The Excitation Spectrum for Weakly Interacting Bosons in a Trap

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Abstract: We investigate the low-energy excitation spectrum of a Bose gas confined in a trap, with weak long-range repulsive interactions. In particular, we prove that the spectrum can be described in terms of the eigenvalues of an effective one-particle operator, as predicted by the Bogoliubov approximation.

1. Introduction and Main Results

1.1. Introduction. Bose-Einstein condensates of dilute atomic gases have been studied extensively in recent years, both from an experimental and a theoretical perspective [1,2]. Many fundamental aspects of quantum mechanics were investigated with the aid of these systems. One of the manifestations of their quantum behavior is superfluidity, leading to the appearance of quantized vortices in rotating systems [3,4]. This property is related to the structure of the low-energy excitation spectrum, via the Landau criterion [5]. Excitation spectra of atomic Bose-Einstein condensates have actually been measured [6], and agreement was found with theoretical predictions based on the Bogoliubov approximation [7].

From the point of view of mathematical physics, starting with the basic underlying many-body Schrödinger equation, it remains a big challenge to understand many features of cold quantum gases [8,9]. While the validity of the Bogoliubov approximation for evaluating the ground state energy has been studied in several cases [10–15], no rigorous results on the excitation spectrum of many-body systems with genuine interactions among the particles are available, with the exception of certain exactly solvable models in one dimension [16–22]. In particular, it remains an open problem to verify Landau's criterion for superfluidity in interacting gases.

In this paper, we shall prove the accuracy of the Bogoliubov approximation for the excitation spectrum of a trapped Bose gas, in the mean-field or Hartree limit [23,24],

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where the interaction is weak and long-range. While the interactions among atoms in the experiments on cold gases are more accurately modeled as strong and short-range, effective long-range interactions can be achieved via application of suitable electromagnetic fields [25]. Our work generalizes the recent results in [26], where the validity of Bogoliubov's approximation was verified for a homogeneous, translation invariant model of interacting bosons. The inhomogeneity caused by the trap complicates the analysis and leads to new features, due to the non-commutativity of the various operators appearing in the effective Bogoliubov Hamiltonian.

1.2. Model and main results. We consider a system of $N \ge 2$ bosons in \mathbb{R}^d , for general $d \ge 1$. The particles are confined by an external potential $V_{\text{ext}}(x)$, and interact via a weak two-body potential, which we write as $(N-1)^{-1}v(x-y)$. The Hamiltonian of the system reads, in suitable units,

$$H_N = \sum_{i=1}^{N} \left(-\Delta_i + V_{\text{ext}}(x_i) \right) + \frac{1}{N-1} \sum_{i < j} v(x_i - x_j), \tag{1}$$

with Δ denoting the standard Laplacian on \mathbb{R}^d . It acts on the Hilbert space of permutation-symmetric square integrable functions on \mathbb{R}^{dN} , as appropriate for bosons. We assume that v is a bounded symmetric function, which is non-negative and of positive type, i.e., has non-negative Fourier transform. The external potential V_{ext} is assumed to be locally bounded and to satisfy $V_{\text{ext}}(x) \to \infty$ as $|x| \to \infty$.

Under these assumptions on V_{ext} and v, the non-linear Hartree equation

$$(-\Delta + V_{\text{ext}})\varphi_0 + (\upsilon * |\varphi_0|^2)\varphi_0 = \varepsilon_0 \varphi_0 \tag{2}$$

admits a unique strictly positive solution φ_0 , normalized as $\int \varphi_0^2 = 1$, which is equal to the ground state of the corresponding Hartree energy functional. In addition, there is a complete set of normalized eigenfunctions $\{\varphi_i\}_{i\in\mathbb{N}}$ for the Hartree operator

$$H_{\rm H} = -\Delta + V_{\rm ext} + v * \varphi_0^2 \,. \tag{3}$$

The corresponding eigenvalues will be denoted by $\varepsilon_0 < \varepsilon_1 \le \varepsilon_2 \dots$. We note that φ_0 is necessarily the ground state of H_H , since it is an eigenfunction that is positive. Moreover, we emphasize that the inequality $\varepsilon_1 > \varepsilon_0$ is strict, since operators of the form (3) have a unique ground state [27]. This will be essential for our analysis.

Let V denote the operator defined by the integral kernel

$$V(x, y) = \varphi_0(x)v(x - y)\varphi_0(y).$$

As shown below, our assumptions on v imply that this defines a positive trace-class operator, whose trace is equal to tr $V = v(0) = ||v||_{\infty}$. Define also

$$D := H_{H} - \varepsilon_{0} = \sum_{i>0} (\varepsilon_{i} - \varepsilon_{0}) |\varphi_{i}\rangle \langle \varphi_{i}|$$
(4)

and let

$$E := \left(D^{1/2}(D+2V)D^{1/2}\right)^{1/2}. (5)$$

Since V is positive and bounded, E is well-defined on the domain of D. We note that both D and E are, by construction, positive operators, with $D\varphi_0 = E\varphi_0 = 0$. The Hartree minimizer φ_0 is the only function in their kernel, all other eigenvalues of D and E are strictly positive.

It turns out that E-D-V is a trace class operator. (We will prove this in Subsect. 5.2 below.) Let $0=e_0< e_1\le e_2\le \dots$ denote the eigenvalues of E. Our main result concerns the spectrum of the Hamiltonian H_N , and reads as follows:

Theorem 1. The ground state energy $E_0(N) = \inf \operatorname{spec} H_N$ equals

$$E_0(N) = N \int_{\mathbb{R}^d} \left(|\nabla \varphi_0(x)|^2 + V_{\text{ext}}(x)\varphi_0(x)^2 \right) dx + \frac{N+1}{2} \int_{\mathbb{R}^{2d}} \varphi_0(x)^2 v(x-y)\varphi_0(y)^2 dx \, dy - \frac{1}{2} \text{tr}(D+V-E) + O(N^{-1/2}) \,.$$
 (6)

Moreover, the spectrum of $H_N - E_0(N)$ below an energy ξ is equal to all finite sums of the form

$$\sum_{i>1} e_i n_i + O(\xi^{3/2} N^{-1/2}), \qquad (7)$$

where $n_i \in \mathbb{N}$ with $\sum_{i>1} n_i \leq N$.

The error term $O(N^{-1/2})$ in (6) stands for an expression which is bounded by a constant times $N^{-1/2}$ for large N, where the constant only depends on the interaction potential v and the gap $\varepsilon_1 - \varepsilon_0$ in the spectrum of $H_{\rm H}$; likewise for the error term $O(\xi^{3/2}N^{-1/2})$ in (7). The dependence on v is relatively complicated but could in principle be computed explicitly by following our proof; all our bounds are quantitative.

Our result is a manifestation of the fact that the Bogoliubov approximation becomes exact in the Hartree limit $N \to \infty$. In particular, as long as $\xi \ll N$, each individual excitation energy ξ is of the form $\sum_{i\geq 1} e_i n_i (1+o(1))$. This result is expected to be optimal in the following sense: if $\xi \ll N$ fails to hold then there is a non-negligible number of particles outside the condensate, violating a key assumption of Bogoliubov's approximation [7,8,26]. Hence there is no reason why the Bogoliubov approximation should predict the correct spectrum for excitation energies of order N or larger.

Remark 1. The emergence of the effective operator E in (5) can also be understood as follows. One considers the time-dependent Hartree equation $\mathrm{i}\partial_t \varphi = (-\Delta + V_\mathrm{ext} + |\varphi|^2 * v)\varphi$ and looks for solutions of the form $\varphi = e^{-\mathrm{i}\varepsilon_0 t}(\varphi_0 + u \, e^{-\mathrm{i}\omega t} + \overline{y} \, e^{\mathrm{i}\omega t})$ for some $\omega > 0$. Expanding to first order in u and y leads to the Bogoliubov-de-Gennes equations (see, e.g., [28], Eq. (5.68))

$$\begin{pmatrix} D+V & V \\ -V & -(D+V) \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \omega \begin{pmatrix} u \\ y \end{pmatrix}. \tag{8}$$

The positive values which can be assumed by ω are then interpreted as excitation energies. This is in agreement with our result: We will see below that the values for ω obtained this way are precisely the eigenvalues of E. (Compare with Remark 4 in Sect. 4.)

Theorem 1 states that the low-energy spectrum of $H_N - E_0(N)$ is, up to small errors, equal to the one of the effective operator

$$\sum_{i=1}^{N} \hat{E}_i, \quad \hat{E} = \sum_{j \ge 1} e_j |\varphi_j\rangle \langle \varphi_j|, \tag{9}$$

where the subscript i in \hat{E}_i stands for the action of the operator \hat{E} on the ith variable. Note that \hat{E} is unitarily equivalent to the operator E defined in (5). The proof of Theorem 1 actually consists of constructing an explicit unitary operator that relates $H_N - E_0(N)$ and (9). In other words, we shall bound $H_N - E_0(N)$ from above and below by a suitable unitary transform (cf. Eq. (31) below) of (9), with error terms that are small in the subspace of low energy. As a byproduct of the proof we obtain the following corollary.

Corollary 1. Let P_H^j be the projection onto the subspace spanned by the eigenfunctions corresponding to the j lowest eigenvalues of H_N (counted with multiplicity). Similarly, let $P_K^j = \sum_{k=1}^j |\psi_k\rangle \langle \psi_k|$ be the projection onto the subspace spanned by the eigenfunctions corresponding to the j lowest eigenvalues of

$$K := \mathcal{U}^{\dagger} \left(\sum_{i=1}^{N} \hat{E}_{i} \right) \mathcal{U} + 1 =: \sum_{i=1}^{\infty} k_{i} |\psi_{i}\rangle \langle \psi_{i}|$$

 $(k_1 \le k_2 \le ...)$, where \mathcal{U} is the unitary operator defined in (31). Then there is a constant C, depending only on v and $\varepsilon_1 - \varepsilon_0$, such that if $k_{j+1} > k_j$ then

$$\|P_K^j - P_H^j\|_2^2 \le C(k_j/N)^{1/2} \frac{\sum_{l=1}^j k_l}{k_{j+1} - k_j},$$

with $\|\cdot\|_2$ denoting the Hilbert-Schmidt norm.

The corollary implies, in particular, that the ground state wave function Ψ_0 of H_N satisfies

$$\|\Psi_0 - \mathcal{U}^{\dagger} \otimes_{i=1}^{N} \varphi_0\|^2 \le CN^{-1/2}$$
 (10)

(for a suitable choice of the phase factor). The presence of the unitary operator \mathcal{U} in (10) is important; we do not expect that Ψ_0 is close to $\bigotimes_{i=1}^N \varphi_0$ in an L^2 -sense for large N. (Compare with Remark 6 in Sect. 7.)

In addition, the corollary states that the eigenfunctions of H_N near the bottom of the spectrum are approximately given by \mathcal{U}^{\dagger} applied to the eigenfunctions of (9), which are symmetrized products of the eigenfunctions φ_i of $H_{\rm H}$ in (3). These functions can be obtained by applying a number, n, of raising operators $a^{\dagger}(\varphi_i)$ to the N-n particle ground state, which is simply the product $\prod_{i=1}^{N-n} \varphi_0(x_i)$. (Here we use the convenient Fock space notation of creation operators, which will be recalled in the next section.) In Subsect. 5.1, we shall also calculate $\mathcal{U}^{\dagger}a^{\dagger}(\varphi_i)\mathcal{U}$ (up to small error terms), and hence arrive at a convenient alternative characterization of the excited eigenstates of H_N . (See Remark 5 in Sect. 7.)

1.3. The translation-invariant case. It is instructive to compare Theorem 1 with the translation invariant case studied in [26], where the Bose gas is confined to the flat unit torus \mathbb{T}^d . Up to an additive constant, the Hartree operator equals the Laplacian in this case, whose eigenfunctions are conveniently labeled by the quantized momentum $p \in (2\pi\mathbb{Z})^d$, and are given explicitly by the plane waves $\varphi_p(x) = e^{\mathrm{i} p \cdot x}$. In this basis, the operators D and V can be written as

$$D = \sum_{p \in (2\pi\mathbb{Z})^d} p^2 |\varphi_p\rangle \langle \varphi_p|,$$

$$V = \sum_{p \in (2\pi\mathbb{Z})^d} \hat{v}(p) |\varphi_p\rangle \langle \varphi_p|,$$

with $\hat{v}(p) = \int_{\mathbb{T}^d} v(x)e^{-\mathrm{i}p\cdot x}dx = \hat{v}(-p)$. Since D and V commute in this case, we further have

$$E = \sum_{p \in (2\pi\mathbb{Z})^d} \sqrt{p^4 + 2p^2 \hat{v}(p)} |\varphi_p\rangle \langle \varphi_p|.$$

Hence

$$\operatorname{tr}(D+V-E) = \sum_{p \in (2\pi\mathbb{Z})^d} \left(p^2 + \hat{v}(p) - \sqrt{p^4 + 2p^2 \hat{v}(p)} \right),$$

and the eigenvalues of E are given by

$$e_p = \sqrt{p^4 + 2p^2 \hat{v}(p)},$$

yielding the well-known Bogoliubov spectrum of elementary excitations, which is linear in |p| for small momentum.

