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RESEARCH ARTICLE

Second-order energy expansion of Bose gases with three-body interactions

Morris Brooks

Department of Mathematics, University of Zurich, Institute of Mathematics, 8057 Zurich, Switzerland;
E-mail: morris.brooks@math.uzh.ch

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Abstract

We provide a second-order energy expansion for a gas of N bosonic particles with three-body interactions in the Gross-Pitaevskii regime. We especially confirm a conjecture by Nam, Ricaud, and Triay in [25], where they predict the subleading term in the asymptotic expansion of the ground state energy to be of the order $\sqrt{N}$. In addition, we show that low-energy states satisfy Bose-Einstein condensation with a rate of the order $N^{-\frac{3}{4}}$.

Contents

1. Introduction

In this manuscript we study a dilute Bose gas consisting of N quantum particles subject to Bose-Einstein statistics, in which the individual particles interact with each other via a three-body potential

$$V_N(x,y,z) := NV\Big(\sqrt{N}(x-y), \sqrt{N}(x-z)\Big), \tag{1}$$

defined in terms of a given bounded and non-negative function $V : \mathbb{R}^3\times\mathbb{R}^3 \longrightarrow \mathbb{R}$ with compact support. The quantum gas is then described by the self-adjoint operator

$$H_N := -\sum_{1\leq k\leq N} \Delta_{x_k} + \sum_{1\leq i<j<k\leq N} V_N(x_i,x_j,x_k), \tag{2}$$

acting on the space of permutation-symmetric functions $L^2_{\mathrm{sym}}(\Lambda^N)$, where $\Lambda := \left[-\frac{1}{2}, \frac{1}{2}\right]^3$ is the three-dimensional periodic torus, that is, $\sum_{1\leq k\leq N}\Delta_{x_k}$ is defined as the closure of the Laplace operator acting on permutations symmetric and periodic C^2 functions and $x-y$ as well as $x-z$ in Eq. (1) refer to the distance on the torus. We further assume that V_N defined in Eq. (1) is permutation symmetric in order to assure that H_N preserves permutation symmetry. The particular scaling in Eq. (1) with the number of particles N is referred to as the Gross-Pitaevskii regime and yields a short-range, but strong, interaction on the scale $r = \frac{1}{\sqrt{N}}$. This especially means that we are dealing with a dilute gas taking up a volume of the order $Nr^3 = \frac{1}{\sqrt{N}}$. Due to the physical relevance of three-body interactions, which are for example responsible for 2% of the binding energy of liquid He^4 [21] and 14% for water [20], Dilute Bose gases with three-particle interactions have been studied extensively in [23, 24, 25, 26, 15], where the leading-order asymptotics of the ground state energy in the limit $N \to \infty$ has been established as well as Bose-Einstein condensation (BEC) in the Gross-Pitaevskii regime. Here (BEC) refers to the observation that most of the particles occupy the state with zero momentum. Following this body of work, we will focus for the sake of simplicity on gases without two-body interactions and a repulsive three-body interaction, which is precisely the setting of [25, Conjecture 5].

In the Gross-Pitaevskii regime, the leading-order term in the asymptotics of the ground state energy has been derived in [23]

$$E_N := \inf \sigma(H_N) = \frac{1}{6} b_{\mathcal{M}}(V) N + o_{N\to\infty}(N), \tag{3}$$

which is proportional to the number of particles N with a rather explicit constant $b_{\mathcal{M}}(V)$. Applying naive first-order perturbation theory, with $-\sum_{1\leq k\leq N}\Delta_{x_k}$ as the unperturbed operator, would suggest the value $\widehat{V}(0)$ for the constant $b_{\mathcal{M}}(V)$. It is, however, due to the singular nature of the scaling in Eq. (1) that we cannot ignore the presence of three particle correlations leading to a renormalized constant $b_{\mathcal{M}}(V) < \widehat{V}(0)$. In the following we will address a conjecture in [25], which claims that the subleading term in the asymptotic expansion of E_N is proportional to $\sqrt{N}$, see our main Theorem 1. The contributions to the ground state energy E_N of the order $\sqrt{N}$ arise based on two-particle, three-particle, and four-particle correlations in the ground state. As a byproduct from the proof of Theorem 1, we obtain in addition that the ground state Ψ_N^{GS} of the operator H_N satisfies (BEC) with a rate $\frac{1}{\sqrt{N}}$, that is, we show that the ratio of particles outside the state with zero momentum compared to the total number of particles N is of the order $O_{N\to\infty}\left(\frac{1}{\sqrt{N}}\right)$. This is an improvement of the (BEC) result in [23], where the authors showed that the ratio is of the order $o_{N\to\infty}(1)$.

It is worth pointing out that much more is known for Bose gases with two-particle interactions, where the expansion of the ground state energy to second order is well known in the Gross-Pitaevskii regime, the thermodynamic limit, and interpolating regimes, see, for example, [3, 7, 8, 10, 11, 13, 22]. Furthermore, (BEC) is well known for the Gross-Pitaevskii regime and regular enough interpolating regimes, even with an (optimal) rate, see, for example, [1, 2, 4, 5, 6, 9, 12, 18], and the subleading term in the expansion of the ground state energy is known to be of the order $O_{N\to\infty}(1)$. This resolution of the energy is sharp enough to see the spectral gap, which is of the order $O_{N\to\infty}(1)$ as well. For a Bose gas with three-particle interaction in the Gross-Pitaevskii regime we expect the spectral gap to be of the magnitude $O_{N\to\infty}(1)$, see the conjecture in [25]; however, the second-order expansion of the energy only allows for a resolution of the order $O_{N\to\infty}\left(\sqrt{N}\right)$, which is not sharp enough to see the spectral gap.

As it is not the goal of this manuscript to optimize the regularity of V, we will assume $V \in C^\infty(\mathbb{R}^6)$ for the sake of convenience (although assuming, e.g., $V \in H^9(\mathbb{R}^6)$ would certainly be sufficient).

The correct constant $b_{\mathcal{M}}(V)$ in the energy asymptotics Eq. (3) can be derived formally by making a translation-invariant ansatz for the correlation structure $\varphi(x-u, y-u)$ between three particles at positions x, y, and u, where $\varphi : \mathbb{R}^6 \longrightarrow \mathbb{R}$. Utilizing the matrix

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$$\mathcal{M} := \sqrt{\frac{1}{2}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}}$$

and the modified Laplace operator $\Delta_{\mathcal{M}} := (\mathcal{M}\nabla_{\mathbb{R}^3\times\mathbb{R}^3})^2$, let us first express the action of the Laplace operator in relative coordinates as

$$(\Delta_x + \Delta_y + \Delta_u)\varphi(x-u, y-u) = (2\Delta_{\mathcal{M}}\varphi)(x-u, y-u).$$

For three particles, the energy of the trial state $\Phi_\varphi(x-u, y-u) := 1 - \varphi(x-u, y-u)$ is then given by

$$\langle \Phi_\varphi, (-2\Delta_{\mathcal{M}} + V)\Phi_\varphi \rangle = \int_{\mathbb{R}^6} \left\{ 2\left|\mathcal{M}\nabla\varphi(X)\right|^2 + V(X)|1 - \varphi(X)|^2 \right\} \mathrm{d}X.$$

Optimizing in φ leads to the definition

$$b_{\mathcal{M}}(V) := \inf_{\varphi \in \dot{H}^1(\mathbb{R}^6)} \int_{\mathbb{R}^6} \left\{ 2\left|\mathcal{M}\nabla\varphi(X)\right|^2 + V(X)|1 - \varphi(X)|^2 \right\} \mathrm{d}x, \tag{4}$$

where $\dot{H}^1(\mathbb{R}^d)$ refers to the space of functions $g : \mathbb{R}^d \longrightarrow \mathbb{C}$ vanishing at infinity with $|\nabla g| \in L^2(\mathbb{R}^d)$, see [17, Section 8.3] where the notion $D^1(\mathbb{R}^d)$ is used instead. It has been verified in [23] that a unique minimizer ω to the variational problem in Eq. (4) exists satisfying the associated Euler–Lagrange equation

$$(-2\Delta_{\mathcal{M}} + V)\omega = V,$$

and the (modified) scattering length $b_{\mathcal{M}}(V)$ describes the leading-order asymptotics of the ground state energy correctly, see Eq. (3). Notably, the solution ω can formally be interpreted as a second-order correction to the condensate wavefunction $\Psi \equiv 1$, taking $-2\Delta_{\mathcal{M}} + V$, acting on functions vanishing at infinity, as the unperturbed operator and V, acting on the condensate $\Psi \equiv 1$, as the perturbation. Our main Theorem 1 confirms that the next term in the energy asymptotics in Eq. (3) is of the order $O_{N\to\infty}\left(\sqrt{N}\right)$ due to contributions from the three-particle correlation ω, as well as from two-particle and four-particle correlations.

In order to quantify the impact of two-particle correlations, we make a translation-invariant ansatz $\xi(x-u)$ with $\xi : \mathbb{R}^3 \longrightarrow \mathbb{R}$. Since $(\Delta_x + \Delta_u)\xi(x-u) = (2\Delta\xi)(x-u)$, we identify the kinetic energy of ξ as

$$\langle \xi, (-2\Delta)\xi \rangle = \int_{\mathbb{R}^3} 2|\nabla\xi(x)|^2 \mathrm{d}x.$$

Furthermore, the interaction energy of the wavefunction Φ_ω introduced above Eq. (4) with the state $\Phi(x-u, y-u) := \xi(x-u)$, which describes two correlated particles at position $(x, u) \in \mathbb{R}^6$ and a particle in the condensate at position $y \in \mathbb{R}^3$, reads

$$\langle \Phi, V\Phi_\omega \rangle + \langle \Phi_\omega, V\Phi \rangle = \int_{\mathbb{R}^6} 2V(x, y)(1 - \omega(x, y))\xi(x)\mathrm{d}y\mathrm{d}x = \int_{\mathbb{R}^3} 2V_{\mathrm{eff}}(x)\xi(x)\mathrm{d}x,$$

where we have introduced the effective two-particle interaction

$$V_{\mathrm{eff}} : \begin{cases} \mathbb{R}^3 \longrightarrow \mathbb{R}, \\ x \mapsto \int_{\mathbb{R}^3} V(x, y)(1 - \omega(x, y))\, \mathrm{d}y. \end{cases}$$

Adding up kinetic and interaction energy, and optimizing in ξ, immediately gives rise to the energy correction $-\mu(V)$ with the proportionality constant $\mu(V)$ defined as

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$$\mu(V) := -\inf_{\xi\in\dot H^1(\mathbb{R}^3)}\left\{\int_{\mathbb{R}^3}2|\nabla\xi(x)|^2\mathrm{d}x-\int_{\mathbb{R}^3}2V_{\mathrm{eff}}(x)\xi(x)\mathrm{d}x\right\}$$
$$=\int_{\mathbb{R}^6}\frac{V_{\mathrm{eff}}(x)V_{\mathrm{eff}}(y)}{8\pi|x-y|}\mathrm{d}x\mathrm{d}y. \tag{5}$$

