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MANY-BODY EXCITATIONS IN TRAPPED BOSE GAS: A NON-HERMITIAN APPROACH

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Abstract. We study a physically motivated model for a trapped dilute gas of Bosons with repulsive pairwise atomic interactions at zero temperature. Our goal is to describe aspects of the excited many-body quantum states of this system by accounting for the scattering of atoms in pairs from the macroscopic state. We start with an approximate many-body Hamiltonian, $\mathcal{H}_{\rm app}$, in the Bosonic Fock space. This $\mathcal{H}_{\rm app}$ conserves the total number of atoms. Inspired by Wu [J. Math. Phys. **2** (1961), 105–123], we apply a *non-unitary* transformation to $\mathcal{H}_{\rm app}$. Key in this procedure is the pair-excitation kernel, which obeys a nonlinear integro-partial differential equation. In the stationary case, we develop an existence theory for solutions to this equation by a variational principle. We connect this theory to a system of partial differential equations for one-particle excitation ("quasiparticle"-) wave functions derived by Fetter [Ann. Phys. **70** (1972), 67–101], and prove existence of solutions for this system. These wave functions solve an eigenvalue problem for a J-self-adjoint operator. From the non-Hermitian Hamiltonian, we derive a one-particle nonlocal equation for low-lying excitations, describe its solutions, and recover Fetter's energy spectrum. We also analytically provide an explicit construction of the excited eigenstates of the reduced Hamiltonian in the N-particle sector of Fock space.

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1. Introduction. In Bose-Einstein condensation (BEC) integer-spin particles (Bosons) occupy en masse a single-particle macroscopic quantum state, known as the condensate, at extremely low temperatures. The first experimental realizations of BEC in trapped atomic gases in 1995 [5,27] – nearly 80 years after its first prediction by Bose and Einstein – were the subject of the 2001 Nobel Prize in Physics [23,47]. Since 1995, the experimental and theoretical research in harnessing ultracold atomic gases has grown considerably. An emergent and far-reaching advance in applied physics is the highly precise manipulation of atoms by various means [20,21,25,34,73].

The dilute atomic gas is amenable to a systematic analysis mainly because of the length scale separation inherent to this system [55]. The following length scales are involved in this problem: (i) The low-energy scattering length, a, which expresses the strength of the atomic interactions and is positive for repulsively interacting atoms. (ii) The mean interatomic distance, ℓ, which is set by the mean density of the gas. (iii) The de Broglie wavelength, ℓ_{dB}, of each atom. For many experimental situations, it is reasonable to assume that $a \ll \ell \ll \ell_{\mathrm{dB}}$. If a trapping potential is applied externally, another length scale is the linear size of the trap, which can be of the same order as or larger than ℓ_{dB}. The gas diluteness is usually implied by the condition $a \ll \ell$, and a macroscopic quantum state may exist if $\ell \lesssim \ell_{\mathrm{dB}}$.

The realization of BEC in atomic gases has sparked various investigations in the modeling and analysis of nonlinear dynamics and out-of-equilibrium phenomena in Boson systems [17,20,56,57,59,64,72]. The usual mean field approach [68], which exclusively relies on the macroscopic wave function for the condensate, is often (but not always) employed. Despite the success of this approach for many phenomena, its limitations have been early recognized [75,76]. This mean field theory cannot capture, for example, the condensate depletion [78]. The modeling of such an effect requires a systematic description of many-body dynamics, in particular pair excitation [16,45,49,70,76,77].

In this paper, our goal is to describe the excited many-body eigenstates of an interacting system of Bosons in an external trapping potential by methods of partial differential equations (PDEs) and operator theory. Our approach yields results for spectral properties of non-self-adjoint operators and existence of solutions to previously unexplored PDEs for quantum excitations. We employ a physically motivated model: A Hamiltonian, denoted as $\mathcal{H}_{\mathrm{app}}$, that is quadratic in field operators for noncondensate atoms [76]. This $\mathcal{H}_{\mathrm{app}}$ commutes with the particle number operator; thus, the total number of particles is conserved. We formally construct $\mathcal{H}_{\mathrm{app}}$ from the full many-body Hamiltonian with a regularized interaction potential. By adopting the formulation of Wu [76,77] from the physics literature, we apply a non-unitary transformation to $\mathcal{H}_{\mathrm{app}}$. For stationary states, we rigorously study the *pair excitation kernel* k, a function of two spatial variables introduced by this transformation. This k expresses the scattering of atoms from the condensate in pairs; and obeys a nonlinear integro-partial differential equation which in operator form is a Riccati equation.

Notably, we develop an *existence theory* for the equation for k by a variational principle. Our treatment reveals a previously unnoticed connection of k to the one-particle excitation wave functions, u_j and v_j, introduced by Fetter [32]. These functions obey a system of linear PDEs, which had not been rigorously studied until now. Our analysis

sheds light on the existence of the eigenfunctions u_j and v_j, and eigenvalues E_j, for this system. By the non-Hermitian Hamiltonian that results from the transformed $\mathcal{H}_{\rm app}$, we derive a nonlocal PDE for phonon-like excitations; and express its solutions in terms of u_j and v_j. We relate the eigenvalues of this nonlocal PDE with E_j; and recover the excitation spectrum [32]. Our approach yields an explicit construction of the many-body eigenstates of $\mathcal{H}_{\rm app}$ in the sector of Fock space with a fixed number (N) of atoms.

Our tasks and results can be outlined as follows:

- Starting from a many-body Hamiltonian with positive and smooth interaction and trapping potentials, we formally apply an approximation scheme that leads to a simplified Hamiltonian, $\mathcal{H}_{\rm app}$. This Hamiltonian is a regularized version of a model invoked in physics [77].
- For stationary states, we apply a non-unitary transformation to $\mathcal{H}_{\rm app}$. A key ingredient is the pair excitation kernel, k.
- By constructing a functional of k and applying a variational principle, we prove the existence of solutions to the operator Riccati equation for k in an appropriate space. We indicate the possibility of multiple solutions, and distinguish the physically relevant, *unique* solution via a restriction on the operator norm of k.
- We provide an explicit construction of the eigenstates of $\mathcal{H}_{\rm app}$ in the N-particle sector of Fock space. We show that the spectrum of $\mathcal{H}_{\rm app}$ is positive and discrete.
- We show that the existence of solutions to the equation for k implies existence of solutions to the eigenvalue problem for the one-particle excitation wave functions u_j and v_j with a regularized interaction in [32]. For this purpose, we employ the theory of J-self-adjoint operators by Albeverio and coworkers [1–3, 24].
- Using the above non-unitary transformation, we derive a one-particle PDE ("phonon PDE") for excitations in the trapped Bose gas. We show that the point spectrum of the Schrödinger operator of the phonon PDE coincides with physically admissible eigenvalues E_j of the PDEs for (u_j, v_j), in agreement with [32].

A highlight of our work is the existence proof for the PDE system satisfied by the one-particle excitation wave functions u_j and v_j [32]. The pair excitation kernel k is a crucial ingredient of this proof. We believe that our analysis sheds light on the notion of the "quasiparticle" introduced in [32]. We describe a nontrivial connection between the non-Hermitian formulation of Wu [76] to the Hermitian view of Fetter [32] for low-lying excitations via the operator theory of Albeverio and coworkers [1–3, 24]; see Fig. 1.

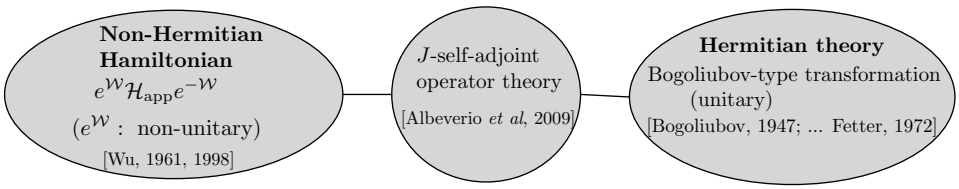

FIG. 1. Schematic on our results. We connect two physically inspired approaches (left and right panels) to the problem of excitations in the Bose gas via J-self-adjoint operator theory (central panel).

Our focus is on the analysis of PDEs that formally result from a non-unitary transformation of the approximate many-body Hamiltonian $\mathcal{H}_{\rm app}$ [76, 77]. This Hamiltonian is a starting point of our analysis, and can be derived heuristically from the full many-particle Hamiltonian. Our analysis invokes a regularized interaction potential and an external trapping potential which yields a decaying condensate wave function. The cases with delta function and Fermi pseudopotential interactions appear harder to address rigorously, and are not studied here. We also do not address the absence of a trap. We fix the total number of atoms at the value N, where N is large but finite. A rigorous justification for $\mathcal{H}_{\rm app}$ lies beyond our scope. We provide a plausibility argument for the extraction of the equation for k, but the analysis of solutions is placed on mathematically firm grounds. The thermodynamic limit ($N \to \infty$) is not treated here; see, e.g., [19, 54].

The non-unitarily transformed Hamiltonian, $\widetilde{\mathcal{H}}_{\rm app}$, has space-time reflection ($\mathcal{PT}$-) symmetry. We believe that there is an interesting connection of this non-Hermitian $\widetilde{\mathcal{H}}_{\rm app}$ to the $\mathcal{PT}$-symmetric quantum theories of Bender and coworkers; see, e.g., [6–12]. This connection should be further explored. Our analysis shows how $\widetilde{\mathcal{H}}_{\rm app}$ defines a physical theory of the Bose system. In particular, the spectrum of $\widetilde{\mathcal{H}}_{\rm app}$ is bounded below (thus, it is physically acceptable) if the operator norm of k is appropriately restricted (section 6). This key spectral property follows naturally from the existence and uniqueness of k.

In the remainder of this section, we discuss the motivation for and some particulars of our approach. The formalism of Fock space is outlined in section 2. The reader who wishes to skip these topics and directly read our main results is deferred to section 3.

1.1. *Motivation for the non-Hermitian view.* The following question may be raised: Why would one pursue a non-unitary transformation of a many-body Hamiltonian? After all, non-unitary transformations are often deemed as mathematically hard to deal with.

Our motivation is twofold. First, from a physics perspective, the formulation with the pair-excitation kernel is a natural extension of the systematic treatment by Lee, Huang and Yang for the setting of translation invariance and periodic boundary conditions [49]; see also [75]. The eigenvectors of the many-body Hamiltonian can be approximately described via the application of a non-unitary operator, $e^{-\mathcal{K}}$, to finite superpositions of tensor products of one-particle momentum ($\boldsymbol{p}$) states on the lattice [37, 49]. The operator $\mathcal{K}$ has the form [76]

$$\mathcal{K} = \frac{1}{2} \sum_{\boldsymbol{p} \neq 0} \alpha(\boldsymbol{p})\, a^*_{\boldsymbol{p}} a^*_{-\boldsymbol{p}} \,, \tag{1.1}$$

where $a_{\boldsymbol{p}}$ ($a^*_{\boldsymbol{p}}$) is the annihilation (creation) operator at one-particle momentum $\boldsymbol{p}$, $\boldsymbol{p} \in (2\pi/L)\mathbb{Z}^3$ and L is the linear size of the periodic box. The function $\alpha(\boldsymbol{p})$, where $\alpha : (2\pi/L)\mathbb{Z}^3 \to \mathbb{R}_+$, yields the phonon spectrum. The operator a_0 for the state of zero momentum (condensate) was replaced by $\sqrt{N}$ times the identity operator, which amounts to the Bogoliubov approximation [70].

Inspired by Wu's extension to the non-translation invariant setting [76, 77], for stationary states we consider a Hamiltonian that conserves the total number of atoms. We replace the exponent $\mathcal{K}$ by

$$\mathcal{W} = -(2N)^{-1} \iint_{\mathbb{R}^6} \mathrm{d}x\, \mathrm{d}y\; a^*_x a^*_y\, k(x,y)\, a(\overline{\phi})^2 \;.$$

Here, a_x^* is the Boson field creation operator at position x, ϕ denotes the wave function of the condensate, $a(\bar{\phi})$ is the Boson field annihilation operator for the state ϕ, $k(x,y) = k(y,x)$, and ϕ is assumed to be orthogonal to k. Since the operator $\mathcal{W}$ commutes with the particle number operator, $\mathcal{W}$ acts on the N-particle sector of Fock space. Thus, for fixed N, $e^{\mathcal{W}}$ *is a well-defined and bounded operator.* The kernel k obeys a nonlocal PDE [76,77]. We will prove the existence of stationary solutions to this PDE (section 5).

We also prove that the $\mathcal{W}$-based formulation, in conjunction with the effective Hamiltonian $\mathcal{H}_{\rm app}$ for pairs, yields the known excitation energy spectrum for the Bose gas, in agreement with other works, e.g., [32,54]. By using the kernel k, we transform the Hamiltonian $\mathcal{H}_{\rm app}$ non-unitarily and explicitly construct the excited many-body eigenstates in the N-particle sector of Fock space. We show that the non-unitary transformation implies a diagonalization scheme that has *upper triangular structure.* Our analysis clarifies how this structure emerges from the use of the operator $\mathcal{W}$ and the equation for k; see section 4.4 for a heuristic argument, and section 6 for more technical details.

Another reason for our non-Hermitian view is that this reveals previously unnoticed connections of the J-self-adjoint operator theory to phonon-like excitations in the trapped Bose gas. We identify the governing equation for k with an operator Riccati equation. This has been studied extensively by Albeverio and coworkers [1–3]; see also [24,48,74]. Our existence theory for k differs from the existence proofs in these works, which use a fixed-point argument. We establish that the excitation spectrum in [32] comes from the eigenvalue problem for a J-self-adjoint operator intimately connected to k (section 7).

1.2. *Related past works.* The quantum dynamics of the Bose gas has been the subject of numerous studies. It is impossible to exhaustively list the bibliography. For a broad view on Boson dynamics, the interested reader may consult [25,45,52,55,64,65,68,70,80].

Mean field limits of Boson dynamics are usually captured by nonlinear Schrödinger-type equations for the condensate wave function [36, 46, 64–66, 76]. Such limits have been rigorously derived from kinetic hierarchies in distinct scaling regimes for the atomic interactions [31, 68]. Our focus in the present paper is different. We primarily address the analysis of low-order PDEs that aim to provide corrections to mean field dynamics.

Second-order corrections to the mean field evolution have been studied through a Bogoliubov-type transformation [43, 44]. Although these works are inspired by Wu's theory [76,77], they are not strictly faithful to his formulation: In [43,44] the Hamiltonian is transformed unitarily; in contrast, in [76,77] the transformation is non-unitary.

The use of the pair-excitation kernel k can also be viewed as a means of improving error estimates for the time evolution of Bosons [45]. It was shown that a unitary transformation of the many-body Hamiltonian that involves k yields considerably improved Fock space estimates [40–44]. Because of the unitary transformation in [40–44], their PDE for k is different from the one in [76,77].

There are many other papers that tackle the problem of quantum fluctuations around the mean field limit and the excitation spectrum of the Bose gas in the mathematics literature [14, 15, 18, 22, 28–30, 53, 54, 58–62, 69, 71, 79]. A review of the challenges for the periodic setting is given in [70]. Regarding the ground state, an ansatz comes from applying the operator $\exp(-N^{-1}\mathcal{K}a_\phi^2)$, where $\mathcal{K}$ is defined in (1.1), to the tensor product $\otimes^N\phi$; see [30,71,79]. Central roles in many treatments of the excitation spectrum are

played by the Bogoliubov approximation and the Bogoliubov transformation [38, 54, 61]. In particular, in [54] Lewin and coworkers tackle aspects of this problem by use of an approximate Hamiltonian with a trapping potential via Fock space techniques in the limit $N \to \infty$. These works adopt a Hermitian view. In [29] the expectation of a quadratic many-body Hamiltonian is minimized over pure Gaussian states. This procedure causes elimination of terms that do not preserve the number of particles and leaves solely quasiparticle excitations [29]. However, there is no notion of a kernel in this formulation; thus, the connection of the exponential structure of the many-body eigenstates to the one-particle excitation wave functions u_j and v_j introduced in [32], which is an ingredient of our work here, is absent in [29].

In physics, the excitation spectrum of the Bose gas in non-translation invariant settings has been described by many authors; for reviews see, e.g. [4, 25, 36, 39, 51, 63–65, 67]. We are tempted to single out the works in [32–34] which use an intriguing PDE system relevant to our work here. The underlying many-body formulation relies on a unitary, Bogoliubov-type transformation of Boson field operators for noncondensate particles. This leads to a formula for the excitation spectrum in terms of the eigenvalues E_j of the PDE system [32]. This formalism is invoked in the modeling of phenomena such as phonon scattering [26] and condensate fluctuations [39].

1.3. *Paper organization.* In section 2, we introduce some notation and terminology. In section 3 we summarize our results. Section 4 focuses on the formal construction of the Hamiltonian $\mathcal{H}_{\text{app}}$, and the derivation of the equation for k. In section 5 we develop an existence theory for this equation. In section 6 we describe the excitation spectrum and construct the associated eigenvectors of $\mathcal{H}_{\text{app}}$. Section 7 addresses the connection of our theory to the PDEs derived heuristically in [32] and related properties of J-self-adjoint operators [2]. In section 8 we conclude our paper by discussing some implications.

2. Notation and terminology. In this section, we describe the basic formalism. In particular, we outline ingredients of the Fock space formalism, and the language of "second quantization" [13]. The interested reader may also consult [45].

- The symbol $\overline{f}$ denotes the complex conjugate of f, while A^* stands for the Hermitian adjoint of operator A. The symbol $\overline{A}$ indicates the operator which acts according to $\overline{A}[f] = \overline{\{A[f]\}}$ for all functions f in the domain of A.
- In the symbol $\int$ the integration region is $\mathbb{R}^3$ (for $\int \mathrm{d}x$) or $\mathbb{R}^3 \times \mathbb{R}^3$ (for $\int \mathrm{d}x\,\mathrm{d}y$).
- The (symmetric) inner product of complex-valued $f, g \in L^2(\mathbb{R}^3)$ is defined by

$$\langle \overline{f}, g \rangle = \int \mathrm{d}x \, \left\{ \overline{f(x)}\, g(x) \right\} .$$

  The respective inner product of complex-valued $f, g \in L^2_V(\mathbb{R}^3)$ is $\langle \overline{f}, Vg \rangle$ for positive external potential $V(x)$. The L^2-norm of f is denoted $\|f\|_2$. For some operator k, the (symmetric) inner product of $f(x)$ and $k(x, g)$ is denoted $\big\langle f, k(\cdot, g) \big\rangle$.
- Function spaces on $\mathbb{R}^d$ (e.g., $d = 3$) are denoted by lowercase gothic letters, viz.,

$$\mathfrak{h}(\mathbb{R}^d) := L^2(\mathbb{R}^d) , \quad \mathfrak{h}^1(\mathbb{R}^d) := H^1(\mathbb{R}^d) , \quad \mathfrak{h}^1_V(\mathbb{R}^d) := H^1(\mathbb{R}^d) \cap L^2_V(\mathbb{R}^d) .$$

  We write $\mathfrak{h}$, $\mathfrak{h}^1$, $\mathfrak{h}^1_V$ for these spaces if $d = 3$. As an exception to this notation, we define $\phi^\perp := \left\{ e \in \mathfrak{h}^1_V \;\middle|\; e \perp \phi \right\}$ where $\phi \in \mathfrak{h}^1$ is the condensate wave function.

