked in this context need to be better understood on the grounds of the underlying microscopic dynamics.

References

[1] R. Adami, C. Bardos, F. Golse, and A. Teta, *Towards a rigorous derivation of the cubic NLSE in dimension one*, Asymptot. Anal. **40** (2004), no. 2, 93–108. MR2104130

[2] R. Adami, F. Golse, and A. Teta, *Rigorous derivation of the cubic NLS in dimension one*, J. Stat. Phys. **127** (2007), no. 6, 1193–1220, DOI 10.1007/s10955-006-9271-z. MR2331036

[3] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Observation of Bose-Einstein condensation in a dilute atomic vapor*, Science **269** (1995), 198–201.

[4] V. Bach, S. Breteaux, T. Chen, J. Fröhlich, and I. M. Sigal, *The time-dependent Hartree-Fock-Bogoliubov equation for Bosons*, arXiv:math-ph/1602.05171 (36pp).

[5] W. Bao and Y. Cai, *Mathematical theory and numerical methods for Bose-Einstein condensation*, Kinet. Relat. Models **6** (2013), no. 1, 1–135, DOI 10.3934/krm.2013.6.1. MR3005624

[6] G. Ben Arous, K. Kirkpatrick, and B. Schlein, *A central limit theorem in many-body quantum dynamics*, Comm. Math. Phys. **321** (2013), no. 2, 371–417, DOI 10.1007/s00220-013-1722-1. MR3063915

[7] N. Benedikter, G. de Oliveira, and B. Schlein, *Quantitative derivation of the Gross-Pitaevskii equation*, Comm. Pure Appl. Math. **68** (2015), no. 8, 1399–1482, DOI 10.1002/cpa.21542. MR3366749

[8] A. Bensoussan, J.-L. Lions, and G. Papanicolaou, *Asymptotic analysis for periodic structures*, Studies in Mathematics and its Applications, vol. 5, North-Holland Publishing Co., Amsterdam-New York, 1978. MR503330

[9] F. A. Berezin, *The method of second quantization*, Translated from the Russian by Nobumichi Mugibayashi and Alan Jeffrey. Pure and Applied Physics, Vol. 24, Academic Press, New York-London, 1966. MR0208930

[10] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics*, Wiley, New York, NY, 1952.

[11] C. Boccato, N. Cenatiempo, and B. Schlein, *Quantum many-body fluctuations around nonlinear Schrödinger dynamics*, arXiv:math-ph/1509.03837 (78pp).

[12] N. Bogolubov, *On the theory of superfluidity*, Acad. Sci. USSR. J. Phys. **11** (1947), 23–32. MR0022177

[13] S. N. Bose, *Plancks Gesetz und Lichtquantenhypothese*, Z. Phys. **26** (1924), 178–181.

[14] I. Carusotto and C. Ciuti, *Quantum fluids of light*, Rev. Mod. Phys. **85** (2013), 299–366.

[15] T. Chen, C. Hainzl, N. Pavlović, and R. Seiringer, *On the well-posedness and scattering for the Gross-Pitaevskii hierarchy via quantum de Finetti*, Lett. Math. Phys. **104** (2014), no. 7, 871–891, DOI 10.1007/s11005-014-0693-2. MR3210237

[16] T. Chen and N. Pavlović, *Derivation of the cubic NLS and Gross-Pitaevskii hierarchy from many-body dynamics in $d = 3$ based on spacetime norms*, Ann. Henri Poincaré **15** (2014), no. 3, 543–588, DOI 10.1007/s00023-013-0248-6. MR3165917

[17] T. Chen, N. Pavlović, and N. Tzirakis, *Multilinear Morawetz identities for the Gross-Pitaevskii hierarchy*, Recent advances in harmonic analysis and partial differential equations, Contemp. Math., vol. 581, Amer. Math. Soc., Providence, RI, 2012, pp. 39–62, DOI 10.1090/conm/581/11491. MR3013052

[18] X. Chen, *Second order corrections to mean field evolution for weakly interacting bosons in the case of three-body interactions*, Arch. Ration. Mech. Anal. **203** (2012), no. 2, 455–497, DOI 10.1007/s00205-011-0453-8. MR2885567

[19] X. Chen, *Collapsing estimates and the rigorous derivation of the 2d cubic nonlinear Schrödinger equation with anisotropic switchable quadratic traps* (English, with English and French summaries), J. Math. Pures Appl. (9) **98** (2012), no. 4, 450–478, DOI 10.1016/j.matpur.2012.02.003. MR2968164

[20] X. Chen, *On the rigorous derivation of the 3D cubic nonlinear Schrödinger equation with a quadratic trap*, Arch. Ration. Mech. Anal. **210** (2013), no. 2, 365–408, DOI 10.1007/s00205-013-0645-5. MR3101788

[21] X. Chen and J. Holmer, *On the rigorous derivation of the 2D cubic nonlinear Schrödinger equation from 3D quantum many-body dynamics*, Arch. Ration. Mech. Anal. **210** (2013), no. 3, 909–954, DOI 10.1007/s00205-013-0667-z. MR3116008

[22] X. Chen and J. Holmer, *Correlation structures, many-body scattering processes and the derivation of the Gross-Pitaevskii hierarchy*, Int. Math. Res. Notices **2016** (2016), 3051–3110.