1.4. Short-range interactions. In Theorem 1, we assumed that v(x) is a bounded function. If we replace v(x) by $g\delta(x)$, then D+V-E will, in general, fail to be trace class (in fact, it is not for the above model of bosons on \mathbb{T}^d for $d \geq 2$). However, Formula (7) for the excitation spectrum still makes sense. Since all our bounds are quantitative, our proof thus shows that if v is allowed to depend on N in such a way that it converges to a δ -function, and v(0) increases with N slow enough, then the excitation spectrum is still of the form $\sum_i e_i n_i$, where e_i are the non-zero eigenvalues of E in (5), and V is now the multiplication operator $g\varphi_0(x)^2$. If v(0) increases too fast with N, though, our error bounds cease to be good enough to allow this conclusion.

Consider now the case d=3. If we write the interaction potential as $(N-1)^{-1}\lambda_N^3v_0(\lambda_Nx)$ for some fixed, N-independent v_0 , with $\lambda_N\to\infty$ as $N\to\infty$, we expect that the Bogoliubov approximation yields the correct excitation spectrum as long as λ_N increases slower than N, i.e., $\lambda_N\ll N$. If $\lambda_N\sim N$, the scattering length of the interaction potential is of the same order as the range of the interactions. This corresponds to the Gross-Pitaevskii scaling [8] of a dilute gas. In this latter case, the scattering length becomes the physically relevant parameter quantifying the interacting strength, instead of $\int_{\mathbb{R}^3} v(x) dx$. Hence we expect the following to be true.

Conjecture 1. Consider the Hamiltonian

$$H_N^{\text{GP}} := \sum_{i=1}^N (-\Delta_i + V_{\text{ext}}(x_i)) + N^2 \sum_{i < j} v(N(x_i - x_j)),$$

on $L^2(\mathbb{R}^3)^{\otimes_s N}$, with v non-negative, bounded and integrable at infinity, and denote its ground state energy by $E_0(N)$. The spectrum of $H_N^{GP}-E_0(N)$ below an energy $\xi \ll N$ is equal to finite sums of the form

$$\sum_{i>1} e_i n_i (1 + o(1))$$

for large N. Here, e_i is defined as in the Hartree case with the replacements

$$H_{\rm H} \rightsquigarrow H_{\rm GP} := -\Delta + V_{\rm ext} + 8\pi a_0 \varphi_0^2,$$

 $V \rightsquigarrow 8\pi a_0 \varphi_0^2,$

where φ_0 is now the minimizer of the Gross-Pitaevskii energy functional, and a_0 is the zero energy scattering length of the interaction potential v(x).

We expect the proof of Conjecture 1 to be more complicated than that of Theorem 1. In particular, the Bogoliubov approximation would have to be modified in such a way to account for the detailed structure of the wave function when particles are close, which gives rise to the scattering length a_0 (instead of merely its first-order Born approximation $(8\pi)^{-1} \int_{\mathbb{R}^3} v(x) dx$).

1.5. Outline. The remainder of the paper is organized as follows. In Sect. 2 we establish bounds on the number of particles outside the condensate, the N-body Hartree operator $\sum_{i=1}^{N} D_i$, and their product for a low-energy state. Section 3 shows how H_N can be bounded from above and below by what we call the Bogoliubov Hamiltonian, which is formally close to Bogoliubov's approximate quadratic Hamiltonian on Fock space, yet is particle number conserving. The diagonalization of the quadratic Hamiltonian can be achieved by a Bogoliubov transformation, which is carried out in Sect. 4. To diagonalize the actual Bogoliubov Hamiltonian we use a modification thereof, which involves the estimation of various error terms (Sect. 5). Finally, we shall complete the proof of Theorem 1 (Sect. 6) and Corollary 1 (Sect. 7).

Throughout this work a multiplicative constant C in an estimate is understood to be generic: it can have different values on each appearance. By $\|\cdot\|$ we denote the operator or vector norm, depending on context; $\|\cdot\|_1$ and $\|\cdot\|_2$ denote the trace class and Hilbert-Schmidt norms of operators, respectively.

2. Bounds on the Condensate Depletion

It is convenient to regard the N-particle Hilbert space $\mathcal{F}^{(N)} := L^2(\mathbb{R}^d)^{\otimes_s N}$, the symmetric tensor product of N one-particle Hilbert spaces $L^2(\mathbb{R}^d)$, as a subspace of the bosonic Fock space $\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)}$. The Hamiltonian H_N can then be written in second quantized form as

$$H_N = \sum_{i,j} h_{ij} a_i^{\dagger} a_j + \frac{1}{2(N-1)} \sum_{i,j,k,l} v_{ijkl} a_j^{\dagger} a_i^{\dagger} a_k a_l, \tag{11}$$

where

$$h_{ij} := \langle \varphi_i | -\Delta + V_{\text{ext}} | \varphi_j \rangle$$
 and $v_{ijkl} := \langle \varphi_i, \varphi_j | v | \varphi_k, \varphi_l \rangle$.

Recall that the set $\{\varphi_i\}_{i\in\mathbb{N}}$ denotes the orthonormal basis of eigenfunctions of H_H in (3), which we can all assume to be chosen *real* without loss of generality. The operators a_i^{\dagger} and a_i in (11) are the usual creation and annihilation operators corresponding to these functions, i.e., $a_i := a(\varphi_i)$.

To be precise, H_N in (1) agrees with the right side of (11) on the subspace $\mathcal{F}^{(N)}$. We shall always work on this subspace, and use Fock space notation only for convenience. In particular, unless stated otherwise, all subsequent identities and inequalities involving operators on Fock space are understood as holding on $\mathcal{F}^{(N)}$ only.

We introduce the rank-one projection $P = |\varphi_0\rangle \langle \varphi_0|$ and the complementary projection Q = 1 - P. The operator that counts the number of particles outside the Hartree ground state is the second quantization $d\Gamma(Q)$ of Q and will be denoted by $N^>$, i.e.

$$N^{>} = \sum_{i=1}^{N} Q_i = \sum_{i} a_i^{\dagger} a_i.$$

Here and in the following, \sum' denotes a sum over all nonzero indices. Another important quantity is the following *N*-body Hartree operator,

$$T_{H} := \sum_{i=1}^{N} \left(-\Delta_{i} + V_{\text{ext}}(x_{i}) + (v * \varphi_{0}^{2})(x_{i}) - \varepsilon_{0} \right) = d\Gamma(D), \tag{12}$$

with D defined in (4).

The following lemma gives simple bounds on the ground state energy of H_N , as well as on the expectation values of $N^>$ and T_H in low-energy states.

Lemma 1. The ground state energy $E_0(N)$ of H_N satisfies the bounds

$$0 \ge E_0(N) - Nh_{00} - \frac{N}{2}v_{0000} \ge \frac{1}{2}v_{0000} - \frac{N}{2(N-1)}v(0).$$

Moreover, for any N-particle state Ψ with $\langle \Psi | H_N | \Psi \rangle \leq Nh_{00} + \frac{N}{2}v_{0000} + \mu$, we have

$$(\varepsilon_1 - \varepsilon_0) \langle \Psi | N^> | \Psi \rangle \le \langle \Psi | T_H | \Psi \rangle \le \mu + \frac{N}{2(N-1)} v(0) - \frac{v_{0000}}{2}. \tag{13}$$

Recall that ε_0 and ε_1 denote the lowest two eigenvalues of the Hartree operator H_H in (3). We emphasize that $\varepsilon_1 - \varepsilon_0 > 0$.

Proof. For the upper bound we use the trial function $|N, 0, ...\rangle$ denoting a state where all particles occupy the ground state of the Hartree operator H_H . This yields

$$E_{0}(N) \leq \sum_{i,j} h_{ij} \langle N, 0, \dots | a_{i}^{\dagger} a_{j} | N, 0, \dots \rangle$$

$$+ \frac{1}{2(N-1)} \sum_{i,j,k,l} v_{ijkl} \langle N, 0, \dots | a_{j}^{\dagger} a_{i}^{\dagger} a_{k} a_{l} | N, 0, \dots \rangle$$

$$= Nh_{00} + \frac{N}{2} v_{0000}.$$

For the lower bound we exploit the positive definiteness of the interaction potential v in the following way. With $\psi(x) = \varphi_0^2(x) - \frac{1}{N-1} \sum_{i=1}^N \delta(x - x_i)$, we have

$$0 \le \int_{\mathbb{R}^{2d}} \psi(x)v(x-y)\psi(y)dxdy$$

$$= v_{0000} - \frac{2}{N-1} \sum_{i=1}^{N} (v * \varphi_0^2)(x_i) + \frac{1}{(N-1)^2} \sum_{i=1}^{N} v(x_i - x_j). \tag{14}$$

Put differently, this inequality reads

$$\frac{1}{N-1} \sum_{i < j} v(x_i - x_j) \ge -\frac{N-1}{2} v_{0000} + \sum_{i=1}^{N} (v * \varphi_0^2)(x_i) - \frac{N}{2(N-1)} v(0). \tag{15}$$

Since $\varepsilon_0 = h_{00} + v_{0000}$, we hence have

$$H_N \ge \sum_{i=1}^{N} \left(-\Delta_i + V_{\text{ext}}(x_i) + (v * \varphi_0^2)(x_i) \right) - \frac{N-1}{2} v_{0000} - \frac{N}{2(N-1)} v(0)$$

$$= T_{\text{H}} + N h_{00} + \frac{N+1}{2} v_{0000} - \frac{N}{2(N-1)} v(0).$$

The asserted bounds now follow, since $T_{\rm H} \ge (\varepsilon_1 - \varepsilon_0) N^> \ge 0$.

Remark 2. The proof actually shows the operator inequality

$$T_{\rm H} \le H_N - Nh_{00} - \frac{N+1}{2}v_{0000} + \frac{N}{2(N-1)}v(0)$$

from which (13) readily follows.

In our analysis we shall also need bounds on the expectation value of the product $N^{>}T_{\rm H}$ for a low-energy state. Such a bound is the content of Lemma 2.

Lemma 2. Let Ψ be an N-particle wave function in the spectral subspace of H_N corresponding to an energy $E \leq E_0(N) + \mu$. Then

$$\begin{split} (\varepsilon_1 - \varepsilon_0) \left< \Psi \right| N^> T_H \left| \Psi \right> & \leq (\mu - v_{0000} + 3v(0)) \left(\mu + \frac{N}{2(N-1)} v(0) - \frac{v_{0000}}{2} \right) \\ & + \frac{1}{4} (2v(0) + \mu)^2. \end{split}$$

Remark 3. A slight modification of the proof yields the operator inequality

$$(\varepsilon_1 - \varepsilon_0)N^{>}T_{\rm H} \le (3v(0) - v_{0000})T_{\rm H} + 2v(0)^2 + 2(H_N - E_0(N))^2$$
.

Proof. We write

$$\langle \Psi | N^{>} T_{\mathrm{H}} | \Psi \rangle = \langle \Psi | N^{>} S | \Psi \rangle + \left\langle \Psi \left| N^{>} \left(H_{N} - E_{0}(N) - \frac{\mu}{2} \right) \right| \Psi \right\rangle,$$

where $S = \sum_{i=1}^{N} (v * \varphi_0^2)(x_i) - N\varepsilon_0 - \frac{1}{N-1} \sum_{i < j} v(x_i - x_j) + \frac{\mu}{2} + E_0(N)$. The second term can be bounded by Schwarz's inequality as

$$\left|\left\langle \Psi \left| N^{>} \left(H_{N} - E_{0}(N) - \frac{\mu}{2} \right) \right| \Psi \right\rangle \right| \leq \frac{\mu}{2} \left\langle \Psi \right| (N^{>})^{2} \left| \Psi \right\rangle^{1/2}.$$

For the first we use the permutation symmetry of Ψ and get

$$\langle \Psi | N^{>} S | \Psi \rangle = N \langle \Psi | Q_1 S | \Psi \rangle$$
.

