# ABSTRACT

Title of dissertation: NON-HERMITIAN APPROACHES
FOR PAIR-EXCITATION
IN QUANTUM BOSON DYNAMICS

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The topic of this thesis is the mathematical analysis of physically motivated models for a trapped dilute Bose gas with repulsive pairwise atomic interactions at zero temperature. Our goal is to develop the spectral theory for excited many-body quantum states of these systems by accounting for the scattering of atoms in pairs from the macroscopic state (condensate). This general methodology, known as *pair-excitation*, was introduced in the physics literature in the 1960s – the work of this thesis provides the first comprehensive mathematical treatment of many aspects of pair-excitation. This includes, e.g., the spectral theory for pair-transformed approximate Hamiltonians, a general existence theory for the pair-excitation kernel, and the connection between the pair-excitation formalism to quasiparticle excitations in the Bose gas.

We formulate the method of pair-excitation for several historical models of the Bose gas from the physics literature. In particular, we focus on the seminal works of Wu, Fetter,

Griffin, and Lee, Huang, and Yang. Each of these models introduce unique features to the mathematical analysis, but the general strategy remains the same: transform the approximate Hamiltonian using a suitably-defined *pair-excitation operator*. This operator is not determined a priori, but is chosen as part of the problem in order to simplify the expression of excited states of the transformed system.

The study begins with models for the Bose gas in the non-translation-invariant setting, where the particles are spatially-confined in an external trapping potential. In this setting, formulating the pair-excitation method entails solving a nonlinear integro-partial-differential equation for the pair-excitation kernel. We provide a general existence theory for this kernel via a variational approach. The kernel which we find allows us to connect the pair-excitation method to the more widely-studied unitary transformation of quadratic Hamiltonians via Bogoliubov rotation. The theory for the kernel also allows us to write a simple formula for excited many-body states, which can be adapted to the various models which we consider in this work.

We then study the problem for the pair-excited transformed approximate Hamiltonian for Bosons in a periodic box. In this setting, the description of the effective Hamiltonian in the momentum basis is particularly simple. However, the lack of particle conservation means that the pair-excitation transform is unbounded in operator norm, and spectral methods developed in earlier chapters are enriched with new tools.

# NON-HERMITIAN APPROACHES FOR PAIR-EXCITATION IN QUANTUM BOSON DYNAMICS

by

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# Chapter 1

# Introduction

The subject of this thesis is the analysis of time-independent systems which model excitations of the weakly-interacting dilute Bose gas at zero temperature. We consider several distinct models of the Bose gas in the chapters that follow, and connections between these models that can be discovered through the mathematical framework of *pair excitation*. The physical phenomenon underlying our investigation is the Bose-Einstein condensation (BEC) in which particles of integer-spin (Bosons) occupy a single quantum state macroscopically. This single state is the condensate.

The general physical theme motivating this work is that pair-excitation provides a *minimal* framework for representing excited states of the Bose gas — this formalism describes a physical process whereby pairs of particles scatter from the condensate into non-condensate single-particle states, thereby depleting the condensate. Including pair-processes in the approximation of many-body dynamics of the Bose gas allows for the modeling of effects beyond the well-studied mean-field theory for BEC, which seeks to describe the many-body ground state for the interacting Bose gas by a single effective quantum wavefunction, the macroscopic condensate.

The mathematical content of the thesis seeks to place the theory of pair-excitation into a rigorous framework, and demonstrate the effective representation of many-body states using this theory. The central component of the pair-excitation method involves the

similarity transformation of an approximate Hamiltonian by a *non-unitary* 'pair-excitation operator,' first suggested by Wu in his study of the non-translation-invariant gas [60]. This is counter-intuitive from the physical perspective; quantum mechanical observables are prescribed by Hermitian operators, and only the *unitary* transformation of a Hermitian operator preserves the expectation of a physical observable. Additionally, the use of a non-unitary pair-excitation operator in this formalism has perhaps made it less desirable for mathematicians to work with compared to unitary transform methods. The benefit of using the non-unitary pair-excitation operator in this work is that it allows us to derive new, physically-transparent formulas for excited many-body states of the model systems under consideration; these formulas offer a clear picture of the scattering processes inherent in the production of low-lying excitations. In the non-translation-invariant setting, developing the theory of pair excitation entails proving the existence of the *pair excitation kernel*, which satisfies a nonlinear integro-differential equation. This kernel then defines the non-unitary pair excitation operator on the bosonic Fock space. We will see that this kernel is intimately related to the unitary Bogoliubov-type transformation (or rotation) of a quadratic Hamiltonian describing the Bose gas, which will be familiar to many physicists. In this sense, we consider the pair-excitation kernel to be a minimal quantity in the description of excitations.

While we will provide a rigorous formulation for pair excitation in several physical models, this work does not address the accuracy of the various approximations for the Bose gas presented here (compared, e.g., to the 'exact' dynamics dictated by the linear many-body Schrödinger equation for $N$ particles). Nor does it treat the time evolution of many-body states. These topics are the subject of intense mathematical interest;

for an introduction to the convergence of mean-field theory to exact dynamics, see the work of Lieb, Seiringer [43, 57], Erdös, Schlein, and Yau [19], as well as the review article by Margetis, Machedon and Grillakis [29]. The intent of this thesis is to elaborate the mathematical features and interconnections between several models for the weakly-interacting Bose gas presented in the physics literature; and to show how these models can be analyzed within a singular (and well-posed) mathematical framework involving non-Hermitian operators and the pair-excitation kernel.

The model systems covered in these chapters describe low-lying excitations of dilute Bose gases, and the many-body states belonging to these systems generalize the tensor product ground state provided by mean-field theory. A brief review of the mean-field theory for BEC is given at the beginning of Chapter 3 (see Section 3.1.1). The systems treated in the next chapters are represented in the physics literature by the works of Lee, Huang, Yang [37, 38], Wu [60, 61], Fetter [20, 21], and Griffin [25]. While these models are well-known among physicists, many of their mathematical details, as well as their common features, have not been explored thoroughly until now.

We refer to the models studied in the following chapters by their approximate (Fock space) Hamiltonians, denoted generically by $\mathscr{H}$. These will be heuristic but physically motivated approximations to the exact many-body Hamiltonian for repulsively-interacting bosons, which governs the quantum dynamics via the linear Schrödinger equation for a system of $N$ particles, where $N$ is finite but large ($N \gg 1$). An example of the exact

Hamiltonian for $N$ particles is given by

$$H = \sum_{j=1}^{N} \Big( -\Delta_j + V_{\text{trap}}(x_j) \Big) + \frac{1}{2} \sum_{\substack{j,k=1 \\ j \neq k}}^{N} \upsilon(x_j - x_k). \tag{1.0.1}$$

Here, $\Delta_j$ denotes the Laplace operator in the coordinate $x_j \in \mathbb{R}^3$, $V_{\text{trap}}(x_j)$ is a trapping potential, and $\upsilon$ denotes the two-particle interaction. The specific assumptions that we make for the trapping and interaction potentials will be covered in the chapters that follow.

As stated, this thesis does not rigorously address the accuracy of the model Hamiltonians $\mathscr{H}$ compared to the exact dynamics, or the domain of validity in which their approximations hold. Rather, our aim is to describe how pair-excitation can be given a rigorous formulation for each model. This formalism utilizes the *non-unitary pair excitation operator* on the Bosonic Fock space, denoted generally by the exponential $\exp(\mathscr{P})$, where $\mathscr{P}$ is a suitable operator in Fock space that describes the depletion of the condensate into pairs of non-condensate particles.

Each of the Chapters 3, 4, 5 begins by introducing a heuristic derivation of the model Fock space Hamiltonian $\mathscr{H}$ studied in that chapter from exact many-body dynamics prescribed, e.g., by exact Hamiltonian $H$. We then define, in each particular setting, a non-unitary pair-excitation operator, $\exp(\mathscr{P})$, and transform the approximate Hamiltonian according to

$$\widetilde{\mathscr{H}} = \exp(\mathscr{P}) \mathscr{H} \exp(-\mathscr{P}).$$

A specific choice of the operator $\mathscr{P}$ in each case will allow us to develop the spectral theory for the transformed approximate Hamiltonian $\widetilde{\mathscr{H}}$. In each chapter, the transformation $\exp(\mathscr{P}) \mathscr{H} \exp(-\mathscr{P})$ will involve a free parameter, which choose so that the resulting operator $\widetilde{\mathscr{H}}$ takes a particularly simple form – in particular, we choose this parameter so

that $\widetilde{\mathscr{H}}$ contains no terms that create pairs of particles. This is analogous to $\widetilde{\mathscr{H}}$ being an upper-triangular matrix, although $\widetilde{\mathscr{H}}$ is defined on an infinite-dimensional Hilbert space (i.e., the Bosonic Fock space $\mathbb{F}$). This particular choice poses constraints for the operator $\mathscr{P}$, which results in a nonlinear intrgro-partial-differential equation for the integral kernel of $\mathscr{P}$, i.e., an equation for the *pair-excitation kernel* $k_{\text{pair}}(x,y)$. The upper-triangular structure of the transformed approximate Hamiltonian allows for its spectrum to be determined from its diagonal part (analogous to the result for finite-dimensional upper-triangular matrices). We will also derive concise formulas for many-body eigenstates of $\widetilde{\mathscr{H}}$ in the Bosonic Fock space. In the chapters where we consider a quadratic model for the Bose gas, this offers an alternative viewpoint to the 'quasiparticle' description familiar to the study of quadratic Hamiltonians.

The body of work presented in Chapters 2, 3, 4, and 5 considers rigorous mathematical features of several model Hamiltonians (denoted by $\mathscr{H}$ here) which describe the weakly-interacting trapped Bose gas. To our knowledge, this work is new.

We begin in Chapter 2 with a motivating example that offers the most concise description of our general methodology; the model considered in this chapter is the Bose gas in a periodic box with a particle-conserving approximate Hamiltonian. In this setting, we are able to utilize the momentum basis to factor the eigenvalue problem for excited states over subspaces with fixed total momentum. We are also able to consider many-body excited states which have a fixed total number of particles. The pair-excitation operator in this model is formulated as a bounded operator; the similarity transformation of the approximate Hamiltonian by the pair-excitation operator therefore preserves the spectrum. This means that we are able to study the eigenvalue problem for the transformed Hamilto-

nian, and infer results about the spectrum of original system. In particular, we choose the pair-excitation operator so that the resulting many-body states of the transformed system take a simple form – the transformation will be chosen so that all states of the transformed system are *finite linear combinations of momentum eigenstates*. We subsequently derive concise formulas for excited many-body states of the approximate Hamiltonian, by transforming these finite-superposition states by the pair-excitation operator.

Chapter 2 serves as a general motivation for later chapters – we will seek results for many-body excited states for a family of approximate Hamiltonians in Chapters 3, 4, and 5. We will see that the system described in Chapter 2 is the simplest model in which to study pair-excitation, for several reasons. Chapters 3, 4, 5 describe the nontrivial extension of these fundamental results to non-translation-invariant settings, where the condensate and excited states may affect each other in complicated ways, and to approximate Hamiltonians which do not conserve the number of particles.

Chapters 3 and 4 study the weakly-interacting Bose gas in a generic trapping potential $V_{\text{trap}}(x)$. Throughout the work, the assumptions on $V_{\text{trap}}(x)$ are kept minimal; the emphasis is on developing a mathematically rigorous theory of pair-excitation in a non-translation-invariant setting with minimal assumptions. In general, we will assume that $V_{\text{trap}}(x)$ is defined so that the single-particle Schrödinger operator $-\Delta + V_{\text{trap}}(x)$ has a discrete spectrum and a gap between its lowest and first excited state. See the introductions to Chapters 3 and 4 for details.

Chapter 3 considers a model for the particle-conserving Bose gas in a generic trapping potential, $V_{\text{trap}}(x)$, based on the model developed by Wu (1960) [60]. The trapping potential confines the particles so that the system is no longer translation-invariant. It is

therefore not possible to simplify the eigenvalue problem for the approximate Hamiltonian by representing it in the momentum basis. Similar to the model of Chapter 2, though, the approximate Hamiltonian in Chapter 3 is particle-conserving. The pair-excitation operator which we formulate is bounded on the Fock space for $N$ particles, but non-translation-invariant. A new quantity – the pair-excitation kernel – describes the spatial variation of the pair-scattering process. We develop the spectral theory for the transformed Hamiltonian $\widetilde{\mathscr{H}}$ of this system, based on our explicit construction of the pair excitation kernel. This kernel solves a nonlinear operator Riccati equation, which results from choosing the pair-excitation transform in a similar way as was done in Chapter 2, so that the resulting transformed operator does not create pairs of particles. We then seek to construct many-body eigenstates of $\widetilde{\mathscr{H}}$ as finite superpositions by determining a single-particle basis which plays the role that the momentum basis did in Chapter 2. We discover that this basis is intimately related to the pair-excitation kernel $k_{\text{pair}}(x,y)$, as well as a non-orthogonal basis which describes the *unitary* rotation of a related quadratic many-body Hamiltonian first used by Fetter (1970) [20]. The discovery of this connection is new to our work, and closely parallels developments in the mathematical theory of $J-$self adjoint operators and operator Riccati equations [2,3,13,58]. The main mathematical results in this chapter are an existence proof for the pair-excitation kernel, the discovery of the single-particle (non-orthogonal) basis which describes the 'phonon' spectrum of $\mathscr{H}$, the connection between this basis and the unitary rotation of a quadratic Hamiltonian, and the construction of many-body eigenstates of $\mathscr{H}$ using this new basis.

In Chapter 4, we demonstrate the utility of the pair-excitation method for a model of the Bose gas which includes additional effects of particle correlations not present in the

models of Chapters 2 or 3. We focus on the model of Griffin (1995) [25], which describes a non-particle-conserving, non-translation-invariant system in a trapping potential $V_{\text{trap}}$. The additional correlations present in this model modify the equation for the condensate in a nontrivial way – coupling the condensate to the basis of elementary excitations. We exploit the results of Chapter 3 to recast this system into a coupled system for the condensate, along with a pair-excitation kernel. The kernel equation can be written in a way which formally resembles the Riccati equation of Chapter 3, although it contains additional nonlinear terms. We construct a solution to this kernel equation by iterating from the known solution to the Riccati equation produced in Chapter 3. An important element of this iteration is the small parameter $g > 0$, which describes the strength of the interaction. In this sense, the nonlinear terms introduced in this model are treated as small perturbations to the system of Chapter 3 when the particle interactions are weak.

In Chapter 5, we return to the physical setting of the periodic box to analyze the celebrated model of Lee Huang and Yang. The approximate Hamiltonian of this model factors over pairs of equal-and-opposite momenta, similar to the model of Chapter 2. However, in distinction to Chapter 2, the Lee-Huang-Yang approximate Hamiltonian does not conserve the number of particles. The pair-excitation operator that we introduce in Chapter 5 is consequently an unbounded operator, defined on the Fock space $\mathbb{F}$. Thus, we extend the method of pair-excitation to study eigenstates of a quadratic approximate Hamiltonian. Transforming the Lee-Huang-Yang Hamiltonian by an unbounded, non-Hermitian operator means that we cannot immediately use the spectral theory for the transformed Hamiltonian to derive the spectrum of the Lee-Huang-Yang Hamiltonian. Indeed, we find that the (point) spectrum of the transformed Hamiltonian is the whole

complex plane, $\mathbb{C}$. The major result of Chapter 5 describes how we can identify a special subset of eigenstates of the transformed Hamiltonian with 'physical' eigenstates of the Lee-Huang-Yang Hamiltonian. We do this, in principle, without any prior knowledge about the spectrum of the Lee-Huang-Yang Hamiltonian (which is derived in the seminal paper [37]). The perspective of this chapter is to show that the analysis of the quadratic Hamiltonian can be carried out via its non-unitary transformation (i.e., by 'forgetting' the original Hermitian problem). We do this in order to demonstrate how the pair-excitation method is capable of reproducing all the usual results of achievable by other methods. We then derive new formulas for excited many-body eigenstates of the Lee-Huang-Yang system in the momentum basis by making use of the pair excitation operator, as was done in previous chapters. The many-body excited states of the transformed system are not necessarily finite superpositions of momentum states; however, we find that eigenstates which correspond to the Lee-Huang-Yang Hamiltonian are precisely the transformation of finite superposition states.

We conclude the thesis with an overview in Chapter 6, where we discuss the consequences of this work for understanding the phonon spectrum and quasiparticles in the Bose gas. We then discuss possible extensions of the work to physically relevant settings.

We will describe the formalism of pair excitation independently in each of the chapters, as it builds on the core methods of mean-field theory.

# Chapter 2

# Common Mathematical themes and a Motivating Example

## 2.1 Periodic Box

We now describe a simplified model system which illustrates significant features of the models in chapters to come, while avoiding many of their technical complications. This section will also be an opportunity to introduce notation that will be present throughout the rest of the work, and familiarize the reader with the kinds of heuristic approximation that we employ in Chapters 3, 4, and 5.

Consider $N$ particles, where $N$ is finite but large, in the box with size $L$, denoted $B_L$, which has volume $|B_L| := L^3$, with periodic boundary conditions and repulsive pairwise particle interactions specified by the potential $\upsilon(x-y) := g\delta(x-y)$, $x, y \in \mathbb{R}^3$. Here, as in what follows, $\delta$ denotes the Dirac delta function, and the parameter $g > 0$ describes the stregth of the repulsive interaction. On the Hilbert space $L^2_{\text{sym}}(\mathbb{R}^{3N})$ of symmetric $N-$particle wavefunctions, the quantum many-body Hamiltonian for this system reads :

$$H_N = -\sum_{j=1}^{N} \Delta_j + g\sum_{i<j}^{N} \delta(x_i - x_j), \quad x_i, x_j \in \mathbb{R}^3. \tag{2.1.1}$$

Here we choose units such that $\hbar = 2m = 1$, where $\hbar$ is Planck's constant, and $m$ is the atomic mass.

The Bosonic Fock space $\mathbb{F}$ is the natural domain for the approximation of $H_N$. We define $\mathbb{F}$ as the infinite direct sum of $N-$particle Fock subspaces, i.e.,

$$\mathbb{F} := \bigoplus_{n=0}^{\infty} \mathbb{F}_n, \quad \text{for} \quad \mathbb{F}_0 := \mathbb{C}, \quad \mathbb{F}_n := L^2_{\text{sym}}(\mathbb{R}^{3n}).$$

Vectors on $\mathbb{F}$ will be represented in bra-ket notation, e.g.,

$$|u\rangle \in \mathbb{F} \implies |u\rangle = \{u^n\}, \quad u^n \in \mathbb{F}_n, \quad n = 0, 1, 2 \ldots,$$

and the inner product on $\mathbb{F}$ is defined using the inherited inner-product from each of the $n-$particle fibres; for $|u\rangle, |v\rangle \in \mathbb{F}$, their inner product is

$$\langle u, v\rangle := \sum_{n=0}^{\infty} \langle u^n, v^n\rangle_{\mathbb{F}_n}.$$

Given a single-particle wavefunction $f \in L^2_{\text{sym}}(\mathbb{R}^3)$, we define the creation and annihilation operators, $\{a(\overline{f}), a^*(f)\}$ for the state $f$ on the vector $|u\rangle \in \mathbb{F}$ component-wise by the formulae:

$$\left(a(\overline{f})|u\rangle\right)^n := \sqrt{n+1} \int \mathrm{dx} \left\{ \overline{f(x)}\, u^{n+1}(x, x_2, \ldots, x_n) \right\},$$

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

Thus, for $n \in \mathbb{N}$ fixed, $a(\overline{f})$ takes elements of $\mathbb{F}_{n+1}$ to $\mathbb{F}_n$ when we consider both as subspaces of the Fock space $\mathbb{F}$. The operator $a^*(f)$ takes elements of $\mathbb{F}_n$ to $\mathbb{F}_{n+1}$. It can be verified that $a^*(f)$ is the Hermitian adjoint of $a(f)$ on $\mathbb{F}$, and that for $f, g \in L^2(\mathbb{R}^3)$, the following canonical commutation relations hold:

$$[a(f), a^*(g)] = \langle f, g\rangle_{L^2}, \quad [a(f), a(g)] = 0 = [a^*(f), a^*(g)].$$

Given an orthonormal basis of single-particle states, $\{e_k(x)\} \subset L^2(\mathbb{R}^3)$ (where $k$ ranges over some index set $\mathbb{I}$), we define the basis of creation/annihilation operators

$$a_k := a(\overline{e_k}), \quad a_k^* := a^*(e_k). \tag{2.1.2}$$

It is immediate that the operator basis $\{a_k, a_k^*\}_{k\in\mathbb{I}}$ satisfies the collection of canonical relations

$$[a_k, a_{k'}^*] = \delta_{k,k'}, \quad [a_k, a_{k'}] = 0 = [a_k^*, a_{k'}^*],$$

where $k, k \in \mathbb{I}$, and $\delta_{k,k'}$ is Kronecker's delta. The particular orthonormal basis that we work with in this section consists of the momentum eigenfunctions on the domain $B_L$:

$$e_k(x) := \frac{e^{ik\cdot x}}{\sqrt{|B_L|}}, \quad \text{where} \quad k := \frac{2\pi n}{L}, \quad n \in \mathbb{Z}^3. \tag{2.1.3}$$

These are periodic functions (of spatial variable $x \in B_L$) with period $L$ and the index set $\mathbb{I}$ is the dual lattice:

$$\mathbb{I} = \mathbb{Z}_L^3 := \{k = 2\pi n/L \,\big|\, n \in \mathbb{Z}^3\}.$$

We also define the momentum half-space, $\mathbb{Z}_L^+$, which will make the description of pair-excited states simpler:

$$\mathbb{Z}_L^+ := \{k = 2\pi n/L \,\big|\, n \in \mathbb{Z}^3, n_3 > 0\}.$$

Finally, the field operators $a_x$, $a_x^*$ are defined for $x \in \mathbb{R}^3$ as operator-valued distributions:

$$a_x := \sum_{k\in\mathbb{I}} \overline{e_k(x)} a_k, \quad a_x^* := \sum_{k\in\mathbb{I}} e_k(x) a_k^*. \tag{2.1.4}$$

These operators satisfy:

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

The Hamiltonian $H_N$ can be lifted to the Bosonic Fock space via the field operators:

$$\mathscr{H} = \int dx \{a_x^*(-\Delta_x) a_x\} + \frac{g}{2} \int dx \{a_x^* a_x^* a_x a_x\}. \tag{2.1.5}$$

Inserting (2.1.4) into the expression (2.1.5), and expanding in the momentum basis yields exact many-body Hamiltonian in the momentum-basis creation/annihilation operators:

$$\mathscr{H} = \sum_{k\in\mathbb{Z}^3_L} |k|^2 a^*_k a_k + \frac{g}{2|B_L|} \sum_{k_1+k_2=k_3+k_4} a^*_{k_1} a^*_{k_2} a_{k_3} a_{k_4}. \tag{2.1.6}$$

We consider in this section a *particle-conserving* approximation $\mathscr{H}_{\text{approx}} \approx \mathscr{H}$, and the resulting construction of many-body excited states for $\mathscr{H}_{\text{approx}}$. The approximation is heuristic, which means that we do not, e.g., compute error in using the resulting eigenstates in place of the eigenstates belonging to $\mathscr{H}$. By particle-conserving, we mean that both $\mathscr{H}$ as well as the resulting approximate Fock space Hamiltonian $\mathscr{H}_{\text{approx}}$ commute with the number operator $\mathscr{N} : \mathbb{F} \to \mathbb{F}$, defined by

$$\mathscr{N} := a^*_0 a_0 + \sum_{k\neq 0} a^*_k a_k.$$

As written, this definition singles-out the particle-number operator for the zero-momentum condensate, $e_0(x) = 1/\sqrt{|B_L|}$. Since $[\mathscr{H}, \mathscr{N}] = 0$, we can restrict the problem to the $N-$particle fiber of $\mathbb{F}$, for $N$ finite but large, so that

$$\mathscr{N}|\Psi\rangle = \Big(a^*_0 a_0 + \sum_{k\neq 0} a^*_k a_k\Big)|\Psi\rangle = N|\Psi\rangle, \quad \text{for all} \quad |\Psi\rangle \in \mathbb{F}_N. \tag{2.1.7}$$

The approximation is now described [45]. The fundamental assumption is the condition for small fluctuation around the condensate occupation number. The assumption may be considered as a restriction on the domain of the resulting approximate Hamiltonian – we consider only states $|\Psi\rangle \in \mathbb{F}_N$ such that, for fixed $0 < \xi < 1$, the following inequality holds:

$$\Big|\big\langle \Psi, (N\xi - a^*_0 a_0)\Psi\big\rangle_{\mathbb{F}}\Big| \ll N, \tag{2.1.8}$$

where $\xi$ is (loosely) defined as the fraction of particles in the condensate.

We rewrite the interaction part of the Hamiltonian, separating the different powers of condensate operators $\{a_0, a_0^*\}$:

$$\frac{g}{2|B_L|}\sum_{\substack{k_1,k_2,k_3,k_4\in\mathbb{Z}_L^3\\ k_1+k_2=k_3+k_4}} a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4} := \mathscr{H}_0+\mathscr{H}_2+\mathscr{H}_3+\mathscr{H}_4. \tag{2.1.9}$$

The operators $\mathscr{H}_0, \mathscr{H}_2, \mathscr{H}_3, \mathscr{H}_4$ refer to

$$\begin{aligned}
\mathscr{H}_0 &= \frac{g}{2|B_L|}(a_0^*)^2(a_0)^2,\\
\mathscr{H}_2 &= \frac{g}{2|B_L|}\sum_{k\neq 0}\Big((a_0^*)^2 a_k a_{-k} + a_k^* a_{-k}^* (a_0)^2 + 4(a_0^* a_0) a_k^* a_k\Big),\\
\mathscr{H}_3 &= \frac{g}{|B_L|}\sum_{\substack{k_1,k_2\neq 0\\ k_1+k_2\neq 0}}\Big(a_0^* a_{k_1+k_2}^* a_{k_1} a_{k_2} + a_{k_1}^* a_{k_2}^* a_0 a_{k_1+k_2}\Big)\\
\mathscr{H}_4 &= \frac{g}{2|B_L|}\sum_{\substack{k_1,k_2,k_3,k_4\neq 0\\ k_1+k_2=k_3+k_4}} a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4}.
\end{aligned} \tag{2.1.10}$$

Particle conservation and the restriction of the problem to $\mathbb{F}_N$ implies the relation

$$a_0^* a_0 = N - \sum_{k\neq 0} a_k^* a_k = N\xi + \Big[N(1-\xi) - \sum_{k\neq 0} a_k^* a_k\Big], \quad \text{on} \quad \mathbb{F}_N, \tag{2.1.11}$$

and the assumption of the approximation allows us to treat higher powers of $\Big[N(1-\xi)-\sum_{k\neq 0} a_k^* a_k\Big]$ as negligible. Thus as an example, the term $\mathscr{H}_0$ is rewritten under this approximation as

$$\begin{aligned}
\mathscr{H}_0 = \frac{g}{2|B_L|}(a_0^* a_0)^2 &= \frac{g}{2|B_L|}\Big\{N\xi + \Big[N(1-\xi) - \sum_{k\neq 0} a_k^* a_k\Big]\Big\}^2\\
&\approx \frac{g}{2|B_L|}\Big\{N^2\xi^2 + 2N\xi\Big[N(1-\xi) - \sum_{k\neq 0} a_k^* a_k\Big]\Big\}\\
&= \frac{g}{2|B_L|}\Big\{N^2\xi(2-\xi) - 2N\xi\sum_{k\neq 0} a_k^* a_k\Big\}.
\end{aligned} \tag{2.1.12}$$

In a similar fashion, dropping the higher powers of $\left[N(1-\xi)-\sum_{k\neq 0} a_k^* a_k\right]$, we write

$$\begin{aligned}\mathscr{H}_2 \approx \frac{g}{2|B_L|}\sum_{k\neq 0}(a_0^*)^2 a_k a_{-k} + a_k^* a_{-k}^* a_0^2 \\ + \frac{2g}{|B_L|}\Big\{N^2(1-\xi)^2 - N(1-2\xi)\sum_{k\neq 0} a_k^* a_k\Big\}\end{aligned} \tag{2.1.13}$$

as well as

$$\mathscr{H}_4 \approx \frac{g}{|B_L|}\Big\{-N^2(1-\xi)^2 + 2N(1-\xi)\sum_{k\neq 0} a_k^* a_k\Big\}. \tag{2.1.14}$$

Assembling the approximations above, and including the diagonal part of $\mathscr{H}$, results in the particle-conserving approximation

$$\begin{aligned}\mathscr{H} \approx \mathscr{H}_{\text{approx}} := \frac{g\rho N}{2}\Big[(1-\xi)^2+1\Big] \\ + \sum_{k\neq 0}\Big(k^2 + g\rho\xi\Big)a_k^* a_k + \frac{g}{2|B_L|}\sum_{k\neq 0}\Big((a_0^*)^2 a_k a_{-k} + a_k^* a_{-k}^* a_0^2\Big).\end{aligned} \tag{2.1.15}$$

The quantity $\rho = N/|B_L|$ is the total particle-density. When $\xi \to 1$, i.e., when the condensation is complete, The approximation reads:

$$\mathscr{H}_{\text{approx}}(\xi = 1) := \frac{g\rho N}{2} + \sum_{k\neq 0}\Big(k^2 + g\rho\Big)a_k^* a_k + \frac{g}{2|B_L|}\sum_{k\neq 0}\Big((a_0^*)^2 a_k a_{-k} + a_k^* a_{-k}^* a_0^2\Big). \tag{2.1.16}$$

We will see that this approximate Hamiltonian is similar to the models of the following chapters in several ways. In particular, $\mathscr{H}_{\text{approx}}$ represents a restriction of the model in Chapter 3 to the spatial domain of the periodic box $B_L$. Our use of the momentum basis here, which reduces the off-diagonal terms of $\mathscr{H}_{\text{approx}}$ to couplings between pairs of equal-and-opposite momenta, $(k,-k)$, is special to the translation-invariant system. Compared to the model in Chapter 4, this model and approximation scheme only includes the effects of specific terms coming from the interaction – that is, the model of Chapter 4 retains more terms from the interaction compared to this approximation. Finally, compared

to the Lee-Huang-Yang model of Chapter 5, the model (2.1.16) is particle-conserving. The pair-excitation transform which we now introduce will therefore be bounded on the $N-$particle Fock space $\mathbb{F}_N$. This significantly simplifies the analysis of the spectrum for the operator $\mathscr{H}_{\text{approx}}$ here (see the equation (2.1.18) in the next paragraph).

We now introduce the transformation of the approximate Hamiltonian, $\exp(\mathscr{W})\mathscr{H}_{\text{approx}}\exp(-\mathscr{W})$, in order to derive a formula for eigenstates of $\mathscr{H}_{\text{approx}}$ in the Fock space $\mathbb{F}_N$. The operator $\mathscr{W}$ is defined via

$$\mathscr{W} := \frac{1}{N}\sum_{k\in\mathbb{Z}_L^+} -\alpha(k)a_k^* a_{-k}^* (a_0)^2, \quad \text{for} \quad 0 \leq \alpha(k) < 1 \quad \forall k \in \mathbb{Z}_L^+. \tag{2.1.17}$$

The general strategy for introducing the transformation by $\exp(\mathscr{W})$ is to determine the coefficients $\alpha(k)$ in such a way as to simplify the expression of the transformed operator. On the $N-$particle fiber, $\mathbb{F}_N$, the operators $\mathscr{W}$, and therefore $\exp(-\mathscr{W})$, are bounded. Thus, even through the operator $\mathscr{W}$ is non-Hermitian, the following equivalence of spectra holds:

$$\sigma(\mathscr{H}_{\text{approx}}) = \sigma\big(\exp(\mathscr{W})\mathscr{H}_{\text{approx}}\exp(-\mathscr{W})\big). \tag{2.1.18}$$

The conjugations of the momentum basis operators with $\exp(\mathscr{W})$ are given by:

$$\begin{aligned}
&\exp(\mathscr{W})a_0\exp(-\mathscr{W}) = a_0,\\
&\exp(\mathscr{W})a_k^*\exp(-\mathscr{W}) = a_k^*,\\
&\exp(\mathscr{W})a_k\exp(-\mathscr{W}) = a_k + \frac{\alpha(k)}{N}a_{-k}^* a_0^2,\\
&\exp(\mathscr{W})a_0^*\exp(-\mathscr{W}) = a_0^* - \frac{2}{N}\sum_{k\in\mathbb{Z}_L^+}\alpha(k)\big(a_k^* a_{-k}^*\big)a_0.
\end{aligned} \tag{2.1.19}$$

In particular, the transformed approximate Hamiltonian $\exp(\mathscr{W})\mathscr{H}_{\text{approx}}\exp(-\mathscr{W})$ will contain cubic and quartic terms in momentum state creation/annihilation operators; these

terms must be dropped on the basis of the approximation scheme. The result of the formulae (2.1.19), after dropping the terms just described, is:

$$\begin{aligned}\exp(\mathscr{W})\mathscr{H}_{\text{approx}}\exp(-\mathscr{W}) \approx \frac{g\rho N}{2} + \frac{g}{2\rho}\sum_{k\in\mathbb{Z}_L^3}\alpha(k) + \frac{g}{2|B_L|}\sum_{k\in\mathbb{Z}_L^3} a_k a_{-k}(a_0^*)^2 \\ + \sum_{k\in\mathbb{Z}_L^3}\Big(k^2 + g\rho + g\rho\,\alpha(k)\Big)(a_k^* a_k) \\ + \sum_{k\in\mathbb{Z}_L^3}\Big(\big(k^2+g\rho\big)\alpha(k) + \frac{g\rho}{2} + \frac{g\rho}{2}\big(\alpha(k)\big)^2\Big)a_k^* a_{-k}^* \frac{a_0^2}{N}.\end{aligned} \tag{2.1.20}$$

The last line of this approximation, which contains the terms proportional to $(a_k^* a_{-k}^*)$, will vanish provided that the following equation holds for $\alpha(k)$,

$$\alpha(k) = \frac{1}{g\rho}\Big\{-(k^2+g\rho) \pm k\sqrt{k^2+2g\rho}\Big\}, \tag{2.1.21}$$

Choosing the solution which corresponds to the plus sign in this expression entails

$$\begin{aligned}\exp(\mathscr{W})\mathscr{H}_{\text{approx}}\exp(-\mathscr{W}) \approx \frac{g}{2\rho N} + \frac{g}{2\rho}\sum_{k\in\mathbb{Z}_L^3}\alpha(k) \\ + \sum_{k\in\mathbb{Z}_L^3}\Big(k\sqrt{k^2+2g\rho}\Big)\big(a_k^* a_k\big) + \frac{g}{2|B_L|}\sum_{k\in\mathbb{Z}_L^3} a_k a_{-k}(a_0^*)^2.\end{aligned} \tag{2.1.22}$$

We consider eigenstates $|\Psi(k)\rangle \in \mathbb{F}_N$ which are linear combinations of tensor product states containing only the momenta $(k,-k)$, and which solve the equation

$$\exp(\mathscr{W})\mathscr{H}_{\text{approx}}\exp(-\mathscr{W})|\Psi(k)\rangle = E|\Psi(k)\rangle. \tag{2.1.23}$$

For this purpose, states $|\Psi\rangle \in \mathbb{F}_N$ are most succinctly described as vectors :

$$|\Psi\rangle = \Big(\Psi_0, \Psi_1, \ldots, \Psi_n, \ldots, \Psi_{N-1}, \Psi_N\Big)^T; \tag{2.1.24}$$

the component $\Psi_n$ in this vector refers to the symmetric tensor product that contains $N-n$ particles in the condensate $e_0(x)$, and $n$ particles in a state orthogonal to the condensate,

denoted $\Psi_n^{\perp} \in \phi^{\perp}(\mathbb{R}^{3n})$, viz.,

$$\Psi_n := \Psi_n^{\perp} \otimes_s (e_0)^{\otimes_s N-n}.$$

In $|\Psi(k)\rangle$, we assume that the component $\Psi_n^{\perp}$ is a linear combination of momentum states $e_k(x)$ and $e_{-k}(x)$ for every $n$. In this notation, the eigenvalue problem (2.1.23) translates to an upper triangular matrix eigenvalue problem for the vectors $(\Psi_0, \ldots, \Psi_N)^T$. This is because the terms in the transformed Hamiltonian (2.1.22) that correspond to momentum $k \in \mathbb{Z}_L^+$ either: **(a)** transform a component $\Psi_n$ to $\widetilde{\Psi}_n$ with the same number of particles in the condensate, or **(b)** transform $\Psi_n$ to a $\widetilde{\Psi}_{n-2}$, with 2 additional particles in the condensate.

The eigenvalues $E$ of this upper-triangular matrix equation are equal to the diagonal elements of the matrix, which are

$$E = \big(k\sqrt{k^2+2g\rho}\big)n, \quad n = 0, 1, \ldots, N-1, N. \tag{2.1.25}$$

These are energies of the diagonal operator $k\sqrt{k^2+2g\rho}\big(a_k^* a_k + a_{-k}^* a_{-k}\big)$ on $\mathbb{F}_N$. The off-diagonal terms of (2.1.22) couple states of the form $\Psi_n^{\perp} \otimes_s (e_0)^{\otimes_s N-n}$ to states $\Psi_{n-2}^{\perp} \otimes_s (e_0)^{\otimes_s N-n+2}$ where $\Psi_{n-2}^{\perp}$ is the result of annihilating one particle with momentum $k$ and one particle with momentum $-k$ from $\Psi_n^{\perp}$. Using the integer $p$ as before to denote the difference in the particle number between states with momentum $k$ and those with momentum $-k$, we can write the (non-normalized) eigenstates as

$$|\Psi_{p,N}(k)\rangle := \sum_{s=0}^{(N-p)/2} \tilde{y}(k)^{-s} \binom{N}{s} \left(\binom{p+s}{s}\right)^{-1/2} \left(\binom{2N}{2s}\right)^{-1/2} \left(\frac{1}{2s!}\right)^{-1/2} |s+p, s\rangle_{\mathbb{F}_N}, \tag{2.1.26}$$

for

$$|s+p, s\rangle_{\mathbb{F}_N} := \Big((e_k)^{\otimes_s s+p} \otimes_s (e_{-k})^{\otimes_s s} \otimes_s (e_0)^{\otimes_s N-2s-p}\Big)$$

and

$$\tilde{y}(k) := \frac{g}{|B_L|k\sqrt{k^2+2g\rho}}.$$

Note that for every state in $|\Psi_{p,N}(k)\rangle$ there is a degenerate state $|\Psi^{(-)}_{p,N}(k)\rangle$ involving a linear combination of the tensor products $(e_k)^{\otimes_s s} \otimes_s (e_{-k})^{\otimes_s s+p} \otimes_s (e_0)^{\otimes_s N-2s-p}$. Therefore, the degeneracy of states with energy $E$ is $2N+1$, exactly the same as the degenerate subspaces of $\mathscr{H}_{\mathrm{LHY}}$. The expression $\exp(\mathscr{W})|\Psi_{p.N}(k)\rangle$ then gives the eigenstates of $\mathscr{H}_{\mathrm{Wu}}$.

## 2.2 Overview of mathematical themes

We conclude this introduction by discussing how the model introduced here will be altered in the chapters that follow, and the more complicated analysis that the pair-excitation method will entail.

In Chapter 3 we extend the approximation scheme for the exact Hamiltonian to the non-translation-invariant setting, where the condensate is trapped in an external potential $V_{\mathrm{trap}}(x)$. This means that we will no longer represent the Hamiltonian using the momentum basis operators $\{a_k, a_k^*\}$; instead we employ the position space field operators orthogonal to the condensate, $\{a_{\perp,x}, a^*_{\perp,x}\}$, and approximate the exact Fock space Hamiltonian by, e.g., dropping terms which are cubic/quartic in these operators. The parameter $\alpha(k)$ in the pair-excitation operator $\mathscr{W}$ of equation (2.1.17) will become a spatially-dendent pair-exctation kernel, denoted by $k(x,y)$. This kernel will be chosen by imposing a similar constraint on the transformed approximate Hamiltonian, in order to cancel out terms proportional to field operators $a^*_{\perp,x}a^*_{\perp,y}$. The quadratic equation (2.1.21) for $\alpha(k)$ will translate to a nonlinear operator Riccati equation for the kernel $k(x,y)$. Indeed, $\alpha(k)$

corresponds to the inverse Fourier transform of a kernel $k(x,y)$, which is a translation-invariant function of $|x-y|$ in the periodic box.

In order to derive a formula for the spectrum and eigenstates of the approximate Hamiltonian in the non-translation-invariant setting – analogous to the formula (2.1.25) for elementary excitations, and formula (2.1.26) for the eigenstates – we must determine some single-particle basis such that finite collections of tensor product states of these these basis elements form invariant subspaces of the transformed Hamiltonian. This new basis will be determined as part of a non-Hermitian eigenvalue problem for the single-particle operator in the diagonal of the transformed Hamiltonian. We will see that this basis has an intimate connection to the pair-excitation kernel $k(x,y)$.

Finally, in Chapter 5, we return to the periodic box, to extend the method described here to the Lee-Huang-Yang approximate Hamiltonian. This model for low-lying excitations does not conserve the total number of particles. We will have to take exceptional care to formulate the theory for many-body states on the Fock space $\mathbb{F}$ as a result. The spectral theory for the unbounded, non-Hermitian transformed Hamiltonian will have several different cases, which correspond to the momentum subspaces that we consider eigenstates to live in. One case (i.e., range of momenta) will correspond to a simple extension of the results displayed here. We treat Chapter 5 as the first step in formulating a pair-excitation method for general quadratic Hamiltonians.

## Disclaimer on Notation

We will be dealing with several different models in this work. So as to not introduce an inordinate number of symbols, each chapter defines its own notation. This comes at the risk of re-using certain symbols to refer to different quantities across different chapters (for example, the Hamiltonian $\mathscr{H}$ will be different between two different chapters).

# Chapter 3

# Pair-excitation in non-translation-invariant systems

## 3.1 Background

In this chapter, our goal is to describe the excited many-body eigenstates of an interacting Bose system in an external trapping potential. We employ a simplified effective model: a Hamiltonian, called $\mathscr{H}_{\text{app}}$, that is quadratic in the Boson field operators for non-condensate atoms and captures pair creation [60]. This $\mathscr{H}_{\text{app}}$ commutes with the particle number operator; thus, the total number of particles is conserved in Fock space. We formally construct $\mathscr{H}_{\text{app}}$ from the full many-body Hamiltonian with a regularized interaction potential. By invoking the formalism of Wu, [60, 61] we apply a non-unitary transformation to $\mathscr{H}_{\text{app}}$. For stationary states, we analyze the role of 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 satisfies a nonlinear integro-differential equation. We develop an *existence theory* for this equation by a variational approach. Our treatment reveals a previously unnoticed connection of $k$ to the one-particle excitation wave functions, $u_j$ and $v_j$, introduced independently by Fetter via Bogoliubov-type rotations [20]. These functions obey a system of linear partial differential equations (PDEs). 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 $\mathscr{H}_{\text{app}}$, we derive a nonlocal PDE for phonon-like excitations in the trap; and

express its solutions in terms of $u_j$ and $v_j$. We firmly relate the eigenvalues of this nonlocal PDE with $E_j$; and recover the excitation spectrum obtained in Ref. [20]. Our approach yields an explicit construction of the excited many-body eigenstates of $\mathscr{H}_{\rm app}$ in the sector of Fock space with a fixed number of particles.

Our tasks and results can be outlined as follows (see also Section 3.2):

- Starting from a many-body Hamiltonian with positive and smooth interaction and trapping potentials, we formally apply an approximation scheme that leads to a Hamiltonian, $\mathscr{H}_{\rm app}$, quadratic in the Boson field operator for noncondensate atoms. $\mathscr{H}_{\rm app}$ is a regularized version of the model in Ref. [61]. The total number of particles is conserved.

- For stationary states, we invoke the concept of pair excitation [60]. A key ingredient is the pair excitation kernel, $k$, which is involved in a *non-unitary* transformation of $\mathscr{H}_{\rm app}$. In operator form this $k$ satisfies a Riccati equation.

- By constructing a functional of $k$, we prove the existence of solutions to the operator Riccati equation in an appropriate space. Our analysis, based on a variational principle, differs from many previous treatments of the operator Riccati equation. We indicate the possibility of multiple solutions for $k$, 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 $\mathscr{H}_{\rm app}$ in the $N$-particle sector of Fock space. We show that the spectrum of $\mathscr{H}_{\rm app}$ 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 Ref. [20]. We employ the theory of $J$-self-adjoint operators by Albeverio and coworkers [2–4, 13]. Hence, we connect the apparently disparate approaches for low-lying (phonon-like) excitations by Fetter [20] and Wu [60, 61].

- As a consequence of the non-unitarily transformed $\mathscr{H}_{\text{app}}$, we formally derive a one-particle PDE ("phonon PDE") for single-particle excitations in the trapped Bose gas. By restricting the operator norm of $k$, 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 Ref. [20].

A highlight of our work is the existence proof that we develop for the one-particle excitation wave functions $u_j$ and $v_j$ corresponding to 'quasiparticles' in a trapped Bose gas [20]. The pair excitation kernel $k$, introduced through the non-unitary transformation of $\mathscr{H}_{\text{app}}$, provides a crucial ingredient of this proof. Our work reveals a nontrivial connection between the non-Hermitian framework of Wu [60] to the Hermitian view of Fetter [20] for low-lying excitations via the operator theory of Albeverio and coworkers; [2–4, 13] see Fig. 3.1. Another highlight of our analysis is the explicit construction of excited many-body eigenstates in the $N$-particle sector of the Bosonic Fock space by use of the kernel $k$.

Our main focus is on the analysis of low-dimensional PDEs that formally result from a non-unitary transformation of the approximate many-body Hamiltonian $\mathscr{H}_{\text{app}}$ [60, 61]. This Hamiltonian is a starting point of our analysis, and can be derived heuristically


Figure 3.1: Schematic for the connection of two main physical approaches (left and right panels) to the problem of excitations in the Bose gas via abstract operator theory (central panel).

from the full many-particle Hamiltonian, as we show by using a regularized interaction potential. In our procedure, we fix the (conserved) total number of atoms at the value $N$ ($N \gg 1$). A rigorous justification for $\mathscr{H}_{\rm app}$ lies beyond our scope. In a similar vein, in this work we restrict ourselves to a plausibility argument for the extraction of the equation for $k$. On the other hand, the analysis of solutions is placed on mathematically firm grounds. The thermodynamic limit ($N \to \infty$) is not treated here. For this limit, see, e.g., Refs. [11, 42].

The non-unitarily transformed Hamiltonian considered here has space-time reflection symmetry. The systematic study of the pair-excitation kernel in the framework of space-time-reflection-symmetric quantum theories [6] lies beyond our scope.

Our motivation for the non-Hermitian view is outlined in Section 3.1.2. Previous related works are discussed in Section 3.1.3. The underlying mathematical formalism is reviewed in Section 5.1.3. The chapter organization is sketched in Section 3.1.5. (The reader who wishes to skip the remaining introduction and read result highlights is deferred to Section 3.2.)

### 3.1.1 A review of the mean field theory for BEC

Mathematical models for BEC aim to predict macroscopic quantities – such as the transition temperature, density of particles occupying the condensate, ground-state energy, as well as the scattering of condensate particles to other states – from the microscopic quantum dynamics of bosons. The underlying physical system is described by the (non-relativistic) many-body Schrödinger equation for bosons, viz.,

$$H\Psi = i\partial_t \Psi, \quad (i^2 = -1), \tag{3.1.1}$$

where $H$ is the (self-adjoint) system Hamiltonian, $t$ is time, and $\Psi$ is the symmetric many- (N-) body wavefunction. Notably, the solution $\Psi$ to this equation lives in a high-dimensional space,

$$\Psi(t, x_1, ..., x_N) : \mathbb{R} \times \mathbb{R}^{3N} \to \mathbb{C},$$

by virtue of the large number of particles involved. The presence of particle-particle interactions in the mathematical expression for $H$ renders the problem of solving the equation for $\Psi$ intractable in realistic systems. Importantly though, extracting information about many macroscopic quantities from the (microscopic) Schrödinger dynamics does not require solving equation (3.1.1) for all particles. It is possible to make predictions for the macroscopic behavior of the system via solutions of simpler, effective low-dimensional equations of motion.