- For a given ordered set $\{e_j(x)\}_j \subset \mathfrak{h}$, we occasionally use the symbol $\langle A\rangle_j$ for the inner product $\langle e_j, a(\cdot, e_j)\rangle$, taking $A := a(x,y)$.
- The symbol $(\upsilon * g)(x)$ denotes the convolution integral $\int \mathrm{d}y\, \upsilon(x-y)g(y)$.
- The space of bounded linear operators on $\mathfrak{h}$ is denoted $\mathfrak{B}(\mathfrak{h})$, with norm $\|\cdot\|_{\mathrm{op}}$. Also, the space of trace-class operators on $\mathfrak{h}$ is denoted $\mathfrak{B}_1(\mathfrak{h})$ with norm

$$\|A\|_{\mathfrak{B}_1(\mathfrak{h})} = \|A\|_1 = \mathrm{tr}\,|A| \ , \quad \forall, A \in \mathfrak{B}_1(\mathfrak{h}) \ .$$

  Similarly, the space of Hilbert-Schmidt operators on $\mathfrak{h}$ is $\mathfrak{B}_2(\mathfrak{h})$ with norm

$$\|A\|_{\mathfrak{B}_2(\mathfrak{h})} = \|A\|_2 = (\mathrm{tr}\,|A^*A|)^{1/2} \ , \quad \forall A \in \mathfrak{B}_2(\mathfrak{h}) \ .$$

  The space of compact operators on $\mathfrak{h}$ is $\mathfrak{B}_0(\mathfrak{h})$. Note the inequalities

$$\|A\|_{\mathrm{op}} \leq \|A\|_2 \leq \|A\|_1 \ ,$$

  and the inclusions $\mathfrak{B}_1(\mathfrak{h}) \subseteq \mathfrak{B}_2(\mathfrak{h}) \subseteq \mathfrak{B}_0(\mathfrak{h}) \subseteq \mathfrak{B}(\mathfrak{h})$.
- We express operators on $\mathfrak{h}$ by use of their integral kernels which we denote by lowercase greek or roman letters. For example, we employ the expression $\delta(x,y)$, in place of $\delta(x-y)$, of the Dirac mass for the identity operator. In this vein, an effective one-particle Hamiltonian of interest is denoted by the singular kernel

$$h(x,y) := \big\{ -\Delta + V(x) + N(\upsilon * |\phi|^2)(x)\big\}\delta(x,y) + N\phi(x)\upsilon(x-y)\overline{\phi(y)} - \mu\delta(x,y) \ ,$$

  where $\phi(x)$ is the condensate wave function, $V(x)$ is the trapping potential, $\upsilon(x)$ is the two-body interaction potential, and μ is a constant. Another example of notation is $k(x,y)$ for the pair-excitation operator. We use the superscript 'T' for a kernel to denote its transpose. The star $(*)$ as a superscript indicates the adjoint kernel, $k^*(x,y) = \overline{k(y,x)}$. We write $k \in \mathfrak{S}$ to mean that the operator with integral kernel k belongs to the space $\mathfrak{S}$, e.g., for $\mathfrak{S} = \mathfrak{B}_2(\mathfrak{h})$.
- The composition of operators h and k is expressed by

$$(h \circ k)(x,y) := \int \mathrm{d}x' \left\{h(x,x')k(x',y)\right\} \ .$$

- If a bounded operator $k \in \mathfrak{B}(\mathfrak{h})$ acts on $f \in \mathfrak{h}$, the result is the function

$$k(x\,, f) := \int \mathrm{d}x' \left\{k(x,x')f(x')\right\} \ , \quad \text{or} \quad k(f,x') := \int \mathrm{d}x \left\{f(x)k(x,x')\right\} \ .$$

  The same notation is used for kernels corresponding to unbounded operators, with the understanding that the domain of such an operator is defined properly.
- For $f, g \in \mathfrak{h}$ the tensor-product operator corresponding to integral kernel $f(x)\overline{g(x')}$ is sometimes expressed as $f \otimes g$. The symmetrized tensor product of f, g is

$$f \otimes_{\mathrm{s}} g := \frac{1}{\sqrt{2}}\big\{f \otimes g + g \otimes f\big\} \ .$$

- For the condensate wave function $\phi \in \mathfrak{h}$ with L^2-norm $\|\phi\|_2 = 1$, the projection operator $\widehat{\delta} : \mathfrak{h} \to \mathfrak{h}$ is defined by

$$\widehat{\delta}(x,y) = \delta(x,y) - \phi(x)\overline{\phi(y)} \ .$$

- The Bosonic Fock space $\mathbb{F}$ is a direct sum of n-particle symmetric L^2-spaces, viz.,

$$\mathbb{F} = \bigoplus_{n=0}^{\infty} \mathbb{F}_n \ ; \quad \mathbb{F}_0 = \mathbb{C} \ , \quad \mathbb{F}_n = L^2_s(\mathbb{R}^{3n}) \text{ if } n \geq 1 \ .$$

  Hence, vectors in $\mathbb{F}$ are described as sequences $\{u^n\}$ of n-particle wave functions where $u^n \in L^2_s(\mathbb{R}^{3n})$, $n \geq 0$. The inner product of $|u\rangle = \{u^n\}, |w\rangle = \{w^n\} \in \mathbb{F}$ is

$$\langle u, w\rangle_{\mathbb{F}} := \sum_{n=0}^{\infty} \langle \overline{u}^n, w^n \rangle_{L^2(\mathbb{R}^{3n})} \ ,$$

  which induces the norm $\||u\rangle\| = \sqrt{\langle u, u\rangle_{\mathbb{F}}}$. We employ the braket notation for Schrödinger state vectors in $\mathbb{F}$ to distinguish them from wave functions in $L^2_s(\mathbb{R}^{3n})$. We often write the inner product of $|u\rangle$ with $\mathcal{A}|w\rangle$ ($\mathcal{A} : \mathbb{F} \mapsto \mathbb{F}$) as $\langle u|\mathcal{A}|w\rangle$. The vacuum state in $\mathbb{F}$ is $|vac\rangle := \{1, 0, 0, \dots\}$, where the unity is placed in the zeroth slot. A symmetric N-particle wave function, $\psi_N \in L^2_s(\mathbb{R}^{3N})$, has a natural embedding into $\mathbb{F}$ given by $|\psi\rangle_N = \{0, 0, \dots, \psi_N(x), 0, \dots\}$, where $\psi_N(x)$ is in the N-th slot. The set of such state vectors $|\psi\rangle_N$ is $\mathbb{F}_N$, the 'N-th fiber' (N-particle sector) of $\mathbb{F}$. We sometimes omit the subscript 'N' in $|\psi\rangle_N$.
- A Hamiltonian on $L^2_s(\mathbb{R}^{3N})$ admits an extension to an operator on $\mathbb{F}$. This extension is carried out via the Bosonic field operator a_x and its adjoint, a^*_x, which are indexed by the spatial coordinate $x \in \mathbb{R}^3$. To define these field operators, first consider the annihilation and creation operators for a one-particle state $f \in \mathfrak{h}$, denoted by $a(\overline{f})$ and $a^*(f)$. These operators act on $|u\rangle = \{u^n\} \in \mathbb{F}$ according to

$$\big(a(\overline{f})|u\rangle\big)^n := \sqrt{n+1} \int \mathrm{d}x \, \overline{f(x)} \, u^{n+1}(x, x_2, \dots, x_n) \ ,$$

$$\big(a^*(f)|u\rangle\big)^n := \frac{1}{\sqrt{n}} \sum_{j \leq n} f(x_j) \, u^{n-1}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n) \ .$$

  We often use the symbols $a_{\overline{f}} := a(\overline{f})$ and $a^*_f := a^*(f)$. Also, given an orthonormal basis, $\{e_j(x)\}_j \subset \mathfrak{h}$, we will write a^*_j in place of $a^*(e_j)$ and a_j in place of $a(\overline{e_j})$.
- The Boson field operators a^*_x, a_x are implicitly defined via the integrals

$$a^*_f = \int \mathrm{d}x \left\{ f(x) \, a^*_x \right\} \ , \quad a_{\overline{f}} = \int \mathrm{d}x \left\{ \overline{f(x)} \, a_x \right\} \ .$$

  By the orthonormal basis $\{e_j(x)\}_j$, the field operators are expressed by

$$a^*_x = \sum_j e_j(x) \, a^*_j \ , \quad a_x = \sum_j \overline{e_j(x)} \, a_j \ .$$

  The canonical commutation relations $[a_x, a^*_y] = \delta(x-y)$, $[a_x, a_y] = 0$ then follow.
- The Boson field operators orthogonal to the condensate $\phi \in \mathfrak{h}$ are defined by

$$a_{\perp,x} = \int \mathrm{d}y \left\{ \widehat{\delta}(x,y) a_y \right\} = \int \mathrm{d}y \left\{ a_y \widehat{\delta}^T(y,x) \right\} \ ,$$

$$a^*_{\perp,x} = \int \mathrm{d}y \left\{ \widehat{\delta}^T(x,y) a^*_y \right\} = \int \mathrm{d}y \left\{ a^*_y \widehat{\delta}(y,x) \right\} \ .$$

  We can decompose the Boson field operators according to the equations

$$a_x = a_{\perp,x} + \phi(x) a_{\overline{\phi}} \ , \quad a^*_x = a^*_{\perp,x} + \overline{\phi(x)} a^*_{\phi} \ . \tag{2.1}$$

It is worthwhile to notice the commutation relations

$$\left[a_{\perp,x}, a^*_{\perp,y}\right] = \widehat{\delta}(x,y)\ ,\ \left[a^*_{\perp,x}, a_{\perp,y}\right] = -\widehat{\delta}^T(x,y)\ ,\ \left[a_{\overline{\phi}}, a^*_{\perp,x}\right] = \left[a_{\perp,x}, a^*_{\phi}\right] = 0\ .$$

- Fock space operators such as $\mathcal{H}$ are primarily denoted by calligraphic letters. Exceptions include annihilation and creation operators such as a_x, a^*_x, $a_{\perp,x}$, $a^*_{\perp,x}$; and $a_{\overline{\phi}}, a^*_{\phi}$ as well as a_j, a^*_j associated with the basis $\{e_j(x)\}_j \subset \mathfrak{h}$.
- We use symbols such as $h(a^*_\perp, a_\perp)$ and $\overline{f_\phi}(a_\perp, a_\perp)$ to denote operators on $\mathbb{F}$ of the form $\int \mathrm{d}x\,\mathrm{d}y\,\{a^*_{\perp,x} h(x,y) a_{\perp,y}\}$ and $\int \mathrm{d}x\,\mathrm{d}y\,\{a_{\perp,x}\overline{f_\phi(x,y)}a_{\perp,y}\}$, respectively, for suitably defined kernels $h(x,y)$ and $f_\phi(x,y)$.
- Functionals on Banach spaces are often denoted also by calligraphic letters.

3. Hamiltonian model and main results. In this section, we define the many-body Hamiltonian, and summarize our results and approach. The starting point is the many-body Hamiltonian on $\mathbb{F}$, viz.,

$$\mathcal{H} = \int \mathrm{d}x\,\mathrm{d}y\,\left\{a^*_x \epsilon(x,y) a_y + \frac{1}{2} a^*_x a^*_y \upsilon(x-y) a_x a_y\right\}\ , \tag{3.1}$$

where $\epsilon(x,y) = \{-\Delta_x + V(x)\}\,\delta(x,y)$ is the kinetic part, $\upsilon(x)$ is the pairwise interaction potential, and $V(x)$ is the trapping potential. We set $d = 3$, and assume that $\upsilon(x)$ is positive, symmetric, integrable and bounded on $\mathbb{R}^3$. The trapping potential $V(x)$ is positive, smooth and grows as $|x|^s$ for sufficiently large $|x|$ where $s > 0$. This assumption about V implies that the one-particle Schrödinger operator $-\Delta + V$ has discrete spectrum.

3.1. *Reduced Hamiltonian and operator Riccati equation for k.* Section 4 describes Wu's approach [77] in a language closer to operator theory, which serves our objectives. By heuristics, we reduce Hamiltonian (3.1) to the quadratic form

$$\mathcal{H}_{\mathrm{app}} = N E_{\mathrm{H}} + h(a^*_\perp, a_\perp) + \frac{1}{2N} f_\phi(a^*_\perp, a^*_\perp) a^2_{\overline{\phi}} + \frac{1}{2N}\overline{f_\phi}(a_\perp, a_\perp) {a^*_\phi}^2\ ,$$

where E_H is the (mean field) Hartree energy per particle and ϕ is the condensate wave function; see section 4.1. Our derivation of the reduced Hamiltonian $\mathcal{H}_{\mathrm{app}}$ relies on (2.1) and the conservation of the total number of particles. Our goal is to solve the eigenvalue problem $\mathcal{H}_{\mathrm{app}}|\psi\rangle = E_N|\psi\rangle$.

We transform $\mathcal{H}_{\mathrm{app}}$ non-unitarily according to $\widetilde{\mathcal{H}}_{\mathrm{app}} := e^{\mathcal{W}} \mathcal{H}_{\mathrm{app}} e^{-\mathcal{W}}$ where the operator $\mathcal{W}$ is of the form $-(2N)^{-1}\int \mathrm{d}x\,\mathrm{d}y\ \{k(x,y)\, a^*_{\perp,x} a^*_{\perp,y}\} a^2_{\overline{\phi}}$ which conserves the total number of particles; see section 4.2. The Riccati equation for kernel k is extracted via the requirement that the non-Hermitian operator $\widetilde{\mathcal{H}}_{\mathrm{app}}$ does *not* contain any terms with the product $a^*_\perp a^*_\perp$; see section 4.3. If $k(x,\overline{\phi}) = 0$, the Riccati equation for k reads

$$h \circ k + k \circ h^T + f_\phi + k \circ \overline{f_\phi} \circ k = \lambda \otimes_{\mathrm{s}} \phi\ .$$

The Lagrange multiplier λ is determined self-consistently.

3.2. *Existence theory for k.* In section 5, we introduce a functional of $\overline{k}$ and k by use of which we develop an existence theory. This functional, $\mathcal{E}[\overline{k}, k] : \mathrm{dom}(\mathcal{E}) \to \mathbb{R}$, reads

$$\mathcal{E}[\overline{k}, k] := \mathrm{tr}\left\{\left(\delta - \overline{k} \circ k\right)^{-1} \circ \left(\overline{k} \circ h \circ k + \frac{1}{2}\overline{k} \circ f_\phi + \frac{1}{2}\overline{f_\phi} \circ k\right)\right\}\ ;$$

see section 5.1 for the definition of $\mathrm{dom}(\mathcal{E})$. Setting the functional derivative of $\mathcal{E}[\overline{k}, k]$ with respect to $\overline{k}$ equal to zero yields the Riccati equation for k.

We prove the existence of solutions to the Riccati equation for k by assuming that

$$h(\overline{e}, e) - \left|f_\phi(\overline{e}, \overline{e})\right| \geq c\|e\|_{L^2}^2 \qquad \forall e \in \phi^\perp = \left\{e \in \mathfrak{h}_V^1 \;\middle|\; e \perp \phi\right\} .$$

This condition is satisfied if ϕ is a minimizer of the Hartree energy, E_H. The aforementioned inequality is employed as a hypothesis in the main existence theorem, Theorem 5.7 (section 5.2). In fact, Theorem 5.7 states that the above inequality and the property that f_ϕ is Hilbert-Schmidt imply that the functional $\mathcal{E}$ restricted to $\mathrm{dom}(\mathcal{E})_\perp = \mathrm{dom}(\mathcal{E}) \cap \{k \in \mathfrak{B}_2(\mathfrak{h}_V^1) \,\big|\, k(x, \overline{\phi}) = 0\}$ attains a minimum for some $k \in \mathrm{dom}(\mathcal{E})_\perp$ which is a weak solution to the operator Riccati equation. We emphasize that ϕ does not need to be a minimizer of the Hartree energy. Our proof makes use of a basis of $\phi^\perp$, the theory of complex ($\mathcal{C}$-) symmetric operators and a variational principle based on functional $\mathcal{E}$. Notably, in section 5.3 we discuss the possible non-uniqueness of solutions to the Riccati equation.

3.3. *Spectrum and eigenvectors of reduced non-Hermitian Hamiltonian.* In section 6, we study the eigenvectors and spectrum of the non-unitarily transformed Hamiltonian $\widetilde{\mathcal{H}}_{\mathrm{app}}$, under the assumptions of Theorem 5.7 for k. A highlight of our analysis is the explicit construction of these eigenvectors in $\mathbb{F}_N$ by Fock space techniques. We write $\widetilde{\mathcal{H}}_{\mathrm{app}} = NE_H + \mathcal{H}_{\mathrm{ph}}$ where

$$\mathcal{H}_{\mathrm{ph}} := h_{\mathrm{ph}}(a_\perp^*, a_\perp) + \frac{1}{N}(a_\phi^*)^2 \overline{f_\phi}(a_\perp, a_\perp) \; ;$$
$$h_{\mathrm{ph}}(a_\perp^*, a_\perp) := \int \mathrm{d}x\, \mathrm{d}y \; \{a_{\perp,x}^*(h + k \circ \overline{f_\phi})(x, y) a_{\perp,y}\} \; .$$

Evidently, $h_{\mathrm{ph}}(a_\perp^*, a_\perp)$ forms the diagonal part of $\widetilde{\mathcal{H}}_{\mathrm{app}}$. We show that h_{ph} is responsible for the discrete phonon-like excitation spectrum of the trapped Bose gas.

The main result is captured by Theorem 6.1, which asserts an equality of spectra, viz.,

$$\sigma\left(\mathcal{H}_{\mathrm{ph}}\big|_{\mathbb{F}_N}\right) = \sigma\left(h_{\mathrm{ph}}(a_\perp^*, a_\perp)\big|_{\mathbb{F}_N}\right) \; .$$

Furthermore, in this theorem we show that for every eigenvector of $h_{\mathrm{ph}}(a_\perp^*, a_\perp)$ with eigenvalue E there is a unique eigenvector of $\mathcal{H}_{\mathrm{ph}}$ with the same eigenvalue, E.

Our analysis is based on the following steps. First, we provide a formalism for the decomposition of $\mathbb{F}_N$ into appropriate orthogonal subspaces (section 6.1). Our technique is similar in spirit to that in the construction by Lewin, Nam, Serfaty and Solovej [54]. However, here we consider the eigenvectors of a Hamiltonian that conserves the number of particles as opposed to the Bogoliubov Hamiltonian studied in [54]. Second, we invoke k explicitly and show that by the restriction $\|k\|_{\mathrm{op}} < 1$, the spectrum of the one-particle Schrödinger-type operator h_{ph} is positive and discrete, and the corresponding eigenfunctions form a non-orthogonal Riesz basis of $\phi^\perp$ (section 6.2). The proof of the main theorem (Theorem 6.1) relies on the above steps to show that the eigenvalue problem for $\mathcal{H}_{\mathrm{ph}}$ can be reduced to a finite-dimensional system of equations that has an upper triangular structure (section 6.3).

3.4. *Connection to Hermitian approach.* In section 7, we compare our approach to Fetter's formulation [32] which makes use of Bogoliubov rotations. We prove the existence of solutions to a PDE system for one-particle excitation wave functions, which reduces to the system in [32] when the pairwise interaction potential $v(x)$ is replaced by $g\delta(x)$ for some constant $g > 0$. We discuss the connection of the Riccati equation for k to the theory of J-self-adjoint matrix operators by Albeverio and coworkers [1–3].

Starting with the relevant Bogoliubov Hamiltonian [32], we discuss that its diagonalization via quasiparticle operators (in Fetter's terminology) leads to the PDE system

$$\begin{pmatrix} h_\perp^T & -f_{\phi\perp} \\ \overline{f_{\phi\perp}} & -h_\perp \end{pmatrix} \circ \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} = E_j \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} \qquad (j = 1, 2, \ldots)$$

for the one-particle wave functions u_j and v_j and respective eigenvalues E_j (section 7.1). Here, $q_\perp$ ($q = h, f_\phi$) is the projection of operator q on space $\phi^\perp$. We show that the existence of solutions to the Riccati equation for k implies the solvability of the above system for (u_j, v_j); see section 7.2. We also prove that the completeness relations between u_j and v_j, posed heuristically in [32], directly follow from our approach. In section 7.3, we invoke ideas from J-self-adjoint operator theory to show that the restriction $\|k\|_{\mathrm{op}} < 1$ yields a positive spectrum $\{E_j\}_{j=1}^\infty$ for the symplectic matrix of the system for (u_j, v_j).

4. Formal construction of reduced many-body Hamiltonian. In this section, we formally construct the (Hermitian) Hamiltonian $\mathcal{H}_{\mathrm{app}}$ for pair excitation which is quadratic in the Boson field operators for noncondensate atoms, and transform it non-unitarily. A core ingredient of this approach is that the number of atoms is strictly conserved, in the sense that $[\mathcal{H}_{\mathrm{app}}, \mathcal{N}] = 0$ where $\mathcal{N}$ is the particle number operator on $\mathbb{F}$. We follow the physics model of Wu [77] but replace the delta function potential $\delta(x-y)$ for repulsive atomic interactions by the smooth potential $v(x-y)$; cf. (3.1).

Section 4.1 focuses on heuristic approximations in the Hermitian setting. Section 4.2 concerns the non-unitary transformation of the approximate Hamiltonian $\mathcal{H}_{\mathrm{app}}$. In section 4.3, we derive an operator Riccati equation for the kernel of the transformation. Section 4.4 provides some remarks on validity of the approximations involved.

4.1. *Heuristics: Approximation of many-body Hamiltonian.* We start with Hamiltonian (3.1). Let ϕ denote the (one-particle) condensate wave function, which has L^2-norm $\|\phi\|_2 = 1$. Recall decomposition (2.1) for the Boson field operators a_x, a_x^*. The operator $\mathcal{N}$ on $\mathbb{F}$ can thus be decomposed as

$$\mathcal{N} = \int \mathrm{d}x \, \{a_x^* a_x\} = a_\phi^* a_{\overline{\phi}} + \int \mathrm{d}x \, \{a_{\perp,x}^* a_{\perp,x}\} =: \mathcal{N}_\phi + \mathcal{N}_\perp \ ,$$

where $\mathcal{N}_\phi := a_\phi^* a_{\overline{\phi}}$ is the number operator for condensate atoms; $\mathcal{N}_\phi$ and $\mathcal{N}_\perp$ commute, and $\mathcal{H}$ commutes with $\mathcal{N}$. We use the N-th fiber, $\mathbb{F}_N$, of the Bosonic Fock space, considering state vectors $|\psi\rangle_N$ that satisfy

$$\mathcal{N}|\psi\rangle_N = N|\psi\rangle_N \ ; \qquad \langle\psi|\psi\rangle = 1 \ .$$

Following Wu [76] we first expand $\mathcal{H}$ is powers of $a_{\perp,x}$, $a^*_{\perp,x}$ by applying decomposition (2.1) for a_x, a^*_x. The Hamiltonian $\mathcal{H}$ reads

$$\begin{aligned}
\mathcal{H} = &\int \mathrm{d}x\,\mathrm{d}y\ \left\{\overline{\phi(x)}\epsilon(x,y)\phi(y) + \frac{1}{2}(\mathcal{N}_\phi - 1)|\phi(x)|^2 \upsilon(x-y)|\phi(y)|^2\right\}\mathcal{N}_\phi \\
&+ \int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}\Big(\epsilon(x,y)\phi(y) + (\mathcal{N}_\phi - 1)\phi(x)\upsilon(x-y)|\phi(y)|^2\Big)a_{\overline{\phi}}\right\} \\
&+ \int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\phi}\Big(\overline{\phi(x)}\epsilon(x,y) + (\mathcal{N}_\phi - 1)\overline{\phi(y)}\upsilon(x-y)|\phi(x)|^2\Big)a_{\perp,y}\right\} \\
&+ \int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}\Big(\epsilon(x,y) + \mathcal{N}_\phi\,(\upsilon * |\phi|^2)(x)\,\delta(x,y) + \mathcal{N}_\phi\phi(x)\upsilon(x-y)\overline{\phi(y)}\Big)a_{\perp,y}\right\} \\
&+ \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}a^*_{\perp,y}\phi(x)\upsilon(x-y)\phi(y)a^2_{\overline{\phi}} + {a^*_\phi}^2\overline{\phi(x)}\upsilon(x-y)\overline{\phi(y)}a_{\perp,x}a_{\perp,y}\right\} \\
&+ \int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}a^*_{\perp,y}\upsilon(x-y)\phi(y)a_{\perp,x}a_{\overline{\phi}} + a^*_\phi a^*_{\perp,x}\overline{\phi(y)}\upsilon(x-y)a_{\perp,x}a_{\perp,y}\right\} \\
&+ \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}a^*_{\perp,y}\upsilon(x-y)a_{\perp,x}a_{\perp,y}\right\}\ .
\end{aligned}$$

Recall that $\epsilon(x,y) = \{-\Delta_x + V(x)\}\,\delta(x,y)$.