We split S into two parts, $S = S_a + S_b$, where

$$S_a := \sum_{i=2}^{N} (v * \varphi_0^2)(x_i) - N\varepsilon_0 - \frac{1}{N-1} \sum_{2 \le i < j} v(x_i - x_j) + \frac{\mu}{2} + E_0(N),$$

$$S_b := (v * \varphi_0^2)(x_1) - \frac{1}{N-1} \sum_{i=2}^{N} v(x_1 - x_i).$$

Using positive definiteness of v as in (14), this time for $\psi(x) = \varphi_0^2(x) - \frac{1}{N-1} \sum_{i=2}^{N} \delta(x - x_i)$, we obtain

$$\frac{1}{N-1} \sum_{2 \le i < j} v(x_i - x_j) \ge -\frac{(N-1)}{2} v_{0000} + \sum_{i=2}^{N} (v * \varphi_0^2)(x_i) - \frac{v(0)}{2}.$$

In combination with the upper bound on $E_0(N)$ in Lemma 1 this implies that

$$S_a \le \frac{1}{2} \left(v(0) - v_{0000} + \mu \right) .$$

In particular, since S_a commutes with Q_1 , we have

$$N \left\langle \Psi \right| Q_1 S_a \left| \Psi \right\rangle \leq \frac{1}{2} \left(v(0) - v_{0000} + \mu \right) \left\langle \Psi \right| N^{>} \left| \Psi \right\rangle.$$

To bound the contribution of S_b , we compute

$$\begin{split} \langle \Psi | \, Q_1 S_b \, | \Psi \rangle &= \langle \Psi | \, Q_1 \left[(v * \varphi_0^2)(x_1) - v(x_1 - x_2) \right] | \Psi \rangle \\ &= \langle \Psi | \, Q_1 Q_2 \left[(v * \varphi_0^2)(x_1) - v(x_1 - x_2) \right] | \Psi \rangle \\ &+ \langle \Psi | \, Q_1 P_2 \left[(v * \varphi_0^2)(x_1) - v(x_1 - x_2) \right] P_2 \, | \Psi \rangle \\ &+ \langle \Psi | \, Q_1 P_2 \left[(v * \varphi_0^2)(x_1) - v(x_1 - x_2) \right] Q_2 \, | \Psi \rangle \, . \end{split}$$

The second term on the right side of the last equation vanishes. For the first and the third, we use Schwarz's inequality and $|(v*\varphi_0^2(x_1)-v(x_1-x_2)|\leq v(0)$ to conclude

$$|\left\langle \Psi\right|\,Q_{1}S_{b}\,|\Psi\rangle\,|\leq v(0)\,\langle\Psi|\,Q_{1}Q_{2}\,|\Psi\rangle^{1/2}+v(0)\,\langle\Psi|\,Q_{1}\,|\Psi\rangle\,.$$

Since

$$N^2 \langle \Psi | Q_1 Q_2 | \Psi \rangle \le \langle \Psi | (N^>)^2 | \Psi \rangle$$

we have thus shown that

$$\begin{split} \langle \Psi | \, N^{>} T_{\rm H} \, | \Psi \rangle & \leq \frac{1}{2} \left(\mu - v_{0000} + 3 v(0) \right) \langle \Psi | \, N^{>} \, | \Psi \rangle \\ & + \frac{1}{2} \left(2 v(0) + \mu \right) \langle \Psi | \, (N^{>})^{2} \, | \Psi \rangle^{1/2} \, . \end{split}$$

Using $T_{\rm H} \ge (\varepsilon_1 - \varepsilon_0) N^{>}$ this implies

$$\langle \Psi | N^{>} T_{\rm H} | \Psi \rangle \le (\mu - v_{0000} + 3v(0)) \langle \Psi | N^{>} | \Psi \rangle + \frac{1}{4} \frac{(2v(0) + \mu)^{2}}{\varepsilon_{1} - \varepsilon_{0}}.$$

The result then follows from Lemma 1. \Box

3. The Bogoliubov Hamiltonian

The well-known Bogoliubov approximation [7] consists of replacing the operators a_0 and a_0^{\dagger} in (11) by \sqrt{N} , and dropping all terms higher than quadratic in the a_i and a_i^{\dagger} for $i \geq 1$. The resulting Bogoliubov Hamiltonian does not preserve particle number and is thus not suitable as an approximation to the full Hamiltonian H_N , as far as operator inequalities are concerned. To circumvent this problem, we work with the following modification of the Bogoliubov Hamiltonian. For $i \geq 1$, we introduce the operators

$$b_i := \frac{a_i a_0^{\dagger}}{\sqrt{N-1}},$$

and we define the Bogoliubov Hamiltonian as

$$H_{\text{Bog}} := \sum_{i} \left(\varepsilon_{i} - \varepsilon_{0} \right) b_{i}^{\dagger} b_{i} + \frac{1}{2} \sum_{i,j} \left(2b_{i}^{\dagger} b_{j} + b_{i} b_{j} + b_{j}^{\dagger} b_{i}^{\dagger} \right), \tag{16}$$

where $V_{ij} = v_{00ij} = \langle \varphi_i | V | \varphi_j \rangle$. Note that this operator preserves the number of particles, hence we can study its restriction to $\mathcal{F}^{(N)}$, the sector of N particles. The price to pay, as compared with the usual Bogoliubov Hamiltonian, is that the b_i , b_i^{\dagger} do not satisfy canonical commutation relations, making it harder to determine the spectrum of H_{Bog} .

In the following, we shall investigate the relation between H_N and H_{Bog} . In particular, we shall derive upper and lower bounds on H_N in terms of H_{Bog} , which are stated in Eqs. (19) and (21), respectively. The error terms in (20) and (22) are small in the low-energy sector.

3.1. Lower bound. Using the positivity of the interaction potential v, a Schwarz inequality on $\mathcal{F}^{(2)}$ yields

$$(P \otimes Q + Q \otimes P)vQ \otimes Q + Q \otimes Qv(P \otimes Q + Q \otimes P)$$

$$> -\varepsilon(P \otimes Q + Q \otimes P)v(P \otimes Q + Q \otimes P) - \varepsilon^{-1}Q \otimes QvQ \otimes Q.$$

Consequently,

$$v \geq P \otimes PvP \otimes P + P \otimes PvQ \otimes Q + Q \otimes QvP \otimes P + (1 - \varepsilon)(P \otimes Q + Q \otimes P)v(P \otimes Q + Q \otimes P) + (1 - \varepsilon^{-1})Q \otimes QvQ \otimes Q + P \otimes PvP \otimes Q + P \otimes PvQ \otimes P + P \otimes QvP \otimes P + Q \otimes PvP \otimes P$$
(17)

for any $\varepsilon > 0$. The last term in the second line can be bounded from below by $(1 - \varepsilon^{-1})v(0)Q \otimes Q$ as long as $\varepsilon \leq 1$ which we shall assume henceforth. We remark that in the case of translation invariance the terms in the last line vanish due to momentum conservation, but this is not the case here.

In second quantized language, the bound (17) implies that H_N is bounded from below by the operator

$$\sum_{i,j}' h_{ij} a_i^{\dagger} a_j + \sqrt{N-1} \sum_{i}' h_{i0} \left(b_i^{\dagger} + b_i \right) + h_{00}(N-N^{>}) + v_{0000} \frac{(N-N^{>})(N-N^{>}-1)}{2(N-1)} + \frac{1}{2} \sum_{i,j}' V_{ij} \left(b_i b_j + b_j^{\dagger} b_i^{\dagger} \right)$$

$$+\frac{1-\varepsilon}{N-1} \sum_{i,j} \left(v_{0i0j} + V_{ij} \right) a_i^{\dagger} a_0^{\dagger} a_j a_0 + (1-\varepsilon^{-1}) \frac{N^{>}(N^{>}-1)v(0)}{2(N-1)} + \sum_i \left(\frac{v_{i000}}{\sqrt{N-1}} \left(b_i(N-N^{>}) + (N-N^{>})b_i^{\dagger} \right) \right),$$
(18)

restricted to the N-particle sector. We note that

$$\sum_{i,j}' (h_{ij} - \varepsilon_0 \delta_{ij}) b_i^{\dagger} b_j = \sum_{i,j}' (h_{ij} - \varepsilon_0 \delta_{ij}) a_i^{\dagger} a_j \frac{N - N^{>} + 1}{N - 1}$$

$$= \sum_{i,j}' (h_{ij} - \varepsilon_0 \delta_{ij}) a_i^{\dagger} a_j + \frac{2 - N^{>}}{N - 1} \sum_{i,j}' (h_{ij} - \varepsilon_0 \delta_{ij}) a_i^{\dagger} a_j.$$

Since $D - v(0) \le -\Delta + V_{\text{ext}} - \varepsilon_0 \le D$, we can bound the last term as

$$\frac{2-N^{>}}{N-1} \sum_{i,j} (h_{ij} - \varepsilon_0 \delta_{ij}) a_i^{\dagger} a_j \leq \frac{1}{N-1} T_{\rm H} + v(0) \frac{(N^{>})^2}{N}.$$

This bound can be easily verified by investigating separately the sectors of different values of $N^>$. (In particular, note that $T_{\rm H}=0$ on the subspace where $N^>=0$, for instance.)

We also have

$$\begin{split} &\frac{1-\varepsilon}{N-1} \sum_{i,j}^{'} \left(v_{0i0j} + V_{ij} \right) a_i^{\dagger} a_0^{\dagger} a_j a_0 \\ &= \sum_{i,j}^{'} \left(v_{0i0j} + V_{ij} \right) b_i^{\dagger} b_j - \frac{1+\varepsilon(N-N^{>})}{N-1} \sum_{i,j}^{'} \left(v_{0i0j} + V_{ij} \right) a_i^{\dagger} a_j \\ &\geq \sum_{i,j}^{'} \left(v_{0i0j} + V_{ij} \right) b_i^{\dagger} b_j - 2v(0) \frac{N^{>} + \varepsilon N^{>} (N-N^{>})}{N-1}, \end{split}$$

where we have used that V as well as multiplication with $v * \varphi_0^2$ are bounded operators with norm bounded by v(0). Using $\varepsilon_0 = h_{00} + v_{0000}$ one verifies that

$$\begin{split} \varepsilon_0 N^> + h_{00}(N-N^>) + v_{0000} \frac{(N-N^>)(N-N^>-1)}{2(N-1)} + (1-\varepsilon^{-1}) \frac{N^>(N^>-1)v(0)}{2(N-1)} \\ &= N h_{00} + \frac{N}{2} v_{0000} + ((1-\varepsilon^{-1})v(0) + v_{0000}) \frac{N^>(N^>-1)}{2(N-1)} \,. \end{split}$$

The Hartree equation (2) implies $h_{i0} + v_{i000} = 0$ for $i \neq 0$, hence we have

$$\sqrt{N-1} \sum_{i}' h_{i0} \left(b_{i}^{\dagger} + b_{i} \right) + \sum_{i}' \frac{v_{i000}}{\sqrt{N-1}} \left(b_{i} (N-N^{>}) + (N-N^{>}) b_{i}^{\dagger} \right)
= \sum_{i}' \frac{v_{i000}}{\sqrt{N-1}} \left(b_{i} (1-N^{>}) + (1-N^{>}) b_{i}^{\dagger} \right).$$

This last expression can be bounded by Schwarz's inequality: for any $\zeta > 0$ one has

$$\begin{split} -\frac{(1-N^{>})^{2}}{\zeta\sqrt{N-1}} - \zeta v(0)^{2} \frac{NN^{>}}{(N-1)^{3/2}} &\leq \sum_{i} \frac{v_{i000}}{\sqrt{N-1}} \left(b_{i}(1-N^{>}) + (1-N^{>})b_{i}^{\dagger} \right) \\ &\leq \frac{(1-N^{>})^{2}}{\zeta\sqrt{N-1}} + \zeta v(0)^{2} \frac{NN^{>}}{(N-1)^{3/2}}. \end{split}$$

Here we made use of

$$\sum_{i} |v_{i000}|^2 = \langle \varphi_0 | v * \varphi_0 Q v * \varphi_0^2 | \varphi_0 \rangle \le v(0)^2.$$

What these computations show is that

$$H_N \ge H_{\text{Bog}} + Nh_{00} + \frac{N}{2}v_{0000} - E_{\varepsilon},$$
 (19)

where

$$E_{\varepsilon} = -\left((1 - \varepsilon^{-1})v(0) + v_{0000}\right) \frac{N^{>}(N^{>} - 1)}{2(N - 1)} + \frac{1}{N - 1}T_{H} + v(0)\frac{(N^{>})^{2}}{N} + \frac{(1 - N^{>})^{2}}{\zeta\sqrt{N - 1}} + \zeta v(0)^{2}N^{>}\frac{N}{(N - 1)^{3/2}} + 2v(0)\frac{1 + \varepsilon N}{N - 1}N^{>}$$

$$\leq C\left(\left(\varepsilon^{-1}N^{-1} + \zeta^{-1}N^{-1/2}\right)(N^{>} + 1)(T_{H} + 1) + (N^{-1} + \varepsilon + \zeta N^{-1/2})(T_{H} + 1)\right).$$
(20)