This thesis takes a knowledge of the mean-field theory for BEC for granted as the starting point of many of the approximations. In this vein, the mean-field approximation for BEC is capable of reproducing many observed quantities of interacting bosonic systems with a drastic reduction in complexity [31, 43]. The core assumption for (time-

independent) mean-field models is that the many-body ground state wavefunction takes the following form:

$$\Psi(t,x_1,...,x_N) = e^{-itE_{\text{tot}}} \prod_{i=1}^{N} \phi(x_i), \quad \phi : \mathbb{R}^3 \to \mathbb{C}$$

where $E_{\text{tot}}$ is the total ground state energy of the system. Furthermore, the many-body Hamiltonian $H$ is approximated in a way consistent with the above assumption for $\Psi$. The macroscopic or condensate (one-particle) wavefunction $\phi(x)$ involved in the above tensor product for $\Psi$ satisfies a (low-dimensional) nonlinear Schrödinger equation in $\mathbb{R}^3$ with cubic nonlinearity, known as the "Gross-Pitaevskii equation" [32, 53]. For a system with an external trapping potential $V_{\text{trap}}(x) : \mathbb{R}^3 \to \mathbb{R}$ and hard-sphere, repulsive particle-particle interactions, the Gross-Pitaevskii equation reads

$$-\Delta\phi(x) + V_{\text{trap}}(x)\phi(x) + g|\phi(x)|^2\phi(x) = E\phi(x), \quad g > 0.$$

The constant $E$ measures the energy per particle of the condensate and g is the strength of the interactions. This mean field theory provides a ground state energy $E$ per particle that approaches the actual ground state energy per particle of the many-body system in the limit $N \to \infty$ [43]. For a system with a more general interaction potential $\upsilon$ (as in (1.0.1)), the mean-field approximation yields a Hartree equation, viz.,

$$-\Delta\phi(x) + V_{\text{trap}}(x)\phi(x) + g(\upsilon * |\phi(x)|^2)(x)\phi(x) = E\phi(x), \quad g > 0,$$

where $\upsilon * |\phi(x)|^2$ denotes the convolution integral of the potential $\upsilon(x)$ with the condensate density $|\phi(x)|^2$.

### 3.1.2 Why a non-Hermitian view?

The reader may raise the following question: What is the motivation for pursuing 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, it can be argued that the formalism involving the pair-excitation kernel is a natural extension of the systematic treatment by Lee, Huang and Yang for the setting with translation invariance and periodic boundary conditions [37]. In their case, the eigenvectors of the many-body Hamiltonian can be approximately expressed in terms of the action of a non-unitary operator, $e^{-\mathscr{K}}$, on finite superpositions of tensor products of one-particle momentum ($\boldsymbol{p}$) states [37]. The exponent $\mathscr{K}$ is of the form [37, 60]

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

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 $a_0$ was replaced by $\sqrt{N}$ times the identity operator, which amounts to the Bogoliubov approximation [57].

Inspired by Wu's extension to the non-translation invariant setting, [60, 61] for stationary states we consider a Hamiltonian that conserves the total number of atoms. We also replace the exponent $\mathscr{K}$ by an integral $\mathscr{W}$ over $\mathbb{R}^3 \times \mathbb{R}^3$. This integral involves the pair excitation kernel $k$, a symmetric function of two spatial variables, viz.,

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

Here, $a^*_x$ is the Boson field creation operator at position $x$, $\phi$ denotes the condensate wave

function, $a(\bar{\phi})$ is the Boson field annihilation operator for the single-particle state $\phi$, and $\phi$ is assumed to be orthogonal to $k$; see Section 5.1.3. We stress that the operator $\mathscr{W}$ commutes with the particle number operator, and therefore is restricted to the $N$-particle sector of Fock space. Thus, *$\mathscr{W}$ is a well-defined and bounded operator in our formulation*. The kernel $k$ must obey a nonlocal PDE [60,61]. We will prove the existence of stationary solutions to this PDE and explore its implications. Note that $a(\overline{\phi})$ is not replaced by a $c$-number in our approach. The existence of $k$ paves the way to addressing physically tangible properties of the Bose gas in a meaningful way. For example, in Section 3.7 we outline the explicit fashion by which one can describe particle-particle correlations by invoking $k$.

We prove that the $\mathscr{W}$-based formalism, in conjunction with the effective Hamiltonian $\mathscr{H}_{\rm app}$ for pairs, yields the known excitation energy spectrum for the Bose gas, in agreement with other works, e.g., Ref. [20, 42]. In particular, Fetter's approach [20] employs a Bogoliubov-type rotation of Boson field operators in the space orthogonal to $\phi$. The underlying Hamiltonian does not commute with the particle number operator. Here, we place emphasis on the role of the pair-excitation kernel $k$, in the context of a Hamiltonian ($\mathscr{H}_{\rm app}$) that conserves the total number of particles. By using $k$, we transform the effective Hamiltonian non-unitarily and explicitly construct the excited many-body eigenstates in the $N$-particle sector of Fock space. The use of a non-unitary transformation with $k$ here results in a diagonalization scheme that has upper triangular structure.

Another reason for pursuing a non-Hermitian view is that this spells out previously unnoticed connections of abstract operator theory to phonon-like excitations in the trapped Bose gas. We identify the governing equation for $k$ with an operator Riccati equa-

tion. The latter has been studied extensively by Albeverio and coworkers; [2–4] see also Refs. [13, 36, 58]. Our existence theory for $k$, based on a variational approach, differs from existence proofs found in these works. Our formalism has a different flavor from the variational approaches for operator matrices in Ref. [58]. We exploit the connection of pair excitations to the operator Riccati equation to prove existence of solutions to the PDE system for the quasiparticle-related excitation wave functions derived heuristically in Ref. [20]. The Riccati equation for $k$ is inherent to the non-Hermitian formalism [60]. We establish that the excitation spectrum by Fetter's approach [20] comes from the eigenvalue problem for a $J$-self-adjoint operator intimately connected to $k$. We use a regularized interaction potential in the place of the delta-function potential of Refs. [20, 60, 61]. Our findings for the excitation spectrum are independent of the particle-conserving (or not) character of the Hamiltonian. In contrast, the construction of the many-body eigenstates relies on particle conservation.

### 3.1.3 On related past works

The quantum dynamics of the Bose gas has been the subject of numerous studies. It is impossible to exhaustively list this bibliography. Here, we make an attempt to place our work in the appropriate context of the existing literature. For a broad view on Boson dynamics, the interested reader may consult, e.g., Refs. [15, 31, 40, 43, 55, 57, 62].

Mean field limits of Boson dynamics are usually captured by nonlinear Schrödinger-type equations for the condensate wave function [32, 53, 60]. Such limits have been rigorously derived from kinetic hierarchies in distinct scaling regimes for the atomic inter-

actions; see, e.g., Ref. [19]. Our focus in this chapter is different. We primarily address the analysis of low-order PDEs that aim to provide corrections to the mean field dynamics. We also describe connections of the PDE solutions to the excitation spectrum and many-body eigenstates of an approximate Hamiltonian for pair creation.

Second-order corrections to the mean field time evolution have been studied through a Bogoliubov-type transformation [29,30]. Although these works are inspired by Wu's approach, [60,61] they are not strictly faithful to his formalism. In Refs. [29,30], the many-body Hamiltonian is transformed *unitarily* whereas in Refs. [60, 61] the corresponding transformation is *non-unitary*. Here, we take a firm step towards showing the importance of the latter approach via a minimal model, applying a non-unitary transformation to an effective approximate Hamiltonian in the stationary setting.

Wu's formal treatment of the interacting Bose system in non-translation invariant settings aims to transcend the mean field limit [60, 61]. This approach has motivated the use of the pair-excitation kernel $k$ as a means of improving error estimates for the time evolution of Bosons. [31] It has been shown that a unitary, Bogoliubov-type transformation of the many-body Hamiltonian that involves $k$ yields considerably improved Fock space estimates [26–30]. A price to pay for this improvement is that $k$ satisfies a non-local evolution PDE coupled with the condensate wave function. Because of the use of a unitary transformation in Refs. [26–30], their PDE for $k$ is different from the one in Refs. [60, 61].

There are many other papers that tackle the problems of quantum fluctuations around the mean field limit and the excitation spectrum of the Bose gas in the mathematics literature [7, 8, 10, 12, 17, 18, 41, 42, 46–50, 56]. A review of the challenges for the periodic

setting is given by Seiringer [57]. Central roles in many treatments of the excitation spectrum are played by the Bogoliubov approximation and the Bogoliubov transformation. In particular, in Ref. [42] Lewin and coworkers tackle aspects of this problem by use of a quadratic Hamiltonian with a trapping potential via Fock space techniques in the limit $N \to \infty$. These works adopt a Hermitian view, and thus differ from our work. Note that in Ref. [18] 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 [18]. However, because of the lack of the notion of a kernel in this formulation, the connection of the exponential structure of the many-body eigenstates to Fetter's one-particle excitation wave functions $u_j$ and $v_j$, [20] which is pointed out here, is absent in Ref. [18]. To the best of our knowledge, the PDE system for $u_j$ and $v_j$ has not been rigorously studied until now.

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., Refs [5, 15, 24, 25, 39, 51, 54]. We single out the work by Fetter [20–22] who formally addresses the excitation problem through an intriguing PDE system. The existence of solutions to this system has not been studied until now. The underlying many-body formalism 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 [20]. This formalism has been invoked in the modeling of phonon scattering [16] and condensate fluctuations [25].

Our analysis brings forth an intimate mathematical connection of Fetter's theory [20] to Wu's approach [60]. Regarding the existence theory for the operator Riccati equation

obeyed by $k$, we develop a variational approach which significantly differs from the previously invoked fixed-point argument [4,13]. We show that this theory naturally implies the existence of solutions to Fetter's PDE system for a regularized interaction potential [20]. We also construct through $k$ the eigenvectors of the approximate Hamiltonian $\mathscr{H}_{\text{app}}$ in the $N$-particle sector of Fock space. The particle-conserving character of the model is key in this construction.

### 3.1.4 Notation and terminology

- 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 limits are omitted. The corresponding 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 $\phi^\perp := \{ e \in \mathfrak{h}^1_V \mid e \perp \phi \}$ 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 $\mu$ 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 (complex conjugate and transpose) kernel; e.g., $k^*(x,y) = \overline{k(y,x)}$. 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 appropriately.

- 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

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

- 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 $\mathscr{A}|w\rangle$ ($\mathscr{A} : \mathbb{F} \mapsto \mathbb{F}$) as $\langle u|\mathscr{A}|w\rangle$. 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 the '$N$-th fiber' ($N$-particle sector) of $\mathbb{F}$, denoted $\mathbb{F}_N$. We sometimes omit the subscript '$N$' in $|\psi\rangle_N$, simply writing $|\psi\rangle$.

- 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 now 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

$$a_x = a_{\perp,x} + \phi(x) a_{\overline{\phi}} , \quad a_x^* = a_{\perp,x}^* + \overline{\phi(x)} a_\phi^* . \tag{3.1.2}$$

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 the Hamiltonian $\mathscr{H}$ are primarily denoted by calligraphic letters. Some exceptions pertain to annihilation and creation operators including $a_x, a_x^*, a_{\perp,x}, a_{\perp,x}^*$; and $a_{\overline{\phi}}, a_\phi^*$ as well as $a_j, a_j^*$ associated with the basis $\{e_j(x)\}_j \subset \mathfrak{h}$.

- Functionals on Banach spaces are often denoted also by calligraphic letters.

### 3.1.5 Chapter organization

The remainder of the chapter is organized as follows. In Section 3.2 we summarize our results. Section 3.3 focuses on the formal construction of the Hamiltonian $\mathscr{H}_{\text{app}}$, and the derivation of the operator Riccati equation for the pair-excitation kernel $k$. In Section 3.4 we develop an existence theory for this Riccati equation. In Section 3.5 we describe the excitation spectrum and construct the associated eigenvectors of $\mathscr{H}_{\text{app}}$. Key in this description is our use of the $N$-particle sector of the Bosonic Fock space. Section 3.6 addresses the connection of our theory for low-lying excitations to Fetter's approach [20] and the properties of $J$-self-adjoint operators [4]. In Section 3.7 we conclude this chapter and discuss some implications.

## 3.2 Hamiltonian model, main results and methodology

In this section, we define the many-body Hamiltonian, and summarize our results and approach. The starting point is the many-body Hamiltonian in Fock space, viz.,

$$\mathscr{H} = \int \mathrm{d}x\mathrm{d}y \left\{ a_x^* \varepsilon(x,y) a_y + \frac{1}{2} a_x^* a_y^* \upsilon(x-y) a_x a_y \right\} , \tag{3.2.1}$$

where $\varepsilon(x,y) = \{-\Delta_x + V(x)\}\,\delta(x,y)$ is the kinetic part, $\upsilon(x)$ is the pairwise interaction potential, and $V(x)$ is the trapping potential. We assume that $\upsilon(x)$ is positive, symmetric, integrable and bounded on $\mathbb{R}^3$. The trapping potential $V(x)$ is positive and such that the one-particle Schrödinger operator $-\Delta + V$ has discrete spectrum.

### 3.2.1 Reduced Hamiltonian and operator Riccati equation for $k$

Section 3.3 describes Wu's approach [61] in a language closer to operator theory, which serves our objectives. By heuristics, we reduce Hamiltonian (3.2.1) to the quadratic form

$$\mathscr{H}_{\text{app}} = NE_{\text{H}} + h(a_\perp^*, a_\perp) + \frac{1}{2N} f_\phi(a_\perp^*, a_\perp^*) a_\phi^2 + \frac{1}{2N} \overline{f_\phi}(a_\perp, a_\perp) a_\phi^{*\,2} \ ,$$

where $E_H$ is the (mean field) Hartree energy per particle, $h(a_\perp^*, a_\perp)$ and $\overline{f_\phi}(a_\perp, a_\perp)$ are operators of the form $\int \mathrm{d}x\,\mathrm{d}y\,\{a_{\perp,x}^* h(x,y) a_{\perp,y}\}$ and $\int \mathrm{d}x\,\mathrm{d}y\,\{a_{\perp,x} \overline{f_\phi(x,y)} a_{\perp,y}\}$ for suitable kernels $h(x,y)$ and $f_\phi(x,y)$, and $\phi$ is the condensate wave function; see Section 3.3.1. Our derivation of the reduced Hamiltonian $\mathscr{H}_{\text{app}}$ relies on (3.1.2) and the conservation of the particle number. Our goal is to solve the eigenvalue problem $\mathscr{H}_{\text{app}} |\psi\rangle = E_N |\psi\rangle$.

Subsequently, we transform $\mathscr{H}_{\text{app}}$ non-unitarily according to $\widetilde{\mathscr{H}_{\text{app}}} := e^{\mathscr{W}}\, \mathscr{H}_{\text{app}} e^{-\mathscr{W}}$ where the operator $\mathscr{W}$ is of the form $-(2N)^{-1} \int \mathrm{d}x\,\mathrm{d}y\ \{k(x,y)\, a_{\perp,x}^* a_{\perp,y}^*\} a_\phi^2$ which conserves the total number of particles; see Section 3.3.2. The Riccati equation for kernel $k$ is extracted via the requirement that the non-Hermitian operator $\widetilde{\mathscr{H}_{\text{app}}}$ does *not* contain any terms with the product $a_\perp^* a_\perp^*$; see Section 3.3.3. If $k(x, \overline{\phi}) = 0$, the Riccati equation for $k$ reads

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

where the Lagrange multiplier $\lambda$ is determined self-consistently.

### 3.2.2 Existence theory for $k$

In Section 3.4, we introduce a functional of $\overline{k}$ and $k$ by use of which we develop an existence theory for $k$. This functional, $\mathscr{E}[\overline{k},k] : \mathrm{dom}(\mathscr{E}) \to \mathbb{R}$, reads

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

see Section 3.4.1 for the definition of $\mathrm{dom}(\mathscr{E})$. Setting the functional derivative of $\mathscr{E}[\overline{k},k]$ 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

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

In particular, this condition is satisfied if $\phi$ is a minimizer of the Hartree energy, $E_H$. The aforementioned inequality is employed as a hypothesis in the main existence theorem, Theorem 1 (Section 3.4.2). In fact, Theorem 1 states that the above inequality and the property that $f_\phi$ is Hilbert-Schmidt imply that the functional $\mathscr{E}$ restricted to $\mathrm{dom}(\mathscr{E})_\perp = \mathrm{dom}(\mathscr{E}) \cap \{k \in \mathfrak{B}_2(\mathfrak{h}_V^1) \,\big|\, k(x,\overline{\phi}) = 0\}$ attains a minimum for some $k \in \mathrm{dom}(\mathscr{E})_\perp$ which is a weak solution to the operator Riccati equation. We emphasize that $\phi$ 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 ($\mathscr{C}$-) symmetric operators and a variational principle based on functional $\mathscr{E}$. In Section 3.4.3, we discuss the possible non-uniqueness of solutions to the Riccati equation.

### 3.2.3 Spectrum and eigenvectors of reduced non-Hermitian Hamiltonian

In Section 3.5, we study the eigenvectors and spectrum of the non-unitarily transformed Hamiltonian $\widetilde{\mathscr{H}}_{\mathrm{app}}$, under the assumptions of Theorem 1 for $k$. A highlight of our

analysis is the explicit construction of these eigenvectors in $\mathbb{F}_N$ by Fock space techniques. We write $\widetilde{\mathscr{H}_{\text{app}}} = NE_H + \mathscr{H}_{\text{ph}}$ where

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

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

The main result is captured by Theorem 2, which asserts the following equality of spectra:

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

Furthermore, in this theorem we show that for every eigenvector of $h_{\text{ph}}(a_\perp^*, a_\perp)$ with eigenvalue $E$ there is a unique eigenvector of $\mathscr{H}_{\text{ph}}$ 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 3.5.1). Our technique is similar in spirit to that in the construction by Lewin, Nam, Serfaty and Solovej [42]. However, here we consider the eigenvectors of a Hamiltonian that conserves the number of particles as opposed to the Bogoliubov Hamiltonian studied in Ref. [42]. Second, we invoke $k$ explicitly and show that by the restriction $\|k\|_{\text{op}} < 1$, the spectrum of the one-particle Schrödinger-type operator $h_{\text{ph}}$ is positive and discrete, and the corresponding eigenfunctions form a non-orthogonal Riesz basis of $\phi^\perp$ (Section 3.5.2). The proof of the main theorem (Theorem 2) relies on the above steps to show that the eigenvalue problem for $\mathscr{H}_{\text{ph}}$ can be reduced to a finite-dimensional system of equations that has an upper triangular form (Section 3.5.3).

### 3.2.4 Connection to Hermitian approach

In Section 3.6, we compare our approach to Fetter's formalism [20] 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 Fetter's system [20] when the pairwise interaction potential $\upsilon$ is replaced by $g\delta$ for some constant $g > 0$. To this end, we assume that a solution to the operator Riccati equation exists. We discuss the connection of the Riccati equation for $k$ to the theory of $J$-self-adjoint matrix operators by Albeverio and coworkers [2–4] .

Starting with the relevant Bogoliubov Hamiltonian, [20] we indicate that its diagonalization via "quasiparticle" operators (in Fetter's terminology) leads to the PDE system $(j = 1, 2, \ldots)$

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

for the one-particle wave functions $u_j$ and $v_j$ and respective eigenvalues $E_j$ (Section 3.6.1). 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 3.6.2. We also prove that the completeness relations between $u_j$ and $v_j$, previously posed by Fetter, [20] directly follow from our approach. In Section 3.6.3 we invoke ideas from $J$-self-adjoint operator theory to show that the restriction $\|k\|_{\text{op}} < 1$ yields a positive spectrum $\{E_j\}_{j=1}^{\infty}$ for the symplectic matrix involved in the system for $(u_j, v_j)$.

## 3.3 Construction of many-body Hamiltonian for pairs

In this section, we formally construct the (Hermitian) Hamiltonian $\mathscr{H}_{\text{app}}$ 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. We follow the treatment of Wu [60,61] but replace his delta-function potential for repulsive pairwise atomic interactions by a smooth potential.

Section 3.3.1 focuses on heuristic approximations in the Hermitian setting. Section 3.3.2 concerns the non-unitary transformation of the approximate Hamiltonian $\mathscr{H}_{\text{app}}$. In Section 3.3.3, we derive a Riccati equation for the pair excitation kernel of the transformation. Section 3.3.4 provides some discussion on the procedure.

### 3.3.1 Reduction of Hamiltonian in Hermitian setting

In this subsection, we formally reduce the many-body Hamiltonian to an approximate Hermitian operator that is quadratic in the Boson field operators for noncondensate atoms. The total number of particles is conserved. Our main result is described by (6.2.3)–(3.3.1e) below.

We start with Hamiltonian (3.2.1). Let $\phi$ denote the (one-particle) condensate wave function, which has $L^2$-norm $\|\phi\|_2 = 1$. Recall decomposition (3.1.2) for the Boson field operators $a_x$, $a_x^*$. The particle number operator, $\mathscr{N}$, on $\mathbb{F}$ can thus be decomposed as

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

where $\mathscr{N}_\phi := a_\phi^* a_{\overline{\phi}}$ is the number operator for condensate atoms; $\mathscr{N}_\phi$ and $\mathscr{N}_\perp$ commute, and $\mathscr{H}$ commutes with $\mathscr{N}$, viz., $[\mathscr{H}, \mathscr{N}] = \mathscr{H}\mathscr{N} - \mathscr{N}\mathscr{H} = 0$. We use the $N$-th fiber,

$\mathbb{F}_N$, of the Bosonic Fock space, considering state vectors $|\psi\rangle_N$ that satisfy

$$\mathscr{N}|\psi\rangle_N = N|\psi\rangle_N\ ; \qquad \||\psi\rangle_N\| = 1\ .$$

Following Wu, [60] we first expand $\mathscr{H}$ is powers of $a_{\perp,x}$, $a^*_{\perp,x}$ by applying decomposition (3.1.2) for $a_x$, $a^*_x$. The Hamiltonian $\mathscr{H}$ reads

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

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

The next step is to reduce $\mathscr{H}$ 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 $\mathscr{N}_\phi = \mathscr{N} - \mathscr{N}_\perp$ and replace $\mathscr{N}$ by $N$ ($\mathscr{N} \mapsto N$ with $N \gg 1$) because $|\psi\rangle \in \mathbb{F}_N$. We then drop the term $\mathscr{N}^2_\perp$. We take $N - 1 \simeq N$ and *apply a Hartree-type equation* for the condensate wave function $\phi$ which we write as

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

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

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

The PDE for $\phi$ formally becomes the Gross-Pitaevskii equation [32, 53] if $\upsilon$ is replaced by $g\delta$ for some constant $g > 0$.

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

$$\mathscr{H}_{\text{app}} = NE_{\text{H}} + h(a_\perp^*, a_\perp) + \frac{1}{2N} f_\phi(a_\perp^*, a_\perp^*) a_\phi^2 + \frac{1}{2N} \overline{f_\phi}(a_\perp, a_\perp) a_\phi^{*\,2} \tag{3.3.1a}$$

where, abusing notation slightly, we define the operators

$$h(a_\perp^*, a_\perp) := \int \mathrm{d}x\mathrm{d}y \, \left\{ a_{\perp,x}^* h(x,y) a_{\perp,y} \right\} , \tag{3.3.1b}$$

$$f_\phi(a_\perp^*, a_\perp^*) := \int \mathrm{d}x\mathrm{d}y \, \left\{ a_{\perp,x}^* f_\phi(x,y) a_{\perp,y}^* \right\} , \tag{3.3.1c}$$

along with the corresponding kernels

$$h(x,y) := \varepsilon(x,y) + N(\upsilon * |\phi|^2)(x)\, \delta(x,y) + N\gamma(x,y) - \mu\delta(x,y) , \tag{3.3.1d}$$

$$f_\phi(x,y) := N\phi(x)\upsilon(x-y)\phi(y) , \quad \gamma(x,y) := \phi(x)\upsilon(x-y)\overline{\phi(y)} . \tag{3.3.1e}$$

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

$$E_{\text{H}} = \int \mathrm{d}x\mathrm{d}y \, \left\{ \overline{\phi(x)} \varepsilon(x,y) \phi(y) + \frac{N}{2} |\phi(x)|^2 \upsilon(x-y) |\phi(y)|^2 \right\} .$$

Equation (6.2.3) is the desired reduced Hamiltonian. Note the key property

$$[\mathscr{H}_{\text{app}}, \mathscr{N}] = 0 .$$

### 3.3.2 Non-unitary transformation of Hamiltonian $\mathscr{H}_{\text{app}}$

In this subsection, we transform $\mathscr{H}_{\text{app}}$ non-unitarily by use of the pair-excitation kernel, $k$. The main result is given by (3.3.3a) and (3.3.3b) below.

For this purpose, we invoke the following quadratic operator:

$$\mathscr{K} := -\frac{1}{2} \int \mathrm{d}x\mathrm{d}y \, \left\{ k(x,y) a_{\perp,x}^* a_{\perp,y}^* \right\} , \tag{3.3.2a}$$

where $k = k^T$. This $\mathscr{K}$ does not conserve the number of particles ($[\mathscr{K}, \mathscr{N}] \neq 0$). In addition, following Wu, [60] we introduce the operator

$$\mathscr{W} := -\frac{1}{2N} \int \mathrm{d}x\,\mathrm{d}y\, \{k(x,y) a^*_{\perp,x} a^*_{\perp,y}\} (a_{\overline{\phi}})^2 = \frac{1}{N} \mathscr{K} (a_{\overline{\phi}})^2 \,. \tag{3.3.2b}$$

The kernel $k$ is not known at this stage, but must satisfy certain consistency conditions (see Section 3.3.3). We refrain from specifying the function space of $k$ now. A salient point of this formalism is the identity $[\mathscr{W}, \mathscr{N}] = 0$. Consequently, the operator $e^{\mathscr{W}}$, which is used to define the non-unitary transformation of $\mathscr{H}_{\mathrm{app}}$ below, leaves $\mathbb{F}_N$ invariant, i.e., $e^{\mathscr{W}} : \mathbb{F}_N \mapsto \mathbb{F}_N$. (However, $e^{\mathscr{W}}$ does not respect the Fock space norm.) Our goal here is to describe the non-Hermitian operator $e^{\mathscr{W}} \mathscr{H}_{\mathrm{app}} e^{-\mathscr{W}}$.

The main idea concerning the proposed non-unitary transformation of $\mathscr{H}_{\mathrm{app}}$ 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 $\mathscr{H}_{\mathrm{app}}$ with eigenvalue $E$, viz., $\mathscr{H}_{\mathrm{app}} |\psi\rangle = E |\psi\rangle$. Then, we have

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

Hence, the non-Hermitian, non-unitarily transformed, operator $e^{\mathscr{W}} \mathscr{H}_{\mathrm{app}} e^{-\mathscr{W}}$ has eigenvalue $E$ and eigenvector $e^{\mathscr{W}} |\psi\rangle$. It turns out that it is more tractable to describe the transformed eigenvector $e^{\mathscr{W}} |\psi\rangle$ in $\mathbb{F}_N$ than the original vector $|\psi\rangle$ by exploiting spectral properties of $e^{\mathscr{W}} \mathscr{H}_{\mathrm{app}} e^{-\mathscr{W}}$. A price that one must pay for this option is that the pair-excitation kernel $k$ must satisfy the operator Riccati equation. One of our major goals here is to motivate the equation obeyed by $k$ through the computation of the non-Hermitian operator $e^{\mathscr{W}} \mathscr{H}_{\mathrm{app}} e^{-\mathscr{W}}$.

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

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

where (abusing notation) we define

$$\begin{aligned}\widehat{k}^T(x,y) &:= \int \mathrm{d}z \, \left\{ k(x,z)\widehat{\delta}^T(z,y) \right\} , \\ \widehat{k}^T(a_\perp^*,x) &:= \int \mathrm{d}y\,\mathrm{d}z \, \left\{ a_{\perp,y}^* k(y,z)\widehat{\delta}^T(z,x) \right\} .\end{aligned}$$

In a similar vein, by virtue of (3.3.2a) we compute

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

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

We proceed to carry out the computation of $e^{\mathscr{W}} \mathscr{H}_{\text{app}} e^{-\mathscr{W}}$. To avoid overly cumbersome expressions, we only display the manipulation of key terms of $\mathscr{H}_{\text{app}}$, for illustration purposes. We refrain from presenting the explicit computation of all terms.

The main term that we need to compute reads

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

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

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

Accordingly, we obtain the non-Hermitian quadratic operator

$$
\begin{aligned}
\widetilde{\mathscr{H}_{\mathrm{app}}} \;:=\; e^{\mathscr{W}}\mathscr{H}_{\mathrm{app}}e^{-\mathscr{W}} &= NE_{\mathrm{H}}+\big(h+\widehat{k}^T\circ\overline{f_\phi}\big)(a_\perp^*,a_\perp)+\big(h^T+\overline{f_\phi}\circ\widehat{k}\big)(a_\perp,a_\perp^*)\\
&\quad+\frac{1}{N}\mathrm{Ric}(a_\perp^*,a_\perp^*)\,(a_{\overline{\phi}})^2+\frac{1}{N}(a_\phi^*)^2\,\overline{f_\phi}(a_\perp,a_\perp)\,. \qquad (3.3.3a)
\end{aligned}
$$

In the formal limit $\upsilon\to\delta$, as the interaction potential becomes a delta function, this $\widetilde{\mathscr{H}_{\mathrm{app}}}$

becomes the reduced transformed Hamiltonian derived in Ref. [61]. The 'Riccati kernel' is

$$\mathrm{Ric}(x,y) := h \circ \widehat{\delta} \circ k + k \circ \widehat{\delta}^T \circ h^T + f_\phi + k \circ \widehat{\delta}^T \circ \overline{f_\phi} \circ \widehat{\delta} \circ k \; . \tag{3.3.3b}$$

Recall that the kernel $h(x,y)$ is defined by (3.3.1d) with (3.3.1e), 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 $\widetilde{\mathscr{H}_{\mathrm{app}}}$ is the focus of our analysis. As we anticipated, we have the identity $[\widetilde{\mathscr{H}_{\mathrm{app}}}, \mathscr{N}] = 0$, which enables us to seek eigenvectors of $\widetilde{\mathscr{H}_{\mathrm{app}}}$ in $\mathbb{F}_N$.

### 3.3.3 Riccati equation for $k$

Next, we heuristically outline the rationale for the derivation of an equation for $k$, in the spirit of Wu [60,61]. This equation is described by (3.3.4b) below. In Sections 3.4–3.6, we study properties and implications of solutions to this equation.

By inspection of (3.3.3a), we see that $\widetilde{\mathscr{H}_{\mathrm{app}}} - NE_H$ consists of two types of terms: (i) Terms that contain $a_\perp^*$ and $a_\perp$, and no $a_{\overline{\phi}}$ and $a_\phi^*$. The sum of these terms forms the 'diagonal part' of $\widetilde{\mathscr{H}_{\mathrm{app}}}$, and can be described by use of a (nonlocal) one-particle Schrödinger operator. In the periodic setting, [37] the use of this operator yields the phonon spectrum. (ii) Terms that contain $a_\perp^*$ and $a_{\overline{\phi}}$, or $a_\perp$ and $a_\phi^*$. In the periodic setting, it can be argued that this second part does *not* affect the phonon spectrum *provided* $\mathrm{Ric}(a_\perp^*, a_\perp^*) = 0$. We require that

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

where $\otimes_{\mathrm{s}}$ denotes the symmetrized tensor product. In view of (3.3.3b), 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 $\mathscr{W}$ 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 impose $k(x,\overline{\phi})=0$ [60, 61]. This condition removes $\widehat{\delta}$, $\widehat{\delta}^T$ from the related equations, which is natural since

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

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

$$\mathrm{Ric}(x,y) = h\circ k + k\circ h^T + f_\phi + k\circ\overline{f_\phi}\circ k\,. \tag{3.3.4a}$$

Consequently, the equation for $k$ reads

$$h\circ k + k\circ h^T + f_\phi + k\circ\overline{f_\phi}\circ k = \lambda\otimes_{\mathrm{s}}\phi = \frac{1}{\sqrt{2}}(\lambda\otimes\phi+\phi\otimes\lambda)\,, \tag{3.3.4b}$$

where $\lambda$ 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 3.4.2. We refer to (3.3.4b) as the 'operator Riccati equation' for $k$. In Section 3.5, we show that this equation leads to an excitation spectrum identical to the one from Fetter's formalism [20]. By virtue of (3.3.4b), the transformed Hamiltonian (3.3.3a) becomes

$$\widetilde{\mathscr{H}_{\mathrm{app}}} \;=\; NE_{\mathrm{H}} + \left(h+\widehat{k}^T\circ\overline{f_\phi}\right)(a^*_\perp,a_\perp) + \left(h^T+\overline{f_\phi}\circ\widehat{k}\right)(a_\perp,a^*_\perp) + \frac{1}{N}(a^*_\phi)^2\,\overline{f_\phi}(a_\perp,a_\perp)\,.$$

### 3.3.4 Further comments

We comment on aspects of our heuristic procedure. First, in hindsight, it is of some interest to discuss how (3.3.4b) can be motivated more transparently. The main

observation is that, in regard to $\mathscr{H}_{\rm app}$, we can consider the quadratic matrix form

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

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

$$\begin{pmatrix} \delta & 0 \\ N^{-1}k(a_{\overline{\phi}})^2 & \delta\end{pmatrix}\circ\begin{pmatrix} -h^T & N^{-1}(a^*_\phi)^2\overline{f_\phi} \\ -N^{-1}f_\phi(a_{\overline{\phi}})^2 & h\end{pmatrix}\circ\begin{pmatrix} \delta & 0 \\ -N^{-1}k(a_{\overline{\phi}})^2 & \delta\end{pmatrix}$$

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

where

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

Replace $\mathscr{N}_\phi$ 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 (3.3.4b) then results from the requirement that *the transformed* $2\times 2$ *matrix is upper triangular*. We will show that this property implies that the excitation spectrum of $\mathscr{H}_{\rm app}$ coincides with the one of the diagonal part of $\widetilde{\mathscr{H}_{\rm app}}$, and is identical to the spectrum of Fetter's approach [20]; see Sect. 3.5.

A second comment concerns the Hartree-type equation for $\phi$, which becomes the Gross-Pitaevskii equation if $\upsilon$ is replaced by $g\delta$ for some constant $g>0$. We write the relevant PDE as $\mathbb{H}_{\rm H}\phi=\mu\phi$ where

$$\mathbb{H}_{\rm H} := -\Delta_x + V(x) + N\big(\upsilon * |\phi|^2\big)(x) \tag{3.3.5}$$

is a one-particle Hartree operator. We will consider the interaction potential $\upsilon(x)$ to be

positive, integrable and smooth. For a *trapping* potential $V(x)$, where $V(x) \to \infty$ as $|x| \to \infty$, the condensate wave function $\phi(x)$ is bounded and decays exponentially as $|x| \to \infty$.

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

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

## 3.4 Existence theory for pair excitation kernel: Variational approach

In this section, we address the existence of solutions to (3.3.4b). Our analysis is partly inspired by works of Albeverio, Tretter and coworkers, [2–4, 13] 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. The existence proof for $k$ paves the way to establishing the connection of pair excitation to the phonon spectrum in a trap (Section 3.5).

Our theory invokes an appropriate functional, $\mathscr{E}[\bar{k},k]$, and two related lemmas (Section 3.4.1). A highlight is Theorem 1 on the existence of $k$ (Section 3.4.2). We stress that our existence proof differs significantly from the approach of Refs. [2–4]. First, we utilize a variational approach by seeking stationary points of the functional $\mathscr{E}[\bar{k},k]$ on a Hilbert space, instead of applying the fixed-point argument of Ref. [4]. Note that this fixed-point argument [4] makes use of operator estimates that are not expected to hold for the operator Ric of (3.3.3b). The variational approach developed here is amenable to con-

straints inherent to our problem; thus, the term $\lambda \otimes_{\mathrm{s}} \phi$ of (3.3.4b) emerges as a Lagrange multiplier. Alternate approaches of variational character for block operator matrices (not for the Riccati equation per se) are described in Ref. [58].

Second, our variational approach reveals that Riccati equation (3.3.4b) 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, $\mathscr{E}$. This lack of uniqueness can pose a challenge in the subsequent analysis of the phonon spectrum (Section 3.5). 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 Ref. [2]). By this restriction, the $k$ that solves Riccati equation (3.3.4b) is a minimizer of $\mathscr{E}$.

### 3.4.1 Functional $\mathscr{E}[\overline{k},k]$ and useful lemmas

Next, we define the relevant Hilbert space and the functional $\mathscr{E}[\overline{k},k]$ which yields (3.3.4b). We also prove two lemmas needed for our existence theory.

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

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

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

$$\mathscr{E}[\overline{k},k] := \mathrm{tr}\Big\{ \big(\delta - \overline{k}\circ k\big)^{-1} \circ \Big( \overline{k}\circ h \circ k + \frac{1}{2}\overline{k}\circ f_\phi + \frac{1}{2}\overline{f_\phi}\circ k \Big) \Big\} \tag{3.4.1a}$$

*where*

$$\mathrm{dom}(\mathscr{E}) := \Big\{ k \in \mathfrak{B}_2(\mathfrak{h}^1_V) \,\Big|\, k^T = k \text{ and } \|k\|_{\mathrm{op}} < 1 \Big\} \subset \mathfrak{B}_2(\mathfrak{h}^1_V) \,. \tag{3.4.1b}$$

**Remark 1.** *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,* $\mathrm{dom}(\mathscr{E})$ *is nonempty. The inequality* $\|k\|_2<1$ *implies* $\|k\|_{\mathrm{op}}<1$. *Further remarks on* $\|k\|_{\mathrm{op}}<1$ *are deferred to Section 3.4.3.*

The first lemma of interest can be stated as follows.

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

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

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

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

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

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

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 $\mathscr{E}$ as the sum

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

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

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

and

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

Now combine the above results to obtain the expression

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

where Ric is defined by (3.3.4a). Note that Ric is manifestly symmetric if $k$ is symmetric. This observation completes the proof of Lemma 1. □

**Remark 2.** *The notion of the weak solution as the critical point of the functional $\mathscr{E}[\overline{k},k]$ is relevant to our existence theorem (Theorem 1). Consider the space $\phi^\perp = \big\{e \in \mathfrak{h}_V^1 \;\big|\; e \perp \phi\big\}$. We remind the reader that a bounded operator $k \in \mathfrak{B}(\phi^\perp,\phi^\perp)$ has 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 $\phi^\perp$.*

Before stating the second lemma, we add a remark on the condensate wave function, $\phi$.

**Remark 3.** *By Section 3.3, recall that $\phi$ satisfies $\mathbb{H}_{\mathrm{H}}\phi(x) = \mu\phi(x)$ where the one-particle Hartree operator $\mathbb{H}_{\mathrm{H}}$ is defined in* (3.3.5)*. 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 $\phi$ comes from minimizing the Hartree energy functional, $E_H$, viz.,*

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

*with $\|\phi\|_2 = 1$ then $\mu$ is the lowest eigenvalue of the linear operator that results from fixing $\phi$ in $\mathbb{H}_{\mathrm{H}}$. The existence theorem (Theorem 1) is stated and proved for a condensate $\phi$ that is not necessarily a minimizer of $E_H$. In fact, we replace the assumption of $\phi$ being such a minimizer by a less restrictive hypothesis (see Lemma 2). We assume that the potential $V$ is such that $-\Delta + V$ has discrete spectrum; for example, $V(x) = c|x|^2$ ($c > 0$). The spectrum of $\mathbb{H}_{\mathrm{H}}$ is also discrete since $\mathbb{H}_{\mathrm{H}}$ is a compact perturbation of $-\Delta + V$.*

**Lemma 2.** *If $\upsilon(x)$ has positive Fourier transform $\widehat{\upsilon}(\xi)$, $\widehat{\upsilon}(\xi) \geq 0$, and $\phi$ is a minimizer of the functional $E_H(\phi)$, then for some $c > 0$ the following inequality holds:*

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

*where $h(\cdot,\cdot)$ and $f_\phi(\cdot,\cdot)$ are defined from* (3.3.1b)–(3.3.1e)*.*

*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

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

Since $\phi$ is the minimizer of the Hartree functional, $E_H(\phi)$, we can assert that $\phi$ is the eigenfunction with the lowest eigenvalue of the operator $\mathbb{H}_{\mathrm{H}}$ and is therefore simple. If $e \perp \phi$ then $\langle \overline{e}, \mathbb{H}_H e\rangle \geq c\|e\|_{L^2}$ for some $c > 0$ because the spectrum of the Hartree operator $\mathbb{H}_H$ is discrete (see Remark 3). □

Lemma 2 motivates the inequality involving $h$ and $f_\phi$ as a key assumption of Theorem 1, which replaces the requirement that $\phi$ is a minimizer of $E_H(\cdot)$.

### 3.4.2 Existence theorem and proof

The existence theorem can be stated as follows:

**Theorem 1.** *Suppose that the kernels $h(x,y)$ and $f_\phi(x,y)$ satisfy the inequality*

$$h(\overline{e},e) - \big|f_\phi(\overline{e},\overline{e})\big| \geq c\|e\|_{L^2}^2 \qquad \forall e \in \phi^\perp = \big\{e \in \mathfrak{h}_V^1 \ \big|\ e \perp \phi\big\}\ , \tag{3.4.2}$$

*for some constant $c > 0$. Moreover, let us assume that $f_\phi$ is Hilbert-Schmidt.*

*Consider the functional $\mathscr{E}[\overline{k},k]$, defined in* (3.4.1a)*, with domain*

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

*which consists of the compact $\mathscr{C}$-symmetric Hilbert-Schmidt operators $k \in \mathfrak{B}_2(\mathfrak{h}_V^1)$ satisfying $k(x,\overline{\phi}) = 0$. Then the functional $\mathscr{E}$ restricted to $\mathrm{dom}(\mathscr{E})_\perp$ attains a minimum for some $k \in \mathrm{dom}(\mathscr{E})_\perp$ which is a weak solution of the operator Riccati equation* (3.3.4b)*. The function $\lambda(x)$ entering this equation is a Lagrange multiplier and equals*

$$\lambda(x) = \sqrt{2}\,\big\{\big(k\circ\gamma\big)\big(x,\overline{\phi}\big) + f_\phi\big(x,\overline{\phi}\big) - \tfrac{1}{2}f_\phi(\overline{\phi},\overline{\phi})\phi(x)\big\}\ . \tag{3.4.3}$$

At this stage, two remarks are in order.

**Remark 4.** *We seek stationary points of $\mathscr{E}[\overline{k},k]$ 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 1. Let $\mathscr{C}$ denote the operator of complex conjugation on $\mathfrak{h}$ where*

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

*An operator $\mathscr{T}$ on $\mathfrak{h}$ is called complex-symmetric ("$\mathscr{C}$-symmetric") if it satisfies*

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

*where $\mathscr{T}^*$ is the Hermitian conjugate of $\mathscr{T}$ ($\mathscr{T}^*(x,y) = \overline{\mathscr{T}(y,x)}$). Clearly, integral operators whose kernels are symmetric in their arguments are $\mathscr{C}$-symmetric. An important property is that any compact complex-symmetric operator $\mathscr{T}$ such that $\mathscr{T}^* \circ \mathscr{T}$ has* simple spectrum *admits the decomposition*

$$\mathscr{T} = \sum_{n=1}^{\infty} a_n (u_n \otimes \mathscr{C} u_n) \ , \tag{3.4.4}$$

*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 $(\mathscr{C}\mathscr{T}) \circ (\mathscr{C}\mathscr{T}) = \mathscr{T}^* \circ \mathscr{T}$, which implies the commutation relation $[\mathscr{C}\mathscr{T}, \mathscr{T}^* \circ \mathscr{T}] = 0$. In particular, $\mathscr{C}\mathscr{T}$ commutes with the spectral measure (and any eigenprojector) of the positive operator $\mathscr{T}^* \circ \mathscr{T}$. 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 $(\mathscr{T}^* \circ \mathscr{T})(u_n,x) = c_n u_n(x)$ to the eigenvalue equation $\mathscr{C}\mathscr{T}(u_n,x) = a_n u_n(x)$; thus, $|a_n|^2 = c_n$. It can be directly shown that all $\mathscr{C}$-symmetric tensor products $u \otimes v$ must have $v(x) = \mathscr{C}u(x)$. Hence, we can also pass*

*from the spectral representation*

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

*to expression* (3.4.4)*. This result amounts to a version of the spectral theorem for compact $\mathscr{C}$-symmetric operators; see, e.g., Ref. [23].*

**Remark 5.** *The reader should compare* (3.4.3)*, regarding the Lagrange multiplier $\lambda$, with equation (3.24) in Ref. [61] 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 prove Theorem 1. Notably, we consider a condensate $\phi$ that is not necessarily a minimizer of the Hartree energy, $E_H$.

*Proof.* We split the proof of Theorem 1 into three main steps.

**Step 1.** We now express the functional $\mathscr{E}$ in terms of a suitable basis and describe critical points, by taking into account the theory of $\mathscr{C}$-symmetric operators. By Remark 4, 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 (3.4.1a) for the energy furnishes

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

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

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

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

$$z_j^{\pm}=\frac{-h(\overline{e}_j,e_j)\pm\sqrt{h^2(\overline{e}_j,e_j)-|f_\phi(\overline{e}_j,\overline{e}_j)|^2}}{f_\phi(\overline{e}_j,\overline{e}_j)}\,. \tag{3.4.5}$$

The assumption stated by (3.4.2) 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 $\mathscr{E}(\{e_j\},\{z_j\})$, 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 $f(z_j^{-};e_j)=-h(\overline{e}_j,e_j)-\sqrt{h^2(\overline{e}_j,e_j)-|f_\phi(\overline{e}_j,\overline{e}_j)|^2}$ 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 (3.4.5) the evaluation of $\mathscr{E}$ with the roots $z_j^{\pm}$ yields

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

In light of the preceding discussion, we choose the root $z_j^+$ where $|z_j^+| < 1$ and define

$$\mathscr{F}(e) := h(\overline{e}, e) - \sqrt{h^2(\overline{e}, e) - |f_\phi(\overline{e}, \overline{e})|^2} \,,$$

so that the value of the functional $\mathscr{E}$ reads

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

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

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

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 $\sum_{j=1}^{\infty} \mathscr{F}(e_j)$ is bounded above. The following inequality holds:

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

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

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

which entails an upper bound for $\sum_{j=1}^{\infty} \mathscr{F}(e_j)$. 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 $\mathscr{E}$.

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

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

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

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

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 $\mathscr{F}(e)$ 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 $\mathfrak{h}_V^1(\mathbb{R}^3)$.

In the above, we use the norm (see also Section 5.1.3 for definition of function space $\mathfrak{h}_V^1$)

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

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 $\mathfrak{h}_V^1(\mathbb{R}^3)$ is compactly embedded in $L^2(\mathbb{R}^3)$ (for $d=3$).

Next, we check that the overall minimum is finite. Condition (3.4.2) implies that $h(\overline{e},e)$ is bounded below. This means that the the overall minimum is finite provided

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

The last condition indeed holds. Note that $z_j^+$ is recast to the expression

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

Accordingly, we 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 $\mathrm{dom}(\mathscr{E})_\perp$. We must now take into account the 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, $\phi$ is the condensate wave function and $\lambda(x)$ is to be determined. Hence, the modified energy functional to be minimized has the form

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

In view of Lemma 1, setting equal to zero the functional derivative of $\tilde{\mathscr{E}}$ with respect to $\overline{k}$ yields Riccati equation (3.3.4b). Given that $h = \mathbb{H}_{\mathrm{H}}\delta + N\gamma - \mu$ and $\mathbb{H}_{\mathrm{H}}\phi = \mu\phi$, we compute $\lambda$ by contracting the above equation for $k$ with $\overline{\phi}$. Thus, we obtain (3.4.3).