[23] X. Chen and J. Holmer, *Focusing quantum many-body dynamics: the rigorous derivation of the 1D focusing cubic nonlinear Schrödinger equation*, Arch. Ration. Mech. Anal. **221** (2016), no. 2, 631–676, DOI 10.1007/s00205-016-0970-6. MR3488534

[24] X. Chen and J. Holmer, *Focusing quantum many-body dynamics: the rigorous derivation of the 1D focusing cubic nonlinear Schrödinger equation*, Arch. Ration. Mech. Anal. **221** (2016), no. 2, 631–676, DOI 10.1007/s00205-016-0970-6. MR3488534

[25] X. Chen and J. Holmer, *The rigorous derivation of the 2D cubic focusing NLS from quantum many-body evolution*, arXiv:math-ph/1508.07675 (36pp).

[26] X. Chen and J. Holmer, *On the Klainerman–Machedon conjecture for the quantum BBGKY hierarchy with self-interaction*, J. Eur. Math. Soc. (JEMS) **18** (2016), no. 6, 1161–1200, DOI 10.4171/JEMS/610. MR3500833

[27] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, *Feshbach resonances in ultracold gases*, Rev. Mod. Phys. **82** (2010), 1225–1286.

[28] E. A. Cornell and C. E. Wieman, *Nobel lecture: Bose-Einstein condensation in a dilute gas, the first 70 years and some recent experiments*, Rev. Mod. Phys. **74** (2002), 875–893.

[29] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Bose-Einstein condensation in a gas of sodium atoms*, Phys. Rev. Lett. **75** (1995), 3969–3973.

[30] P. A. M. Dirac, *The Principles of Quantum Mechanics*, Clarendon Press, 4th. Ed., Oxford, 1958.

[31] F. J. Dyson, *Ground-state energy of a hard sphere gas*, Phys. Rev. **106** (1957), 20–26.

[32] A. Einstein, *Quantentheorie des Einatomigen Idealen Gases*, Sitzungsber. Kgl. Preuss. Akad. Wiss. **22** (1924), 261–267.

[33] A. Einstein, *Quantentheorie des Einatomigen Idealen Gases. 2. Abhandlung*, Sitzungsber. Kgl. Preuss. Akad. Wiss. **23** (1925), 3–14.

[34] A. Elgart, L. Erdős, B. Schlein, and H.-T. Yau, *Gross-Pitaevskii equation as the mean field limit of weakly coupled bosons*, Arch. Ration. Mech. Anal. **179** (2006), no. 2, 265–283, DOI 10.1007/s00205-005-0388-z. MR2209131

[35] L. Erdős, B. Schlein, and H.-T. Yau, *Derivation of the Gross-Pitaevskii hierarchy for the dynamics of Bose-Einstein condensate*, Comm. Pure Appl. Math. **59** (2006), no. 12, 1659–1741, DOI 10.1002/cpa.20123. MR2257859

[36] L. Erdős, B. Schlein, and H.-T. Yau, *Derivation of the cubic non-linear Schrödinger equation from quantum dynamics of many-body systems*, Invent. Math. **167** (2007), no. 3, 515–614, DOI 10.1007/s00222-006-0022-1. MR2276262

[37] L. Erdős, B. Schlein, and H.-T. Yau, *Rigorous derivation of the Gross-Pitaevskii equation*, Phys. Rev. Lett. **98** (2007), 040404.

[38] L. Erdős, B. Schlein, and H.-T. Yau, *The ground state energy of a low density Bose gas: a second order upper bound.* Phys. Rev. A **78** (2008), 053627.

[39] L. Erdős, B. Schlein, and H.-T. Yau, *Derivation of the Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensate*, Ann. of Math. (2) **172** (2010), no. 1, 291–370, DOI 10.4007/annals.2010.172.291. MR2680421

[40] G. Fibich, Y. Sivan, and M. I. Weinstein, *Bound states of nonlinear Schrödinger equations with a periodic nonlinear microstructure*, Phys. D **217** (2006), no. 1, 31–57, DOI 10.1016/j.physd.2006.03.009. MR2234239

[41] J. Ginibre, *On the asymptotic exactness of the Bogoliubov approximation for many boson systems*, Comm. Math. Phys. **8** (1968), 26–51. MR0225552