3.2. Upper bound. The upper bound on H_N follows essentially the same lines as the lower bound in the previous subsection. By Schwarz's inequality,

$$(P \otimes Q + Q \otimes P)vQ \otimes Q + Q \otimes Qv(P \otimes Q + Q \otimes P)$$

$$\leq \varepsilon(P \otimes Q + Q \otimes P)v(P \otimes Q + Q \otimes P) + \varepsilon^{-1}Q \otimes QvQ \otimes Q,$$

and hence

$$v \leq P \otimes PvP \otimes P + P \otimes PvQ \otimes Q + Q \otimes QvP \otimes P$$
$$+(1+\varepsilon)(P \otimes Q + Q \otimes P)v(P \otimes Q + Q \otimes P) + (1+\varepsilon^{-1})v(0)Q \otimes Q$$
$$+P \otimes PvP \otimes Q + P \otimes PvQ \otimes P + P \otimes QvP \otimes P + Q \otimes PvP \otimes P$$

for any $\varepsilon > 0$. This means that H_N is bounded from above by the expression (18) with ε exchanged for $-\varepsilon$. Using

$$\sum_{i,j}' \left(h_{ij} - \varepsilon_0 \delta_{ij} \right) a_i^{\dagger} a_j = \sum_{i,j}' \left(h_{ij} - \varepsilon_0 \delta_{ij} \right) b_i^{\dagger} b_j + \frac{N^{>} - 2}{N - 1} \sum_{i,j}' \left(h_{ij} - \varepsilon_0 \delta_{ij} \right) a_i^{\dagger} a_j$$

$$\leq \sum_{i,j}' \left(h_{ij} - \varepsilon_0 \delta_{ij} \right) b_i^{\dagger} b_j + \frac{N^{>} T_{\mathrm{H}}}{N} + v(0) \frac{N^{>}}{N - 1},$$

we obtain

$$H_N \le H_{\text{Bog}} + Nh_{00} + \frac{N}{2}v_{0000} + F_{\varepsilon},$$
 (21)

where

$$F_{\varepsilon} = \frac{N^{>}T_{\rm H}}{N} + v(0)\frac{3 + 2\varepsilon N}{N - 1}N^{>} + ((1 + \varepsilon^{-1})v(0) + v_{0000})\frac{N^{>}(N^{>} - 1)}{2(N - 1)}$$

$$+ \frac{(1 - N^{>})^{2}}{\zeta\sqrt{N - 1}} + \zeta v(0)^{2}N^{>}\frac{N}{(N - 1)^{3/2}}$$

$$\leq C\left(\left(N^{-1} + \zeta^{-1}N^{-1/2} + \varepsilon^{-1}N^{-1}\right)(N^{>} + 1)(T_{\rm H} + 1)$$

$$+ \left(\varepsilon + \zeta N^{-1/2} + N^{-1}\right)(N^{>} + 1)^{1/2}(T_{\rm H} + 1)^{1/2}\right). \tag{22}$$

Here we have again used that $N^>$ can be bounded by T_H , and similarly for their square roots. To proceed with the analysis in Sect. 6.2, it is convenient to work with the bound (22) on F_{ε} , involving only the operator $(N^> + 1)(T_H + 1)$ and its square root.

4. Symplectic Diagonalization

In order to investigate the spectrum of the Bogoliubov Hamiltonian H_{Bog} in (16), it is useful to consider first the usual Bogoliubov Hamiltonian, which is the formal quadratic expression

$$\tilde{H}_{\text{Bog}} = \frac{1}{2} \left((a^{\dagger})^{\mathsf{T}}, a^{\mathsf{T}} \right) \begin{pmatrix} D + V & V \\ V & D + V \end{pmatrix} \begin{pmatrix} a \\ a^{\dagger} \end{pmatrix}. \tag{23}$$

It is convenient to use a matrix notation where

$$a = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}, \quad a^{\dagger} = \begin{pmatrix} a_1^{\dagger} \\ a_2^{\dagger} \\ \vdots \end{pmatrix},$$

and ${}^\intercal$ denotes transposition; e.g., $a{}^\intercal D a^\dagger$ stands for $\sum_{i,j}' \langle \varphi_i | D | \varphi_j \rangle a_i a_j^\dagger$, $(a^\dagger){}^\intercal V a$ stands for $\sum_{i,j}' V_{ij} a_i^\dagger a_j$, etc. The operator \tilde{H}_{Bog} is symmetric since V has real matrix elements with respect to the basis $\{\varphi_i\}_{i\in\mathbb{N}}$. Equation (23) is only a formal expression; in particular, it has an infinite ground state energy. It also does not preserve the particle number and hence cannot be restricted to the sector of N particles. Nevertheless, it serves as a useful device to motivate our analysis below leading to an approximate diagonalization of the actual Bogoliubov Hamiltonian H_{Bog} .

We introduce the Segal field operators $\phi = (\phi_1, \phi_2, \dots)^T, \pi = (\pi_1, \pi_2, \dots)^T$, which are given by

$$\begin{pmatrix} a \\ a^{\dagger} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{i} \\ 1 & -\mathrm{i} \end{pmatrix} \begin{pmatrix} \phi \\ \pi \end{pmatrix} =: T \begin{pmatrix} \phi \\ \pi \end{pmatrix}.$$

They satisfy the commutation relations

$$[\phi_i, \phi_j] = [\pi_i, \pi_j] = 0, \quad [\phi_i, \pi_j] = i\delta_{ij}.$$

These remain invariant under symplectic transformations S, which satisfy

$$S^{\mathsf{T}}JS = J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

We can write

$$\tilde{H}_{\mathrm{Bog}} = \left(\phi^{\mathsf{T}}, \pi^{\mathsf{T}}\right) M \begin{pmatrix} \phi \\ \pi \end{pmatrix},$$

where

$$M:=\frac{1}{2}\,T^*\begin{pmatrix}D+V&V\\V&D+V\end{pmatrix}T=\frac{1}{2}\begin{pmatrix}D+2V&0\\0&D\end{pmatrix}.$$

Here and in the following, we shall use * for the adjoint of an operator on the one-particle space $\mathcal{F}^{(1)}$ or the doubled space $\mathcal{F}^{(1)} \oplus \mathcal{F}^{(1)}$, while we use † for the adjoint of an operator on Fock space.

In order to diagonalize \tilde{H}_{Bog} we thus have to symplectically diagonalize M. To do so we introduce a real unitary operator U_0 such that

$$\hat{E} = U_0^* E U_0$$

is diagonal with ordered eigenvalues, i.e. $\hat{E} = \sum_{i}' e_{i} |\varphi_{i}\rangle \langle \varphi_{i}|$ with $0 < e_{1} \le e_{2} \le \ldots$ On the subspace $QL^{2}(\mathbb{R}^{d})$, the operators D, E and \hat{E} are invertible, and we denote their inverse by D^{-1} , E^{-1} and \hat{E}^{-1} for simplicity, i.e., $D^{-1} = Q(QD)^{-1}$, etc.

With

$$S = \begin{pmatrix} D^{1/2} & 0 \\ 0 & D^{-1/2} \end{pmatrix} \begin{pmatrix} U_0 & 0 \\ 0 & U_0 \end{pmatrix} \begin{pmatrix} \hat{E}^{-1/2} & 0 \\ 0 & \hat{E}^{1/2} \end{pmatrix} = \begin{pmatrix} AU_0 & 0 \\ 0 & BU_0 \end{pmatrix}, \quad (24)$$

where $A := D^{1/2}E^{-1/2}$ and $B := (A^{-1})^*$, we then have $S^{T} = S^*$ and

$$S^*MS = \frac{1}{2} \begin{pmatrix} \hat{E} & 0 \\ 0 & \hat{E} \end{pmatrix}.$$

This corresponds to a Hamiltonian consisting of sums of independent harmonic oscillators of the form $\phi_i^2 + \pi_i^2$, and hence yields the desired diagonalization of \tilde{H}_{Bog} .

Remark 4. As claimed in Remark 1 in Sect. 1.2, it is not difficult to see that the positive eigenvalues ω in (8) are precisely the eigenvalues of E. With

$$I := \begin{pmatrix} -\mathbf{i} & 0 \\ 0 & \mathbf{i} \end{pmatrix},$$

Eq. (8) can be written as

$$2iITMT^*\psi = \omega\psi$$
,

where we denote $\psi = (u, y)^{\mathsf{T}}$ for short. If we multiply this from the left with ITS^*JT^* , using $T^*I = JT^*$ and $S^*J = JS^{-1}$, we obtain the equation

$$2iITS^*MST^*\chi = \omega\chi,$$

with $\chi = T S^{-1} T^* \psi$. This latter equation is simply

$$\begin{pmatrix} \hat{E} & 0 \\ 0 & -\hat{E} \end{pmatrix} \chi = \omega \chi \,,$$

hence ω is indeed an eigenvalue of \hat{E} , as claimed.

The formal considerations above serve as a starting point of our analysis. Using S in (24), we define particle number preserving operators $c = (c_1, c_2, ...)$ by

$$\begin{pmatrix} b \\ b^{\dagger} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \begin{pmatrix} AU_0 & 0 \\ 0 & BU_0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} c \\ c^{\dagger} \end{pmatrix}$$
$$= \frac{1}{2} \begin{pmatrix} AU_0 + BU_0 & AU_0 - BU_0 \\ AU_0 - BU_0 & AU_0 + BU_0 \end{pmatrix} \begin{pmatrix} c \\ c^{\dagger} \end{pmatrix}. \tag{25}$$

Note that the operators A, B and U_0 are all real, hence c_j^{\dagger} is indeed the adjoint of c_j . By inverting S one easily obtains the inverse transformation law

$$\begin{pmatrix} c \\ c^{\dagger} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} U_0^* A^{-1} + U_0^* B^{-1} & U_0^* A^{-1} - U_0^* B^{-1} \\ U_0^* A^{-1} - U_0^* B^{-1} & U_0^* A^{-1} + U_0^* B^{-1} \end{pmatrix} \begin{pmatrix} b \\ b^{\dagger} \end{pmatrix}. \tag{26}$$

We can rewrite the Bogoliubov Hamiltonian

$$H_{\text{Bog}} = (b^{\dagger})^{\mathsf{T}} (D + V) b + \frac{1}{2} b^{\mathsf{T}} V b + \frac{1}{2} (b^{\dagger})^{\mathsf{T}} V b^{\dagger}$$
 (27)

as a quadratic operator in these c, c^{\dagger} . Here, $(b^{\dagger})^{\mathsf{T}} V b = \sum_{i,j}' V_{ij} b_i^{\dagger} b_j$, etc. We insert (25) into (27) and obtain

$$H_{\text{Bog}} = \sum_{i} {'e_{i}c_{i}^{\dagger}c_{i}} - \sum_{i,j} {'\left(U_{0}^{*}\left(Y - \frac{E}{2}\right)U_{0}\right)_{ij}} [c_{i}, c_{j}^{\dagger}]$$

$$-\frac{1}{2} \sum_{i,j} {'Z_{ij}\left([c_{j}, c_{i}] + [c_{i}^{\dagger}, c_{j}^{\dagger}]\right)} =: \text{(I)+(II)+(III)},$$
(28)

where

$$Y := \frac{1}{4}E^{1/2}D^{-1/2}(D+V)D^{1/2}E^{-1/2} + \text{h.c.}$$

and

$$Z := \frac{1}{4} U_0^* \left[(A - B)^* (D + V) (A + B) + \frac{1}{2} (A + B)^* V (A + B) + \frac{1}{2} (A - B)^* V (A - B) \right] U_0$$

$$= \frac{1}{4} U_0^* \left[A^* (D + 2V) A - B^* D B - B^* (D + V) A + A^* (D + V) B \right] U_0$$

$$= \frac{1}{4} U_0^* \left[A^* (D + V) B - B^* (D + V) A \right] U_0.$$

Note that Z is antisymmetric and hence

$$\sum_{i,j} Z_{ij} c_i c_j = \frac{1}{2} \sum_{i,j} Z_{ij} c_i c_j - \frac{1}{2} \sum_{i,j} Z_{ji} c_i c_j = -\frac{1}{2} \sum_{i,j} Z_{ji} [c_i, c_j].$$

To arrive at (28), we have used that

$$\frac{1}{4} \left[(A+B)^*(D+V)(A+B) + \frac{1}{2}(A-B)^*V(A+B) + \frac{1}{2}(A+B)^*V(A-B) \right]
= \frac{1}{4} \left[(A+B)^*(D+V)(A+B) + A^*VA - B^*VB \right]
= \frac{1}{4} \left[A^*(D+2V)A + B^*DB + B^*(D+V)A + A^*(D+V)B \right]
= \frac{1}{2}E + \frac{1}{4} \left[B^*(D+V)A + A^*(D+V)B \right]
= \frac{1}{2}E + Y$$

and

$$\begin{split} &\frac{1}{4} \left[(A - B)^* (D + V)(A - B) + \frac{1}{2} (A + B)^* V(A - B) + \frac{1}{2} (A - B)^* V(A + B) \right] \\ &= \frac{1}{4} \left[(A - B)^* (D + V)(A - B) + A^* V A - B^* V B \right] \\ &= \frac{1}{4} \left[A^* (D + 2V)A + B^* D B - B^* (D + V)A - A^* (D + V)B \right] \\ &= \frac{1}{2} E - \frac{1}{4} \left[B^* (D + V)A + A^* (D + V)B \right] \\ &= \frac{1}{2} E - Y \,. \end{split}$$