Proceeding with the four-particle correlations, let us again commit to a translation-invariant ansatz $\eta(x-u,y-u,z-u)$ with $\eta:\mathbb{R}^9\longrightarrow\mathbb{R}$. Defining $\mathbb{V}:\mathbb{R}^9\longrightarrow\mathbb{R}$ and the matrix $\mathcal{M}_*$ as

$$\mathbb{V}(x_1,x_2,x_3):=V(x_1-x_3,x_2-x_3)+V(x_1,x_2)+V(x_1,x_3)+V(x_2,x_3),$$
$$\mathcal{M}_*:=\sqrt{\frac{1}{2}\begin{bmatrix}2&1&1\\1&2&1\\1&1&2\end{bmatrix}},$$

we can identify the action of the Laplace operator as

$$\begin{aligned}&(\Delta_{x_1}+\Delta_{x_2}+\Delta_{x_3}+\Delta_{x_4})\eta(x_1-x_4,x_2-x_4,x_3-x_4)\\&=\left(\left[\nabla_1^2+\nabla_2^2+\nabla_3^2+(-\nabla_1-\nabla_2-\nabla_3)^2\right]\eta\right)(x_1-x_4,x_2-x_4,x_3-x_4)\\&=\left((\nabla_1,\nabla_2,\nabla_3)\begin{bmatrix}2&1&1\\1&2&1\\1&1&2\end{bmatrix}\begin{pmatrix}\nabla_1\\\nabla_2\\\nabla_3\end{pmatrix}\eta\right)(x_1-x_4,x_2-x_4,x_3-x_4)\\&=(2\Delta_{\mathcal{M}_*}\eta)(x_1-x_4,x_2-x_4,x_3-x_4)\end{aligned} \tag{6}$$

and the action of the potential on η as

$$\begin{aligned}&\sum_{1\le i<j<k\le 4}V(x_i-x_k,x_j-x_k)\eta(x_1-x_4,x_2-x_4,x_3-x_4)\\&=[V(x_1-x_3,x_2-x_3)+V(x_1-x_4,x_2-x_4)+V(x_1-x_4,x_3-x_4)+V(x_2-x_4,x_3-x_4)]\\&\quad\times\eta(x_1-x_4,x_2-x_4,x_3-x_4)\\&=(\mathbb{V}\eta)(x_1-x_4,x_2-x_4,x_3-x_4).\end{aligned} \tag{7}$$

Adding up the kinetic and potential energy of the four-particle correlation η, therefore yields

$$\langle\eta,(-2\Delta_{\mathcal{M}_*}+\mathbb{V})\eta\rangle=\int_{\mathbb{R}^9}\left\{2\left|\mathcal{M}_*\nabla\eta(x)\right|^2+\mathbb{V}(x)|\eta(x)|^2\right\}\mathrm{d}x.$$

Moreover, the interaction energy $V_*(x,y,z):=V(x,y)$ of η with the state

$$\Phi(x-u,y-u,z-u):=\omega(y-u,z-u),$$

which describes three correlated particles at position $(y,z,u)\in\mathbb{R}^9$ and a particle in the condensate at position $x\in\mathbb{R}^3$, reads

$$\langle\eta,V_*\Phi\rangle+\langle\Phi,V_*\eta\rangle=2\int_{\mathbb{R}^9}V(x,y)\eta(x,y,z)\omega(y,z)\mathrm{d}x\mathrm{d}y\mathrm{d}z=2\int_{\mathbb{R}^9}\eta(X)f(X)\mathrm{d}X,$$

where we have introduced the function $f(x,y,z):=V(x,y)\omega(y,z)$. Combining kinetic, potential and interaction energy, yields

$$\int_{\mathbb{R}^9}\left\{2\left|\mathcal{M}_*\nabla\eta(x)\right|^2+\mathbb{V}(x)\eta(x)^2-2f(x)\eta(x)\right\}\mathrm{d}x=\mathcal{Q}(\eta)-\mathcal{Q}(0),$$

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where we have introduced the functional

$$\mathcal{Q}(\eta) := \int_{\mathbb{R}^9} \left\{ 2\left|\mathcal{M}_* \nabla \eta(x)\right|^2 + \mathbb{V}(x) \left| \frac{f(x)}{\mathbb{V}(x)} - \eta(x) \right|^2 \right\} \mathrm{d}x. \tag{8}$$

Note that $\frac{f}{\mathbb{V}}$ is well defined and bounded on the support of $\mathbb{V}$, due to the sign of $V \geq 0$. Consequently, the corresponding energy correction is given by $-\sigma(V)$ with

$$\sigma(V) := \mathcal{Q}(0) - \inf_{\eta \in \dot{H}^1(\mathbb{R}^9)} \mathcal{Q}(\eta). \tag{9}$$

Finally, we observe in the presence of an additional particle at position z further interaction terms between ω and itself. Utilizing again the potential $V_*(x, y, z) := V(x, z)$, and defining the states $\Phi_1(x - u, y - u, z - u) := \omega(y - u, z - u)$ and $\Phi_2(x - u, y - u, z - u) := \omega(x - u, z - u)$, there are two relevant terms

$$\langle \Phi_1, V_* \Phi_1 \rangle = \int_{\mathbb{R}^9} V(x, y)\omega(y, z)^2 \mathrm{d}x\mathrm{d}y\mathrm{d}z,$$

$$\langle \Phi_1, V_* \Phi_2 \rangle = \int_{\mathbb{R}^9} V(x, y)\omega(x, z)\omega(y, z)\mathrm{d}x\mathrm{d}y\mathrm{d}z,$$

giving rise to the energy correction $\gamma(V)$

$$\gamma(V) := \int_{\mathbb{R}^9} V(x, y)\omega(x, z)\omega(y, z)\mathrm{d}x\mathrm{d}y\mathrm{d}z + \frac{1}{2}\int_{\mathbb{R}^9} V(x, y)\omega(y, z)^2 \mathrm{d}x\mathrm{d}y\mathrm{d}z. \tag{10}$$

It is the content of our main Theorem 1, that $\gamma(V)$, $\mu(V)$, and $\sigma(V)$ describe the second-order correction to the leading-order asymptotics of the ground state energy E_N in Eq. (3), which is of the order $O_{N\to\infty}\left(\sqrt{N}\right)$. The mathematically precise implementation of the correlation structures ω, ξ, and η will be based on modified creation and annihilation operators, see, for example, [8], and generalized (unitary) Bogoliubov transformations, see, for example, [2, 3]. Furthermore, we show that the order $O_{N\to\infty}\left(\sqrt{N}\right)$ term comes with a nonzero prefactor for a large class of potentials V.

Theorem 1. *Let $V \in C^\infty(\mathbb{R}^6)$ be a bounded and non-negative function with compact support, such that the function V_N defined in Eq. (1) is permutation symmetric. Furthermore, let $\gamma(V), \mu(V)$, and $\sigma(V) \in \mathbb{R}$ be as in Eq. (10), Eq. (5) and Eq. (9) respectively, and let $b_{\mathcal{M}}(V)$ be as in Eq. (4). Then the ground state energy $E_N := \inf \sigma(H_N)$ satisfies*

$$E_N = \frac{1}{6} b_{\mathcal{M}}(V) N + \Big(\gamma(V) - \mu(V) - \sigma(V)\Big)\sqrt{N} + O_{N\to\infty}\left(N^{\frac{1}{4}}\right). \tag{11}$$

Furthermore, there exists a $\lambda(V) > 0$, such that for all $0 < \lambda \leq \lambda(V)$

$$\gamma(\lambda V) - \mu(\lambda V) - \sigma(\lambda V) < 0.$$

Remark 1. While Theorem 1 concerns Bose gases in the ultra-dilute Gross-Pitaevskii regime occupying a volume of the order $\frac{1}{\sqrt{N}}$, the leading-order behavior of the ground state energy per unit volume $e(\rho)$ is known in the thermodynamic regime as well as a function of the density ρ, see [24], and given in analogy to the leading-order asymptotics in Eq. (3) by

$$e(\rho) = \frac{1}{6} b_{\mathcal{M}}(V)\rho^3 + o_{\rho\to 0}\left(\rho^3\right).$$

It is remarkable that the coefficients $\gamma(V)$, $\mu(V)$, and $\sigma(V)$ from Theorem 1 are defined in terms of variational problems on the unconfined space $\mathbb{R}^{3d}$ and do not depend on the boundary conditions of the

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box Λ^d. Substituting ρ with $\frac{1}{\sqrt{N}}$ in Theorem 1 we therefore expect the second-order expansion of $e(\rho)$, as $\rho \longrightarrow 0$, to be given by

$$e(\rho) = \rho^3\left(\frac{1}{6}b_{\mathcal{M}}(V) + \Big(\gamma(V) - \mu(V) - \sigma(V)\Big)\rho\right) + o_{\rho\to 0}\Big(\rho^4\Big).$$

This would be in contrast with the second-order expansion of a Bose gas with two-body interactions, where in the celebrated Lee-Huang-Yang formula, see, for example, [14, 10] and [3] specifically for the periodic torus Λ, a summation of Fourier coefficients in the Pontryagin dual $(2\pi\mathbb{Z})^3$ of the locally compact group Λ appears. It is, however, expected that there is a corresponding Lee-Huang-Yang term for gases with three-body interactions, which should appear in a third-order expansion of the energy as a term of the order $O_{N\to\infty}(1)$.

Proof strategy of Theorem 1. Following the ideas in [23], respectively [2, 3, 10, 11], which have been developed in the context of Bose gases with two-body interactions, we are going to unveil the correlation structure of the ground state with the help of a suitable coordinate transformation. Based on the strategy presented in [8], our initial coordinate transformation will be of algebraic nature, that is, we introduce a new set of operators and observe that the many-body operator H_N is almost diagonal in these new variables. The algebraic approach immediately allows us to find satisfactory lower bounds on the ground state energy E_N. Furthermore, we show that this coordinate transformation can be realized in terms of a unitary map, at least in an approximate sense, which yields the corresponding upper bound on E_N.

In order to find a suitable transformation bringing H_N into a diagonal form, we observe that collisions between at most three particles will occur much more frequently compared to collisions between four or more particles, as we are in the dilute regime where the gas occupies only a volume of the magnitude $\frac{1}{\sqrt{N}}$. Consequently, we first look for a diagonalization of a gas with only three particles $N = 3$, which will involve the three-particle correlation structure ω, and subsequently lift it to a diagonalization of the full many-body problem. As it turns out, including the three-particle correlation structure is enough to identify the leading-order behavior of the ground state energy. To be more precise, utilizing the a priori information in Eq. (14), we are able to show at this point

$$E_N = \frac{1}{6}b_{\mathcal{M}}(V)N + O_{N\to\infty}\Big(\sqrt{N}\Big). \tag{12}$$

We want to emphasize that the proof of Eq. (12) depends on our ability to neglect collisions between four or more particles, and we note that the correlation structure involves mostly particles outside the state with zero-momentum. It is therefore crucial to have strong a priori information regarding the number of particles outside the state with zero momentum, which we will refer to as excited particles. In the language of second quantization, the number of excited particles can naturally be expressed as

$$\mathcal{N} := N - \mathcal{N}_0 := N - a_0^\dagger a_0, \tag{13}$$

where N is the total number of particles, $\mathcal{N}_0$ counts the number of particles with zero momentum and a_0 is the annihilation operator corresponding to the zero-momentum state, see also Section 2 for a more comprehensive introduction. The following result, which has been verified in [23], tells us that the number of excited particles is indeed small compared to the total number of particles N, that is,

$$\frac{1}{N}\langle\Psi_N, \mathcal{N}\Psi_N\rangle = o_{N\to\infty}(1), \tag{14}$$

for any sequence of states Ψ_N satisfying $\langle\Psi_N, H_N\Psi_N\rangle = E_N + O_{N\to\infty}(1)$. Notably, the results in [23] concern particles in $\mathbb{R}^3$ subject to a confining external potential, which can be generalized to our setting on the periodic torus without significant modifications as is explained in [25, Eq. (19)]. Using the a

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priori information in Eq. (14) then allows us to identify the leading-order asymptotics of the ground state energy E_N in Eq. (12). In addition, we obtain at this point an improved (BEC) result

$$\frac{1}{N}\langle \Psi_N^{\mathrm{GS}}, \mathcal{N}\Psi_N^{\mathrm{GS}}\rangle = O_{N\to\infty}\left(\frac{1}{\sqrt{N}}\right) \tag{15}$$

for any sequence of states Ψ_N satisfying $\langle \Psi_N, H_N\Psi_N\rangle = E_N + O_{N\to\infty}\left(N^{\frac{1}{4}}\right)$, see also the subsequent Theorem 2 where we further improve this result up to a rate of the order $N^{-\frac{3}{4}}$, which we believe to be of independent interest. Based on the observation that our constructed unitary maps create an order $O_{N\to\infty}(1)$ amount of excited particles, we conjecture that the optimal rate of condensation is of the magnitude $\frac{1}{N}$.