[42] J. Ginibre and G. Velo, *The classical field limit of scattering theory for nonrelativistic many-boson systems. I*, Comm. Math. Phys. **66** (1979), no. 1, 37–76. MR530915

[43] J. Ginibre and G. Velo, *The classical field limit of scattering theory for nonrelativistic many-boson systems. II*, Comm. Math. Phys. **68** (1979), no. 1, 45–68. MR539736

[44] M. G. Grillakis, M. Machedon, and D. Margetis, *Second-order corrections to mean field evolution of weakly interacting bosons. I*, Comm. Math. Phys. **294** (2010), no. 1, 273–301, DOI 10.1007/s00220-009-0933-y. MR2575484

[45] M. Grillakis, M. Machedon, and D. Margetis, *Second-order corrections to mean field evolution of weakly interacting bosons. II*, Adv. Math. **228** (2011), no. 3, 1788–1815, DOI 10.1016/j.aim.2011.06.028. MR2824569

[46] M. Grillakis and M. Machedon, *Pair excitations and the mean field approximation of interacting bosons, I*, Comm. Math. Phys. **324** (2013), no. 2, 601–636, DOI 10.1007/s00220-013-1818-7. MR3117522

[47] M. Grillakis and M. Machedon, *Beyond mean field: on the role of pair excitations in the evolution of condensates*, J. Fixed Point Theory Appl. **14** (2013), no. 1, 91–111, DOI 10.1007/s11784-013-0150-3. MR3202027

[48] M. Grillakis and M. Machedon, *Pair excitations and the mean field approximation of interacting bosons, I*, Comm. Math. Phys. **324** (2013), no. 2, 601–636, DOI 10.1007/s00220-013-1818-7. MR3117522

[49] E. P. Gross, *Structure of a quantized vortex in boson systems* (English, with Italian summary), Nuovo Cimento (10) **20** (1961), 454–477. MR0128907

[50] K. Hepp, *The classical limit for quantum mechanical correlation functions*, Comm. Math. Phys. **35** (1974), 265–277. MR0332046

[51] K. Huang, C. N. Yang, and J. M. Luttinger, *Imperfect Bose gas with hard-sphere interaction*, Phys. Rev. (2) **105** (1957), 776–784. MR0084264

[52] Y. Kawaguchi and M. Ueda, *Spinor Bose-Einstein condensates*, Phys. Rep. **520** (2012), no. 5, 253–381, DOI 10.1016/j.physrep.2012.07.005. MR3006185

[53] W. Ketterle, *Nobel lecture: When atoms behave as waves: Bose-Einstein condensation and the atom laser*, Rev. Mod. Phys. **74** (2002), 1131–1151.

[54] K. Kirkpatrick, B. Schlein, and G. Staffilani, *Derivation of the two-dimensional nonlinear Schrödinger equation from many body quantum dynamics*, Amer. J. Math. **133** (2011), no. 1, 91–130, DOI 10.1353/ajm.2011.0004. MR2752936

[55] S. Klainerman and M. Machedon, *On the uniqueness of solutions to the Gross-Pitaevskii hierarchy*, Comm. Math. Phys. **279** (2008), no. 1, 169–185, DOI 10.1007/s00220-008-0426-4. MR2377632

[56] A. Knowles and P. Pickl, *Mean-field dynamics: singular potentials and rate of convergence*, Comm. Math. Phys. **298** (2010), no. 1, 101–138, DOI 10.1007/s00220-010-1010-2. MR2657816

[57] E. Kuz, *Rate of convergence to mean field for interacting bosons*, Comm. Partial Differential Equations **40** (2015), no. 10, 1831–1854, DOI 10.1080/03605302.2015.1053568. MR3391830

[58] E. Kuz, *Exact evolution versus mean field with second-order correction for Bosons interacting via short-range two-body potential*, arXiv:1511.00487 (38pp).

[59] T. D. Lee, K. Huang, and C. N. Yang, *Eigenvalues and eigenfunctions of a Bose system of hard spheres and its low-temperature properties*, Phys. Rev. (2) **106** (1957), 1135–1145. MR0088176

[60] T. D. Lee and C. N. Yang, *Low-temperature behavior of a dilute Bose system of hard spheres. I. Equilibrium properties*, Phys. Rev. (2) **112** (1958), 1419–1429. MR0127865

[61] T. D. Lee and C. N. Yang, *Low-temperature behavior of a dilute Bose system of hard spheres. II. Nonequilibrium properties*, Phys. Rev. (2) **113** (1959), 1406–1413. MR0135530

[62] M. Lewin, P. T. Nam, and B. Schlein, *Fluctuations around Hartree states in the mean-field regime*, Amer. J. Math. **137** (2015), no. 6, 1613–1650, DOI 10.1353/ajm.2015.0040. MR3432269

[63] E. H. Lieb, *The Bose fluid*, in Lecture Notes in Theoretical Physics VIIC, W. E. Brittin, ed., University of Colorado Press, Boulder, CO, 1964, pp. 175–224.