5. Bounds on the Bogoliubov Hamiltonian

To prove Theorem 1 we derive upper and lower bounds for the various terms (I)–(III) in (28). This yields a bound on H_{Bog} in terms of an operator whose spectrum is explicit, as well as errors which are small for large N in the low-energy sector. More specifically we shall prove:

Proposition 1. The three terms in (28) have the following properties. There exists a unitary operator $\mathcal{U}: \mathcal{F}^{(N)} \to \mathcal{F}^{(N)}$ (explicitly given in (31) below) such that the following bounds hold on $\mathcal{F}^{(N)}$:

(I): For arbitrary $\lambda > 0$ we have

$$\sum_{i}' e_{i} c_{i}^{\dagger} c_{i} \geq (1 - \lambda) \mathcal{U}^{\dagger} \left(\sum_{i}' e_{i} a_{i}^{\dagger} a_{i} \right) \mathcal{U} - C(1 + \lambda^{-1}) N^{-1} (N^{>} + 1) (T_{H} + 1) ,$$

$$\sum_{i}' e_{i} c_{i}^{\dagger} c_{i} \leq (1 + \lambda) \mathcal{U}^{\dagger} \left(\sum_{i}' e_{i} a_{i}^{\dagger} a_{i} \right) \mathcal{U} + C(1 + \lambda^{-1}) N^{-1} (N^{>} + 1) (T_{H} + 1) .$$

(II): D + V - E is a trace class operator, and

$$\begin{split} &-CN^{-1}(T_H+1) \\ &\leq 2\sum_{i,j}{'} \left(U_0^* \left(Y-\frac{E}{2}\right) U_0\right)_{ij} [c_i,c_j^{\dagger}] - \operatorname{tr}(D+V-E) + v_{0000} \\ &\leq CN^{-1}(T_H+1) \,. \end{split}$$

(III):

$$-CN^{-1}T_H \leq \sum_{i,j}' Z_{ij} \left([c_j, c_i] + [c_i^{\dagger}, c_j^{\dagger}] \right) \leq CN^{-1}T_H.$$

The following three subsections contain the proof of this proposition.

5.1. Proof of Proposition 1 (I). We first refine the symplectic transformation S. By polar decomposition there is a unitary W_0 such that $A = |A^*|W_0 = W_0|A|$. Since

$$|B^*| = |A^{-1}| = |A^*|^{-1}, (29)$$

also $B = |B^*|W_0$. Hence

$$S = \begin{pmatrix} |A^*|W_0U_0 & 0 \\ 0 & |B^*|W_0U_0 \end{pmatrix} =: \tilde{S} \begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix},$$

where $W = W_0 U_0$. The transformation

$$\begin{pmatrix} W & 0 \\ 0 & W \end{pmatrix}$$
(30)

is implementable on \mathcal{F} by a unitary $\mathcal{W} = \Gamma(W)$, as it corresponds to a change of basis of the one-particle Hilbert space $L^2(\mathbb{R}^d)$. We define the real, bounded, and positive operator

$$\alpha := \log\left(|A^*|^{-1}\right).$$

Note that $\log |B^*| = \alpha$ due to (29). One can show that for any $t \in \mathbb{R}$ the symplectic transformation

$$\tilde{S}_t := \begin{pmatrix} e^{-t\alpha} & 0 \\ 0 & e^{t\alpha} \end{pmatrix}$$

is implemented on Fock space \mathcal{F} by $\mathrm{e}^{X_a t}$ where

$$X_a := \frac{1}{2} \sum_{i,j} \alpha_{ij} (a_i^{\dagger} a_j^{\dagger} - a_i a_j).$$

However, it is important to note that $e^{X_a t}$ does not preserve the particle number, and hence we shall instead work with e^{Xt} , where

$$X := \frac{1}{2} \sum_{i,j} \alpha_{ij} (b_i^{\dagger} b_j^{\dagger} - b_i b_j).$$

We will repeatedly need the following facts.

Lemma 3. (i) *V* is a positive trace class operator.

- (ii) A 1 and B 1 are Hilbert-Schmidt operators.
- (iii) α is a Hilbert-Schmidt operator.
- (iv) iX : $\mathcal{F}^{(N)} \to \mathcal{F}^{(N)}$ is a symmetric bounded operator.

The proof of this lemma will be given at the end of this subsection. The lemma implies that

$$\mathcal{U} := \mathcal{W}^{\dagger} e^{X} \tag{31}$$

(with \mathcal{W} defined just after (30)) is a particle number preserving unitary transformation on the Fock space \mathcal{F} , and hence we can study its restriction to the N-particle sector $\mathcal{F}^{(N)}$. With $\nu := \frac{a_0^2}{N-1}$, $G := \cosh(\alpha)W$, and $H := \sinh(\alpha)W$, we define the operators $d_i : \mathcal{F}^{(N)} \to \mathcal{F}^{(N-1)}$ by

$$d_i := a(G\varphi_i) + \nu a^{\dagger}(H\varphi_i). \tag{32}$$

Note that (26) implies

$$\begin{split} c_i &= \frac{1}{\sqrt{N-1}} \sum_j {'} \left(\left(W^* \cosh(\alpha) \right)_{ij} a_j a_0^\dagger + \left(W^* \sinh(\alpha) \right)_{ij} a_j^\dagger a_0 \right) \\ &= \frac{a(G\varphi_i) a_0^\dagger}{\sqrt{N-1}} + \frac{a(H\varphi_i) a_0^\dagger}{\sqrt{N-1}}, \end{split}$$

from which we derive

$$d_{i}^{\dagger}d_{i} = c_{i}^{\dagger}c_{i} + a^{\dagger}(G\varphi_{i})a(G\varphi_{i})\left(1 - \frac{a_{0}a_{0}^{\dagger}}{N - 1}\right) + a(H\varphi_{i})a^{\dagger}(H\varphi_{i})\left(\frac{(a_{0}^{\dagger})^{2}a_{0}^{2}}{(N - 1)^{2}} - \frac{a_{0}^{\dagger}a_{0}}{N - 1}\right) = c_{i}^{\dagger}c_{i} + a^{\dagger}(G\varphi_{i})a(G\varphi_{i})\frac{N^{2} - 2}{N - 1} - (a^{\dagger}(H\varphi_{i})a(H\varphi_{i}) + \|H\varphi_{i}\|^{2})\frac{N^{2}(N - N^{2})}{(N - 1)^{2}}.$$
(33)

The first step towards the proof of Proposition 1 (I) is the following lemma.

Lemma 4.

$$\sum_{i}' e_{i} d_{i}^{\dagger} d_{i} - CN^{-1} T_{H} N^{>} \leq \sum_{i}' e_{i} c_{i}^{\dagger} c_{i} \leq \sum_{i}' e_{i} d_{i}^{\dagger} d_{i} + CN^{-1} (N^{>} + 1) (T_{H} + 1).$$

Proof. By (33) we have

$$\sum_{i}' e_i c_i^{\dagger} c_i \ge \sum_{i}' e_i d_i^{\dagger} d_i - \frac{N^{>}}{N} \sum_{i}' e_i a^{\dagger} (G\varphi_i) a(G\varphi_i), \tag{34}$$

and similarly

$$\sum_{i}' e_{i} c_{i}^{\dagger} c_{i} \leq \sum_{i}' e_{i} d_{i}^{\dagger} d_{i} + \sum_{i}' e_{i} \left(\frac{2}{N-1} a^{\dagger} (G\varphi_{i}) a(G\varphi_{i}) + \frac{NN^{>}}{(N-1)^{2}} \left(a^{\dagger} (H\varphi_{i}) a(H\varphi_{i}) + \|H\varphi_{i}\|^{2} \right) \right).$$

$$(35)$$

Hence the lemma follows from the following three estimates:

$$\sum_{i}' e_{i} a^{\dagger} (G\varphi_{i}) a(G\varphi_{i}) \leq CT_{H},$$

$$\sum_{i}' e_{i} a^{\dagger} (H\varphi_{i}) a(H\varphi_{i}) \leq CN^{>},$$

$$\sum_{i}' e_{i} \|H\varphi_{i}\|^{2} < \infty.$$
(36)

For the proof of the first estimate note that the operator on the left side is the second quantization of $GU_0^*EU_0G^*$, which we can write as

$$\begin{split} GU_0^* E U_0 G^* &= \cosh(\alpha) W_0 E W_0^* \cosh(\alpha) \\ &= \frac{1}{4} \left(D^{-1/2} E^{1/2} + D^{1/2} E^{-1/2} \right) E \left(E^{1/2} D^{-1/2} + E^{-1/2} D^{1/2} \right) \\ &= \frac{1}{4} D^{1/2} \left(D^{-1} E^{1/2} + E^{-1/2} \right) E \left(E^{1/2} D^{-1} + E^{-1/2} \right) D^{1/2} \,. \end{split}$$

Since $T_{\rm H} = \mathrm{d}\Gamma(D)$ it suffices to show boundedness of the operator

$$D^{-1}E^2D^{-1} + D^{-1}E + ED^{-1} + 1$$

which follows from

$$||D^{-1}E^2D^{-1}|| = ||1 + 2D^{-1/2}VD^{-1/2}|| < \infty.$$

The second estimate in (36) follows from the third, for which we note that

$$\sum_{i}' e_{i} \|H\varphi_{i}\|^{2} = \operatorname{tr}(HU_{0}^{*}EU_{0}H^{*})$$

$$= \|E^{1/2}W_{0}^{*}\sinh(\alpha)\|_{2}^{2}$$

$$= \frac{1}{4}\|(D - E)D^{-1/2}\|_{2}^{2}.$$

To bound the Hilbert-Schmidt norm of the operator $(D-E)D^{-1/2}$, we use the integral representation $x^{1/2}=\pi\int_0^\infty t^{1/2}\left(\frac{1}{t}-\frac{1}{x+t}\right)dt$, which implies that

$$\begin{split} \|(D-E)D^{-1/2}\|_{2} &= \pi \left\| \int_{0}^{\infty} t^{1/2} \left((t+D^{2})^{-1} - (t+E^{2})^{-1} \right) D^{-1/2} dt \right\|_{2} \\ &= 2\pi \left\| \int_{0}^{\infty} t^{1/2} (t+E^{2})^{-1} D^{1/2} V(t+D^{2})^{-1} dt \right\|_{2} \\ &\leq 2\pi \|V\|_{2} \int_{0}^{\infty} t^{1/2} \|(t+E^{2})^{-1} D^{1/2} \| \|(t+D^{2})^{-1} \| dt \,. \end{split}$$
(37)

Using $D \le E$ and the spectral theorem one verifies that $\|(t+E^2)^{-1}D^{1/2}\| \le \|(t+E^2)^{-1}E^{1/2}\| \le C(1+t^{3/4})^{-1}$. Since also $\|(t+D^2)^{-1}\| \le 1/t$, the integrand in the last line in (37) falls off like $t^{-5/4}$ at infinity, making the integral finite. \square

Proposition 1 (I) is now a direct consequence of the following lemma.