Finally, we use an additional coordinate transformation, which implements the two-particle and four-particle correlation structure ξ and η, together with the improved control on the number of excited particles in Eq. (15), in order to identify the coefficient C in front of the $\sqrt{N}$ term in the energy asymptotics

$$C = \gamma(V) - \mu(V) - \sigma(V).$$

Notably, collisions between four particles do contribute to the subleading term in the energy expansion in Eq. (11); however, in analogy to Eq. (12) we can dismiss collisions between five or more particles.

Theorem 2. *Let V satisfy the assumptions of Theorem 1 and let Ψ_N be a sequence of elements in $L^2_{\mathrm{sym}}(\Lambda^N)$ satisfying $\|\Psi_N\| = 1$ and*

$$\langle \Psi_N, H_N\Psi_N\rangle \leq E_N + DN^{\frac{1}{4}},$$

for some constant $D > 0$. Furthermore let $\mathcal{N}$ be the operator counting the number of excitations introduced in Eq. (13). Then there exists a constant $C > 0$, such that

$$\frac{1}{N}\langle \Psi_N, \mathcal{N}\Psi_N\rangle \leq CN^{-\frac{3}{4}}.$$

Outline. In Subsection 1.1 we are first deriving the three-particle correlation structure for a model where the total number of particles is $N = 3$. Following the strategy proposed in [8], we are implementing in a systematic way the correlation structures from Subsection 1.1 for gases with many particles $N \gg 1$ in Section 2. Using Bose-Einstein condensation of the ground state as an input, this allows us to immediately recover the leading-order behavior of E_N as a lower bound and, in the subsequent Section 3, also as an upper bound. Furthermore, we obtain at this point an improved version of (BEC) with a rate. In Section 4, we are going to describe the two-particle and four-particle correlation structure, which gives rise to the correction $\mu(V)$ and the correction $\sigma(V)$ defined in Eq. (5) and Eq. (9) respectively. It is the purpose of Subsection 4.2 to verify the lower bound in our main Theorem 1, wherein we use the improved (BEC) result, and the purpose of Section 5 to verify the corresponding upper bound. In the following Section 6, we can then provide (BEC) with a rate of the order $N^{-\frac{3}{4}}$, which concludes the proof of Theorem 2. The sign of $\gamma(\lambda V) - \mu(\lambda V) - \sigma(\lambda V)$ is established in Section 7 for small $\lambda > 0$, alongside other useful properties of the scattering solutions that describe the correlation structure. Finally Appendix A contains a collection of operator inequalities.

1.1. The three-body Problem

While naive first-order perturbation theory would tell us that the ground state energy E_N is to leading order given by the energy of the uncorrelated wavefunction $\Gamma_0(x_1, \ldots, x_N) := 1$

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$$\langle \Gamma_0, H_N \Gamma_0 \rangle = \frac{N(N-1)(N-2)}{6N^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} V(x,y)\, \mathrm{d}x\mathrm{d}y = \frac{N}{6} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} V(x,y)\, \mathrm{d}x\mathrm{d}y + o_{N\to\infty}(N),$$

it is due to the presence of correlations in the ground state of the operator H_N, that the leading-order coefficient $b_{\mathcal{M}}(V)$ in the energy asymptotics of E_N in Eq. (3) satisfies

$$b_{\mathcal{M}}(V) < \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} V(x,y)\, \mathrm{d}x\mathrm{d}y.$$

In order to quantify the correlation energy $\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} V(x,y)\, \mathrm{d}x\mathrm{d}y - b_{\mathcal{M}}(V)$, we are going to follow the frame work developed in [8], and investigate first the corresponding three-particle operator $H_{(3)} := -\Delta_3 + V_N$ acting on $L^2(\Lambda^3)$, where $\Delta_3 := \Delta_{x_1} + \Delta_{x_2} + \Delta_{x_3}$, before we study the many particle operator H_N defined in Eq. (2). It will be our goal to find a transformation

$$T : L^2(\Lambda^3) \longrightarrow L^2(\Lambda^3)$$

that removes correlations between states with low momenta and states with high momenta, that is, we want to bring $H_{(3)}$ into a block-diagonal form, which allows us to extract the correlation energy. It is content of Section 2 to lift the block-diagonalization from the three-particle problem, described by the transformation T, to a block-diagonalization of the many-particle operator H_N, which will allow us to identify the correlation energy for the many-particle problem.

Let us first specify the set of low momenta as either the set where all three particles occupy the zero-momentum state

$$\mathcal{L}_0 := \{(0,0,0)\} \subseteq (2\pi\mathbb{Z})^9 \tag{16}$$

or the set where at most one of the three particles is allowed to have non-zero momentum

$$\mathcal{L}_K := \bigcup_{|k|\leq K} \{(k,0,0),(0,k,0),(0,0,k)\} \subseteq (2\pi\mathbb{Z})^9,$$

where $0 \leq K < \infty$ is a parameter that we are going to specify later. For the purpose of extracting the correlation energy, it is enough to consider $K := 0$, however, for technical reasons it is going to be convenient later to consider positive values $K > 0$ as well. Having the set $\mathcal{L}_K$ at hand, we can define the projection π_K onto states with low momenta as

$$\pi_K(\Psi) := \sum_{(k_1 k_2 k_3)\in \mathcal{L}_K} \langle u_{k_1} u_{k_2} u_{k_3}, \Psi \rangle u_{k_1} u_{k_2} u_{k_3}, \tag{17}$$

where $u_k(x) := e^{ikx}$ for $k \in (2\pi\mathbb{Z})^3$ and $u_{k_1} u_{k_2} u_{k_3}$ has to be understood as the function $u_{k_1}(x_1) u_{k_2}(x_2) u_{k_3}(x_3)$. Let us furthermore introduce the projection Q acting on $L^2(\Lambda)$ as

$$Q(\phi) := \sum_{k\neq 0} \langle u_k, \phi \rangle u_k. \tag{18}$$

Following the strategy in [8], let R be the pseudoinverse of the operator $Q^{\otimes 3}(-\Delta_3 + V_N)Q^{\otimes 3}$, that is, using the function $h(t) := \frac{1}{t}$ for $t \neq 0$ and $h(0) := 0$ the operator R is given as

$$R = h\Big(Q^{\otimes 3}(-\Delta_3 + V_N)Q^{\otimes 3}\Big),$$

and let us define the Feshbach-Schur like transformation

$$T := 1 + R V_N \pi_K. \tag{19}$$

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Note that T would be a proper Feshbach-Schur map, in case we would exchange $Q^{\otimes 3}$ with the projection $1-\pi_K$; however, we prefer to work with $Q^{\otimes 3}$ for technical reasons. Using the notation $\{A+\mathrm{H.c.}\} := A+A^*$ and the observation $T^{-1} = 1 - RV_N\pi_K$, yields

$$H_{(3)}T^{-1} = H_{(3)} - H_{(3)}RV_N\pi_K = H_{(3)} - Q^{\otimes 3}H_{(3)}RV_N\pi_K - (1-Q^{\otimes 3})H_{(3)}RV_N\pi_K$$
$$= H_{(3)} - Q^{\otimes 3}V_N\pi_K - (1-Q^{\otimes 3})V_N RV_N\pi_K,$$

and by taking the adjoint we furthermore obtain

$$(T^{-1})^\dagger H_{(3)} = H_{(3)} - \pi_K V_N Q^{\otimes 3} - \pi_K V_N RV_N(1-Q^{\otimes 3}).$$

Combining both equations yields

$$\begin{aligned}(T^{-1})^\dagger H_{(3)}T^{-1} &= H_{(3)}T^{-1} - \pi_K V_N Q^{\otimes 3} - \pi_K V_N RV_N(1-Q^{\otimes 3}) + \pi_K V_N RV_N\pi_K\\ &= H_{(3)} - Q^{\otimes 3}V_N\pi_K - \pi_K V_N Q^{\otimes 3} - (1-Q^{\otimes 3})V_N RV_N\pi_K\\ &\quad - \pi_K V_N RV_N(1-Q^{\otimes 3}) + \pi_K V_N RV_N\pi_K\\ &= -\Delta_3 + V_N - Q^{\otimes 3}V_N\pi_K - \pi_K V_N Q^{\otimes 3} - (1-\pi_K-Q^{\otimes 3})V_N RV_N\pi_K\\ &\quad - \pi_K V_N RV_N(1-\pi_K-Q^{\otimes 3}) - \pi_K V_N RV_N\pi_K\\ &= -\Delta_3 + \pi_K(V_N - V_N RV_N)\pi_K + (1-\pi_K)V_N(1-\pi_K)\\ &\quad + \left\{\pi_K(V_N - V_N RV_N)\left(1-\pi_K-Q^{\otimes 3}\right) + \mathrm{H.c.}\right\},\end{aligned} \tag{20}$$

where we have used in the final identity Eq. (20) the decomposition

$$V_N = \pi_K V_N\pi_K + (1-\pi_K)V_N(1-\pi_K) + \left\{\pi_K V_N(1-\pi_K-Q^{\otimes 3}) + \pi_K V_N Q^{\otimes 3} + \mathrm{H.c.}\right\}.$$

Defining the almost block-diagonal renormalized potential $\widetilde{V}_N$ as

$$\begin{aligned}\widetilde{V}_N &:= \pi_K(V_N - V_N RV_N)\pi_K + (1-\pi_K)V_N(1-\pi_K)\\ &\quad + \left\{\left(1-\pi_K-Q^{\otimes 3}\right)(V_N - V_N RV_N)\pi_K + \mathrm{H.c.}\right\},\end{aligned} \tag{21}$$

and multiplying Eq. (20) from the left by $T^\dagger$ and from the right by T, therefore yields the algebraic identity

$$H_{(3)} = T^\dagger\left(-\Delta_3 + \widetilde{V}_N\right)T. \tag{22}$$

The presence of $\{(1-\pi_K-Q^{\otimes 3})(V_N - V_N RV_N)\pi_K + \mathrm{H.c.}\}$ in $\widetilde{V}_N$, which are the terms that violate the block-diagonal structure, is due to the usage of $Q^{\otimes 3}$ instead of $1-\pi_K$; however, it turns out that these terms do not contribute to the correlation energy to leading order. One therefore expects to read off the leading-order coefficient $b_{\mathcal{M}}(V)$ in the asymptotic expansion of the ground state energy E_N in Eq. (3) from the matrix entries of the renormalized potential

$$\left(\widetilde{V}_N\right)_{000,000} = \langle u_0u_0u_0, \widetilde{V}_N u_0u_0u_0\rangle = \langle u_0u_0u_0, (V_N - V_N RV_N)u_0u_0u_0\rangle.$$