The next step is to reduce $\mathcal{H}$ to a Hermitian operator quadratic in $a_\perp$, $a^*_\perp$. First, we drop the terms that are cubic or quartic in $a_\perp$, $a^*_\perp$. Second, we make the substitution $\mathcal{N}_\phi = \mathcal{N} - \mathcal{N}_\perp$ and replace $\mathcal{N}$ by N ($\mathcal{N} \mapsto N$ with $N \gg 1$) because $|\psi\rangle \in \mathbb{F}_N$. We then drop the term $\mathcal{N}_\perp^2$. We take $N - 1 \simeq N$ and *apply a Hartree-type equation* for the condensate wave function ϕ which we write as

$$\int \mathrm{d}y\ \left\{\epsilon(x,y)\phi(y) + N\phi(x)\upsilon(x-y)|\phi(y)|^2\right\} - \mu\phi(x) = 0\ .$$

This results in the elimination of terms linear in $a_\perp$, $a^*_\perp$ in the Hamiltonian $\mathcal{H}$. The multiplier μ enables us to impose the normalization constraint $\|\phi\|_2 = 1$; thus,

$$\mu = \int \mathrm{d}x\,\mathrm{d}y\ \left\{\overline{\phi(x)}\epsilon(x,y)\phi(y) + N|\phi(x)|^2\upsilon(x-y)|\phi(y)|^2\right\}\ .$$

The PDE for ϕ formally becomes the Gross-Pitaevskii equation [46,65,66] if υ is replaced by $g\delta$, the delta function interaction, for some constant $g > 0$.

Consequently, the original Hamiltonian $\mathcal{H}$ is reduced to the quadratic form

$$\mathcal{H}_{\mathrm{app}} = NE_{\mathrm{H}} + h(a^*_\perp, a_\perp) + \frac{1}{2N}f_\phi(a^*_\perp, a^*_\perp)a^2_{\overline{\phi}} + \frac{1}{2N}\overline{f_\phi}(a_\perp, a_\perp){a^*_\phi}^2, \tag{4.1a}$$

where, abusing notation slightly, we define the operators

$$h(a^*_\perp, a_\perp) := \int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}h(x,y)a_{\perp,y}\right\}\ , \tag{4.1b}$$

$$f_\phi(a^*_\perp, a^*_\perp) := \int \mathrm{d}x\,\mathrm{d}y\ \left\{a^*_{\perp,x}f_\phi(x,y)a^*_{\perp,y}\right\}\ , \tag{4.1c}$$

along with the corresponding kernels

$$h(x,y) := \epsilon(x,y) + N(\upsilon * |\phi|^2)(x)\,\delta(x,y) + N\gamma(x,y) - \mu\,\delta(x,y)\ , \tag{4.1d}$$

$$f_\phi(x,y) := N\phi(x)\upsilon(x-y)\phi(y)\ , \quad \gamma(x,y) := \phi(x)\upsilon(x-y)\overline{\phi(y)}\ . \tag{4.1e}$$

In the above, the Hartree energy functional, $E_{\rm H}$, is defined by

$$E_{\rm H} = \int {\rm d}x\, {\rm d}y\ \left\{ \overline{\phi(x)} \epsilon(x,y) \phi(y) + \frac{N}{2} |\phi(x)|^2 v(x-y) |\phi(y)|^2 \right\}\ .$$

Equation (4.1a) is the desired reduced Hamiltonian. Note the key property $[\mathcal{H}_{\rm app}, \mathcal{N}] = 0$.

4.2. *Non-unitary transformation.* In this subsection, we transform $\mathcal{H}_{\rm app}$ non-unitarily by use of the pair-excitation kernel, k. The result is given by (4.3a) and (4.3b) below.

For this purpose, we invoke the following quadratic operator:

$$\mathcal{K} := -\frac{1}{2} \int {\rm d}x\, {\rm d}y\ \left\{ k(x,y) a^*_{\perp,x} a^*_{\perp,y} \right\}\ , \tag{4.2a}$$

where $k = k^T$. This $\mathcal{K}$ does not conserve the number of particles ($[\mathcal{K}, \mathcal{N}] \neq 0$). In addition, following Wu, [76] we introduce the operator

$$\mathcal{W} := -\frac{1}{2N} \int {\rm d}x\, {\rm d}y\ \{ k(x,y) a^*_{\perp,x} a^*_{\perp,y} \} (a_{\overline{\phi}})^2 = \frac{1}{N} \mathcal{K} (a_{\overline{\phi}})^2\ . \tag{4.2b}$$

The kernel k is not known at this stage, but must satisfy certain consistency conditions (see section 4.3). We refrain from specifying the function space of k now. A salient point of this formulation is the identity $[\mathcal{W}, \mathcal{N}] = 0$. Consequently, the operator $e^{\mathcal{W}}$, which is used to define the non-unitary transformation of $\mathcal{H}_{\rm app}$ below, leaves $\mathbb{F}_N$ invariant, i.e., $e^{\mathcal{W}} : \mathbb{F}_N \mapsto \mathbb{F}_N$. In addition, $e^{\mathcal{W}}$ is bounded on $\mathbb{F}_N$. (However, $e^{\mathcal{W}}$ does not respect the Fock space norm.) Our goal here is to describe the non-Hermitian operator $e^{\mathcal{W}} \mathcal{H}_{\rm app} e^{-\mathcal{W}}$.

The main idea concerning the proposed non-unitary transformation of $\mathcal{H}_{\rm app}$ can be described as follows. Assume that $|\psi\rangle_N = |\psi\rangle$ ($|\psi\rangle \in \mathbb{F}_N$) is an eigenvector of the (Hermitian) Hamiltonian $\mathcal{H}_{\rm app}$ with eigenvalue E, viz., $\mathcal{H}_{\rm app} |\psi\rangle = E |\psi\rangle$. We have

$$\left\{ e^{\mathcal{W}} \mathcal{H}_{\rm app} e^{-\mathcal{W}} \right\} \left(e^{\mathcal{W}} |\psi\rangle \right) = E \left(e^{\mathcal{W}} |\psi\rangle \right)\ .$$

Hence, the non-Hermitian, non-unitarily transformed, operator $e^{\mathcal{W}} \mathcal{H}_{\rm app} e^{-\mathcal{W}}$ has eigenvalue E and eigenvector $e^{\mathcal{W}} |\psi\rangle$. It turns out that the description of the transformed eigenvector $e^{\mathcal{W}} |\psi\rangle$ in $\mathbb{F}_N$ leads to an upper triangular system, which offers an interesting alternative to the approach based on the Bogoliubov transformation [70]. To understand this point, we will study spectral properties of $e^{\mathcal{W}} \mathcal{H}_{\rm app} e^{-\mathcal{W}}$. A price that one must pay for this option is that the kernel k must satisfy the operator Riccati equation. One of our goals here is to motivate the equation obeyed by k through the explicit computation of the non-Hermitian operator $e^{\mathcal{W}} \mathcal{H}_{\rm app} e^{-\mathcal{W}}$.

Next, we organize our calculation. First, we readily compute the conjugation

$$e^{\mathcal{W}} a_{\perp,x} e^{-\mathcal{W}} = a_{\perp,x} + \frac{1}{N} \widehat{k^T}(a^*_\perp, x) \left(a_{\overline{\phi}} \right)^2\ ,$$

where (abusing notation) we define

$$\widehat{k^T}(x,y) := \int {\rm d}z\ \left\{ k(x,z) \widehat{\delta^T}(z,y) \right\}\ ,$$

$$\widehat{k^T}(a^*_\perp, x) := \int {\rm d}y\, {\rm d}z\ \left\{ a^*_{\perp,y} k(y,z) \widehat{\delta^T}(z,x) \right\}\ .$$

In a similar vein, by virtue of (4.2a) we compute

$$e^{\mathcal{W}} a^*_{\phi} e^{-\mathcal{W}} = a^*_{\phi} + \frac{2}{N} \mathcal{K} a_{\overline{\phi}}\ .$$

In order to obtain a symmetric equation in the end, we symmetrize $h(a_\perp^*, a_\perp)$ as

$$h(a_\perp^*, a_\perp) = \frac{1}{2}\left\{h(a_\perp^*, a_\perp) + h^T(a_\perp, a_\perp^*)\right\} + c_\infty \ ,$$

where c_∞ is an (infinite) immaterial constant. This constant is harmless since it is added and subtracted. In fact, we remove this c_∞ after we perform the calculation.

We proceed to carry out the computation of $e^{\mathcal{W}}\mathcal{H}_{\rm app}e^{-\mathcal{W}}$. To avoid cumbersome expressions, we only display the manipulation of key terms of $\mathcal{H}_{\rm app}$.

The main operator on $\mathbb{F}_N$ that we need to compute reads

$$\begin{aligned}
&\int \mathrm{d}x\,\mathrm{d}y\ \left\{e^{\mathcal{W}}\Big((a_\phi^*)^2 a_{\perp,x}a_{\perp,y}\Big)e^{-\mathcal{W}}\frac{1}{N}\overline{f_\phi(x,y)}\right\}\\
&= \left\{(a_\phi^*)^2 + \frac{2}{N}\mathcal{K}(2\mathcal{N}_\phi - 1) + \frac{4}{N^2}\mathcal{K}^2(a_{\overline{\phi}})^2\right\}\\
&\times \int \mathrm{d}x\,\mathrm{d}y\ \left(a_{\perp,x} + \frac{1}{N}\widehat{k}^T(a_\perp^*, x)(a_{\overline{\phi}})^2\right)\frac{1}{N}\overline{f_\phi(x,y)}\left(a_{\perp,y} + \frac{1}{N}\widehat{k}(y, a_\perp^*)(a_{\overline{\phi}})^2\right)\\
&= \left\{(a_\phi^*)^2 + \frac{2}{N}\mathcal{K}(2\mathcal{N}_\phi - 1) + \frac{4}{N^2}\mathcal{K}^2(a_{\overline{\phi}})^2\right\}\\
&\times \left\{\frac{1}{N}\overline{f_\phi}(a_\perp, a_\perp) + \frac{1}{N^2}\left((\widehat{k}^T\circ\overline{f_\phi})(a_\perp^*, a_\perp) + (\overline{f_\phi}\circ\widehat{k})(a_\perp, a_\perp^*)\right)(a_{\overline{\phi}})^2\right.\\
&\qquad \left. + \frac{1}{N^3}(\widehat{k}^T\circ\overline{f}\circ\widehat{k})(a_\perp^*, a_\perp^*)(a_{\overline{\phi}})^4\right\}\\
&= (a_\phi^*)^2\frac{1}{N}\overline{f_\phi}(a_\perp, a_\perp) + \frac{1}{N^2}\left\{(\widehat{k}^T\circ\overline{f_\phi})(a_\perp^*, a_\perp) + (\overline{f_\phi}\circ\widehat{k})(a_\perp, a_\perp^*)\right\}\mathcal{N}_\phi(\mathcal{N}_\phi - 1)\\
&\quad + \frac{1}{N^3}(\widehat{k}^T\circ\overline{f_\phi}\circ\widehat{k})(a_\perp^*, a_\perp^*)(a_{\overline{\phi}})^2(\mathcal{N}_\phi - 2)(\mathcal{N}_\phi - 3)\\
&\qquad + \text{higher order terms in } a_\perp,\ a_\perp^* \ .
\end{aligned}$$

The above operator can be further simplified, without distortion of its commutability with $\mathcal{N}$, via the replacement $\mathcal{N}_\phi = \mathcal{N} - \mathcal{N}_\perp \mapsto N - \mathcal{N}_\perp$. Subsequently, we drop terms higher than quadratic in $a_\perp$, $a_\perp^*$; and treat N as large so that $N - l \simeq N$ if the number l is fixed. The other relevant computations are

$$\begin{aligned}
e^{\mathcal{W}}h(a_\perp^*, a_\perp)e^{-\mathcal{W}} &= h(a_\perp^*, a_\perp) + \frac{1}{N}\big(h\circ\widehat{k}\big)(a_\perp^*, a_\perp^*)\,(a_{\overline{\phi}})^2 \ ,\\
e^{\mathcal{W}}h^T(a_\perp, a_\perp^*)e^{-\mathcal{W}} &= h^T(a_\perp, a_\perp^*) + \frac{1}{N}\big(\widehat{k}^T\circ h^T\big)(a_\perp^*, a_\perp^*)\,(a_{\overline{\phi}})^2 \ .
\end{aligned}$$

Accordingly, we obtain the non-Hermitian operator

$$\begin{aligned}
\widetilde{\mathcal{H}}_{\rm app} := e^{\mathcal{W}}\mathcal{H}_{\rm app}e^{-\mathcal{W}} &= NE_{\rm H} + \big(h + \widehat{k}^T\circ\overline{f_\phi}\big)(a_\perp^*, a_\perp) + \big(h^T + \overline{f_\phi}\circ\widehat{k}\big)(a_\perp, a_\perp^*)\\
&\quad + \frac{1}{N}\mathrm{Ric}(a_\perp^*, a_\perp^*)\,(a_{\overline{\phi}})^2 + \frac{1}{N}(a_\phi^*)^2\,\overline{f_\phi}(a_\perp, a_\perp) \ .
\end{aligned} \tag{4.3a}$$

In the formal limit $\upsilon \to \delta$, as the interaction potential becomes a delta function, $\widetilde{\mathcal{H}}_{\rm app}$ becomes the reduced transformed Hamiltonian derived in [77]. The 'Riccati kernel' is

$$\mathrm{Ric}(x,y) := h\circ\widehat{\delta}\circ k + k\circ\widehat{\delta}^T\circ h^T + f_\phi + k\circ\widehat{\delta}^T\circ\overline{f_\phi}\circ\widehat{\delta}\circ k \ . \tag{4.3b}$$

Recall that the kernel $h(x,y)$ is defined by (4.1d) with (4.1e), viz.,

$$h(x,y) = \{-\Delta_x + V(x)\}\delta(x,y) + N(\upsilon * |\phi|^2)(x)\delta(x,y) + N\phi(x)\upsilon(x-y)\overline{\phi(y)} - \mu\delta(x,y) \ .$$

The operator $\widetilde{\mathcal{H}}_{\rm app}$ will be the focus of our analysis. As we anticipated, we have the identity $[\widetilde{\mathcal{H}}_{\rm app}, \mathcal{N}] = 0$, which enables us to seek eigenvectors of $\widetilde{\mathcal{H}}_{\rm app}$ in $\mathbb{F}_N$.

4.3. *Operator Riccati equation for k.* Next, we outline the rationale for the derivation of an integro-partial differential equation for k, in the spirit of Wu [76, 77]. This equation is described by (4.4b) below. In sections 5, 6, and 7, we study implications of this equation.

By inspection of (4.3a), we see that $\widetilde{\mathcal{H}}_{\rm app} - NE_H$ consists of two types of terms: (i) Terms that contain $a_\perp^*$ and $a_\perp$, and no $a_{\overline{\phi}}$ and a_ϕ^*. The sum of these terms forms the 'diagonal part' of $\widetilde{\mathcal{H}}_{\rm app}$, and can be described by use of a (nonlocal) one-particle Schrödinger operator. In the periodic setting [49], the use of this operator yields the excitation spectrum. (ii) Terms that contain $a_\perp^*$ and $a_{\overline{\phi}}$, or $a_\perp$ and a_ϕ^*. For the periodic setting, it can be argued that this second part does *not* affect the excitation spectrum *provided* $\mathrm{Ric}(a_\perp^*, a_\perp^*) = 0$ [77].

Therefore, we require that

$$\mathrm{Ric} = \lambda \otimes_{\rm s} \phi \ ,$$

where $\otimes_{\rm s}$ denotes the symmetrized tensor product. In view of (4.3b), we thus have an equation for k. Here, $\lambda(x)$ is arbitrary and can be chosen to satisfy a prescribed constraint involving the inner product $k(x,\overline{\phi})$. Notably, the operator $\mathcal{W}$ is invariant under changes of this constraint. In other words, physical predictions are not affected by the choice of $k(x,\overline{\phi})$. For example, we can conveniently impose $k(x,\overline{\phi}) = 0$ [76, 77]. This condition removes $\widehat{\delta}$, $\widehat{\delta}^T$ from the related equations, which is natural since

$$\int \mathrm{d}x\,\mathrm{d}y\ \left\{\mathrm{Ric}(x,y)a_{\perp,x}^* a_{\perp,y}^*\right\} = \int \mathrm{d}x\,\mathrm{d}y\ \left\{\big(\widehat{\delta}\circ\mathrm{Ric}\circ\widehat{\delta}^T\big)(x,y)\ a_x^* a_y^*\right\} \ .$$

The expression for $\mathrm{Ric}(x,y)$ becomes

$$\mathrm{Ric}(x,y) = h\circ k + k\circ h^T + f_\phi + k\circ\overline{f_\phi}\circ k \ . \tag{4.4a}$$

Consequently, the equation for k reads

$$h\circ k + k\circ h^T + f_\phi + k\circ\overline{f_\phi}\circ k = \lambda\otimes_{\rm s}\phi = \frac{1}{\sqrt{2}}(\lambda\otimes\phi + \phi\otimes\lambda) \ , \tag{4.4b}$$

where λ should be determined self-consistently. In fact, $\lambda(x)$ obeys the equation

$$\lambda(x) = C_1\phi(x) + \sqrt{2}(h\circ k + k\circ h^T + f_\phi + k\circ\overline{f_\phi}\circ k)(x,\overline{\phi}) = C_1\phi(x) + \sqrt{2}(k\circ h^T + f_\phi)(x,\overline{\phi})$$

with $C_1 = -\langle\overline{\phi},\lambda\rangle$; see section 5.2.

Equation (4.4b) amounts to an integro-partial differential equation for the function $k(x,y)$. We refer to (4.4b) as the operator Riccati equation for k. By virtue of (4.4b), the transformed Hamiltonian (4.3a) becomes

$$\widetilde{\mathcal{H}}_{\rm app} = NE_{\rm H} + \big(h + \widehat{k}^T\circ\overline{f_\phi}\big)(a_\perp^*, a_\perp) + \big(h^T + \overline{f_\phi}\circ\widehat{k}\big)(a_\perp, a_\perp^*) + \frac{1}{N}(a_\phi^*)^2\,\overline{f_\phi}(a_\perp, a_\perp) \ .$$

4.4. *On the non-unitary transformation and heuristic procedure.* In hindsight, we now discuss how (4.4b), and thus the underlying non-Hermitian approach, can be motivated more transparently. The main observation is that, in regard to $\mathcal{H}_{\rm app}$, we can consider the quadratic matrix form

$$\int \mathrm{d}x\,\mathrm{d}y\ \begin{pmatrix} a_{\perp,x} & a^*_{\perp,x}\end{pmatrix} \begin{pmatrix} -h^T(x,y) & N^{-1}(a^*_\phi)^2\overline{f_\phi}(x,y) \\ -N^{-1}f_\phi(x,y)(a_{\overline{\phi}})^2 & h(x,y)\end{pmatrix} \begin{pmatrix} -a^*_{\perp,y} \\ a_{\perp,y}\end{pmatrix}\ .$$

In view of the commutability of $a_\perp$, $a^*_\perp$ with $a_{\overline{\phi}}$, a^*_ϕ we can perform the following conjugation of the above 2×2 matrix, assuming for simplicity that $k(x,\overline{\phi})=0$:

$$\begin{aligned} &\begin{pmatrix} \delta & 0 \\ N^{-1}k(a_{\overline{\phi}})^2 & \delta\end{pmatrix} \circ \begin{pmatrix} -h^T & N^{-1}(a^*_\phi)^2\overline{f_\phi} \\ -N^{-1}f_\phi(a_{\overline{\phi}})^2 & h\end{pmatrix} \circ \begin{pmatrix} \delta & 0 \\ -N^{-1}k(a_{\overline{\phi}})^2 & \delta\end{pmatrix} \\ = \ &\begin{pmatrix} -h^T - N^{-2}\overline{f_\phi}\circ k\mathcal{N}_\phi(\mathcal{N}_\phi-1) & N^{-1}(a^*_\phi)^2\overline{f_\phi} \\ -N^{-1}\widetilde{\mathrm{Ric}}(a_{\overline{\phi}})^2 & h + N^{-2}k\circ\overline{f_\phi}\mathcal{N}_\phi(\mathcal{N}_\phi-1)\end{pmatrix}, \end{aligned}$$

where

$$\widetilde{\mathrm{Ric}} = h\circ k + k\circ h^T + f_\phi + \frac{1}{N^2}k\circ\overline{f_\phi}\circ k\,\mathcal{N}_\phi(\mathcal{N}_\phi-1)\ .$$

Replace $\mathcal{N}_\phi$ with N in the last expression and take $N-1\simeq N$; thus, $\widetilde{\mathrm{Ric}}$ is reduced to Ric (with the $\widehat{\delta}$ and $\widehat{\delta}^T$ removed). Equation (4.4b) then results from the requirement that *the transformed* 2×2 *matrix is upper triangular*. We will show that this property implies that the excitation spectrum of $\mathcal{H}_{\rm app}$ coincides with the one of the diagonal part of $\widetilde{\mathcal{H}}_{\rm app}$, and is identical to the spectrum found in [32]; see section 6.