Lemma 5. For arbitrary $\lambda > 0$ we have the bounds

$$\sum_{i}' e_{i} d_{i}^{\dagger} d_{i} \geq (1 - \lambda) \mathcal{U}^{\dagger} \left(\sum_{i}' e_{i} a_{i}^{\dagger} a_{i} \right) \mathcal{U} - C \lambda^{-1} N^{-1} (N^{>} + 1)^{2},$$

$$\sum_{i}' e_{i} d_{i}^{\dagger} d_{i} \leq (1 + \lambda) \mathcal{U}^{\dagger} \left(\sum_{i}' e_{i} a_{i}^{\dagger} a_{i} \right) \mathcal{U} + C (1 + \lambda^{-1}) N^{-1} (N^{>} + 1)^{2}.$$

Proof. We define $K_i := \mathcal{U}^{\dagger} a_i \mathcal{U} - d_i$ and hence, by Schwarz's inequality,

$$(1-\lambda)\mathcal{U}^{\dagger}a_{i}^{\dagger}a_{i}\mathcal{U}-\lambda^{-1}K_{i}^{\dagger}K_{i}\leq d_{i}^{\dagger}d_{i}\leq (1+\lambda)\mathcal{U}^{\dagger}a_{i}^{\dagger}a_{i}\mathcal{U}+(1+\lambda^{-1})K_{i}^{\dagger}K_{i}$$

for arbitrary $\lambda > 0$. We have to show that $\sum_i e_i K_i^{\dagger} K_i \leq C N^{-1} (N^{>} + 1)^2$. To simplify notation we define also $g_t := \cosh(\alpha t)$, $h_t := \sinh(\alpha t)$ and the quantity

$$\kappa_f(t) := e^{-tX} a(f) e^{tX} - a(g_t f) - \nu a^{\dagger} (h_t \overline{f}) \text{ for } f \perp \varphi_0,$$

which is related to K_i by $K_i = \kappa_{W\omega_i}(1)$. We claim

$$\kappa_f(1)^{\dagger} \kappa_f(1) \le C N^{-1} (N^{>} + 1)^2 \langle f | \alpha^2 | f \rangle.$$
(38)

Assuming this for the moment, we can use $\hat{E} = U_0^* E U_0$ as well as $W_0^* \alpha^2 W_0 = (\log |A|)^2$ to conclude that

$$\sum_{i}' e_{i} K_{i}^{\dagger} K_{i} \leq CN^{-1} (N^{>} + 1)^{2} \sum_{i}' e_{i} \langle W \varphi_{i} | \alpha^{2} W \varphi_{i} \rangle$$

$$= CN^{-1} (N^{>} + 1)^{2} \sum_{i}' \langle E^{1/2} (\log |A|)^{2} E^{1/2} U_{0} \varphi_{i} | U_{0} \varphi_{i} \rangle$$

$$= CN^{-1} (N^{>} + 1)^{2} ||E^{1/2} (\log |A|)^{2} E^{1/2} ||_{1}.$$

The claim of the lemma then follows if $||E^{1/2}(\log |A|)^2 E^{1/2}||_1 < \infty$. To see this observe that

$$0 \le -\log|A| \le |A|^{-1} - 1$$

$$\le |A|^{-2} - 1 = E^{1/2}D^{-1}E^{1/2} - 1,$$
 (39)

which leads to

$$\begin{split} \|E^{1/2}(\log|A|)^2 E^{1/2}\|_1 &\leq \|E^{1/2}(E^{1/2}D^{-1}E^{1/2}-1)^2 E^{1/2}\|_1 \\ &= \|(ED^{-1}-1)E^{1/2}\|_2^2 \\ &= \|(E-D)D^{-1}E^{1/2}\|_2^2 \\ &\leq \|(E-D)D^{-1/2}\|_2^2 \|D^{-1/2}E^{1/2}\|^2 \,. \end{split}$$

The claim thus follows from (37) and boundedness of $B = D^{-1/2}E^{1/2}$. The proof of (38) is a bit more elaborate. With

$$[X, a(f)] = -\nu a^{\dagger}(\alpha \overline{f})$$

we easily obtain

$$\kappa_f''(t) = \kappa_{\alpha^2 f}(t) - r_{\alpha, \alpha f}(t),$$

where

$$r_{\alpha,\varphi}(t) := \mathrm{e}^{-tX} \left[(1 - \nu \nu^{\dagger}) a(\alpha \varphi) - [X, \nu] a^{\dagger}(\overline{\varphi}) \right] \mathrm{e}^{tX}.$$

Using $\kappa_f(0) = \kappa_f'(0) = 0$, a second order Taylor expansion yields

$$\kappa_f(t) = \int_0^t (t - s) \left(\kappa_{\alpha^2 f}(s) - r_{\alpha, f}(s) \right) ds.$$

For any $|\psi\rangle \in \mathcal{F}^{(N)}$ we introduce

$$\begin{split} \hat{\kappa}_{\psi}(t) &:= \sup_{\|\alpha f\| \le 1} \|\kappa_f(t) |\psi\rangle \|, \\ \hat{r}_{\alpha,\psi} &:= \frac{1}{2} \sup_{s < 1} \sup_{\|\alpha f\| \le 1} \|r_{\alpha,f}(s) |\psi\rangle \|. \end{split}$$

Note that

$$\sup_{\|\alpha f\| \leq 1} \|\kappa_{\alpha^2 f}(t) |\psi\rangle\| = \|\alpha\|^2 \sup_{\|\alpha f\| \leq 1} \|\kappa_{\alpha^2 f/\|\alpha\|^2}(t) |\psi\rangle\| \leq \|\alpha\|^2 \hat{\kappa}_{\psi}(t)$$

which yields

$$\hat{\kappa}_{\psi}(t) \leq \hat{r}_{\alpha,\psi} + \|\alpha\|^2 \int_0^t \hat{\kappa}_{\psi}(s) ds$$

for $t \le 1$. It follows from Grönwall's lemma (see, e.g., [29, Thm. III.1.1]) that

$$\hat{\kappa}_{\psi}(1) \leq \mathrm{e}^{\|\alpha\|^2} \hat{r}_{\alpha,\psi}(1).$$

If $f \in \ker \alpha$ then $\kappa_f(t) = 0$. For $f \notin \ker \alpha$,

$$\frac{\|\kappa_f(1) |\psi\rangle\|}{\|\alpha f\|} \le e^{\|\alpha\|^2} \hat{r}_{\alpha,\psi}(1),$$

from which (38) follows if we can show that

$$\hat{r}_{\alpha,\psi}(1) \le CN^{-1/2} \| (N^{>} + 1) | \psi \rangle \|. \tag{40}$$

To see (40) we define $g = \alpha f$ and first show that for $||g|| \le 1$,

$$a^{\dagger}(\alpha\overline{g})(1-\nu\nu^{\dagger})^{2}a(\alpha\overline{g}) \le CN^{-1}(N^{>}+1)^{2} \tag{41}$$

and

$$a(g)[X, \nu]^{\dagger}[X, \nu]a^{\dagger}(g) \le CN^{-1}(N^{>} + 1)^{2}.$$
 (42)

The first bound follows directly from

$$1 - \nu \nu^{\dagger} = \frac{(2N+3)N^{>} - (N^{>})^{2} - 5N - 1}{(N-1)^{2}}$$

and $a^{\dagger}(\alpha \overline{g})a(\alpha \overline{g}) < \|\alpha\|^2 N^>$. To show (42) we write

$$\begin{split} a(g)[X,\nu]^{\dagger}[X,\nu]a^{\dagger}(g) &\leq \left(\frac{[(a_0^{\dagger})^2,a_0^2]}{2(N-1)^2}\right)^2 a(g) \left(\sum_{i,j,k,l}{}'\alpha_{ij}\alpha_{kl}a_k^{\dagger}a_l^{\dagger}a_ia_j\right) a^{\dagger}(g) \\ &\leq \left(\frac{2(N-N^{>})+1}{(N-1)^2}\right)^2 a(g)\|\alpha\|_2^2 N^{>}(N^{>}-1)a^{\dagger}(g) \\ &\leq CN^{-2}\|\alpha\|_2^2\|g\|^2 N^{>}(N^{>}-1)(N^{>}+1) \\ &\leq CN^{-1}(N^{>}+1)^2. \end{split}$$

To conclude the proof of (38) it remains to show that the inequality

$$e^{-tX}(N^{>}+1)^{2}e^{tX} < e^{Ct}(N^{>}+1)^{2}$$
 (43)

holds for t = 1. To that end we compute

$$\begin{split} [X, N^{>}] &= -\frac{1}{2} \sum_{i,j} \left(v^{\dagger} \alpha_{ij} [a_i a_j, N^{>}] - v \alpha_{ij} [a_i^{\dagger} a_j^{\dagger}, N^{>}] \right) \\ &= -\sum_{i,j} \alpha_{ij} (b_i b_j + b_i^{\dagger} b_j^{\dagger}). \end{split}$$

Taking the square of this expression yields

$$\begin{split} [X,N^{>}]^{2} &\leq 2 \left(\sum_{i,j} {'} \alpha_{ij} b_{i} b_{j} \right) \left(\sum_{k,l} {'} \alpha_{kl} b_{k}^{\dagger} b_{l}^{\dagger} \right) + 2 \left(\sum_{i,j} {'} \alpha_{ij} b_{i}^{\dagger} b_{j}^{\dagger} \right) \left(\sum_{k,l} {'} \alpha_{kl} b_{k} b_{l} \right) \\ &\leq 2 v^{\dagger} v \sum_{i,j,k,l} {'} \alpha_{ij} \alpha_{kl} a_{i} a_{j} a_{k}^{\dagger} a_{l}^{\dagger} + 2 \|\alpha\|_{2}^{2} v v^{\dagger} N^{>} (N^{>} - 1) \\ &\leq 2 \frac{(N - N^{>})(N - N^{>} - 1)}{(N - 1)^{2}} \left(\sum_{i,j,k,l} {'} \alpha_{ij} \alpha_{kl} a_{i}^{\dagger} a_{j}^{\dagger} a_{k} a_{l} + 4 \sum_{i,j} {'} (\alpha^{2})_{ij} a_{i}^{\dagger} a_{j} + 2 \|\alpha\|_{2}^{2} \right) \\ &+ 2 \|\alpha\|_{2}^{2} \frac{(N - N^{>})(N - N^{>} + 3) + 2}{(N - 1)^{2}} N^{>} (N^{>} - 1) \\ &\leq 2 \frac{(N - N^{>})(N - N^{>} - 1)}{(N - 1)^{2}} \left(\|\alpha\|_{2}^{2} N^{>} (N^{>} - 1) + 4 \|\alpha\|^{2} N^{>} + 2 \|\alpha\|_{2}^{2} \right) \\ &+ 2 \|\alpha\|_{2}^{2} \frac{(N - N^{>})(N - N^{>} + 3) + 2}{(N - 1)^{2}} N^{>} (N^{>} - 1) \\ &\leq C \|\alpha\|_{2}^{2} (N^{>} + 1)^{2} . \end{split} \tag{44}$$

By Schwarz's inequality we obtain

$$[X, (N^{>} + 1)^{2}] = (N^{>} + 1)[X, N^{>}] + [X, N^{>}](N^{>} + 1)$$

$$\leq C(N^{>} + 1)^{2},$$

and hence it follows that

$$e^{tX}(N^{>} + 1)^{2}e^{-tX} = (N^{>} + 1)^{2} + \int_{0}^{t} e^{sX}[X, (N^{>} + 1)^{2}]e^{-sX}ds$$

$$\leq (N^{>} + 1)^{2} + C\int_{0}^{t} e^{sX}(N^{>} + 1)^{2}e^{-sX}ds.$$

Grönwall's lemma then yields (43). This completes the proof of the lemma.

We conclude this section with the proof of Lemma 3.

Proof of Lemma 3. (i): The positivity of V follows directly from the assumption that v is of positive type:

$$\langle \psi | V | \psi \rangle = \int_{\mathbb{R}^{2d}} \varphi_0(x) \varphi_0(y) v(x-y) \overline{\psi(x)} \psi(y) dx dy \ge 0.$$

In particular, the trace norm of V equals its trace, which is equal to

tr
$$V = \int_{\mathbb{R}^d} \varphi_0(y)^2 v(0) dy = v(0) < \infty$$
.

(ii): With $A - 1 = (D^{1/2} - E^{1/2})E^{-1/2}$ and the integral representation $x^{1/4} - y^{1/4} = \sqrt{2}\pi \int_0^\infty t^{1/4} \left(\frac{1}{y+t} - \frac{1}{x+t}\right) dt$

$$||A - 1||_{2} \leq \sqrt{2}\pi \int_{0}^{\infty} t^{1/4} || \left((t + D^{2})^{-1} - (t + E^{2})^{-1} \right) E^{-1/2} ||_{2} dt$$

$$= 2^{3/2}\pi \int_{0}^{\infty} t^{1/4} || (t + D^{2})^{-1} D^{1/2} V D^{1/2} (t + E^{2})^{-1} E^{-1/2} ||_{2} dt$$

$$\leq 2^{3/2}\pi ||V||_{2} \int_{0}^{\infty} t^{1/4} || (t + D^{2})^{-1} D^{1/2} || ||D^{1/2} (t + E^{2})^{-1} E^{-1/2} || dt.$$

$$(45)$$

Since D < E we can further bound

$$\begin{split} \|D^{1/2}(t+E^2)^{-1}E^{-1/2}\| &= \|E^{-1/2}(t+E^2)^{-1}D(t+E^2)^{-1}E^{-1/2}\|^{1/2} \\ &\leq \|(t+E^2)^{-1}\| \leq \frac{1}{t} \,. \end{split}$$

Using the spectral theorem we conclude that $\|(t+D^2)^{-1}D^{1/2}\| \le C(1+t^{3/4})^{-1}$ and hence the integrand in (45) falls off like $t^{-3/2}$ at infinity, making the integral finite. The estimate for $B-1=D^{-1/2}(E^{1/2}-D^{1/2})$ is obtained along the same lines.

(iii): We apply the integral representation $\log x = \frac{1}{2} \int_0^\infty \left(\frac{1}{x+t} - \frac{1}{x^{-1}+t} \right) dt$ and the resolvent identity to obtain

$$2\|\alpha\|_{2} \leq \int_{0}^{\infty} \|(|A^{*}| + t)^{-1} - (|B^{*}| + t)^{-1}\|_{2} dt$$

$$\leq \||A^{*}| - |B^{*}|\|_{2} \int_{0}^{\infty} \|(|A^{*}| + t)^{-1}\|\|(|B^{*}| + t)^{-1}\| dt < \infty,$$

since $||A^*| - |B^*||_2 = ||A - B||_2 \le ||A - 1||_2 + ||B - 1||_2 < \infty$ by (i).