As we are going to verify in Lemma 16, we have indeed the asymptotic result

$$b_{\mathcal{M}}(V) = N^2\langle u_0u_0u_0, (V_N - V_N RV_N)u_0u_0u_0\rangle + O_{N\to\infty}\left(\frac{1}{N}\right).$$

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2. First-order lower bound

It is the goal of this Section to bring, in analogy to Eq. (22), the many-particle operator H_N in an approximate block-diagonal form, which allows us to obtain an asymptotically correct lower bound on the ground state energy E_N in Corollary 2. First, we are going to rewrite the operator H_N defined in Eq. (2) in the language of second quantization. For this purpose let $a_k^\dagger$ denote the operator that creates a particle in the mode u_k, that is, for $\Phi_n \in L^2_{\mathrm{sym}}(\Lambda^n)$ we define $a_k^\dagger \Phi_n \in L^2_{\mathrm{sym}}(\Lambda^{n+1})$ as

$$a_k^\dagger \Phi_n := \frac{1}{\sqrt{n+1}} \Xi_{n+1}(u_k \otimes \Phi_n),$$

where Ξ_{n+1} is the orthogonal projection onto $L^2_{\mathrm{sym}}(\Lambda^{n+1}) \subseteq L^2(\Lambda^{n+1})$, and we write a_k for its adjoint, which annihilates a particle in the mode $u_k(x) := e^{ik\cdot x}$. With creation and annihilation operators at hand, we can write

$$H_N = \sum_{k\in(2\pi\mathbb{Z})^3} |k|^2 a_k^\dagger a_k + \frac{1}{6} \sum_{ijk,\ell mn\in(2\pi\mathbb{Z})^3} (V_N)_{ijk,\ell mn} a_i^\dagger a_j^\dagger a_k^\dagger a_\ell a_m a_n, \tag{23}$$

where $(V_N)_{ijk,\ell mn}$ are the matrix elements of V_N w.r.t. to the basis $u_i u_j u_k$ defined below Eq. (17). If not indicated otherwise, we will always assume that indices run in the set $(2\pi\mathbb{Z})^3$, which we will usually neglect in our notation, and we write $k \neq 0$ in case the index runs in the set $(2\pi\mathbb{Z})^3 \setminus \{0\}$. Note that the operator on the right hand side of Eq. (23) is naturally defined on the full Fock space

$$\mathcal{F}\left(L^2(\Lambda)\right) := \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\Lambda^n),$$

while the left-hand side is only defined on $L^2_{\mathrm{sym}}(\Lambda^N) \subseteq \mathcal{F}(L^2(\Lambda))$, and therefore Eq. (23) has to be understood as being restricted to the subspace $L^2_{\mathrm{sym}}(\Lambda^N)$. Furthermore, we observe that V_N is a translation-invariant multiplication operator, and therefore the matrix elements of V_N satisfy $(V_N)_{ijk,\ell mn} = 0$ in case $i + j + k \neq \ell + m + n$ and otherwise

$$(V_N)_{ijk,\ell mn} = (V_N)_{(i-\ell)(j-m)(k-n),000} = N^{-2}\widehat{V}\left(\frac{j-m}{\sqrt{N}}, \frac{k-n}{\sqrt{N}}\right). \tag{24}$$

Following the strategy proposed in [8], we are going to introduce a many-particle counterpart to the three particle map T defined in Eq. (19), which is realized by the set of operators

$$c_k := a_k + \frac{1}{2} \sum_{ij,\ell mn} (T-1)_{ijk,\ell mn}\, a_i^\dagger a_j^\dagger a_\ell a_m a_n, \tag{25}$$

$$\psi_{ijk} := \sum_{\ell mn} T_{ijk,\ell mn}\, a_\ell a_m a_n. \tag{26}$$

Here $T_{ijk,\ell mn} := \langle u_i u_j u_k, T u_\ell u_m u_n\rangle$ denotes the matrix elements of T. The following Lemma 1 is the many-particle counterpart to Eq. (22), in the sense that it provides an (approximate) block-diagonal representation of the operator H_N in terms of the new variables c_k and ψ_{ijk}.

Lemma 1. *Let $\widetilde{V}_N$ be the operator defined in Eq. (21). Then we have*

$$H_N = \sum_k |k|^2 c_k^\dagger c_k + \frac{1}{6} \sum_{ijk,\ell mn} \left(\widetilde{V}_N\right)_{ijk,\ell mn} \psi_{ijk}^\dagger \psi_{\ell mn} - \mathcal{E}, \tag{27}$$

where the residual term $\mathcal{E}$ is defined as

$$\mathcal{E} := \frac{1}{4} \sum_{ijk,\ell mn;i'j',\ell'm'm'} |k|^2 \overline{(T-1)_{i'j'k,\ell'm'n'}} (T-1)_{ijk,\ell mn}\, a^\dagger_{\ell'} a^\dagger_{m'} a^\dagger_{n'} \times \left(a_{i'} a_{j'} a^\dagger_i a^\dagger_j - \delta_{ii'}\delta_{jj'} - \delta_{ij'}\delta_{ji'} \right) a_\ell a_m a_n.$$

Proof. Using the permutation symmetry of T, we first identify $\sum_k |k|^2 (c_k - a_k)^\dagger (c_k - a_k)$ as

$$\begin{aligned}
&\frac{1}{4} \sum_{ijk,\ell mn;i'j',\ell'm'm'} |k|^2 \overline{(T-1)_{i'j'k,\ell'm'n'}} (T-1)_{ijk,\ell mn}\, a^\dagger_{\ell'} a^\dagger_{m'} a^\dagger_{n'} a_{i'} a_{j'} a^\dagger_i a^\dagger_j a_\ell a_m a_n \\
&= \frac{1}{2} \sum_{ijk,\ell mn} \left\{ (T-1)^\dagger (-\Delta_{x_3})(T-1) \right\}_{ijk,\ell mn} a^\dagger_i a^\dagger_j a^\dagger_k a_\ell a_m a_n + \mathcal{E} \\
&= \frac{1}{6} \sum_{ijk,\ell mn} \left\{ (T-1)^\dagger (-\Delta_3)(T-1) \right\}_{ijk,\ell mn} a^\dagger_i a^\dagger_j a^\dagger_k a_\ell a_m a_n + \mathcal{E},
\end{aligned}$$

where Δ_3 is the Laplace operator on $L^2(\Lambda)^{\otimes 3}$. Similarly

$$\begin{aligned}
\sum_k |k|^2 a^\dagger_k (c_k - a_k) + \text{H.c.} &= \frac{1}{6} \sum_{ijk,\ell mn} \left\{ (-\Delta_3)(T-1) + \text{H.c.} \right\}_{ijk,\ell mn} a^\dagger_i a^\dagger_j a^\dagger_k a_\ell a_m a_n, \\
\sum_{ijk,\ell mn} \left(\widetilde{V}_N \right)_{ijk,\ell mn} \psi^\dagger_{ijk} \psi_{\ell mn} &= \sum_{ijk,\ell mn} \left(T^\dagger \widetilde{V}_N T \right)_{ijk,\ell mn} a^\dagger_i a^\dagger_j a^\dagger_k a_\ell a_m a_n.
\end{aligned}$$

Since

$$(T-1)^\dagger \Delta_3 (T-1) + \{\Delta_3(T-1) + \text{H.c.}\} = T^\dagger \Delta_3 T - \Delta_3$$

we obtain

$$\begin{aligned}
&\sum_k |k|^2 c^\dagger_k c_k + \frac{1}{6} \sum_{ijk,\ell mn} \left(\widetilde{V}_N \right)_{ijk,\ell mn} \psi^\dagger_{ijk} \psi_{\ell mn} \\
&= \sum_k |k|^2 a^\dagger_k a_k + \frac{1}{6} \sum_{ijk,\ell mn} \left\{ T^\dagger \left(-\Delta_3 + \widetilde{V}_N \right) T + \Delta_3 \right\}_{ijk,\ell mn} a^\dagger_i a^\dagger_j a^\dagger_k a_\ell a_m a_n + \mathcal{E}.
\end{aligned}$$

We observe that $T^\dagger \left(-\Delta_3 + \widetilde{V}_N \right) T + \Delta_3 = V_N$ by Eq. (22), which concludes the proof by the representation of H_N in second quantization, see Eq. (23). □

Making use of the sign $(1-\pi_K) V_N (1-\pi_K) \geq 0$, we immediately obtain that

$$\sum_{ijk,\ell mn} ((1-\pi_K) V_N (1-\pi_K))_{ijk,\ell mn} \psi^\dagger_{ijk} \psi_{\ell mn} \geq 0.$$

Therefore Lemma 1 allows us to bound H_N from below by

$$\begin{aligned}
H_N &\geq \sum_k |k|^2 c^\dagger_k c_k + \frac{1}{6} \sum_{ijk,\ell mn} \left(\widetilde{V}_N - (1-\pi_K) V_N (1-\pi_K) \right)_{ijk,\ell mn} \psi^\dagger_{ijk} \psi_{\ell mn} - \mathcal{E} \\
&= \sum_k |k|^2 c^\dagger_k c_k + \frac{1}{6} \sum_{ijk,\ell mn} \left(\widetilde{V}_N - (1-\pi_K) V_N (1-\pi_K) \right)_{ijk,\ell mn} a^\dagger_i a^\dagger_j a^\dagger_k a_\ell a_m a_n - \mathcal{E}, \qquad (28)
\end{aligned}$$

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where we have used the fact that $\psi_{ijk} = a_i a_j a_k$ in case one of the indices is zero, which is a direct consequence of the observation that $(T-1)_{ijk,\ell mn} = 0$ in case one of the indices in $\{i, j, k\}$ is zero. Note that we can write

$$\widetilde{V}_N - (1-\pi_K)V_N(1-\pi_K) = A + B + B^*$$

with A and B defined as

$$A := \pi_K(V_N - V_N R V_N)\pi_K,$$
$$B := \left(1 - \pi_K - Q^{\otimes 3}\right)(V_N - V_N R V_N)\pi_K.$$

Using the sets $\mathcal{L}^{(z)} := \{(z,0,0),(0,z,0),(0,0,z)\}$, let us first analyze the term involving A

$$\frac{1}{6}\sum_{ijk,\ell mn}(A)_{ijk,\ell mn} a_i^\dagger a_j^\dagger a_k^\dagger a_\ell a_m a_n = \frac{1}{6}\sum_{(ijk),(\ell mn)\in\mathcal{L}_K}(V_N - V_N R V_N)_{ijk,\ell mn} a_i^\dagger a_j^\dagger a_k^\dagger a_\ell a_m a_n$$
$$= \frac{1}{6}(V_N - V_N R V_N)_{000,000}(a_0^\dagger)^3 a_0^3 + \sum_{0<|z|<K}\left\{\frac{1}{6}\sum_{(ijk),(\ell mn)\in\mathcal{L}^{(z)}}(V_N - V_N R V_N)_{ijk,\ell mn}\right\} a_0^{2\dagger} a_0^2 a_z^\dagger a_z.$$