*Note on k as a weak solution:* We conclude the proof by showing that $k$ satisfies the definition of a weak solution (Remark 2). The condition that $\mathscr{E}$ is minimized implies that the first variation with respect to $\overline{k}$ vanishes, i.e.,

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

for all $\overline{k}_1 \in \mathrm{dom}(\mathscr{E})$. 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

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

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

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

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. □

### 3.4.3 On the non-uniqueness of the solution for $k$

Next, we discuss the important issue of the non-uniqueness of solutions for $k$ by our variational approach. The energy functional $\mathscr{E}[\overline{k},k]$ 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 1. We can show that these different 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 $X(e_1) := \text{span}(e_1) = \{z_1 e_1(x) \in \mathfrak{h} \mid z_1 \in \mathbb{C}\}$. Accordingly, we set up the min-max problem expressed by

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

By repetition of the above argument (proof of Theorem 1), this min-max problem generates the (saddle type) critical point of the functional $\mathscr{E}(\overline{k},k)$. 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 $\|k\|_{\text{op}} < 1$ is the one given in the proof of Theorem 1. 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 6.** *If $z_j$ is chosen in* (3.4.5) *such that $z_j = z_j^+$ for all $j > 0$ (i.e., $\|k\|_{\text{op}} < 1$) then*

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

*This property will be relevant for the spectrum of the reduced Hamiltonian (Section 3.5.2).*

## 3.5 Spectrum and eigenvectors of reduced Hamiltonian

In this section, we describe the spectrum and eigenvectors of the reduced transformed Hamiltonian $\widetilde{\mathscr{H}_{\text{app}}}$ in the $N$-th sector of Fock space, $\mathbb{F}_N$ (see Section 3.3.3). For this purpose, we decompose $\mathbb{F}_N$ into suitable orthogonal subspaces. A similar technique is used in Ref. [42] in connection to the Bogoliubov Hamiltonian which does not conserve the particle number.

We start by writing the transformed, approximate non-Hermitian Hamiltonian as

$$\widetilde{\mathscr{H}_{\text{app}}} = NE_H + \mathscr{H}_{\text{ph}} , \quad \mathscr{H}_{\text{ph}} := h_{\text{ph}}\big(a_\perp^*, a_\perp\big) + \frac{1}{N}(a_\phi^*)^2\,\overline{f_\phi}\big(a_\perp, a_\perp\big) \tag{3.5.1a}$$

where $f_\phi(a_\perp^*, a_\perp^*)$ (and thus $\overline{f_\phi}(a_\perp, a_\perp)$) is defined by (3.3.1b) with (3.3.1d), and

$$h_{\text{ph}} := h + k \circ \overline{f_\phi} \, . \tag{3.5.1b}$$

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

The main result of this section is expressed by the following theorem.

**Theorem 2.** *Consider the operators $\mathscr{H}_{\text{ph}}$ and $h_{\text{ph}}(a_\perp^*, a_\perp)$ restricted on $\mathbb{F}_N$. Then*

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

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

$$\mathscr{H}_{\text{ph}}|\Psi(\Omega)\rangle_N = E|\Psi(\Omega)\rangle_N \, .$$

Before we give a proof of Theorem 2, we need to provide a few useful results. In Section 3.5.1, we develop a formalism for the decomposition of $\mathbb{F}_N$ into orthogonal

subspaces. A key ingredient of our approach is the use of Fock space techniques. In Section 3.5.2, we show that the spectrum of $h_{\rm ph}$ is discrete. In Section 3.5.3, we use this machinery (theory of Sections 3.5.1 and 3.5.2) to prove Theorem 2. In our proof, we describe an explicit construction of the eigenvectors of $\mathscr{H}_{\rm ph}$ restricted on $\mathbb{F}_N$ in terms of eigenvectors of $h_{\rm ph}(a_\perp^*, a_\perp)$. This construction invokes the discrete spectrum of $h_{\rm ph}$.

### 3.5.1 Decomposition of $\mathbb{F}_N$ and two related lemmas

Next, we set the stage for the proof of Theorem 2. We use the symbol $|\psi\rangle_n$ to denote the vector of $\mathbb{F}$ with entry $\psi_n(x_1, \ldots, x_n)$ in the $n$-th slot and zero elsewhere. Let us also introduce the projection $\mathscr{P}_N \,:\, \mathbb{F} \mapsto \mathbb{F}_N$.

The vector $\psi_N(x_1, \ldots, x_N)$ 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 $\psi_{N,n}(x_1, \ldots, x_n)$ satisfy the orthogonality relations ($n = 1, 2 \ldots N$)

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

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

$$|\psi^{\perp}\rangle := \left(\psi_{N,0}, \psi_{N,1}, \ldots, \psi_{N,N}, 0, \ldots\right)$$

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

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

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

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

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

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

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

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

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

At this stage, we can state the first lemma of this section as follows.

**Lemma 3.** *The operator $\mathscr{P}_{n,n} = P_n(\mathscr{N}_\phi)$ satisfies the factorization*

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

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

*Proof.* First, we note the useful identities

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

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

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

Moreover, we have the following formulas:

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

By using the above relations, we write

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

We can show that $\mathscr{P}_{n,n}$ is a projection. Indeed, notice that $\mathscr{N}_\phi P_n(\mathscr{N}_\phi)\big|_{\mathbb{F}_n} = 0$, and if $|\psi\rangle_n \in \mathbb{F}_n$ then $\mathscr{P}_{n,n}|\psi\rangle_n = |\psi_{n,n}\rangle_n$. 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 $\mathscr{P}_{n,n}$ 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 $p = 0, 1 \ldots n$. □

For later algebraic convenience, we give the following definition (cf. Ref. [42]).

**Definition 2.** *Consider the operators $\mathscr{U}_n, \mathscr{U}_n^* : \mathbb{F}_N \mapsto \mathbb{F}_N$ given by*

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

By Definition 2, the result of Lemma 3 implies that

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

The key relations following from this decomposition are

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

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

**Lemma 4.** *The operators $\{\mathscr{U}_n\}_{n=0}^N$ (see Definition 2) satisfy the relation*

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

*Proof.* First, we make the observation that

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

If $m < n$ (thus, $N-m > N-n$), in view of the property $a_{\overline{\phi}} \mathscr{P}_{n,n}\big|_{\mathbb{F}_n} = 0$ we have

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

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

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

□

### 3.5.2 On the spectrum of $h_{\mathrm{ph}}$

Next, we discuss 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. As such, many important spectral properties of self-adjoint operators carry over to $h_{\mathrm{ph}}$.

**Lemma 5.** *Assume that the pair-excitation kernel $k$ solves the operator Riccati equation* (3.3.4b) *with $\|k\|_{\mathrm{op}} < 1$.*

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

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

$$\sum_{j=1}^{\infty} \overline{\omega_j(x)} u_j(y) = \widehat{\delta}(x,y) \ . \tag{3.5.2}$$

*Proof.* The following relation holds on $\phi^\perp$ by use of the Riccati equation (3.3.4b):

$$(h + k\circ\overline{f_\phi})\circ(\widehat{\delta} - k\circ\overline{k}) = (\widehat{\delta} - k\circ\overline{k})\circ(h + f_\phi\circ\overline{k}) \ . \tag{3.5.3}$$

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 (3.5.3), 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 6). 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

$$\omega_j(x) = (\widehat{\delta} - k\circ\overline{k})^{1/2}(x,\eta_j) \ , \tag{3.5.4a}$$

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

$$u_j(x) := (\widehat{\delta} - k \circ \overline{k})^{-1/2}(x, \eta_j) \tag{3.5.4b}$$

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

The resolution of the identity by the eigenvectors $\eta_j$ 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 (3.5.2), by use of (3.5.4). □

### 3.5.3 Proof of Theorem 2

We are now in position to prove Theorem 2. Our argument for the construction of eigenvectors of $\mathscr{H}_{\rm ph}$ relies on the fact the $h_{\rm ph}$ has discrete spectrum. Let $|\psi\rangle := |\psi\rangle_N$.

*Proof.* **Step 1.** We decompose $\mathscr{H}_{\rm ph}\big|\psi\big\rangle$, where $\mathscr{H}_{\rm ph}$ is given in (3.5.1). We show that

$$\begin{aligned}
&\sum_{m=0}^{N} \mathscr{U}_m^* \mathscr{U}_m \mathscr{H}_{\rm ph} \sum_{n=0}^{N} \mathscr{U}_n^* \mathscr{U}_n |\psi\rangle = \sum_{m,n=0}^{N} \mathscr{U}_m^* \left\{ \mathscr{U}_m \mathscr{H}_{\rm ph} \mathscr{U}_n^* \right\} \left( \mathscr{U}_n \big| \psi \big\rangle \right) \\
&= \sum_{n=0}^{N} \mathscr{U}_n^* h_{\rm ph}(a_{\perp}^*, a_{\perp}) \mathscr{U}_n |\psi\rangle + \sum_{n=0}^{N-2} b_{N,n} \mathscr{U}_n^* \overline{f_{\phi}}(a_{\perp}, a_{\perp}) \mathscr{U}_{n+2} |\psi\rangle \ .
\end{aligned} \tag{3.5.5}$$

Here, $b_{N,n}$ is a numerical constant. Regarding the operators $\mathscr{U}_n$, see Definition 2.

In order to derive (3.5.5), we invoke Lemma 4. In this vein, we notice the relations

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

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

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 $\mathscr{U}_n|\psi\rangle = |\psi_{N,n}\rangle_n$ 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 $\psi_n$ 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 $\psi_{n+2}$ to $\psi_n$. 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

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

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 $\mathscr{H}_{\rm ph}|\psi\rangle = E|\psi\rangle$ reduces to a finite system, viz.,

$$h_{\rm ph}\circ\psi_{N,N} = E\,\psi_{N,N}\ , \tag{3.5.6a}$$

$$h_{\rm ph}\circ\psi_{N,N-2} + \overline{f_\phi}:\psi_{N,N} = E\,\psi_{N,N-2}\ , \tag{3.5.6b}$$

$$h_{\rm ph}\circ\psi_{N,N-4} + \overline{f_\phi}:\psi_{N,N-2} = E\,\psi_{N,N-4}\ ,\ldots\ . \tag{3.5.6c}$$

This system has upper triangular form and manifests the effect of pair excitation, since the number of non-condensate particles is reduced in pairs. The even and odd values of $N$ should be considered separately. 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, (3.5.6a) implies the equality of the spectra, $\sigma\left(\mathscr{H}_{\rm ph}\right) = \sigma\left(h_{\rm ph}(a_\perp^*, a_\perp)\right)$, on $\mathbb{F}_N$. Indeed, if (3.5.6a) 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. Note that the top equation has infinitely many possible solutions corresponding to the spectrum of $h_{\rm ph}$ – but choosing 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 (3.5.6). For example, start with (see Lemma 5)

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

for given $j_p$ ($p = 0,\, 1,\, \ldots,\, N$) so that $\Omega_N$ 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 $\Omega_N$ 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 (3.5.6b), 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, $\Omega_{N-4}$, is a linear combination of $\omega_{j_k}$ where four terms have been removed from the original collection. The idea of computation is similar. One can proceed until all

non-condensate particles are removed. This argument concludes our explicit construction of the eigenvectors of $\mathscr{H}_{\rm ph}$ in terms of eigenvectors of $h_{\rm ph}$. □

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

## 3.6 Connections to a 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 [20, 42]. This Hamiltonian results from the Bogoliubov approximation and has the same spectrum as our non-Hermitian $\widetilde{\mathscr{H}_{\rm app}}$ 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 [2–4] (see also Refs. [13, 58]). 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 by Fetter, if his delta-function interaction potential is regularized [20].

### 3.6.1 On a reduced Hamiltonian via the Bogoliubov approximation

Recall our reduced Hamiltonian with a smooth interaction potential (Section 3.3.1), viz.,

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

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

$$\mathscr{H}_{\text{Bog}} := NE_{\text{H}} + h(a_{\perp}^{*}, a_{\perp}) + \frac{1}{2} f_{\phi}(a_{\perp}^{*}, a_{\perp}^{*}) + \frac{1}{2} \overline{f_{\phi}}(a_{\perp}, a_{\perp}) \ , \tag{3.6.1}$$

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

Next, we discuss the diagonalization of $\mathscr{H}_{\text{Bog}}$ by using eigenstates of the operator $h_{\text{ph}} : \mathfrak{h}_V^1 \cap \phi^{\perp} \to \mathfrak{h}$ defined by (3.5.1b) (Section 3.5). We proceed in the spirit of Fetter, [20] who diagonalizes $\mathscr{H}_{\text{Bog}} - NE_H$ via (unitary) Bogoliubov-type rotations of the Boson field operators in the space orthogonal to $\phi$; see equation (2.14) for a delta-function interaction potential in Ref. [20]. In this vein, let us consider Fetter's quasiparticle operators $\gamma_j, \gamma_j^{*}$ which are defined as follows [20] .

**Definition 3.** *The operators $\gamma_j, \gamma_j^{*} : \mathbb{F} \mapsto \mathbb{F}$ ($j = 1, 2, \dots$) 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 $\gamma_j$ and $\gamma_j^{*}$ satisfy the canonical commutation relations.*

One can verify that $\gamma_j, \gamma_j^{*}$ satisfy the canonical commutation relations provided

$$\begin{aligned} \int \mathrm{d}x \, \{u_j(x) v_{j'}(x) - v_j(x) u_{j'}(x)\} &= 0 \ , \\ \int \mathrm{d}x \, \{u_j(x) \overline{u_{j'}(x)} - v_j(x) \overline{v_{j'}(x)}\} &= \delta_{jj'} \ . \end{aligned} \tag{3.6.2}$$

We proceed to show that the diagonalization of $\mathscr{H}_{\rm Bog}$ in terms of $\gamma_j$ and $\gamma_j^*$ implies that $\{u_j(x), v_j(x)\}_{j=1}^{\infty}$ must solve a linear system of PDEs. Following Fetter's procedure, [20] let us momentarily assume the following completeness relations:

$$\begin{aligned}
&\sum_{j=1}^{\infty} \{u_j(x)\overline{u_j(x')} - \overline{v_j(x)}v_j(x')\} = \widehat{\delta}(x,x') \ , \\
&\sum_{j=1}^{\infty} \{u_j(x)\overline{v_j(x')} - \overline{v_j(x)}u_j(x')\} = 0, \quad \forall x, x' \in \mathbb{R}^3 \ .
\end{aligned} \tag{3.6.3}$$

In view of Definition 3, these relations 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 3 amount to a Bogoliubov-type (unitary) transformation in the space orthogonal to the condensate $\phi$. The substitution of these expressions into (3.6.1) along with the requirement that the terms proportional to $\gamma_j\gamma_l$ and $\gamma_j^*\gamma_l^*$ vanish (for all $j, l = 1, 2, \ldots$) yields the following eigenvalue problem involving a symplectic matrix:

$$\begin{pmatrix} h_\perp^T & -f_{\phi\perp} \\ \overline{f_{\phi\perp}} & -h_\perp \end{pmatrix} \circ \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} = E_j \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} \ ; \quad j = 1, 2, \ldots . \tag{3.6.4}$$

In the above, $h_\perp$ and $f_{\phi\perp}$ are the projections of operators $h$ and $f_\phi$ on space $\phi^\perp$. Equation (3.6.4) should be compared to equations (2.21a,b) in Ref. [20]. 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 3.5.2. In fact, the corresponding quantities turn out to be identical in the two eigenvalue problems, as we discuss below.

### 3.6.2 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 5 (Section 3.5.2). We should also add that this theory relies on the existence of solutions to the Riccati equation for $k$, Theorem 1 (Section 3.4). To make a connection to system (3.6.4), consider the solutions $\omega_j$ 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

$$h_{\rm ph}(x,\omega_j) = (h + k \circ \overline{f_\phi})(x,\omega_j) = E_j \omega_j(x) \ ,$$

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

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 (3.6.4). We can show that this definition for $v_j$ also gives the second equation in system (3.6.4) by employing the conjugate Riccati equation (for $\overline{k}$). Indeed, notice that

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

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 (3.6.4).

**Remark 7.** ***(i)*** *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* (3.6.4) *coming from Fetter's Hermitian view. A direct comparison to the results in Ref. [20] is meaningful if Fetter's delta-function interaction is appropriately regularized. This connection is in*

*fact a manifestation of a deeper theory which links the Riccati equation to J-self-adjoint matrix operators [2–4]. We briefly discuss aspects of this theory in Section 3.6.3.*

***(ii)*** *In Fetter's work [20], an ansatz for the many-body ground state* $|\psi_0\rangle$ *of the quadratic Hamiltonian* $\mathscr{H}_{\mathrm{Bog}}$ *on* $\mathbb{F}$ *is*

$$|\psi_0\rangle = Ze^{\mathscr{G}}\{a_{\phi}^{*N}\}|vac\rangle \; ; \quad \mathscr{G} := \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\; b(x,y)\, a_{\perp,x}^{*} a_{\perp,y}^{*} \; .$$

*However, a single governing equation for the associated kernel* $b(x,y)$ *is not provided in Ref. [20]. 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:*

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

*By comparison of this formalism to our approach, we realize that kernel b coincides with k, and the above integral relations are already a consequence of our solution for k. In fact, in Ref. [20] 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* (3.6.4) *under a delta-function interaction. The kernel k is expressed as a bilinear form involving* $\phi$*-orthogonal projections of the wave functions* $v_j$*; [20] see also Ref. [18]. Our existence proof for k furnished in the context of Theorem 1 shows that the ground state* $|\psi_0\rangle$ *is self-consistent, in the sense that the integral system stemming from* $|\psi_0\rangle$ *and* (3.6.4) *is well-posed if a solution to the Riccati equation for k exists.*

At this stage, we find it compelling to give the following corollary for system (3.6.4).

**Corollary 1.** *For* $\{u_j(x), v_j(x)\}_{j=1}^{\infty}$ *that solve* (3.6.4)*, completeness relations* (4.3.2) *and orthogonality relations* (3.6.2) *hold.*

*Proof.* We resort to the spectral theory of operator $h_{\rm ph}$ on space $\phi^{\perp}$, particularly the proof of Lemma 5 (Section 3.5.2). 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

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

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 (4.3.2).

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 (4.3.2) 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 (3.6.2), the manipulation of system (3.6.4) 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 (3.6.2), 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 (3.6.2) follows by a similar procedure which we omit here. □

### 3.6.3 On the $J$-self-adjoint system

Next, we discuss the connection between Riccati equation (3.3.4b) and main ideas from the theory of $J$-self-adjoint operators found in, e.g., Refs. [2–4]. A link between these two theories is suggested by the eigenvalue problem (3.6.4), which involves the symplectic matrix

$$M := \begin{pmatrix} h_\perp^T & -f_{\phi\perp} \\ \overline{f_{\phi\perp}} & -h_\perp \end{pmatrix}; \quad \mathrm{dom}(M) := \mathfrak{h}_V^1 \oplus \mathfrak{h}_V^1 \,. \tag{3.6.5}$$

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 1 (Section 3.4.2). 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, [4] 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 $\sigma(\overline{h_{\rm ph}}) \cup \sigma(-h_{\rm ph})$, which under the assumptions of Theorem 1 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 (3.6.5). 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 $h_{\rm ph}$, and another type is of the form $\big(0, \overline{\omega_j(x)}\big)$ (see Section 3.5.2). 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 should be excluded since they yield a negative spectrum.

**Remark 8.** *So far, we assumed that the Riccati equation for k is satisfied (and solutions to this equation exist by Theorem 1). Conversely, if we assume that the integral system* $v_j = -\bar{k}(x, u_j)$ *as well as PDE system* (3.6.4) *hold then k must obey the Riccati equation. This claim can be proved by use of the methods that we already developed.*

## 3.7 Conclusion and discussion

In concluding this chapter, we stress the intimate, and perhaps surprising, mathematical connection between two apparently disparate approaches (those of Fetter [20] and Wu [60]) for the problem of low-lying Boson excitations via the theory of $J$-self-adjoint operators [4]. 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 (quasiparticles) in Fetter's far-reaching formalism [20]. In addition, we explicitly constructed the eigenvectors of the approximate many-body Hamiltonian $\mathscr{H}_{\text{app}}$ for pair excitations, given by (6.2.3), in the $N$-particle sector of Fock space. Some of our results can be viewed as an application of the powerful theory of $J$-self-adjoint operators to a physics-inspired problem.

Let us outline implications of our analysis. The similarity relation $WMW^{-1} = D$, discussed in Section 3.6.3, shows that the spectrum of $h_{\text{ph}}$ 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 $\sigma(h_{\rm ph})$ will change under different choices of solutions for $k$. In light of our analysis, the only possible change induced by $\sigma(h_{\rm ph}(k)) \mapsto \sigma(h_{\rm ph}(k'))$ for two different solutions $k$ and $k'$ ($k' \neq k$) is such that a finite collection of eigenvalues $\{E_j\} \subset \sigma(h_{\rm phon}(k))$ is mapped to $\{-E_j\} \subset \sigma(h_{\rm phon}(k'))$ while the rest of the eigenvalues remain unchanged.

The kernel $k$ is directly related to the pair correlation function $C_2 : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}$ at the ground state $\Psi$ (at zero temperature), which for our purposes is defined by $C_2(x,y) := N^{-1}\langle\Psi|a^*_{\perp,x}a_{\perp,y}a^*_{\phi}a_{\overline{\phi}}|\Psi\rangle$. An asymptotic calculation of $C_2$ for large $N$ to the order of approximation consistent with the reduced Hamiltonian $\widetilde{\mathscr{H}_{\rm app}}$ yields [20, 60]

$$C_2(x,y) = \frac{k \circ \overline{k}}{\widehat{\delta} - k \circ \overline{k}} \, .$$

This formula can be extracted from the analysis of Ref. [60] under the restriction $\|k\|_{\rm op} < 1$ which ensures uniqueness of the solution to the operator Riccati equation for $k$. Hence, the existence of a unique $k$ directly implies a well-defined pair correlation function $C_2(x,y)$. The investigation of the connection between $k$ and $C_2$ is the subject of future work.

We are tempted to also mention a few other open problems motivated by our work. For example, given the existence of the kernel $k$ with $\|k\|_{\rm op} < 1$, it is of interest to consider the effect of a non-unitary transformation analogous to $e^{\mathscr{W}}$ 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. Furthermore, it is conceivable that the non-Hermitian approach involving $k$ can be extended to the setting of finite (positive) temperatures below the phase transition in the presence of a trapping potential. In the

spirit of the periodic case, [38] we could construct an effective approximate Hamiltonian for pair excitation that involves a parameter expressing the average fraction of particles at the condensate, and subsequently transform it non-unitarily. Alternatively, one may use a Hermitian approach at finite temperatures akin to Fetter's formalism, e.g., the approach taken up in Ref. [25].

# Chapter 4

# Non-translation-invariant systems: pairs coupled with mean field

## 4.1 Background

In the previous chapter, we connected the theory for pair-excitation kernel $k(x,y)$ to the diagonalization of a quadratic many-body Hamiltonian. In that chapter, the quadratic Hamiltonian was derived by the method of Fetter [20], and resulted in a system for the condensate $\phi(x)$ and excitation kernel $k(x,y)$ (which we review here in equations (4.1.4) and (4.1.14)). That model had the particular feature that the Hartree equation for $\phi$ was decoupled from the Riccati equation for $k$, so that we could solve them independently by different variational methods.

In the present chapter, we analyze a more complicated quadratic approximate Hamiltonian for the trapped Bose gas, which contains effective mean-field potentials arising from the density of non-condensate particles. The model of Fetter tacitly ignored the contribution of these terms in the approximation scheme for the exact many-body Hamiltonian.

The starting point of this chapter is the exact many-body Hamiltonian, $\mathscr{H}$, for $N$ bosons with a repulsive, mean-field, pairwise interaction $\upsilon_N$, in the trapping potential $V_{\text{trap}}(x)$, given by the Fock space operator:

$$\mathscr{H} = \int \mathrm{d}x \left\{ a_x^* \big( -\Delta + V_{\text{trap}}(x) \big) a_x \right\} + \frac{1}{2} \iint \mathrm{d}x \mathrm{d}y \left\{ a_x^* a_y^* \frac{1}{N} \upsilon_N(x-y) a_x a_y \right\}, \quad \mathbb{F}_N \to \mathbb{F}_N. \tag{4.1.1}$$

A feature of this system which was not present in the previous chapters is the mean-field interaction, $\frac{1}{N}\upsilon_N(x)$. Here, we require that $\upsilon_N(x) = N^{3\beta}\upsilon(N^{\beta}x)$, where $\upsilon$ is a smooth, positive, radially symmetric function, with $\int \mathrm{d}x\{\upsilon(x)\} = g$, for $g > 0$, and $\beta \leq 1/6$. In particular, $\frac{1}{N}\upsilon_N(x-y) \leq \|\upsilon\|_{L^\infty}$, and $\|\frac{1}{N}(\upsilon_N * f)\|_{L^2} \leq g\|f\|_{L^2}$, by Young's inequality. We assume that $V_{\mathrm{trap}}(x)$ is positive, and that the operator $(-\Delta_x + V_{\mathrm{trap}}(x))$ has a positive spectrum with a gap between it's lowest and first excited states. It is useful to take the concrete example $V_{\mathrm{trap}}(x) = |x|^2$ for $x \in \mathbb{R}^3$ as the prototypical trapping potential.

As in previous chapters, the goal is to write an approximation to $\mathscr{H}$ (denoted generically by $\mathscr{H}_{\mathrm{approx}}$) which describes important features of the many-body system for states close to the ground state. The previous chapter emphasized the utility of an approximation $\mathscr{H}_{\mathrm{approx}}$ which is quadratic in field operators orthogonal to the condensate; since quadratic Hamiltonians can be diagonalized by unitary rotation, finding a quadratic system which approximates (5.2.5) is of great value. Here we describe a systematic approximation scheme motivated by Griffin [25], which generalizes the quadratic approximation of the previous chapter, represented by the work of Fetter [20]. Compared to the previous chapter, the scheme here includes additional quadratic terms coming from non-condensate densities. The new terms alter the analysis in a qualitative way; giving rise to a nonlinear system for elementary excitations in place of the corresponding linear system of Chapter 3.

We first translate the approximation of Fetter (1970) [20] to this new context. The operator $\mathscr{H} - \mu\mathscr{N}$, (where $\mathscr{N} = \int \mathrm{d}x\{a_x^* a_x\}$, and $\mu > 0$ is the chemical potential), is

rewritten using the Bogoliubov approximation:

$$\begin{aligned} a_x &\approx N\phi(x)\overline{\phi(x)} + b_x \\ a_x^* &\approx N\phi(x)\overline{\phi(x)} + b_x^*, \end{aligned} \tag{4.1.2}$$

where, as before, the operators $b_x$, $b_x^*$ are understood to satisfy the canonical commutation relations on the space orthogonal to the condensate. In particular,

$$[b_x, b_y^*] = \delta(x-y) - \phi(x)\overline{\phi(y)}.$$

The macroscopic condensate wavefunction $\phi(x)$, with $\|\phi\| = 1$, is determined self-consistently as part of the scheme. Making the above substitutions in $\mathscr{H}$, and ignoring cubic and quartic terms in the operators $b_x$, $b_x^*$, the reduced Hamiltonian is given by:

$$\begin{aligned} \mathscr{H}_{\text{Fetter}} &= \text{const} + \int dx \{\overline{A_{\text{Fetter}}(x)} b_x + A_{\text{Fetter}}(x) b_x^*\} \\ &+ \int dxdy \Big\{ (b_x, b_x^*) \begin{pmatrix} -h_{\text{Fet}}^T(x,y) & \overline{f_\phi}(x,y) \\ -f_\phi(x,y) & h_{\text{Fet}}(x,y) \end{pmatrix} \begin{pmatrix} -b_y^* \\ b_y \end{pmatrix} \Big\}. \end{aligned} \tag{4.1.3}$$

Here, $A_{\text{Fetter}}(x)$, $h_{\text{Fet}}(x,y)$, and $f_\phi(x,y)$ are defined by:

$$A_{\text{Fetter}}(x) := (-\Delta_x + V_{\text{trap}}(x) - \mu)\phi(x) + \int dy \{\upsilon_N(x-y)|\phi(y)|^2\}\phi(x),$$

$$h_{\text{Fet}}(x,y) := (-\Delta_x + V_{\text{trap}}(x) - \mu)\delta(x-y) + \overline{\phi(y)}\upsilon_N(x-y)\phi(x) + (\upsilon_N * |\phi|^2)(x)\delta(x-y),$$

$$f_\phi(x,y) := \phi(y)\upsilon_N(x-y)\phi(x).$$

The equation for the mean-field condensate $\phi(x)$ of Fetter results by enforcing the condition $A_{\text{Fetter}}(x) = 0$, i.e.,

$$(-\Delta_x + V_{\text{trap}}(x))\phi(x) + (\upsilon_N * |\phi|^2)(x)\phi(x) = \mu\phi(x). \tag{4.1.4}$$

With $\phi(x)$ specified by equation (4.1.4), the operator matrix in $\mathscr{H}_{\text{Fetter}}$ (equation (4.1.3)) is then well-defined. The method outlined by Fetter [20, 21] for diagonalizing the operator

$\mathscr{H}_{\text{Fetter}}$ is equivalent to solving the eigenvalue problem for this matrix, for the basis of single-particle states $\{U_j(x), P_j(x)\}_{j=1}^{\infty}$, i.e.,

$$\int \mathrm{d}y \Big\{ \begin{pmatrix} h_{\text{Fet}}(x,y) & -f_\phi(x,y) \\ \overline{f_\phi(x,y)} & -h_{\text{Fet}}^T(x,y) \end{pmatrix} \begin{pmatrix} U_j(y) \\ P_j(y) \end{pmatrix} \Big\} = E_j \begin{pmatrix} U_j(x) \\ P_j(x) \end{pmatrix}, \quad \|U_j\|^2 - \|P_j\|^2 = 1. \tag{4.1.5}$$

This system is the result of defining the quasiparticle operators $\alpha_j$, $\alpha_j^*$ by the formula

$$\begin{aligned} b_x &= \sum_j \{U_j(x)\alpha_j - \overline{P_j(x)}\alpha_j^*\} \\ b_x^* &= \sum_j \{\overline{U_j(x)}\alpha_j^* - P_j(x)\alpha_j\}. \end{aligned} \tag{4.1.6}$$

The operators $\alpha_j$, $\alpha_j^*$ in (4.3.1) are taken to satisfy the canonical commutation relations

$$[\alpha_j, \alpha_k^*] = \delta_{jk}, \quad [\alpha_j, \alpha_k] = [\alpha_j^*, \alpha_k^*] = 0,$$

which gives the normalization condition for $\{U_j(x), P_j(x)\}_{j=1}^{\infty}$ in (4.1.5). The spectrum $\{E_j\}_{j=1}^{\infty}$ describes the elementary excitations of $\mathscr{H}_{\text{Fetter}}$.

Griffin (1996) [25] extended the analysis of (4.1.3) by including higher order terms within a quadratic scheme, introducing the two-particle correlation functions for non-condensate particles, denoted $n^{\text{pair}}(x,y)$, $m^{\text{pair}}(x,y)$, $\rho^{\text{pair}}(x) := n^{\text{pair}}(x,x)$. The setup is similar to the derivation of $\mathscr{H}_{\text{Fetter}}$; the Bogoliubov approximation (4.1.2) is made in the exact Hamiltonian $\mathscr{H}$. Now, instead of ignoring cubic and quartic terms in $\{b_x, b_x^*\}$, the following replacements are made:

$$\begin{aligned} b_x^* b_y^* b_x b_y &\approx \; 2n^{\text{pair}}(x,y) b_y^* b_x + 2\rho^{\text{pair}}(x) b_y^* b_y + \overline{m^{\text{pair}}(x,y)} b_x b_y + m^{\text{pair}}(x,y) b_x^* b_y^* \,, \\ b_x^* b_x b_y &\approx \; \rho^{\text{pair}}(x) b_y + n^{\text{pair}}(x,y) b_x + m^{\text{pair}}(x,y) b_x^* \,. \end{aligned} \tag{4.1.7}$$

The reduced Hamiltonian is a generalization of (4.1.3), which reads:

$$\begin{aligned}\mathscr{H}_{\text{Grif}} &= \text{const} + \int dx\{\overline{A_{\text{Grif}}(x)}b_x + A_{\text{Grif}}(x)b_x^*\} \\ &+ \int dxdy\Big\{(b_x, b_x^*)\begin{pmatrix} -h^T(x,y) & (\upsilon_N\overline{m})(x,y) \\ -(\upsilon_N m)(x,y) & h(x,y)\end{pmatrix}\begin{pmatrix} -b_y^* \\ b_y\end{pmatrix}\Big\},\end{aligned} \tag{4.1.8}$$

where the operators in this expresssion are defined by

$$\begin{aligned}A_{\text{Grif}}(x) &:= \big(-\Delta_x + V_{\text{trap}}(x) + \frac{1}{N}(\upsilon_N * \rho)(x) - \mu\big)\phi(x) + \\ &\quad + \frac{1}{N}\int dy\{\upsilon_N(x-y)n(x,y)\phi(y)\} + \int dy\{\upsilon_N(x-y)m(x,y)\overline{\phi(y)}\}, \\ n(x,y) &:= \phi(x)\overline{\phi(y)} + \frac{1}{N}n^{\text{pair}}(x,y), \\ m(x,y) &:= \phi(x)\phi(y) + \frac{1}{N}m^{\text{pair}}(x,y), \\ \rho(x) &:= n(x,x), \quad \rho^{\text{pair}}(x) := n^{\text{pair}}(x,x), \\ h(x,y) &:= \{-\Delta_x + V_{\text{trap}}(x) + (\upsilon_N * \rho^{\text{pair}})(x) - \mu\}\delta(x-y) + \upsilon_N(x-y)n(x,y).\end{aligned} \tag{4.1.9}$$

The apparent problem with this formulation is that it is unclear how to determine the functions $n^{\text{pair}}(x,y)$, $m^{\text{pair}}(x,y)$, $\phi(x)$ consistently, which would require enforcing more equations than just $A_{\text{Grif}}(x) = 0$. Griffin, making an implicit assumption on the structure of eigenstates of $\mathscr{H}_{\text{Grif}}$, diagonalizes $\mathscr{H}_{\text{Grif}}$ using a basis of states $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$ (which play the same role as $\{U_j(x), P_j(x)\}_{j=1}^{\infty}$ in (4.1.5)), thereby providing a "closure" to the system that determines all correlation functions. The system for condensate $\phi(x)$, and the basis $\{u_j(x), p_j(x)\}$ reads:

$$\begin{aligned}\mu\phi(x) &= (-\Delta_x + V_{\text{trap}}(x))\phi(x) + (\upsilon_N * |\phi|^2)(x)\phi(x) + \frac{1}{N}(\upsilon_N * \rho^{\text{pair}})(x)\phi(x) \\ &\quad + \frac{1}{N}\int dy\{\upsilon_N(x-y)n^{\text{pair}}(x,y)\phi(y)\} + \frac{1}{N}\int dy\{\upsilon_N(x-y)m^{\text{pair}}(x,y)\phi(y)\},\end{aligned} \tag{4.1.10}$$

and

$$\int \mathrm{d}y \Big\{ \begin{pmatrix} -h^T(x,y) & (\upsilon_N \overline{m})(x,y) \\ -(\upsilon_N m)(x,y) & h(x,y) \end{pmatrix} \begin{pmatrix} u_j(y) \\ p_j(y) \end{pmatrix} \Big\} = E_j \begin{pmatrix} u_j(x) \\ p_j(x) \end{pmatrix}, \quad \|u_j\|^2 - \|p_j\|^2 = 1. \tag{4.1.11}$$

The normalization condition for the basis in (4.1.11) ensures that the spectrum $\{E_j\}$ that we find is positive. An implicit assumption on the structure of eigenstates allows for the correlation functions to be given by the formulas (see Remark 9):

$$\begin{aligned} m^{\text{pair}}(x,y) &= -\sum_j u_j(x)\overline{p_j(y)} \\ n^{\text{pair}}(x,y) &= \sum_j p_j(x)\overline{p_j(y)}. \end{aligned} \tag{4.1.12}$$

### 4.1.1 Synopsis of the theory of $J-$self-adjoint operators

In Chapter 3, it was also shown that there is a connection between the unitary rotation of quadratic bosonic Hamiltonians, and the non-Hermitian formalism of *pair-excitation*. These methods are represented in the physics literature by the works of Lee, Huang, Yang [37, 38], Fetter [20, 21], and Wu [60, 61], respectively.

More precisely, the theory of $J$-self-adjoint operators, motivated by the work of Albeverio, Tretter, et. al [2, 3, 13, 58] can be applied to any quadratic Hamiltonian. In the context of equation (4.1.4) for the condensate and the linear system (4.1.13) for $\{U_j(x), P_j(x)\}_{j=1}^{\infty}$, a solution to any one of the following systems can be used to construct a solution to the other two:

**(i)** The Bogoliubov de-Gennes system for the basis $\{U_j(x), P_j(x)\}_{j=1}^{\infty}$:

$$\int \left\{ \begin{pmatrix} h_{\text{Fet}}(x,y) & -f_\phi(x,y) \\ \overline{f_\phi(x,y)} & -h_{\text{Fet}}^T(x,y) \end{pmatrix} \begin{pmatrix} U_j(y) \\ P_j(y) \end{pmatrix} \right\} \mathrm{d}y = E_j \begin{pmatrix} U_j(x) \\ P_j(x) \end{pmatrix}, \quad \|U_j\|^2 - \|P_j\|^2 = 1. \tag{4.1.13}$$

**(ii)** The nonlinear Riccati equation for kernel $k(x,y)$:

$$h_{\text{Fet}} \circ k + k \circ h_{\text{Fet}}^T + f_\phi + k \circ \overline{f_\phi} \circ k = 0, \quad k : (\phi)_\perp \to (\phi)_\perp, \quad \|k\|_{\text{op}} < 1. \tag{4.1.14}$$

This approach is used, e.g., in [60] to describe a spatially-dependent process whereby pairs of particles escape the condensate.

**(iii)** The 'phonon' equation for a (non-orthogonal) basis of single-particle excitations $\omega_j(x)$:

$$h_{\text{ph}}(x, \omega_j) := (h_{\text{Fet}} + k \circ f_\phi)(x, \omega_j) = E_j \omega_j(x). \tag{4.1.15}$$

In particular, the operator matrix in (4.1.13) is diagonalized by a boundedly-invertible matrix which depends on the kernel $k$, via:

$$\begin{pmatrix} h_{\text{Fet}}^T + k \circ \overline{f_\phi} & 0 \\ 0 & -h_{\text{Fet}} - \overline{k} \circ f_\phi \end{pmatrix} = W \circ \begin{pmatrix} h_{\text{Fet}} & -f_\phi \\ \overline{f_\phi} & -h_{\text{Fet}}^T \end{pmatrix} \circ W^{-1}, \tag{4.1.16}$$

for

$$W := \begin{pmatrix} \widehat{\delta} & k \\ \overline{k} & \widehat{\delta} \end{pmatrix},$$

and

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

The diagonalized matrix in (4.1.16) features the phonon operator of (4.1.15).

We extend the equivalence of systems (4.1.13) and (4.1.14) to the nonlinear system of equations (4.1.10), (4.1.11), (4.1.12). This allows us to consider the equation (for operators $h, m$ defined in equation (4.1.9))

$$h \circ k + k \circ h^T + (\upsilon_N m) + k \circ \overline{(\upsilon_N m)} \circ k = 0, \quad k : (\phi)_\perp \to (\phi)_\perp, \tag{4.1.17}$$

*in lieu* of the coupled nonlinear system (4.1.11). In this reformulation, we have the formulas

$$\begin{aligned} -\sum_j u_j(x)\overline{p_j(y)} &= \left(k \circ (\delta - k \circ \bar{k})^{-1}\right)(x,y), \\ \sum_j p_j(x)\overline{p_j(y)} &= \left((k \circ \bar{k}) \circ (\delta - k \circ \bar{k})^{-1}\right)(x,y). \end{aligned} \tag{4.1.18}$$

This allows us to rewrite the densities $n^{\text{pair}}(x,y), m^{\text{pair}}(x,y)$, in terms of the operator $k(x,y)$. The equation for $\phi(x)$ is therefore coupled to the equation for $k(x,y)$, via these densities. This approach has the benefit of solving a single equation for $k(x,y)$, instead of the infinite, nonlinear, coupled system for $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$.

In this chapter, we solve the nonlinear system (4.1.10), (4.1.17), (4.1.18) using techniques developed for solving the linear system (4.1.13). Our construction is perturbative—we introduce the small parameter $g > 0$ which describes the strength of the interaction (i.e., $\upsilon_N(x) := gN^{3\beta}\upsilon(N^\beta x)$ where $\upsilon(x) \geq 0$ is a symmetric, smooth function, such that $\upsilon_N(x-y) \to g\delta(x-y)$ as $N \to \infty$), and show that solutions to the nonlinear system exist which are close to the unperturbed solutions of (4.1.13) and (4.1.14).

The translation of the system (4.1.10), (4.1.11), (4.1.12), to a coupled system for $\phi(x)$ and $k(x,y)$ also helps us to understand the spectrum $E_j$ in the context of the nonlinear system (4.1.11). Our main result is:

**Theorem 3.** *Suppose the single-particle operator* $\big(-\Delta+V_{\rm trap}(x)\big)$ *contains a gap between its ground state and first excited state. Then for* $g>0$ *small enough and* $0\le\beta\le 1/6$*, there exist* $\phi\in\mathfrak{h}^1_V$*, with* $\|\phi\|_{L^2}=1$*, and* $k\in\mathfrak{B}_2(\phi_\perp,\phi_\perp)$*, with* $\|k\|_{\rm op}<1$ *which solve the coupled system consisting of the equation for* $\phi$*:*

$$(-\Delta_x+V_{\rm trap}(x))\phi(x)+(v_N*|\phi|^2)(x)\phi(x)+\frac{1}{N}(v_N*\rho^{\rm pair})(x)\phi(x)$$
$$+\frac{1}{N}\int dy\{v_N(x-y)n^{\rm pair}(x,y)\phi(y)\}+\frac{1}{N}\int dy\{v_N(x-y)m^{\rm pair}(x,y)\phi(y)\}=\mu\phi(x),$$

*the nonlinear equation for* $k(x,y)$*:*

$$h\circ k+k\circ h^T+(v_N m)+k\circ\overline{(v_N m)}\circ k=0,\quad k:(\phi)_\perp\to(\phi)_\perp,$$

*for particle densities* $n^{\rm pair}(x,y)$ *and* $m^{\rm pair}(x,y)$ *given by:*

$$n^{\rm pair}(x,y):=\Big((\delta-k\circ\bar{k})^{-1}\circ(k\circ\bar{k})\Big)(x,y),\quad m^{\rm pair}(x,y):=\Big((\delta-k\circ\bar{k})^{-1}\circ k\Big)(x,y),$$

*and* $\rho^{\rm pair}(x):=n^{\rm pair}(x,x)$.

## 4.2 Many-body system and approximation scheme

We derive the coupled system for the condensate wavefunction and pair-excitation kernel via the heuristic approximation scheme of Griffin [25]. The starting point is the operator $\mathscr{H}-\mu\mathscr{N}$, where $\mathscr{H}$ is the many-body Fock space Hamiltonian (5.2.5). We write this using the definition

$$\varepsilon(x,y):=\big(-\Delta+V_{\rm trap}(x)-\mu\big)\delta(x-y),$$

so that,

$$\mathscr{H}-\mu\mathscr{N}=\iint {\rm d}x{\rm d}y\,\big\{a_x^*\varepsilon(x,y)a_y+\frac{1}{2}a_x^*a_y^*\frac{1}{N}v_N(x-y)a_xa_y\big\}. \tag{4.2.1}$$

The function $V_{\text{trap}}(x) > 0$ represents the effect of a generic trapping potential. It suffices for our purposes to consider, for example, $V_{\text{trap}}(x) = |x|^2$, or any trapping potential that makes the Schrödinger operator $(-\Delta - V_{\text{trap}}(x))$ positive, with a gap between its lowest and first excited state. The constant $\mu > 0$ represents the chemical potential of the system, and is included because the total particle number is not conserved in the resulting quadratic approximate Hamiltonian. We understand $\mu$ as a Lagrange multiplier which fixes the average number of particles $N > 0$ in the system; its value must be determined as part of the approximation. The two-particle interaction potential is given by $\upsilon_N(x) := gN^{3\beta}\upsilon(N^{\beta}x)$ where $\upsilon(x)$ is a positive, symmetric, and $\int \mathrm{d}x\{\upsilon(x)\} = 1$. The constant $g > 0$ is a small parameter, such that $\upsilon_N(x-y) \to g\delta(x-y)$ as $N \to \infty$. In what follows, we will assume $\beta \leq 1/6$, so that, in particular, $\frac{1}{N}\upsilon_N(x) \leq g\|\upsilon\|_{L^\infty}$ for all $x \in \mathbb{R}^3$. To avoid unnecessary complications, we also assume that the Fourier transform of $\upsilon$ is positive, i.e., $\widehat{\upsilon} \geq 0$, although this is not strictly necessary in order for the argument to hold.

The operators $a_x, a_x^*$ denote the bosonic field operators on $\mathbb{F}(\mathfrak{h})$ which satisfy the usual commutation relations,

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

The scheme consists in replacing $\mathscr{H} - \mu\mathscr{N}$ by the 'approximation' $\mathscr{K}'$, which is described by the expression

$$\mathscr{K}' = K_0 + \tilde{K}_1 + \tilde{K}_2.$$

The three operators $K_0, \tilde{K}_1, \tilde{K}_2$ contain, respectively, constant, linear, and quadratic terms in the bosonic field operators for the noncondensate (see (4.2.2)). The goal of this descrip-

tion is to derive effective equations for two quantities: **(i)** the macroscopic condensate wavefunction $\Phi \in L^2(\mathbb{R}^3)$ (this results from enforcing the condition $\tilde{K}_1 \equiv 0$), and **(ii)** a quantity that describes low-lying excitations of the Bose gas that can be attributed to particles outside the condensate. We will show that there are two equivalent descriptions of this second quantity. The first comes from diagonalizing the operator $\tilde{K}_2$ via a unitary transformation of field operators, and yields the basis of single-particle states $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$. The second description utilizes the pair-excitation kernel $k(x,y)$, which solves a nonlinear Riccati-type equation (equation (4.4.9)), and describes a spatially-dependent process whereby pairs of particles scatter from the condensate.

The macroscopic wavefunction is normalized according to

$$\|\Phi\|^2 = N,$$

where $N > 0$ is the total number of particles of the system with Hamiltonian $\mathscr{H}$, or the average number of particles of the system with Hamiltonian $\mathscr{K}'$. More generally, the normalization can be taken to be $N\xi$ where the parameter $0 < \xi < 1$ represents the condensate fraction, although we do not pursue this currently. Furthermore, we employ the *Bogoliubov approximation*, writing the field operators as

$$a_x \approx \Phi(x) + b_x, \quad a_x^* \approx \overline{\Phi(x)} + b_x^*. \tag{4.2.2}$$

Here the operators $b_x^*, b_x$ are taken to satisfy canonical commutation relations on the space orthogonal to the condensate, $(\Phi)_\perp$. That is,

$$[b_x, b_y^*] = \delta(x-y) - \frac{1}{N}\overline{\Phi(x)}\,\Phi(y) := \widehat{\delta}(x-y).$$

We will not justify the approximation (4.2.2) in the current work. Our aim is rather to

explore consequences of the model that results from this heuristic approximation. For relevant mathematical work on the validity of the Bogoliubov approximation for interacting Bosonic Hamiltonians, see [57].