(iv): On $\mathcal{F}^{(N)}$ we have the bound

$$\sum_{i,j} \overline{\alpha}_{ij} b_i^{\dagger} b_j^{\dagger} \sum_{i,j} \alpha_{ij} b_i b_j \leq \frac{a_0^2 (a_0^{\dagger})^2}{(N-1)^2} \sum_{i,j,k,l} \overline{\alpha}_{ij} \alpha_{kl} a_i^{\dagger} a_j^{\dagger} a_k a_l \\
\leq \left(\frac{N+2}{N-1}\right)^2 \|\alpha\|_2^2 N(N-1),$$

which shows that X is a bounded operator. Its anti-symmetry follows directly from its definition. \square

This completes the proof of part (I) of Proposition 1.

5.2. Proof of Proposition 1 (II). We abbreviate the symplectic transformation (26) by

$$\begin{pmatrix} c \\ c^{\dagger} \end{pmatrix} =: \begin{pmatrix} L & M \\ M & L \end{pmatrix} \begin{pmatrix} b \\ b^{\dagger} \end{pmatrix}. \tag{46}$$

A straightforward computation shows that

$$[c_i, c_j^{\dagger}] + [c_j, c_i^{\dagger}] = 2 \frac{N - N^{\dagger}}{N - 1} \delta_{ij} - \frac{1}{N - 1} \sum_{k,l} \left(L_{jl} L_{ik} - M_{jl} M_{ik} \right) \left(a_k^{\dagger} a_l + a_l^{\dagger} a_k \right).$$

We will show below that Y - E/2 and D - E are trace class, with

$$\operatorname{tr}\left(Y - \frac{E}{2}\right) = \frac{1}{2}\operatorname{tr}\left(D + QV - E\right). \tag{47}$$

Given that, we have

$$\begin{split} &2\sum_{i,j}{}^{'}\left(U_{0}^{*}\left(Y-\frac{E}{2}\right)U_{0}\right)_{ij}[c_{i},c_{j}^{\dagger}]\\ &=\frac{N-N^{>}}{N-1}\mathrm{tr}\left(D+QV-E\right)\\ &-\frac{1}{N-1}\sum_{k,l}{}^{'}\left(L^{*}U_{0}^{*}\left(Y-\frac{E}{2}\right)U_{0}L-M^{*}U_{0}^{*}\left(Y-\frac{E}{2}\right)U_{0}M\right)_{kl}\left(a_{k}^{\dagger}a_{l}+a_{l}^{\dagger}a_{k}\right)\,. \end{split}$$

Since tr $QV = \text{tr } V - v_{0000}$, Proposition 1 (II) then follows if we can show that

$$-CD \le L^* U_0^* \left(Y - \frac{E}{2} \right) U_0 L - M^* U_0^* \left(Y - \frac{E}{2} \right) U_0 M \le CD. \tag{48}$$

We compute

$$4L^*U_0^* \left(Y - \frac{E}{2}\right) U_0 L - 4M^* U_0^* \left(Y - \frac{E}{2}\right) U_0 M$$

$$= \frac{1}{2} D^{1/2} \left(1 + D^{-1/2} V D^{-1/2} + D^{-1} E (1 + D^{-1/2} V D^{-1/2}) D E^{-1} - 2D^{-1} E + \text{h.c.}\right) D^{1/2}$$

$$=: D^{1/2} R D^{1/2}.$$

Now R is a bounded operator since DE^{-1} and $D^{-1}E$ are bounded, which follows from

$$||DE^{-1}||^2 = ||DE^{-2}D|| < 1, (49)$$

$$\|D^{-1}E\|^2 = \|D^{-1}E^2D^{-1}\| = \|1 + 2D^{-1/2}VD^{-1/2}\| < \infty.$$
 (50)

This proves (48).

We now turn to (47). Note that

$$2(2Y - E) = B^* (D + V - D^{1/2}ED^{-1/2}) A + A^* (D + V - D^{-1/2}ED^{1/2}) B.$$

We claim that

$$||D^{1/2}(E-D)D^{-1/2}||_2 < \infty, \tag{51}$$

$$||D^{1/2}(E-D)D^{-1/2} + \text{h.c.}||_{1} < \infty, \tag{52}$$

$$||D + QV - E||_1 < \infty.$$
 (53)

Since by Lemma 3 A-1, B-1, are Hilbert-Schmidt and, in addition, V is trace class by Lemma 3, it follows from (51)–(53) that

$$B^* \left(D + V - D^{1/2} E D^{-1/2} \right) A + \text{h.c.} = D + QV - D^{1/2} E D^{-1/2} + \text{h.c.} + \text{Rest}$$

with $\|\text{Rest}\|_1 < \infty$; hence 2Y - E is trace class. Moreover,

$$tr(2Y - E) = \frac{1}{2}tr\left(D^{1/2}(D - E)D^{-1/2} + h.c.\right) + tr QV$$

= tr (D + QV - E),

where the first equality holds by cyclicity of the trace and the second is seen to be true by computing the trace in the eigenbasis of D.

To show (51)–(53) we compute

$$D^{1/2}(E-D)D^{-1/2} = \pi D^{1/2} \int_0^\infty \sqrt{t} \left((t+D^2)^{-1} - (t+E^2)^{-1} \right) D^{-1/2} dt$$

$$= 2\pi \int_0^\infty \sqrt{t} D(t+D^2)^{-1} V D^{1/2} (t+E^2)^{-1} D^{-1/2} dt$$

$$= 2\pi \int_0^\infty \sqrt{t} D(t+D^2)^{-1} V (t+D^2)^{-1} dt$$

$$-4\pi \int_0^\infty \sqrt{t} D(t+D^2)^{-1} V D^{1/2} (t+E^2)^{-1} D^{1/2} V (t+D^2)^{-1} dt ,$$
(54)

where we applied the resolvent identity twice. The expression on the last line is trace class. This follows from the bound

$$\begin{split} & \left\| D(t+D^2)^{-1} V D^{1/2} (t+E^2)^{-1} D^{1/2} V (t+D^2)^{-1} \right\|_1 \\ & \leq \left\| D(t+D^2)^{-1} \right\|^2 \left\| (t+D^2)^{-1} \right\| \left\| V \right\|_1^2 \,, \end{split}$$

where we have used that $E^2 \ge D^2$ in the second factor. The latter expression falls off like t^{-2} for large t, making the integral finite. For the first term on the right side of (54), we compute its matrix elements. With $D_i = \varepsilon_i - \varepsilon_0$ the eigenvalues of D,

$$\begin{split} \left\langle \varphi_i \left| \pi \int_0^\infty \sqrt{t} D(t+D^2)^{-1} V(t+D^2)^{-1} dt \right| \varphi_j \right\rangle \\ &= V_{ij} \pi \int_0^\infty \sqrt{t} \frac{D_i}{t+D_i^2} \frac{1}{t+D_j^2} dt = V_{ij} \frac{D_i}{D_i+D_j}. \end{split}$$

In particular, since

$$\left| V_{ij} \frac{D_i}{D_i + D_j} \right| \le |V_{ij}|,$$

the Hilbert-Schmidt property (51) follows. Moreover,

$$V_{ij}\frac{D_i}{D_i + D_i} + (i \leftrightarrow j) = V_{ij},$$

which implies (52). To prove (53), one simply computes the trace of the operator in (52) in the basis of D, which leads to the conclusion that $\sum_{i}' \langle \varphi_i | E - D | \varphi_i \rangle < \infty$. Since E - D is a positive operator, this implies that E - D is trace class. Since also V is trace class, this proves (53).

5.3. Proof of Proposition 1 (III). Recall the notation introduced in (46). A straightforward computation shows

$$[c_j, c_i] = \frac{1}{N-1} \sum_{k,l} \left(M_{jk} L_{il} a_l a_k^{\dagger} - L_{jk} M_{il} a_k a_l^{\dagger} \right)$$

and

$$\sum_{i,j} Z_{ij} \left([c_j, c_i] + [c_i^{\dagger}, c_j^{\dagger}] \right) = \frac{1}{N-1} \sum_{k,l} \left(L^* Z M - M^* Z L \right)_{kl} \left(a_k^{\dagger} a_l + a_l^{\dagger} a_k \right).$$

Hence what we need to show is

$$-CD < L^*ZM - M^*ZL < CD.$$

We observe that

$$\begin{split} &8\left(L^*ZM - M^*ZL\right) \\ &= \frac{1}{2}(B-A)\left(B^*\left(D+V\right)A - A^*\left(D+V\right)B\right)\left(A^* + B^*\right) + \text{h.c.} \\ &= \left[D^{-1/2}ED^{-1/2}(D+V)D^{1/2}E^{-1}D^{1/2} - D - V\right] + \text{h.c.} \\ &= D^{1/2}\left(\left[D^{-1}E(1+D^{-1/2}VD^{-1/2})DE^{-1} - 1 - D^{-1/2}VD^{-1/2}\right] + \text{h.c.}\right)D^{1/2}. \end{split}$$

The operator in square brackets is bounded because of (49) and (50), hence the claim follows.

6. Proof of Theorem 1

This section contains the proof of Theorem 1. We split the proof into two parts, corresponding to the lower and upper bounds on the eigenvalues of H_N , respectively.

6.1. Lower bound. By combining the estimate (19) with Proposition 1, we obtain the inequality

$$H_{N} \geq Nh_{00} + \frac{N+1}{2}v_{0000} + (1-\lambda)\mathcal{U}^{\dagger}\left(\sum_{i}'e_{i}a_{i}^{\dagger}a_{i}\right)\mathcal{U} + \frac{1}{2}\operatorname{tr}(E-D-V)$$

$$-C\left(\left(N^{-1}\varepsilon^{-1} + N^{-1}\lambda^{-1} + \zeta^{-1}N^{-1/2}\right)(N^{>} + 1)(T_{H} + 1)\right)$$

$$+(N^{-1} + \varepsilon + \zeta N^{-1/2})(T_{H} + 1)\right), \tag{55}$$

which holds for any $\lambda > 0$, $\zeta > 0$ and $0 < \varepsilon < 1$. Since the spectrum of $\sum_i' e_i a_i^{\dagger} a_i$ consists of finite sums of the form $\sum_i' e_i n_i$ with $\sum_i' n_i \leq N$, the desired lower bound follows directly from the min-max principle. In fact, for any function Ψ in the spectral subspace of H_N corresponding to energy $E \leq E_0(N) + \xi$, Lemmas 1 and 2 imply that

$$\langle \Psi | (T_{\mathrm{H}} + 1) | \Psi \rangle \leq C(\xi + 1)$$

and

$$\langle \Psi | (N^{>} + 1)(T_{\rm H} + 1) | \Psi \rangle \leq C(\xi + 1)^2$$
.

Choosing $\varepsilon = O(\sqrt{\xi/N}) = \lambda$ and $\zeta = \sqrt{\xi}$, we conclude that the spectrum of H_N below an energy $E_0(N) + \xi$ is bounded from below by the corresponding spectrum of

$$Nh_{00} + \frac{N+1}{2}v_{0000} + \sum_{i}{}^{'}e_{i}a_{i}^{\dagger}a_{i} - \frac{1}{2}\mathrm{tr}(D+V-E) - O(\xi^{\frac{3}{2}}N^{-1/2}).$$

This completes the desired lower bound.

6.2. Upper bound. A combination of (21) and Proposition 1 implies that

$$H_{N} \leq Nh_{00} + \frac{N+1}{2}v_{0000} + (1+\lambda)\mathcal{U}^{\dagger}\left(\sum_{i}{}'e_{i}a_{i}^{\dagger}a_{i}\right)\mathcal{U} - \frac{1}{2}\operatorname{tr}(D+V-E)$$

$$+C\left(N^{-1}\varepsilon^{-1} + N^{-1}\lambda^{-1} + N^{-1} + \zeta^{-1}N^{-1/2}\right)(N^{>} + 1)(T_{H} + 1)$$

$$+C\left(\varepsilon + \zeta N^{-1/2} + N^{-1}\right)(N^{>} + 1)^{1/2}(T_{H} + 1)^{1/2},$$

$$(56)$$

for any $\lambda>0,\,\zeta>0$ and $\varepsilon>0$. To apply the min-max principle we need the following bound.