[64] E. H. Lieb and R. Seiringer, *Proof of Bose-Einstein condensation for dilute trapped gasses*, Phys. Rev. Lett. **88** (2002), 170409.

[65] E. H. Lieb, R. Seiringer, J. P. Solovej, and J. Yngvanson, *The mathematics of the Bose gas and its condensation*, Oberwolfach Seminars, vol. 34, Birkhäuser Verlag, Basel, 2005. MR2143817

[66] E. H. Lieb, R. Seiringer, and J. Yngvanson, *Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional*, Phys. Rev. A **61** (2006), 043602.

[67] E. H. Lieb and J. P. Solovej, *Ground state energy of the one-component charged Bose gas*, Comm. Math. Phys. **217** (2001), no. 1, 127–163, DOI 10.1007/s002200000353. MR1815028

[68] D. Margetis, *Solvable model for pair excitation in trapped boson gas at zero temperature*, J. Phys. A **41** (2008), no. 38, 385002, 18, DOI 10.1088/1751-8113/41/38/385002. MR2438468

[69] D. Margetis, *Bose-Einstein condensation beyond mean field: many-body bound state of periodic microstructure*, Multiscale Model. Simul. **10** (2012), no. 2, 383–417, DOI 10.1137/110826576. MR2968845

[70] P. T. Nam, M. Napiórkowski, and J. P. Solovej, *Diagonalization of bosonic quadratic Hamiltonians by Bogoliubov transformations*, J. Funct. Anal. **270** (2016), no. 11, 4340–4368, DOI 10.1016/j.jfa.2015.12.007. MR3484973

[71] O. Penrose and L. Onsager, *Bose-Einstein condensation and liquid helium*, Phys. Rev. **104** (1956), 576–584.

[72] P. Pickl, *Derivation of the time dependent Gross-Pitaevskii equation without positivity condition on the interaction*, J. Stat. Phys. **140** (2010), no. 1, 76–89, DOI 10.1007/s10955-010-9981-0. MR2651439

[73] P. Pickl, *A simple derivation of mean field limits for quantum systems*, Lett. Math. Phys. **97** (2011), no. 2, 151–164, DOI 10.1007/s11005-011-0470-4. MR2821235

[74] L. P. Pitaevskii, *Vortex lines in an imperfect Bose gas*, Soviet Phys. JETP **13** (1961), 451–454.

[75] I. Rodnianski and B. Schlein, *Quantum fluctuations and rate of convergence towards mean field dynamics*, Comm. Math. Phys. **291** (2009), no. 1, 31–61, DOI 10.1007/s00220-009-0867-4. MR2530155

[76] D. Shale, *Linear symmetries of free boson fields*, Trans. Amer. Math. Soc. **103** (1962), 149–167. MR0137504

[77] V. Sohinger, *A rigorous derivation of the defocusing cubic nonlinear Schrödinger equation on* $\mathbb{T}^3$ *from the dynamics of many-body quantum systems*, Ann. Inst. H. Poincaré Anal. Non Linéaire **32** (2015), no. 6, 1337–1365, DOI 10.1016/j.anihpc.2014.09.005. MR3425265

[78] J. P. Solovej, *Many Body Quantum Mechanics*, Lecture Notes, Summer (2007). Available at http://www. mathematik.uni-muenchen.de/∼sorensen/Lehre/SoSe2013/MQM2/skript.pdf

[79] H. Spohn, *Kinetic equations from Hamiltonian dynamics: Markovian limits*, Rev. Modern Phys. **52** (1980), no. 3, 569–615, DOI 10.1103/RevModPhys.52.569. MR578142

[80] B. Vacchini and K. Hornberger, *Quantum linear Boltzmann equation*, Phys. Rep. **478** (2009), no. 4-6, 71–120, DOI 10.1016/j.physrep.2009.06.001. MR2562278

[81] J. von Neumann, *Mathematical foundations of quantum mechanics*, Princeton University Press, Princeton, 1955. Translated by Robert T. Beyer. MR0066944

[82] T. T. Wu, *Some nonequilibrium properties of a Bose system of hard spheres at extremely low temperatures*, J. Mathematical Phys. **2** (1961), 105–123. MR0121200

[83] T. T. Wu, *Bose-Einstein condensation in an external potential at zero temperature: General theory*, Phys. Rev. A **58** (1998), 1465–1474.

[84] K. Xu, Y. Liu, D. E. Miller, J. K. Chin, W. Setiawan, and W. Ketterle, *Observation of strong quantum depletion in a gaseous Bose-Einstein condensate*, Phys. Rev. Lett. **96** (2006), 180405 (4pp).