Using the Bogoliubov approximation (4.2.2) in Hamiltonian (4.2.1) yields an operator $\mathscr{K}_{\mathrm{Bog}} : \mathbb{F}(\Phi_\perp) \to \mathbb{F}(\Phi_\perp)$ which is quartic in field operators $b_x, b_x^*$:

$$\begin{aligned}\mathscr{K}_{\mathrm{Bog}} &:= \iint \mathrm{d}x\mathrm{d}y \Big\{ \big(\overline{\Phi(x)} + b_x^*\big)\varepsilon(x,y)\big(\Phi(y)+b_y\big)\Big\} \\ &\quad + \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y \Big\{ \big(\overline{\Phi(x)} + b_x^*\big)\big(\overline{\Phi(y)} + b_y^*\big)\frac{1}{N}\upsilon_N(x-y)\big(\Phi(x)+b_x\big)\big(\Phi(y)+b_y\big)\Big\} \\ &:= K_0 + K_1 + K_2 + K_3 + K_4,\end{aligned} \tag{4.2.3}$$

The operators $K_i$ for $i = 0,1,2,3$ contain all terms with $i$ factors of the field operators $b^*, b$. More precisely,

$$\begin{aligned}K_0 &= \iint \mathrm{d}x\mathrm{d}y \Big\{ \overline{\Phi(x)}\varepsilon(x,y)\Phi(y) + \frac{1}{2N}|\Phi(x)|^2\upsilon_N(x-y)|\Phi(y)|^2\Big\}, \\ K_1 &= \iint \mathrm{d}x\mathrm{d}y\; b_x^*\Big\{\varepsilon(x,y)\Phi(y) + |\Phi(y)|^2\frac{1}{N}\upsilon_N(x-y)\Phi(x)\Big\} + \mathrm{h.c.}, \\ K_3 &= \iint \mathrm{d}x\mathrm{d}y\; b_x^*\Big\{\overline{\Phi(y)}\frac{1}{N}\upsilon_N(x-y)\Big\}b_x b_y + \mathrm{h.c.}, \\ K_4 &= \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y\; b_x^* b_y^*\big\{\frac{1}{N}\upsilon_N(x-y)\big\}b_x b_y\,.\end{aligned} \tag{4.2.4}$$

We write $K_2 = K_{diag} + K_2'$, where

$$\begin{aligned}K_{diag} &= \iint \mathrm{d}x\mathrm{d}y\; b_x^*\Big\{\varepsilon(x,y) + \overline{\Phi(y)}\frac{1}{N}\upsilon_N(x-y)\Phi(x)\Big\}b_y \\ &\quad + \iint \mathrm{d}x\mathrm{d}y\; b_x^*\Big\{|\Phi(y)|^2\frac{1}{N}\upsilon_N(x-y)\Big\}b_x\end{aligned} \tag{4.2.5}$$

and

$$K_2' = \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y\; b_x^* b_y^*\Big\{\Phi(x)\frac{1}{N}\upsilon_N(x-y)\Phi(y)\Big\} + \mathrm{h.c.} \tag{4.2.6}$$

Next, the Hamiltonian $\mathscr{K}_{\mathrm{Bog}}$ is replaced by $\mathscr{K}'$, by replacing the operators $K_3$ and $K_4$ with combinations of quadratic operators. This is done by replacing products of field

operators, $(b_x^* b_y)$, $(b_x b_y)$, or $(b_x^* b_y^*)$, by the averages $\langle b_x^* b_y \rangle$, $\langle b_x b_y \rangle$, or $\langle b_x^* b_y^* \rangle$. **Note:** We will remark on the meaning of these averages shortly, and link them to a *quasifree* hypothesis. Thus, we make the replacements:

$$\begin{aligned} b_x^* b_y^* b_x b_y \approx\ & 2\langle b_x^* b_y \rangle b_y^* b_x + 2\langle b_x^* b_x \rangle b_y^* b_y + \langle b_x^* b_y^* \rangle b_x b_y + \langle b_x b_y \rangle b_x^* b_y^* \,, \\ b_x^* b_x b_y \approx\ & \langle b_x^* b_x \rangle b_y + \langle b_x^* b_y \rangle b_x + \langle b_x b_y \rangle b_x^* \,. \end{aligned} \tag{4.2.7}$$

Defining the quantities

$$\rho^{\text{pair}}(x) := \langle b_x^* b_x \rangle, \quad n^{\text{pair}}(x,y) := \langle b_x^* b_y \rangle, \quad m^{\text{pair}}(x,y) := \langle b_x b_y \rangle, \tag{4.2.8}$$

we arrive at the approximate Hamiltonian,

$$\mathscr{K}' = K_0 + \tilde{K}_1 + \tilde{K}_2,$$

where

$$\begin{aligned} \tilde{K}_1 &= K_1 + \iint \mathrm{d}x\mathrm{d}y\ \{\overline{\Phi(y)} \frac{1}{N} \upsilon_N(x-y)\} \Big( \rho^{\text{pair}}(x) b_y + n^{\text{pair}}(x,y) b_x + m^{\text{pair}}(x,y) b_x^* \Big) \\ &\quad + \iint \mathrm{d}x\mathrm{d}y \{\Phi(y) \frac{1}{N} \upsilon_N(x-y)\} \Big( \rho^{\text{pair}}(x) b_y^* + n^{\text{pair}}(x,y) b_x^* + \overline{m^{\text{pair}}}(x,y) b_x \Big) \\ &= K_1 + \frac{1}{N} \iint \mathrm{d}x\mathrm{d}y\ b_x^* \upsilon_N(x-y) \{\overline{\Phi(y)} m^{\text{pair}}(x,y) + \Phi(x) \rho^{\text{pair}}(y) + \Phi(y) n^{\text{pair}}(x,y)\} + \text{h.c.} \end{aligned}$$

and $\tilde{K}_2 = \tilde{K}_{diag} + \tilde{K}_2'$, with

$$\begin{aligned} \tilde{K}_{diag} &= K_{diag} + \frac{1}{N} \iint \mathrm{d}x\mathrm{d}y\ b_x^* \{n^{\text{pair}}(x,y) \upsilon_N(x-y)\} b_y + \frac{1}{N} \iint \mathrm{d}x\mathrm{d}y\ b_y^* \{\upsilon_N(x-y) \rho^{\text{pair}}(x)\} b_y, \\ \tilde{K}_2' &= \frac{1}{2} \iint \mathrm{d}x\mathrm{d}y\ b_x^* b_y^*\ \frac{1}{N} \upsilon_N(x-y) \Big\{ \Phi(x)\Phi(y) + m^{\text{pair}}(x,y) \Big\} + \text{h.c.} \end{aligned}$$

For the remainder of this work, we work with the normalized condensate wavefunction,

$$\phi(x) := \frac{1}{\sqrt{N}} \Phi(x), \quad \|\phi\|^2 = 1.$$

The equation for $\phi$ emerges by imposing the constraint $\tilde{K}_1 = 0$, which yields:

$$\begin{aligned} \mu\phi(x) = & \Big( -\Delta + V_{\text{trap}}(x) + (\upsilon_N * |\phi|^2)(x) \Big) \phi(x) + \frac{1}{N} (\upsilon_N * \rho^{\text{pair}})(x) \phi(x) \\ & + \frac{1}{N} \int \mathrm{d}y \Big\{ n^{\text{pair}}(x,y) \upsilon_N(x-y) \phi(y) + m^{\text{pair}}(x,y) \upsilon_N(x-y) \overline{\phi(y)} \Big\}. \end{aligned} \tag{4.2.9}$$

Define the operators

$$\begin{aligned} h(x,y) &:= \varepsilon(x,y) + \overline{\phi(y)}\upsilon_N(x-y)\phi(x) + (\upsilon_N * |\phi|^2)(y)\delta(x-y) \\ &\quad + \frac{1}{N}\upsilon_N(x-y)n^{\text{pair}}(x,y) + (\frac{1}{N}\upsilon_N * \rho^{\text{pair}})(x)\delta(x-y), \\ \Theta(x,y) &:= \upsilon_N(x-y)\big\{\phi(x)\phi(y) + \frac{1}{N}m^{\text{pair}}(x,y)\big\}. \end{aligned} \tag{4.2.10}$$

Then, Hamiltonian $\mathscr{K}'$ reads $\mathscr{K}' = K_0 + \tilde{K}_2$, for

$$\tilde{K}_2 = \iint \mathrm{d}x\mathrm{d}y\; b_x^*\big\{h(x,y)\big\}b_y + \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y\; b_x\big\{\overline{\Theta(x,y)}\big\}b_y + \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y\; b_x^*\big\{\Theta(x,y)\big\}b_y^*.$$

## 4.3 Diagonalization of $\tilde{K}_2$ and the coupled system for $\phi, k$ :

Assume that $\phi$ satisfies equation (4.2.9). We now diagonalize the Hamiltonian $\mathscr{K}'$ via a unitary rotation of the field operators $b_x, b_x^*$. This introduces the basis of single-particle states $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$, which satisfy a block operator matrix problem (4.3.4) involving the densities $n^{\text{pair}}(x,y)$, $\rho^{\text{pair}}(x)$, $m^{\text{pair}}(x,y)$.

The most concise way to represent this unitary rotation is via the formula:

$$\begin{aligned} b_x &= \sum_j \{u_j(x)\alpha_j - \overline{p_j(x)}\alpha_j^*\} \\ b_x^* &= \sum_j \{\overline{u_j(x)}\alpha_j^* - p_j(x)\alpha_j\}. \end{aligned} \tag{4.3.1}$$

The operators $\alpha_j$, $\alpha_j^*$ in (4.3.1) are taken to satisfy the canonical commutation relations

$$[\alpha_j, \alpha_k^*] = \delta_{jk}, \quad [\alpha_j, \alpha_k] = [\alpha_j^*, \alpha_k^*] = 0,$$

and the canonical relations on the operators $b_x, b_x^*$ imply the following relations for the basis $\{u_j(x), p_j(x)\}$:

$$\begin{aligned} &\sum_{j=1}^{\infty} \{u_j(x)\overline{u_j(x')} - \overline{p_j(x)}p_j(x')\} = \widehat{\delta}(x,x') \ , \\ &\sum_{j=1}^{\infty} \{u_j(x)\overline{p_j(x')} - \overline{p_j(x)}u_j(x')\} = 0, \quad \forall x, x' \in \mathbb{R}^3 \ . \end{aligned} \tag{4.3.2}$$

By an elementary calculation, identical to the one carried out in Chapter 3, it is found that $\tilde{K}_2$ becomes diagonal in the $\{\alpha_j, \alpha_j^*\}$ operators, i.e.,

$$\tilde{K}_2 = \sum_j E_j \alpha_j^* \alpha_j, \tag{4.3.3}$$

provided the following block operator matrix eigenvalue equation holds for all $j$:

$$\int \mathrm{d}y \left\{ \begin{pmatrix} h(x,y) & -\Theta(x,y) \\ \overline{\Theta(x,y)} & -h^T(x,y) \end{pmatrix} \begin{pmatrix} u_j(y) \\ p_j(y) \end{pmatrix} \right\} = E_j \begin{pmatrix} u_j(x) \\ p_j(x) \end{pmatrix}. \tag{4.3.4}$$

At this point, the operator matrix in (4.3.4) contains contributions from the unknown operators $\rho^{\mathrm{pair}}(x), n^{\mathrm{pair}}(x,y), m^{\mathrm{pair}}(x,y)$. A solution to the system will therefore require us to interpret these quantities.

The contribution of this chapter is to solve the system (4.3.4) in the case where the parameter $g$ is very small. In particular, we must characterize the spectrum $\{E_j\}$ and determine the single-particle wavefunctions $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$. The operators $h(x,y)$ and $\Theta(x,y)$ contain contributions from densities $\rho^{\mathrm{pair}}(x)$, $n^{\mathrm{pair}}(x,y)$ and $m^{\mathrm{pair}}(x,y)$, which have been left undetermined up to this point; these quantities must be determined self-consistently as part of the solution. This complication was not present in our analysis of system (4.1.13) & (4.1.14), which is a special case of equation (4.3.4) that results from setting $\rho^{\mathrm{pair}}(x), n^{\mathrm{pair}}(x,y), m^{\mathrm{pair}}(x,y)$ equal to zero. Our solution takes the operators $h(x,y), \Theta(x,y)$ to depend on the solutions $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$, thus equation (4.3.4) is actually nonlinear.

We take the densities $n^{\mathrm{pair}}$, $m^{\mathrm{pair}}$ to be given by the formulas:

$$\begin{aligned} n^{\mathrm{pair}}(x,y) &= \sum_j p_j(x)\overline{p_j(y)}, \\ m^{\mathrm{pair}}(x,y) &= -\sum_j u_j(x)\overline{p_j(y)}. \end{aligned} \tag{4.3.5}$$

The reason for this is given in the next remark (which is part of the argument of Griffin [25]):

**Remark 9.** *We now derive the formulas for the densities* $\rho^{\text{pair}}(x), n^{\text{pair}}(x,y), m^{\text{pair}}(x,y)$ *under several assumptions on the operators* $\alpha_j, \alpha_j^*$. *This follows the derivation of Griffin. Using equation* (4.3.1)*,*

$$\begin{aligned}\langle b_x^* b_y\rangle = &\sum_{jk}\{\overline{u_j(x)}u_k(y) + \overline{p_j(x)}p_k(y)\}\langle\alpha_j^*\alpha_k\rangle + \sum_j p_j(x)\overline{p_j(y)} \\ &-\sum_{jk} p_j(x)u_k(y)\langle\alpha_j\alpha_k\rangle + \overline{u_j(x)}\;\overline{p_k(y)}\langle\alpha_j^*\alpha_k^*\rangle\end{aligned} \tag{4.3.6}$$

*and*

$$\begin{aligned}\langle b_x b_y\rangle = &\sum_{jk}\{-\overline{p_j(x)}u_k(y) - \overline{p_j(y)}u_k(x)\}\langle\alpha_j^*\alpha_k\rangle - \sum_j u_j(x)\overline{p_j(y)} \\ &+\sum_{jk} u_j(x)u_k(y)\langle\alpha_j\alpha_k\rangle + \overline{p_j(x)}\;\overline{p_k(y)}\langle\alpha_j^*\alpha_k^*\rangle.\end{aligned} \tag{4.3.7}$$

*We have not yet interpreted the meaning of the averages* $\langle b_x^* b_y\rangle$, $\langle b_x b_y\rangle$, *or* $\langle\alpha_j^*\alpha_k\rangle, \langle\alpha_j\alpha_k\rangle$. *Apparently, Griffin makes the assumption:*

$$\sum_{jk}\{p_j(x)u_k(y)\langle\alpha_j\alpha_k\rangle + \overline{u_j(x)}\;\overline{p_k(y)}\langle\alpha_j^*\alpha_k^*\rangle\} = 0, \tag{4.3.8}$$

*as well as*

$$\sum_{jk}\{u_j(x)u_k(y)\langle\alpha_j\alpha_k\rangle + \overline{p_j(x)}\;\overline{p_k(y)}\langle\alpha_j^*\alpha_k^*\rangle\} = 0. \tag{4.3.9}$$

*(Note: the approximation also works in the same way by making the more strict assumption* $\langle\alpha_j\alpha_k\rangle = 0$.*) In addition, Griffin takes the averages* $\langle\alpha_j^*\alpha_k\rangle$ *to follow the Bose distribution, i.e.,*

$$\langle\alpha_j^*\alpha_k\rangle = N_0(E_j)\delta_{jk}, \quad N_0(E_j) := \Big(\frac{1}{e^{\beta(T)E_j} - 1}\Big), \quad \beta(T) := 1/k_B T, \quad T \geq 0. \tag{4.3.10}$$

*Equations* (4.3.8)*,* (4.3.9)*, and* (4.3.10) *then imply*

$$\langle b_x^* b_y \rangle = \sum_j \{\overline{u_j(x)} u_j(y) + \overline{p_j(x)} p_j(y)\} N_0(E_j) + p_j(x)\overline{p_j(y)}, \tag{4.3.11}$$

*and*

$$\langle b_x b_y \rangle = \sum_j -2N_0(E_j)\overline{p_j(x)} u_k(y) - u_j(x)\overline{p_j(y)}. \tag{4.3.12}$$

*Taking* $N_0(E_j) = 0$ *for all* $j$*, which corresponds to the limit* $T \to 0$*, or* $\beta \to \infty$*, then gives the formulas* (4.3.5)*.*

The coupled system therefore consists of the formulas:

$$\begin{aligned} n^{\text{pair}}(x,y) &= \sum_j p_j(x)\overline{p_j(y)}, \\ m^{\text{pair}}(x,y) &= -\sum_j u_j(x)\overline{p_j(y)}, \end{aligned} \tag{4.3.13}$$

the equation for $\phi(x)$:

$$\begin{aligned} \mu\phi(x) = \Big( -\Delta + V_{\text{trap}}(x) + (\upsilon_N * |\phi|^2)(x) \Big)\phi(x) + \frac{1}{N}(\upsilon_N * \rho^{\text{pair}})(x)\phi(x) \\ + \frac{1}{N}\int \mathrm{d}y \left\{ n^{\text{pair}}(x,y)\upsilon_N(x-y)\phi(y) + m^{\text{pair}}(x,y)\upsilon_N(x-y)\overline{\phi(y)} \right\}, \end{aligned} \tag{4.3.14}$$

and the matrix system for $\{u_j(x),\, p_j(x)\}_{j=1}^{\infty}$:

$$\int \mathrm{d}y \Big\{ \begin{pmatrix} h(x,y) & -\Theta(x,y) \\ \overline{\Theta(x,y)} & -h^T(x,y) \end{pmatrix} \begin{pmatrix} u_j(y) \\ p_j(y) \end{pmatrix} \Big\} = E_j \begin{pmatrix} u_j(x) \\ p_j(x) \end{pmatrix}, \quad \|u_j\|^2 - \|p_j\|^2 = 1. \tag{4.3.15}$$

**Remark 10.** *Since the system of equation* (4.3.15) *is formally identical to the matrix system of Fetter [20] covered in the previous chapter, the spectrum*

$$\sigma_{\text{p}}\Big( \begin{pmatrix} h(x,y) & -\Theta(x,y) \\ \overline{\Theta(x,y)} & -h^T(x,y) \end{pmatrix} \Big),$$

*will have two 'sheets,' one of which is bounded below, the other bounded above. The normalization condition in* (4.3.15) *specifies the sheet which is bounded below. For details of this choice, we refer to the previous chapter.*

## 4.4 Variational formalism for the nonlinear system

The operator matrix in (4.3.15) has an associated Riccati equation for operator $k$ : $(\phi)_\perp \to (\phi)_\perp$, which reads as

$$h \circ k + k \circ h^T + \Theta + k \circ \overline{\Theta} \circ k = 0, \quad k : (\phi)_\perp \to (\phi)_\perp. \tag{4.4.1}$$

This is a nonlinear integro-differential equation, which we solve for Hilbert-Schmidt kernel $k(x,y) \in \mathfrak{B}_2(\mathfrak{h}_V^1)$. The link between block operator matrices and operator Riccati equations has an extensive mathematical background which was discussed in depth in Chapter 3 (see also the works of Tretter, Albeverio, et. al. [2,3,13,58]). We state the relevant facts as they apply to the matrix system (4.3.15) in the following theorem:

**Theorem 4.** ***(a)*** *Suppose $k \in \mathfrak{B}_2(\mathfrak{h}_V^1)$ is a symmetric solution to equation* (4.5.6) *with $\|k\|_{\text{op}} < 1$. Then there exists basis $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$ solving* (4.3.15) *with normalization $\|u_j\|^2 - \|p_j\|^2 = 1$. The spectrum $\{E_j\}$ in this case is positive and the following integral relation holds:*

$$k(x, u_j) = p_j(x). \tag{4.4.2}$$

***(b)*** *Suppose $\{u_j(x), p_j(x)\}_{j=1}^{\infty}$ solves* (4.3.15)*, where $\{u_j\}$ is a basis of $\phi_\perp$, and that the integral relation* (4.4.2) *holds for some $k$ with $\|k\|_{\text{op}} < 1$ and all $j$. Then $k$ solves the Riccati equation* (4.5.6)*.*

The proof of this theorem is an adaptation of the spectral theory of J-self-adjoint operator matrices [58]; our proof is the same here as it was in the case $\rho^{\text{pair}}, n^{\text{pair}}, m^{\text{pair}} = 0$, which was handled in Chapter 3. We include the proof here, adapted to the current system, for the reader's convenience.

*Proof.* The matrix in equation (4.3.15) is diagonalized by an operator matrix constructed using $k$ which solves (4.5.6). In particular, define the operator matrices

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

and

$$D := \begin{pmatrix} h^T + k \circ \overline{\Theta} & 0 \\ 0 & -h - \overline{k} \circ \Theta \end{pmatrix}.$$

A direct calculation, which uses the fact that $k$ satisfies the Riccati equation, shows that the following holds:

$$\begin{pmatrix} h^T + k \circ \overline{\Theta} & 0 \\ 0 & -h - \overline{k} \circ \Theta \end{pmatrix} = W \circ \begin{pmatrix} h & -\Theta \\ \overline{\Theta} & -h^T \end{pmatrix} \circ W^{-1}.$$

In order for both $W$ and $W^{-1}$ to be bounded, we require that $(\delta - k \circ \overline{k})^{-1}$ be a bounded operator, which is true if $\|k\|_{\text{op}} < 1$. The operator $h^T + k \circ \overline{\Theta}$, while not self-adjoint, is similar to the self-adjoint operator (a consequence of the equation (4.4.1) for $k$):

$$(\delta - k \circ \overline{k})^{-1/2} \circ (h^T + k \circ \overline{\Theta}) \circ (\delta - k \circ \overline{k})^{1/2}. \tag{4.4.3}$$

The spectrum $\sigma\left(h^T + k \circ \overline{\Theta}\right)$ is therefore real, discrete, and bounded below (as a compact perturbation of $-\Delta + V_{\text{trap}}(x) - \mu$), and the system of eigenvectors of (4.4.3), denoted

$\{\eta_j(x)\}$, is orthogonal and complete in the space $(\phi)_\perp$. Given the solutions $\eta_j(x)$, we can construct $u_j(x)$, $p_j(x)$ which solve the matrix system via

$$u_j(x) = (\delta - k \circ \overline{k})^{-1/2}(x, \eta_j), \quad p_j(x) = k(x, u_j).$$

The spectrum of $D$ consists of two discrete and semi-bounded parts: $\sigma(h^T + k \circ \overline{\Theta})$ is bounded below (since $\sigma(h^T)$ is bounded below), and $-\sigma(h^T + k \circ \overline{\Theta})$ is bounded above. The normalization condition for $\{u_j, p_j\}$, which comes from the fact that these functions represent Bogoliubov rotations, implies that the Bogoliubov spectrum of the quadratic Hamiltonian $K_0 + \tilde{K}_2$ consists of one part only, namely $\sigma(h^T + k \circ \overline{\Theta})$. □

**Corollary 2.** *Assume that* $\{u_j, p_j\}$ *satisfy equation* (4.3.15)*, and that k solves the Ricatti equation. Then the following formulas hold for the density operators:*

$$\begin{aligned} m^{\text{pair}}(x,y) &= -\sum_j u_j(x)\overline{p_j(y)} = \Big(k \circ (\delta - \overline{k} \circ k)^{-1}\Big)(x,y) \\ n^{\text{pair}}(x,y) &= \sum_k p_j(x)\overline{p_j(y)} = \Big((k \circ \overline{k}) \circ (\delta - \overline{k} \circ k)^{-1}\Big)(x,y). \end{aligned} \tag{4.4.4}$$

Corollary 2 shows that the nonlinear terms of the Riccati equation (4.4.1) can be rewritten exclusively in terms of the kernel $k$. In particular, the operators $h(x,y), \Theta(x,y)$ are written using this kernel (recall $\varepsilon(x,y) = (-\Delta_x + V_{\text{trap}}(x) - \mu)\delta(x-y)$):

$$\begin{aligned} h[\phi,k](x,y) &= \varepsilon(x,y) + \overline{\phi(y)}\upsilon_N(x-y)\phi(x) + (\upsilon_N * |\phi|^2)(y)\delta(x-y) \\ &+ \frac{1}{N}\upsilon_N(x-y)\Big\{\frac{k \circ \overline{k}}{\delta - k \circ \overline{k}}\Big\}(x,y) + \frac{1}{N}\int \mathrm{d}x'\, \upsilon_N(x-x')\Big\{\frac{k \circ \overline{k}}{\delta - k \circ \overline{k}}\Big\}(x',x')\delta(x-y). \end{aligned} \tag{4.4.5}$$

Note: The fraction notation $k \circ \overline{k}/(\delta - k \circ \overline{k})$ is justified here because of the commutation

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

and

$$\Theta[\phi,k](x,y) = \upsilon_N(x-y)\Big\{\phi(x)\phi(y) + \frac{1}{N}\big(k\circ(\delta-\overline{k}\circ k)^{-1}\big)(x,y)\Big\}. \tag{4.4.6}$$

By Theorem 4, solving the system consisting of equation (4.3.14) for $\phi$, and equation (4.4.1) for $k$ is equivalent to the system (4.3.5), (4.3.14), (4.3.15).

**Remark 11.** *The system for $\phi$ and $k$ can be rewritten in an illustrative way. Let $h_0 := h+\mu$, i.e.,*

$$\begin{aligned} h_0[\phi,k](x,y) &= \varepsilon_0(x,y) + \overline{\phi(y)}\upsilon_N(x-y)\phi(x) + (\upsilon_N * |\phi|^2)(y)\delta(x-y) \\ &+ \frac{1}{N}\upsilon_N(x-y)\Big\{\frac{k\circ\overline{k}}{\delta-k\circ\overline{k}}\Big\}(x,y) + \frac{1}{N}\int \mathrm{d}x'\upsilon_N(x-x')\Big\{\frac{k\circ\overline{k}}{\delta-k\circ\overline{k}}\Big\}(x',x')\delta(x-y). \end{aligned} \tag{4.4.7}$$

*and define the operator $\theta$ by the formula:*

$$\theta := \upsilon_N(x-y)\big\{\phi(x)\phi(y) - \frac{1}{N}\big(k\circ(\delta-\overline{k}\circ k)^{-1}\big)(x,y)\big\}. \tag{4.4.8}$$

*(Note the difference between $\Theta$ and $\theta$.) Then the system for $\phi$, $k$ is:*

$$\begin{cases} \begin{pmatrix} h_0(x,y) & -\theta(x,y) \\ -\overline{\theta(x,y)} & h_0^T(x,y) \end{pmatrix} \circ \begin{pmatrix} \phi(y) \\ \overline{\phi(y)} \end{pmatrix} = \mu \begin{pmatrix} \phi(y) \\ \overline{\phi(y)} \end{pmatrix}, \\ \\ h\circ k + k\circ h^T + \Theta + k\circ\overline{\Theta}\circ k = 0. \end{cases} \tag{4.4.9}$$

In the spirit of the previous chapter, we adopt a variational approach to find solutions to the system (4.4.9). The functions $\phi$ and $k$ are sought as minimizers of the total energy, $\mathscr{E}_{\mathrm{tot}}[\phi,k]$.

**Definition 4.** *For the operator $\varepsilon_0 := (-\Delta + V_{\text{trap}}(x))$, the Hartree energy functional, denoted $E_{\text{H}}$, is defined for all $\phi \in \mathfrak{h}^1_V$, by*

$$E_{\text{H}}[\phi] := \iint \mathrm{d}x\mathrm{d}y \big\{ \overline{\phi(x)} \varepsilon_0(x,y)\phi(y) + \frac{1}{2}|\phi(x)|^2 \upsilon_N(x-y)|\phi(y)|^2 \big\}. \tag{4.4.10}$$

*Given the operators $h, \Theta : \mathfrak{h}^1_V \to \mathfrak{h}^1_V$ (which have a dependence on $k, \phi$ via equations* (4.4.6), (4.4.7)*), the functional $\mathscr{E}[k; h, \Theta]$ is defined on the set of kernels*

$$\big\{ k \in \mathfrak{B}_2(\mathfrak{h}^1_V), \quad \|k\|_{\text{op}} < 1 \big\},$$

*by the trace*

$$\mathscr{E}[k; h_0, \Theta] := \mathrm{tr}\Big\{ (\delta - \overline{k} \circ k)^{-1} \circ \Big( \overline{k} \circ h_0 \circ k + \frac{1}{2}\overline{k} \circ \Theta + \frac{1}{2}\overline{\Theta} \circ k \Big) \Big\}. \tag{4.4.11}$$

*The total energy, $\mathscr{E}_{\text{tot}}$ is defined for all $\phi \in \mathfrak{h}^1_V$ and $\big\{ k \in \mathfrak{B}_2(\mathfrak{h}^1_V), \quad \|k\|_{\text{op}} < 1 \big\}$ by the sum*

$$\mathscr{E}_{\text{tot}}[\phi, k; N] := \Big\{ E_{\text{H}}[\phi] + \frac{1}{N}\mathscr{E}\big[k; h_0, \Theta\big] \Big\}, \tag{4.4.12}$$

$$\mathrm{dom}(\mathscr{E}_{\text{tot}}) = \{ \phi \in \mathfrak{h}^1_V, \quad k \in \mathfrak{B}_2(\mathfrak{h}^1_V), \quad \|k\|_{\text{op}} < 1 \}.$$

**Lemma 6.** *Let $h[\phi, k], \Theta[\phi, k]$ be given by* (4.4.5), (4.4.6)*, and let the total energy $\mathscr{E}_{\text{tot}}$ be given by formula* (4.4.12) *with $h_0 = h_0[\phi, k]$, $\Theta = \Theta[\phi, k]$, i.e.,*

$$\mathscr{E}_{\text{tot}}[\phi, k; N] := \Big\{ E_{\text{H}}[\phi] + \frac{1}{N}\mathscr{E}\big[k; h_0[\phi, k], \Theta[\phi, k]\big] \Big\}.$$

***(i):*** *For fixed $k, \overline{k}$, critical points of the total energy with respect to constrained variations $\overline{\phi} \in L^2(\mathbb{R}^3)$, $\|\phi\|^2 = 1$, i.e., points satisfying $\delta\mathscr{E}_{\text{tot}}/\delta\overline{\phi} = \mu\phi$, where $\mu$ is the Lagrange multiplier enforcing the constraint, are solutions to the nonlinear Hartree-type equation* (4.4.9)*.*

***(ii):*** *For fixed $\phi$, $\overline{\phi}$ and $\mu$ satisfying* (4.4.9)*, critical points of the total energy*

$$E_{\mathrm{H}}[\phi]+\frac{1}{N}\mathscr{E}\big[k;h_0-\mu,\Theta\big]$$

*with respect to symmetric variations of $\overline{k}\in\mathfrak{B}_2(\mathfrak{h}_V)$, i.e., points satisfying $\delta\mathscr{E}_{\mathrm{tot}}/\delta\overline{k}=0$, are solutions to the nonlinear Riccati equation* (4.4.9)*.*

*Proof.* For assertion **(i)**, It suffices to show that the functional derivative

$$\frac{\delta}{\delta\overline{\phi}}\mathscr{E}\big[k;h[\phi,k],\Theta[\phi,k]\big],$$

yields the terms proportional to $k$ in the equation for $\phi$ in system (4.4.9). The relevant terms of $\mathscr{E}$ are the trace

$$\iint \mathrm{d}x\mathrm{d}y\Big\{\Big(\overline{\phi(y)}\upsilon_N(x-y)\phi(x)+(\upsilon_N*|\phi|^2)(y)\delta(x-y)\Big)\Big(\frac{k\circ\overline{k}}{\delta-k\circ\overline{k}}\Big)(x,y)\Big\},\quad(4.4.13)$$

as well as the trace

$$\mathrm{tr}\Big\{(\delta-\overline{k}\circ k)^{-1}\circ\Big(\frac{1}{2}\overline{\mathscr{G}}\circ k+\frac{1}{2}\overline{k}\circ\mathscr{G}\Big)\Big\},\quad(4.4.14)$$

where $\mathscr{G}:=\upsilon_N(x-y)\phi(x)\phi(y)$. Replacing $\overline{\phi}$ by $\overline{\phi}+\delta\overline{\phi}$ in the (4.4.13), and collecting terms proportional to $\delta\overline{\phi}$ yields

$$\begin{aligned}&\iint \mathrm{d}x\mathrm{d}y\Big\{\Big((\delta\overline{\phi})(y)\upsilon_N(x-y)\phi(x)+(\upsilon_N*(\delta\overline{\phi})\phi)(y)\delta(x-y)\Big)\Big(\frac{k\circ\overline{k}}{\delta-k\circ\overline{k}}\Big)(x,y)\Big\}\\&\quad=\int \mathrm{d}y\,\delta\overline{\phi}(y)\Big\{\int \mathrm{d}x\upsilon_N(x-y)n^{\mathrm{pair}}(x,y)\phi(x)\Big\}+\int \mathrm{d}y\,\delta\overline{\phi}(y)\Big\{\phi(y)(\upsilon_N*\rho^{\mathrm{pair}})(y)\Big\}.\end{aligned}\quad(4.4.15)$$

Replacing $\overline{\phi}$ by $\overline{\phi}+\delta\overline{\phi}$ in (4.4.14), and collecting relevant terms yields

$$\iint \mathrm{d}x\mathrm{d}y\Big(\frac{k}{\delta-\overline{k}\circ k}\Big)(x,y)\upsilon_N(x,y)\Big\{\delta\overline{\phi}(x)\overline{\phi}(y)\Big\}=\int \mathrm{d}y\delta\overline{\phi}(y)\Big\{\int \mathrm{d}x m(x,y)\upsilon_N(x,y)\overline{\phi}(x)\Big\}.\quad(4.4.16)$$

adding the terms (4.4.15) and (4.4.16) to $N\delta E_{\mathrm{H}}[\phi]/\delta\overline{\phi}$ gives exactly equation (4.4.9) for $\phi$.

**(ii)** We show that the variation with respect to $k$ is

$$\delta\mathscr{E}/\delta\overline{k} = \frac{1}{2}(\delta - k\circ\overline{k})^{-1}\circ\Big\{h\circ k + k\circ h^T + \Theta + k\circ\overline{\Theta}\circ k\Big\}\circ(\delta - \overline{k}\circ k)^{-1}.$$

For a Hilbert-Schmidt operator $\mathscr{O}$ with the integral kernel $\mathscr{O}(x,y)$, define the shorthand $(\upsilon\cdot\mathscr{O})$, which is the Hilbert-Schmidt operator with the integral kernel

$$\big(\upsilon\cdot\mathscr{O}\big)(x,y) := \frac{1}{N}\upsilon_N(x-y)\mathscr{O}(x,y).$$

Additionally, define $h_1[\phi]$, $\Theta_1[\phi]$:

$$h_1[k] := \frac{1}{N}\upsilon_N(x-y)\Big\{\frac{k\circ\overline{k}}{\delta - k\circ\overline{k}}\Big\}(x,y) + \frac{1}{N}\int \mathrm{d}x'\upsilon_N(x-x')\Big\{\frac{k\circ\overline{k}}{\delta - k\circ\overline{k}}\Big\}(x',x')\delta(x-y),$$

$$\Theta_1[k] := \frac{1}{N}\upsilon_N(x-y)\big(k\circ(\delta - k\circ\overline{k})^{-1}\big)(x,y),$$

so that we can write the decomposition $h[\phi,k] := h_0[\phi] + h_1[k]$ and $\Theta[\phi,k] := \Theta_0[\phi] + \Theta_1[k]$. We have that

$$\begin{aligned}\frac{\delta\mathscr{E}}{\delta\overline{k}} =& \frac{1}{2}(\delta - k\circ\overline{k})^{-1}\circ\Big\{h_0[\phi]\circ k + k\circ h_0^T[\phi] + \Theta_0[\phi] + k\circ\overline{\Theta}_0[\phi]\circ k\Big\}\circ(\delta - \overline{k}\circ k)^{-1} \\ &+ \frac{\delta}{\delta\overline{k}}\mathrm{tr}\Big\{(\delta - \overline{k}\circ k)^{-1}\Big(\overline{k}\circ h_1[k]\circ k + \frac{1}{2}\overline{k}\circ\Theta_1[k] + \frac{1}{2}\overline{\Theta_1}[k]\circ k\Big)\Big\}\end{aligned} \tag{4.4.17}$$

where

$$\begin{aligned}\frac{\delta}{\delta\overline{k}}\mathrm{tr}\Big\{(\delta - \overline{k}\circ k)^{-1}\Big(\overline{k}\circ h_1[k]\circ k\Big)\Big\} =& \ 2(\delta - k\circ\overline{k})^{-1}\circ\Big[\upsilon\cdot\Big(\frac{k\circ\overline{k}}{\delta - k\circ\overline{k}}\Big)\Big]\circ(\delta - \overline{k}\circ k)^{-1} \\ &+ 2(\delta - k\circ\overline{k})^{-1}\circ\Big[\frac{1}{N}\Big(\upsilon_N * \frac{k\circ\overline{k}}{\delta - k\circ\overline{k}}\Big)(x)\delta(x-y)\Big]\circ k\circ(\delta - \overline{k}\circ k)^{-1}\end{aligned} \tag{4.4.18}$$

and

$$\frac{\delta}{\delta\overline{k}}\mathrm{tr}\Big\{(\delta-\overline{k}\circ k)^{-1}\Big(\overline{k}\circ\Theta_1[k]\Big)\Big\}=\frac{\delta}{\delta\overline{k}}\mathrm{tr}\Big\{(\delta-\overline{k}\circ k)^{-1}\Big(\overline{\Theta_1[k]}\circ k\Big)\Big\}$$
$$=(\delta-k\circ\overline{k})^{-1}\circ\Big[\upsilon\cdot(\delta-k\circ\overline{k})^{-1}\circ k\Big]\circ(\delta-\overline{k}\circ k)^{-1}$$
$$+(\delta-k\circ\overline{k})^{-1}\circ k\circ\Big[\upsilon\cdot(\delta-\overline{k}\circ k)^{-1}\circ\overline{k}\Big]\circ k\circ(\delta-\overline{k}\circ k)^{-1}. \tag{4.4.19}$$

Substituting (4.4.18), (4.4.19) back into (4.4.17) yields

$$\delta\mathscr{E}/\delta\overline{k}=\frac{1}{2}(\delta-k\circ\overline{k})^{-1}\circ\Big\{h\circ k+k\circ h^T+\Theta+k\circ\overline{\Theta}\circ k\Big\}\circ(\delta-\overline{k}\circ k)^{-1},$$

which shows that saddle points of $\mathscr{E}$ must satisfy (4.4.9).

□

Integrating the equation for $\phi(x)$ against $\overline{\phi(x)}$ gives the formula for $\mu$:

$$\begin{aligned}\mu=\iint \mathrm{d}x\mathrm{d}y\{&\overline{\phi(x)}\varepsilon_0(x,y)\phi(y)+|\phi(x)|^2\upsilon_N(x-y)|\phi(y)|^2\\&+\frac{1}{N}(\upsilon_N*\rho^{\mathrm{pair}}[k])(y)\delta(x-y)|\phi(x)|^2+\frac{1}{N}n^{\mathrm{pair}}[k](x,y)\upsilon_N(x-y)\overline{\phi(x)}\phi(y)\\&+\frac{1}{N}m^{\mathrm{pair}}[k](x,y)\upsilon_N(x-y)\overline{\phi(x)}\,\overline{\phi(y)}\}.\end{aligned} \tag{4.4.20}$$

## 4.5 Solving the nonlinear system

Griffin [25] suggests solving the nonlinear matrix system (4.3.4) by iteration, beginning with solutions to the non-interacting system (i.e., $g=0$). Here, we adopt an iterative approach to construct solutions, but with several differences. First, we have reformulated the system for the condensate $\phi$ and the basis $\{u_j,\,p_j\}$ into the a system for $\phi$ and the new quantity, $k$. Second, the starting point of the iterative method is not the non-interacting system ($g=0$), but the system for $\{\phi_{\mathrm{Fet}},k_{\mathrm{Fet}}\}$ which we solved in Chapter 3. This corresponds to setting the densities $n^{\mathrm{pair}}$, $m^{\mathrm{pair}}$ to zero, but retaining the densities associated

with the condensate — $n^{\mathrm{cond}}(x,y) = \phi(x)\overline{\phi(y)}$, and $\rho^{\mathrm{cond}}(x) = |\phi(x)|^2$. The main result is stated in Theorem 5.

**Theorem 5.** *Suppose the single-particle operator* $\big(-\Delta + V_{\mathrm{trap}}(x)\big)$ *contains a gap between its ground state and first excited state, and the interaction* $\upsilon_N = N^{3\beta}\upsilon_N(Nx)$ *for* $\beta \leq 1/6$ *where* $\upsilon(x)$ *is smooth and bounded (we also assume that* $\widehat{\upsilon} \geq 0$*). Then for* $g > 0$ *small enough, there exist* $\phi \in \mathfrak{h}^1_V(\phi_\perp)$*, with* $\|\phi\|_{L^2} = 1$*, and* $k \in \mathfrak{B}_2\big(\mathfrak{h}^1_V(\phi_\perp)\big)$*, with* $\|k\|_{\mathrm{op}} < 1$ *which solve the coupled system:*

$$\int \mathrm{d}y \Big\{ \begin{pmatrix} h_0(x,y) & -\theta(x,y) \\ -\overline{\theta(x,y)} & h_0^T(x,y) \end{pmatrix} \begin{pmatrix} \phi(y) \\ \overline{\phi(y)} \end{pmatrix} \Big\} = \mu \begin{pmatrix} \phi(x) \\ \overline{\phi(x)} \end{pmatrix}, \quad \mu > 0, \tag{4.5.1}$$

*for operators* $h$, $\theta$ *given by* (4.4.7)*,* (4.4.8)*, and*

$$h \circ k + k \circ h^T + \Theta + k \circ \overline{\Theta} \circ k = 0, \quad k : \phi_\perp \to \phi_\perp, \tag{4.5.2}$$

*for* $h$, $\Theta$ *given by* (4.4.5)*,* (4.4.6)*.*

**Remark 12.** *For simplicity, we have written the equation for k as it holds on the space* $\phi_\perp$*. This allows us to avoid including the Lagrange multiplier term* $\lambda \otimes_{\mathrm{s}} \phi$ *in the equation* (4.5.2) *for k, as we did in Chapter 3.*

The iteration provides solutions $\{\phi_n, k_n\}_{n=0}^{\infty}$ to a sequence of simpler minimization problems. We show that this sequence converges strongly (in $\mathfrak{h}$ and $\mathfrak{B}(\mathfrak{h})$) to weak solutions $\phi, k$ of the nonlinear system. To this end, define the following shorthand for the operators $h, \Theta$ in this sequence:

$$h[\phi_n, k_n] := h[n],$$

as well as

$$\Theta[\phi_n, k_n] := \Theta[n].$$

The function $\phi_0(x)$ is a constrained minimizer of the Hartree equation (i.e., $\mathrm{E}_H[\phi]$), and the formula for the Lagrange multiplier of this equation, $\mu_0$, is the same as the chemical potential as determined by Fetter's scheme. The kernel $k_1$ is computed by minimizing $\mathscr{E}\left[\phi_0, k\right]$ on the space of Hilbert-Schmidt operators orthogonal to $\phi_0$, $\mathfrak{B}(\phi_\perp)$, so that solutions $\phi_0(x)$, $k_1(x,y)$ are the solutions to the simpler system found in the previous chapter. The general iteration step uses $k_n, \phi_n$ to find minimizer $k_{n+1}$ of $\mathscr{E}\left[k; h[n], \Theta[n]\right]$, $\phi_{n+1}$ as a minimizer of the total functional $\mathscr{E}_{\mathrm{tot}}$, and $\mu_{n+1}$ which depends on both $\phi_{n+1}, k_{n+1}$. The steps of the iteration scheme are summarized below:

- **Zeroth iterate:** Set $k_0 = 0$, and solve the constrained minimization problem

$$\min_{\|\phi\|=1} E_{\mathrm{H}}[\phi], \quad \text{for} \quad \phi_0 \in \mathfrak{h}.$$

  This entails that $\phi_0$ satisfies $\delta E_{\mathrm{H}}/\delta\overline{\phi} = \mu_0\phi$, which gives the Hartree equation

$$\varepsilon_0\phi_0(x) + (\upsilon_N * |\phi_0|^2)(x)\phi_0(x) = \mu_0\phi_0(x).$$

  The constant $\mu_0$ is given by

$$\mu_0 = \iint \mathrm{d}x\mathrm{d}y\{\overline{\phi_0(x)}\varepsilon_0(x,y)\phi_0(y) + |\phi_0(x)|^2\upsilon_N(x-y)|\phi_0(y)|^2\}.$$

- **$(n+1)$-th iterate:** By the previous step, we have $\{\phi_n, k_n, \mu_n\}$, The operators $h[n]$, $\Theta[n]$

are then defined by the formulas

$$
\begin{aligned}
h[n] &:= \big(\varepsilon_0(x,y)-\mu_n\big)+\overline{\phi_n(y)}\upsilon_N(x-y)\phi_n(x)+(\upsilon_N*|\phi_n|^2)(y)\delta(x-y)\\
&\quad+\frac{1}{N}\upsilon_N(x-y)\Big\{\frac{k_n\circ\overline{k_n}}{\delta-k_n\circ\overline{k_n}}\Big\}(x,y)+\frac{1}{N}\int \mathrm{d}x'\,\upsilon_N(x-x')\Big\{\frac{k_n\circ\overline{k_n}}{\delta-k_n\circ\overline{k_n}}\Big\}(x',x')\delta(x-y)\\
\Theta[n] &:= \upsilon_N(x,y)\Big\{\phi_n(x)\phi_n(y)+\frac{1}{N}\left(\frac{k_n}{\delta-k_n\circ\overline{k_n}}\right)\Big\}.
\end{aligned}
\tag{4.5.3}
$$

We solve the variational problem for $k=k_{n+1}$:

$$
\min_{\|k\|_{\mathrm{op}}<1}\Big\{E_{\mathrm{H}}[\phi_n]+\frac{1}{N}\mathscr{E}\big[k;\,h[n],\Theta[n]\big],\quad k\in\mathfrak{B}_2(\mathfrak{h}_V^1)\Big\},
\tag{4.5.4}
$$

and next the variational problem for $\phi=\phi_{n+1}$:

$$
\min_{\|\phi\|=1}\Big\{E_{\mathrm{H}}[\phi]+\frac{1}{N}\mathscr{E}\big[k_{n+1};h[\phi,k_{n+1}],\Theta[\phi,k_{n+1}]\big],\quad \phi\in\mathfrak{h}_V^1\Big\}.
\tag{4.5.5}
$$

The minimization (4.5.4) implies that $k_{n+1}$ solves the Riccati equation

$$
h[n]k_{n+1}+k_{n+1}h[n]^T+\Theta[n]+k\circ\overline{\Theta[n]}\circ k=0,
\tag{4.5.6}
$$

for the operators

$$
n^{\mathrm{pair}}[n+1]:=(\delta-k_{n+1}\circ\overline{k}_{n+1})^{-1}\circ(k_{n+1}\circ\overline{k}_{n+1}),
$$

$$
m^{\mathrm{pair}}[n+1]:=(\delta-k_{n+1}\circ\overline{k}_{n+1})^{-1}\circ k_{n+1}.
$$

The minimization (4.5.5) yields the function $\phi_{n+1}$ which satisfies

$$
\begin{aligned}
\mu_{n+1}\phi_{n+1}(x) &= \big(\varepsilon_0+\frac{1}{N}(\upsilon_N*\rho^{\mathrm{pair}}[n+1])(x)\big)\phi_{n+1}(x)\\
&\quad+\frac{1}{N}\int \mathrm{d}y\{n^{\mathrm{pair}}[n+1](x,y)\phi_{n+1}(y)\}+\frac{1}{N}\int \mathrm{d}y\{m[n+1](x,y)\overline{\phi_{n+1}(y)}\},
\end{aligned}
\tag{4.5.7}
$$

where the constant $\mu_{n+1}$ is given by

$$\begin{aligned}\mu_{n+1} = &\int \mathrm{d}x\mathrm{d}y\, \overline{\phi_{n+1}(x)}\Big(\varepsilon_0(x,y) + (\upsilon_N * |\phi_{n+1}|^2)\delta(x-y)\Big)\phi_{n+1}(y) \\ &+ \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y\{\overline{\phi_{n+1}(x)}\Big(n^{\mathrm{pair}}[n+1](x,y) + (\upsilon_N * \rho^{\mathrm{pair}}[n+1])(x)\delta(x-y)\Big)\phi_{n+1}(y)\} \\ &+ \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y\{\overline{\phi_{n+1}(x)}m^{\mathrm{pair}}[n+1](x,y)\overline{\phi_{n+1}(y)}\}.\end{aligned} \tag{4.5.8}$$

**Remark 13.** *(Solutions to the Riccati equation for $k_n$). Suppose the functions $\phi_n, k_n$ which solve* (4.5.5)*,* (4.5.4) *are given, in addition to the operators $h[n], \Theta[n]$. We review some conclusions about minimizers of the energy functional $\mathscr{E}\big[k; h[n], \Theta[n]\big]$ by which we generate the function $k_{n+1}$ (for a complete treatment of this, see Chapter 3). Namely, if the following operator estimate holds for all $e \in (\phi_n)_\perp$:*

$$\Big\{h[n](e,\overline{e}) - \big|\Theta[n](\overline{e},\overline{e})\big|\Big\} \geq c\|e\|^2, \quad c > 0, \quad e \in (\phi_n)_\perp, \tag{4.5.9}$$

*then a Hilbert-Schmidt minimizer of $\mathscr{E}$, denoted $k_{n+1} \in \mathfrak{B}_2(\mathfrak{h}_V^1)$, with $\|k_{n+1}\|_{\mathrm{op}} < 1$, exists. The proof of this statement consists in constructing an orthonormal basis $\{e_j(n+1)\}_{j=1}^\infty \subset \mathfrak{h}_V^1$ of $(\phi_n)_\perp$, and a sequence $\{z_j(n+1)\}_{j=1}^\infty \subset \ell^2$, such that*

$$k_{n+1}(x,y) = \sum_j z_j(n+1)\{e_j(x)e_j(y)\}. \tag{4.5.10}$$

*(We will refer to the basis as $\{e_j\}_{j=1}^\infty$ since its dependence on $n+1$ is clear from the context and does not play a role in the current argument). Plugging this expansion into the trace formula which defines $\mathscr{E}$, and setting $\partial\mathscr{E}/\partial\overline{z_j} = 0$, yields two possible choices of coefficient, $z_j^{(\pm)}$ for every $j$, where $|z_j^+| < 1$ and $|z_j^-| > 1$. The formula for $z_j^+$ is of interest since this is the solution which guarantees $\|k\|_{\mathrm{op}} < 1$:*

$$z_j^+(n+1) = \frac{\Theta[n](e_j,e_j)}{h[n](e_j,\overline{e_j}) + \sqrt{h[n](e_j,\overline{e_j})^2 - |\Theta[n](e_j,e_j)|^2}}. \tag{4.5.11}$$

*This allows us to write the energy* $\mathscr{E}\left[k_{n+1}; h[n], \Theta[n]\right]$ *as*

$$\mathscr{E}\left[k_{n+1}; h[n], \Theta[n]\right] = \mathscr{E}\Big(\{z_j^+\}, \{e_j\}\Big) = -\frac{1}{2}\sum_{j=1}^{\infty}\left\{h(\overline{e_j}, e_j) - \sqrt{h^2(\overline{e_j}, e_j) - |\Theta(\overline{e_j}, \overline{e_j})|^2}\right\}$$
$$:= -\frac{1}{2}\sum_j \mathscr{F}(e_j). \tag{4.5.12}$$

*The existence proof for* $k_{n+1}$ *proceeds by maximizing* $\sum_j \mathscr{F}(e_j)$ *over all orthogonal frames* $\{e_j\}$. *The expression for* $\mathscr{F}$ *given above implies that* $h(\overline{e}, e)$ *is bounded for any maximizing sequence in* $(\text{span}\{e_i\}_{i=1}^{j})_\perp$, *which allows us to extract a strongly convergent subsequence in* $L^2(\mathbb{R}^3)$ *to produce* $e_j(x)$. *Having constructed the orthonormal basis and coefficients, the proof of existence for* $k_{n+1}$ *is then complete.*

**Remark 14.** *(Solutions to the nonlinear Schrödinger-type equation for* $\phi_{n+1}$*) The existence of constrained minimizer* $\phi_{n+1}$ *of*

$$\min_{\|\phi\|=1}\left\{E_{\text{H}}[\phi] + \frac{1}{N}\mathscr{E}\left[k_{n+1}; h[\phi, k_{n+1}], \Theta[\phi, k_{n+1}]\right], \quad \phi \in \mathfrak{h}_V^1\right\}, \tag{4.5.13}$$

*will follow the usual proof for finding a minimizer of the Hartree functional* $E_{\text{H}}[\phi]$, *noting that the additional terms introduced by the functional* $\mathscr{E}$ *are bounded when* $k_{n+1}$ *is fixed with* $\|k_{n+1}\|_{\text{op}} < 1$.