It is important to realize that the condensate wave function ϕ is determined by a mean field equation, which is of the Hartree type. Hence, at this level of approximation, the kernel k does not modify the mean field description.

Now let us turn our attention to the (mean field) Hartree-type equation for ϕ, which becomes the Gross-Pitaevskii equation if υ is replaced by $g\delta$ for some constant $g>0$. We write the relevant PDE as $\mathbb{H}_{\rm H}\phi=\mu\phi$ where

$$\mathbb{H}_{\rm H} := -\Delta_x + V(x) + N\big(\upsilon * |\phi|^2\big)(x) \tag{4.5}$$

is a one-particle Hartree operator. In view of the trapping potential $V(x)$, the condensate wave function $\phi(x)$ is bounded and decays exponentially as $|x|\to\infty$.

Lastly, we are tempted to comment on the assumptions underlying the (uncontrolled) approximations for the many-body Hamiltonian presented in this section. We expect that the simplifications leading to the reduced Hamiltonian $\widetilde{\mathcal{H}}_{\rm app}$ make sense provided

$$\frac{\langle\psi|\mathcal{N}_\perp^l|\psi\rangle}{N^l} \ll 1 \quad \forall\,|\psi\rangle\in\mathbb{F}_N\ ; \quad l=1,\,2,\,3,\,4\ .$$

This condition loosely expresses the requirement that quantum fluctuations around the condensate should be relatively small.

5. Existence theory for pair excitation kernel. In this section, we address the existence of solutions to (4.4b). Our analysis is partly inspired by works of Albeverio, Tretter and coworkers [1–3,24] who rigorously connected the operator Riccati equation to the spectral theory of J-self-adjoint operators. In our work, we view an existence proof for k as a necessary step towards ensuring the self-consistency of the approximation and non-unitary transform for the Bosonic many-body Hamiltonian. Furthermore, the existence proof for k paves the way to establishing the connection of the non-unitary transformation involving k [76] to the notion of quasiparticle [32] for settings without translation invariance (see section 6).

Our theory invokes an appropriate functional, $\mathcal{E}[\overline{k},k]$, and two related lemmas, Lemmas 5.3 and 5.6 (section 5.1). A highlight is Theorem 5.7 on the existence of k (section 5.2). We stress that our existence proof differs significantly from the approach in [1–3]. First, we utilize a variational approach by seeking stationary points of $\mathcal{E}[\overline{k},k]$ on a Hilbert space, instead of applying the fixed-point argument of [2]. Note that the latter argument [2] makes use of operator estimates that are not expected to hold for the operator Ric corresponding to (4.3b). The variational approach developed here is amenable to constraints inherent to the physical problem; thus, the term $\lambda\otimes_{\mathrm{s}}\phi$ of (4.4b) emerges as a Lagrange multiplier. Alternate approaches of variational character for block operator matrices (not for the Riccati equation per se) are described in [74].

Second, our variational approach reveals that Riccati equation (4.4b) may in principle *not* have a unique solution. Our existence proof indicates how one can construct an infinite number of solutions for k. These correspond to saddle points of the underlying functional, $\mathcal{E}$. This lack of uniqueness can pose a challenge in the subsequent analysis of the excitation spectrum (section 6). As a remedy to this issue, we point out that a restriction on the norm of k, i.e., $\|k\|_{\mathrm{op}}<1$, warrants uniqueness (see also [3]). By this restriction, the k that solves Riccati equation (4.4b) is a minimizer of $\mathcal{E}$.

5.1. *Functional $\mathcal{E}[\overline{k},k]$ and useful lemmas.* Next, we define the relevant Hilbert space and the functional $\mathcal{E}[\overline{k},k]$. We also state and prove lemmas for our existence theory.

Definition 5.1. Let $\mathfrak{h}^1_V(\mathbb{R}^3\times\mathbb{R}^3)$ be the space of functions $k(x,x')$ such that

$$\iint \mathrm{d}x\,\mathrm{d}x'\,\Big\{|\nabla_x k(x,x')|^2+|\nabla_{x'}k(x,x')|^2+\big(V(x)+V(x')\big)|k(x,x')|^2\Big\}<\infty\,.$$

The energy functional $\mathcal{E}[\overline{k},k]:\mathrm{dom}(\mathcal{E})\to\mathbb{R}$ is defined by

$$\mathcal{E}[\overline{k},k]:=\mathrm{tr}\Big\{\big(\delta-\overline{k}\circ k\big)^{-1}\circ\Big(\overline{k}\circ h\circ k+\frac{1}{2}\overline{k}\circ f_\phi+\frac{1}{2}\overline{f_\phi}\circ k\Big)\Big\},\tag{5.1a}$$

where

$$\mathrm{dom}(\mathcal{E}):=\Big\{k\in\mathfrak{B}_2(\mathfrak{h}^1_V)\big|\,k^T=k\text{ and }\|k\|_{\mathrm{op}}<1\Big\}\subset\mathfrak{B}_2(\mathfrak{h}^1_V)\,.\tag{5.1b}$$

Remark 5.2. The space $\mathfrak{h}^1_V(\mathbb{R}^3\times\mathbb{R}^3)$ is the same as the space $\mathfrak{B}_2\big(\mathfrak{h}^1_V\big)$. If $k\in\mathfrak{B}_2(\mathfrak{h}^1_V)$ and $\|k\|_2<1$ then $(\delta-\overline{k}\circ k)^{-1}\in\mathfrak{B}_2(\mathfrak{h}^1_V)$. Thus, $\mathrm{dom}(\mathcal{E})$ is nonempty. The inequality $\|k\|_2<1$ implies $\|k\|_{\mathrm{op}}<1$. Further remarks on $\|k\|_{\mathrm{op}}<1$ are deferred to section 5.3.

The first lemma of interest can now be stated as follows.

LEMMA 5.3. The functional derivative of $\mathcal{E}[\overline{k}, k]$ with respect to symmetric variations of $\overline{k}$ in $\mathfrak{h}^1_V(\mathbb{R}^3 \times \mathbb{R}^3)$, denoted by $\delta\mathcal{E}/\delta\overline{k}$ where $\delta\mathcal{E}/\delta\overline{k} \in \mathfrak{B}^*_2(\mathfrak{h}^1_V) = \mathfrak{B}_2(\mathfrak{h}^1_V)$, is

$$\frac{\delta\mathcal{E}[\overline{k}, k]}{\delta\overline{k}} = \frac{1}{2}(\delta - k \circ \overline{k})^{-1} \circ \left\{h \circ k + k \circ h^T + f_\phi + k \circ \overline{f_\phi} \circ k\right\} \circ (\delta - \overline{k} \circ k)^{-1} \ .$$

Proof. Consider the arbitrary symmetric perturbation $\ell(x, x')$. It suffices to show that

$$\begin{aligned}\Big(\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{E}[\overline{k} + s\overline{\ell}, k]\Big)\Big|_{s=0} \\ = \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}x' \ \big\{\overline{\ell}(x, x')(\delta - k \circ \overline{k})^{-1} \\ \circ\big\{h \circ k + k \circ h^T + f_\phi + k \circ \overline{f_\phi} \circ k\big\} \circ (\delta - \overline{k} \circ k)^{-1}(x, x')\big\} \ .\end{aligned}$$

First, by differentiating the formal identity $\delta = (\delta - \overline{k} \circ k)^{-1} \circ (\delta - \overline{k} \circ k)$ we obtain

$$\Big(\frac{\mathrm{d}}{\mathrm{d}s}\big\{\delta - (\overline{k} + s\overline{\ell}) \circ k\big\}^{-1}\Big)\Big|_{s=0} = \big(\delta - \overline{k} \circ k\big)^{-1} \circ \overline{\ell} \circ k \circ \big(\delta - \overline{k} \circ k\big)^{-1} \ .$$

By using, e.g., the Neumann series for $(\delta - \overline{k} \circ k)^{-1}$, we realize that

$$k \circ \big(\delta - \overline{k} \circ k\big)^{-1} = \big(\delta - k \circ \overline{k}\big)^{-1} \circ k \ .$$

Hence, we also obtain the identity

$$\Big(\frac{\mathrm{d}}{\mathrm{d}s}\big\{\big(\delta - (\overline{k} + s\overline{\ell}) \circ k\big)^{-1} \circ (\overline{k} + s\overline{\ell})\big\}\Big)\Big|_{s=0} = \big(\delta - \overline{k} \circ k\big)^{-1} \circ \overline{\ell} \circ \big(\delta - k \circ \overline{k}\big)^{-1} \ .$$

Now express $\mathcal{E}$ as the sum

$$\mathcal{E} = \mathrm{tr}\left\{(\delta - \overline{k} \circ k)^{-1} \circ \overline{k} \circ \big(h \circ k + \tfrac{1}{2}f_\phi\big)\right\} + \mathrm{tr}\left\{\big(\delta - \overline{k} \circ k\big)^{-1} \circ \tfrac{1}{2}(\overline{f_\phi} \circ k)\right\} =: \mathcal{E}_1 + \mathcal{E}_2 \ .$$

The use of the cyclic property of the trace along with $\ell^T = \ell$ and $(\overline{k} \circ k)^T = k \circ \overline{k}$ yields

$$\begin{aligned}\Big(\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{E}_1[\overline{k} + s\overline{\ell}, k]\Big)\Big|_{s=0} &= \mathrm{tr}\left\{(\delta - \overline{k} \circ k)^{-1} \circ \overline{\ell} \circ (\delta - k \circ \overline{k})^{-1} \circ (h \circ k + \tfrac{1}{2}f_\phi)\right\} \\ &= \mathrm{tr}\left\{\overline{\ell} \circ (\delta - k \circ \overline{k})^{-1} \circ (h \circ k + \tfrac{1}{2}f_\phi) \circ (\delta - \overline{k} \circ k)^{-1}\right\}\end{aligned}$$

and

$$\begin{aligned}\Big(\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{E}_2[\overline{k} + s\overline{\ell}, k]\Big)\Big|_{s=0} &= \mathrm{tr}\left\{\tfrac{1}{2}\big(\delta - \overline{k} \circ k\big)^{-1} \circ \overline{\ell} \circ k \circ \big(\delta - \overline{k} \circ k\big)^{-1} \circ (\overline{f_\phi} \circ k)\right\} \\ &= \mathrm{tr}\left\{\tfrac{1}{2}\overline{\ell} \circ k \circ \big(\delta - \overline{k} \circ k\big)^{-1} \circ (\overline{f_\phi} \circ k) \circ (\delta - \overline{k} \circ k)^{-1}\right\} \\ &= \mathrm{tr}\left\{\tfrac{1}{2}\overline{\ell} \circ \big(\delta - k \circ \overline{k}\big)^{-1} \circ (k \circ \overline{f_\phi} \circ k) \circ (\delta - \overline{k} \circ k)^{-1}\right\} \ .\end{aligned}$$

Now combine the above results to obtain the expression

$$\Big(\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{E}[\overline{k} + s\overline{\ell}, k]\Big)\Big|_{s=0} = \frac{1}{2}\,\mathrm{tr}\left\{\overline{\ell} \circ \Big(\big(\delta - k \circ \overline{k}\big)^{-1} \circ \mathrm{Ric} \circ \big(\delta - \overline{k} \circ k\big)^{-1}\Big)\right\} \ ,$$

where Ric is defined by (4.4a). Note that Ric is manifestly symmetric if k is symmetric. □

REMARK 5.4. The notion of the weak solution as the critical point of the functional $\mathcal{E}[\overline{k}, k]$ is relevant to our existence theorem (Theorem 5.7). Consider the space $\phi^\perp = \{e \in \mathfrak{h}^1_V \mid e \perp \phi\}$. A bounded operator $k \in \mathfrak{B}(\phi^\perp, \phi^\perp)$ is a weak solution to the Riccati equation

$$k \circ h_\perp^T + h_\perp \circ k + k \circ \overline{f_\phi} \circ k + f_\phi = 0$$

provided

$$\langle k \circ h_\perp^T p, r\rangle + \langle kp, h_\perp^T r\rangle + \langle k \circ \overline{f_\phi} \circ kp, r\rangle = \langle -f_\phi p, r\rangle \quad \forall p,\, r \in \mathrm{dom}\{h_\perp^T\}\ ,$$

where $h_\perp$ is the projection of operator h on space $\phi^\perp$.

REMARK 5.5. Recall that ϕ satisfies the Hartree equation $\mathbb{H}_{\mathrm{H}}\phi(x) = \mu\phi(x)$ where the one-particle Hartree operator $\mathbb{H}_{\mathrm{H}}$ is defined in (4.5). We now state a few assumptions, which primarily concern the interaction potential $\upsilon(x)$ and the trapping potential $V(x)$. First, let us assume that $\upsilon(x)$ is positive, symmetric, integrable, and smooth. If the equation for ϕ comes from minimizing the Hartree energy functional, E_H, viz.,

$$E_H(\phi) := \int \mathrm{d}x\, \mathrm{d}y\ \left\{\overline{\phi(x)}\epsilon(x,y)\phi(y) + \frac{N}{2}|\phi(x)|^2\upsilon(x-y)|\phi(y)|^2\right\}\ ,$$

with $\|\phi\|_2 = 1$ then μ is the lowest eigenvalue of the linear operator that results from fixing ϕ in $\mathbb{H}_{\mathrm{H}}$. The existence theorem (Theorem 5.7) is stated and proved for a condensate ϕ that is not necessarily a minimizer of E_H. In fact, we replace the assumption of ϕ being such a minimizer by a less restrictive hypothesis (see Lemma 5.6). Because we assume that the potential V is smooth and behaves as $|x|^s$ when $|x| \to \infty$, where $s > 0$, the operator $-\Delta + V$ has discrete spectrum. The spectrum of $\mathbb{H}_{\mathrm{H}}$ is also discrete since $\mathbb{H}_{\mathrm{H}}$ is a compact perturbation of $-\Delta + V$.

LEMMA 5.6. If $\upsilon(x)$ has positive Fourier transform $\widehat{\upsilon}(\xi)$, $\widehat{\upsilon}(\xi) \geq 0$, and ϕ is a minimizer of the functional $E_H(\phi)$ then for some $c > 0$ the following inequality holds:

$$h(\overline{e}, e) - \left|f_\phi(\overline{e}, \overline{e})\right| \geq c\|e\|_2 \quad \forall e \in \phi^\perp = \{e \in \mathfrak{h}^1_V \mid e \perp \phi\},$$

where $h(\cdot,\cdot)$ and $f_\phi(\cdot,\cdot)$ are defined from (4.1b) and (4.1e).

Proof. Define $g(x) := \overline{\phi(x)}\, e(x)$. Parseval's identity yields

$$\iint \mathrm{d}x\, \mathrm{d}y\ \{\overline{e(x)}\phi(x)N\upsilon(x-y)\overline{\phi}(y)e(y)\} = \int \mathrm{d}\xi\ \{N\widehat{\upsilon}(\xi)|\widehat{g}(\xi)|^2\}\ ,$$

which dominates the integral

$$\iint \mathrm{d}x\, \mathrm{d}y\ \{\overline{e}(x)f_\phi(x,y)\overline{e}(y)\} = \int \mathrm{d}\xi\ \{N\widehat{\upsilon}(\xi)\left(\overline{\widehat{g}(\xi)}\right)^2\}\ .$$

Since ϕ is the minimizer of the Hartree functional, $E_H(\phi)$, we can assert that ϕ is the eigenfunction with the lowest eigenvalue of the operator $\mathbb{H}_{\mathrm{H}}$ and is therefore simple. If $e \perp \phi$ then $\left\langle \overline{e}, \mathbb{H}_H e\right\rangle \geq c\|e\|_{L^2}$ for some $c > 0$ because the spectrum of the Hartree operator $\mathbb{H}_H$ is discrete (see Remark 5.5). □

Lemma 5.6 motivates the inequality involving h and f_ϕ as an assumption of Theorem 5.7, which replaces the requirement that ϕ is a minimizer of $E_H(\cdot)$.

5.2. *Existence theorem and proof.* The existence theorem can be stated as follows.

THEOREM 5.7. Suppose that the kernels $h(x,y)$ and $f_\phi(x,y)$ satisfy the inequality

$$h(\overline{e},e) - \left|f_\phi(\overline{e},\overline{e})\right| \geq c\|e\|_{L^2}^2 \qquad \forall e \in \phi^\perp = \left\{e \in \mathfrak{h}_V^1 \;\middle|\; e \perp \phi\right\}, \tag{5.2}$$

for some constant $c > 0$. Moreover, let us assume that f_ϕ is Hilbert-Schmidt. Consider the functional $\mathcal{E}[\overline{k},k]$, defined in (5.1a), with domain

$$\mathrm{dom}(\mathcal{E})_\perp := \mathrm{dom}(\mathcal{E}) \cap \left\{k \in \mathfrak{B}_2(\mathfrak{h}_V^1) \;\middle|\; k(x,\overline{\phi}) = 0\right\}$$

which consists of the compact $\mathcal{C}$-symmetric Hilbert-Schmidt operators $k \in \mathfrak{B}_2(\mathfrak{h}_V^1)$ satisfying $k(x,\overline{\phi}) = 0$. Then the functional $\mathcal{E}$ restricted to $\mathrm{dom}(\mathcal{E})_\perp$ attains a minimum for some $k \in \mathrm{dom}(\mathcal{E})_\perp$ which is a weak solution of the operator Riccati equation (4.4b). The function $\lambda(x)$ entering this equation is a Lagrange multiplier and equals

$$\lambda(x) = \sqrt{2}\left\{\big(k\circ\gamma\big)\big(x,\overline{\phi}\big) + f_\phi\big(x,\overline{\phi}\big) - \tfrac{1}{2}f_\phi(\overline{\phi},\overline{\phi})\phi(x)\right\} . \tag{5.3}$$

At this stage, before we give a proof, two remarks are in order.

REMARK 5.8. We seek stationary points of $\mathcal{E}[\overline{k},k]$ under the constraint $k^T = k$. We now describe a generalization of the spectral theorem for compact operators with *symmetric* kernels which is invoked in the proof of Theorem 5.7. Let $\mathcal{C}$ denote the operator of complex conjugation on $\mathfrak{h}$ where

$$\mathcal{C}f(x) = \overline{f(x)} \qquad \forall\, f \in \mathfrak{h} .$$

Let us recall that an operator $\mathcal{T}$ on $\mathfrak{h}$ is called *complex-symmetric* ("$\mathcal{C}$-symmetric") if

$$\mathcal{C}\mathcal{T} = \mathcal{T}^*\mathcal{C} ,$$

where $\mathcal{T}^*$ is the Hermitian conjugate of $\mathcal{T}$ ($\mathcal{T}^*(x,y) = \overline{\mathcal{T}(y,x)}$). Clearly, integral operators whose kernels are symmetric in their arguments are $\mathcal{C}$-symmetric. Any compact complex-symmetric operator $\mathcal{T}$ such that $\mathcal{T}^*\circ\mathcal{T}$ has *simple spectrum* is decomposed as

$$\mathcal{T} = \sum_{n=1}^{\infty} a_n(u_n \otimes \mathcal{C}u_n) , \tag{5.4}$$

where $a_n \in \mathbb{C}$ converge to zero as $n \to \infty$ and $\{u_n\}_{n=1}^\infty$ is an orthonormal basis of $\mathfrak{h}$. This property comes from the identity $(\mathcal{C}\mathcal{T})\circ(\mathcal{C}\mathcal{T}) = \mathcal{T}^*\circ\mathcal{T}$, which implies the commutation relation $[\mathcal{C}\mathcal{T}, \mathcal{T}^*\circ\mathcal{T}] = 0$. In particular, $\mathcal{C}\mathcal{T}$ commutes with the spectral measure (and any eigenprojector) of the positive operator $\mathcal{T}^*\circ\mathcal{T}$. Since the latter operator has simple spectrum, it follows that these two operators have the same eigenspace. This fact allows us to pass from the eigenvalue equation $(\mathcal{T}^*\circ\mathcal{T})(u_n,x) = c_n u_n(x)$ to the eigenvalue equation $\mathcal{C}\mathcal{T}(u_n,x) = a_n u_n(x)$; thus, $|a_n|^2 = c_n$. It can be directly shown that all $\mathcal{C}$-symmetric tensor products $u\otimes v$ must have $v(x) = \mathcal{C}u(x)$. Hence, we can also pass from the spectral representation

$$\mathcal{T}^*\circ\mathcal{T} = \sum_{n=1}^{\infty} c_n(u_n\otimes u_n)$$

to expression (5.4). This result amounts to a version of the spectral theorem for compact $\mathcal{C}$-symmetric operators; see [35].