Together with the definition of the coefficients

$$\lambda_{k,\ell} := \frac{1}{18}\langle u_0 u_\ell u_{k-\ell}, (V_N - V_N R V_N)(u_0 u_0 u_k + u_0 u_k u_0 + u_k u_0 u_0)\rangle \tag{29}$$

we can write

$$\frac{1}{6}(V_N - V_N R V_N)_{000,000} = \frac{1}{6}\langle u_0 u_0 u_0, (V_N - V_N R V_N) u_0 u_0 u_0\rangle = \lambda_{0,0},$$

and utilizing the permutation symmetry of $V_N - V_N R V_N$ we furthermore obtain for $z \neq 0$

$$\frac{1}{6}\sum_{(ijk),(\ell mn)\in\mathcal{L}^{(z)}}(V_N - V_N R V_N)_{ijk,\ell mn} = \frac{1}{6}\left\langle \sum_{(ijk)\in\mathcal{L}^{(z)}} u_i u_j u_k, (V_N - V_N R V_N)\sum_{(\ell mn)\in\mathcal{L}^{(z)}} u_\ell u_m u_n\right\rangle$$
$$= \frac{1}{2}\left\langle u_0 u_0 u_z, (V_N - V_N R V_N)\sum_{(\ell mn)\in\mathcal{L}^{(z)}} u_\ell u_m u_n\right\rangle$$
$$= 9\lambda_{z,0}.$$

Therefore,

$$\frac{1}{6}\sum_{ijk,\ell mn}(A)_{ijk,\ell mn} a_i^\dagger a_j^\dagger a_k^\dagger a_\ell a_m a_n = \lambda_{0,0}\,(a_0^\dagger)^3 a_0^3 + 9 a_0^{2\dagger} a_0^2 \sum_{0<|k|\leq K}\lambda_{k,0} a_k^\dagger a_k. \tag{30}$$

To keep the notation light, we do not explicitly indicate the N dependence of $\lambda_{k,\ell}$. Similarly

$$\frac{1}{6}\sum_{ijk,\ell mn}(B)_{ijk,\ell mn} a_i^\dagger a_j^\dagger a_k^\dagger a_\ell a_m a_n = 3 a_0^\dagger a_0^3 \sum_{\ell\neq 0}\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger + 9 a_0^\dagger a_0^2 \sum_{\ell,0<|k|\leq K}\lambda_{k,\ell} a_\ell^\dagger a_{k-\ell}^\dagger a_k. \tag{31}$$

Putting together Eq. (28), Eq. (30) and Eq. (31) yields

$$H_N \geq \lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \sum_k |k|^2 c_k^\dagger c_k + \mathbb{Q}_K + \mathcal{E}' - \mathcal{E}, \tag{32}$$

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where we define the operator $\mathbb{Q}_K$ and the error term $\mathcal{E}'$ as

$$\mathbb{Q}_K := 9a_0^{2\dagger}a_0^2 \sum_{0<|k|\leq K} \lambda_{k,0}a_k^\dagger a_k + 3\left(a_0^\dagger a_0^3 \sum_{0<|\ell|\leq K} \lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger + \text{H.c.}\right), \tag{33}$$

$$\mathcal{E}' := \left(3\sum_{|\ell|>K} \lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger\, a_0^\dagger a_0^3 + 9\sum_{\ell,0<|k|\leq K} \lambda_{k,\ell} a_\ell^\dagger a_{k-\ell}^\dagger a_k\, a_0^\dagger a_0^2 + \text{H.c.}\right). \tag{34}$$

Let us furthermore introduce the particle number operator

$$\mathcal{N} := \sum_{k\neq 0} a_k^\dagger a_k,$$

which counts the number of excited particles, that is, the number of particles with momentum $k \neq 0$. Since we have the operator identity $\sum_k a_k^\dagger a_k = N$ on the Hilbert space $L^2_{\text{sym}}(\Lambda^N) \subseteq \mathcal{F}\big(L^2(\Lambda)\big)$, we observe that $a_0^\dagger a_0 = N - \mathcal{N}$, see also Eq. (13), that is, the number of particles with momentum $k = 0$ is given by the difference between the total number of particles N and the number of excited particles.

In order to control the terms arising in Eq. (32), it is imperative to understand the asymptotic behavior of the coefficients $\lambda_{k,\ell}$ and the matrix entries $T_{ijk,\ell mn}$ defined below Eq. (26). Since we want to focus our attention on the many-body analysis, we will postpone our study of the scattering coefficients to Section 7. For the convenience of the reader, we are going to state the relevant results, which are proven in Lemma 15 and Lemma 16 respectively,

$$|\lambda_{k,\ell}| \leq \frac{C}{N^2}\left(1 + \frac{|\ell|^2}{N}\right)^{-1}, \tag{35}$$

$$\big|(T-1)_{ijk,\ell 00}\big| \leq \frac{C\,\mathbb{1}(i+j+k=\ell)}{N^2(|i|^2+|j|^2+|k|^2)}\left(1 + \frac{|i|^2+|j|^2+|k|^2}{N+|\ell|^2}\right)^{-2}, \tag{36}$$

$$\big|6N^2\lambda_{0,0} - b_{\mathcal{M}}(V)\big| \leq \frac{1}{N}, \tag{37}$$

$$\left|6N^2\frac{\lambda_{k,\ell}}{6} - b_{\mathcal{M}}(V)\right| \leq \frac{C_{k,\ell}}{\sqrt{N}}. \tag{38}$$

Furthermore, we need the following result, which is verified in Lemma A2, see Appendix A, and which allows us to compare the new operators c_k with the annihilation operators a_k,

$$\sum_k |k|^{2\sigma}(c_k - a_k)(c_k - a_k)^\dagger \lesssim \frac{1}{N}\mathcal{N}^2, \tag{39}$$

$$\sum_k |k|^{2\tau} a_k^\dagger \mathcal{N}^s a_k \lesssim \sum_k |k|^{2\tau} c_k^\dagger \mathcal{N}^s c_k + \frac{1}{N}\mathcal{N}^{s+2} + N^\tau(\mathcal{N}+1)^s \tag{40}$$

for $0 \leq \tau \leq 1$, $0 \leq \sigma < \frac{1}{2}$ and integers $s \geq 0$. Utilizing Eq. (35)-(40), the following Lemma 2, Lemma 3 and Lemma 4, provide relevant bounds on the various terms appearing in Eq. (32), which will be instrumental in order to establish that the ground state energy E_N of H_N is, to leading order, bounded from below by $\frac{1}{6}b_{\mathcal{M}}(V)N$, see Corollary 2. In our first Lemma 2 we provide a lower bound on

$$\lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \mathbb{Q}_K$$

for K large enough, which is an operator that is at most quadratic in the variables a_k and $a_k^\dagger$ for $k \neq 0$.

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Lemma 2. *Let $b_{\mathcal{M}}(V)$ be the modified scattering length defined in Eq. (4). Then there exists for all $\tau, \alpha > 0$, a constant $K_0(\tau,\alpha)$ and for all $K \geq K_0(\tau,\alpha)$ a constant $C_K > 0$, such that*

$$\lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \mathbb{Q}_K \geq \frac{1}{6} b_{\mathcal{M}}(V) N - \alpha \sum_k |k|^{2\tau} a_k^\dagger a_k - C_K\left(1 + \frac{\mathcal{N}^2}{N} + \frac{\mathcal{N}}{\sqrt{N}}\right),$$

for $K \geq K_0(\tau,\alpha)$.

Proof. First of all we observe that we can write

$$\begin{aligned}(a_0^\dagger)^3 a_0^3 &= N^3 - 3N^2(\mathcal{N}+3) + N(3\mathcal{N}^2 + 6\mathcal{N} + 2) - \mathcal{N}^3 - 3\mathcal{N}^2 - 2\mathcal{N} \\ &\geq N^3 - 3N^2\mathcal{N} - N^2 D,\end{aligned}$$

for a suitable $D > 0$. Defining

$$\mathcal{N}_> := \mathcal{N} - \sum_{0<|k|\leq K} a_k^\dagger a_k,$$

we therefore obtain in combination with Eq. (37) and Eq. (38)

$$\begin{aligned}&\lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \mathbb{Q}_K - \frac{1}{6} b_{\mathcal{M}}(V) N \\ &\geq \frac{1}{6} b_{\mathcal{M}}(V)\left\{9\frac{(a_0^\dagger)^2 a_0^2}{N^2}\sum_{0<|k|\leq K} a_k^\dagger a_k + 3\left(\frac{a_0^\dagger a_0^3}{N^2}\sum_{0<|k|\leq K} a_k^\dagger a_{-k}^\dagger + \text{H.c.}\right) - 3\mathcal{N} - DN^{-\frac{1}{2}}\mathcal{N}\right\} - D \\ &= \frac{1}{6} b_{\mathcal{M}}(V)\left\{\left(9\frac{(a_0^\dagger)^2 a_0^2}{N^2} - 3 - DN^{-\frac{1}{2}}\right)\sum_{0<|k|\leq K} a_k^\dagger a_k \right. \\ &\quad \left. + 3\left(\frac{a_0^\dagger a_0^3}{N^2}\sum_{0<|k|\leq K} a_k^\dagger a_{-k}^\dagger + \text{H.c.}\right) - 3\mathcal{N}_>\right\} - D,\end{aligned}$$

for a suitable constant $D > 0$. Since

$$3\frac{a_0^\dagger a_0^3}{N^2}\sum_{0<|k|\leq K} a_k^\dagger a_{-k}^\dagger + \text{H.c.} \leq 3\sum_{0<|k|\leq K}\left(2a_k^\dagger a_k + 1\right) \leq 6\sum_{0<|k|\leq K} a_k^\dagger a_k + 3\left(\frac{K}{\pi}+1\right)^3,$$

and since we have

$$\left(9\frac{(a_0^\dagger)^2 a_0^2}{N^2} - 9 - DN^{-\frac{1}{2}}\right)\sum_{0<|k|\leq K} a_k^\dagger a_k \geq -9\frac{\mathcal{N}^2}{N} - D\frac{\mathcal{N}}{\sqrt{N}},$$

we obtain

$$\lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \mathbb{Q}_K \geq \frac{1}{6} b_{\mathcal{M}}(V) N - \frac{1}{2} b_{\mathcal{M}}(V)\mathcal{N}_> - C_K\left(1 + \frac{\mathcal{N}^2}{N} + \frac{\mathcal{N}}{\sqrt{N}}\right)$$

for a suitable, K-dependent, constant C_K. Finally, we choose $K_0(\tau,\alpha)$ large enough such that $\frac{1}{2} b_{\mathcal{M}}(V) K_0(\tau,\alpha)^{-2\tau} \leq \alpha$, and therefore we have for all $K \geq K_0(\tau,\alpha)$

$$\frac{1}{2} b_{\mathcal{M}}(V)\mathcal{N}_> \leq \frac{1}{2} b_{\mathcal{M}}(V) K^{-2\tau}\sum_k |k|^{2\tau} a_k^\dagger a_k \leq \alpha \sum_k |k|^{2\tau} a_k^\dagger a_k. \qquad \square$$

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In the Lemma 3, we will provide estimates on the residual term $\mathcal{E}$ defined in Lemma 1, which will allow us to compare the size of $\mathcal{E}$ with the kinetic energy $\sum_k |k|^2 c_k^\dagger c_k$ in the variables c_k. Before we come to Lemma 3, we need the following Corollary 1, which is a consequence of Eq. (40) and allows us to estimate monomials in the operators a_k and $a_k^\dagger$ by the kinetic energy in the variables c_k and powers of the particle number operator $\mathcal{N}$.