We now utilize the results of these remarks to prove Theorem 5. This is done by constructing the sequence of solutions $\{\phi_n, k_n\}$ to the simpler minimization problems (4.5.5), (4.5.4), and proving that these solutions converge to a solution of the nonlinear system (4.4.9). Several preliminary results are required for this, and are presented in the following order: Lemma 7 is a general result on the stability of spectral gaps for relatively-bounded perturbations of self-adjoint operators. It is an extension of the work

of Kato [35], which we quote from Tretter, Cuenin [14]; the proof of this lemma is not provided here, a concise version of it can be found in [14]. Lemma 8 and its corollary prove that $\rho^{\text{pair}}[n]$ defines $(\upsilon_N * \rho^{\text{pair}}[n])$ as a bounded operator on $L^2$ for all $n$. The discussion which follows Lemma 8 provides the existence of the sequence of functions $\{\phi_n, k_n\}_{n=0}^{\infty}$ which solve (4.5.5), (4.5.4). This requires showing that it is possible go from one step of the iteration to the next, which means we must show that the sequence $\Theta[n]$ remains uniformly bounded in Hilbert-Schmidt and operator norm, and that the gap condition (4.5.9) holds uniformly for all steps. These estimates allow us to take strong limits of the operators $\Theta[n]$, $n^{\text{pair}}[n]$ as $n \to \infty$ in (4.5.5), (4.5.4) to construct solutions to the coupled system in Theorem 5.

The next lemma is given without proof (see [14]).

**Lemma 7.** *Let $T$ be a self-adjoint operator in a Hilbert space $\mathfrak{h}$ and let $A$ be bounded, i.e., $\|Ax\| \leq a\|x\|$ for all $x \in \mathfrak{h}$ with $a \geq 0$. Then if $T$ has a spectral gap $(\alpha_T, \beta_T) \subset \mathbb{R}$, i.e., $\sigma(T) \cap (\alpha_T, \beta_T) = \emptyset$ with $\alpha_T, \beta_T \in \sigma(T)$, and if*

$$2a < \beta_T - \alpha_T,$$

*then $T + A$ has a stable spectral free strip $(\alpha_{T+A}, \beta_{T+A}) + i\mathbb{R} \subset \mathbb{C}$, i.e.,*

$$\sigma(T + sA) \cap \{z \in \mathbb{C} : \alpha_{T+A} < \text{Re}(z) < \beta_{T+A}\} = \emptyset, \quad s \in [0, 1],$$

*with*

$$\alpha_{T+A} := \alpha_T + a, \quad \beta_{T+A} := \beta_T - a.$$

**Lemma 8.** *Suppose that $k_n \in \mathfrak{B}_2(\mathfrak{h}_V^1)$ solves* (4.5.4) *with $\|k_n\|_{\text{op}} < 1$, where the operators $h[n-1]$ and $\Theta[n-1]$ are given by formula* (4.5.20)*. Also, suppose that the operator*

$\Theta[n-1]$ *is Hilbert-Schmidt. Then the density*

$$\rho^{\text{pair}}[n](x) = \Big(\frac{k_n \circ \overline{k_n}}{\delta - k_n \circ \overline{k_n}}\Big)(x,x),$$

*satisfies* $\rho^{\text{pair}}[n](x) \in L^3(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$. *In particular,*

$$\|\rho^{\text{pair}}[n]\|_{L^3} \leq C\Big\|\frac{k_n}{\delta - k_n \circ \overline{k_n}}\Big\|_{\text{HS}} \cdot \Big(\Big\|\Theta[n-1]\Big\|_{\text{HS}} + \mu[n-1]\Big), \tag{4.5.14}$$

*where C is some constant independent of n.*

*Proof.* Define the operator kernel:

$$\psi(x,y) := \Big(\frac{k_n}{(\delta - k_n \circ \overline{k_n})^{1/2}}\Big)(x,y),$$

so that $\rho^{\text{pair}}[n](x) = (\psi \circ \overline{\psi})(x,x)$. Then using Hölder's inequality,

$$\begin{aligned} |\nabla \rho^{\text{pair}}[n](x)|^{(3/2)} &= \Big|\nabla_x \int \mathrm{d}z \{\psi(x,z)\overline{\psi(z,x)}\}\Big|^{3/2} \\ &\leq \Big(\int \mathrm{d}z |\nabla_x \psi(x,z)|^2\Big)^{3/4} \Big(\int \mathrm{d}z |\psi(x,z)|^2\Big)^{3/4} \\ &= \Big(\int \mathrm{d}z |\nabla_x \psi(x,z)|^2\Big)^{3/4} \Big(\rho^{\text{pair}}[n](x)\Big)^{3/4}. \end{aligned} \tag{4.5.15}$$

Using Holder's inequality again, ($p = 4/3$, $q = 4$) gives:

$$\begin{aligned} \int \mathrm{d}x |\nabla \rho^{\text{pair}}[n](x)|^{3/2} &\leq \int \mathrm{d}x \Big(\int \mathrm{d}z |\nabla \psi(x,z)|^2\Big)^{3/4} \Big(\rho^{\text{pair}}[n](x)\Big)^{3/4} \\ &\leq \Big(\iint \mathrm{d}x\mathrm{d}z \big|\nabla_x \psi(x,z)\big|^2\Big)^{3/4} \Big(\int \mathrm{d}x \big(\rho^{\text{pair}}[n](x)\big)^3\Big)^{1/4}, \end{aligned} \tag{4.5.16}$$

The Sobolev embedding $W^{1,3/2}(\mathbb{R}^3) \subseteq L^3(\mathbb{R}^3)$ gives (up to a constant)

$$\Big(\int \mathrm{d}x \rho^{\text{pair}}[n](x)^3\Big)^{1/3} \leq \|\nabla \rho^{\text{pair}}[n]\|_{L^{3/2}}.$$

Combining this with the previous equation, we have

$$\Big(\int \mathrm{d}x \rho^{\text{pair}}[n](x)^3\Big)^{1/3} \leq \Big(\iint \mathrm{d}x\mathrm{d}z \big|\nabla_x \psi(x,z)\big|^2\Big).$$

Now, we know that

$$\mathscr{E}(k_n) = \operatorname{tr}\Big\{ \big(\delta - k_n \circ \overline{k_n}\big)^{-1} \circ \Big( k_n \circ h[n-1] \circ \overline{k_n} + \frac{1}{2} k_n \circ \overline{\Theta[n-1]} + \frac{1}{2} \Theta[n-1] \circ \overline{k_n} \Big) \Big\} \leq 0.$$

So it follows that

$$\begin{aligned} \Big( \iint \mathrm{d}x\mathrm{d}z \big| \nabla_x \psi(x,z) \big|^2 \Big) &\leq \operatorname{tr}\Big[ \psi \circ h[n-1] \circ \overline{\psi} \Big] + \mu[n-1] \operatorname{tr}\Big[ \psi \circ \overline{\psi} \Big] \\ &\leq \Big| \operatorname{tr}\Big\{ \big(\delta - k_n \circ \overline{k_n}\big)^{-1} \circ \Big( \frac{1}{2} k_n \circ \overline{\Theta[n-1]} + \frac{1}{2} \Theta[n-1] \circ \overline{k_n} \Big) \Big\} \Big| \\ &\quad + \mu[n-1] \operatorname{tr}\Big[ \psi \circ \overline{\psi} \Big] \\ &\leq \Big\| \Big( \frac{k_n}{\delta - k_n \circ \overline{k_n}} \Big) \Big\|_{\mathrm{HS}} \cdot \Big\| \Theta[n-1] \Big\|_{\mathrm{HS}} + \mu[n-1] \Big\| \Big( \frac{k_n}{\delta - k_n \circ \overline{k_n}} \Big) \Big\|_{\mathrm{HS}}. \end{aligned} \tag{4.5.17}$$

This completes the proof. □

**Corollary 3.** *Under the assumptions of Lemma 8,* $\rho^{\mathrm{pair}}[n](x) \in L^2$ *with*

$$\|\rho^{\mathrm{pair}}[n]\|_{L^2} \leq \Big\| \frac{k_n}{\delta - k_n \circ \overline{k_n}} \Big\|_{\mathrm{HS}} \cdot \Big( \Big\| \Theta[n-1] \Big\|_{\mathrm{HS}} + \mu[n-1] \Big)^{3/4}. \tag{4.5.18}$$

*Proof.* Interpolation gives

$$\|\rho^{\mathrm{pair}}[n]\|_{L^2} \leq \|\rho^{\mathrm{pair}}[n]\|_{L^3}^{3/4} \|\rho^{\mathrm{pair}}[n]\|_{L^1}^{1/4},$$

and

$$\|\rho^{\mathrm{pair}}[n]\|_{L^1} = \operatorname{tr}\Big( \frac{k_n \circ \overline{k_n}}{\delta - k_n \circ \overline{k_n}} \Big) \leq \|k_n\|_{\mathrm{op}} \Big\| \frac{k_n}{\delta - k_n \circ \overline{k_n}} \Big\|_{\mathrm{HS}},$$

which proves the statement. □

### 4.5.1 Completing the iteration

The iteration depends on verifying the gap condition at every step, i.e., showing that there exists $c > 0$ independent of $n$ such that

$$h[n](e,\overline{e}) - |\Theta[n](\overline{e},\overline{e})| \geq c\|e\|, \quad e \in (\phi_n)_\perp, \quad n = 0,1,2,\ldots. \tag{4.5.19}$$

We start with $\phi_0(x)$, which is a solution to the Hartree equation:

$$\varepsilon_0\phi_0(x) + (v_N * |\phi_0|^2)(x)\phi_0(x) = \mu_0\phi_0(x).$$

The constant $\mu_0$ is given by

$$\mu_0 = \iint \mathrm{d}x\mathrm{d}y\{\overline{\phi_0(x)}\varepsilon_0(x,y)\phi_0(y) + |\phi_0(x)|^2 v_N(x-y)|\phi_0(y)|^2\},$$

and the operators $h[0]$, $\Theta[0]$ are defined by

$$\begin{aligned} h[0] &:= \varepsilon_0(x,y) + \overline{\phi_0(y)}v_N(x-y)\phi_0(x) + (v_N * |\phi_0|^2)(y)\delta(x-y) - \mu_0, \\ \Theta[0] &:= v_N(x,y)\Big\{\phi_0(x)\phi_0(y)\Big\}. \end{aligned} \tag{4.5.20}$$

In particular, the operator $\Theta[0]$ is Hilbert-Schmidt, with norm

$$\|\Theta[0]\|_{\mathrm{HS}} \leq gN^{3\beta}\|v\|_{L^\infty}\|\phi_0\|_{L^2}^2,$$

(we do not require $\Theta[0]$ to be small in this scheme, only that it is bounded; see equation (4.5.40)). We also have – using the assumption $\widehat{v} \geq 0$ for the Fourier transform of $v$:

$$h[0](e,\overline{e}) - |\Theta[0](\overline{e},\overline{e})| \geq \varepsilon_0(e,\overline{e}) + \iint \mathrm{d}x\mathrm{d}y\{v_N(x-y)|\phi_0(x)|^2|e(y)|^2\} - \mu_0\|e\|^2.$$

The gap condition for $h[0]$, $\Theta[0]$ follows from this inequality, because $\phi_0(x)$, as the minimizer of $\mathscr{E}_{\mathrm{Hartree}}(\phi)$, is also the ground state of the linear Hartree operator, $H_{\mathrm{Hartree}}$, defined by

$$H_{\mathrm{Hartree}} := \varepsilon_0(x,y) + (v_N * |\phi_0|^2)(x)\delta(x-y).$$

$H_{\mathrm{Hartree}}$ has a discrete spectrum, with a gap between its lowest and first eigenvalues, since it is a compact perturbation of $\varepsilon_0(x,y)$. More specifically, using Young's convolution inequality, and the compact Sobolev embedding $L^4(\mathbb{R}^3) \subset \mathfrak{h}_V^1$,

$$\|(v_N * |\phi_0|^2)\|_{L^2} \leq \|v_N\|_{L^1}\| \ |\phi_0|^2 \ \|_{L^2} = \|v_N\|_{L^1}\|\phi_0\|_{L^4} \leq \|v_N\|_{L^1}\|\phi_0\|_{\mathfrak{h}_V^1}, \tag{4.5.21}$$

i.e.,

$$\|(\upsilon_N * |\phi_0|^2)\|_{L^2} \leq \|\upsilon_N\|_{L^1} \cdot \mathscr{E}_{\text{Hartree}}(\phi_0) \leq g \cdot \mathscr{E}_{\text{Hartree}}(\phi_0). \tag{4.5.22}$$

This means that the perturbation to $\varepsilon_0$ can be made arbitrarily small in $L^2$ by making $g$ small.

For the induction step, assume that there exists $c > 0$ and $C > 0$ such that for $s = 0, 1, 2, \ldots, n$,

$$\begin{cases} \left\|\Theta[s]\right\|_{\text{HS}} \leq CN^{3\beta}, \\ \mu[s] \leq C, \quad \text{for} \quad s = 0, 1, 2, \ldots, n, \\ h[s](e,\overline{e}) - |\Theta[s](\overline{e},\overline{e})| \geq c\|e\|^2, \quad e \in (\phi_s)_\perp, \end{cases} \tag{4.5.23}$$

From these assumptions, we prove that

$$\begin{cases} \|\Theta[n+1]\|_{\text{HS}} < CN^{3\beta}, \\ \mu[n+1] < C, \\ h[n+1](e,\overline{e}) - \left|\Theta[n+1](e,e)\right| \geq c\|e\|^2, \quad e \in (\phi_{n+1})_\perp. \end{cases} \tag{4.5.24}$$

The equation for $k_{n+1}$ on the space $\mathfrak{h}(\phi_\perp)$ is

$$h[n] \circ k_{n+1} + k_{n+1} \circ h[n]^T + \Theta[n] + k_{n+1} \circ \overline{\Theta[n]} \circ k_{n+1} = 0, \tag{4.5.25}$$

and the equation for $\phi_{n+1}$ is

$$\begin{aligned} \mu_{n+1}\phi_{n+1}(x) = \varepsilon_0(\phi_{n+1}, x) + (\upsilon_N * |\phi_{n+1}|^2)(x)\phi_{n+1}(x) + \frac{1}{N}(\upsilon_N * \rho^{\text{pair}}[n+1])(x)\phi_{n+1}(x) \\ + \frac{1}{N}(\upsilon_N n^{\text{pair}}[n+1])(\phi_{n+1}, x) + \frac{1}{N}(\upsilon_N m^{\text{pair}}[n+1])(\overline{\phi_{n+1}}, x), \end{aligned} \tag{4.5.26}$$

with the operators

$$\begin{aligned} h[n] &:= \varepsilon_0(x,y) + \overline{\phi_n(y)}\upsilon_N(x-y)\phi_n(x) + (\upsilon_N * |\phi_n|^2)(y)\delta(x-y) - \mu_n \\ &\quad + \frac{1}{N}\big(\upsilon_N n^{\mathrm{pair}}[n]\big)(x,y) + \frac{1}{N}\big(\upsilon_N * \rho^{\mathrm{pair}}[n]\big)(x)\delta(x-y), \\ \Theta[n] &:= \upsilon_N(x-y)\Big\{\phi_n(x)\phi_n(y) + \frac{1}{N}m^{\mathrm{pair}}[n](x,y)\Big\}. \end{aligned} \tag{4.5.27}$$

First we show that $\|\Theta[n+1]\|_{\mathrm{HS}} < CN^{3\beta}$. The induction assumption allows us to construct $k_{n+1}$ as a minimizer of $\mathscr{E}\big[\phi_n, k; h[n], \Theta[n]\big]$. The formula for $m^{\mathrm{pair}}[n+1]$ is:

$$m^{\mathrm{pair}}[n+1](x,y) = \sum_j \Big(\frac{z_j}{1-|z_j|^2}\Big) e_j(x) e_j(y). \tag{4.5.28}$$

Here $\{e_j(n+1)\}_{j=1}^{\infty}$ is an orthonormal basis of $(\phi_n)_\perp$, which is determined as part of the construction of $k_{n+1}$. The formula for the coefficient $z_j(n+1)$ gives

$$\Big|\frac{z_j(n+1)}{1-|z_j(n+1)|^2}\Big|^2 = \frac{1}{4}\Big(\frac{|\Theta[n](e_j,e_j)|^2}{h[n]^2(e_j,\overline{e_j}) - |\Theta[n](e_j,e_j)|^2}\Big) \leq \frac{1}{4c^2}|\Theta[n](e_j,e_j)|^2, \tag{4.5.29}$$

where the inequality follows since we assume the gap condition for the operators $h[n]$, $\Theta[n]$. Thus,

$$\|m^{\mathrm{pair}}[n+1]\|_{\mathrm{HS}} \leq \frac{1}{2c}\|\Theta[n]\|_{\mathrm{HS}} \leq \frac{C}{2c}N^{3\beta}.$$

From this, recalling that $\upsilon_N(x) = gN^{3\beta}\upsilon(N^\beta x)$ for $\beta \leq 1/6$, we have

$$\begin{aligned} \|\frac{1}{N}(\upsilon_N m^{\mathrm{pair}})[n+1]\|_{\mathrm{HS}} &\leq g\frac{1}{2c}\frac{N^{3\beta}}{N}\|\upsilon\|_{L^\infty}\|\Theta[n]\|_{\mathrm{HS}} \leq \frac{gC^2}{2c}\|\upsilon\|_{L^\infty}\Big(\frac{N^{6\beta}}{N}\Big), \\ \|\frac{1}{N}(\upsilon_N n^{\mathrm{pair}})[n+1]\|_{\mathrm{HS}} &\leq \|\frac{1}{N}(\upsilon_N m^{\mathrm{pair}})[n+1]\|_{\mathrm{HS}} \leq \frac{gC^2}{2c}\|\upsilon\|_{L^\infty}\Big(\frac{N^{6\beta}}{N}\Big), \end{aligned} \tag{4.5.30}$$

and, using Corollary (3) with Young's convolution inequality:

$$\begin{aligned} \|\frac{1}{N}(\upsilon_N * \rho^{\mathrm{pair}}[n+1])\|_{L^2} &\leq \frac{g}{N}\|\rho^{\mathrm{pair}}[n+1]\|_{L^2} \\ &\leq \frac{gC}{2c}\frac{N^{3\beta}}{N}\cdot\Big(\Big\|\Theta[n-1]\Big\|_{\mathrm{HS}} + \mu[n-1]\Big)^{3/4} \\ &\leq \frac{gC^2}{c}\Big(\frac{N^{6\beta}}{N}\Big). \end{aligned} \tag{4.5.31}$$

It is now clear that for $\beta \leq 1/6$ the constant $g > 0$ can be chosen at the start so that

$$\|\Theta[n+1]\|_{\mathrm{HS}}^2 < CN^{3\beta},$$

because,

$$\begin{aligned}\|\Theta[n+1]\|_{\mathrm{HS}} &\leq gN^{3\beta}\|\upsilon\|_{L^\infty}\|\phi_{n+1}\|_{L^2}^2 + \frac{1}{N}\|(\upsilon_N m^{\mathrm{pair}}[n+1])\|_{\mathrm{HS}} \\ &\leq g\|\upsilon\|_{L^\infty}\Big\{N^{3\beta} + \frac{C^2}{2c}\Big\}.\end{aligned} \tag{4.5.32}$$

We remind the reader that the inductive argument only requires $\Theta[n+1]$ to be bounded (not small), and that the particle number $N$ is large but fixed throughout the entire chapter.

We use this to show that $\mu[n+1] < C$, where

$$\begin{aligned}\mu_{n+1} &= \varepsilon_0(\phi_{n+1}, \overline{\phi_{n+1}}) + \frac{1}{N}(\upsilon_N n^{\mathrm{pair}}[n+1])(\phi_{n+1}, \overline{\phi_{n+1}}) + (\upsilon_N m^{\mathrm{pair}}[n+1])(\overline{\phi_{n+1}}, \overline{\phi_{n+1}}) \\ &+ \iint \mathrm{d}x\mathrm{d}y|\phi_{n+1}(x)|^2\upsilon_N(x-y)|\phi_{n+1}(y)|^2 + \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y|\phi_{n+1}(x)|^2\upsilon_N(x-y)\rho^{\mathrm{pair}}[n+1](y),\end{aligned} \tag{4.5.33}$$

Indeed, $\phi_{n+1}$ minimizes the functional

$$\begin{aligned}\tilde{\mathscr{E}}(\phi) &:= \varepsilon_0(\phi, \overline{\phi}) + \frac{1}{N}(\upsilon_N n^{\mathrm{pair}}[n+1])(\phi, \overline{\phi}) + \frac{1}{2}(\upsilon_N m^{\mathrm{pair}}[n+1])(\overline{\phi}, \overline{\phi}) \\ &+ \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y|\phi(x)|^2\upsilon_N(x-y)|\phi(y)|^2 + \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y|\phi(x)|^2\upsilon_N(x-y)\rho^{\mathrm{pair}}[n+1](y)\end{aligned} \tag{4.5.34}$$

(the functional $\tilde{\mathscr{E}}$ consists of only the terms of $\mathscr{E}_{\mathrm{tot}}[\phi, k]$ with a dependence on $\phi$), and

$$\begin{aligned}\tilde{\mathscr{E}}(\phi_{n+1}) = \mu_{n+1} &- \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y|\phi_{n+1}(x)|^2\upsilon_N(x-y)|\phi_{n+1}(y)|^2 \\ &- \frac{1}{2N}(\upsilon_N m^{\mathrm{pair}}[n+1])(\overline{\phi_{n+1}}, \overline{\phi_{n+1}}).\end{aligned} \tag{4.5.35}$$

Since $\phi_{n+1}$ is the minimizer of $\tilde{\mathscr{E}}$, we have

$$\begin{aligned}
&\tilde{\mathscr{E}}(\phi_{n+1}) \leq \tilde{\mathscr{E}}(\phi_0) \\
&= \mu_0 - \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 v_N(x-y)|\phi_0(y)|^2 + \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 v_N(x-y)\rho^{\mathrm{pair}}[n+1](y) \\
&+ \frac{1}{N}(v_N n^{\mathrm{pair}}[n+1])(\phi_0, \overline{\phi_0}) + \frac{1}{2}\frac{1}{N}(v_N m^{\mathrm{pair}}[n+1])(\overline{\phi_0}, \overline{\phi_0}).
\end{aligned} \tag{4.5.36}$$

Combining (4.5.35) and (4.5.36) gives,

$$\begin{aligned}
\mu_{n+1} &\leq \mu_0 - \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 v_N(x-y)|\phi_0(y)|^2 \\
&+ \frac{1}{2}\iint \mathrm{d}x\mathrm{d}y|\phi_{n+1}(x)|^2 v_N(x-y)|\phi_{n+1}(y)|^2 \\
&+ \frac{1}{2}\frac{1}{N}(v_N m^{\mathrm{pair}}[n+1])(\overline{\phi_0}, \overline{\phi_0}) + \frac{1}{2}\frac{1}{N}(v_N m^{\mathrm{pair}}[n+1])(\overline{\phi_{n+1}}, \overline{\phi_{n+1}}) \\
&+ \frac{1}{N}(v_N n^{\mathrm{pair}}[n+1])(\phi_0, \overline{\phi_0}) + \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 v_N(x-y)\rho^{\mathrm{pair}}[n+1](y).
\end{aligned} \tag{4.5.37}$$

Using (4.5.30) and (4.5.31), we conclude that

$$\begin{aligned}
\mu_{n+1} &\leq \mu_0 + \frac{1}{2}\mathscr{E}_{\mathrm{Hartree}}(\phi_0)\cdot\|(v_N * |\phi_0|^2)\|_{L^2} + \frac{1}{2}\tilde{\mathscr{E}}(\phi_{n+1})\cdot\|(v_N * |\phi_{n+1}|^2)\|_{L^2} \\
&+ \frac{2gC}{c}\|v\|_{L^\infty} + \frac{1}{N}\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 v_N(x-y)\rho^{\mathrm{pair}}[n+1](y) \\
&\leq \mu_0 + \frac{g}{2}\big(\mathscr{E}_{\mathrm{Hartree}}(\phi_0)\big)^2 + \frac{g}{2}\big(\tilde{\mathscr{E}}(\phi_{n+1})\big)^2 + \frac{2gC}{c}\|v\|_{L^\infty} + \frac{gC^2}{Nc}\tilde{\mathscr{E}}_{\mathrm{Hartree}}(\phi_0).
\end{aligned} \tag{4.5.38}$$

where we use (Sobolev and Young)

$$\begin{aligned}
\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 v_N(x-y)|\phi_0(y)|^2 &\leq \mathscr{E}_{\mathrm{Hartree}}(\phi_0)\cdot\|(v_N * |\phi_0|^2)\|_{L^2} \\
\iint \mathrm{d}x\mathrm{d}y|\phi_{n+1}(x)|^2 v_N(x-y)|\phi_{n+1}(y)|^2 &\leq \tilde{\mathscr{E}}(\phi_{n+1})\cdot\|(v_N * |\phi_{n+1}|^2)\|_{L^2},
\end{aligned} \tag{4.5.39}$$

and the following $L^2$ bound (Young's inequality and the Sobolev embedding, see equation (4.5.21))

$$\|(v_N * |\phi_{n+1}|^2)\|_{L^2} \leq \|v_N\|_{L^1}\cdot\|\phi_{n+1}\|_{\mathfrak{h}_V^1} \leq g\cdot\tilde{\mathscr{E}}(\phi_{n+1}),$$

and the last line of (4.5.38) follows from

$$\frac{1}{N}\iint \mathrm{d}x\mathrm{d}y|\phi_0(x)|^2 \upsilon_N(x-y)\rho^{\mathrm{pair}}[n+1])(y) \leq \frac{g}{N}\cdot \mathscr{E}_{\mathrm{Hartree}}(\phi_0)\|\rho^{\mathrm{pair}}[n+1]\|_{L^2}.$$

This shows that $\mu_{n+1}$ modifies $\mu_0$ by a correction of order $\mathscr{O}(g)$. We can also say that $\mu_{n+1}$ modifies the ground state of $\varepsilon_0$ by a correction with order $\mathscr{O}(g)$, using (4.5.22))

Finally, to show estimate (4.5.19), observe that for any $e(x) \in (\phi_n)_\perp$,

$$h[n+1](e,\overline{e}) - |\Theta[n+1](\overline{e},\overline{e})| \geq h'[n+1](e,\overline{e}) - \mu_{n+1} - \frac{1}{N}|(\upsilon_N m^{\mathrm{pair}}[n+1])(\overline{e},\overline{e})|, \tag{4.5.40}$$

for the operator $h'[n+1]$ defined by

$$\begin{aligned} h'[n+1] := \varepsilon_0 + (\upsilon_N * |\phi_{n+1}|^2)(x)\delta(x-y) + \frac{1}{N}(\upsilon_N n^{\mathrm{pair}}[n+1])(x,y) \\ + \frac{1}{N}(\upsilon_N * \rho^{\mathrm{pair}}[n+1])(x)\delta(x-y). \end{aligned} \tag{4.5.41}$$

Also observe that $\phi_{n+1}$ satisfies the self-adjoint operator matrix equation

$$\begin{pmatrix} h'[n+1] & \frac{1}{N}(\upsilon_N m^{\mathrm{pair}}[n+1]) \\ \frac{1}{N}\overline{(\upsilon_N m^{\mathrm{pair}}[n+1])} & h'[n+1] \end{pmatrix} \circ \begin{pmatrix} \phi_{n+1} \\ \overline{\phi_{n+1}} \end{pmatrix} = \mu_{n+1} \begin{pmatrix} \phi_{n+1} \\ \overline{\phi_{n+1}} \end{pmatrix}. \tag{4.5.42}$$

The rest of the argument follows by showing that: **(i)** $\phi_{n+1}$ which minimizes $\tilde{\mathscr{E}}(\phi)$ is the ground state of the operator in (4.5.42); and **(ii)** the higher eigenstates of (4.5.42), which take the form $(e,\overline{e})^T$, for $e(x) \in (\phi_{n+1})_\perp$, and satisfy

$$\begin{pmatrix} h'[n+1] & \frac{1}{N}(\upsilon_N m^{\mathrm{pair}}[n+1]) \\ \frac{1}{N}\overline{(\upsilon_N m^{\mathrm{pair}}[n+1])} & h'[n+1] \end{pmatrix} \circ \begin{pmatrix} e \\ \overline{e} \end{pmatrix} = \lambda(e) \begin{pmatrix} e \\ \overline{e} \end{pmatrix}, \quad \lambda(e) \geq \mu_{n+1}, \tag{4.5.43}$$

are separated from $\mu_{n+1}$, which has no degeneracy, i.e.,

$$\lambda(e) - \mu_{n+1} \geq \delta, \quad e \in (\phi_{n+1})_\perp, \quad \text{for} \quad \delta > 0.$$

The $\lambda(e)$ are given by

$$\lambda(e) = h'[n+1](e,\overline{e}) + \frac{1}{N}(\upsilon_N m^{\text{pair}}[n+1])(\overline{e},\overline{e}). \tag{4.5.44}$$

Both of these arguments follow from the fact that the matrix in equations (4.5.42), (4.5.43) is a perturbation of the diagonal matrix $\text{diag}(\varepsilon_0, \varepsilon_0)$. Specifically,

$$\begin{pmatrix} h'[n+1] & \frac{1}{N}(\upsilon_N m^{\text{pair}}[n+1]) \\ \frac{1}{N}\overline{(\upsilon_N m^{\text{pair}}[n+1])} & h'[n+1] \end{pmatrix} = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{pmatrix} + M'[n+1] \tag{4.5.45}$$

for the matrix $M'[n+1] = M_1[n+1] + M_2[n+1]$ with

$$M_1[n+1] := \text{diag}\Big((\upsilon_N * |\phi_{n+1}|^2) + \frac{1}{N}(\upsilon_N n^{\text{pair}}) + \frac{1}{N}(\upsilon_N * \rho^{\text{pair}})\Big),$$

and

$$M_2[n+1] := \begin{pmatrix} 0 & \frac{1}{N}(\upsilon_N m^{\text{pair}}) \\ \frac{1}{N}\overline{(\upsilon_N m^{\text{pair}})} & 0 \end{pmatrix}.$$

The perturbation $M'[n+1]$ is bounded in operator norm by

$$\|M'[n+1]\|_{\text{op}} \leq g \cdot \tilde{\mathscr{E}}(\phi_{n+1}) + g\|\upsilon\|_{L^\infty} C, \quad \text{for} \quad C < \infty. \tag{4.5.46}$$

The first term of this operator bound comes from Young's inequality (i.e., equation (4.5.38)). The second term in (4.5.46) meanwhile comes from (4.5.30). The important feature is that the operator bound for $M[n+1]$ can be made as small as desired by choosing $g$ small enough.

At this point, we invoke the perturbation lemma, Lemma 7, in order to claim that the spectrum

$$\sigma\begin{pmatrix} h'[n+1] & \frac{1}{N}(\upsilon_N \cdot m^{\text{pair}}[n+1]) \\ \frac{1}{N}\overline{(\upsilon_N \cdot m^{\text{pair}}[n+1])} & h'[n+1] \end{pmatrix} \tag{4.5.47}$$

is a perturbation of the spectrum $\sigma(\varepsilon_0)$. In particular, for $g$ small enough we can guarantee that $\mu_{n+1}$ is the smallest element of this set, since it is the only element which is in a neighborhood of size $gC$ of the ground state of $\varepsilon_0$ (where $C$ is some constant).

It follows that

$$\lambda(e) - \mu_{n+1} \geq \delta - 2\|M'[n+1]\|_{\text{op}},$$

for all $e \in (\phi_{n+1})_\perp$, where $\delta$ is the size of the gap for the operator $\varepsilon_0$. Since $\|M'[n+1]\|_{\text{op}}$ can be made arbitrarily small by making $g$ small enough, we can choose the constants $g$, $c$ to be small enough so that $\lambda(e) - \mu_{n+1} > c$. This completes the proof of existence for the sequence $\{\phi_n, k_n\}$. □

**Theorem 6.** *Suppose the single-particle operator* $\big(-\Delta + V_{\text{trap}}(x)\big)$ *contains a gap between its ground state and first excited state. Then for* $g < 1$ *small enough, and the interaction* $\upsilon_N = N^{3\beta}\upsilon_N(Nx)$ *for* $\beta \leq 1/6$ *where* $\upsilon(x)$ *is smooth and bounded (we also assume that* $\widehat{\upsilon} \geq 0$*), there exists* $\phi \in \mathfrak{h}^1_V$*, with* $\|\phi\|_{L^2} = 1$*, and* $k \in \mathfrak{B}_2(\mathfrak{h}^1_V(\phi_\perp), \mathfrak{h}^1_V(\phi_\perp))$*, with* $\|k\|_{\text{op}} < 1$ *which solve the coupled system*

$$n^{\text{pair}} = (\delta - k \circ \overline{k})^{-1} \circ (k \circ \overline{k}), \tag{4.5.48}$$

$$m^{\text{pair}} = (\delta - k \circ \overline{k})^{-1} \circ k, \tag{4.5.49}$$

$$h \circ k + k \circ h^T + \Theta + k \circ \overline{\Theta} \circ k = 0, \quad k \in \mathfrak{B}(\mathfrak{h}^1_V),\ \|k\|_{\text{op}} < 1, \tag{4.5.50}$$

*and*

$$\int \mathrm{d}y \Big\{ \begin{pmatrix} h_0(x,y) & -\theta(x,y) \\ -\overline{\theta(x,y)} & h_0^T(x,y) \end{pmatrix} \begin{pmatrix} \phi(y) \\ \overline{\phi(y)} \end{pmatrix} \Big\} = \mu \begin{pmatrix} \phi(x) \\ \overline{\phi(x)} \end{pmatrix}, \quad \mu > 0, \quad \|\phi\| = 1. \tag{4.5.51}$$

*Proof.* Since the gap condition holds for every step of the iteration, the sequence $\{\phi_n, k_n\}$ determined by the minimization problems (4.5.5) and (4.5.4) exists, with $\|\phi_n\| = 1$ and $\|k_n\|_{\mathrm{HS}} < C$, $\|(\delta - k_n \circ \overline{k_n})^{-1}\|_{\mathrm{op}} < C$ for all $n$ and some $C$. The sequence $\{\mu_n\}$ is also uniformly bounded as a result of the previous theorem. Since we also have

$$\begin{aligned}\mathrm{tr}\Big\{\overline{k_n} \circ \varepsilon_0 \circ k_n\Big\} &\leq \Big|\mathrm{tr}\Big\{(\delta - \overline{k_n} \circ k_n)^{-1} \circ (\overline{k_n} \circ \varepsilon_0 \circ k_n)\Big\}\Big| \\ &\leq \frac{1}{2}\Big|\mathrm{tr}\Big\{(\delta - \overline{k_n} \circ k_n)^{-1} \circ \{\overline{k_n} \circ \Theta[n-1] + \overline{\Theta[n-1]} \circ k_n\}\Big\}\Big| \\ &\quad + \mu_n \mathrm{tr}\Big\{(\delta - \overline{k_n} \circ k_n)^{-1} \circ (\overline{k_n} \circ k_n)\Big\}\Big|,\end{aligned} \tag{4.5.52}$$

the sequence $\{k_n\}$ is uniformly bounded in $\mathfrak{B}_2(\mathfrak{h}^1_V, \mathfrak{h}^1_V)$. Because $\{\phi_n\}$ and $\{k_n\}$ are uniformly bounded in $\mathfrak{h}^1_V$, $\mathfrak{B}_2(\mathfrak{h}^1_V)$, we can find some subsequence (again denoted $\{\phi_n\}$ and $\{k_n\}$) which converges weakly in $\mathfrak{h}^1_V$, ($\mathfrak{B}_2(\mathfrak{h}^1_V)$ respectively). Since $\mathfrak{h}^1_V$ is compactly embedded in $L^2_V \cap L^4_V$, we conclude that $\phi_n$ converges strongly in $L^2_V \cap L^4_V$ to some $\phi$, and $k_n$ converges strongly in $\mathfrak{B}_2(L^2_V)$ to some $k$.

The following strong limits in $\mathfrak{B}_2(\mathfrak{h})$ therefore hold:

$$\begin{aligned}\upsilon_N(x-y)\phi_n(x)\phi_n(y) &\to \upsilon_N(x-y)\phi(x)\phi(y), \\ \upsilon_N(x-y)\Big\{\frac{k_n}{\delta - \overline{k_n} \circ k_n}\Big\} &\to \upsilon_N(x-y)\Big\{\frac{k}{\delta - \overline{k} \circ k}\Big\}, \\ \upsilon_N(x-y)\Big\{\frac{k_n \circ \overline{k_n}}{\delta - k_n \circ \overline{k_n}}\Big\} &\to \upsilon_N(x-y)\Big\{\frac{k \circ \overline{k}}{\delta - k \circ \overline{k}}\Big\}.\end{aligned} \tag{4.5.53}$$

We also have the strong limits in $L^2(\mathbb{R}^3)$:

$$\begin{aligned}(\upsilon_N * |\phi_n|^2)(y)\delta(x-y) &\to (\upsilon_N * |\phi|^2)(y)\delta(x-y), \\ \int \mathrm{d}x' \upsilon_N(x-x')\Big\{\frac{k_n \circ \overline{k_n}}{\delta - k_n \circ \overline{k_n}}\Big\}(x',x')\delta(x-y) &\to \int \mathrm{d}x' \upsilon_N(x-x')\Big\{\frac{k \circ \overline{k}}{\delta - k \circ \overline{k}}\Big\}(x',x')\delta(x-y).\end{aligned} \tag{4.5.54}$$

The first, $(\upsilon_N * |\phi_n|^2)(y)\delta(x-y) \to (\upsilon_N * |\phi|^2)(y)\delta(x-y)$, follows by noticing (via Young's

convolution inequality),

$$\|(v_N * |\phi_n|^2)\|_{L^2} \leq \|v_N\|_{L^1} \cdot \||\phi_n|^2\|_{L^2} = \|v_N\|_{L^1} \cdot \|\phi_n\|_{L^4},$$

and so $(v_N * |\phi_n|^2)(x) \to (v_N * |\phi|^2)(x)$ strongly in $L^2$, since $\phi_n \to \phi$ strongly in $L^4(\mathbb{R}^3)$. The second of these inequalities follows by the fact that $\rho^{\text{pair}}[n](x) \in L^2(\mathbb{R}^3)$ for all $n$.

Taking $n \to \infty$ in the equations satisfied by $\phi_n, k_n$ therefore gives equations (4.5.48) for $\phi, k$. Finally, we must check that $k \perp \phi$. Since $k_n(\phi_n, x) = 0$ by construction, we have

$$\|k(\phi, x)\|_{L^2} \leq \|k\|_{\text{HS}} \cdot \|\phi - \phi_n\|_{L^2} + \|k - k_n\|_{\text{HS}} \cdot \|\phi_n\|_{L^2}.$$

By picking $n$ sufficiently large, we can bound $\|k(\phi, x)\|$ by an arbitrarily small quantity. This completes the proof. □

# Chapter 5

# Lee-Huang-Yang model for the periodic Bose gas

## 5.1 Introduction

We have seen in the previous chapters that the concept of a macroscopic quantum state plays a key role in deriving effective models for the Bose gas. In particular, the interacting many-body Hamiltonian can be expanded around the macroscopic, mean field state. Heuristically, the macroscopic occupation of a single state makes it reasonable to retain only quadratic terms in non-condensate field operators in an approximation to the exact many-body Hamiltonian. This general strategy of approximation is appealing mathematically, since (as demonstrated in previous chapters) the spectrum of this family of Hamiltonians can be described exactly. In addition, when the gas is confined in a trapping potential, we have shown that pair-excitation can be given a precise mathematical foundation.

The subject of the current chapter is the Bose gas trapped in the box of size $L$, with periodic boundary conditions.

We formulate the non-Hermitian transform for a quadratic approximate Hamiltonian based on the famous model of Lee, Huang and Yang [37, 38]. This model describes low-lying excitations of the hard-sphere Bose gas in a periodic box with volume $L^3$, where the condensate is given by the zero-momentum constant function $\phi(x) = 1/\sqrt{L^3}$. The second-quantized approximate Hamiltonian in the momentum basis, parameterized by $k$

in the momentum dual lattice

$$k \in \mathbb{Z}^3_L := \{k = 2\pi n/L \,\big|\, n \in \mathbb{Z}^3\},$$

is described by:

$$\mathscr{H}_{\mathrm{LHY}} = 4\pi a\rho N + \sum_{k\in\mathbb{Z}^3_L, k\neq 0} \left\{k^2 + 8\pi a\rho\right\} a^*_k a_k + 4\pi a\rho \sum_{k\in\mathbb{Z}^3_L, k\neq 0} \left\{a^*_k a^*_{-k} + a_k a_{-k}\right\}. \tag{5.1.1}$$

To make a connection to the previous chapters, the scattering length $a > 0$ is related to the constant $g$ by the relation $8\pi a = g$. The Hamiltonian $\mathscr{H}_{\mathrm{LHY}}$ acts on the Fock space orthogonal to the condensate $\{k \neq 0\}$. In this setting we introduce the Fock space operator

$$\mathscr{P} := \frac{1}{2} \sum_{k\neq 0} \alpha(k)\, a^*_k a^*_{-k}\,,$$

where the real function $\alpha(k)$ defined on the lattice is the Fourier transform of a translation-invariant kernel $k(x,y)$.

We remark that neither the Hamiltonian $\mathscr{H}_{\mathrm{LHY}}$ nor the operator $\mathscr{P}$ commute with the total number operator, given in the momentum basis by (see Section 5.1.3)

$$\mathscr{N} = \sum_{k\in\mathbb{Z}^3_L} a^*_k a_k.$$

We correspondingly refer to $\mathscr{H}_{\mathrm{LHY}}$ and $\mathscr{P}$ as being *non-particle-conserving*. More generally, the Fock space operator $\mathscr{O}$ is non-particle-conserving if $[\mathscr{O}, \mathscr{N}] \neq 0$. The domains of non-particle-conserving operators must be taken to be the Fock space $\mathbb{F}$, (in contrast to the Fock space with fixed particle number $\mathbb{F}_N$ from previous chapters). The transformed Hamiltonian $\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P})$ is now both non-Hermitian and *unbounded* in the operator norm on $\mathbb{F}$; in Section 5.4.1, it is shown that the point spectrum $\sigma_{\mathrm{p}}\big(\mathscr{H}_{\mathrm{LHY}}\big)$ is

not equal to the point spectrum $\sigma_{\mathrm{p}}\big(\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P})\big)$. Compare this to the more familiar case of a similarity transformation by a bounded (or finite-dimensional) operator, which must preserve the point spectrum of the original operator.