REMARK 5.9. The reader should compare (5.3), regarding the Lagrange multiplier λ, to equation (3.24) in [77] which employs a delta function interaction potential. The respective formulas for $\lambda(x)$ differ by a factor of $\sqrt{2}$ because of the choice of a normalization factor for $\lambda \otimes_{\mathrm{s}} \phi$.

We can now proceed to give a proof of Theorem 5.7. Notably, we consider a condensate ϕ that is not necessarily a minimizer of the Hartree energy, E_H.

Proof. We split the proof of Theorem 5.7 into three main steps.

STEP 1. We express the functional $\mathcal{E}$ in terms of a suitable basis and describe critical points, by taking into account the theory of $\mathcal{C}$-symmetric operators. By Remark 5.8, any k satisfying our assumptions admits the decomposition

$$k(x,x') = \sum_{j=1}^{\infty} z_j e_j(x) e_j(x') \ , \quad e_j \in \phi^{\perp} \ ,$$

where $\{e_j(x)\}_j \subset \mathfrak{h}$ is an orthonormal basis and the coefficients $\{z_j\} \subset \mathbb{C}$ are such that $z_j \to 0$ as $j \to \infty$. For the moment, we assume $|z_j| \neq 1$ for all j so that

$$(\delta - \overline{k} \circ k)^{-1}(x,x') = \sum_{j=1}^{\infty} \Big(\frac{1}{1-|z_j|^2} \Big) \overline{e}_j(x) e_j(x') \ .$$

The substitution of the two preceding expressions into (5.1a) for the energy furnishes

$$\mathcal{E}\Big(\{e_j\},\{z_i\}\Big) = \sum_{j=1}^{\infty} \frac{1}{1-|z_j|^2} \left\{ h(\overline{e}_j, e_j)|z_j|^2 + \frac{1}{2}\Big(f_\phi(\overline{e}_j,\overline{e}_j) z_j + \overline{f_\phi}(e_j,e_j)\overline{z}_j \Big) \right\} ,$$

where $\overline{f_\phi}(e_j,e_j) = \overline{f_\phi(\overline{e}_j,\overline{e}_j)}$. The derivative of $\mathcal{E}\big(\{e_j\},\{z_j\}\big)$ with respect to $\overline{z_j}$ reads

$$\frac{\partial}{\partial \overline{z}_j} \mathcal{E}\Big(\{e_j\},\{z_j\}\Big) = \frac{1}{2} \sum_{j=1}^{\infty} \frac{2h(\overline{e}_j,e_j) z_j + \overline{f_\phi}(e_j,e_j) + f_\phi(\overline{e}_j,\overline{e}_j) z_j^2}{(1-|z_j|^2)^2} \ .$$

Setting $\partial \mathcal{E}/\partial \overline{z}_j = 0$ gives two roots, viz.,

$$z_j^{\pm} = \frac{-h(\overline{e}_j,e_j) \pm \sqrt{h(\overline{e}_j,e_j)^2 - |f_\phi(\overline{e}_j,\overline{e}_j)|^2}}{f_\phi(\overline{e}_j,\overline{e}_j)} \ . \tag{5.5}$$

Condition (5.2) guarantees that $|z_j^{\pm}| \neq 1$ provided e_j is a member of the function space $\phi^{\perp}$; in fact, $|z_j^{+}| < 1$ and $|z_j^{-}| > 1$. Regarding $\mathcal{E}(\{e_j\},\{z_j\})$, notice that the summand (for fixed j and $e_j = e$) is described by the function

$$f(z;e) := \frac{2h(\overline{e},e)|z|^2 + f_\phi(\overline{e},\overline{e})\overline{z} + \overline{f_\phi}(e,e) z}{1-|z|^2}$$

which takes real values with $f(0;e) = 0$, while

$$\lim_{|z|\to 1^-} f(z;e) = +\infty \ .$$

Thus, the function $f(z;e_j)$ attains a minimum at $z = z_j^{+}$. On the other hand, we have

$$\lim_{|z|\to\infty} f(z;e) = -2h(\overline{e},e) \ ,$$

and $f(z_j^-; e_j) = -h(\overline{e}_j, e_j) - \sqrt{h(\overline{e}_j, e_j)^2 - |f_\phi(\overline{e}_j, \overline{e}_j)|^2}$ which implies that $f(z; e_j)$ has a maximum at $z = z_j^-$ in view of

$$\lim_{|z|\to 1^+} f(z; e) = -\infty \ .$$

By (5.5) the evaluation of $\mathcal{E}$ with the roots $z_j^\pm$ yields

$$\mathcal{E}\Big(\{(z_j^\pm\}, \{e_j\}\Big) = -\frac{1}{2}\sum_{j=1}^{\infty}\Big\{h(\overline{e}_j, e_j) \mp \sqrt{h(\overline{e}_j, e_j)^2 - |f_\phi(\overline{e}_j, \overline{e}_j|^2}\Big\} \ .$$

We choose the root z_j^+ where $|z_j^+| < 1$ and define

$$\begin{aligned}\mathcal{F}(e) :=& h(\overline{e}, e) - \sqrt{h(\overline{e}, e)^2 - |f_\phi(\overline{e}, \overline{e})|^2} \\ =& \frac{|f_\phi(\overline{e}, \overline{e})|^2}{h(\overline{e}, e) + \sqrt{h(\overline{e}, e)^2 - |f_\phi(\overline{e}, \overline{e})|^2}} \ .\end{aligned}$$

The value of the functional $\mathcal{E}$ reads

$$\mathcal{E}\big(\{z_j^+\}, \{e_j\}\big) = -\frac{1}{2}\sum_{j=1}^{\infty}\mathcal{F}(e_j) \ .$$

Step 2. The minimization problem can be stated by the following expression:

$$\min_{\{e_j\}_{j=1}^\infty}\left\{-\frac{1}{2}\sum_{j=1}^{\infty}\mathcal{F}(e_j)\right\} = -\frac{1}{2}\max_{\{e_j\}_{j=1}^\infty}\sum_{j=1}^{\infty}\mathcal{F}(e_j) \ ,$$

where $\{e_j\}_{j=1}^\infty$ is an orthonormal frame, i.e.,

$$\big\langle \overline{e}_j, e_k\big\rangle = \delta_{j,k} \quad ; \quad \big\langle \overline{\phi}, e_j\big\rangle = 0 \ .$$

Next, we prove that the overall minimum is attained.
Recall the bilinear expansion

$$k(x, y) = \sum_{j=1}^{\infty} z_j^+ e_j(x) e_j(y),$$

where the coefficients z_j^+ are

$$z_j^+ = \frac{-h(\overline{e}, e) + \sqrt{h(\overline{e}, e)^2 - |f_\phi(\overline{e}, \overline{e})|^2}}{f_\phi(\overline{e}, \overline{e})} = \frac{-f_{\overline{\phi}}(e, e)}{h(\overline{e}, e) + \sqrt{h(\overline{e}, e)^2 - |f_\phi(\overline{e}, \overline{e})|^2}} \ .$$

We will prove that $\sum_{j=1}^\infty \mathcal{F}(e_j)$ is bounded above. The following inequality holds:

$$\mathcal{F}(e) \le \frac{|f_\phi(\overline{e}, \overline{e})|^2}{h(\overline{e}, e)} \le \frac{1}{c_{\text{gap}}}|f_\phi(\overline{e}, \overline{e})|^2,$$

where $c_{\rm gap}$ denotes a positive constant. Subsequently, we have

$$\begin{aligned}\sum_{j=1}^{\infty}|f_\phi(e_j,e_j)|^2 &= \sum_{j=1}^{\infty}\left|\langle e_j(x),\ \int v(x-y)\overline{\phi(x)}\,\overline{\phi(y)}e_j(y)\,\mathrm{d}y\rangle\right|^2\\ &\le \sum_{j=1}^{\infty}\int \mathrm{d}x\ \left|\int v(x-y)\overline{\phi(x)}\,\overline{\phi(y)}e_j(y)\,\mathrm{d}y\right|^2\\ &\le \int \mathrm{d}x\,\mathrm{d}y\ \left\{v(x-y)^2|\phi(x)|^2|\phi(y)|^2\right\} \le \|v\|_{L^3(\mathbb{R}^d)}\|\phi\|^2_{L^6(\mathbb{R}^d)}\ ,\end{aligned}$$

which entails an upper bound for $\sum_{j=1}^{\infty}\mathcal{F}(e_j)$. This result is crucial because it enables us to seek a maximizing sequence $\{e_j^{(n)}\}_j$ of frames ($n\in\mathbb{N}$); and show that such a sequence converges strongly in the domain of definition of the functional $\mathcal{E}$.

Indeed, consider the maximizing sequence of frames $\{e_j^{(n)}\}_{j=1}^{\infty}$, where $n\in\mathbb{N}$, i.e.,

$$\lim_{n\to\infty}\frac{1}{2}\sum_{j=1}^{\infty}\mathcal{F}(e_j^{(n)}) = \max_{\{e_j\}_{j=1}^{\infty}}\frac{1}{2}\sum_{j=1}^{\infty}\mathcal{F}(e_j)\ .$$

A (standard) diagonalization procedure then yields

$$e_j^{(n)}\to e_j \quad \text{weakly in } \mathfrak{h}(\mathbb{R}^3),$$

where $\mathfrak{h}=L^2$. If there exists some constant C_j independent of n such that

$$h(\overline{e}_j^{(n)},e_j^{(n)})\le C_j \quad \forall n\in\mathbb{N}\ ,$$

we conclude that

$$e_j^{(n)}\to e_j \quad \text{strongly in } \mathfrak{h}(\mathbb{R}^3)\ .$$

Otherwise, we have $z_j^{(n)}\to 0$ as $n\to\infty$, and we can ignore this case.

We should add that if the convergence were weak in $\mathfrak{h}^1_V(\mathbb{R}^3)$ then we would have

$$h(\overline{e}_j,e_j) < \lim_{n\to\infty} h(\overline{e}_j^{(n)},e_j^{(n)})\ .$$

Since $\mathcal{F}(e)$ is a decreasing function of $h(\overline{e},e)$, we obtain a contradiction to the fact that $\{e_j^{(n)}\}_{j=1}^{\infty}$ is a maximizing sequence. This proves the strong convergence in $\mathfrak{h}^1_V(\mathbb{R}^3)$.

In the above, we use the norm (see section 2 for definition of function space $\mathfrak{h}^1_V$)

$$\|f\|^2_{\mathfrak{h}^1_V(\mathbb{R}^d)} = \int_{\mathbb{R}^d}\mathrm{d}x\ \left\{|\nabla f(x)|^2+V(x)|f(x)|^2\right\}\ .$$

It is thus necessary that the presence of the trapping potential V controls the $L^2(\mathbb{R}^3)$ norm in such a way that $\mathfrak{h}^1_V(\mathbb{R}^3)$ is compactly embedded in $L^2(\mathbb{R}^3)$ (for $d=3$).

Next, we check that the overall minimum is finite. Condition (5.2) implies that $h(\overline{e},e)$ is bounded below. This means that the the overall minimum is finite provided

$$\begin{aligned}\sum_{j=1}^{\infty}\mathcal{F}(e_j) \le C\sum_{j=1}^{\infty}|f_\phi(\overline{e}_j,e_j)|^2 &= \sum_{j=1}^{\infty}\left|\ \int \mathrm{d}x\,\mathrm{d}y\ \{\overline{e}_j(x)f_\phi(x,y)\overline{e}_j(y)\}\right|^2\\ &\le \int \mathrm{d}x\ \sum_{j=1}^{\infty}\left|\ \int \mathrm{d}y\ \{f_\phi(x,y)\overline{e}_j(y)\}\right|^2 \le \int \mathrm{d}x\,\mathrm{d}y\ \left\{|f_\phi(x,y)|^2\right\}<\infty\ .\end{aligned}$$

The last condition indeed holds. We can see that

$$\sum_{j=1}^{\infty} |z_j^+|^2 \leq C \sum_{j=1}^{\infty} |f_\phi(\overline{e}_j, \overline{e}_j)|^2 \leq \|f_\phi\|^2_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \ .$$

Thus, k is Hilbert-Schmidt.

STEP 3. So far, we showed that the minimum is attained in $\mathrm{dom}(\mathcal{E})_\perp$. We must now take into account the orthogonality constraint $k(x,\overline{\phi}) = 0$ via a Lagrange multiplier. We introduce the Lagrange multiplier as an operator with symmetric kernel $\ell(x,y)$ where

$$\ell(x,y) = \big(\lambda \otimes_{\mathrm{s}} \phi\big)(x,y) := \frac{1}{\sqrt{2}} \left\{\lambda(x)\phi(y) + \lambda(y)\phi(x)\right\} \ .$$

In the above, ϕ is the condensate wave function and $\lambda(x)$ is to be determined. Hence, the modified energy functional to be minimized has the form

$$\tilde{\mathcal{E}}[\overline{k}, k] := \mathcal{E}[\overline{k}, k] - \mathrm{tr}\left\{\overline{\ell} \circ k + \overline{k} \circ \ell\right\} \ .$$

In view of Lemma 5.3, setting equal to zero the functional derivative of $\tilde{\mathcal{E}}$ with respect to $\overline{k}$ yields Riccati equation (4.4b). Given that $h = \mathbb{H}_{\mathrm{H}}\delta + N\gamma - \mu$ and $\mathbb{H}_{\mathrm{H}}\phi = \mu\phi$, we compute λ by contracting the above equation for k with $\overline{\phi}$. Thus, we obtain (5.3).

Note on k as a weak solution: We conclude the proof by showing that k satisfies the definition of a weak solution (Remark 5.4). The condition that the functional $\mathcal{E}$ be minimized implies that the first variation with respect to $\overline{k}$ vanishes, i.e.,

$$\mathrm{tr}\left[\overline{k}_1 \circ (\delta - k\circ\overline{k})^{-1} \circ \left\{h_\perp \circ k + k \circ h_\perp^T + f_\phi + k \circ \overline{f_\phi} \circ k\right\} \circ (\delta - \overline{k}\circ k)^{-1}\right] = 0 \ ,$$

for all $\overline{k}_1 \in \mathrm{dom}(\mathcal{E})$. Without loss of generality, we can make the substitution $\overline{k}_1 \mapsto (\delta - \overline{k}\circ k)^{-1} \circ \overline{k}_1 \circ (\delta - \overline{k}\circ k)^{-1}$ so that the equation for vanishing first variation reads

$$\mathrm{tr}\left[\overline{k}_1 \circ \left\{h_\perp \circ k + k \circ h_\perp^T + f_\phi + k \circ \overline{f_\phi} \circ k\right\}\right] = \mathrm{tr}\left[\overline{k}_1 \circ \mathrm{Ric}\right] = 0 \ .$$

If $\overline{k}_1 := p \otimes_{\mathrm{s}} r$ for $p,\, r \in \mathrm{dom}(h_\perp)$, the condition $\mathrm{tr}\left[\overline{k}_1 \circ \mathrm{Ric}\right] = 0$ translates to

$$\begin{aligned}\mathrm{tr}\left[p \otimes_{\mathrm{s}} r \circ \mathrm{Ric}\right] &= \mathrm{tr}\left[(k\circ p \otimes_{\mathrm{s}} r) \circ h_\perp\right] + \mathrm{tr}\left[(p \otimes_{\mathrm{s}} r) \circ k \circ h_\perp\right] \\ &\quad + \mathrm{tr}\left[(p \otimes_{\mathrm{s}} r) \circ \left(f_\phi + k \circ \overline{f_\phi} \circ k\right)\right] \\ &= \sqrt{2}\big(\langle kp, h_\perp r\rangle + \langle p, (k\circ h_\perp) r\rangle + \langle p, \big(f_\phi + k\circ\overline{f_\phi}\circ k\big) r\rangle\big) \ .\end{aligned}$$

Observe that this expression is defined for any $p,\, r \in \mathrm{dom}(h_\perp)$, which is the space of test functions for the weak formulation of the Riccati equation. □

5.3. *On the non-uniqueness of k.* Next, we discuss the issue of the non-uniqueness of solutions for k by our variational approach. The energy functional $\mathcal{E}[\overline{k}, k]$ has infinitely many critical points which correspond to choosing one of the two roots $z_j^\pm$, at every index j, in the proof of Theorem 5.7. We can show that these choices correspond to minimax points. To this end, pick an arbitrary $e_1(x)$, normalized so that $\|e_1\|_{\mathfrak{h}} = 1$, and let

$$X^\perp(\phi, e_1) := \left\{e(x) \;\middle|\; e \perp \{\phi, e_1\}\right\} \ .$$

Also, consider the subspace $X(e_1) := \mathrm{span}(e_1) = \{z_1 e_1(x) \in \mathfrak{h} \mid z_1 \in \mathbb{C}\}$. Accordingly, we set up the min-max problem expressed by

$$\max_{e \in X(e_1), |z_1|>1} \left\{ \min_{\|k|_{X^\perp(\phi,e_1)}\|_{\mathrm{op}}<1} \mathcal{E}(\overline{k}, k) \right\} .$$

By repetition of the above argument (proof of Theorem 5.7), this min-max problem generates the (saddle type) critical point of the functional $\mathcal{E}(\overline{k}, k)$. More generally, the maximum can be taken over any finite collection of $\{(e_{j_k}, z_{j_k})\}_k$, producing a unique solution for every distinct sequence.

Evidently, the only solution k that obeys $\|k\|_{\mathrm{op}} < 1$ is the one given in the proof of Theorem 5.7. Thus, we single out the choice $\{z_j = z_j^+\}$ with $|z_j^+| < 1$ for all j as the one yielding the unique pair-excitation kernel for our model.

REMARK 5.10. If z_j is chosen in (5.5) such that $z_j = z_j^+ \ \forall j > 0$ (i.e., $\|k\|_{\mathrm{op}} < 1$) then

$$\begin{aligned}(h + k \circ \overline{f_\phi})(\overline{e}_j, e_j) &= h(\overline{e}_j, e_j) + (k\overline{e}_j, \overline{f_\phi} e_j) = h(\overline{e}_j, e_j) + (z_j^+)\overline{f_\phi}(e_j, e_j) \\ &= \sqrt{h^2(\overline{e}_j, e_j) - |f_\phi(\overline{e}_j, \overline{e}_j)|^2} > 0 .\end{aligned}$$

This property is germane to the spectrum of the reduced Hamiltonian (section 6.2).

6. Spectrum and eigenvectors of reduced Hamiltonian. In this section, we describe the spectrum and eigenvectors of the reduced transformed Hamiltonian $\widetilde{\mathcal{H}}_{\mathrm{app}}$ in the N-th sector of Fock space, $\mathbb{F}_N$. To this end, we decompose $\mathbb{F}_N$ into suitable orthogonal subspaces. A similar technique is used in [54] in connection to the Bogoliubov Hamiltonian.

We start by writing

$$\widetilde{\mathcal{H}}_{\mathrm{app}} = NE_H + \mathcal{H}_{\mathrm{ph}} , \quad \mathcal{H}_{\mathrm{ph}} := h_{\mathrm{ph}}\big(a_\perp^*, a_\perp\big) + \frac{1}{N}(a_\phi^*)^2\, \overline{f_\phi}\big(a_\perp, a_\perp\big), \tag{6.1a}$$

where $f_\phi(a_\perp^*, a_\perp^*)$ (and thus $\overline{f_\phi}(a_\perp, a_\perp)$) is defined by (4.1b) with (4.1d), and

$$h_{\mathrm{ph}} := h + k \circ \overline{f_\phi} . \tag{6.1b}$$

The non-Hermitian operator $h_{\mathrm{ph}}\big(a_\perp^*, a_\perp\big)$ forms the diagonal part of $\mathcal{H}_{\mathrm{ph}}$.

The main result is expressed by Theorem 6.1 concerning two spectra.

THEOREM 6.1. Consider the operators $\mathcal{H}_{\mathrm{ph}}$ and $h_{\mathrm{ph}}(a_\perp^*, a_\perp)$ restricted on $\mathbb{F}_N$. Then

$$\sigma\left(\mathcal{H}_{\mathrm{ph}}\big|_{\mathbb{F}_N}\right) = \sigma\left(h_{\mathrm{ph}}(a_\perp^*, a_\perp)\big|_{\mathbb{F}_N}\right) .$$

Moreover, for each eigenvector $|\Omega\rangle_N \in \mathbb{F}_N$ of $h_{\mathrm{ph}}(a_\perp^*, a_\perp)$ with eigenvalue E there exists a unique eigenvector, $|\Psi(\Omega)\rangle_N \in \mathbb{F}_N$, of $\mathcal{H}_{\mathrm{ph}}$ such that

$$\mathcal{H}_{\mathrm{ph}}|\Psi(\Omega)\rangle_N = E|\Psi(\Omega)\rangle_N .$$

To prove Theorem 6.1, we need a few lemmas. In Section 6.1, we develop a formalism for the decomposition of $\mathbb{F}_N$ into orthogonal subspaces by using Fock space techniques. In Section 6.2, we show that the spectrum of h_{ph} is discrete. In Section 6.3, we use this machinery to prove Theorem 6.1. In our proof, we describe an explicit construction of

the eigenvectors of $\mathcal{H}_{\rm ph}$ restricted on $\mathbb{F}_N$ in terms of eigenvectors of $h_{\rm ph}(a_\perp^*, a_\perp)$. This construction invokes the discrete spectrum of $h_{\rm ph}$.