Corollary 1. *Let $\mathcal{K}_{\tau,t} := \sum_{i=1}^t (-\Delta_{x_i})^\tau$. Given $0 \leq \tau \leq 1$, and integers $s,t \geq 1$ and $\alpha,\beta \geq 0$, there exist $\delta > 0$ and $C > 0$, such that for $\epsilon > 0$*

$$\pm\left(\sum_{i_1\dots i_s, j_1\dots j_t} G_{i_1\dots i_s, j_1\dots j_t} a_{j_t}^\dagger \dots a_{j_1}^\dagger X\, a_{i_1}\dots a_{i_s} + \mathrm{H.c.}\right) \leq C\left\|\mathcal{K}_{\tau,t}^{-\frac{1}{2}} G \mathcal{K}_{\tau,s}^{-\frac{1}{2}}\right\| \|\mathcal{N}^{-\frac{\beta}{2}} X \mathcal{N}^{-\frac{\alpha}{2}}\|$$
$$\times\left\{\sum_k |k|^2 c_k^\dagger\left(\epsilon\mathcal{N}^{s+\alpha-1} + \epsilon^{-1}\mathcal{N}^{t+\beta-1}\right)c_k + (\mathcal{N} + N^\tau)\left(\epsilon\mathcal{N}^{s+\alpha-1} + \epsilon^{-1}\mathcal{N}^{t+\beta-1}\right)\right\},$$

where $G : (\mathrm{ran}Q)^{\otimes s} \longrightarrow (\mathrm{ran}Q)^{\otimes t}$ and $X : \mathcal{F}(L^2(\Lambda)) \longrightarrow \mathcal{F}(L^2(\Lambda))$. In case $s = 0$

$$\pm\left(\sum_{j_1\dots j_t} G_{j_1\dots j_t} a_{j_t}^\dagger \dots a_{j_1}^\dagger X + \mathrm{H.c.}\right) \leq C\left\|\mathcal{K}_{\tau,t}^{-\frac{1}{2}} G\right\| \|\mathcal{N}^{-\frac{\beta}{2}} X \mathcal{N}^{-\frac{\alpha}{2}}\|$$
$$\times\left\{\epsilon\mathcal{N}^\alpha + \epsilon^{-1}\sum_k |k|^2 c_k^\dagger \mathcal{N}^{t+\beta-1} c_k + \epsilon^{-1}(\mathcal{N} + N^\tau)\mathcal{N}^{t+\beta-1}\right\}.$$

Proof. Let us define for $s,t \geq 1$ the operator-valued vector and operator-valued matrix

$$\begin{aligned}(\Phi_{\tau,s})_{k_1\dots k_s} &:= \left(|k_1|^{2\tau} + \dots + |k_s|^{2\tau}\right)^{\frac{1}{2}} a_{k_1}\dots a_{k_s}, \\ \Upsilon_{i_1\dots i_s, j_1\dots j_t} &:= \left(\mathcal{K}_{\tau,t}^{-\frac{1}{2}} G\, \mathcal{K}_{\tau,s}^{-\frac{1}{2}}\right)_{i_1\dots i_s, j_1\dots j_t} \mathcal{N}^{-\frac{\beta}{2}} X \mathcal{N}^{-\frac{\alpha}{2}},\end{aligned} \tag{41}$$

which allow us to represent

$$\sum_{i_1\dots i_s, j_1\dots j_t} G_{i_1\dots i_s, j_1\dots j_t} a_{j_t}^\dagger \dots a_{j_1}^\dagger X\, a_{i_1}\dots a_{i_s} = \Phi_{\tau,t}^\dagger \mathcal{N}^{\frac{\beta}{2}} \Upsilon \mathcal{N}^{\frac{\alpha}{2}} \Phi_{\tau,s}.$$

Using the fact that $\|\Upsilon\| \leq \left\|\mathcal{K}_{\tau,t}^{-\frac{1}{2}} G\, \mathcal{K}_{\tau,s}^{-\frac{1}{2}}\right\| \|\mathcal{N}^{-\frac{\beta}{2}} X \mathcal{N}^{-\frac{\alpha}{2}}\|$, we obtain by Cauchy-Schwarz

$$\pm\left(\Phi_t^\dagger \Upsilon \Phi_s + \mathrm{H.c.}\right) \leq \left\|\mathcal{K}_{\tau,t}^{-\frac{1}{2}} G\, \mathcal{K}_{\tau,s}^{-\frac{1}{2}}\right\| \|\mathcal{N}^{-\frac{\beta}{2}} X \mathcal{N}^{-\frac{\alpha}{2}}\| \left(\epsilon\Phi_{\tau,t}^\dagger \mathcal{N}^\beta \Phi_{\tau,t} + \epsilon^{-1}\Phi_{\tau,s}^\dagger \mathcal{N}^\alpha \Phi_{\tau,s}\right)$$
$$= \left\|\mathcal{K}_{\tau,t}^{-\frac{1}{2}} G\, \mathcal{K}_{\tau,s}^{-\frac{1}{2}}\right\| \|\mathcal{N}^{-\frac{\beta}{2}} X \mathcal{N}^{-\frac{\alpha}{2}}\| \left(\epsilon s \sum_k |k|^{2\tau} a_k^\dagger \mathcal{N}^{s+\alpha-1} a_k + \epsilon^{-1}\, t \sum_k |k|^{2\tau} a_k^\dagger \mathcal{N}^{t+\beta-1} a_k\right).$$

Since $\mathcal{N} \leq N$ we furthermore have by Eq. (40)

$$\sum_k |k|^{2\tau} a_k^\dagger \mathcal{N}^{s+\alpha-1} a_k \lesssim \sum_k |k|^2 c_k^\dagger \mathcal{N}^{s+\alpha-1} c_k + (\mathcal{N}+1)^{s+\alpha-1}(N^\tau + \mathcal{N}).$$ □

With Corollary 1 at hand, we can verify the subsequent Lemma 3.

Lemma 3. *For $K \geq 0$, there exists a constant $C_K > 0$, such that*

$$\pm\mathcal{E} \leq C_K \sum_k |k|^2 c_k^\dagger \left(\frac{\mathcal{N}}{N} + N^{-\frac{1}{2}}\right) c_k + C_K\left(\frac{\mathcal{N}}{N} + N^{-\frac{1}{3}}\right)(\mathcal{N} + 1).$$

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Proof. Let us denote with $\mathcal{I} \subseteq (2\pi\mathbb{Z})^{3\times 3}$ the index set

$$\mathcal{I} := \{(0,0,0)\} \cup \bigcup_{0<|\ell|\leq K} \{(\ell,0,0),(0,\ell,0),(0,0,\ell)\}$$

Then we define for $I = (I_1, I_2, I_3), I' = (I'_1, I'_2, I'_3) \in \mathcal{I}$ the operator $K^{(I,I')}$ acting on $L^2(\Lambda)$ and the operator $G^{(I,I')}$ acting on $L^2(\Lambda)^{\otimes 2}$ as

$$K^{(I,I')}_{i,i'} := \frac{1}{2}\sum_{jk} |k|^2 \overline{(T-1)_{i'jk,I'}}\left((T-1)_{ijk,I} + (T-1)_{jik,I}\right),$$

$$G^{(I,I')}_{ij,i'j'} := \frac{1}{4}\sum_{k} |k|^2 \overline{(T-1)_{i'j'k,I'}}(T-1)_{ijk,I},$$

as well as $\mathcal{K}_{\tau,2} := (-\Delta_{x_1})^\tau + (-\Delta_{x_2})^\tau$ acting on $L^2(\Lambda)^{\otimes 2}$. Then we can write $\mathcal{E}$ as

$$\mathcal{E} = \sum_{I,I'\in\mathcal{I}}\left(\sum_{i,i'} K^{(I,I')}_{i,i'} a^\dagger_i \left(a^\dagger_{I_1}a^\dagger_{I_2}a^\dagger_{I_3}a_{I'_1}a_{I'_2}a_{I'_3}\right)a_{i'} + \sum_{ij,i'j'} G^{(I,I')}_{ij,i'j'} a^\dagger_i a^\dagger_j \left(a^\dagger_{I_1}a^\dagger_{I_2}a^\dagger_{I_3}a_{I'_1}a_{I'_2}a_{I'_3}\right)a_{i'}a_{j'}\right). \quad (42)$$

By the weighted Schur test, the operator norm of $\mathcal{K}^{-\frac{1}{2}}_{\tau,2} G^{(I,I')} \mathcal{K}^{-\frac{1}{2}}_{\tau,2}$ is bounded by

$$\|\mathcal{K}^{-\frac{1}{2}}_{\tau,2} G^{(I,I')} \mathcal{K}^{-\frac{1}{2}}_{\tau,2}\| \leq \sqrt{\alpha^{(I,I')}\alpha^{(I',I)}},$$

where we define $\alpha^{(I,I')} := \sup_{i'j'} \sum_{ij} \frac{|G^{(I,I')}_{ij,i'j'}|}{|i|^{2\tau}+|j|^{2\tau}}$. Let us furthermore introduce $s := I_1 + I_2 + I_3$ and $s' := I'_1 + I'_2 + I'_3$. Making use of Eq. (36), we obtain for the concrete choice $\tau := \frac{2}{3}$

$$\alpha^{(I,I')} \leq \sup_{i'j'} \sum_{ijk} \frac{|k|^2 |(T-1)_{i'j'k,I'}|\,|(T-1)_{ijk,I}|}{|i|^{2\tau}+|j|^{2\tau}} \lesssim N^{-4} \sup_{i'j'} \sum_{ijk\neq 0} \frac{\delta_{i'+j'+k=s'}\delta_{i+j+k=s}}{(|i|^{2\tau}+|j|^{2\tau})(|i|^2+|j|^2+|k|^2)}$$
$$\leq N^{-4}\sum_{i\neq 0}\frac{1}{|i|^{2+2\tau}} \lesssim N^{-4}.$$

Consequently $\|\mathcal{K}^{-\frac{1}{2}}_{\tau,2} G^{(I,I')} \mathcal{K}^{-\frac{1}{2}}_{\tau,2}\| \lesssim N^{-4}$. Furthermore, the operator

$$X^{(I,I')} := a^\dagger_{I_1}a^\dagger_{I_2}a^\dagger_{I_3}a_{I'_1}a_{I'_2}a_{I'_3}$$

satisfies $\|X^{(I,I')}\| \leq N^3$. Therefore we obtain by Corollary 1

$$\sum_{ij,i'j'} G^{(I,I')}_{ij,i'j'} a^\dagger_i a^\dagger_j \left(a^\dagger_{I_1}a^\dagger_{I_2}a^\dagger_{I_3}a_{I'_1}a_{I'_2}a_{I'_3}\right)a_{i'}a_{j'} \lesssim \sum_k |k|^2 c^\dagger_k \frac{\mathcal{N}}{N} c_k + (\mathcal{N}+N^\tau)\frac{\mathcal{N}}{N}.$$

Again by Lemma 15 we have $\|K^{(I,I')}\| \lesssim N^{-\frac{7}{2}}$, which concludes the proof by Corollary 1, together with the observation that the set $\mathcal{I}$ in the definition of $\mathcal{E}$ in Eq. (42) is finite. □

The next Lemma 4 will give us sufficient bounds on the error term $\mathcal{E}'$ defined in Eq. (34), which will be responsible for the appearance of an order $O_{N\to\infty}\left(\sqrt{N}\right)$ error in the main results of this Section Theorem 3 and Corollary 2.