A remark is in order. Namely, the exact many-body Hamiltonian $\mathscr{H}$ given in Section 5.2, equation (5.2.5), from which $\mathscr{H}_{\mathrm{LHY}}$ is derived, is manifestly particle-conserving (in the sense that $[\mathscr{H},\mathscr{N}]=0$), and so its associated eigenvalue problem may be considered on the Fock space of fixed particle number, $\mathbb{F}_N$ for $N$ finite but large. By contrast, the effective Hamiltonian of Lee Huang and Yang, $\mathscr{H}_{\mathrm{LHY}}$, does not conserve the total number of particles. We will discuss the implications of this for the model of low-lying excitations after summarizing the steps of the approximation arriving at $\mathscr{H}_{\mathrm{LHY}}$.

In the results that follow, we show how the spectrum of $\mathscr{H}_{\mathrm{LHY}}$ can be identified as a subset of the spectrum of the transformed operator $\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P})$, (i.e., without prior knowledge of $\sigma(\mathscr{H}_{\mathrm{LHY}})$). This is a complication introduced by using a non-Hermitian transformation to analyze the Lee-Huang-Yang system. The benefit to this method lies in the fact that the many-body Fock space eigenstates of $\mathscr{H}_{\mathrm{LHY}}$ have a particularly simple expression by utilizing the operator $\exp(\mathscr{P})$. Wu [60] observed that the ground state for $\mathscr{H}_{\mathrm{LHY}}$ can be written using the operator $\mathscr{P}$ defined above, via

$$|\Psi_0\rangle = \exp(-\mathscr{P})\frac{(a_0^*)^N}{\sqrt{N!}}|\mathrm{vac}\rangle, \quad N>0, \tag{5.1.2}$$

where $a_0^*$ is the creation operator for the zero-momentum condensate, and $|\mathrm{vac}\rangle$ denotes the Fock space vacuum state (see Section 5.1.3 for details). We extend this result to show that all excited states of $\mathscr{H}_{\mathrm{LHY}}$ take the form

$$|\Psi_{E(\vec{n})}\rangle := \exp(-\mathscr{P})|\Psi_{\vec{n}}\rangle, \tag{5.1.3}$$

where $|\Psi_{\vec{n}}\rangle$ is a *finite superposition* of momentum tensor product states (see equation (1)). This is a unique feature of our approach — the pair-excitation hypothesis yields a simple formula for excited many-body states in a physically transparent basis.

### 5.1.1 Comparison with other works

It is necessary to remark on the more common method of 'Bogoliubov rotations' for quadratic Hamiltonians, by which the spectrum and excited states of Hamiltonian $\mathscr{H}_{\mathrm{LHY}}$ can be derived [9, 33, 43]. To this end, if the collection $\{a_k, a_k^*\}_{k\in\mathbb{Z}_L^3}$ denotes the momentum state creation/annihilation operator basis (see Section 5.1.3), then the operators defined by

$$b_k := \cosh(\alpha(k))a_k + \sinh(\alpha(k))a_{-k}^*, \quad \text{for} \quad 0 \leq \alpha(k) < 1$$

satisfy the canonical commutation relations for bosonic operators, and a particular choice of $\alpha(k)$ makes $\mathscr{H}_{\mathrm{LHY}}$ diagonal in this new operator basis $\{b_k^*, b_k\}_{k\in\mathbb{Z}_L^3}$. I.e.,

$$\mathscr{H}_{\mathrm{LHY}} = \sum_{k\in\mathbb{Z}_L^3} \varepsilon(k) b_k^* b_k \,. \tag{5.1.4}$$

Here, $\{\varepsilon(k)\}_{k\in\mathbb{Z}_L^3} = \sigma(\mathscr{H}_{\mathrm{LHY}})$. For fixed $N, L$, the $\varepsilon(k)$ are discrete, positive, with a gap between the ground state energy and first excited state. This transformation can alternatively be expressed as

$$b_k = \exp(\mathscr{X}) a_k \exp(-\mathscr{X}),$$

where $\mathscr{X}$ is the skew-Hermitian operator

$$\mathscr{X} := \sum_{k\in\mathbb{Z}_L^+} \alpha(k)(a_k^* a_{-k}^* - a_k a_{-k}). \tag{5.1.5}$$

Excited many-body states of $\mathscr{H}_{\mathrm{LHY}}$ are given by tensor products of the $b$ operators, viz.

$$|\Psi_{\{n_k\}}\rangle := \prod_{k\in\mathbb{Z}_L^+} (b_k^*)^{n_k}|\Psi_0\rangle, \quad n_k \in \mathbb{N} \quad \forall k, \quad \sum_{k\in\mathbb{Z}_L^+} n_k < \infty. \tag{5.1.6}$$

The ground state in particular exhibits form

$$|\Psi_0\rangle = \exp(\mathscr{X})|0\rangle = \exp(-\mathscr{P})|0\rangle,$$

where $|0\rangle$ is a state such that both $|0\rangle$ and the vacuum state $|\mathrm{vac}\rangle$ project onto the same state in the space orthogonal to the condensate. The choice $|0\rangle = (a_0^*)^N/\sqrt{N!}$ gives exactly the formula derived by Wu, equation (5.1.2) above. The fact that $\mathscr{H}_{\mathrm{LHY}}$ is diagonal in the operators $\{b_k, b_k^*\}$ leads one to attribute physical significance to them as *quasiparticles*. As far as the computation of observables goes, one may use the operator basis $\{b_k, b_k^*\}$ just as easily as the momentum operators $\{a_k, a_k^*\}$.

The quasiparticle approach is equivalent to the method of pair excitation described in this chapter in the sense that it provides formulas for computing all observables of the system. The reason for developing the alternative method of pair-excitation here (besides the new mathematical structures and analysis involved) is that it emphasizes the pair-hypothesis in the structure of many-body states; the non-Hermitian operator involved describes a physical process between the condensate and excited states in momentum space, which stands in contrast to quasiparticle excitations. Equation (5.1.3) holds for all many-body excited states, and emphasizes the role of pairs in the physics of excitations. We discovered in previous chapters that this allowed for an elegant development of the theory for a family of Hamiltonians. The major analogy is with Wu's Hamiltonian in Chapter 3. The eigenstates for that operator were written precisely using pair-excitation.

The case here is harder, and can be seen as the simplest extension of this method to quadratic Hamiltonians.

In pursuing a rigorous analysis of the Lee-Huang-Yang model, we do not address the validity of quadratic models for BEC in this work. See [57] for a detailed discussion of these matters in the periodic setting. As such, we rely on the ubiquity of these approximations in many areas of physics for our motivation.

We choose the particular model of Lee, Huang and Yang as the subject of the current work because in our opinion it captures the essential physics of pair excitation in quadratic systems in the most concise fashion. In this vein, the Lee-Huang-Yang Hamiltonian describes low-energy two-particle collisions via a delta-function interaction potential and a *scattering length*, $a > 0$. We note that this introduces a familiar infinite constant term in the Hamiltonian, which will be ignored. Our argument for recovering the spectrum $\sigma_{\mathrm{p}}\big(\mathscr{H}_{\mathrm{LHY}}\big)$ from $\sigma_{\mathrm{p}}\big(\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P})\big)$ relies on the momentum basis in a non-trivial way — it is unclear how to extend the construction of this chapter, e.g., to the study of $\mathscr{H}_{\mathrm{Fetter}}$ in Chapter 3. Our construction, however, still holds for a variety of quadratic Hamiltonians; for example, Bogoliubov adopted the following quadratic Hamiltonian for bosons in the periodic box with a two-body interaction potential $v(x)$ [9, 43]

$$\mathscr{H}_{\mathrm{Bog}} := \sum_k (k^2 + \frac{N}{2V}\widehat{v}(k))a_k^* a_k + \frac{N}{2V}\sum_k \widehat{v}(k)(a_k^* a_{-k}^* + a_k a_{-k}), \tag{5.1.7}$$

where $\widehat{v}(k)$ denotes the Fourier transform of the interaction potential $v(x)$.

### 5.1.2 Outline of Chapter

In Section 5.2, we introduce the many-body Hamiltonian and describe the heuristic approximation scheme by which the Lee-Huang-Yang Hamiltonian, $\mathscr{H}_{\mathrm{LHY}}$, is derived.

In Section 5.3 we introduce the pair excitation transformation, $\exp(\mathscr{P})$, and provide an exact formula for excited states of the non-unitary transformed Hamiltonian via expansion in the momentum basis.

In Sections (5.4.1) and (5.5) we discuss the spectral theory for the transformed operator

$$\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P}),$$

whose spectrum is *not* identical to the spectrum of $\mathscr{H}_{\mathrm{LHY}}$. This fact necessitates that we take care in identifying the mappings of $\mathscr{H}_{\mathrm{LHY}}$ eigenstates among the eigenstates of the transformed operator; they are exactly those eigenstates of the transformed system which are finite superpositions of momentum states.

### 5.1.3 Preliminaries

Our domain will be the periodic box in 3 dimensions with length $L$, which we denote $B_L = [0,L]^3$, and its volume $|B_L| = L^3$. Unless otherwise noted, all integrals are assumed to be over $B_L$.

Function spaces on $\mathbb{R}^3$ or $B_L$ are denoted by lowercase gothic letters, viz.,

$$\mathfrak{h}(\mathbb{R}^3) := L^2(\mathbb{R}^3)\ .$$

An exception is the definition $\phi^\perp := \left\{ e \in \mathfrak{h} \;\middle|\; e \perp \phi \right\}$ where $\phi \in \mathfrak{h}$ is the condensate wave

function. When considering function spaces for many-particle systems, we will take

$$\mathfrak{h}(\mathbb{R}^{3N}) := L^2_{\text{sym}}(\mathbb{R}^{3N}),$$

where the subscript refers to the fact that the functions in this space are symmetric under permutations of the $N$ coordinates, $x_1, x_2, \ldots, x_N \in \mathbb{R}^3$. Operators on $\mathfrak{h}$ are given by greek or roman letters. For example, $\delta(x,y)$ will denote the Dirac mass of the identity operator and $\Delta$ is the Laplace operator. The many-body Hamiltonian on the configuration space $\mathfrak{h}(\mathbb{R}^{3N})$ is denoted $H_N$ which we define in Section 5.2.

For $f, g \in \mathfrak{h}$ the tensor-product corresponding to $f(x)\overline{g(y)}$ is expressed by $f \otimes g$. The symmetrized tensor product of $f, g$ is

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

## The bosonic Fock space

We define the Bosonic Fock space, $\mathbb{F}$, as a direct sum of $n$-particle Hilbert spaces, via

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

Vectors in $\mathbb{F}$ are described as sequences of $n$-particle wave functions, or using ket notation, as in $|u\rangle = \{u^n\}$ where $u^n \in \mathfrak{h}(\mathbb{R}^{3n})$, for $n \geq 0$. The inner product of $|u\rangle = \{u^n\}$, $|w\rangle = \{w^n\} \in \mathbb{F}$ is

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

This induces the norm $\||u\rangle\|_{\mathbb{F}} = \sqrt{\langle u, u\rangle_{\mathbb{F}}}$. As we already aluded to, we employ the bra-ket notation for Schrödinger state vectors in $\mathbb{F}$ to distinguish them from wave functions in $\mathfrak{h}(\mathbb{R}^{3n})$.

Operators on $\mathbb{F}$ will be denoted by calligraphic letter, an example being the Hamiltonian $\mathscr{H} : \mathbb{F} \to \mathbb{F}$. This, of course, excludes the annihilation and creation operators, including the field operators $a_x$, $a_x^*$, as well as the operators $a_{\overline{\phi}}, a_\phi^*$ and $a_k, a_k^*$ associated with the basis $\{e_k(x)\}$ discussed shortly. 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, $\psi_N \in \mathfrak{h}(\mathbb{R}^{3N})$, 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 all vectors $|\psi\rangle_N$ for $N$ fixed is a linear subspace of $\mathbb{F}$, denoted $\mathbb{F}_N$, and is called the '$N$-th fiber' ($N$-particle sector) of $\mathbb{F}$. We sometimes omit the subscript '$N$' when referring to a $|\psi\rangle_N \in \mathbb{F}_N$ when the context makes it clear .

A Hamiltonian on $\mathfrak{h}(\mathbb{R}^{3N})$ admits an extension to an operator on $\mathbb{F}$. This extension is carried out via the Bosonic field operator $a_x$ and its adjoint, $a_x^*$, for 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

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

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

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 now defined using an orthonormal basis via

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

The canonical commutation relations $[a_x, a_y^*] = \delta(x-y)$, $[a_x, a_y] = 0$ then follow.

An orthonormal basis that we use extensively in this work consists of the momentum eigenfunctions on $B_L$:

$$e_k(x) := \frac{e^{ik\cdot x}}{\sqrt{|B_L|}}, \quad \text{where} \quad k := \frac{2\pi n}{L}, \quad n \in \mathbb{Z}^3. \tag{5.1.8}$$

Thus we consider periodic functions (of spatial variable $x \in B_L$) with period $L$ and denote the dual lattice

$$\mathbb{Z}^3_L := \{k = 2\pi n/L \,\big|\, n \in \mathbb{Z}^3\}.$$

We also define the momentum half-space, $\mathbb{Z}^+_L$, which will make the description of pair-excited states simpler:

$$\mathbb{Z}^+_L := \{k = 2\pi n/L \,\big|\, n \in \mathbb{Z}^3, n_3 > 0\}.$$

By virtue of the commutation relations on $\{a_x, a^*_x\}$, the creation and annihilation operators for the states $\{e_k(x)\}_{k\in\mathbb{Z}^3_L}$, denoted $a(\overline{e_k}) := a_k$ and $a^*(e_k) := a^*_k$ satisfy

$$[a_{k_1}, a^*_{k_2}] = \delta(k_1, k_2), \quad [a_{k_1}, a_{k_2}] = 0 = [a^*_{k_1}, a^*_{k_2}], \quad k_1, k_2 \in \mathbb{Z}^3_L.$$

Vectors $|\Psi\rangle \in \mathbb{F}$ can also be expressed in terms of the occupation number basis for $\{e_k(x)\}$. The orthonormal elements of this Fock space basis consist of tensor product states for every collection of integers $\{n_k \in \mathbb{N}\}_{k\in\mathbb{Z}^3_L}$ with $\sum_{k\in\mathbb{Z}^3_L} n_k < \infty$, given by

$$|n_{k_1}, n_{k_2}, \ldots\rangle := \prod_{k\in\mathbb{Z}^3_L} \frac{\left(a(e_k)^*\right)^{n_k}}{\sqrt{n_k!}} |vac\rangle.$$

The states $|n_{k_1}, n_{k_2}, \ldots, n_{k_n}\rangle$ will also be used to denote the basis of tensor products for a fixed finite collection of momenta, $(k_1, \ldots, k_n)$.

Finally, the symbol "$\approx$" will be used in two senses. The first sense refers the the heuristic approximation of Fock space operators, as in $\mathscr{H}_{\text{LHY}} \approx \mathscr{H}$. The second

sense is the relation of asymptotic equivalence of functions. A function $f(z)$ is said to be asymptotically equivalent to $g(z)$ as $|z| \to \infty$, i.e., $f(z) \approx g(z)$ as $|z| \to \infty$, provided $\lim_{|z|\to\infty} \frac{f(z)}{g(z)} = 1$. We will be careful to clarify in which sense we are using this symbol when it occurs in the text.

**On the operator exponential:** We will make extensive use of the operator $\exp(\mathscr{P}) : \mathbb{F} \to \mathbb{F}$, where

$$\mathscr{P} := \sum_{k\in\mathbb{Z}_L^+} \alpha(k) a_k^* a_{-k}^*, \quad \text{for} \quad 0 \leq \alpha(k) < 1 \quad \forall k \in \mathbb{Z}_L^+.$$

The operator $\mathscr{P}$ is unbounded on $\mathbb{F}$. While it does not have any eigenvalues, its spectrum $\sigma(\mathscr{P})$ (that is, the union of point, continuous and residual spectra) consists of the entire complex plane. A precise definition of $\mathrm{dom}(\exp(\mathscr{P}))$ is not strictly necessary for our purposes; it will suffice to consider this operator as a formal series in powers of $\mathscr{P}$ as long as we are acting on states which remain finite-norm under the action of this formal operator series. Fixing $k \in \mathbb{Z}_L^+$, and defining

$$|0\rangle := \frac{1}{\sqrt{N!}} (a_0^*)^N |\mathrm{vac}\rangle, \quad N < \infty,$$

a state vector of the form:

$$|\Psi(k)\rangle = \sum_{n=0}^{\infty} c_n |n,n\rangle, \quad |n,n\rangle := \frac{(a_k^* a_{-k}^*)^n}{n!} |0\rangle, \quad \sum_{n=0}^{\infty} |c_n|^2 = 1$$

will belong to $\mathrm{dom}\big(\exp(\mathscr{P})\big)$ provided that the sequence

$$\left\{ \tilde{c}_s := \sum_{n=0}^{s} c_n (-\alpha(k))^{s-n} \binom{s}{s-n} \right\}_{s=0}^{\infty} \tag{5.1.9}$$

is square-summable. We note that the use of exponentials involving creation operators such as $\exp(\mathscr{P})$ is quite common the study of generalized coherent states [52].

The following lemma will be crucial [59].

**Lemma 9.** *Any two operators $\mathscr{A}, \mathscr{B}$ in the Fock space satisfy the identity*

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

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

$$ad(\mathscr{A})^n(\mathscr{B}) = [\mathscr{A}, ad(\mathscr{A})^{n-1}(\mathscr{B})], \quad n \geq 1.$$

## 5.2 Many-body Hamiltonian and approximation scheme

We now summarize the bosonic many-body Hamiltonian and discuss the quadratic approximation of Lee, Huang, and Yang. This is included as motivation for the analysis that follows; we do not rigorously justify the derivation of this section.

Consider $N$ bosons inside the box $B_L$, with periodic boundary conditions and repulsive pairwise particle interaction $\upsilon$. On the Hilbert space $\mathfrak{h}(\mathbb{R}^{3N})$ of symmetric $N-$particle wavefunctions, the Hamiltonian for this system reads

$$H_N = \sum_{j=1}^{N} -\Delta_j + \sum_{i<j}^{N} \upsilon(x_i, x_j), \quad x_j \in \mathbb{R}^3. \tag{5.2.1}$$

Here we choose units such that $\hbar = 2m = 1$, where $\hbar$ is Planck's constant, and $m$ is the atomic mass. The interaction potential $\upsilon$ should be understood to be positive, symmetric, and compactly supported.

This Hamiltonian can be lifted to the bosonic Fock space via the field operators $\{a_x, a_x^*\}$:

$$\mathscr{H} = \int dx \{a_x^*(-\Delta_x)a_x\} + \frac{1}{2} \iint dxdy \{\upsilon(x,y) a_x^* a_y^* a_x a_y\}. \tag{5.2.2}$$

In the spirit of Lee, Huang and Yang, we take the interaction $\upsilon$ to be the Fermi pseudopotential, which is an effective operator that reproduces the low-energy limit of

the far field of the exact wavefunction [34]. If $f$ is any two-body wavefunction, we therefore take

$$v(x_i,x_j)f(x_i,x_j) \approx g\delta(x_i-x_j)\frac{\partial}{\partial x_{ij}}\big[x_{ij}f(x_i,x_j)\big], \quad (i\neq j), \tag{5.2.3}$$

where $x_{ij} := |x_i - x_j|$, and $g := 8\pi a$ where $a$ is the scattering length. We further simplify this interaction by omitting $(\partial/\partial x_{ij})x_{ij}$ from (5.2.3), viz.,

$$v(x_i,x_j) \mapsto g\delta(x_i-x_j). \tag{5.2.4}$$

The substitution (5.2.4) will be exact for solutions to the many-body wavefunction with sufficient regularity [34]. Inserting (5.2.4) into (5.2.2), and expanding in the momentum basis yields

$$\mathscr{H} \approx \sum_{k\in\mathbb{Z}^3_L} |k|^2 a_k^* a_k + \frac{4\pi a}{|B_L|}\sum_{k_1+k_2=k_3+k_4} a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4}. \tag{5.2.5}$$

The symbol "$\approx$" denotes the fact that we have approximated the two-body interaction potential with a delta function.

As remarked on in the introduction to this chapter, $\mathscr{H}$ as written in (5.2.5) is manifestly particle conserving (in the sense that $[\mathscr{H},\mathscr{N}]=0$), and so its associated eigenvalue problem may be considered on the Fock space of fixed particle number, $\mathbb{F}_N$ for $N$ finite but large. By contrast, the effective Hamiltonian of Lee Huang and Yang (which we denote by $\mathscr{H}_{\mathrm{LHY}}$ and define shortly), will not conserve the total number of particles. We discuss this after summarizing the remaining steps in the approximation of $\mathscr{H}_{\mathrm{LHY}}$. We proceed by decomposing the interaction part of $\mathscr{H}$ into terms containing like-powers of the condensate operators, $a_0$ and $a_0^*$ ; the second, third, and fourth lines of the expression

below contain quadratic, linear, and zeroth-order terms in these operators respectively:

$$\begin{aligned}\mathscr{H} = &\sum_{k\in\mathbb{Z}^3_L,k\neq 0} k^2 a^*_k a_k + \frac{4\pi a}{|B_L|}(a^*_0)^2 a_0^2 \\ &+ \frac{4\pi a}{|B_L|}\sum_{k\in\mathbb{Z}^3_L,k\neq 0}\Big((a^*_0)^2 a_k a_{-k} + a^*_k a^*_{-k}(a_0)^2 + 4(a^*_0 a_0)a^*_k a_k\Big) \\ &+ \frac{8\pi a}{|B_L|}\sum_{\substack{k_3=k_1+k_2\\ k_1,k_2,k_3\neq 0}}\Big((a^*_{k_1}a^*_{k_2}a_{k_3})a_0 + (a_{k_1}a_{k_2}a^*_{k_3})a^*_0\Big) \\ &+ \frac{4\pi a}{|B_L|}\sum_{\substack{k_1+k_2=k_3+k_4\\ k_1,k_2,k_3,k_4\neq 0}} a^*_{k_1}a^*_{k_2}a_{k_3}a_{k_4}.\end{aligned} \tag{5.2.6}$$

The approximation of Lee Huang and Yang is consistent with the following steps (we use these steps for explanatory purposes): **(i)** replace the condensate occupation number operator by

$$(a^*_0 a_0) \mapsto N - \sum_{k\neq 0} a^*_k a_k, \quad \text{for} \quad N<\infty,$$

and **(ii)** consider the action of Hamiltonian $\mathscr{H}$ on states $\Psi$ satisfying

$$\begin{cases} \langle\Psi|\sum_{k\neq 0}\frac{1}{N}a^*_k a_k|\Psi\rangle \ll 1, \\ \\ \mathscr{H}\Psi = E\Psi, \quad \langle\Psi|\mathscr{N}|\Psi\rangle = N. \end{cases} \tag{5.2.7}$$

In particular, for $\tilde{\mathscr{N}} := \sum_{k\neq 0} a^*_k a_k$, we make the operator approximation

$$(\mathscr{N}-\tilde{\mathscr{N}})^2 - (\mathscr{N}-\tilde{\mathscr{N}}) = \mathscr{N}^2 - \mathscr{N} - 2\mathscr{N}\tilde{\mathscr{N}} + \tilde{\mathscr{N}}^2 + \tilde{\mathscr{N}} \approx \mathscr{N}^2 - \mathscr{N} - 2\mathscr{N}\tilde{\mathscr{N}},$$

where we have dropped the terms $\tilde{\mathscr{N}}^2 + \tilde{\mathscr{N}}$ because $\langle\Psi|\tilde{\mathscr{N}}|\Psi\rangle \ll N$ for all states of interest according to the assumption (5.2.7).

The first line in (5.2.6) is therefore approximated by

$$\begin{aligned}\frac{4\pi a}{|B_L|}(a_0^*)^2 a_0^2 &= \frac{4\pi a}{|B_L|}\big\{(a_0^* a_0)^2 - (a_0^* a_0)\big\} \\ &\approx \frac{4\pi a}{|B_L|}\Big\{(N - \sum_{k\neq 0} a_k^* a_k)^2 - (N - \sum_{k\neq 0} a_k^* a_k)\Big\} \\ &\approx \frac{4\pi a}{|B_L|}\Big\{N(N-1) - 2N\sum_{k\neq 0} a_k^* a_k\Big\} \\ &\approx 4\pi a\rho N - 8\pi a\rho\Big\{\sum_{k\neq 0} a_k^* a_k\Big\}.\end{aligned} \tag{5.2.8}$$

The second line of (5.2.6) consists of three quadratic terms in condensate operators, proportional to $(a_0)^2$, $(a_0^*)^2$ and $(a_0^* a_0)$ respectively. The $(a_0^* a_0)$ term will contribute to the diagonal part of $\mathscr{H}_{\mathrm{LHY}}$, via

$$\begin{aligned}\frac{16\pi a}{|B_L|}\sum_{k\neq 0}(a_0^* a_0)a_k^* a_k &\approx 16\pi a\rho\sum_{k\neq 0} a_k^* a_k - \frac{16\pi a}{|B_L|}\Big(\sum_{k\neq 0} a_k^* a_k\Big)^2 \\ &\approx 16\pi a\rho\sum_{k\neq 0} a_k^* a_k.\end{aligned} \tag{5.2.9}$$

If cubic and quartic terms in the $\{a_k^{(*)}\}$ operators where $k \neq 0$ are now neglected (we will provide a consistent explanation for this in the next paragraph), approximations (5.2.8) and (5.2.9) yield the reduced Hamiltonian

$$\mathscr{H} \approx 4\pi a\rho N + \sum_{k\in\mathbb{Z}_L^3, k\neq 0}\big\{k^2 + 8\pi a\rho\big\}a_k^* a_k + \frac{4\pi a}{|B_L|}\sum_{k\in\mathbb{Z}_L^3, k\neq 0}\big\{(a_0^*)^2 a_k a_{-k} + a_k^* a_{-k}^* (a_0)^2\big\}. \tag{5.2.10}$$

This intermediate approximation to $\mathscr{H}_{\mathrm{LHY}}$ is of independent interest, since it is particle-conserving.

It is now apparent that the only way for off-diagonal terms of (5.2.10) to (formally) contribute, requires that $(a_0)^2$ and $(a_0^*)^2$ be replaced (or be replaceable) by $N$. This also

justifies the dropping of cubic-and-quartic terms in the $\{a_k^{(*)}\}$ operators between (5.2.6) and (5.2.10), since replacing $a_0$, $a_0^*$ by $\sqrt{N}$ and making the above assumptions (5.2.7) will result in these terms formally vanishing. We note that this amounts to a version of the famous Bogoliubov approximation [9], although such terminology was not used explicitly by Lee, Huang and Yang. With this final replacement, we arrive at the Lee-Huang-Yang Hamiltonian

$$\mathscr{H}_{\mathrm{LHY}} := 4\pi a\rho N + \sum_{k\in\mathbb{Z}_L^3, k\neq 0} \left\{k^2 + 8\pi a\rho\right\} a_k^* a_k + 4\pi a\rho \sum_{k\in\mathbb{Z}_L^3, k\neq 0} \left\{a_k^* a_{-k}^* + a_k a_{-k}\right\}. \tag{5.2.11}$$

From this expression, we see that $\mathscr{H}_{\mathrm{LHY}}$ is a sum of terms which involve only the momenta $(k,-k)$. We therefore utilize the *momentum half space*:

$$\mathbb{Z}_L^+ := \{k = 2\pi n/L \,\big|\, n \in \mathbb{Z}^3, n_3 > 0\},$$

in order to write $\mathscr{H}_{\mathrm{LHY}}$ as a sum of operators which commute with $\left(a_k^* a_k + a_{-k}^* a_{-k}\right)$, for $k \in \mathbb{Z}_L^+$, i.e.,

$$\mathscr{H}_{\mathrm{LHY}} = 4\pi a\rho N + \sum_{k\in\mathbb{Z}_L^+} 2\left(k^2 + 8\pi a\rho\right)\left\{\frac{1}{2}\left(a_k^* a_k + a_{-k}^* a_{-k}\right) + y(k)\left(a_k^* a_{-k}^* + a_k a_{-k}\right)\right\}. \tag{5.2.12}$$

where, consistent with [37], we define the constant

$$y(k) := \frac{4\pi a\rho}{k^2 + 8\pi a\rho}, \quad k \in \mathbb{Z}_L^+.$$

The point spectrum of $\mathscr{H}_{\mathrm{LHY}}$ will be called the *Bogoliubov spectrum*, and is given by $\sum_{k\in\mathbb{Z}_L^+}(n_k + n_{-k})\varepsilon_k$ where the set of occupation numbers $\{n_k\}_{k\in\mathbb{Z}_L}$ satisfies

$$\sum_{k\in\mathbb{Z}_L^+} (n_k + n_{-k}) < \infty,$$

and the single particle energies are given by

$$\varepsilon_k := k\sqrt{k^2 + 16\pi a\rho}. \tag{5.2.13}$$

In the analysis of the next section, it will be easier to state results for the generic operator that appears inside the brackets in (5.2.12), where $y(k)$ may take on the range of values $(0, 1/2)$ as $k$ varies over $\mathbb{Z}_L^+$. We therefore conclude this section by defining the quadratic Hamiltonian for two orthogonal momentum states $(a,b)$, denoted $\mathscr{H}_{\text{ab}}(y)$. The notation for this 'core' operator is inspired by Wu [61].

**Definition 5.** *Let the operators $\{a, a^*, b, b^*\}$ satisfy the canonical commutation relations*

$$\begin{aligned} &[a,a^*] = [b,b^*] = 1, \\ &[a,a] = [b,b] = [a^*,a^*] = [b^*,b^*] = 0 \\ &[a,b] = [a^*,b^*] = [a^*,b] = [a,b^*] = 0, \end{aligned} \tag{5.2.14}$$

*and act on the Fock space $\mathbb{F}_{ab}$ which is the linear span of all formal tensor products of the operators $a^*, b^*$, i.e.,*

$$\mathbb{F}_{ab} := \text{span}\{|n_a, n_b\rangle, \quad \text{for} \quad n_a, n_b \in \mathbb{N}\}, \quad |n_a, n_b\rangle := \frac{(a^*)^{n_a}(b^*)^{n_b}}{\sqrt{n_a! n_b!}}|\text{vac}\rangle. \tag{5.2.15}$$

*Define the Hamiltonian $\mathscr{H}_{ab}(y)$ on $\mathbb{F}_{ab}$, where $0 < y < 1/2$, by*

$$\mathscr{H}_{\text{ab}}(y) := \frac{1}{2}\big(a^*a + b^*b\big) + y\big(a^*b^* + ab\big). \tag{5.2.16}$$

*We then define the Bogoliubov spectrum for $\mathscr{H}_{\text{ab}}$ by the formula*

$$(n_a + n_b)\sqrt{1 - 4y^2}, \quad \text{for} \quad n_a + n_b < \infty. \tag{5.2.17}$$

### 5.2.1 Comment on particle conservation versus non-conservation

There is an apparent contradiction in the approximation scheme above, since step **(i)** is a statement of particle-conservation, while we ultimately arrive at $\mathscr{H}_{\mathrm{LHY}}$ which does not conserve the number of particles. We must therefore be more precise, and specify that the steps **(i)** and **(ii)** do not refer to the restriction of the problem to the $N$-particle sector of Fock space, $\mathbb{F}_N$, but rather impose a constraint on the average number of particles for the many-body states of $\mathscr{H}_{\mathrm{LHY}}$. This means that we solve the eigenvalue problem $\mathscr{H}_{\mathrm{LHY}}|\Psi\rangle = E|\Psi\rangle$ for eigenstates $|\Psi\rangle \in \mathbb{F}$ which satisfy the condition

$$\langle\Psi|a_0^* a_0 + \sum_k a_k^* a_k|\Psi\rangle = N. \tag{5.2.18}$$

We will have to verify that the eigenstates $\Psi$ which we construct are self-consistent with this assumption.

## 5.3 Formal construction of many-body excited states

We now construct a family of *formal* solutions to the eigenvalue problem for Hamiltonian $\mathscr{H}_{\mathrm{LHY}}$. This construction makes use of the non-unitary transformation by $\exp(-\mathscr{P})$ : $\mathbb{F} \to \mathbb{F}$, which creates pairs of particles with opposite-momenta, and maps any $\Psi \in \mathbb{F}_n$ to the state $\exp(-\mathscr{P})\Psi$ which has a nonzero component in every $(n+s)-$particle fiber, $\mathbb{F}_{n+s}$, of $\mathbb{F}$, $s = 0,1,2,\ldots$. In defining the operator $\mathscr{P}$, we are inspired by the operator described by Wu (Chapter 3) [60,61]. The operator $\mathscr{P}$ depends on a free parameter, denoted $0 < \alpha(k) < 1$, for every $k \in \mathbb{Z}_L^+$, and is defined by

$$\mathscr{P} := \sum_{k \in \mathbb{Z}_L^+} \alpha(k) a_k^* a_{-k}^*. \tag{5.3.1}$$

We will choose $\alpha(k)$ in the manner of Wu in order to eliminate all terms proportional to $(a_k^* a_{-k}^*)$ in the transformed operator $\exp(\mathscr{P})(\mathscr{H}_{\mathrm{LHY}})\exp(-\mathscr{P})$. The resulting non-Hermitian eigenvalue problem can be solved exactly by considering solutions $|\Psi_{\mathrm{LHY}}(k)\rangle$, for $k \in \mathbb{Z}_L^+$, which are linear combinations of tensor product states containing only the momenta $k$ and $-k$:

$$\Big(\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P})\Big)|\Psi_{\mathrm{LHY}}(k)\rangle = E|\Psi_{\mathrm{LHY}}(k)\rangle. \tag{5.3.2}$$

**Important Note:** The non-Hermitian eigenvalue problem, equation (5.3.2), will not in general yield $E$ that lie in the point spectrum $\sigma_{\mathrm{p}}(\mathscr{H}_{\mathrm{LHY}})$. In fact we will see that the transformed problem can have either a discrete or a continuous point spectrum depending on whether the quantity

$$\tilde{y}(k) := \frac{y(k)}{\sqrt{1-4y(k)^2}}, \quad \text{for} \quad y(k) = \frac{4\pi a\rho}{k^2+8\pi a\rho},$$

satisfies $\tilde{y}(k) < 1$ or $\tilde{y}(k) \geq 1$. We note that for $y(k) \in (0,1/2)$, the quantity $\tilde{y}(k)$ takes on values in the range $(0,\infty)$. This splitting of the problem into the two cases $\tilde{y}(k) < 1$ and $\tilde{y}(k) \geq 1$ is a mathematical *artifact* of using a method which transforms a Hermitian Hamiltonian by an unbounded, non-Hermitian operator. This may suggest that the spectrum for the problem (5.3.2) has no significance for the original physics problem — the following analysis shows otherwise. In the next section, we will provide a characterization of the eigenstates of the transformed Hamiltonian. We will see that the case $\tilde{y}(k) < 1$ corresponds to a regular perturbation of the eigenvalue problem for the diagonal

Hamiltonian $\mathscr{H}_{\text{diag}} := \frac{1}{2}(a_k^* a_k + a_{-k}^* a_{-k})$. The case $\tilde{y}(k) \geq 1$ can be solved exactly, and we will see that it cannot be associated with a regular perturbation of the problem for $\mathscr{H}_{\text{diag}}$. While information about the Hamiltonian $\mathscr{H}_{\text{ab}}$ can be discerned by different means (e.g., Bogoliubov rotation), our goal is to show how analyzing the Hamiltonian via pair excitation can give all the same information as these other methods, without prior knowledge of them.

### 5.3.1 The non-Hermitian transform

For $\mathscr{P}$ given by (5.3.1), a straightforward calculation using Lemma 9 yields the conjugations

$$\exp(\mathscr{P})a_k \exp(-\mathscr{P}) = a_k - \alpha(k)a_{-k}^*, \quad \exp(\mathscr{P})a_k^* \exp(-\mathscr{P}) = a_k^*, \quad \forall k \in \mathbb{Z}_L^3. \tag{5.3.3}$$

We define $\alpha(-k) = \alpha(k)$ for $k \in \mathbb{Z}_L^+$. This yields the transformed Hamiltonian

$$\begin{aligned}\exp(\mathscr{P})\mathscr{H}_{\text{LHY}} \exp(-\mathscr{P}) = {} & 4\pi a\rho N + 4\pi a\rho \sum_{k\in\mathbb{Z}_L^3} \alpha(k) \\ & + \sum_{k\in\mathbb{Z}_L^3} \big(k^2 + 8\pi a\rho - 8\pi a\rho\,\alpha(k)\big)(a_k^* a_k) + 4\pi a\rho \sum_{k\in\mathbb{Z}_L^3} (a_k a_{-k}) \\ & + \sum_{k\in\mathbb{Z}_L^3} \big(4\pi a\rho(\alpha(k))^2 - (k^2 + 8\pi a\rho)\alpha(k) + 4\pi a\rho\big)(a_k^* a_{-k}^*).\end{aligned} \tag{5.3.4}$$

We note that at this point that the term $\sum_{k\in\mathbb{Z}_L^3} \alpha(k)$ introduces an infinite constant (see equation (5.3.5)) to the energy spectrum of the transformed Hamiltonian; this can be attributed to approximating the smooth interaction potential by a delta function and can be removed in a systematic way. For brevity, and since it does not affect the construction that follows in a meaningful way, we will retain this term in the following analysis, and refer to [34] for details regarding its proper analytical remedy. In distinction to the unitary

transformation of $\mathscr{H}_{\mathrm{LHY}}$ exemplified by equation (5.1.5), the exponential transformation by $\mathscr{P}$ has a free parameter $\alpha(k)$ for every $k \in \mathbb{Z}_L^+$ which is not constrained by a requirement of unitarity. We exploit this freedom in order to make the expansion of eigenvectors in the momentum basis particularly simple. The resulting problem (5.3.2) on Fock space will correspond to an (infinite) upper triangular matrix system.

In this vein, we choose $\alpha(k) = \alpha_c(k)$ so that the last line of (5.3.4) vanishes, which implies

$$\alpha_c(k) = \frac{1}{8\pi a\rho}\Big((k^2 + 8\pi a\rho) \pm k\sqrt{k^2 + 16\pi a\rho}\Big), \quad k \in \mathbb{Z}_L^+. \tag{5.3.5}$$

The choice of $\alpha_c(k)$ corresponding to the minus sign in (5.3.5) yields a positive spectrum for (5.3.2). The two possible solutions for $\alpha_c(k)$ in the expansion of $\mathscr{P}$ has an analog in the non-periodic setting, where the quadratic equation for $\alpha_c(k)$ generalizes to an operator Riccati equation for a pair excitation kernel $k(x,y)$. In Chapter 3, we provide a detailed description of this correspondence. With this choice, the transformed Hamiltonian reads

$$\begin{aligned}\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P}) &= 4\pi a\rho N + 4\pi a\rho \sum_{k\in\mathbb{Z}_L^3} \alpha_c(k) \\ &+ \sum_{k\in\mathbb{Z}_L^+} 2\big(k\sqrt{k^2+16\pi a\rho}\big)\Big\{\frac{1}{2}(a_k^* a_k + a_{-k}^* a_{-k}) + \Big(\frac{4\pi a\rho}{k\sqrt{k^2+16\pi a\rho}}\Big)a_k a_{-k}\Big\}.\end{aligned} \tag{5.3.6}$$

For a single term of this sum corresponding to fixed $k \in \mathbb{Z}_L^+$, the operator inside curly brackets is a transformation of the formal Hamiltonian $\mathscr{H}_{\mathrm{ab}}(y) : \mathbb{F}_{\mathrm{ab}} \to \mathbb{F}_{\mathrm{ab}}$ if for each $k \in \mathbb{Z}_L^+$ we identify annihilation operator $a_k$ with operator $a$ and annihilation operator $a_{-k}$ with operator $b$. This is summarized in the following definition:

**Definition 6.** *Define the family of rescaled transformed Hamiltonians, parameterized by* $\alpha \in [0, 1/2y)$*, by:*

$$\begin{aligned} \mathscr{H}_{\mathrm{ab}}^{(\alpha)} &:= \frac{1}{1-2\alpha y}\Big(\exp(\alpha a^* b^*)\mathscr{H}_{\mathrm{ab}}\exp(-\alpha a^* b^*) + \alpha y\Big) \\ &= \frac{1}{2}\big(a^* a + b^* b\big) + y_1(\alpha)ab + y_2(\alpha)a^* b^*, \end{aligned} \tag{5.3.7}$$

*where* $y_1(\alpha), y_2(\alpha)$ *are given by*

$$y_1(\alpha) := \frac{y}{1-2\alpha y}, \quad \text{and} \quad y_2(\alpha) := \frac{y-\alpha+\alpha^2 y}{1-2\alpha y}.$$

*The value*

$$\alpha = \alpha_c := \frac{1-\sqrt{1-4y^2}}{2y},$$

*then induces the transformation:*

$$\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)} = \frac{1}{2}\Big(a^* a + b^* b\Big) + \tilde{y}ab, \tag{5.3.8}$$

*for*

$$\tilde{y} := \Big(\frac{y}{\sqrt{1-4y^2}}\Big).$$

*If* $y = y(k) = \frac{4\pi a\rho}{k^2+8\pi a\rho}$*, the operator* (5.5.2) *acts on* $\mathbb{F}_{\mathrm{ab}}$ *in precisely the same way as the operator inside curly brackets in equation* (5.3.6) *acts on the Fock subspace formed by tensor product states with momentum* $(k,-k)$*.*

### 5.3.2 Constructing eigenstates

The formal eigenstates of $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ are now described, where $\alpha = \alpha_c$, the critical parameter which cancels terms proportional to $a^* b^*$ in the transformed Hamiltonian. The choice of the critical parameter allows us to derive a particularly simple formula for the

eigenstates. First we explain the setup. By *formal*, we mean that the formula given in this section (equation (5.3.13)) does not specify whether the states have finite norm in the space $\mathbb{F}_{\text{ab}}$. We nonetheless write the general formula for all eigenstates before discussing the issue of normalizability. This is an abuse of notation, but neatly encompasses all of the cases involved in the spectral analysis of the family of operators $\mathscr{H}_{\text{ab}}^{(\alpha_c)}(y)$ for $0 \leq y \leq 1/2$.

The structure of the Hamiltonian $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ for the critical value $\alpha_c$ is important for this construction. Since this Hamiltonian contains no term proportional to the operator $a^*b^*$, the effect of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ on any $\Psi_n \in \mathbb{F}_n$ for $1 \leq n < \infty$ is to create a linear combination:

$$\mathscr{H}_{\text{ab}}^{(\alpha_c)}\Psi_n = \tilde{\Psi}_n + \tilde{\Psi}_{n-2},$$

where $\tilde{\Psi}_n \in \mathbb{F}_n$ and $\tilde{\Psi}_{n-2} \in \mathbb{F}_{n-2}$. This is analogous to the action of an upper-triangular matrix in finite dimensions, which preserves subspaces of the underlying linear space $\mathbb{X}$ spanned by unit vectors $\{e_1, e_2, \ldots, e_n\}$, for $n \leq \dim(\mathbb{X})$. This observation motivates finding a solution to the eigenvalue problem

$$\mathscr{H}_{\text{ab}}^{(\alpha_c)}|\Psi_E\rangle = E|\Psi_E\rangle,$$

via a difference scheme for the coefficients of $|\Psi_E\rangle$ when expanded in the momentum basis. For the critical value $\alpha_c$, the iteration will be a backward scheme, which can be solved exactly to give a formula for the coefficients.

The specifics of this scheme are given in Appendix A.1; we write the conclusion for general $\alpha \in [0, \alpha_c]$ for convenience in equation (5.3.10). We work in the occupation number basis of $\mathbb{F}_{\text{ab}}$; this basis is represented by states $|m_a, m_b\rangle \in \mathbb{F}_{\text{ab}}$, for $m_a, m_b \in \mathbb{N}$, which

are simultaneous eigenvectors of the operators $a^*a$ and $b^*b$, satisfying the equations

$$(a^*a)|m_a,m_b\rangle = m_a|m_a,m_b\rangle, \quad (b^*b)|m_a,m_b\rangle = m_b|m_a,m_b\rangle. \tag{5.3.9}$$

In the Appendix, we explain how eigenstates $|\Psi_E\rangle$ satisfying $\mathscr{H}_{\text{ab}}^{(\alpha)}|\Psi_E\rangle = E|\Psi_E\rangle$ (where $\alpha \in [0,\alpha_c]$), with $E \in \mathbb{C}$ can be reduced to expansions in the occupation number basis which take one of the the two forms:

$$|\Psi_E\rangle = \sum_{s=0}^{\infty} c_s|p+s,s\rangle, \quad \text{or} \quad |\Psi_E\rangle = \sum_{s=0}^{\infty} c_s|s,p+s\rangle \quad \text{for} \quad p \in \mathbb{N}.$$

From either of these expressions, we arrive at the difference scheme for the coefficients $\{c_s\}_{s=0}^{\infty}$ in the expansion of $|\Psi_E\rangle$:

$$\left(\frac{p}{2}+s\right)c_s + y_1(\alpha)c_{s+1}\sqrt{(p+s+1)(s+1)} + y_2(\alpha)c_{s-1}\sqrt{(p+s)s} = Ec_s. \tag{5.3.10}$$

Solving this scheme for $\alpha = \alpha_c$ (see Appendix) shows that the states are uniquely described by two parameters $p \in \mathbb{N}$ and $\Theta \in \mathbb{C}$; we call the corresponding state $|\Psi_{p,\Theta}\rangle \in \mathbb{F}_{\text{ab}}$. The index $p$ describes the fact that $|\Psi_{p,\Theta}\rangle$ is an element of the linear subspace of states $|\Psi\rangle \in \mathbb{F}_{\text{ab}}$ such that $(a^*a - b^*b)|\Psi\rangle = p|\Psi\rangle$ holds, i.e., $|\Psi_{p,\Theta}\rangle$ corresponds to a state with fixed total momentum if we assosciate the operator $a$ with $a_k$ and the operator $b$ with $a_{-k}$ for some $k \in \mathbb{Z}_L^+$. In the occupation number basis, $|\Psi_{p,\Theta}\rangle$ belongs to the closed linear span

$$|\Psi_{p,\Theta}\rangle \in \text{span}\big\{|p+s,s\rangle, s \in \mathbb{N}\big\}.$$

For every $p \in \mathbb{N}$, it is also possible to consider solutions which satisfy $(b^*b - a^*a)|\Psi\rangle = p|\Psi\rangle$, and construct eigenstates in the span of vectors $|s,s+p\rangle$. Thus every state $|\Psi_{p,\Theta}\rangle$ will be associated with a degenerate state denoted $|\Psi_{p,\Theta}^{(-)}\rangle$. Indeed, the only difference

between $|\Psi_{p,\Theta}\rangle$ and $|\Psi^{(-)}_{p,\Theta}\rangle$ will be whether the expansion is formed from states $|s+p,s\rangle$ versus $|s,p+s\rangle$. We therefore write formulas explicitly for the first kind of eigenstate, implying that equivalent formulas can be derived for $|\Psi^{(-)}_{p,\Theta}\rangle$ by the appropriate substitution. The state $|\Psi_{p,\Theta}\rangle$ satisfies the formal eigenvalue problem

$$\mathscr{H}^{(\alpha_c)}_{\text{ab}}|\Psi_{p,\Theta}\rangle = \big(\frac{p}{2}+\Theta\big)|\Psi_{p,\Theta}\rangle. \tag{5.3.11}$$

The complex value $\Theta$ enters into the expansion for the state $|\Psi_{p,\Theta}\rangle$ via the generalized binomial coefficients $\binom{\Theta}{s}$ for $s = 0,1,2,\ldots$. We now give the precise formula for the (unnormalized) states $|\Psi_{p,\Theta}\rangle$ which result from solving the iteration scheme (5.3.10) for the critial parameter $\alpha = \alpha_c$ (see the Appendix for a complete derivation):

**Proposition 1.** *Let $p \in \mathbb{N}$ and $\Theta \in \mathbb{C}$, and define $\tilde{y}$ by*

$$\tilde{y} := \frac{y}{\sqrt{1-4y^2}}, \quad \text{for} \quad 0 < y < 1/2.$$

*In the occupation number basis for the $a,b$ operators, define the formal expansion*

$$|\Psi_{p,\Theta}\rangle := \sum_{s=0}^{\infty} (\tilde{y})^{-s} \binom{\Theta}{s} \left( \binom{p+s}{s} \right)^{-1/2} |p+s,s\rangle. \tag{5.3.12}$$

*(If $\Theta \in \mathbb{C}\setminus\mathbb{N}$, the binomial coefficient in formula* (5.3.12) *is understood in the generalized sense; see, for example [1]). The state $|\Psi_{p,\Theta}\rangle$ satisfies the eigenvalue problem* (5.3.11) *with energy $E = \frac{p}{2}+\Theta$. A second collection of states, denoted $|\Psi^{(-)}_{p,\Theta}\rangle$, are constructed in an identical way, replacing $|p+s,s\rangle$ by $|s,p+s\rangle$ in* (5.3.12).