6.1. *Decomposition of $\mathbb{F}_N$ and two related lemmas.* Next, we set the stage for the proof of Theorem 6.1. The symbol $|\psi\rangle_n$ denotes the vector of $\mathbb{F}$ with entry $\psi_n(x_1, \dots, x_n)$ in the n-th slot and zero elsewhere. Let us also employ the projection $\mathcal{P}_N : \mathbb{F} \mapsto \mathbb{F}_N$.

The vector $\psi_N(x_1, \dots, x_N)$ can be decomposed as a direct sum according to

$$\psi_N = \sum_{n=0}^{N} \psi_{N,n} \otimes_{\rm s} \left(\otimes^{N-n} \phi \right) =: \sum_{n=0}^{N} \psi_{N,n}^{\phi} \ , \qquad \otimes^p \phi := \prod_{j=1}^{p} \phi(x_j) \ ,$$

where the vectors $\psi_{N,n}(x_1, \dots, x_n)$ satisfy the orthogonality relations $(n = 1, 2 \dots N)$

$$\int \mathrm{d}x \ \left\{ \overline{\phi}(x) \psi_{N,n}(x, x_2, \dots, x_n) \right\} = 0 \ .$$

We also define $|\psi_{N,n}^{\phi}\rangle_N := \big(0, \dots, 0, \psi_{N,n}^{\phi}, \dots\big) \in \mathbb{F}_N$. Hence, the vector

$$|\psi^{\perp}\rangle := \big(\psi_{N,0}, \psi_{N,1}, \dots, \psi_{N,N}, 0, \dots\big)$$

describes fluctuations around $\otimes^N \phi$ (pure condensate). This means that we can decompose the space $\mathbb{F}_N$ into the following direct sum of orthogonal subspaces:

$$\mathbb{F}_N = \oplus_{n=0}^{N} \mathbb{F}_{N,n} \ ; \qquad \mathbb{F}_{N,n} = \mathrm{span}_{\psi_n \perp \phi} \big(0, \dots, 0, \psi_n \otimes_{\rm s} (\otimes^{N-n} \phi), 0 \dots\big) \ .$$

To describe this decomposition, we consider the number operator $\mathcal{N}_\phi = a_\phi^* a_{\bar{\phi}}$ for the condensate. We have

$$\mathcal{N}_\phi \big|_{\mathbb{F}_{N,n}} = (N - n) \mathcal{I} \big|_{\mathbb{F}_{N,n}} \quad , \quad 0 \leq n \leq N \ ,$$

where $\mathcal{I}$ is the identity operator on $\mathbb{F}$. In other words, $\mathbb{F}_{N,n}$ are the eigenspaces of $\mathcal{N}_\phi$ restricted to $\mathbb{F}_N$. To see how the decomposition works, we invoke the identity

$$\mathcal{P}_N = \sum_{n=0}^{N} \frac{(-1)^{N-n}}{(N-n)! n!} \prod_{\substack{p=0 \\ p \neq N-n}}^{N} \big(\mathcal{N}_\phi - p\mathcal{I}\big) \mathcal{P}_N \ ,$$

which can be understood as a resolution of the identity on $\mathbb{F}_N$. By introducing the projection operator (projection on $\mathbb{F}_n$) via the polynomial

$$P_n(z) := \frac{(-1)^n}{n!} \prod_{j=1}^{n} (z - j) \ ,$$

we define

$$\mathcal{P}_{n,n} := P_n(\mathcal{N}_\phi) = \frac{(-1)^n}{n!} \prod_{j=1}^{n} \left(\mathcal{N}_\phi - j\mathcal{I}\right) \ .$$

Thus, $\mathcal{P}_{n,n}$ is the projection $\mathcal{P}_{n,n} : \mathbb{F}_n \mapsto \mathbb{F}_{n,n}$.

We state the first lemma as follows.

LEMMA 6.2. The operator $\mathcal{P}_{n,n} = P_n(\mathcal{N}_\phi)$ satisfies the factorization

$$\sum_{n=0}^{N} \frac{(-1)^N}{(N-n)!}\, a_\phi^{*\,N-n} \mathcal{P}_{n,n} a_\phi^{N-n} = \sum_{n=0}^{N} \frac{(-1)^{N-n}}{(N-n)!\, n!} \prod_{\substack{p=0 \\ p\neq N-n}}^{N} \big(\mathcal{N}_\phi - p\mathcal{I}\big)$$

which, restricted to $\mathbb{F}_N$, describes a resolution of $\mathbb{F}_N$ into orthogonal subspaces.

Proof. First, we note the useful identities

$$a_\phi^{\,p} \mathcal{N}_\phi = \big(\mathcal{N}_\phi + p\mathcal{I}\big) a_\phi^{\,p} \ , \quad a_\phi^{*\,p} \mathcal{N}_\phi = \big(\mathcal{N}_\phi - k\mathcal{I}\big) a_\phi^{*\,p} \qquad (p = 0,\, 1,\, \dots N) \ .$$

Subsequently, for any polynomial $P(z)$ we can assert that

$$P(\mathcal{N}_\phi) a_\phi^{\,p} = a_\phi^{\,p} P\big(\mathcal{N}_\phi - p\mathcal{I}\big) \ , \quad P(\mathcal{N}_\phi) a_\phi^{*\,p} = a_\phi^{*\,p} P\big(\mathcal{N}_\phi + p\mathcal{I}\big) \ .$$

Moreover, we have the following formulas:

$$a_\phi^{n} a_\phi^{*\,n} = \prod_{p=1}^{n} \big(\mathcal{N}_\phi + p\mathcal{I}\big) \ , \quad a_\phi^{*\,n} a_\phi^{n} = \prod_{p=0}^{n-1} \big(\mathcal{N}_\phi - p\mathcal{I}\big) \ .$$

By using the above relations, we write

$$\begin{aligned}
&\sum_{n=0}^{N} \frac{(-1)^N}{(N-n)!} a_\phi^{*\,N-n} P_n(\mathcal{N}_\phi) a_\phi^{N-n} = \sum_{n=0}^{N} \frac{(-1)^N}{(N-n)!} a_\phi^{*\,N-n} a_\phi^{\,N-n} P_n\big(\mathcal{N}_\phi - (N-n)\mathcal{I}\big) \\
&= \sum_{n=0}^{N} \frac{(-1)^N (-1)^n}{(N-n)! n!} \prod_{j=0}^{N-n-1} \big(\mathcal{N}_\phi - j\mathcal{I}\big) \prod_{p=1}^{n} \big(\mathcal{N}_\phi + (n-p-N)\mathcal{I}\big) \\
&= \sum_{n=0}^{N} \frac{(-1)^{N-n}}{(N-n)!\, n!} \prod_{\substack{j=0 \\ j\neq N-n}}^{N} \big(\mathcal{N}_\phi - j\mathcal{I}\big) = \mathcal{P}_N \ .
\end{aligned}$$

We can show that $\mathcal{P}_{n,n}$ is a projection. Indeed, notice that $\mathcal{N}_\phi P_n(\mathcal{N}_\phi)\big|_{\mathbb{F}_n} = 0$, and if $|\psi\rangle_n \in \mathbb{F}_n$ then $\mathcal{P}_{n,n}|\psi\rangle_n = |\psi_{n,n}\rangle_n$. If we consider the decomposition

$$\psi_n = \sum_{p=0}^{n} \psi_{n,p} \otimes_s \big(\otimes^{n-p} \phi\big) = \sum_{p=0}^{n} \psi_{n,p}^{\phi}$$

then $\mathcal{P}_{n,n}$ applied to $\big|\psi\big\rangle_n$ produces a vector in $\mathbb{F}_{n,n}$, where $\mathbb{F}_{n,p}$ is the decomposition of $\mathbb{F}_n$ for $p = 0, 1 \dots n$. □

For later algebraic convenience, we give the following definition (cf. [54]).

DEFINITION 6.3. Consider the operators $\mathcal{U}_n, \mathcal{U}_n^* : \mathbb{F}_N \mapsto \mathbb{F}_N$ given by

$$\mathcal{U}_n := \mathcal{P}_{n,n} \frac{a_\phi^{N-n}}{\sqrt{(N-n)!}} \ , \quad \mathcal{U}_n^* := \frac{a_\phi^{*\,N-n}}{\sqrt{(N-n)!}} \mathcal{P}_{n,n} \ ; \quad n = 0,\, 1,\, \dots,\, N \ .$$

By Definition 6.3, the result of Lemma 6.2 implies that

$$\mathcal{P}_N = \sum_{n=0}^{N} \frac{(-1)^N}{(N-n)!} a_\phi^{*\,N-n} \mathcal{P}_{n,n} \mathcal{P}_{n.n} a_{\overline{\phi}}^{N-n} \mathcal{P}_N = (-1)^N \sum_{n=0}^{N} \frac{a_\phi^{*\,N-n} \mathcal{P}_{n,n}}{\sqrt{(N-n)!}} \frac{\mathcal{P}_{n,n} a_{\overline{\phi}}^{N-n}}{\sqrt{N-n)!}} \mathcal{P}_N$$
$$= (-1)^N \sum_{n=0}^{N} \mathcal{U}_n^* \mathcal{U}_n \Big|_{\mathbb{F}_N} .$$

The key relations following from this decomposition are

$$\mathcal{U}_n |\psi\rangle_N = |\psi_{N,n}\rangle_n \ , \quad \mathcal{U}_n^* |\psi_{N,n}\rangle_n = |\psi_{N,n}^\phi\rangle_N \quad \text{and} \quad \sum_{n=0}^{N} |\psi_{N,n}^\phi\rangle_N = |\psi\rangle_N \ .$$

Hence, we have $\mathcal{U}_n : \mathbb{F}_N \mapsto \mathbb{F}_{n,n}$ and $\mathcal{U}_n^* : \mathbb{F}_n \mapsto \mathbb{F}_{N,n}$.

LEMMA 6.4. The operators $\{\mathcal{U}_n\}_{n=0}^N$ satisfy the relation

$$\mathcal{U}_m \mathcal{U}_n^* = \delta_{m,n} \mathcal{P}_{m,m} \mathcal{P}_{n,n} \ .$$

Proof. First, we make the observation that

$$\mathcal{U}_m \mathcal{U}_n^* = \mathcal{P}_{m,m} \frac{a_{\overline{\phi}}^{N-m}}{\sqrt{(N-m)!}} \frac{a_\phi^{*\,N-n}}{\sqrt{(N-n)!}} \mathcal{P}_{n,n} \ .$$

If $m < n$ then in view of the property $a_{\overline{\phi}} \mathcal{P}_{n,n}\big|_{\mathbb{F}_n} = 0$ we have

$$\mathcal{U}_m \mathcal{U}_n^* = \frac{\prod_{j=n-m}^{N-m-1} (\mathcal{N}_\phi + j\mathcal{I})}{\sqrt{(N-m)!(N-n)!}} \mathcal{P}_{m,m} a_{\overline{\phi}}^{n-m} \mathcal{P}_{n,n} = 0 \ .$$

In this vein, if $n < m$ then $\mathcal{U}_m \mathcal{U}_n^* = 0$. By $\mathcal{N}_\phi \mathcal{P}_{n,n} = 0$ we assert that if $m = n$ then

$$\mathcal{U}_n \mathcal{U}_n^* = \mathcal{P}_{n,n} \frac{\prod_{j=1}^{N-n} (\mathcal{N}_\phi + j\mathcal{I})}{(N-n)!} \mathcal{P}_{n,n} = \mathcal{P}_{n,n} \ .$$

This relation concludes the proof. □

6.2. *On the spectrum of* h_{ph}. Next, we address key properties of the diagonal part, $h_{\mathrm{ph}}(a_\perp^*, a_\perp)$, of the reduced Hamiltonian. Interestingly, $h_{\mathrm{ph}}(x,y)$ is similar to a self-adjoint operator.

LEMMA 6.5. Assume that the pair-excitation kernel k solves the operator Riccati equation (4.4b) with $\|k\|_{\mathrm{op}} < 1$.

(i) Then the spectrum of $h_{\mathrm{ph}} : \mathfrak{h}_V^1 \cap \phi^\perp \mapsto \mathfrak{h}$ is real and discrete. The corresponding eigenfunctions $\omega_j(x)$, which satisfy $h_{\mathrm{ph}}(x, \omega_j) = E_j \omega_j(x)$ where $E_j > 0$ are the eigenvalues $(j = 1, \dots)$, form a non-orthogonal Riesz basis of $\phi^\perp$.

(ii) Also, suppose that the functions $u_j(x)$ solve the adjoint problem, i.e., $h_{\mathrm{ph}}^*(x, u_j) = E_j u_j(x)$ on $\phi^\perp$ $(j = 1, 2, \dots)$. Then the following completeness relation holds:

$$\sum_{j=1}^{\infty} \overline{\omega_j(x)} u_j(y) = \widehat{\delta}(x,y) \ . \tag{6.2}$$

Proof. The following relation holds on $\phi^\perp$ by use of the Riccati equation (4.4b):

$$(h + k \circ \overline{f_\phi}) \circ (\widehat{\delta} - k \circ \overline{k}) = (\widehat{\delta} - k \circ \overline{k}) \circ (h + f_\phi \circ \overline{k}) \ . \tag{6.3}$$

If $\|k\|_{\rm op} < 1$ then $(\widehat{\delta} - k \circ \overline{k})^{-1}$ and $(\widehat{\delta} - k \circ \overline{k})^{1/2}$ exist and are bounded operators on $\phi^\perp$. By (6.3), the operator $\varkappa := (\widehat{\delta} - k \circ \overline{k})^{-1/2} \circ (h + k \circ \overline{f_\phi}) \circ (\widehat{\delta} - k \circ \overline{k})^{1/2}$ is self-adjoint. Recall that h has discrete spectrum; thus, $h + k \circ \overline{f_\phi}$ has discrete spectrum because $k \circ \overline{f_\phi}$ is compact. Moreover, the eigenvalues of $h + k \circ \overline{f_\phi}$ are positive (see Remark 5.10). By the spectral theorem, the eigenvalues of $\varkappa$ are then positive and discrete, and the respective eigenvectors form an orthonormal basis of $\phi^\perp$.

(i) Let the eigenvalues of $\varkappa$ be $\{E_j\}_{j=1}^\infty$, with eigenvectors $\{\eta_j\}_{j=1}^\infty$. Since the mapping $(h + k \circ \overline{f_\phi}) \mapsto (\widehat{\delta} - k \circ \overline{k})^{-1/2}(h + k \circ \overline{f_\phi})(\widehat{\delta} - k \circ \overline{k})^{1/2}$ is a similarity transformation, the operator $h_{\rm ph}$ also has real spectrum $\{E_j\}_{j=1}^\infty$. From the relation

$$\omega_j(x) = (\widehat{\delta} - k \circ \overline{k})^{1/2}(x, \eta_j) \ , \tag{6.4a}$$

we conclude that $\{\omega_j(x)\}_{j=1}^\infty$ forms a Riesz basis as a bounded perturbation of an orthonormal basis of $\phi^\perp$.

(ii) In a similar vein, the family $\{u_j(x)\}_{j=1}^\infty$ defined by

$$u_j(x) := (\widehat{\delta} - k \circ \overline{k})^{-1/2}(x, \eta_j) \tag{6.4b}$$

forms a Riesz basis for the adjoint problem on $\phi^\perp$.

The resolution of the identity by the eigenvectors η_j of the operator $\varkappa$ reads

$$\sum_{j=1}^\infty \eta_j(x)\overline{\eta_j(y)} = \widehat{\delta}(x, y) \ .$$

This equation yields completeness relation (6.2) by use of (6.4). □

6.3. *Proof of Theorem* 6.1. We are now in position to prove Theorem 6.1. Our argument for the construction of eigenvectors of $\mathcal{H}_{\rm ph}$ relies on the fact the $h_{\rm ph}$ has discrete spectrum. Let $|\psi\rangle := |\psi\rangle_N$.

Proof. We provide the proof in two stages.

Step 1. We decompose $\mathcal{H}_{\rm ph}|\psi\rangle$, where $\mathcal{H}_{\rm ph}$ is given in (6.1). We will show that

$$\begin{aligned}
&\sum_{m=0}^N \mathcal{U}_m^* \mathcal{U}_m \mathcal{H}_{\rm ph} \sum_{n=0}^N \mathcal{U}_n^* \mathcal{U}_n |\psi\rangle = \sum_{m,n=0}^N \mathcal{U}_m^* \left\{\mathcal{U}_m \mathcal{H}_{\rm ph} \mathcal{U}_n^*\right\} \left(\mathcal{U}_n |\psi\rangle\right) \\
&= \sum_{n=0}^N \mathcal{U}_n^* h_{\rm ph}(a_\perp^*, a_\perp) \mathcal{U}_n |\psi\rangle + \sum_{n=0}^{N-2} b_{N,n} \mathcal{U}_n^* \overline{f_\phi}(a_\perp, a_\perp) \mathcal{U}_{n+2} |\psi\rangle \ .
\end{aligned} \tag{6.5}$$

Here, $b_{N,n}$ is a numerical constant. Regarding the operators $\mathcal{U}_n$, see Definition 6.3.

In order to derive (6.5), we invoke Lemma 6.4. In this vein, we notice the relations

$$h_{\rm ph}(a_\perp^*, a_\perp)|\psi\rangle = \sum_{n,m=0}^{N} \mathcal{U}_n^* \mathcal{U}_n h_{\rm ph}(a_\perp^*, a_\perp) \mathcal{U}_m^* \mathcal{U}_m |\psi\rangle = \sum_{n=0}^{N} \mathcal{U}_n^* h_{\rm ph}(a_\perp^*, a_\perp) \mathcal{U}_n |\psi\rangle \ ,$$

$$\begin{aligned}
\frac{a_\phi^{*\,2}}{N} \overline{f_\phi}(a_\perp, a_\perp)|\psi\rangle &= \sum_{n,m=0}^{N} \mathcal{U}_n^* \mathcal{U}_n \frac{a_\phi^{*\,2}}{N} \overline{f_\phi}(a_\perp, a_\perp) \mathcal{U}_m^* \mathcal{U}_m |\psi\rangle \\
&= \sum_{n,m=0}^{N} \mathcal{U}_n^* \mathcal{P}_{n,n} \frac{a_\phi^{N-n}}{\sqrt{(N-n)!}} \frac{a_\phi^{*\,2}}{N} \frac{a_\phi^{*\,N-m}}{\sqrt{(N-m)!}} \mathcal{P}_{m,m} \overline{f_\phi}(a_\perp, a_\perp) \mathcal{U}_m |\psi\rangle \\
&= \sum_{n=0}^{N-2} b_{N,n} \mathcal{U}_n^* \overline{f_\phi}(a_\perp, a_\perp) \mathcal{U}_{n+2} |\psi\rangle \ , \quad b_{N,n} = \frac{\sqrt{(N-n)(N-n+1)}}{N} \ ,
\end{aligned}$$

since only the terms with $n = m - 2$ survive in the last double sum.

Step 2. Next, we describe the finite system that results from the above decomposition. The first observation is that $\mathcal{U}_n|\psi\rangle = |\psi_{N,n}\rangle_n$ where $\psi_{N,n}(x_1, \ldots, x_n)$ is a function orthogonal to the condensate. Let $\psi_n := \psi_{N,n}$, a function of n variables where $n = 0, 1, \ldots, N$. The operator $h_{\rm ph}$ acts on each of these functions ψ_n for $n = 1, 2, \ldots, N$ by preserving the number of variables. On the other hand, the operator $\overline{f_\phi}(a_\perp, a_\perp)$ maps ψ_{n+2} to ψ_n. Denote the first action by $h_{\rm ph} \circ \psi_n$ and the second one by $\overline{f_\phi} : \psi_{n+2}$.

We elaborate on these actions. For a symmetric function $\psi_n(x_1, \ldots, x_n)$, we have

$$h_{\rm ph} \circ \psi_n := d_n \sum_{j=1}^{n} \int \mathrm{d}y \ \{h_{\rm ph}(x_j, y) \psi_n(x_1, \ldots, x_{j-1}, y, x_{j+1}, \ldots, x_n)\} \ .$$

Similarly, $\overline{f_\phi}$ acts on $\psi_{n+2}(x_1 \ldots x_{n+2})$ as follows:

$$\overline{f_\phi} : \psi_{n+2} := b_n \int \mathrm{d}y_1 \, \mathrm{d}y_2 \ \left\{\overline{f_\phi}(y_1, y_2) \psi_{n+2}(y_1, y_2, x_1, \ldots, x_n)\right\} \ .$$

In the above, d_n and b_n are some (immaterial) numerical constants.