Lemma 6. One has the bound

$$\mathcal{U}(N^{>} + 1)(T_H + 1)\mathcal{U}^{\dagger} \le C\left(\sum_{i}' e_i a_i^{\dagger} a_i + 1\right)^2.$$
 (57)

Note that by operator monotonicity of the square root it follows immediately from Lemma 6 that

$$\mathcal{U}(N^> + 1)^{1/2} (T_{\mathrm{H}} + 1)^{1/2} \mathcal{U}^{\dagger} \le C \left(\sum_{i} e_{i} a_{i}^{\dagger} a_{i} + 1 \right).$$

Hence we obtain from (56),

$$\mathcal{U}H_{N}\mathcal{U}^{\dagger} \leq Nh_{00} + \frac{N+1}{2}v_{0000} + (1+\lambda)\sum_{i}'e_{i}a_{i}^{\dagger}a_{i} - \frac{1}{2}\operatorname{tr}(D+V-E)
+ C\left(N^{-1}\varepsilon^{-1} + N^{-1}\lambda^{-1} + N^{-1} + \zeta^{-1}N^{-1/2}\right)\left(\sum_{i}'e_{i}a_{i}^{\dagger}a_{i} + 1\right)^{2}
+ C\left(\varepsilon + \zeta N^{-1/2} + N^{-1}\right)\left(\sum_{i}'e_{i}a_{i}^{\dagger}a_{i} + 1\right).$$
(58)

Given an eigenvalue of $\sum_{i}^{'}e_{i}a_{i}^{\dagger}a_{i}$ with value ξ , we choose $\varepsilon=O(\sqrt{\xi/N})=\lambda$ and $\zeta=\sqrt{\xi}$ to obtain $Nh_{00}+\frac{N+1}{2}v_{0000}+\xi-\frac{1}{2}\mathrm{tr}(D+V-E)+O(\xi^{3/2}N^{-1/2})$ for the right side of (58). Hence the desired upper bound follows from the min-max principle. It remains to prove (57).

Proof of Lemma 6. If we can show that

$$e^{X}(N^{>}+1)(T_{H}+1)e^{-X} < C(N^{>}+1)(T_{H}+1)$$
 (59)

and

$$W^*DW = U_0^* W_0^* DW_0 U_0 \le C\hat{E} , \qquad (60)$$

the claim follows since then

$$\mathcal{U}(N^{>}+1)(T_{\rm H}+1)\mathcal{U}^{\dagger} \leq C\mathcal{W}^{\dagger}(N^{>}+1)^{1/2}(T_{\rm H}+1)(N^{>}+1)^{1/2}\mathcal{W}$$

$$= C(N^{>}+1)^{1/2}\mathcal{W}^{\dagger}(T_{\rm H}+1)\mathcal{W}(N^{>}+1)^{1/2}$$

$$\leq C(N^{>}+1)\left(\sum_{i}{'e_{i}a_{i}^{\dagger}a_{i}}+1\right),$$

where we have used (59) for the first inequality, and (60) for the second. We start with the proof of (59). In fact we shall show that

$$e^{X}(N^{>}+1)^{2}(T_{H}+1)^{2}e^{-X} \le C(N^{>}+1)^{2}(T_{H}+1)^{2},$$
 (61)

from which the claim follows by operator monotonicity of the square root. We compute

$$[X, (N^{>} + 1)^{2}(T_{H} + 1)^{2}] = (N^{>} + 1)(T_{H} + 1)[X, (N^{>} + 1)(T_{H} + 1)] + [X, (N^{>} + 1)(T_{H} + 1)](N^{>} + 1)(T_{H} + 1).$$
 (62)

With

$$\begin{split} A_{1} &:= [X, N^{>}] = \sum_{i,j} '\alpha_{ij} \left(b_{i}b_{j} + b_{j}^{\dagger}b_{i}^{\dagger}\right), \\ A_{2} &:= [X, T_{\mathrm{H}}] = \sum_{i,j} '\alpha_{ij} (\varepsilon_{i} - \varepsilon_{0}) \left(b_{i}b_{j} + b_{j}^{\dagger}b_{i}^{\dagger}\right), \end{split}$$

we can bound

$$\begin{split} [X,(N^>+1)(T_{\rm H}+1)]^2 &= \left(A_1(T_{\rm H}+1) + (N^>+1)A_2\right)^2 \\ &= \left(A_1(T_{\rm H}+1) + A_2(N^>+1) + [N^>,A_2]\right)^2 \\ &\leq C\left((T_{\rm H}+1)A_1^2(T_{\rm H}+1) + (N^>+1)A_2^2(N^>+1) + [N^>,A_2]^2\right) \,. \end{split}$$

By (44) we have

$$A_1^2 \le C \|\alpha\|_2^2 (N^> + 1)^2$$

and similarly

$$A_2^2 \le C \|D\alpha\|_2^2 (N^> + 1)^2$$
.

Furthermore, since

$$[N^{>}, A_{2}] = 2 \sum_{i,j} \alpha_{ij} (\varepsilon_{i} - \varepsilon_{0}) \left(b_{j}^{\dagger} b_{i}^{\dagger} - b_{i} b_{j} \right)$$

one checks that

$$[N^>, A_2]^2 \le C \|D\alpha\|_2^2 (N^> + 1)^2$$
.

To see that $||D\alpha||_2 < \infty$, we can proceed as in (39) and bound

$$D\alpha^2 D < D(D^{-1/2}ED^{-1/2}-1)^2 D = D^{1/2}(E-D)D^{-1}(E-D)D^{1/2}$$
.

Hence we have

$$||D\alpha||_2 < ||D^{1/2}(E-D)D^{-1/2}||_2$$

which is finite due to (51). Applying Schwarz's inequality to (62), we have thus shown that

$$[X, (N^> + 1)^2 (T_{\rm H} + 1)^2] \le C(N^> + 1)^2 (T_{\rm H} + 1)^2$$
.

We further have

$$\begin{aligned} e^{tX}(N^{>} + 1)^{2}(T_{H} + 1)^{2}e^{-tX} &= (N^{>} + 1)^{2}(T_{H} + 1)^{2} \\ &+ \int_{0}^{t} e^{sX}[X, (N^{>} + 1)^{2}(T_{H} + 1)^{2}]e^{-sX}dx \\ &\leq (N^{>} + 1)^{2}(T_{H} + 1)^{2} \\ &+ C \int_{0}^{t} e^{sX}(N^{>} + 1)^{2}(T_{H} + 1)^{2}e^{-sX}ds \end{aligned}$$

which by Grönwall's inequality implies (61).

For the proof of (60) we need to show that

$$W_0^*DW_0 \le CE$$

or, equivalently, that

$$D^{1/2}W_0E^{-1/2} = DE^{-1/2}(E^{-1/2}DE^{-1/2})^{-1/2}E^{-1/2}$$
$$= \pi D \int_0^\infty t^{-1/2}(Et + D)^{-1}dt$$
(63)

is a bounded operator. Observe that, by (49),

$$\left\| D(Et+D)^{-1} \right\| \le \|DE^{-1}\| \|Q(t+DE^{-1})^{-1}\| \le \|Q(t+DE^{-1})^{-1}\|. \tag{64}$$

With the aid of a Neumann expansion, one sees that the right side of (64) can be bounded by $2t^{-1}$ for $t > 2 \| DE^{-1} \|$, which gives a bounded contribution to the integral in (63). For $t \le 2 \| DE^{-1} \|$, one can argue that by analyticity of the resolvent map $t \mapsto (t+DE^{-1})^{-1}$, as well as the fact that ED^{-1} is bounded, we get a uniform bound on $\| Q(t+DE^{-1})^{-1} \|$. This argument does not yield a quantitative bound, however, since DE^{-1} is not a self-adjoint operator. To obtain an explicit bound, we make use of the fact that $DE^{-1} - 1$ is a Hilbert-Schmidt operator. In fact, it is even trace class, since by (49) and (53),

$$||DE^{-1} - 1||_1 = ||DE^{-1}(D - E)D^{-1}||_1 < ||(D - E)D^{-1}||_1 < \infty.$$

We shall apply the following result.

Lemma 7 (Theorem 6.4.1 in [30]). Let A be a Hilbert-Schmidt operator. Then for $z \notin \sigma(A)$ (the spectrum of A),

$$\|(A-z)^{-1}\| \le \sum_{k=0}^{\infty} \frac{\|A\|_2^k}{(\inf_{t \in \sigma(A)} |z-t|)^{k+1} \sqrt{k!}}.$$

Define a to be the infimum of the spectrum of DE^{-1} on the space $Q\mathcal{F}^{(1)}$. It equals the infimum of the spectrum of $E^{-1/2}DE^{-1/2}$ on that space, hence

$$a = ||E^{1/2}D^{-1}E^{1/2}||^{-1} > 0.$$

By Lemma 7 we thus have

$$\begin{split} \|Q(t+DE^{-1})^{-1}\| &= \|Q(t+1+DE^{-1}-1)^{-1}\| \\ &\leq \sum_{k=0}^{\infty} \frac{\|DE^{-1}-1\|_2^k}{(t+a)^{k+1}\sqrt{k!}} \\ &\leq \frac{\sqrt{2}}{t+a} \exp\left(\frac{\|DE^{-1}-1\|_2}{t+a}\right). \end{split}$$

Here we have used the bound $\sum_{k=0}^{\infty} x^k / \sqrt{k!} \le \sqrt{2} e^{x^2}$ for $x \ge 0$ (cf. p. 84 in [30]). This yields the desired quantitative bound, and concludes the proof of the boundedness of (63). \square

7. Consequences for Eigenvectors

7.1. Proof of Corollary 1. We abbreviate

$$H := H_N - E_0(N) + 1 =: \sum_{i=1}^{\infty} h_i |\chi_i\rangle \langle \chi_i|,$$

with $h_i \le h_{i+1}$. For $h_i \le \xi$, it follows from (55) and Lemmas 1–2 that

$$\langle \chi_j | K | \chi_j \rangle \leq h_j \left(1 + C(\xi/N)^{1/2} \right).$$

From (58) we further deduce that $h_j \le k_j (1 + C(\xi/N)^{1/2})$, and thus

$$\langle \chi_j | K | \chi_j \rangle \leq k_j \left(1 + C(\xi/N)^{1/2} \right).$$

A simple application of the min-max principle [31, Lem. 2] then shows that if $k_{j+1} > k_j$ then

$$\sum_{k,l=1}^{j} |\langle \chi_k, \psi_l \rangle|^2 \ge j - C(\xi/N)^{1/2} \frac{\sum_{l=1}^{j} k_l}{k_{j+1} - k_j}.$$

In other words, with $P_K^j:=\sum_{k=1}^j|\psi_k\rangle\,\langle\psi_k|$ and $P_H^j:=\sum_{k=1}^j|\psi_k\rangle\,\langle\psi_k|$,

$$\|P_K^j - P_H^j\|_2^2 \le C(\xi/N)^{1/2} \frac{\sum_{l=1}^j k_l}{k_{i+1} - k_i}.$$

This completes the proof. \Box

Remark 5. Note that the (normalized) eigenfunctions of K can be written as

$$\left(\mathcal{U}^{\dagger} \prod_{i \geq 1} \frac{(a_i^{\dagger})^{n_i}}{\sqrt{n_i!}} \mathcal{U}\right) \mathcal{U}^{\dagger} | N-n, 0, \ldots \rangle = \prod_{i \geq 1} \frac{(d_i^{\dagger} + K_i^{\dagger})^{n_i}}{\sqrt{n_i!}} \mathcal{U}^{\dagger} | N-n, 0, \ldots \rangle, \quad (65)$$

where $n = \sum_{i \geq 1} n_i \leq N$, and $|N-n,0,\ldots\rangle$ denotes the function $\bigotimes_{i=1}^{N-n} \varphi_0 \in \mathcal{F}^{(N-n)}$. The operators d_i are explicitly defined in (32). The operators K_i are small in the lowenergy subspace, as shown in the proof of Lemma 5. The eigenfunctions of K (and, hence, the ones of H_N) are thus approximately obtained by applying the raising-type operators d_i^{\dagger} to the N-n-particle ground state. To explicitly estimate the difference of the functions (65) and

$$\prod_{i\geq 1} \frac{(d_i^{\dagger})^{n_i}}{\sqrt{n_i!}} \mathcal{U}^{\dagger} | N-n, 0, \ldots \rangle ,$$

however, it would be necessary to give bounds on products of powers of the operators K_i^{\dagger} and d_i^{\dagger} , which are more involved than the ones used in Lemma 5.

Remark 6. As noted in Sect. 1.2, Corollary 1 implies that the ground state Ψ_0 of H_N is close, in L^2 -norm, to $\mathcal{U}^{\dagger} | N, 0, \ldots \rangle$. To see the importance of the unitary operator \mathcal{U} , one can calculate the matrix element

$$\langle N, 0, \dots | \mathcal{U}^{\dagger} | N, 0, \dots \rangle = \langle N, 0, \dots | e^{-X} | N, 0, \dots \rangle.$$
 (66)

This equality follows from the fact that W leaves the Hartree ground state φ_0 invariant. One readily checks that $\frac{d}{dt}\langle N,0,\ldots | e^{-tX}|N,0,\ldots \rangle|_{t=0}=0$. However,

$$\frac{d^2}{dt^2} \langle N, 0, \ldots | e^{-tX} | N, 0, \ldots \rangle |_{t=0} = \langle N, 0, \ldots | X^2 | N, 0, \ldots \rangle = -\frac{N}{2(N-1)} \|\alpha\|_2^2,$$

which is not small for large N. Hence we expect that the matrix element (66) differs significantly from 1.

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