*A special case occurs when $\Theta = N \in \mathbb{N}$. The resulting states are then finite linear combinations, and formula* (5.3.12) *is replaced by*

$$|\Psi_{p,N}\rangle := \sum_{s=0}^{N} (\tilde{y})^{-s} \binom{N}{s} \left( \binom{p+s}{s} \right)^{-1/2} |p+s,s\rangle. \tag{5.3.13}$$

### 5.3.3 Remarks

The derivation of formula (5.3.12) is elaborated in the appendix, and follows from a direct expansion in the occupation number basis. A remark on notation is in order: since we will carry out the analysis for the model Hamiltonian in $\mathbb{F}_{\text{ab}}$, we will use $N$ from now on to refer to the integer quantum number for the states $|\Psi_{p,n}\rangle$, at risk of confusing it with the total number of particles for the Hamiltonian $\mathscr{H}_{\text{LHY}}$ written in the momentum operators. Some key points are now emphasized:

1. All eigenstates of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ (as well as $\mathscr{H}_{\text{ab}}$) must be superpositions of states with fixed momentum $p$, either given by $|p+s,s\rangle$, or $|s,p+s\rangle$ for $s \in \mathbb{N}$. This is because the operator (Casimir's operator [52])

$$\mathscr{C} := \frac{1}{4} - \frac{1}{4}(a^*a - b^*b)^2 \tag{5.3.14}$$

commutes with $a^*b^*$, $ab$, and $\frac{1}{2}(a^*a + b^*b + 1)$. Casimir's operator is constant on each of the subspaces $\text{span}\{|p+s,s\rangle|\ s \in \mathbb{N}\} \subset \mathbb{F}_{\text{ab}}$ for $p \in \mathbb{N}$.

2. Definition 1 suggests that every complex number $E \in \mathbb{C}$ is an eigenvalue of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$. This is sometimes, but not always, the case — the subject of the following sections will be to describe constraints on the states $|\Psi_{p,\Theta}\rangle$ (i.e., constraints on $p, \Theta$) for all values of $y \in [0,\infty)$ so that the spectrum $\{\frac{p}{2} + \Theta\}$ corresponds (under scaling) to the spectrum of the operator $\mathscr{H}_{\text{ab}}$ for certain 'allowed' values of $p, \Theta$ under these constraints.

3. In particular, for $\tilde{y} < 1$, the only normalizable states $|\Psi_{p,\Theta}\rangle$ will be $|\Psi_{p,N}\rangle$ for $N \in \mathbb{N}$, while for $1 \leq \tilde{y}$, the states $|\Psi_{p,\Theta}\rangle$ are normalizable for all $\Theta \in \mathbb{C}$. Thus, additional

constraints on the states $|\Psi_{p,\Theta}\rangle$ will be necessary when $\tilde{y} \geq 1$, in order to connect them to the eigenvalue problem for $\mathscr{H}_{\mathrm{ab}}$.

4. When $\Theta = N \in \mathbb{N}$, the energy of state $|\Psi_{p,N}\rangle$ is $E = N + \frac{p}{2}$. The states $|\Psi_{p,N}\rangle$ have the same energies as the tensor product eigenstates of the Hamiltonian $\frac{1}{2}(a^*a + b^*b)$, which is the limit of the operator $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ as $y \to 0$.

The remainder of this work is devoted to analyzing the spectrum of $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ (and more generally $\mathscr{H}_{\mathrm{ab}}^{(\alpha)}$ for $\alpha \in [0, \alpha_c]$) in the two regimes $\tilde{y} < 1$ and $1 \leq \tilde{y}$. We undertake this in order to answer the physically pertinent questions: **(i)** which of the states $|\Psi_{p,\Theta}\rangle$ defined in Proposition 1 determine eigenstates $|\Psi_E\rangle$ of $\mathscr{H}_{\mathrm{ab}}$ by means of the transform

$$|\Psi_E\rangle = \exp(-\alpha_c a^* b^*)|\Psi_{p,\Theta}\rangle \ ? \tag{5.3.15}$$

Of course, since we can already determine the spectrum $\sigma_{\mathrm{p}}(\mathscr{H}_{\mathrm{ab}})$ by direct means, this question may seem trivial. The perspective we take in developing the method here is that we may start from the transformed Hamiltonian $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$, and derive all relevant quantities for $\mathscr{H}_{\mathrm{ab}}$, 'forgetting' the direct methods which exist for the Hermitian problem.

**(ii)** If the point spectrum of $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ is the entire complex plane (which we see shortly to be the case for $\alpha = \alpha_c$ and $\tilde{y} \geq 1$ in Proposition 2) is there an easy way to distinguish among $|\Psi_{p,\Theta}\rangle$ those states which correspond to members of the spectrum of $\mathscr{H}_{\mathrm{ab}}$? **(iii)** Finally, can all of the eigenstates of $\mathscr{H}_{\mathrm{ab}}$ be identified with unique eigenstates of $\mathscr{H}_{\mathrm{ab}}$?

As stated, we handle the cases $\tilde{y} < 1$ and $\tilde{y} \geq 1$ separately. The three questions **(i)** – **(iii)** are answered definitively for $\tilde{y} < 1$ in the next theorem, and provide a glimpse of the difficulties we will have to address in the case $\tilde{y} \geq 1$. When $\tilde{y} < 1$, the result of Proposition 2 says that only the states $\{\Psi_{p,N}\}_{p,N\in\mathbb{N}}$ will be normalizable in $\mathbb{F}_{\mathrm{ab}}$ and

in this sense the eigenvalue problem for $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ is a regular perturbation of the problem for $\frac{1}{2}(a^*a+b^*b)$. Sections (5.4.1) and (5.5) are devoted to the case $\tilde{y} \geq 1$. We make the disclaimer that while this condition on $\tilde{y}$ changes the analysis for the transformed operator, the spectral problem for $\mathscr{H}_{\mathrm{ab}}$ remains the same. In this sense, the fact that the different cases $\tilde{y} < 1$ and $\tilde{y} \geq 1$ must be handled differently is solely a mathematical artifact of using the non-Hermitian pair-excitation transform.

### 5.3.4 Discrete spectrum in the Case $0 < \tilde{y} < 1$:

When $\tilde{y} < 1$, the eigenstates of $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ will be $|\Psi_{p,N}\rangle$ of formula (1), where $N \in \mathbb{N}$. Energies of these states are equal to the energies of tensor products $|p+N,N\rangle$ as eigenstates of the operator $\frac{1}{2}(a^*a+b^*b)$. The condition $0 < \tilde{y} < 1$ in $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ translates to the condition $|k|^2 > 4\pi a\rho(\sqrt{5}-2) > 0$ in the $k-$momentum component of $\mathscr{H}_{\mathrm{LHY}}$. Thus, this case represents an infinite collection of momenta in the Lee-Huang-Yang Hamiltonian.

**Proposition 2.** *Suppose* $0 < \tilde{y} < 1$. *Then the point spectrum of* $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ *is*

$$\sigma_{\mathrm{p}}\big(\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}\big) = \Big\{\frac{p}{2}+N, \text{ for } p,N \in \mathbb{N}\Big\}. \tag{5.3.16}$$

*The eigenstates are given by* $|\Psi_{p,N}\rangle$, $|\Psi_{p,N}^{(-)}\rangle$ *of Definition* (1), *for* $N \in \mathbb{N}$, *and exhibit the same degeneracy as the momentum states* $\big\{|N,N+p\rangle \text{ or } |N+p,N\rangle\big\}$ *as eigenstates of the operator* $\frac{1}{2}(a^*a+b^*b)$ *for* $p,N \in \mathbb{N}$.

*Proof.* It is clear that the states $|\Psi_{p,N}\rangle$ with $N \in \mathbb{N}$ have finite norm in $\mathbb{F}_{\mathrm{ab}}$ as finite superpositions in the particle number basis.

Now suppose $\Theta \in \mathbb{C} \setminus \mathbb{N}$, so the coefficients

$$c_s := (\tilde{y})^{-s} \binom{\Theta}{s} \sqrt{\binom{p+s}{s}}^{-1},$$

are nonzero for all $s \geq 0$. We proceed to show that $\{c_s\}_{s=0}^{\infty}$ cannot be square summable.

Indeed, using the Gamma function [44] to describe the generalized binomial coefficient, we have

$$|c_s|^2 = \tilde{y}^{-2s} \frac{\Gamma(1+p)}{\Gamma(-\Theta)^2} \cdot \frac{\Gamma(s-\Theta)^2}{\Gamma(s+p+1)\Gamma(s+1)} |c_0|^2.$$

Let us write *Stirling's approximation* as follows [44]

$$\log(\Gamma(z)) \approx \big(z - \frac{1}{2}\big) \log(z) - z + \frac{1}{2} \log(2\pi), \quad \text{as} \quad |z| \to \infty, \quad \text{Re}(z) > 0. \tag{5.3.17}$$

Here, the symbol "$\approx$" denotes asymptotic equivalence. Thus

$$\log\big(\Gamma(s-\Theta)\big) \approx s\log(s) - (\Theta + 1/2)\log(s) - s + C, \quad \text{as} \quad s \to \infty, \tag{5.3.18}$$

where $C$ is a constant whose specific value does not matter. Similarly

$$\log(\Gamma(s+p+1)) \approx s\log(s) + (p+1/2)\log(s) - s, \quad \text{as} \quad s \to \infty. \tag{5.3.19}$$

Putting the two lines above together gives

$$\frac{\Gamma(s-\Theta)}{\Gamma(s+p+1)\Gamma(s+1)} \approx \frac{e^{2\log s} e^{-2(\Theta+1/2)\log(s)} e^{-2s}}{e^{s\log s} e^{(p+1/2)\log s} e^{-s} e^{s\ln s} e^{1/2\log s} e^{-s}} = \frac{1}{s^{2\Theta+2+p}}, \quad \text{as} \quad s \to \infty. \tag{5.3.20}$$

Therefore

$$|c_{p+s,s}|^2 \approx K \frac{\tilde{y}^{-2s}}{s^{2\Theta+2+p}} |c_{p,0}|^2, \quad \text{for} \quad K = \frac{\Gamma(1+p)}{\Gamma(-\Theta)^2} \quad \text{as} \quad s \to \infty. \tag{5.3.21}$$

If $|\tilde{y}| < 1$, then it follows that $\sum_{s=0}^{\infty} |c_s|^2$ cannot be finite if $\Theta \in \mathbb{C} \setminus \mathbb{N}$. This concludes the proof. $\square$

When $\tilde{y} \geq 1$, the estimates in the above proof show that the states $|\Psi_{p,\Theta}\rangle$ are normalizable for all values $\Theta \in \mathbb{C}$. Answering the questions **(i) – (iii)** of Section 5.3.3 becomes more difficult in this case. This is the subject of the next section.

### 5.3.5 A Geometric Picture of Degeneracies

We conclude this section with a geometric description of the degenerate eigenspaces of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ in $\mathbb{F}_{ab}$ when $\tilde{y} < 1$. The Fock space $\mathbb{F}_{ab}$ is the orthogonal direct sum of the following subspaces:

$$\mathbb{F}_{ab} = \bigoplus_{p=-\infty}^{\infty} \mathbb{F}^{(p)}, \quad \mathbb{F}^{(+p)} := \text{span}\{|p+s,s\rangle : s \in \mathbb{N}\}, \quad \mathbb{F}^{(-p)} := \text{span}\{|s,p+s\rangle : s \in \mathbb{N}\}.$$

On the two-dimensional lattice describing occupation numbers $(n_a, n_b)$ of the states $|n_a, n_b\rangle$, the subspace $\mathbb{F}^{(\pm p)}$ describes an infinite line segment terminating at a point $(0,p)$ (for '+' sign) or $(p,0)$ (for '$-$' sign). The states $|\Psi_{p,N}\rangle$ are elements of $\mathbb{F}^{(+p)}$, while the states $|\Psi_{p,N}^{(-)}\rangle$ are elements of $\mathbb{F}^{(-p)}$.

It was established that the state $|\Psi_{p,N}\rangle$ has energy $E = \frac{p}{2} + N$, identical to the energy of the tensor product $|p+N,N\rangle$ as an eigenstate of $\frac{1}{2}(a^*a + b^*b)$, and that within the subspace $\mathbb{F}^{(p)}$ it is the unique state with this energy. Accordingly, on $\mathbb{N} \times \mathbb{N}$, the line segment $\{(p,N) \big| \frac{p}{2} + N = E\}$ connecting endpoints $(p+N,N)$ and $(N,p+N)$ intersects all ordered pairs corresponding to degenerate states $|\Psi_{p,N}\rangle$ with energy $E$ (see Figure 5.1).

Finally, consider the limit $\tilde{y} \to 0$ in the state $|\Psi_{p,N}\rangle$ with energy $E = \frac{p}{2} + N$ given by equation (5.3.13) (the limit $\tilde{y} \to 0$ amounts to $|k| \to \infty$ in the momentum space, where the model $\mathscr{H}_{\text{LHY}}$ is no longer expected to hold). In this limit, the state can no longer be

normalized; although the finite sum corresponding to the state reduces to a single term

$$|\Psi_{p,N}\rangle \to |N+s,s\rangle, \quad \text{as } \tilde{y} \to 0.$$

This is expected by the fact that $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ approaches $\frac{1}{2}(a^*a + b^*b)$ in this limit.

## 5.4 Bogoliubov spectrum for $\tilde{y} \geq 1$

In the previous section, we showed that when $\tilde{y} < 1$ and $\alpha = \alpha_c$, the eigenstates of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ are given by $|\Psi_{p,N}\rangle$ for $N \in \mathbb{N}$. In this section, we address the spectral theory for the non-Hermitian transformed Hamiltonian $\mathscr{H}_{\text{ab}}^{(\alpha)}$ in the case where $\tilde{y} \geq 1$ and $\alpha \in [0, \alpha_c]$. We saw, in the proof of Proposition 2, that when $\tilde{y} \geq 1$ and $\alpha = \alpha_c$, the states $\{|\Psi_{p,\Theta}\rangle\}$ are normalizable in the Fock space $\mathbb{F}_{\text{ab}}$ for all $p \in \mathbb{Z}$ and all $\Theta \in \mathbb{C}$. Thus, we wish to answer which states in $\sigma\big(\mathscr{H}_{\text{ab}}^{(\alpha)}\big)$ map to eigenstates of $\sigma\big(\mathscr{H}_{\text{ab}}\big)$ by taking the transform $|\Psi_{p,\Theta}\rangle \mapsto \exp(-\alpha a^* b^*)|\Psi_{p,\Theta}\rangle$ — without using our prior knowledge of $\sigma(\mathscr{H}_{\text{ab}})$. Momentarily returning to the momentum space, the pair-excitation formalism means that we analyze the non-Hermitian eigenvalue problem for state $|\Psi(k)\rangle$:

$$\big(\exp(\mathscr{P})\mathscr{H}_{\text{LHY}}\exp(-\mathscr{P})\big)|\Psi(k)\rangle = E|\Psi(k)\rangle,$$

in order to discover information about the the Hermitian eigenvalue problem for state $|\tilde{\Psi}(k)\rangle$:

$$\mathscr{H}_{\text{LHY}}|\tilde{\Psi}(k)\rangle = E|\tilde{\Psi}(k)\rangle.$$

Since $\mathscr{H}_{\text{LHY}}$ contains contributions from all $k \in \mathbb{Z}_L^3$, recalling the formula

$$\tilde{y}(k) := \frac{y(k)}{\sqrt{1-4y(k)^2}}, \quad \text{for} \quad y(k) = \frac{4\pi a\rho}{k^2 + 8\pi a\rho},$$

we see that $\tilde{y}(k)$ can take on all values in $(0,\infty)$ for $k \in \mathbb{Z}_L^3$. The method that we develop will have a direct consequence for identifying eigenstates in the spectrum $\sigma\big(\exp(\mathscr{P})\mathscr{H}_{\mathrm{LHY}}\exp(-\mathscr{P})\big)$ with 'physical' states in $\sigma(\mathscr{H}_{\mathrm{LHY}})$.

This difference in the spectra is a consequence of using an unbounded, non-unitary operator to transform $\mathscr{H}_{\mathrm{LHY}}$. We emphasize that the problem which we address here may seem artificial since we already know the spectrum of $\mathscr{H}_{\mathrm{LHY}}$ by other means (for example, by Bogoliubov rotation). The emphasis in the analysis that follows is that we can discern all the information for states of $\mathscr{H}_{\mathrm{LHY}}$ by starting from the *transformed* quadratic Hamiltonian.

The method that we introduce for identifying the Bogoliubov spectrum as a subset of $\sigma\big(\mathscr{H}_{\mathrm{ab}}^{(\alpha)}\big)$ will be provided by analysis of the formal generating function $G(z;|\Psi_E\rangle)$ for eigenstate $|\Psi_E\rangle$ of $\mathscr{H}_{\mathrm{ab}}^{(\alpha)}$. The generating function $G(z;|\Psi_E\rangle)$ can be seen as a transformation which takes the sequence of coefficients for the expansion of $|\Psi_E\rangle$ in the occupation number basis to a formal Taylor series. In the opposite direction, given the generating function $G(z;|\Psi_E\rangle)$ for state $|\Psi_E\rangle$, we can determine the coefficients for $|\Psi_E\rangle$ in the occupation number basis from the terms in the Taylor expansion of $G(z;|\Psi_E\rangle)$. The most important fact about generating functions, which we will exploit, is that the analyticity in the unit disk of the generating function $G(z;|\Psi_E\rangle)$ is connected to the normalizability of $|\Psi_E\rangle$ in the Fock space $\mathbb{F}_{\mathrm{ab}}$.

We proceed by considering the operator family $\mathscr{H}_{\mathrm{ab}}^{(\alpha)}$ for $0 < \alpha \leq \alpha_c$. When $\alpha = \alpha_c$, the (formal) statement:

$$\mathscr{H}_{\mathrm{ab}}\big(e^{-\alpha_c a^* b^*}|\Psi_{p,\Theta}\rangle\big) = \Big((1+2\alpha_c y)(\frac{p}{2}+\Theta)+\alpha_c y\Big)(e^{-\alpha_c a^* b^*}|\Psi_{p,\Theta}\rangle), \quad p\in\mathbb{N}, \Theta\in\mathbb{C},$$

implies that states in the set $\{e^{-\alpha_c a^* b^*}|\Psi_{p,\Theta}\rangle\}_{p,\Theta}$ are also eigenstates of $\mathscr{H}_{\mathrm{ab}}$, provided that $|\Psi_{p,\Theta}\rangle \in \mathrm{dom}\big(e^{-\alpha_c a^* b^*}\big)$. More specifically, given $\tilde{y}\geq 1$ we will show that the only states $|\Psi_{p,\Theta}\rangle \in \mathrm{dom}\big(e^{-\alpha_c a^* b^*}\big)$ occur for $\Theta\in\mathbb{N}$, and that the collection $\{|\Psi_{p,N}\rangle\}_{p,N\in\mathbb{N}}$ constitutes a basis of $\mathbb{F}_{\mathrm{ab}}$. We conduct the first of these two tasks in the present section.

### 5.4.1 Method of generating functions

Inspired by Lee, Huang, and Yang [37], we define the generating function $G(z;|\Psi_E\rangle): \mathbb{C}\to\mathbb{C}$ for eigenstate $|\Psi_E\rangle$ of $\mathscr{H}_{\mathrm{ab}}^{(\alpha)}$, where $0<\alpha\leq\alpha_c$, and demonstrate how the singularities of $G(z;|\Psi_E\rangle)$ in the complex plane furnish a criterion for constructing eigenstates of the Hamiltonian $\mathscr{H}_{\mathrm{ab}}=\mathscr{H}_{\mathrm{ab}}^{(\alpha=0)}$. More specifically, in Proposition 5, we show that the action of the exponential map

$$|\Psi_E\rangle \mapsto e^{-\alpha a^* b^*}|\Psi_E\rangle$$

induces the following transformation of the generating function:

$$G(z;|\Psi_E\rangle) \mapsto G(z;e^{-\alpha a^* b^*}|\Psi_E\rangle) = \Big(\frac{1}{1+\alpha z}\Big)G\Big(\frac{z}{1+\alpha z};|\Psi_E\rangle\Big).$$

We exploit this fact when $\tilde{y}\geq 1$; the function

$$\frac{1}{1+\alpha z}G(\frac{z}{1+\alpha z};|\Psi_E\rangle)$$

cannot have a singularity in the unit disk if $|\Psi_E\rangle\in\mathrm{dom}(e^{-\alpha a^* b^*})$, which will only be possible for discrete energies $E$ corresponding to the Bogoliubov spectrum.

When $0 \leq \alpha \leq \alpha_c(y)$, both of the constants $y_1(\alpha)$ and $y_2(\alpha)$ in the transformed Hamiltonian $\mathscr{H}_{\text{ab}}^{(\alpha)}$ will be nonzero, and are given by

$$y_1(\alpha) := \frac{y}{1-2\alpha y}, \quad \text{and} \quad y_2(\alpha) := \frac{y-\alpha+\alpha^2 y}{1-2\alpha y}.$$

We consider the range of values $0 \leq y_1(\alpha) < \infty$, so that eigenstates of $\mathscr{H}_{\text{ab}}^{(\alpha)}$ are no longer finite superpositions in the occupation number basis. The operator $(a^*a - b^*b)$ still commutes with $\mathscr{H}_{\text{ab}}^{(\alpha)}$, so we know that eigenstates of $\mathscr{H}_{\text{ab}}^{(\alpha)}$ will remain superpositions of the states $|s+p,s\rangle$ or $|s,s+p\rangle$ for fixed $p \in \mathbb{N}$.

**Definition 7.** *Let $|\Psi\rangle \in \mathbb{F}_{\text{ab}}$ have expansion in the occupation number basis given by*

$$|\Psi\rangle = \sum_{s=0}^{\infty} c_s |p+s,s\rangle, \quad \text{for} \quad \{c_s\}_{s=0}^{\infty} \in \ell^2(\mathbb{C}),$$

*where $\ell^2(\mathbb{C})$ denotes the space of square-summable complex sequences, and define the rescaled coefficients*

$$C_s := \sqrt{\frac{s!}{(p+s)!}} c_s, \tag{5.4.1}$$

*(this will make the algebra with generating functions easier.) Alternatively $|\Psi\rangle$ can have an exapnsion in the states $|s,s+p\rangle$.*

*The generating function which corresponds to state $|\Psi\rangle$ is a formal power series in complex variable $z$ defined by*

$$G(z;|\Psi\rangle) := \sum_{s=0}^{\infty} C_s z^s.$$

It is clear that for fixed $p \in \mathbb{N}$, the sequence $\{C_s\}_{s=0}^{\infty}$ is square summable if and only if $\{c_s\}_{s=0}^{\infty}$ is as well. Since,

$$|\sum_s C_s z^s|^2 \leq \sum_s |C_s|^2 \sum_s |z|^{2s},$$

the condition that $\||\Psi\rangle\|_{\mathbb{F}_{\text{ab}}} = 1$ means that $G(z;|\Psi\rangle)$ will be analytic in the unit disk, $\{z \in \mathbb{C} : |z| < 1\}$.

The following proposition follows by standard arguments of analytic continuation in the complex plane. The proof is omitted.

**Proposition 3.** *Let $|\Psi_E\rangle \in \mathbb{F}_{\text{ab}}$ be an eigenstate of $\mathscr{H}_{\text{ab}}^{(\alpha)}$ for $0 < \alpha \leq \alpha_c \leq 1$, with energy $E \in \mathbb{C}$, e.g.,*

$$\mathscr{H}_{\text{ab}}^{(\alpha)}|\Psi_E\rangle = E|\Psi_E\rangle,$$

*and let $G(z;|\Psi_E\rangle)$ be the generating function for $|\Psi_E\rangle$ according to definition* (7)*. Then*

1. *$G(z;|\Psi_E\rangle)$ satisfies the first-order ordinary differential equation (coming from the difference scheme* (5.3.10)*):*

$$\begin{aligned} &z\Big\{y_2(\alpha)z^2 + z + y_1(\alpha)\Big\}\big(G(z;|\Psi_E\rangle)\big)' \\ &+\Big\{y_2(\alpha)z^2 + \Big(\frac{p}{2} - E\Big)z + y_1(\alpha)p\Big\}G(z;|\Psi_E\rangle) = C_0 y_1(\alpha)p, \end{aligned} \tag{5.4.2}$$

   *where $C_0$ is the zeroth rescaled coefficient in the definition of $G(z;|\Psi_E\rangle)$.*

2. *The general solution to* (5.4.2) *is given by*

$$G(z;|\Psi_E\rangle) = G_{hom}(z;|\Psi_E\rangle) + I(z;|\Psi_E\rangle), \tag{5.4.3}$$

   *where the solution to the homogeneous equation reads*

$$G_{hom}(z;|\Psi_E\rangle) = Kz^{-p}(z - z_+(\alpha))^B(z - z_-(\alpha))^{(p-1-B)}, \tag{5.4.4}$$

   *for $K, B \in \mathbb{C}$, and the constants $z_\pm(\alpha)$ are the nonzero roots of the polynomial*

$$Q(z) := z\big(y_2(\alpha)z^2 + z + y_1(\alpha)\big).$$

*In particular, we obtain*

$$z_{\pm}(\alpha) := \frac{-1 \pm \sqrt{1-4y_1(\alpha)y_2(\alpha)}}{2y_2(\alpha)}, \quad \text{assuming} \quad y_2(\alpha) \neq 0. \tag{5.4.5}$$

*The term $I(z;|\Psi_E\rangle)$ is the particular solution to* (5.4.2)*, and is given by*

$$I(z;|\Psi_E\rangle) := \frac{C_0 y_1(\alpha) p}{y_2(\alpha)} (z-z_+)^B (z-z_-)^{(p-1-B)} \int_0^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{B-p} du. \tag{5.4.6}$$

*The integral in this expression has an integration path lying within a simply-connected region of analyticity so that it is uniquely specified by the endpoints.*

3. *The constant K is arbitrary, while the constant B is related to the energy $E \in \mathbb{C}$ via*

$$B = \frac{(p/2-E-1)z_+(\alpha) + y_1(\alpha)(p-1)}{z_+(\alpha) + 2y_1(\alpha)}. \tag{5.4.7}$$

4. *For $p > 0$ (which represents the eigen-subspace of $(a^*a - b^*b)$ that we construct the solution $|\Psi_E\rangle$ in), $G_{hom}(z;|\Psi_E\rangle)$ has a pole of order p at $z = 0$, but $I(z;|\Psi_E\rangle)$ does not. It follows that we must set $K = 0$, so that $G(z;|\Psi_E\rangle) = I(z;|\Psi_E\rangle)$. The function $I(z;|\Psi_E\rangle)$ manifests a possible singularity at $z = z_+$ depending on the value of B.*

It is well-known that singularities of solutions to (5.4.2) can occur only at roots of the leading polynomial $Q(z) := z\big(y_2(\alpha)z^2 + z + y_1(\alpha)\big)$, which are given by $z = \{0, z_{\pm}(\alpha)\}$ for

$$z_{\pm}(\alpha) := \frac{-1 \pm \sqrt{1-4y_1(\alpha)y_2(\alpha)}}{2y_2(\alpha)}, \quad \text{assuming} \quad y_2(\alpha) \neq 0. \tag{5.4.8}$$

Let us now state a few properties of $z_{\pm}(\alpha)$ of (5.4.8). Recall that $\alpha_c = \frac{1-\sqrt{1-4y^2}}{2y}$:

- For any $\alpha \in [0, \alpha_c]$, we have $1 - 2\alpha y > 0$.

- For any $\alpha \in [0, \alpha_c]$, the polynomial $P(\alpha) = y - \alpha + \alpha^2 y$ is strictly positive. Hence, both $y_1(\alpha)$, $y_2(\alpha)$ given in Definition 6 are strictly positive for $\alpha \in [0, \alpha_c]$.

- The discriminant, $1 - 4y_1(\alpha)y_2(\alpha)$ of equation (5.4.8) is strictly positive for any $\alpha \in [0, \alpha_c]$. Hence, $z_\pm(\alpha)$ are real for $\alpha$ in the prescribed range.

- $z_+(\alpha)z_-(\alpha) = 1$ with $|z_+(0)| < 1$. Hence, $|z_-(0)| > 1$. In addition, $|z_-(\alpha)| > 1$ for any $\alpha \in \big(0, \alpha_c\big)$, with $z_-(\alpha) \to -\infty$ as $\alpha \uparrow \alpha_c$.

- By contrast, $z_+(\alpha)$ may or may not be inside the unit circle. Indeed, the condition $|z_+(\alpha)| < 1$ implies $y_1(\alpha) + y_2(\alpha) < 1$, which is true for all $\alpha \in [0, \alpha_c]$ only if

$$\tilde{y} = \frac{y}{\sqrt{1 - 4y^2}} < 1.$$

  Otherwise there exists some $\alpha_{max} < \alpha_c$ such that $|z_+(\alpha)| < 1$ for $\alpha < \alpha_{max}$ and $|z_+(\alpha)| \geq 1$ for $\alpha_{max} < \alpha < \alpha_c$. We handle these two cases separately.

### 5.4.2 The Bogoliubov spectrum for $|z_+(\alpha)| < 1$:

Summarizing the problem so far: When $\tilde{y} \geq 1$ and $\alpha = \alpha_c$, we wish to identify a subset of states $|\Psi_{p,\Theta}\rangle$ that correspond to the physical states of $\mathscr{H}_{\text{ab}}$ (after transforming by the exponential operator). More generally, for $\tilde{y} \geq 1$, and $\alpha \in [0, \alpha_c]$, we wish to identify some set of eigenstates $|\Psi_E\rangle$ of $\mathscr{H}_{\text{ab}}^{(\alpha)}$ with eigenstates of $\mathscr{H}_{\text{ab}}$. We have introduced the formal generating function $G(z; |\Psi_E\rangle)$ for the eigenstate $|\Psi_E\rangle$ of the transformed operator $\mathscr{H}_{\text{ab}}^{(\alpha)}$ for this matter. This function satisfies an ordinary differential equation in the complex variable $z$ (equation (5.4.2)), which is a consequence of the difference scheme

(5.3.10) for the coefficients of $|\Psi_E\rangle$ in the occupation number basis. The function $G$ has singular points $z_\pm(\alpha)$, which determine possible singularities in the unit disk.

We continue the argument as follows: since $G(z;|\Psi_E\rangle)$ must be analytic in the unit disk if $|\Psi_E\rangle$ is to be normalizable, we must restrict the real parameter $B$ in the solution for $G(z;|\Psi_E\rangle)$, which translates to restricting the possible values of the energy $E$ (equation (5.4.7)).

Consider first the case $|z_+(\alpha)|<1$. We remind the reader that for $\mathscr{H}_{\rm ab}^{(\alpha)}|\Psi_E\rangle = E|\Psi_E\rangle$, and for $\tilde{y}\geq 1$, it is possible that $z_+(\alpha)$ lies inside or outside the unit disk depending on whether $\alpha<\alpha_{max}$ or $\alpha_{max}<\alpha<\alpha_c$. As an example, when $\alpha\leq\alpha_c$ and $p=0$,

$$G(z;|\Psi_E\rangle) = K\big(z-z_+(\alpha)\big)^B\big(z-z_-(\alpha)\big)^{-1-B}.$$

Since $z_+(\alpha)$ lies inside the unit disk by assumption, $G(z;|\Psi_E\rangle)$ is analytic in this region *if and only if* $B\in\mathbb{N}$. It follows that the allowed energies $E$ must be discrete. This is extended to $p\neq 0$ in the following proposition.

**Proposition 4.** *For $\alpha$ such that $|z_+(\alpha)|<1$ (which implies $|z_-(\alpha)|>1$), and $p>0$, the function $G(z;|\Psi_E\rangle)$ defined by*

$$G(z;|\Psi_E\rangle) = \frac{C_0 y_1(\alpha) p}{y_2(\alpha)}(z-z_+)^B(z-z_-)^{p-1-B}\int_0^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du \tag{5.4.9}$$

*is analytic if and only if $B\in\mathbb{N}$ and $B\geq p$. This implies that the energies $E\in\sigma_{\rm p}(\mathscr{H}_{\rm ab}^{(\alpha)})$ must be discrete. In this case we have*

$$(1-2\alpha y)\sigma_{\rm p}(\mathscr{H}_{\rm ab}^{(\alpha)}) - \alpha y = \sigma_{\rm p}(\mathscr{H}_{\rm ab}).$$

*Proof.* The proof consists of two parts. First, it must be shown that there is a singularity of $G(z;|\Psi_E\rangle)$ inside the unit disk which is removable under the condition $B \in \mathbb{N}$, $B \geq p$. This pertains to the analyticity of $G$ in $\mathbb{C}$ and is a standard argument, but technical. It is delegated to the Appendix.

For the second part, we show that $(1-2\alpha y)E - \alpha y$ must take values in the Bogoliubov spectrum (5.2.17) for $B = m \in \mathbb{N}$. Suppose first that $p = 0$. Then equation (5.4.7) reads

$$\frac{(E+1)z_+(\alpha) + y_1(\alpha)}{z_+(\alpha) + 2y_1(\alpha)} = -m. \tag{5.4.10}$$

Using equation (5.4.8) for $z_+(\alpha)$ and manipulating yields

$$E = \sqrt{1-4y_1(\alpha)y_2(\alpha)}(m+1) - \frac{2y_1(\alpha)y_2(\alpha)}{1-\sqrt{1-4y_1(\alpha)y_2(\alpha)}}. \tag{5.4.11}$$

Recall the values of $y_1(\alpha) = \frac{y}{1-2\alpha y}$ and $y_2(\alpha) = \frac{y-\alpha+\alpha^2 y}{1-2\alpha y}$. Thus

$$(1-2\alpha y)E - \alpha y = (m+1)\sqrt{1-4y^2} - \alpha y - \frac{2y(y-\alpha+\alpha^2 y)}{1-2\alpha y - \sqrt{1-4y^2}}. \tag{5.4.12}$$

Interestingly, we can show that the quantity

$$Q := \alpha y + \frac{2y(y-\alpha+\alpha^2 y)}{1-2\alpha y - \sqrt{1-4y^2}} \tag{5.4.13}$$

is independent of $\alpha$, which follows by factorizing the numerator. In fact, $Q = \frac{1}{2}\big(1 + \sqrt{1-4y^2}\big)$. Hence, if $|\Psi_E\rangle$ is the eigenstate of $\mathscr{H}_{\text{ab}}^{(\alpha)}$ with energy $E$ and generating function $G(z;|\Psi_E\rangle)$, then $e^{-\alpha a^* b^*}|\Psi_E\rangle$ is an eigenstate of Hamiltonian $\mathscr{H}_{\text{ab}}^{(0)}$ with energy

$$(1-2\alpha y)E - \alpha y = \frac{1}{2}\sqrt{1-4y^2}(2m+1) - \frac{1}{2}. \tag{5.4.14}$$

This is exactly the result of Bogoliubov. The case $p \neq 0$ is similar, so we skip many details. We now solve for $E$ the equation

$$\frac{(p/2-E-1)z_+(\alpha) + y_1(\alpha)(p-1)}{z_+(\alpha) + 2y_1(\alpha)} = m, \tag{5.4.15}$$

which comes from relation (5.4.7), and will give a formula for the energies of the eigenstates $|\Psi_E\rangle$ of $\mathscr{H}_{\text{ab}}^{(\alpha)}$. We get

$$(1-2\alpha y)E-\alpha y=\sqrt{1-4y^2}(m-\frac{p}{2})+\frac{1}{2}\sqrt{1-4y^2}-\frac{1}{2}, \tag{5.4.16}$$

The interpretation of this is that the energies $E$ for $\mathscr{H}_{\text{ab}}^{(\alpha)}$ must give the Bogoliubov spectrum in this case. □

### 5.4.3 Bogoliubov spectrum for $|z_+(\alpha)| \geq 1$:

We now consider the range of parameters $\alpha \in [\alpha_{max}, \alpha_c]$, and $\tilde{y} \geq 1$. Let us review how this comes about, and why it must be treated separately from the case of the previous subsection. For clarity of the argument, consider the case $\tilde{y} \geq 1$ and $\alpha = \alpha_c$ first. Here, the eigenvalue problem

$$\mathscr{H}_{\text{ab}}^{(\alpha_c)}|\Psi_{p,\Theta}\rangle = E|\Psi_{p,\Theta}\rangle,$$

is solved by the difference scheme for $|\Psi_{p,\Theta}\rangle$ and has the exact formula (5.3.12), with $E = p/2+\Theta$. Formula (5.3.12) shows that $|\Psi_{p,\Theta}\rangle$ is normalizable in $\mathbb{F}_{\text{ab}}$ for all $p \in \mathbb{N}$ and $\Theta \in \mathbb{C}$; This poses a problem for if we want to use the transformed system $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ to answer questions about the system $\mathscr{H}_{\text{ab}}$. We also face the additional complication that the generating function $G(z;|\Psi_{p,\Theta}\rangle)$ has no singularity inside the unit disk (in the previous subsection we showed that for $\tilde{y} \geq 1$ there remains an interval $0 \leq \alpha < \alpha_{max}$, for $\alpha_{max} < \alpha_c$, such that the singularity at $z_+(\alpha)$ is inside the unit disk, which we used to restrict the energy $E$ of state $|\Psi_E\rangle$ for $\mathscr{H}_{\text{ab}}^{(\alpha)}$). We therefore require a new method to deal with this possibility.

Translating this problem to the more general case of the eigenvalue equation

$$\mathscr{H}_{\text{ab}}^{(\alpha)}|\Psi_E\rangle = E|\Psi_E\rangle, \quad \alpha_{max} < \alpha \leq \alpha_c,$$

we find similarly, that the function $G(z;|\Psi_E\rangle)$ which solves the differential equation (5.4.2) is analytic in the unit disk for all values $B \in \mathbb{R}$ (see Proposition 3 for the discussion of this parameter).

It is therefore impossible to pose a constraint on $B$ and the energy $E$ directly, as we did before. We will instead show that $|\Psi_E\rangle \notin \text{dom}(e^{-\alpha a^* b^*})$ for these states, which means that they cannot be transformed, via the exponential operator, into states which solve an eigenvalue problem for $\mathscr{H}_{\text{ab}}$. We show this by analyzing the generating function for the state $\exp(-\alpha a^* b^*)|\Psi_E\rangle$ — it contains singularities in the unit disk when $B \notin \mathbb{N}$.

We introduce a new notation that will aid in the proof that $|\Psi_E\rangle \notin \text{dom}(e^{-\alpha a^* b^*})$ for certain values of $B$. Given a sequence $\{a_s\}_{s=0}^{\infty}$, its *ordinary generating function*, denoted $\text{ogf}\{a_s\}(z)$ is a formal power series defined by

$$\text{ogf}\{a_s\}(z) := \sum_{s=0}^{\infty} a_s z^s.$$

Thus, $G(z;|\Psi_E\rangle) = \text{ogf}\{C_s\}$ where $\{C_s\}_{s=0}^{\infty}$ are the rescaled coefficients for the expansion of $|\Psi_E\rangle$ in the occupation number basis (Definition 7).

The *exponential generating function* for the same sequence is defined as

$$\text{egf}\{a_s\}(z) := \sum_{s=0}^{\infty} a_s \frac{z^s}{s!}.$$

The following facts hold for exponential generating functions:

**Lemma 10.** ***(i)*** *The product of exponential generating functions is itself the exponential*

*function given by*

$$\mathrm{egf}\{c_m\}(z)\cdot\mathrm{egf}\{d_m\}(z)=\mathrm{egf}\left\{\sum_{s=0}^{m}c_m d_{m-s}\binom{m}{s}\right\}(z).$$

***(ii)*** *We can convert between ordinary and exponential generating functions by means of the Borel transform, which is defined for an analytic function $f(z)$ by*

$$\mathscr{L}'[f](z):=\int_0^\infty f(zt)e^{-t}dt.$$

*The relevant fact for generating functions is*

$$\mathscr{L}'\big[\mathrm{egf}\{d_m\}\big](z)=\mathrm{ogf}\{d_m\}(z).$$

Proof of these properties are direct and follow by manipulation of Taylor series. For the second part of Lemma 10, note that for $f(z)=\sum_{m=0}^{\infty}f_m z^m$, the action of $\mathscr{L}'$ on $f$ results in the formal multiplication of coefficient $f_m$ by $m!$.

It is important to note that the generating function

$$G\big(z;e^{-\alpha a^*b^*}|\Psi_E\rangle\big),$$

will in principle have a region of analyticity that is different from the region of analyticity of $G(z;|\Psi_E\rangle)$. The next proposition describes this phenomenon precisely.

**Proposition 5.** *Let $0<\alpha\leq\alpha_c\leq 1$ and $|\Psi_E\rangle\in\mathbb{F}_{ab}$ be a solution to the eigenvalue problem*

$$\mathscr{H}_{\mathrm{ab}}^{(\alpha)}|\Psi_E\rangle=E|\Psi_E\rangle.$$

*Additionally, suppose that $|\Psi_E\rangle\in\mathrm{dom}(e^{-\alpha a^*b^*})$. If $G(z;|\Psi_E\rangle)$ is the generating function associated with $|\Psi_E\rangle$ (as per Definition 7), then*

$$G\Big(z;e^{-\alpha a^*b^*}|\Psi_E\rangle\Big)=\frac{1}{1+\alpha z}G\Big(\frac{z}{1+\alpha z};|\Psi_E\rangle\Big).$$

*Proof.* We return to the generating function $G(z;|\Psi_E\rangle) = \mathrm{ogf}\{C_s\}$. Consider first the case $p=0$, so that $|\Psi_E\rangle$ lies in $\mathrm{span}\{|s,s\rangle\}_{s=0}^{\infty}$, and the rescaled coefficients of Definition 7 are the coefficients of $|\Psi_E\rangle$ in the occupation number basis, $C_s = c_s$. Then by the assumption that $|\Psi_E\rangle \in \mathrm{dom}(e^{-\alpha a^* b^*})$, we compute

$$e^{-\alpha a^* b^*}|\Psi_E\rangle = \sum_{m=0}^{\infty}\left(\sum_{s=0}^{m} c_s \alpha^{m-s}\binom{m}{s}\right)|m,m\rangle,$$

and so

$$G\big(z; e^{-\alpha a^* b^*}|\Psi_E\rangle\big) = \mathrm{ogf}\left\{\sum_{s=0}^{m} c_s(-\alpha)^{m-s}\binom{m}{s}\right\}(z). \quad (5.4.17)$$

The first part of Lemma 10 shows that

$$\mathrm{egf}\left\{\sum_{s=0}^{m} c_s(-\alpha)^{m-s}\binom{m}{s}\right\}(z) = \mathrm{egf}\{c_m\}(z)\cdot\mathrm{egf}\{(-\alpha)^m\}(z) = \mathrm{egf}\{c_m\}(z)\cdot e^{-\alpha z}.$$

while the second part of Lemma 10 shows,

$$\begin{aligned}
G\big(z; e^{-\alpha a^* b^*}|\Psi_E\rangle\big) &= \mathrm{ogf}\left\{\sum_{s=0}^{m} c_s(-\alpha)^{m-s}\binom{m}{s}\right\} = \mathscr{L}'[e^{-\alpha z}\mathrm{egf}\{c_m\}](z)\\
&= \int_{t=0}^{\infty}\mathrm{egf}\{c_m\}(tz)e^{-t(\alpha z+1)}dt\\
&= \frac{1}{1+\alpha z}\int_{\eta=0}^{\infty}\mathrm{egf}\{c_m\}\left(\frac{z\eta}{\alpha z+1}\right)e^{-\eta}d\eta \quad (\text{for } \eta := t(\alpha z+1))\\
&= \frac{1}{1+\alpha z}\mathscr{L}'[\mathrm{egf}\{c_m\}]\left(\frac{z}{1+\alpha z}\right)\\
&= \frac{1}{1+\alpha z}\mathrm{ogf}\{c_m\}\left(\frac{z}{1+\alpha z}\right)\\
&= \frac{1}{1+\alpha z}G\big(\frac{z}{1+\alpha z};|\Psi_E\rangle\big).
\end{aligned}$$

This shows the proof for $p=0$. When $p\neq 0$, the transformed state vector reads

$$e^{-\alpha a^* b^*}|\Psi_E\rangle = \sum_{m=0}^{\infty}\Big(\frac{(p+m)!}{m!}\Big)^{1/2}\sum_{s=0}^{m} c_s(-\alpha)^{m-s}\binom{m}{s}|m+p,m\rangle. \quad (5.4.18)$$

It is straightforward to verify that the above computations hold using the rescaled coefficients $\{C_m\}_{m=0}^{\infty}$ and the generating functions

$$\begin{aligned} G(z;|\Psi_E\rangle) &= \sum_{m=0}^{\infty} C_m z^m \quad \text{and} \\ G\big(z;e^{-\alpha a^* b^*}|\Psi_E\rangle\big) &= \sum_{m=0}^{\infty}\left(\sum_{s=0}^{m} C_s(-\alpha)^{m-s}\binom{m}{s}\right) z^m. \end{aligned} \tag{5.4.19}$$

This concludes the proof. □

Finally, we use the result of Proposition 5 to show that, in the case $|z_+(\alpha)|>1$ (i.e., $\tilde{y}\geq 1$ and $\alpha_{max}\leq\alpha\leq\alpha_c$), we must restrict the parameter $B$ in the formula for $G(z;|\Psi_E\rangle)$, viz.,

$$G(z;|\Psi_E\rangle) = \frac{C_0 y_1(\alpha) p}{y_2(\alpha)}(z-z_+)^B(z-z_-)^{p-1-B}\int_0^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du.$$

This restriction will result from the requirement that

$$|\Psi_E\rangle \in \mathrm{dom}\big(e^{-\alpha a^* b^*}\big).$$

Indeed, if the state $e^{-\alpha a^* b^*}|\Psi_E\rangle$ exists as a vector in $\mathbb{F}_{\mathrm{ab}}$, it must have generating function

$$G\big(z;e^{-\alpha a^* b^*}|\Psi_E\rangle\big) = \frac{1}{1+\alpha z}G\left(\frac{z}{1+\alpha z};|\Psi_E\rangle\right).$$

The singularity of $G(z;|\Psi_E\rangle)$ at $z=z_+(\alpha)$ is therefore transformed to a singularity of $G\big(z;e^{-\alpha a^* b^*}|\Psi_E\rangle\big)$ at

$$\frac{z}{1+\alpha z} = z_+(\alpha),$$

i.e.,

$$z = \frac{z_+(\alpha)}{\big(1-\alpha z_+(\alpha)\big)}.$$

Therefore, if $\left|\frac{z_+(\alpha)}{1-\alpha z_+(\alpha)}\right|<1$ it will be necessary that $B\in\mathbb{N}$ using the reasoning of Proposition 4.