Hence, the eigenvalue equation $\mathcal{H}_{\rm ph}|\psi\rangle = E|\psi\rangle$ reduces to a finite system, viz.,

$$h_{\rm ph} \circ \psi_{N,N} = E \psi_{N,N} \ , \tag{6.6a}$$

$$h_{\rm ph} \circ \psi_{N,N-2} + \overline{f_\phi} : \psi_{N,N} = E \psi_{N,N-2} \ , \tag{6.6b}$$

$$h_{\rm ph} \circ \psi_{N,N-4} + \overline{f_\phi} : \psi_{N,N-2} = E \psi_{N,N-4} \ , \ldots \ . \tag{6.6c}$$

This system is upper triangular and manifests the effect of pair excitation, since the number of noncondensate particles is reduced in pairs. The even and odd values of N should be considered separately. We do not give such details here. These equations describe how to compute the fluctuation vector $|\psi_\perp\rangle = \big(\psi_{N,0}, \psi_{N,1}, \ldots, \psi_{N,N}, 0, \ldots\big)$.

Notably, (6.6a) implies the equality of the spectra, $\sigma\left(\mathcal{H}_{\rm ph}\right) = \sigma\left(h_{\rm ph}(a_\perp^*, a_\perp)\right)$, on $\mathbb{F}_N$. Indeed, if (6.6a) has only the trivial solution then all the subsequent equations have trivial solutions. The upper triangular form suggests that we can construct the eigenvalues explicitly. The top equation has infinitely many possible solutions corresponding to the spectrum of $h_{\rm ph}$. The choice of one of them results in a finite system of equations.

We now give the relevant construction, which serves as a proof of existence for system (6.6). For example, start with (see Lemma 6.5)

$$\Omega_N = \prod_{p=1}^{N} \omega_{j_p}(x_p)$$

for given j_p ($p = 0, 1, \ldots, N$) so that Ω_N is an eigenvector of $h_{\rm ph}(a_\perp^*, a_\perp)$, viz.,

$$h_{\rm ph} \circ \Omega_N = \left(\sum_{p=0}^{N} E_{j_p} \right) \Omega_N \ .$$

The action of $\overline{f_\phi}$ on the state Ω_N produces the collection of states

$$\Omega_{l,m} := \prod_{\substack{p=0 \\ p \neq l,m}}^{N} \omega_{j_p}(x_p) \ ; \qquad l, m = 0, 1, \ldots, N \ .$$

We can determine $\Omega_{N-2} := \sum_{l,m} c_{l,m} \Omega_{l,m}$ which plays the role of $\psi_{N,N-2}$. By substituting into (6.6b), we obtain the system $c_{l,m}\big(E_{j_l} + E_{j_m}\big) = b_2 \overline{f_\phi}(\omega_{j_l}, \omega_{j_m})$ which yields $c_{l,m}$. The next state, Ω_{N-4}, is a linear combination of ω_{j_k} where four terms have been removed from the original collection. The idea of computation is similar. One can proceed until all noncondensate particles are removed. This argument concludes our construction of the eigenvectors of $\mathcal{H}_{\rm ph}$ in terms of eigenvectors of $h_{\rm ph}$.

□

It is of some interest to observe that the eigenvectors of $\mathcal{H}_{\rm ph}$ contain (in part) the condensate wave function, in contrast to the eigenvectors of $h_{\rm ph}(a_\perp^*, a_\perp)$.

7. Hermitian approach and J-self-adjoint system. In this section, we focus on how our existence theory for kernel k is connected to another approach, namely, the direct diagonalization of a Hermitian Hamiltonian that does not conserve the number of particles [32, 54]. This Hamiltonian results from the Bogoliubov approximation and has the same spectrum as our non-Hermitian $\widetilde{\mathcal{H}}_{\rm app}$ when restricted to $\mathbb{F}_N$. Our analysis reveals a connection between (unitary) Bogoliubov-type rotations of Hamiltonians that are quadratic in Boson field operators for noncondensate atoms, the operator Riccati equation for k, and the theory of J-self-adjoint operators developed by Albeverio and coworkers [1–3] (see also [24, 74]). These works, however, appear not to address the possible presence of infinitely many solutions to the Riccati equation which is suggested by our existence theory. We also point out that our results so far imply the existence of solutions to the eigenvalue problem for Boson excitations (quasiparticles) formulated in [32], if the delta function interaction potential is regularized.

7.1. *On a reduced Hamiltonian via the Bogoliubov approximation.* Recall our reduced Hamiltonian with a smooth interaction potential (Section 4.1), viz.,

$$\mathcal{H}_{\rm app} = N E_{\rm H} + h(a_\perp^*, a_\perp) + \frac{1}{2N} f_\phi(a_\perp^*, a_\perp^*) a_\phi^2 + \frac{1}{2N} \overline{f_\phi}(a_\perp, a_\perp) a_\phi^{*\,2} \ .$$

Let us now apply the Bogoliubov approximation to this $\mathcal{H}_{\rm app}$ by formally replacing the operators $a_{\overline{\phi}}$, $a^*_{\overline{\phi}}$ with $\sqrt{N}$. This results in the Hamiltonian $\mathcal{H}_{\rm Bog} : \mathbb{F} \mapsto \mathbb{F}$ where

$$\mathcal{H}_{\rm Bog} := NE_{\rm H} + h(a^*_\perp, a_\perp) + \frac{1}{2} f_\phi(a^*_\perp, a^*_\perp) + \frac{1}{2}\overline{f_\phi}(a_\perp, a_\perp) \ , \tag{7.1}$$

which does not commute with the number operator $\mathcal{N}$.

Next, we discuss the diagonalization of $\mathcal{H}_{\rm Bog}$ by using eigenstates of the operator $h_{\rm ph} : \mathfrak{h}^1_V \cap \phi^\perp \to \mathfrak{h}$ defined by (6.1b) (section 6). We proceed similarly to the approach in [32], where $\mathcal{H}_{\rm Bog}$ is diagonalized via (unitary) Bogoliubov-type rotations of the Boson field operators in the space orthogonal to ϕ; see equation (2.14) in [32], for a delta function interaction potential. Consider the quasiparticle operators γ_j, γ^*_j defined as follows [32].

DEFINITION 7.1. The operators γ_j, $\gamma^*_j : \mathbb{F} \mapsto \mathbb{F}$ ($j = 1, 2, \dots$) are defined by

$$\gamma_j := \int \mathrm{d}x \ \{\overline{u_j(x)} a_{\perp,x} + \overline{v_j(x)} a^*_{\perp,x}\} \ , \quad \gamma^*_j := \int \mathrm{d}x \ \{u_j(x) a^*_{\perp,x} + v_j(x) a_{\perp,x}\} \ .$$

In the above, $\{u_j(x)\}_{j=1}^\infty$ is a Riesz basis of $\phi^\perp$ and $\{v_j(x)\}_{j=1}^\infty$ are chosen such that γ_j and γ^*_j satisfy the canonical commutation relations.

One can verify that γ_j, γ^*_j satisfy the canonical commutation relations provided

$$\begin{aligned} &\int \mathrm{d}x \ \{u_j(x) v_{j'}(x) - v_j(x) u_{j'}(x)\} = 0 \ , \\ &\int \mathrm{d}x \ \{u_j(x) \overline{u_{j'}(x)} - v_j(x) \overline{v_{j'}(x)}\} = \delta_{jj'} \ . \end{aligned} \tag{7.2}$$

We proceed to show that the diagonalization of $\mathcal{H}_{\rm Bog}$ in terms of γ_j and γ^*_j implies that $\{u_j(x), v_j(x)\}_{j=1}^\infty$ must solve a linear system of PDEs [32]. Let us momentarily assume the following completeness relations:

$$\begin{aligned} &\sum_{j=1}^\infty \{u_j(x) \overline{u_j(x')} - \overline{v_j(x)} v_j(x')\} = \widehat{\delta}(x, x') \ , \\ &\sum_{j=1}^\infty \{u_j(x) \overline{v_j(x')} - \overline{v_j(x)} u_j(x')\} = 0, \quad \forall x, \, x' \in \mathbb{R}^3 \ . \end{aligned} \tag{7.3}$$

In view of Definition 7.1, these allow us to decompose the operators $a_{\perp,x}$ and $a^*_{\perp,x}$ as

$$a_{\perp,x} = \sum_{j=1}^\infty \{u_j(x) \gamma_j - \overline{v_j(x)} \gamma^*_j\} \ , \quad a^*_{\perp,x} = \sum_{j=1}^\infty \{\overline{u_j(x)} \gamma^*_j - v_j(x) \gamma_j\} \ .$$

These two relations together with Definition 7.1 amount to a Bogoliubov-type (unitary) transformation in the space orthogonal to the condensate ϕ. The substitution of these expressions into (7.1) along with the requirement that the terms proportional to $\gamma_j \gamma_l$ and $\gamma^*_j \gamma^*_l$ vanish (for all $j, l = 1, 2, \dots$) yields the following eigenvalue problem:

$$\begin{pmatrix} h^T_\perp & -f_{\phi\perp} \\ \overline{f_{\phi\perp}} & -h_\perp \end{pmatrix} \circ \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} = E_j \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} \ ; \quad j = 1, 2, \dots \ . \tag{7.4}$$

In the above, the 2×2 matrix is symplectic, and $h_\perp$ and $f_{\phi\perp}$ are the projections of operators h and f_ϕ on space $\phi^\perp$. Equation (7.4) should be compared to equations (2.21a,b) in [32]. Note that the notation for u_j and E_j here is the same as the one used for the

eigenvectors and eigenvalues of $h^*_{\rm ph}$ in section 6.2. In fact, the corresponding quantities turn out to be identical in the two eigenvalue problems, as we discuss below.

7.2. *On the existence of solutions to eigenvalue problem for* $(u_j,\, v_j)$. Let us recall the spectral theory for $h_{\rm ph}$, particularly Lemma 6.5 (section 6.2). We should also stress that this theory relies on the existence of solutions to the Riccati equation for k, Theorem 5.7 (section 5). To make a connection to system (7.4), consider the solutions ω_j and u_j $(j = 1,\, 2,\, \ldots)$ to the eigenvalue problem for $h_{\rm ph}$ and its adjoint. This problem is expressed by the equations

$$\begin{aligned} h_{\rm ph}(x,\omega_j) &= (h + k \circ \overline{f_\phi})(x,\omega_j) = E_j \omega_j(x)\ , \\ h^*_{\rm ph}(x,u_j) &= (h^T + f_\phi \circ \overline{k})(x,u_j) = E_j u_j(x) \qquad (j = 1,\, 2,\, \ldots)\ . \end{aligned}$$

Notice that if we define $v_j(x) := -\overline{k}(x,u_j)$ then the (adjoint) equation for $u_j(x)$ here immediately takes the form of the first equation in system (7.4). We can show that this definition for v_j also gives the second equation in system (7.4) by employing the conjugate Riccati equation (for $\overline{k}$). Indeed, notice that

$$\begin{aligned} -h_\perp(x,v_j) &= (h_\perp \circ \overline{k})(x,u_j) = (-\overline{k} \circ h_\perp^T - \overline{f_\phi} - \overline{k} \circ f_\phi \circ \overline{k})(x,u_j) \\ &= -\overline{k} \circ \big[E_j u_j(x) - f_\phi \circ \overline{k}(x,u_j)\big] - \overline{f_\phi}(x,u_j) - (\overline{k} \circ f_\phi \circ \overline{k})(x,u_j) \\ &= -E_j v_j(x) - \overline{f_\phi}(x,u_j)\ . \end{aligned}$$

Hence, the existence of eigenvectors $\{\omega_j, u_j\}_{j=1}^\infty$ and spectrum $\{E_j\}_{j=1}^\infty$ in regard to $h_{\rm ph}$ entails the existence of solutions to system (7.4).

A few remarks are in order at this stage.

Remark 7.2. We showed an intimate connection of the eigenvalue problem for $h_{\rm ph}$ and its adjoint, based on the Riccati equation for kernel k, to PDE system (7.4) coming from the Hermitian view. A direct comparison to the results in [32] is meaningful if the delta function interaction used in that work is regularized. This connection is in fact a manifestation of a deeper theory which links the Riccati equation to J-self-adjoint matrix operators [1–3]. We briefly discuss aspects of this theory in section 7.3.

Remark 7.3. In [32], an ansatz for the many-body ground state $|\psi_0\rangle$ of the quadratic Hamiltonian $\mathcal{H}_{\rm Bog}$ on $\mathbb{F}$ is

$$|\psi_0\rangle = Z e^{\mathcal{G}} \{a^{*N}_\phi\} |vac\rangle\ ; \quad \mathcal{G} := \frac{1}{2} \int {\rm d}x\, {\rm d}y\ b(x,y)\, a^*_{\perp,x} a^*_{\perp,y}\ .$$

However, a single governing equation for the associated kernel $b(x,y)$ is not provided in [32]. Instead, the condition $\gamma_j |\psi_0\rangle = 0$ is applied for all $j = 1, 2, \ldots$, which yields the following system of integral relations:

$$\int {\rm d}y\ \big\{b(x,y)\overline{u}_j(y)\big\} = -\overline{v_j(x)} \qquad (j = 1,\, 2,\, \ldots)\ .$$

By comparison of this formulation to our approach, we realize that the kernel $b(x,y)$ coincides with $k(x,y)$, and the above integral relations are already a consequence of our solution for k. In fact, in [32] the above integral system is used to define the kernel $b(x,y) = k(x,y)$ when $\{u_j(x), v_j(x)\}$ solve the matrix eigenvalue problem (7.4) under a delta function interaction. The kernel k is expressed as a bilinear form involving ϕ-orthogonal projections of the wave functions v_j [32]; see also [29]. Our existence proof

for k furnished in the context of Theorem 5.7 shows that the ground state $|\psi_0\rangle$ is self-consistent, in the sense that the integral system stemming from $|\psi_0\rangle$ and (7.4) is well posed if a solution to the Riccati equation for k exists.

We find it compelling to give the following corollary for system (7.4).

COROLLARY 1. For the set $\{u_j(x), v_j(x)\}_{j=1}^{\infty}$ of functions that solve (7.4), completeness relations (7.3) and orthogonality relations (7.2) must hold.

Proof. We resort to the spectral theory of operator $h_{\rm ph}$ on space $\phi^{\perp}$, particularly the proof of Lemma 6.5 (section 6.2). Recall the completeness relation for the basis $\{\eta_j\}_{j=1}^{\infty}$ of $\phi^{\perp}$, as well as the relation $\eta_j(x) = (\widehat{\delta} - k \circ \overline{k})^{1/2}(x, u_j)$.

Hence, on $\phi^{\perp}$ we have

$$\widehat{\delta}(x,x') = (\widehat{\delta} - k \circ \overline{k})^{1/2} \left\{ \sum_{j=1}^{\infty} \eta_j(x) \overline{\eta_j(x')} \right\} (\widehat{\delta} - k \circ \overline{k})^{-1/2}$$

$$= (\widehat{\delta} - k \circ \overline{k}) \left\{ \sum_{j=1}^{\infty} u_j(x) \overline{\eta_j(x')} \right\} (\widehat{\delta} - k \circ \overline{k})^{-1/2} = (\widehat{\delta} - k \circ \overline{k}) \sum_{j=1}^{\infty} u_j(x) \overline{u_j(x')} \ .$$

Thus, we obtain

$$\sum_{j=1}^{\infty} u_j(x) \overline{u_j(x')} = \frac{\widehat{\delta}(x,x')}{\widehat{\delta} - k \circ \overline{k}} \ .$$

By use of the relation $v_j(x) = -\overline{k}(x, u_j)$, we can therefore assert that

$$\sum_{j=1}^{\infty} \overline{v_j(x)} v_j(x') = \sum_{j=1}^{\infty} k(\overline{u_j}, x) \overline{k}(x', u_j) = \frac{k \circ \overline{k}}{\widehat{\delta} - k \circ \overline{k}} \ .$$

The last two equations entail the first relation of (7.3).

Next, we invoke the equation just derived to write

$$\sum_{j=1}^{\infty} u_j(x) \overline{v_j(x')} = -\sum_{j=1}^{\infty} u_j(x) k(x', \overline{u_j}) = -(\widehat{\delta} - k \circ \overline{k})^{-1} \circ k \ .$$

Alternatively, we have

$$\sum_{j=1}^{\infty} \overline{v_j(x)} u_j(x') = -\sum_{j=1}^{\infty} k(x, \overline{u_j}) u_j(x') = -k \circ (\widehat{\delta} - \overline{k} \circ k)^{-1} \ .$$

Thus, we obtain the second completeness relation of (7.3) by using the identity $(\widehat{\delta} - k \circ \overline{k})^{-1} \circ k = k \circ (\widehat{\delta} - \overline{k} \circ k)^{-1}$.

Regarding orthogonality relations (7.2), the manipulation of system (7.4) yields the following equations:

$$(E_j - \overline{E_{j'}}) \int \mathrm{d}x \ \{u_j(x) \overline{u_{j'}(x)}\} = \int \mathrm{d}x \ \{-\overline{u_{j'}(x)} f_{\phi}(x, v_j) + u_j(x) \overline{f_{\phi}}(x, \overline{v_{j'}})\} \ ,$$

$$(E_j - \overline{E_{j'}}) \int \mathrm{d}x \ \{v_j(x) \overline{v_{j'}(x)}\} = \int \mathrm{d}x \ \{\overline{v_{j'}(x)}\, \overline{f_{\phi}}(x, u_j) - v_j(x) f_{\phi}(x, \overline{u_{j'}})\} \ .$$

By subtracting the second equation from the first one, we obtain the second orthogonality relation of (7.2), if $\|u_j\|_2^2 - \|v_j\|_2^2 \neq 0$ and this normalization for u_j and v_j is chosen to give unity. The first orthogonality relation of (7.2) follows by a similar procedure. □

7.3. *On the J-self-adjoint system.* Next, we discuss the connection between Riccati equation (4.4b) for the pair excitation kernel and main ideas from the theory of J-self-adjoint operators found in, e.g., [1–3]. A link between these two theories is suggested by the eigenvalue problem (7.4), which involves the symplectic matrix

$$M := \begin{pmatrix} h_\perp^T & -f_{\phi\perp} \\ \overline{f_{\phi\perp}} & -h_\perp \end{pmatrix}; \quad \mathrm{dom}(M) := \mathfrak{h}_V^1 \oplus \mathfrak{h}_V^1 \ . \tag{7.5}$$

Note that the matrix

$$\widetilde{M} := \begin{pmatrix} h^T & -f_\phi \\ \overline{f_\phi} & -h \end{pmatrix}$$

has the zero eigenvalue with eigenvector $(\phi, \overline{\phi})$.

Suppose that $\phi(x)$, $h(x,y)$ and $f_\phi(x,y)$ satisfy the assumptions of Theorem 5.7 (section 5.2). Let k be the unique solution to the Riccati equation with $\|k\|_{\mathrm{op}} < 1$. Then the operator matrix

$$W := \begin{pmatrix} \widehat{\delta} & k \\ \overline{k} & \widehat{\delta} \end{pmatrix} : \phi^\perp \oplus \phi^\perp \mapsto \phi^\perp \oplus \phi^\perp$$

is boundedly invertible, [2] with inverse

$$W^{-1} = \begin{pmatrix} (\widehat{\delta} - k \circ \overline{k})^{-1} & -k \circ (\widehat{\delta} - \overline{k} \circ k)^{-1} \\ -\overline{k} \circ (\widehat{\delta} - k \circ \overline{k})^{-1} & (\widehat{\delta} - \overline{k} \circ k)^{-1} \end{pmatrix} \ .$$

Now let us consider the diagonal matrix

$$D := \begin{pmatrix} h_\perp^T + k \circ \overline{f_{\phi\perp}} & 0 \\ 0 & -h_\perp - \overline{k} \circ f_{\phi\perp} \end{pmatrix} \ .$$

The spectrum of D is $\sigma(\overline{h_{\mathrm{ph}}}) \cup \sigma(-h_{\mathrm{ph}})$, which under the assumptions of Theorem 5.7 consists of two disjoint parts. Since k obeys the Riccati equation on $\phi^\perp$, we have

$$DW = \begin{pmatrix} h_\perp^T + k \circ \overline{f_{\phi\perp}} & -k \circ h_\perp - f_{\phi\perp} \\ \overline{k} \circ h_\perp^T + \overline{f_{\phi\perp}} & -h_\perp - \overline{k} \circ f_{\phi\perp} \end{pmatrix} = WM \ ,$$

where M is defined by (7.5). Thus, the matrix M is similar to the diagonal matrix D.

We proceed to describe implications of this similarity relation. Eigenvectors of the diagonal operator matrix D are of two types. One type is of the form $\big(\omega_j(x), 0\big)$ where $\omega_j(x)$ is an eigenvector of h_{ph}, and another type is of the form $\big(0, \overline{\omega_j(x)}\big)$ (see section 6.2). This fact yields two types of eigenvectors for M after transformation by W^{-1}, viz.,

$$W^{-1} \begin{pmatrix} \omega_j(x) \\ 0 \end{pmatrix} = \begin{pmatrix} (\widehat{\delta} - k \circ \overline{k})^{-1}(x, \omega_j) \\ -\overline{k} \circ (\widehat{\delta} - k \circ \overline{k})^{-1}(x, \omega_j) \end{pmatrix} \ ,$$

and

$$W^{-1} \begin{pmatrix} 0 \\ \overline{\omega_j(x)} \end{pmatrix} = \begin{pmatrix} -k \circ (\widehat{\delta} - \overline{k} \circ k)^{-1}(x, \overline{\omega_j}) \\ (\widehat{\delta} - \overline{k} \circ k)^{-1}(x, \overline{\omega_j}) \end{pmatrix} \ .$$

For the second type of eigenvector, we make the identifications

$$u_j(x) := (\widehat{\delta} - k \circ \overline{k})^{-1}(x, \omega_j) \quad \text{and} \quad v_j(x) := -\overline{k} \circ (\widehat{\delta} - k \circ \overline{k})^{-1}(x, \omega_j) = -\overline{k}(x, u_j) \ .$$

The eigenvectors of the second type are excluded since they yield a negative spectrum.