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Lemma 4. *There exist constants $C, C_K > 0$ such that for $K \leq \sqrt{N}$, where K is as in the definition of π_K below Eq. (17), and $\epsilon > 0$*

$$\pm\left(\sum_{|\ell|>K} \lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger\, a_0^\dagger a_0^3 + \text{H.c.}\right) \leq \epsilon \sum_\ell |\ell|^2 c_\ell^\dagger c_\ell + \epsilon \mathcal{N} + C\frac{\mathcal{N}}{\sqrt{N}} + \frac{C}{\epsilon}\left(\sqrt{N} + \frac{\mathcal{N}}{\sqrt{K+1}}\right), \quad (43)$$

$$\pm\left(\sum_{0<|k|\leq K,\ell} \lambda_{k,\ell} a_\ell^\dagger a_{k-\ell}^\dagger a_k\, a_0^\dagger a_0^2 + \text{H.c.}\right) \lesssim \epsilon \sum_\ell |\ell|^2 c_\ell^\dagger c_\ell + \epsilon\frac{\mathcal{N}^2}{N} + C_K\frac{\mathcal{N}}{N} + \frac{C_K}{\epsilon}\left(\frac{\mathcal{N}}{\sqrt{N}} + \frac{\mathcal{N}^2}{N}\right). \quad (44)$$

Furthermore, we have

$$\pm\left(\sum_{|\ell|>K} \lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger\, a_0^\dagger a_0^3 \frac{\mathcal{N}}{N} + \text{H.c.}\right) \leq N^{-\frac{1}{2}}\left(\sum_\ell |\ell|^2 c_\ell^\dagger c_\ell + \mathcal{N}\right) + N^{-\frac{3}{2}}\mathcal{N}^2\left(\mathcal{N} + \sqrt{N}\right). \quad (45)$$

Proof. Given $m \in \{0,1\}$, let us define the operator $X := a_0^\dagger a_0^3 \frac{\mathcal{N}^m}{N^m}$ and the coefficients

$$\Lambda_{\ell,k}^{(n)} := \overline{(T-1)_{(n-k)(k-\ell)\ell,n00}} + \overline{(T-1)_{(n-k)(k-\ell)\ell,0n0}} + \overline{(T-1)_{(n-k)(k-\ell)\ell,00n}},$$

and observe that by Eq. (36) there exists a constant $C > 0$ such that

$$|\Lambda_{\ell,k}^{(n)}| \leq \frac{C}{N^2(|\ell|^2 + |k|^2)}\left(1 + \frac{|\ell|^2 + |k|^2}{N}\right)^{-1}, \quad (46)$$

where we have assumed w.l.o.g. that $|n| \leq \sqrt{N}$, since $\Lambda_{\ell,k}^{(n)} = 0$ in case $|n| > K$ and $K \leq \sqrt{N}$. In order to verify Eq. (43), respectively Eq. (45), let us write

$$\begin{aligned}\sum_{|\ell|>K} \lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger a_0^\dagger a_0^3 \frac{\mathcal{N}^m}{N^m} &= \sum_{|\ell|>K} \lambda_{0,\ell}\, c_\ell^\dagger a_{-\ell}^\dagger X - \sum_{|\ell|>K} \lambda_{0,\ell}\, (c_\ell - a_\ell)^\dagger a_{-\ell}^\dagger X \\ &= \sum_{|\ell|>K} \lambda_{0,\ell}\, c_\ell^\dagger a_{-\ell}^\dagger X - \sum_{|\ell|>K} \lambda_{0,\ell}\, a_{-\ell}^\dagger (c_\ell - a_\ell)^\dagger X - \sum_{|\ell|>K}\sum_{n\neq 0} \lambda_{0,\ell}\, \Lambda_{\ell,0}^{(n)} a_0^{2\dagger} a_n^\dagger a_n X. \end{aligned} \quad (47)$$

Regarding the first term in Eq. (47), note that we have for $\epsilon > 0$ the estimate

$$\pm \sum_{|\ell|>K} \lambda_{0,\ell}\, c_\ell^\dagger a_{-\ell}^\dagger X \pm \text{H.c.} \leq \epsilon \sum_\ell |\ell|^2 c_\ell^\dagger c_\ell + \frac{1}{\epsilon} X^\dagger \left(\sum_{|\ell|>K} \frac{|\lambda_{0,\ell}|^2}{\ell^2} a_\ell^\dagger a_\ell + \sum_{|\ell|>K} \frac{|\lambda_{0,\ell}|^2}{\ell^2}\right) X.$$

Using $|\lambda_{k,\ell}| \lesssim N^{-2}(1 + \frac{|\ell|^2}{N})^{-1}$, see Eq. (35), we have $\sum_{|\ell|>K} \frac{|\lambda_{0,\ell}|^2}{\ell^2} \lesssim N^{-\frac{7}{2}}$ and $\frac{|\lambda_{0,\ell}|^2}{\ell^2} \leq \frac{1}{N^4(K^2+1)}$ for $|\ell| > K$, and therefore we obtain for such K

$$\begin{aligned}\pm \sum_{|\ell|>K} \lambda_{0,\ell}\, c_\ell^\dagger a_{-\ell}^\dagger X \pm \text{H.c.} &\lesssim \epsilon \sum_\ell |\ell|^2 c_\ell^\dagger c_\ell + \frac{1}{\epsilon N^4} X^\dagger \left(\frac{\mathcal{N}}{K^2+1} + \sqrt{N}\right) X \\ &\lesssim \epsilon \sum_\ell |\ell|^2 c_\ell^\dagger c_\ell + \frac{1}{\epsilon}\frac{\mathcal{N}^{2m}}{N^{2m}}\left(\frac{\mathcal{N}}{K^2+1} + \frac{\sqrt{N}}{\epsilon}\right),\end{aligned}$$

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where we have used $X^\dagger X \lesssim N^2 \frac{\mathcal{N}^{2m}}{N^{2m}}$ and $[X, \mathcal{N}] = 0$. Regarding the second term in Eq. (47), let us use $\sum_{|\ell|>K} |\ell|^{-\frac{1}{2}} |N^4 \lambda_{0,\ell}|^2 a_\ell^\dagger a_\ell \lesssim \frac{\mathcal{N}}{\sqrt{K+1}}$ as well as the fact that

$$\sum_\ell \sqrt{|\ell|}(c_\ell - a_\ell)(c_\ell - a_\ell)^\dagger \lesssim \mathcal{N}$$

by Eq. (39), to estimate for $\kappa > 0$

$$\pm \sum_{|\ell|>K} \lambda_{0,\ell}\, a_{-\ell}^\dagger (c_\ell - a_\ell)^\dagger X \pm \text{H.c.} \lesssim \frac{1}{\kappa\sqrt{K+1}}\mathcal{N} + \frac{\kappa}{N^4} X^\dagger \mathcal{N} X \leq \frac{1}{\kappa\sqrt{K+1}}\mathcal{N} + \kappa \frac{\mathcal{N}^{2m}}{N^{2m}}\mathcal{N}.$$

Regarding the final term in Eq. (47) we have that $\sum_\ell |\Lambda_{\ell,0}^{(n)}| \lesssim N^{-\frac{3}{2}}$ by Eq. (46), and hence

$$\pm \sum_{|\ell|>K} \sum_{n\neq 0} \lambda_{0,\ell}\, \Lambda_{\ell,0}^{(n)} a_0^{2\dagger} a_n^\dagger a_n X \pm \text{H.c.} \lesssim N^{-\frac{1}{2}}\mathcal{N}.$$

For $m = 0$, the choice $\kappa := \epsilon$ yields Eq. (43) and for $m = 1$ the choice $\kappa := \sqrt{N}$ and $\epsilon := \frac{1}{\sqrt{N}}$ yields Eq. (45).

Regarding the proof of Eq. (44), let us define the operators $d_{k,\ell} := \lambda_{k,\ell} N^{\frac{3}{2}} a_{k-\ell}^\dagger a_k$ and write $a_\ell^\dagger d_{k,\ell} = c_\ell^\dagger d_{k,\ell} + d_{k,\ell}(c_\ell - a_\ell)^\dagger + [(c_\ell - a_\ell)^\dagger, d_{k,\ell}]$. We compute

$$\begin{aligned}
\sum_\ell [(c_\ell - a_\ell)^\dagger, d_{k,\ell}] &= \frac{1}{2} N^{\frac{3}{2}} \Big(a_0^{3\dagger} \sum_{ij\ell} \frac{1}{3} \Lambda_{\ell,-i}^{(0)} \lambda_{k,\ell} [a_i a_{-i-\ell}, a_{k-\ell}^\dagger a_k] \\
&\quad + a_0^{2\dagger} \sum_{|n|\leq K} \sum_{i\ell} \Lambda_{\ell,n-i}^{(n)} \lambda_{k,\ell} [a_n^\dagger a_i a_{n-i-\ell}, a_{k-\ell}^\dagger a_k] \Big) \frac{a_0^\dagger a_0^2}{N^{\frac{3}{2}}} \\
&= \frac{a_0^{3\dagger}}{N^{\frac{3}{2}}} \mu_k^{(1)} a_k a_{-k} \frac{a_0^\dagger a_0^2}{N^{\frac{3}{2}}} + \frac{a_0^{2\dagger}}{N} \sum_{|n|\leq K} \mu_{k,n}^{(2)} a_n^\dagger a_k a_{n-k} \frac{a_0^\dagger a_0^2}{N^{\frac{3}{2}}} - \frac{a_0^{2\dagger}}{N} \sum_{i,\ell} \mu_{k,i,\ell}^{(3)} a_{k-\ell}^\dagger a_i a_{k-i-\ell} \frac{a_0^\dagger a_0^2}{N^{\frac{3}{2}}},
\end{aligned}$$

where we define the coefficients

$$\begin{aligned}
\mu_k^{(1)} &:= N^3 \sum_\ell \frac{1}{3} \Lambda_{\ell,k}^{(0)} \lambda_{k,\ell}, \\
\mu_{k,n}^{(2)} &:= N^{\frac{5}{2}} \sum_\ell \Lambda_{\ell,k}^{(n)} \lambda_{k,\ell}, \\
\mu_{k,i,\ell}^{(3)} &:= N^{\frac{5}{2}} \Lambda_{\ell,k-i}^{(k)} \lambda_{k,\ell}.
\end{aligned}$$

Using again Eq. (46) and $|\lambda_{k,\ell}| \lesssim N^{-2}(1 + \frac{|\ell|^2}{N})^{-1}$, we immediately obtain $|\mu_k^{(1)}| \lesssim \frac{1}{\sqrt{N}}$, $|\mu_{k,n}^{(2)}| \lesssim \frac{1}{N}$, $|\mu_{k,i,\ell}^{(3)}| \lesssim N^{-\frac{3}{2}}$ and $\sum_i |\mu_{k,i,\ell}^{(3)}| \lesssim \frac{1}{N}$, and therefore by Cauchy-Schwarz

$$\sum_\ell \left([(c_\ell - a_\ell)^\dagger, d_{k,\ell}] \frac{a_0^\dagger a_0^2}{N^{\frac{3}{2}}} + \text{H.c.} \right) \lesssim \frac{\mathcal{N}}{\sqrt{N}}.$$

Consequently,

$$\pm\left(\sum_{0<|k|\le K,\ell}\lambda_{k,\ell}a_\ell^\dagger a_{k-\ell}^\dagger a_k\, a_0^\dagger a_0^2+\text{H.c.}\right)=\left(\sum_\ell a_\ell^\dagger d_{k,\ell}\frac{a_0^\dagger a_0^2}{N^{\frac{3}{2}}}+\text{H.c.}\right)$$
$$\lesssim\sum_{0<|k|\le K}\left(\frac{\epsilon}{K^3}\sum_\ell|\ell|^2c_\ell^\dagger c_\ell+\frac{K^3}{\epsilon}\sum_\ell\frac{1}{|\ell|^2}d_{k,\ell}^\dagger d_{k,\ell}+\frac{\epsilon}{K^3}\sum_\ell d_{k,\ell}d_{k,\ell}^\dagger\right.$$
$$\left.+\frac{K^3}{\epsilon}\sum_\ell\frac{a_0^{3\dagger}a_0}{N^2}(c_\ell-a_\ell)(c_\ell-a_\ell)^\dagger\frac{a_0^\dagger a_0^3}{N^2}+\frac{\mathcal{N}}{\sqrt{N}}\right)$$
$$\lesssim\epsilon\sum_\ell|\ell|^2c_\ell^\dagger c_\ell+\frac{K^3}{\epsilon}\sum_{0<|k|\le K,\ell}\frac{1}{|\ell|^2}d_{k,\ell}^\dagger d_{k,\ell}+\frac{\epsilon}{K^3}\sum_{0<|k|\le K,\ell}d_{k,\ell}d_{k,\ell}^\dagger$$
$$+\frac{K^3}{\epsilon}\sum_{0<|k|\le K,\ell}\frac{a_0^{3\dagger}a_0}{N^2}(c_\ell-a_\ell)(c_\ell-a_\ell)^\dagger\frac{a_0^\dagger a_0^3}{N^2}+K^3\frac{\mathcal{N}}{\sqrt{N}}.$$