Since $z_+(\alpha) < 0$ and $\alpha > 0$ this is the same as showing that $\frac{1}{|z_+(\alpha)|} + \alpha > 1$ or $|z_+(\alpha)| < \frac{1}{1-\alpha}$. Indeed, recall

$$z_+(\alpha) = \frac{1}{2}\frac{(-1+2\alpha y+\sqrt{1-4y^2})}{(y-\alpha+\alpha^2 y)}, \tag{5.4.20}$$

and

$$y-\alpha+\alpha^2 y = y\left(\alpha - \frac{1-\sqrt{1-4y^2}}{2y}\right)\left(\alpha - \frac{1+\sqrt{1-4y^2}}{2y}\right),$$

so that

$$z_+(\alpha) = \left(\alpha - \frac{1+\sqrt{1-4y^2}}{2y}\right)^{-1}. \tag{5.4.21}$$

For $0 \le y \le \frac{1}{2}$ we have $\frac{1+\sqrt{1-4y^2}}{2y} \ge 1$, hence

$$|z_+(\alpha)| = \left(\left(\frac{1+\sqrt{1-4y^2}}{2y}\right) - \alpha\right)^{-1} \le \frac{1}{1-\alpha}. \tag{5.4.22}$$

The zero $z_+(\alpha)$ therefore lies inside the unit disk.

Note the relation for the $E$ of the eigenvalue problem

$$\mathscr{H}_{\text{ab}}^{(\alpha)}|\Psi_E\rangle = E|\Psi_E\rangle, \quad \alpha_{max} \le \alpha \le \alpha_C, \quad \tilde{y} \ge 1,$$

in terms of the exponent $B$:

$$E+1-\frac{p}{2} = B + \frac{y_1(\alpha)}{z_+(\alpha)}(2B+p-1). \tag{5.4.23}$$

Using the expression for $z_+(\alpha)$ just derived and $y_1(\alpha) = \frac{y}{1-2\alpha y}$, we get

$$\frac{y_1(\alpha)}{z_+(\alpha)} = \frac{1}{2}\big(-1+\sqrt{1-4y^2}\big), \tag{5.4.24}$$

and so

$$E = -\frac{1}{2} + \sqrt{1+4y^2}\Big(B+\frac{p-1}{2}\Big). \tag{5.4.25}$$

In the case that $\alpha = \alpha_c$, we have $y_1(\alpha_c) = 0$ and so using expression (5.4.23)

$$E = B - 1 + \frac{p}{2}.$$

Thus the spectrum of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ (after restricting the spectrum via analyticity arguments for $G(z;|\Psi_E\rangle)$) is the same as the spectrum of $\frac{1}{2}(a^*a + b^*b)$. Otherwise, the energy is given by expression (5.4.25).

Note that the singularity due to $z_-(\alpha)$ remains outside the disk under the transformation $|\Psi_E\rangle \mapsto e^{-\alpha a^* b^*}|\Psi_E\rangle$. Indeed,

$$z_-(\alpha) = \left(\alpha - \frac{1-\sqrt{1-4y^2}}{2y}\right)^{-1}, \tag{5.4.26}$$

and $\alpha \leq \frac{1-\sqrt{1-4y^2}}{2y}$, so $\frac{1}{|z_-(\alpha)|} = |\alpha - \frac{1-\sqrt{1-4y^2}}{2y}| < 1-\alpha$. This shows that the singularity due to $z_-(\alpha)$ does not affect the analyticity of $G\big(z; e^{-\alpha a^* b^*}|\Psi_E\rangle\big)$ inside the unit disk.

## 5.5 Completeness of the states $\{e^{(-\alpha_c a^* b^*)}|\Psi_{p,N}\rangle\}_{p,N\in\mathbb{N}}$

We recall the analysis so far. We wish to study the non-Hermitian transformed model Hamiltonian $\mathscr{H}_{\text{ab}}^{(\alpha)}$ on the Fock space $\mathbb{F}_{\text{ab}}$, given by:

$$\mathscr{H}_{\text{ab}}^{(\alpha)} = \frac{1}{2}\big(a^*a + b^*b\big) + y_1(\alpha)ab + y_2(\alpha)a^*b^*,$$

where

$$y_1(\alpha) := \frac{y}{1-2\alpha y}, \quad \text{and} \quad y_2(\alpha) := \frac{y - \alpha + \alpha^2 y}{1-2\alpha y}.$$

This operator is studied in place of the Hermitian Hamiltonian given by

$$\mathscr{H}_{\text{ab}}(y) := \mathscr{H}_{\text{ab}}^{(\alpha=0)} = \frac{1}{2}\big(a^*a + b^*b\big) + y\big(a^*b^* + ab\big), \quad \text{for} \quad 0 \leq y < 1/2. \tag{5.5.1}$$

We distinguished a particular case in the continuous parameter family, namely,

$$\alpha = \alpha_c := \frac{1-\sqrt{1-4y^2}}{2y},$$

since the model Hamiltonian for this value has an 'upper triangular' form:

$$\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)} = \frac{1}{2}\Big(a^*a + b^*b\Big) + \tilde{y}ab, \quad \text{for} \quad \tilde{y} := \Big(\frac{y}{\sqrt{1-4y^2}}\Big). \tag{5.5.2}$$

The eigenvalue problem for $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ reads:

$$\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}|\Psi_{p,\Theta}\rangle = (p/2+\Theta)|\Psi_{p,\Theta}\rangle, \quad p \in \mathbb{N}, \Theta \in \mathbb{C},$$

where the states $\{|\Psi_{p,\Theta}\rangle\}$ are given by the expression (5.3.12). Let us discuss the existing results for this critical parameter $\alpha = \alpha_c$. We have shown how for all $0 < \tilde{y} < \infty$, the point spectrum $\sigma\big(\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}\big)$ must either be discrete, or else, if $\sigma\big(\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}\big) = \mathbb{C}$, then we can restrict our attention to a discrete subset of $\sigma\big(\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}\big)$, which corresponds to those eigenstates that map to eigenstates of $\mathscr{H}_{\mathrm{ab}}$ under the inverse transform $\exp(-\alpha a^*b^*)$ (we actually demonstrated this for all $0 < \alpha \leq \alpha_c$ when $\tilde{y} \geq 1$). This was accomplished using several different methods in the previous sections. In Section 5.3, the case $\tilde{y} < 1$, and $\alpha = \alpha_c$ was handled, where it was shown by direct estimates on the coefficients of $|\Psi_{p,\Theta}\rangle$ that the eigenstates of $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ consist only of the states with $p \in \mathbb{N}$ and $\Theta \in \mathbb{N}$.

In Section 5.4.3, we discussed the case $\tilde{y} \geq 1$. In order to determine which $|\Psi_{p,\Theta}\rangle \in \mathrm{dom}\big(\exp(-\alpha_c a^*b^*)\big)$, we turned to studying the location of singularities of the generating function

$$G\big(z; \exp(-\alpha_c a^*b^*)|\Psi_{p,\Theta}\rangle\big).$$

It was found that this generating function is related to the generating function $G(z; |\Psi_{p,\Theta}\rangle)$ by a simple transform. In particular, $G(z; |\Psi_{p,\Theta}\rangle)$ has two singular points that will re-

strict the spectrum if one of these points lies inside the disk. We also discovered that if $G(z;|\Psi_{p,\Theta}\rangle)$ has no singular point inside the unit disk, then for the function $G\big(z;\exp(-\alpha_c a^* b^*)|\Psi_{p,\Theta}\rangle\big)$, this point will lie inside the disk.

We now prove the completeness of eigenstates $\{e^{(-\alpha_c)a^*b^*}|\Psi_{p,N}\rangle\}_{p,N\in\mathbb{N}}$ in the Fock space $\mathbb{F}_{ab}$ for critical parameter $\alpha_c$. The completeness of these states is not obvious, for several reasons. First, the operator $e^{(-\alpha_c)a^*b^*}$ is unbounded, so the relation

$$\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)} = \frac{1}{1-2(\alpha_c)y}\Big(e^{\alpha_c a^* b^*}\,\mathscr{H}_{\mathrm{ab}} e^{(-\alpha_c)a^*b^*} + \alpha_c y\Big)$$

does not imply that the spectra of the two operators are the same. It is likewise not clear that our formula for eigenstates recovers the same degeneracy of eigenstates for $\mathscr{H}_{\mathrm{ab}}$ given in terms of tensor products of quasiparticle operators (equation (5.1.6)). Finally, in Proposition 5 of Section 5.4.3 we have determined that infinitely many eigenstates $|\Psi_{p,\Theta}\rangle$ corresponding to $\frac{p}{2}+\Theta \in \sigma(\mathscr{H}_{\mathrm{ab}}^{\alpha_c})$ cannot be in the domain of $e^{-\alpha_c a^* b^*}$ when $\tilde{y} \geq 1$.

This chapter takes the approach of analyzing the spectral problem for $\mathscr{H}_{\mathrm{ab}}^{(\alpha_c)}$ without any necessary prior knowledge about the spectrum of $\mathscr{H}_{\mathrm{ab}}$. The completeness result of this section implies that eigenstates of $\mathscr{H}_{\mathrm{ab}}$ are *exactly* the non-Hermitian transforms of states $|\Psi_{p,\Theta}\rangle$ with $\Theta \in \mathbb{N}$. The following density argument also gives an alternative proof to the claim that the degeneracy of the $E = \frac{p}{2}+N$ eigenspace matches the degeneracy of the momentum eigenstates $|p+N,N\rangle$, or $|N,p+N\rangle$, represented by the Figure 5.1.

In order to show the completeness of the states

$$\{e^{-\alpha_c a^* b^*}|\Psi_{p,N}^{(\pm)}\rangle\}_{p,N\in\mathbb{N}} \quad \in \mathbb{F}_{ab},$$

it suffices to consider the completeness of states

$$\{e^{-\alpha_c a^* b^*}|\Psi_{p,N}\rangle\}_{N=0}^{\infty} \quad \in \mathrm{span}\{|s+p,s\rangle, s\in\mathbb{N}\} \quad \text{for fixed } p.$$

We make use of the well-known fact that a collection of elements $|\psi_j\rangle_{j\in\mathbb{N}}$ in a separable Hilbert space is complete if the only element $|f\rangle$ that satisfies

$$\langle f|\psi_j\rangle = 0, \quad \forall j \in \mathbb{N}$$

is the zero element, $|f\rangle \equiv 0$.

We therefore fix $p \geq 0$ without loss of generality. For $N \geq 0$, a straightforward calculation gives:

$$e^{(-\alpha_c a^* b^*)}|\Psi_{p,N}\rangle = \sum_{m=0}^{\infty} (-\alpha_c)^m S(m,N)|p+m,m\rangle. \tag{5.5.3}$$

for

$$S(m,N) := \sum_{s=0}^{\min\{m,N\}} (-\alpha_c \tilde{y})^{-s} \binom{N}{s} \left(\binom{p+s}{s}\right)^{-1/2} \left(\binom{p+m}{p+s}\binom{m}{s}\right)^{1/2}.$$

If $|f\rangle$ is an arbitrary vector in $\mathbb{F}_{\text{ab}}$ with expansion $|f\rangle := \sum_m d_m|p+m,m\rangle$ and coefficients $\{d_m\}_{m=0}^{\infty} \in \ell^2$, the inner product of $|f\rangle$ with the state (5.5.3) reads:

$$\langle f|e^{-\alpha_c a^* b^*}\Psi_{p,N}\rangle = \sum_m \overline{d_m}(-\alpha_c)^m S(m,N). \tag{5.5.4}$$

We will also use relations among Hypergeometric functions [44] $F(a,b,c;z)$ as a central tool in the proof, which are defined (using the Pochhammer symbols) by the power series

$$F(a,b,c;z) \equiv \sum_{m=0}^{\infty} \frac{z^m}{m!} \frac{(a)_m (b)_m}{(c)_m}, \quad a,b,c \in \mathbb{R}, \quad c \neq 0, \quad |z| < 1.$$

We alert the reader that the conventional notation for the Hypergeometric function $F$ uses parameters $a, b\,c$, which should not be confused with the annihilation operators on the Fock space $\mathbb{F}_{\text{ab}}$. We risk this confusion in order to retain the standard notation for $F$. We also remark that for the parameters considered in the proof, the Hypergeometric

function $F$ will reduce to a polynomial. The properties of $F$ which we use are listed in the lemma below. They are proved in the Appendix A.3.

**Lemma 11.** *(Properties for Hypergeometric functions) Let $m,N,p \in \mathbb{N}$. Then*

***(i)*** *$F$ at index $-m$ is related to $F$ at index $-m+1$ via:*

$$\begin{aligned}(mz)F\big(-m+1,-N,p+1;z\big) = &-(p+1+2N)F\big(-m,-N,p+1;z\big)\\ &+(p+1+N)F\big(-m,-N-1,p+1;z\big)\\ &+NF\big(-m,-N+1,p+1;z\big)\end{aligned} \tag{5.5.5}$$

*with the exceptional case $N=0$:*

$$(mz)F\big(-m+1,0,p+1,z\big) = -(p+1)F\big(-m,0,p+1,z\big)+(p+1)F\big(-m,-1,p+1,z\big). \tag{5.5.6}$$

***(ii)*** *For $a<0, z\in\mathbb{C}$*

$$\frac{d}{dz}z^aF\big(a,b,c,\frac{1}{z}\big) = az^{a-1}F(a+1,b,c,\frac{1}{z}). \tag{5.5.7}$$

Note: We will use the conventional shorthand for the contiguous hypergeometric functions when the parameters $a,b,c$ are clear from the context,

$$F = F(a,b,c;z), \quad F(a\pm) = F(a\pm 1,b,c;z), \tag{5.5.8}$$

with similar definitions holding for $F(b\pm)$, $F(c\pm)$.

**Proposition 6.** *(Completeness of eigenstates $|\Psi_{p,N}\rangle$ for critical parameter) Let $\alpha=\alpha_c = \frac{1-\sqrt{1-4y^2}}{2y}$. Then the collection*

$$\{e^{-\alpha_c a^*b^*}|\Psi^{(\pm)}_{p,N}\rangle\}_{p\in\mathbb{Z},N\in\mathbb{N}}$$

*is complete in the Bosonic Fock space $\mathbb{F}_{ab}$.*

*Proof.* It suffices to prove the statement for fixed $p$. Let $|f\rangle$ be a vector in $\mathbb{F}_{\text{ab}}$ which satisfies

$$\langle f|e^{(-\alpha_c a^* b^*)}\Psi_{p,N}\rangle = 0 \quad \forall N.$$

We write this inner product in the form of the expansion (5.5.4) above. Using equation (5.5.4) to write the inner product $\langle f|e^{-\alpha_c a^* b^*}\Psi_{p,N}\rangle$, the claim is that the infinite linear system for $\{d_m\}_{m=0}^{\infty} \in \ell^2$ which corresponds to the problem $\langle f|e^{(-\alpha_c a^* b^*)}\Psi_{p,N}\rangle = 0 \quad \forall N$ has only the trivial solution $\{d_m = 0\}_{m=0}^{\infty} \in \ell^2$.

Summarizing the steps of the proof: The family of functions defined by

$$f_N(z) := \langle f|e^{z a^* b^*}\Psi_{p,N}\rangle$$

are shown to be analytic for $z$ in the unit disk. The main assumption, namely,

$$\langle f|e^{(-\alpha_c) a^* b^*}\Psi_{p,N}\rangle = 0 \quad \text{for all} \quad N,$$

translates to the collection of point evaluatons $f_N(-\alpha_c) = 0 \ \forall N$. Next, the derivatives $\frac{d^n}{dz^n} f_N(z)$ are written as linear combinations of $f_{N+j}(z)$ for $0 \le j \le N+n$. Therefore the restriction $f_N(-\alpha_c) = 0$ for all $N$ translates to the restriction of all derivatives, $\frac{d^n}{dz^n} f_N(-\alpha_c) = 0$ for $n, N \ge 0$. Finally, since $f_N(z)$ is analytic in the unit disk and $|\alpha_c| < 1$ we conclude that $f_N(z) \equiv 0$ for all $N$, which gives the proof.

Assume first $\tilde{y} = 1$ (this condition will be removed later). Define the family of functions $f_N : \mathbb{C} \to \mathbb{C}, N \in \mathbb{N}$ by making the substitution $-\alpha \mapsto z$ in (5.5.4), i.e.,

$$\begin{aligned} f_N(z) &:= \sum_{m=0}^{\infty} \overline{d_m} z^m \left[ \sum_{s=0}^{\min\{m,N\}} z^{-s} \binom{N}{s} \left( \binom{p+s}{s} \right)^{-1/2} \sqrt{\binom{p+m}{p+s}\binom{m}{s}} \right] \\ &= \sum_{m=0}^{\infty} \overline{d_m} z^m \left( \binom{p+m}{m} \right)^{1/2} \left[ \sum_{s=0}^{\min\{m,N\}} z^{-s} \binom{N}{s} \binom{m}{s} \binom{p+s}{s}^{-1} \right] \\ &= \sum_{m=0}^{\infty} \overline{d_m} z^m \left( \binom{p+m}{m} \right)^{1/2} F\left( -m, -N, p+1; \frac{1}{z} \right). \end{aligned} \tag{5.5.9}$$

Here $F(a,b,c;z)$ is the Hypergeometric function, and equation (5.5.9) is a consequence of the factorization

$$\binom{p+m}{p+s} = \binom{m}{s}\binom{p+s}{s}^{-1}\binom{p+m}{m}.$$

Note that $f_0(z) \equiv \sum_{m=0}^{\infty} \overline{c_m}\sqrt{\binom{p+m}{m}}z^m$ is consistent with this definition since $F(\cdot,0,\cdot,z) = 1$. It is easy to verify that the series defining $f_N(z)$ is convergent (and therefore $f_N$ is analytic) for $|z| < 1$.

Now assume that $\langle f|e^{-\alpha_c a^* b^*}\Psi_{p,N}\rangle = 0 \quad \forall N$, which translates to the point evaluation

$$f_N\big(-\alpha_c\big) = 0 \quad \forall N \geq 0. \tag{5.5.10}$$

The remainder of the proof describes how this condition implies $f_N(z) \equiv 0 \quad \forall N$ and hence $d_m \equiv 0$ for all $m$

Using formulas of Lemma 11 we now show that $\frac{d^n}{dz^n}f_N(z)$ is a finite linear combination of $f_0(z), f_1(z), \ldots, f_{N+n}(z)$ for every $n$. Since we have $f_n(-\alpha_c) = 0$ for all $n$, i.e., equation (5.5.10), this shows that $\frac{d^n}{dz^n}f_N(-\alpha_c) = 0$ for all $n$.

Indeed,

$$\begin{aligned}
\frac{d}{dz}f_N^{(p)}(z) &= \sum_{m=0}^{\infty}\sqrt{\binom{p+m}{m}}\overline{d_m}\frac{d}{dz}\Big[z^m F\left(-m,-N,p+1,\frac{1}{z}\right)\Big] \\
&= \sum_{m=0}^{\infty}\sqrt{\binom{p+m}{m}}\overline{d_m}\Big[mz^{m-1}F\left(-m+1,-N,p+1,\frac{1}{z}\right)\Big] \\
&= \sum_{m=0}^{\infty}\sqrt{\binom{p+m}{m}}\overline{d_m}z^m\Big[m\frac{1}{z}F\left(-m+1,-N,p+1,\frac{1}{z}\right)\Big] \\
&= \sum_{m=0}^{\infty}\sqrt{\binom{p+m}{m}}\overline{d_m}z^m\Big[-(p+1+2N)F+(p+1+N)F(-N-1)+NF(-N+1)\Big] \\
&= -(p+1+2N)f_N^{(p)}(z)+(p+1+N)f_{N+1}^{(p)}(z)+Nf_{N-1}^{(p)}(z).
\end{aligned} \tag{5.5.11}$$

Iterating this same procedure, it is clear that we can write a corresponding formula for any number of derivatives of $f_N$. This formula is written as a vector equation for convenience:

$$\frac{d^n}{dz^n}f_N^{(p)}(z) = \mathbf{L}\big(f_0^{(p)}(z),\ldots,f_N^{(p)}(z),f_{N+1}^{(p)}(z),\ldots,f_{N+n}^{(p)}(z)\big)^T,$$

where $\mathbf{L}$ is a $1\times(N+n+1)$ dimensional vector. The precise entries of $\mathbf{L}$ are irrelevant to us, except for the fact that they generally involve the constants $p,N$ but not $\alpha_c$. We should remark on the derivative of $f_0^{(p)}(z)$. In this case, equation (5.5.6) is used and Formula **(ii)** becomes trivial, so $\frac{d^n}{dz^n}f_0^{(p)}(z)$ will be a linear combination of the functions $f_0^{(p)},f_1^{(p)},\ldots,f_n^{(p)}$.

Collecting like powers of $z$ in $f_N(z)$ gives

$$f_N(z) = \sum_{q=0}^{\infty}\left[\sum_{m=q}^{q+N}\overline{d_m}\binom{N}{m-q}\binom{m}{q}\right]z^q, \quad \text{for} \quad q=m-s, \tag{5.5.12}$$

so indeed, $f_N\equiv 0$ implies that $d_m=0$ for all $m=0,1,2,\ldots$ .

Finally, the restriction $\tilde{y}=1$ is now removed via a change of variables. We show this for $p=0$ for clarity – the other cases follow analogously. The function $f_N(z)$ is now

defined by

$$f_N(z) := \sum_{m=0}^{\infty} \overline{d_m} z^m F\Big(-m,-N,1,\frac{1}{\tilde{y}z}\Big), \quad \tilde{y} \neq 0. \tag{5.5.13}$$

We now have

$$\frac{d}{dz} f_N(z) = \tilde{y} \sum_{m=0}^{\infty} \overline{d_m} z^m \Big[ m \frac{1}{\tilde{y}z} F\big(-m+1,-N,1,\frac{1}{\tilde{y}z}\big)\Big], \tag{5.5.14}$$

and the derivative formula in Lemma 11 again applies to give

$$\frac{d}{dz} f_N(z) = \tilde{y}\Big[-(1+2N) f_N(z) + (p+1) f_{N+1}(z) + N f_{N-1}(z)\Big], \tag{5.5.15}$$

Following the above reasoning we conclude that $d_m = 0$ for $m = 0,1,2,\ldots$ and the proof is complete. □

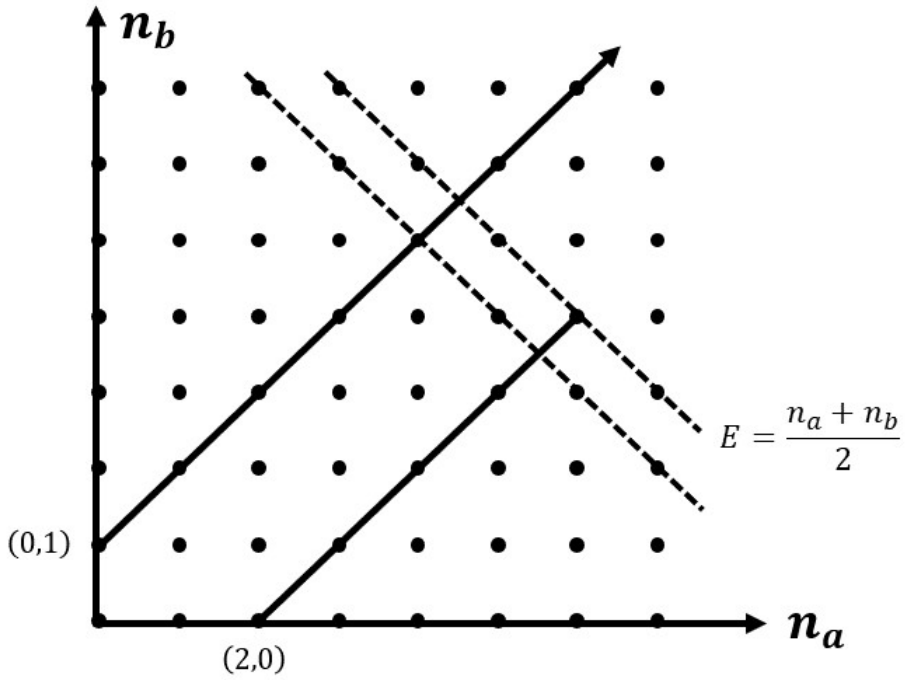


Figure 5.1: Schematic of the dependence of quantum states $|\Psi_{p,\Theta}\rangle$ on the occupation numbers $n_a, n_b$. The lattice points represent the occupation-number eigenstates $|n_a, n_b\rangle$, and the dotted lines (labeled $E = 4.5$ and $E = 5$) represent hypersurfaces on which $\frac{1}{2}(n_a + n_b) = 4.5, 5$ respectively; the lattice points lying on these hypersurfaces thus represent the degenerate eigenstates of the operator $\frac{1}{2}(a^*a + b^*b)$. The two solid lines (beginning at the points $(0,1)$ and $(2,0)$) contain the lattice points which appear in the formula for two example states $|\Psi_{p,\Theta}\rangle$ elaborated in Proposition 1. The line starting at $(0,1)$ represents a state $|\Psi_{-1,\Theta}\rangle$, where $2\Theta \notin \mathbb{N}$ – this state is an infinite sum, which is represented by the fact that the arrow extends indefinitely. The line starting at the point $(2,0)$ represents the state $|\Psi_{2,4}\rangle$ – this state is a linear combination of the basis states $\{|2,0\rangle, |3,1\rangle, |4,2\rangle, |5,3\rangle, |6,4\rangle\}$.

# Chapter 6

## Overview and Extensions

In this thesis, we have rigorously developed the method of pair-excitation as it relates to several models for excitations of the interacting Bose gas at zero temperature. These models vary significantly in their mathematical details; we have expanded the formulation of pair-excitation to account for non-translation-invariant systems as well as systems which do not conserve the number of particles. We construct many-body excited states in each of these settings.

## 6.1 Overview

We now discuss some of the themes, with broad scientific appeal, that this work touches upon.

### The phonon spectrum spectrum

A major element of this work pertains to the construction of many-body excited states which correspond to the phonon spectrum of the Bose gas in a physically transparent form involving spatial coordinates. We have found that the pair-excitation formalism can offer a concise description of many-body states in spatial coordinates in both the periodic and non-translation-invariant systems. In the periodic box, we discovered that states belonging to the phonon spectrum (of the Lee-Huang-Yang model, for example)

are finite linear combinations of momentum tensor product states after transforming the system by the pair-excitation operator. The states of the transformed system correspond in a direct way to the eigenstates of an upper-triangular finite-dimensional matrix. In the non-translation-invariant setting, we must replace the description in terms of the single-particle momentum states by utilizing a new basis of single-particle states; we found that this basis consists of eigenstates of the single-particle (non-Hermitian) 'phonon' operator $h_{\mathrm{ph}}$ of Chapter 3. The procedure for constructing many-body excitations of the transformed approximate Hamiltonian using this new basis also corresponds to solving an upper-triangular eigenvalue problem in finite dimensions. Moreover, energies corresponding to these excitations are sums of energies of the phonon operator. This leads us to consider the pair-excitation method as a direct method for determining the phonon spectrum of the Bose gas in general systems, in the sense that low-lying energies of the many-body system appear as sums of energies from the spectrum of the effective single-particle operator $h_{\mathrm{ph}}$.

## The notion of quasiparticle

Also in relation to the spectrum of elementary excitations, we believe that our analysis sheds light on the notion of the "quasiparticle" introduced for the Bose gas in [20], and which is related to the notion of the phonon [37]. Fetter heuristically introduces the quasiparticle operators $\gamma_j$, $\gamma_j^*$ which satisfy canonical commutation relations and appear in the diagonal form of a quadratic (Hermitian) Hamiltonian which does not conserve the number of particles. In Chapter 3, we showed that the non-orthogonal basis $\{u_j(x), v_j(x)\}$

appearing in the definition of the quasiparticle operators is directly related to the pair-excitation kernel $k(x,y)$. In particular, $u_j(x)$ can be defined by applying the bounded operator $(\delta - k \circ \overline{k})^{-1/2}$ to eigenfunction $\eta_j(x)$ of the single-particle, self-adjoint operator $\varkappa$ (see Chapter 3, Lemma 5 proof). The function $v_j(x)$ is then defined via $v_j(x) = -\overline{k}(x, u_j)$. In light of this, we suggest an alternative notion for quasiparticle – as an excitation of a quadratic Hamiltonian which corresponds to the spectrum of an effective single-particle operator (e.g., $h_{\text{ph}}$ in our notation). Such an excitation is related to both a non-orthogonal basis in the position space, (e.g., $\{u_j(x), v_j(x)\}$) and also an orthogonal basis (e.g., $\{\eta_j\}$) via the pair excitation kernel $k$. We can construct many-body excited states as finite superpositions in tensor products involving the eigenstates of the operator $h_{\text{ph}}$.

## Connection of pair-excitation to Bogoliubov rotations

Another insight which is new to this thesis is the connection between the unitary Bogoliubov rotation of quadratic Hamiltonians, which gives the matrix system (3.6.4) for the single-particle basis $\{u_j(x), v_j(x)\}$ of Chapter 3, and the non-Hermitian pair-excitation transform, which gives the Riccati equation for the kernel $k$ of equation (3.3.4b). This connection reflects fundamental results from the theory of $J-$self-adjoint operators [2–4, 13], and is represented schematically in the Figure 3.1 of Chapter 3. The translation of these results in operator theory to the setting of the Bose gas is new to our work. It is of interest to note that, historically, the two sides of this connection appear independently in the works of Wu [60], who formulated the theory of the pair-excitation kernel, and Fetter [20], who developed the theory for the Bogoliubov rotation of a non-translation-invariant Bose

gas. In terms of the fundamental physics, connecting these two distinct methods allows us to claim that processes of pair-excitation are fundamental to the energetics of quadratic systems. Pair-excitation and Bogoliubov rotation represent two equivalent representations of the same physics.

## 6.2 Extensions

We conclude by suggesting a few extensions of the framework and results introduced in this thesis. These extensions pertain to the study of the Bose gas in more general, and physically relevant settings.

### Time-evolution problems for pair-excited states

The problems considered in this thesis pertain to the stationary theory of the Bose gas, but much work has been done on the evolution of pair-excited states [26, 27]. Wu originally introduced the kernel $k$ in a time-dependent setting [60]. The results here serve as an important first step in understanding the time evolution problem for the approximate systems of the previous chapters. The stationary solutions for $k$ given in this work can be used to generate solutions to Wu's equation for the excitation kernel with the simple time dependence:

$$k(x,y,t) := e^{-i\mu t}k(x,y).$$

The time-dependent pair-excitation kernel means that the resulting pair-excitation operator will be time-dependent. An important question is whether the time-dependence of many-body excited states can be described solely in terms of a time dependent kernel.

That is, can many-body states be described by a time-dependent pair-excitation operator acting on a simple stationary state?

## Pair excitation at small positive temperatures

The system of Chapter 4 included the mean-field effect of pair-correlations involving field operators for the non-condensate. In [25], Griffin wrote these correlations to include general nonzero-temperature effects, via the expressions :

$$\begin{aligned}\rho_1(x) &= \sum_j \left\{ |u_j(x)|^2 + |p_j(x)|^2 \right\} (e^{\beta(\varepsilon_j-\mu)}-1)^{-1} + |p_j(x)|^2 \\ \rho_2(x) &= \sum_j u_j(x)\overline{p_j(x)}[2(e^{\beta(\varepsilon_j-\mu)}-1)^{-1}+1].\end{aligned} \tag{6.2.1}$$

Here, $\{u_j(x), p_j(x)\}$ solve the nonlinear matrix system of Chapter 4, with energies $\varepsilon_j$. These formulas contain the average occupation number for particles with energies $\varepsilon_j$ satisfying Bose statistics,

$$\langle n_{\varepsilon j}\rangle = \frac{1}{e^{\beta(\varepsilon_j-\mu)}-1}.$$

The equations of Chapter 4 therefore have an extension to finite temperatures within Griffin's scheme. As it relates to this thesis, the question is whether a solution $\{\phi_{T>0}, k_{T>0}\}$ can be found to this new system as a perturbation of the system found in Chapter 4. Additionally, it is of interest to derive these equations self-consistently from a variational approach using quantum statistical ensembles.

## Generalizations on quadratic Hamiltonians

Finally, we consider an extension of the work presented here in the domain of the periodic box. Instead of reducing the system using the Fermi pseudopotential (which al-

lowed us to factor the model Hamiltonian over momentum subspaces), we can consider keeping the generic interaction potential $\upsilon(x,y)$ in the approximation of Chapter 5, simplifying the system by means of a compact cut-off for $\widehat{\upsilon}$ in momentum space. Carrying out the steps of the approximation scheme, we will end up studying a quadratic Hamiltonian of the form

$$\mathscr{H}_{\text{app1}} := \sum_k (k^2 + \frac{N}{2V}\widehat{\upsilon}(k)) a_k^* a_k + \frac{N}{2V} \sum_{k\in\mathbb{Z}_L^+,\, p\in I(k)} \widehat{\upsilon}(k,p)(a_k^* a_p^* + a_k a_p). \tag{6.2.2}$$

Here, $I(k)$ is a finite set in $-\mathbb{Z}_L^+$ that contains $-k$ for every $k \in \mathbb{Z}_L^+$. The more complicated coupling means that we cannot use the model Fock space $\mathbb{F}_{\text{ab}}$ of Chapter 5 to describe eigenstates of $\mathscr{H}_{\text{app1}}$. We nonetheless hypothesize that the essential results of this thesis (regarding the structure (5.1.3) of eigenstates for $\mathscr{H}_{\text{LHY}}$) hold, by introducing a non-unitary pair-excitation operator of the form

$$\exp(\mathscr{Q}), \quad \text{for} \quad \mathscr{Q} := \sum_{k\in\mathbb{Z}_L^+,\, p\in I(k)} \{-\alpha(k,p) a_k^* a_p^*\}, \quad 0 < \alpha(k,p) < 1.$$

In Chapter 3, we described the eigenstates of a particle conserving Hamiltonian on $\mathbb{F}_N$, containing the trapping potential $V_{\text{trap}}(x)$. The approximate Hamiltonian reads:

$$\mathscr{H}_{\text{app2}} := NE_H + h(a_\perp^*, a_\perp) + \frac{(a_{\overline{\phi}})^2}{2N} f_\phi(a_\perp^*, a_\perp^*) + \frac{(a_\phi^*)^2}{2N} \overline{f_\phi}(a_\perp, a_\perp) \tag{6.2.3}$$

where, e.g., $h(a_\perp^*, a_\perp) = \iint dxdy \{h(x,y) a_{\perp,x}^* a_{\perp,y}\}$, and the corresponding kernels are

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

for $\mu > 0$, and

$$f_\phi(x,y) := N\phi(x)\upsilon(x,y)\phi(y).$$

We showed that there is a *non-orthogonal* basis $\{u_j(x)\}_{j\in\mathbb{N}}$ that plays the role of the momentum states $\{e_k(x)\}_{k\in\mathbb{Z}_L}$ in the construction of eigenstates of $\mathscr{H}_{\text{app2}}$. It remains an

open question as to whether these states can be utilized, in the spirit of Chapter 5, to write many body excitations of the *quadratic* approximation $\mathscr{H}_{\text{app2}}$:

$$\mathscr{H}_{\text{app2}} \approx NE_{\text{H}} + h(a_{\perp}^{*}, a_{\perp}) + \frac{1}{2} f_{\phi}(a_{\perp}^{*}, a_{\perp}^{*}) + \frac{1}{2}\overline{f_{\phi}}(a_{\perp}, a_{\perp}). \tag{6.2.4}$$

# Appendix A

This Appendix contains complete proofs for several of the propositions of Chapter 5. First, we give the details of the difference scheme, which we solve in order to derive the formula for many-body excited states. We then complete the proof of Proposition 4 in Chapter 5, which describes the analyticity properties of the generating function for a state $|\Psi_E\rangle$. Finally, we prove several properties of the Hypergeometric functions which we use in Theorem 6 of Chapter 5. These properties can be found in any standard treatment of Hypergeometric functions, e.g., Ref. [44]. We include their proofs here for completeness.

## A.1 Derivation of many-body eigensates $|\Psi_{p,\Theta}\rangle$

Let $E \in \mathbb{C}$ denote the eigenvalue of $\mathscr{H}_{\text{ab}}^{(\alpha_c)}$ associated with eigenvector $|\Psi_E\rangle \in \mathbb{F}_{ab}$. Expanding $|\Psi_E\rangle$ in the occupation number basis, i.e.,

$$|\Psi_E\rangle = \sum_{\{m_a,m_b\in\mathbb{N}\}} c_{m_a m_b}|m_a,m_b\rangle, \tag{A.1.1}$$

yields the following relation between coefficients

$$\frac{1}{2}(m_a+m_b)c_{m_a,m_b} + \tilde{y}\sqrt{(m_a+1)(m_b+1)}c_{m_a+1,m_b+1} = Ec_{m_a,m_b}. \tag{A.1.2}$$

Next define $E_{m_a,m_b} := \frac{1}{2}(m_a+m_b)$, which is the energy of the state $|m_a,m_b\rangle$ as an eigenvector of the operator $\frac{1}{2}(a^*a+b^*b)$, so that

$$c_{m_a+1,m_b+1} = \frac{\left(E-E_{m_a,m_b}\right)}{\tilde{y}\sqrt{(m_a+1)(m_b+1)}}c_{m_a,m_b}. \tag{A.1.3}$$

Repeating this relation $s$ times results in the formula

$$c_{m_a+s,m_b+s} = \tilde{y}^{-s} \frac{(E - E_{m_a+s-1,m_b+s-1}) \cdot \cdots \cdot (E - E_{m_a,m_b})}{\sqrt{(m_a+s) \cdot \cdots \cdot (m_a+1)(m_b+s) \cdot \cdots \cdot (m_b+1)}} c_{m_a,m_b}. \tag{A.1.4}$$

We now fix $\vec{m} := (m_a, m_b)$, and define the energy difference $\Theta := E - E_{\vec{m}}$ as well as the shorthand $\vec{m} + s := (m_a + s, m_b + s)$. Equation (A.1.4) can be rewritten using the generalized binomial coefficient $\binom{\Theta}{s} := \frac{\Gamma(\Theta+1)}{\Gamma(s+1)\Gamma(\Theta-s+1)}$ via

$$\begin{aligned} c_{\vec{m}+s} &= \tilde{y}^{-s} \frac{(\Theta - s + 1) \cdot \cdots \cdot (\Theta - 1)\Theta}{\sqrt{(m_a+1) \cdot \cdots \cdot (m_a+s)(m_b+1) \cdot \cdots \cdot (m_b+s)}} c_{\vec{m}} \\ &= \tilde{y}^{-s} \binom{\Theta}{s} \frac{s!}{\sqrt{(m_a+1) \cdot \cdots \cdot (m_a+s)(m_b+1) \cdot \cdots \cdot (m_b+s)}} c_{\vec{m}} \\ &= \tilde{y}^{-s} \binom{\Theta}{s} \sqrt{\binom{m_a+s}{s}\binom{m_b+s}{s}}^{-1} c_{\vec{m}}. \end{aligned} \tag{A.1.5}$$

With the quantities $\Theta, \vec{m}$ fixed, the single coefficient $c_{\vec{m}}$ uniquely determines all other coefficients $c_{\vec{m}\pm s}$. Imposing the normalization condition

$$\sum_{s=-\min(m_a,m_b)}^{\infty} |c_{m_a+s,m_b+s}|^2 = 1, \tag{A.1.6}$$

then determines $c_{\vec{m}}$ uniquely. Without loss of generality, we take $\vec{m} = 0$.

## Difference scheme for eigenstates of $\mathscr{H}_{\text{ab}}^{(\alpha)}$

An iteration scheme can be written in the occupation number basis for eigenstates of $\mathscr{H}_{\text{ab}}^{(\alpha)}$ when $0 \leq \alpha \leq \alpha_c$. We again assume that the state $|\Psi_E\rangle$ with energy $E \in \mathbb{C}$ has the expansion (A.1.1). It suffices to fix $p \in \mathbb{N}$ and consider only linear combinations of states $|m_a, m_b\rangle = |p+s, s\rangle$ for $s = 0, 1, 2, \ldots$, so that we can write $c_s := c_{p+s,s}$ and the

eigenvalue equation reads:

$$\begin{aligned}\frac{1}{2}\sum_{s=0}^{\infty} c_s(p+2s)|p+s,s\rangle + y_1(\alpha)\sum_{s=0}^{\infty} c_s\sqrt{(p+s)s}|p+s-1,s-1\rangle \\ + y_2(\alpha)\sum_{s=0}^{\infty} c_s\sqrt{(p+s+1)(s+1)}|p+s+1,s+1\rangle \\ = E\sum_{s=0}^{\infty} c_s|p+s,s\rangle.\end{aligned}$$

For $E \in \mathbb{C}$ we arrive at the difference scheme

$$\left(\frac{p}{2}+s\right)c_s + y_1(\alpha)c_{s+1}\sqrt{(p+s+1)(s+1)} + y_2(\alpha)c_{s-1}\sqrt{(p+s)s} = Ec_s. \quad \text{(A.1.7)}$$

## A.2 Properties of the generating function $G(z;|\Psi_E\rangle)$

Here we complete the proof of analyticity in Proposition 4, which is restated below.

**Proposition 7.** *For $\alpha$ such that $|z_+(\alpha)| < 1$, and $p > 0$, the function $G(z;|\Psi_E\rangle)$ defined by*

$$G(z;|\Psi_E\rangle) = \frac{C_0 y_1(\alpha)p}{y_2(\alpha)}(z-z_+)^B(z-z_-)^{p-1-B}\int_0^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du \quad \text{(A.2.1)}$$

*is analytic if and only if $B \in \mathbb{N}$.*

*Proof.* It is shown that there is a singularity of $G(z;|\Psi_E\rangle)$ inside the unit disk which is removable under the condition $B \in \mathbb{N}$. Let us start with $\mathrm{Re}(B) < 0$. The results can be analytically continued to $\mathrm{Re}(B) > 0$ by standard techniques (e.g., integration by parts).

We want to know how $G(z)$ behaves as $z \to_+$. For this we write the integral of

(A.2.1) as

$$\int_0^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du = \int_0^{z_+} u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du + \int_{z_+}^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du. \tag{A.2.2}$$

The first of these integrals can be written

$$\int_0^{z_+} u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du = (-1)^{-1-B}z_+^{p-1-B}(-z_-)^{B-p}\int_0^1 t^{p-1}(-t+1)^{-(1+B)}(1-\frac{z_+}{z_-}t)^{B-p}dt. \tag{A.2.3}$$

This is compared to the integral of the Hypergeometric function,

$$F(a,b,c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}dt, \quad \mathrm{Re}(c) > \mathrm{Re}(b) > 0.$$

The second integral in (A.2.2) is written, taking $z = z_+ + \varepsilon$ for $|\varepsilon| \ll 1$, and making the change of variables $u = v + z_+$:

$$\int_{z_+}^z u^{p-1}(u-z_+)^{-(1+B)}(u-z_-)^{(p-B)}du = \int_0^{\varepsilon}(v+z_+)^{p-1}v^{-(1+B)}(v-z_+-z_-)^{(p-B)}du. \tag{A.2.4}$$

Expanding in powers of $v = u - z_+$ by a typical argument shows that this integral takes the form

$$\int_0^{\varepsilon}(v+z_+)^{p-1}v^{-(1+B)}(v-z_+-z_-)^{(p-B)}du = \int_0^{\varepsilon}v^{-(1+B)}\Big(\sum_{m=0}^{\infty}d_m v^m\Big)dv, \tag{A.2.5}$$

where the expansion in the powers $v^m$ is analytic. The integral in the above equation is carried out to give

$$\int_0^{\varepsilon}(v+z_+)^{p-1}v^{-(1+B)}(v-z_+-z_-)^{(p-B)}du = \varepsilon^{-B}\sum_{m=0}^{\infty}\Big(\frac{d_m}{m-B}\Big)\varepsilon^m. \tag{A.2.6}$$

When $\mathrm{Re}(B) < 0$ (which we assume at the current point in the argument), it follows that the expression (A.2.6) is analytic in $\varepsilon$ if and only if $-B \in \mathbb{N}$; otherwise the function in (A.2.6) exhibits a singularity as $\varepsilon \to 0$. This proof can be extended to $B \geq 0$ by standard techniques. For example, we can use integration by parts to increase $B$ by integer values in the integral of (A.2.6). □

## A.3 Properties of the hypergeometric functions

Here we provide direct proofs of the properties for Hypergeometric functions used in the proof of Theorem 6.

**Property (i)** For $p = 0, 1, 2, \ldots$ ,

$$mzF(-m+1) = -(p+1+2N)F + (p+1+N)F(-N-1) + NF(-N+1).$$

*Proof.* Using the definition of the hypergeometric function, the left-hand-side of the above relation reads

$$\begin{aligned} & mz \sum_{s=0}^{\infty} \frac{z^s}{s!} \frac{(-m+1)_s (-N)_s}{(p+1)_s} = \\ & \sum_{s=0}^{\infty} \frac{z^{s+1}}{(s+1)!} \frac{(-m)_{s+1}(-N)_{s+1}}{(p+1)_{s+1}} \left\{ \frac{m(-m+1)_s}{(-m)_{s+1}} \cdot \frac{(-N)_s}{(-N)_{s+1}} \cdot \frac{(p+1)_{s+1}}{(p+1)_s} \right\} \\ & = \sum_{s=0}^{\infty} \frac{z^{s+1}}{(s+1)!} \frac{(-m)_{s+1}(-N)_{s+1}}{(p+1)_{s+1}} \left\{ \frac{-(s+1)(p+s+1)}{(-N+s)} \right\}. \end{aligned}$$

The right-hand-side of **(i)** meanwhile reads

$$\sum_{s=0}^{\infty} \frac{z^s}{s!} \frac{(-m)_s (-N)_s}{(p+1)_s} \left\{ -(p+1+2N) + (p+1+N) \frac{(-N-1)}{(-N+s-1)} + N \frac{(-N+s)}{-N} \right\}.$$

It must be shown that the $(s+1)^{th}$ term of the RHS agrees with the $s^{th}$ term of the LHS,

and that the $s=0$ term on the RHS vanishes. Indeed

$$\frac{(-m)_0(-N)_0}{(p+1)_0}\{-(p+1+2N)+(p+1+N)+N\}=0. \tag{A.3.1}$$

This shows the second statement, while the coefficient of $\frac{z^{s+1}}{(s+1)!}\frac{(-m)_{s+1}(-N)_{s+1}}{(p+1)_{s+1}}$ on the RHS is

$$\begin{aligned}
&-(p+1+2N)+(p+1+N)\frac{-N-1}{-N+s}+N\frac{(-N+s+1)}{-N}\\
&=\frac{-(p+N+s+2)(-N+s)-(p+1+N)(N+1)}{(-N+s)}\\
&=\frac{-(s+1)(p+s+1)}{(-N+s)}
\end{aligned}$$

The case $N=0$ follows by comparing the LHS

$$mz\sum_{s=0}^{\infty}\frac{(-m+1)_s(0)_s}{(p+1)_s}\frac{z^s}{s!}=mz \tag{A.3.2}$$

to the RHS

$$-(p+1)\cdot 1+(p+1)\sum_s\frac{(-m)_s(-1)_s}{(p+1)_s}\frac{z^s}{s!}=-(p+1)+(p+1)\left\{1+\frac{(-m)(-1)}{(p+s)}z\right\}=mz$$

□

**Property (ii):** For $a<0$,

$$\frac{d}{dz}z^aF\left(a,b,c,\frac{1}{z}\right)=az^{a-1}F\left(a+1,b,c,\frac{1}{z}\right). \tag{A.3.3}$$

*Proof.* The LHS reads

$$z^{a-1}\sum_{s=0}^{\infty}\frac{(a)_s(b)_s}{(c)_s}\frac{z^{-s}}{s!}\{a-s\} \tag{A.3.4}$$

while the RHS reads

$$az^{m-s}\sum_{s=0}^{\infty}\frac{(a+s)_s(b)_s}{(c)_s}\frac{z^{-s}}{s!}. \tag{A.3.5}$$

Proving the formula then follows from the relation $(a-s)(a)_s = a(a+1)_s$. The exceptional case $b = 0$ is handled by

$$\frac{d}{dz}\left\{z^m F(-a,0,c,\frac{1}{z})\right\} = \frac{d}{dz}z^m. \tag{A.3.6}$$

□

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