REMARK 7.4. So far, we assumed that the Riccati equation for k is satisfied and solutions to this equation exist by Theorem 5.7. Conversely, if we assume that the integral system $v_j = -\overline{k}(x, u_j)$ as well as PDE system (7.4) hold then k must obey the Riccati equation. This claim can be proved by the methods that we already developed.

8. Conclusion and discussion. We stress the intimate connection between two apparently disparate approaches (those of Fetter [32] and Wu [76]) for the problem of low-lying Boson excitations via the theory of J-self-adjoint operators of Albeverio and coworkers [2]. This connection sheds light on the concept of the quasiparticle [32]. By exploiting this connection, we were able to prove existence of solutions to the PDE system for the single-particle wave functions u_j and v_j pertaining to elementary excitations in [32]. In addition, we explicitly constructed the eigenvectors of the approximate (reduced) many-body Hamiltonian $\mathcal{H}_{\text{app}}$ for pairs in the N-particle sector of Fock space. Some of our results can be viewed as an application of the theory of J-self-adjoint operators to Boson quantum dynamics.

Let us outline implications of our analysis. Our treatment suggests an alternate view of the concept of the quasiparticle in a Bose gas. In [32], this notion is heuristically introduced via the operator γ_j and its adjoint, γ_j^*. These operators satisfy canonical commutation relations and are manifest in the diagonal form of a quadratic (Hermitian) Hamiltonian that does not conserve the number of particles. In the present work, we show that the corresponding one-particle wave functions u_j and v_j are directly related to the kernel k through the following manipulations. First, $u_j(x)$ can be defined by application of the bounded operator $(\widehat{\delta} - k \circ \overline{k})^{-1/2}$ to the eigenfunction $\eta_j(x)$ of the one-particle self-adjoint operator $\varkappa$ (see proof of Lemma 6.5). Second, $v_j(x)$ can be defined as $v_j(x) = -\overline{k}(x, u_j)$. This treatment, based on a well-defined non-unitary transformation of a quadratic Hamiltonian in the N-sector of Fock space via the pair excitation kernel k, circumvents the need for introducing γ_j and γ_j^*.

Another implication is that the similarity relation $WMW^{-1} = D$, discussed in section 7.3, shows that the spectrum of h_{ph} can change for different solutions to the Riccati equation, but in a predictable way. In particular, since we have the spectrum $\sigma(M) = \sigma(D) = \sigma(h_{\text{ph}}) \cup \sigma(-h_{\text{ph}})$, the (double) spectrum $\sigma(h_{\text{ph}}) \cup \sigma(-h_{\text{ph}})$ is unaffected by the choice of kernel k solving the Riccati equation. However, the spectrum $\sigma(h_{\text{ph}})$ will change under different choices of solutions for k. In light of our analysis, the only possible change induced by $\sigma(h_{\text{ph}}(k)) \mapsto \sigma(h_{\text{ph}}(k'))$ for two different solutions k and k' ($k' \neq k$) is such that a finite collection of eigenvalues $\{E_j\} \subset \sigma(h_{\text{phon}}(k))$ is mapped to $\{-E_j\} \subset \sigma(h_{\text{phon}}(k'))$ while the rest of the eigenvalues remain unchanged.

The kernel k can be invoked in the computation of the pair correlation function $C_2 : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}$ at the ground state Ψ (at zero temperature), which for our purposes is defined by $C_2(x, y) := N^{-1} \langle \Psi | a^*_{\perp,x} a_{\perp,y} a^*_{\phi} a_{\overline{\phi}} | \Psi \rangle$. A calculation of C_2 to the order of

approximation consistent with the reduced Hamiltonian $\widetilde{\mathcal{H}}_{\text{app}}$ yields [32, 76]

$$C_2(x,y) = (k \circ \overline{k}) \left(\widehat{\delta} - k \circ \overline{k}\right)^{-1} .$$

This formula can be extracted from the analysis of [76] if $\|k\|_{\text{op}} < 1$. Hence, the existence of a unique k directly implies a well-defined pair correlation function $C_2(x,y)$. The study of the connection between k and C_2 will be the subject of future work.

We are tempted to mention a few other open problems motivated by our work. For example, given the existence of the kernel k with $\|k\|_{\text{op}} < 1$, it is of interest to consider the effect of a non-unitary transformation analogous to $e^{\mathcal{W}}$ by including contributions from higher-order (cubic and quartic terms) in the reduced many-body Hermitian Hamiltonian. This consideration would plausibly require the introduction of additional kernels, which must satisfy several consistency conditions [77]. Furthermore, it is conceivable that the non-Hermitian approach can be extended to nonzero temperatures below the phase transition in the presence of a trapping potential. In the spirit of the periodic case [50], it is plausible to construct an effective approximate Hamiltonian for pair excitation that involves a parameter for the average fraction of particles at the condensate, and transform the Hamiltonian non-unitarily. Alternatively, one may use a Hermitian approach at nonzero temperatures, e.g., the approach taken up by Griffin [39].

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References

[1] S. Albeverio and A. K. Motovilov, *Solvability of the operator Riccati equation in the Feshbach case* (Russian, with Russian summary), Mat. Zametki **105** (2019), no. 4, 483–506, DOI 10.4213/mzm12061; English transl., Math. Notes **105** (2019), no. 3-4, 485–502. MR3942805

[2] S. Albeverio, A. K. Motovilov, and A. A. Shkalikov, *Bounds on variation of spectral subspaces under J-self-adjoint perturbations*, Integral Equations Operator Theory **64** (2009), no. 4, 455–486, DOI 10.1007/s00020-009-1702-1. MR2534029

[3] S. Albeverio, A. K. Motovilov, and C. Tretter, *Bounds on the spectrum and reducing subspaces of a J-self-adjoint operator*, Indiana Univ. Math. J. **59** (2010), no. 5, 1737–1776, DOI 10.1512/iumj.2010.59.4225. MR2865428

[4] O. E. Alon, R. Beinke, and L. S. Cederbaum, *Many-body effects in the excitations and dynamics of trapped Bose-Einstein condensates*, `arXiv:2101.11615v1` (106pp).

[5] 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), no. 5221, 198–201.

[6] C. M. Bender, *Making sense of non-Hermitian Hamiltonians*, Rep. Progr. Phys. **70** (2007), no. 6, 947–1018, DOI 10.1088/0034-4885/70/6/R03. MR2331294

[7] C. M. Bender, *$\mathcal{PT}$-symmetric quantum theory*, J. Phys. Conf. Ser. **631** (2015), 012002.

[8] C. M. Bender, *$\mathcal{PT}$-symmetric quantum field theory*, J. Phys. Conf. Ser. **1586** (2020), 012004.

[9] C. M. Bender, M. V. Berry, and A. Mandilara, *Generalized PT symmetry and real spectra*, J. Phys. A **35** (2002), no. 31, L467–L471, DOI 10.1088/0305-4470/35/31/101. MR1928842

[10] C. M. Bender and S. Boettcher, *Real spectra in non-Hermitian Hamiltonians having $\mathcal{PT}$ symmetry*, Phys. Rev. Lett. **80** (1998), no. 24, 5243–5246, DOI 10.1103/PhysRevLett.80.5243. MR1627442

[11] C. M. Bender, M. DeKieviet, and S. P. Klevansky, *$\mathcal{PT}$ quantum mechanics*, Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. **371** (2013), no. 1989, 20120523, 4, DOI 10.1098/rsta.2012.0523. MR3035410

[12] C. M. Bender and G. V. Dunne, *Large-order perturbation theory for a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian*, J. Math. Phys. **40** (1999), no. 10, 4616–4621, DOI 10.1063/1.532991. MR1715272
[13] F. A. Berezin, *The method of second quantization*, Pure and Applied Physics, Vol. 24, Academic Press, New York-London, 1966. Translated from the Russian by Nobumichi Mugibayashi and Alan Jeffrey. MR0208930
[14] C. Boccato, *The excitation spectrum of the Bose gas in the Gross-Pitaevskii regime*, Rev. Math. Phys. **33** (2021), no. 1, Paper No. 2060006, 11, DOI 10.1142/S0129055X20600065. MR4205369
[15] C. Boccato, C. Brennecke, S. Cenatiempo, and B. Schlein, *The excitation spectrum of Bose gases interacting through singular potentials*, J. Eur. Math. Soc. (JEMS) **22** (2020), no. 7, 2331–2403, DOI 10.4171/JEMS/966. MR4107508
[16] N. Bogolubov, *On the theory of superfluidity*, Acad. Sci. USSR. J. Phys. **11** (1947), 23–32. MR0022177
[17] L. Boßmann, N. Pavlović, P. Pickl, and A. Soffer, *Higher order corrections to the mean-field description of the dynamics of interacting Bosons*, J. Stat. Phys. **178** (2020), no. 6, 1362–1396, DOI 10.1007/s10955-020-02500-8. MR4081233
[18] C. Brennecke, P. T. Nam, M. Napiórkowski, and B. Schlein, *Fluctuations of N-particle quantum dynamics around the nonlinear Schrödinger equation*, Ann. Inst. H. Poincaré C Anal. Non Linéaire **36** (2019), no. 5, 1201–1235, DOI 10.1016/j.anihpc.2018.10.007. MR3985542
[19] L. S. Cederbaum, *Exact many-body wave function and properties of trapped Bosons in the infinite-particle limit*, Phys. Rev. A **96** (2017), no. 1, 013615.
[20] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, *Feshbach resonances in ultracold gases*, Rev. Mod. Phys. **82** (2010), no. 2, 1225–1286.
[21] N. R. Cooper, J. Dalibard, and I. B. Spielman, *Topological bands for ultracold atoms*, Rev. Mod. Phys. **91** (2019), no. 1, 015005, 55, DOI 10.1103/RevModPhys.91.015005. MR3942980
[22] H. D. Cornean, J. Dereziński, and P. Ziń, *On the infimum of the energy-momentum spectrum of a homogeneous Bose gas*, J. Math. Phys. **50** (2009), no. 6, 062103, 49, DOI 10.1063/1.3129489. MR2541168
[23] 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), no. 3, 875–893.
[24] J.-C. Cuenin and C. Tretter, *Non-symmetric perturbations of self-adjoint operators*, J. Math. Anal. Appl. **441** (2016), no. 1, 235–258, DOI 10.1016/j.jmaa.2016.03.070. MR3488056
[25] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Theory of Bose-Einstein condensation in trapped gases*, Rev. Mod. Phys. **71** (1999), no. 3, 463–512.
[26] I. Danshita, N. Yokoshi, and S. Kurihara, *Phase dependence of phonon tunnelling in bosonic superfluid-insulator-superfluid junctions*, New J. Phys. **8** (2006), 44.
[27] 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), no. 22, 3969–3973.
[28] J. Dereziński and M. Napiórkowski, *Excitation spectrum of interacting bosons in the mean-field infinite-volume limit*, Ann. Henri Poincaré **15** (2014), no. 12, 2409–2439, DOI 10.1007/s00023-013-0302-4. MR3272826
[29] J. Dereziński, M. Napiórkowski, and J. P. Solovej, *On the minimization of Hamiltonians over pure Gaussian states*, Complex Quantum Systems, Lect. Notes Ser. Inst. Math. Sci. Natl. Univ. Singap., vol. 24, World Sci. Publ., Hackensack, NJ, 2013, pp. 151–161, DOI 10.1142/9789814460156_0004. MR3331491
[30] L. Erdős, B. Schlein, and H-T Yau, *Ground-state energy of a low-density Bose gas: A second-order upper bound*, Phys. Rev. A **78** (2008), 053627.
[31] L. Erdős, B. Schlein, and H.-T. Yau, *Derivation of the Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensate*, Ann. of Math. **172** (2010), no. 1, 291–370, DOI 10.4007/annals.2010.172.291. MR2680421
[32] A. L. Fetter, *Nonuniform states of an imperfect Bose gas*, Annals Phys. **70** (1972), no. 1, 67–101.
[33] A. L. Fetter, *Ground state and excited states of a confined condensed Bose gas*, Phys. Rev. A **53** (1996), no. 6, 4245–4249.
[34] A. L. Fetter, *Rotating trapped Bose-Einstein condensates*, Rev. Mod. Phys. **81** (2009), no. 2, 647–691.
[35] S. R. Garcia and M. Putinar, *Complex symmetric operators and applications*, Trans. Amer. Math. Soc. **358** (2006), no. 3, 1285–1315, DOI 10.1090/S0002-9947-05-03742-6. MR2187654

[36] C. W. Gardiner, *Particle-number-conserving Bogoliubov method which demonstrates the validity of the time-dependent Gross-Pitaevskii equation for a highly condensed Bose gas*, Phys. Rev. A **56** (1997), no. 2, 1414–1423.
[37] M. Girardeau and R. Arnowitt, *Theory of many-Boson systems: Pair theory*, Phys. Rev. (2) **113** (1959), 755–761. MR129365
[38] P. Grech and R. Seiringer, *The excitation spectrum for weakly interacting Bosons in a trap*, Comm. Math. Phys. **322** (2013), no. 2, 559–591, DOI 10.1007/s00220-013-1736-8. MR3077925
[39] A. Griffin, *Conserving and gapless approximations for an inhomogeneous Bose gas at finite temperatures*, Phys. Rev. B **53** (1996), no. 14, 9341–9347.
[40] 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
[41] 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
[42] M. Grillakis and M. Machedon, *Pair excitations and the mean field approximation of interacting Bosons, II*, Comm. Partial Differential Equations **42** (2017), no. 1, 24–67, DOI 10.1080/03605302.2016.1255228. MR3605290
[43] 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
[44] 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
[45] M. Grillakis, M. Machedon, and D. Margetis, *Evolution of the Boson gas at zero temperature: mean-field limit and second-order correction*, Quart. Appl. Math. **75** (2017), no. 1, 69–104, DOI 10.1090/qam/1455. MR3580096
[46] E. P. Gross, *Structure of a quantized vortex in boson systems* (English, with Italian summary), Nuovo Cimento (10) **20** (1961), 454–477. MR128907
[47] W. Ketterle, *Nobel lecture: When atoms behave as waves: Bose-Einstein condensation and the atom laser*, Rev. Mod. Phys. **74** (2002), no. 4, 1131–1151.
[48] V. Kostrykin, K. A. Makarov, and A. K. Motovilov, *Existence and uniqueness of solutions to the operator Riccati equation. A geometric approach*, Advances in differential equations and mathematical physics (Birmingham, AL, 2002), Contemp. Math., vol. 327, Amer. Math. Soc., Providence, RI, 2003, pp. 181–198, DOI 10.1090/conm/327/05814. MR1991541
[49] 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. MR88176
[50] 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. MR127865
[51] A. J. Leggett, *Bose-Einstein condensation in the alkali gases: Some fundamental concepts*, Rev. Mod. Phys. **73** (2001), no. 2, 307–356.
[52] M. Lewin, P. T. Nam, and N. Rougerie, *The mean-field approximation and the non-linear Schrödinger functional for trapped Bose gases*, Trans. Amer. Math. Soc. **368** (2016), no. 9, 6131–6157, DOI 10.1090/tran/6537. MR3461029
[53] 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
[54] M. Lewin, P. T. Nam, S. Serfaty, and J. P. Solovej, *Bogoliubov spectrum of interacting Bose gases*, Comm. Pure Appl. Math. **68** (2015), no. 3, 413–471, DOI 10.1002/cpa.21519. MR3310520
[55] E. H. Lieb, R. Seiringer, J. P. Solovej, and J. Yngvason, *The mathematics of the Bose gas and its condensation*, Oberwolfach Seminars, vol. 34, Birkhäuser Verlag, Basel, 2005. MR2143817
[56] 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
[57] O. Morsch and M. Oberthaler, *Dynamics of Bose-Einstein condensates in optical lattices*, Rev. Mod. Phys. **78** (2006), no. 1, 179–215.

[58] P. T. Nam and M. Napiórkowski, *Bogoliubov correction to the mean-field dynamics of interacting bosons*, Adv. Theor. Math. Phys. **21** (2017), no. 3, 683–738, DOI 10.4310/ATMP.2017.v21.n3.a4. MR3695801

[59] P. T. Nam and M. Napiórkowski, *Norm approximation for many-body quantum dynamics and Bogoliubov theory*, Advances in Quantum Mechanics, Springer INdAM Ser., vol. 18, Springer, Cham, 2017, pp. 223–238. MR3588052

[60] P. T. Nam and M. Napiórkowski, *A note on the validity of Bogoliubov correction to mean-field dynamics* (English, with English and French summaries), J. Math. Pures Appl. (9) **108** (2017), no. 5, 662–688, DOI 10.1016/j.matpur.2017.05.013. MR3711470

[61] 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

[62] P. T. Nam and R. Seiringer, *Collective excitations of Bose gases in the mean-field regime*, Arch. Ration. Mech. Anal. **215** (2015), no. 2, 381–417, DOI 10.1007/s00205-014-0781-6. MR3294406

[63] R. Ozeri, N. Katz, J. Steinhauer, and N. Davidson, *Colloquium: Bulk Bogoliubov excitations in a Bose-Einstein condensate*, Rev. Mod. Phys. **77** (2005), no. 1, 187–205.

[64] C. J. Pethick and H. Smith, *Bose-Einstein condensation in dilute gases*, 2nd ed., Cambridge University, Cambridge, UK, 2008.

[65] L. Pitaevskii and S. Stringari, *Bose-Einstein condensation*, International Series of Monographs on Physics, vol. 116, The Clarendon Press, Oxford University Press, Oxford, 2003. MR2012737

[66] L. P. Pitaevskii, *Vortex lines in an imperfect Bose gas*, Soviet Phys. JETP **13** (1961), no. 2, 451–454.

[67] A. Rovenchak, *Effective Hamiltonian and excitation spectrum of harmonically trapped bosons*, Low Temp. Phys. **42** (2016), no. 1, 36–41.

[68] B. Schlein, *Gross-Pitaevskii evolution for Bose-Einstein condensates*, Macroscopic Limits of Quantum Systems (D. Cadamuro, M. Duell, W. Dybalski, and S. Simonella, eds.), Springer Proceedings in Mathematics and Statistics, vol. 270, Springer International Publishing, Cham, Switzerland, 2018, pp. 171–184.

[69] R. Seiringer, *The excitation spectrum for weakly interacting bosons*, Comm. Math. Phys. **306** (2011), no. 2, 565–578, DOI 10.1007/s00220-011-1261-6. MR2824481

[70] R. Seiringer, *Bose gases, Bose-Einstein condensation, and the Bogoliubov approximation*, J. Math. Phys. **55** (2014), no. 7, 075209, 18, DOI 10.1063/1.4881536. MR3390687

[71] J. P. Solovej, *Upper bounds to the ground state energies of the one- and two-component charged Bose gases*, Comm. Math. Phys. **266** (2006), no. 3, 797–818, DOI 10.1007/s00220-006-0020-6. MR2238912

[72] D. M. Stamper-Kurn and M. Ueda, *Spinor Bose gases: Symmetries, magnetism, and quantum dynamics*, Rev. Mod. Phys. **85** (2013), no. 3, 1191–1244.

[73] M. Tomza, K. Jachymski, R. Gerritsma, A. Negretti, T. Calarco, Z. Idziaszek, and P. S. Julienne, *Cold hybrid ion-atom systems*, Rev. Mod. Phys. **91** (2019), no. 3, 035001, 57, DOI 10.1103/RevModPhys.91.035001. MR4015929

[74] C. Tretter, *Spectral theory of block operator matrices and applications*, Imperial College Press, London, 2008, DOI 10.1142/9781848161122. MR2463978

[75] T. T. Wu, *Ground state of a Bose system of hard spheres*, Phys. Rev. **115** (1959), 1390–1404. MR127866

[76] T. T. Wu, *Some nonequilibrium properties of a Bose system of hard spheres at extremely low temperatures*, J. Math. Phys. **2** (1961), 105–123, DOI 10.1063/1.1724205. MR121200

[77] T. T. Wu, *Bose-Einstein condensation in an external potential at zero temperature: General theory*, Phys. Rev. A **58** (1998), no. 2, 1465–1474.

[78] 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), no. 18, 180405.

[79] H.-T. Yau and J. Yin, *The second order upper bound for the ground energy of a Bose gas*, J. Stat. Phys. **136** (2009), no. 3, 453–503, DOI 10.1007/s10955-009-9792-3. MR2529681

[80] V. A. Zagrebnov and J.-B. Bru, *The Bogoliubov model of weakly imperfect Bose gas*, Phys. Rep. **350** (2001), no. 5-6, 291–434, DOI 10.1016/S0370-1573(00)00132-0. MR1853206