Similar to the proof of Eq. (43), we observe that $\frac{1}{K^3}\sum_{0<|k|\le K,\ell}d_{k,\ell}d_{k,\ell}^\dagger\lesssim\frac{\mathcal{N}}{N}\mathcal{N}$ and, using Eq. (39),

$$\sum_{0<|k|\le K,\ell}\frac{a_0^{3\dagger}a_0}{N^2}(c_\ell-a_\ell)(c_\ell-a_\ell)^\dagger\frac{a_0^\dagger a_0^3}{N^2}\lesssim K^3\frac{a_0^{3\dagger}a_0}{N^2}\frac{\mathcal{N}^2}{N}\frac{a_0^\dagger a_0^3}{N^2}\le K^3\frac{\mathcal{N}^2}{N},$$
$$\sum_{0<|k|\le K,\ell}\frac{1}{|\ell|^2}d_{k,\ell}^\dagger d_{k,\ell}\lesssim K^3\frac{\mathcal{N}}{\sqrt{N}}+K^3N^3\sum_\ell\frac{1}{|\ell|^2}|\lambda_{k,\ell}|^2a_k^\dagger a_{k-\ell}^\dagger a_{k-\ell}a_k\lesssim K^3\frac{\mathcal{N}}{\sqrt{N}}+K^3\frac{\mathcal{N}^2}{N}.\qquad\square$$

Having Lemma 2, Lemma 3 and Lemma 4 at hand, we can use the lower bound in Eq. (32) in order to derive the following Theorem 3, which provides strong lower bounds on the quantity $\langle\Psi,H_N\Psi\rangle$. Note, however, that Theorem 3 is only applicable for states Ψ which satisfy the strong condition that Ψ is in the spectral subspace $\mathcal{N}\le\epsilon N$, that is,

$$\mathbb{1}(\mathcal{N}\le\epsilon N)\Psi=\Psi,\tag{48}$$

where the orthogonal projection $\mathbb{1}(\mathcal{N}\le\epsilon N)$ is defined by means of functional calculus. In the following we will refer to the property in Eq. (48) as (BEC) in the spectral sense $\mathbb{1}(\mathcal{N}\le\epsilon N)\Psi=\Psi$. Furthermore, we refer to a Hilbert space element Ψ as a state, in case it satisfies $\|\Psi\|=1$.

Theorem 3. *There exist constants $\delta,C,N_0>0$ and $\epsilon>0$, such that*

$$\langle\Psi,H_N\Psi\rangle\ge\frac{1}{6}b_{\mathcal{M}}(V)N+\delta\langle\Psi,\sum_k|k|^2c_k^\dagger c_k\Psi\rangle+\delta\langle\Psi,\mathcal{N}\Psi\rangle-C\sqrt{N}$$

for any state Ψ satisfying $\mathbb{1}(\mathcal{N}\le\epsilon N)\Psi=\Psi$ and $N\ge N_0$, where $\mathcal{N}:=\sum_{k\neq0}a_k^\dagger a_k$.

Proof. By Eq. (32) together with the estimates in Lemma 2, Lemma 3 and Lemma 4 we have for $\alpha,\tau,\epsilon'>0$ and $K\ge K_0(\alpha,\tau)$

$$H_N\ge\frac{1}{6}b_{\mathcal{M}}(V)N+(1-\epsilon')\sum_k|k|^2c_k^\dagger c_k-C_{K,\epsilon'}\sum_k|k|^2c_k^\dagger\left(\frac{\mathcal{N}}{N}+N^{-\frac{1}{2}}\right)c_k\tag{49}$$
$$-\alpha\sum_k|k|^{2\tau}a_k^\dagger a_k-\left(\epsilon'+C_{K,\epsilon'}\frac{\mathcal{N}}{N}+C_{K,\epsilon'}N^{-\frac{1}{3}}+\frac{C}{\epsilon'\sqrt{K+1}}\right)\mathcal{N}-C_{K,\epsilon'}\sqrt{N},$$

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where $C, C_{K,\epsilon'}$ and $K_0(\alpha,\tau)$ are suitable constants. In the following let Ψ be a state satisfying $\mathbb{1}_{[0,\epsilon N)}(\mathcal{N})\Psi = \Psi$ and define $\Psi_k := c_k\Psi$. By the definition of c_k it is clear that $\mathbb{1}_{[0,\epsilon N+2)}(\mathcal{N})\Psi_k = \Psi_k$, and therefore

$$\left\langle \Psi, \sum_k |k|^2 c_k^\dagger \left(\frac{\mathcal{N}}{N} + N^{-\frac{1}{2}}\right) c_k \Psi\right\rangle = \sum_k |k|^2 \left\langle \Psi_k, \left(\frac{\mathcal{N}}{N} + N^{-\frac{1}{2}}\right)\Psi_k\right\rangle$$
$$= \sum_k |k|^2 \left\langle \Psi_k, \left(\frac{\mathcal{N}}{N} + N^{-\frac{1}{2}}\right)\mathbb{1}_{[0,\epsilon N+2)}(\mathcal{N})\Psi_k\right\rangle \le \sum_k |k|^2 \left\langle \Psi_k, \left(\frac{\epsilon N+2}{N} + N^{-\frac{1}{2}}\right)\Psi_k\right\rangle$$
$$= \left(\frac{\epsilon N+2}{N} + N^{-\frac{1}{2}}\right)\left\langle \Psi, \sum_k |k|^2 c_k^\dagger c_k \Psi\right\rangle. \tag{50}$$

In a similar fashion we have

$$\langle \Psi, \mathcal{N}^2\Psi\rangle \le \epsilon N \langle \Psi, \mathcal{N}\Psi\rangle. \tag{51}$$

Furthermore, note that for a suitable constant $D_1 > 0$

$$\sum_k |k|^{2\tau} a_k^\dagger a_k \le D_1 \sum_k |k|^2 c_k^\dagger c_k + D_1 \frac{\mathcal{N}^2}{N} + D_1 N^{\frac{1}{2}} \tag{52}$$

by Eq. (40) for $\tau < \frac{1}{2}$, and by Eq. (39) we have

$$\mathcal{N}\left(1 - R\frac{\mathcal{N}}{N}\right) \le R \sum_k |k|^2 c_k^\dagger c_k + R$$

for a suitable constant $R > 0$. Using $\mathbb{1}(\mathcal{N} \le \epsilon N)\Psi = \Psi$ with ϵ small enough such that $R\epsilon < 1$, we therefore obtain

$$\langle \Psi, \mathcal{N}\Psi\rangle \le D_2 \left\langle \Psi, \sum_k |k|^2 c_k^\dagger c_k \Psi\right\rangle + D_2, \tag{53}$$

for a suitable constant $D_2 > 0$. Combining Eq. (49)-(53), therefore yields for suitable constants D and $D_{K,\epsilon',\alpha}$, and $0 < \epsilon < \frac{1}{R}$,

$$\langle \Psi, H_N\Psi\rangle \ge \left[1 - D\left(\epsilon' + \alpha + \frac{D}{\epsilon'\sqrt{K+1}}\right) - D_{K,\epsilon',\alpha}\left(\epsilon + N^{-\frac{1}{3}}\right)\right]\langle \Psi, \sum_k |k|^2 c_k^\dagger c_k \Psi\rangle$$
$$+ \frac{1}{6} b_{\mathcal{M}}(V) N - D_{K,\epsilon',\alpha}\sqrt{N}.$$

We can now make our choice of parameters concrete. First we take choose τ such that $0 < \tau < \frac{1}{2}$ and $\alpha, \epsilon' > 0$ small enough, such that $D(\epsilon' + \alpha) < \frac{1}{2}$, and then we take $K \ge K_0(\alpha,\tau)$ large enough, such that

$$D\left(\epsilon' + \alpha + \frac{D}{\epsilon'\sqrt{K+1}}\right) \le \frac{1}{2}.$$

Finally, we take $0 < \epsilon < \frac{1}{R}$ small enough and N large enough, such that

$$D_{K,\epsilon',\alpha}\left(\epsilon + N^{-\frac{1}{3}}\right) \le \frac{1}{2}. \qquad \square$$

It has been verified in [23], for the more general setting of particles being confined by an additional external potential, that any approximate ground state Ψ_N of the operator H_N satisfies complete Bose-Einstein condensation

$$\langle \Psi_N, \mathcal{N}\Psi_N \rangle = o_{N\to\infty}(N). \tag{54}$$

Adapting the localization procedure presented in [19, Theorem A.1] in the form stated in [16, Proposition 6.1] for the following Lemma 5 allows us to lift Bose-Einstein condensation in the sense of Eq. (54), to Bose-Einstein condensation in the spectral sense, which is a crucial assumption of the previous Theorem 3.

Lemma 5. *Let Ψ satisfy $\langle \Psi, H_N \Psi\rangle = E_N + \delta$ with $\delta \leq N$. Then there exists a constant $C > 0$, such that there exists for all $1 \leq M \leq N$ states Φ satisfying $\mathbb{1}(\mathcal{N} \leq M)\Phi = \Phi$ and*

$$\langle \Phi, H_N \Phi\rangle \leq E_N + C\left(1 - \frac{2\langle \Psi, \mathcal{N}\Psi}{\rangle} M\right)^{-1}\left(\frac{\sqrt{N}}{M} + \frac{N}{M^2} + \delta\right). \tag{55}$$

Furthermore, there exists a state $\widetilde{\Phi}$ such that $\mathbb{1}\left(\mathcal{N} > \frac{M}{2}\right)\widetilde{\Phi} = \widetilde{\Phi}$ and

$$\langle \Psi, \mathcal{N}\Psi\rangle \leq \langle \Phi, \mathcal{N}\Phi\rangle + \frac{CN}{\langle \widetilde{\Phi}, H_N \widetilde{\Phi}} - E_N\rangle\left(\frac{\sqrt{N}}{M} + \frac{N}{M^2} + \delta\right). \tag{56}$$

Proof. In the following let $f, g : \mathbb{R} \to [0, 1]$ be smooth functions satisfying $f^2 + g^2 = 1$ and $f(x) = 1$ for $x \leq \frac{1}{2}$, as well as $f(x) = 0$ for $x \geq 1$, and let us define $m := \|f\left(\frac{\mathcal{N}}{M}\right)\Psi\|^2$ and

$$\Phi := \frac{1}{\sqrt{m}} f\left(\frac{\mathcal{N}}{M}\right)\Psi,$$
$$\widetilde{\Phi} := \frac{1}{\sqrt{1-m}} g\left(\frac{\mathcal{N}}{M}\right)\Psi.$$

Note that $\|\Phi\| = \|\widetilde{\Phi}\| = 1$, $0 \leq m \leq 1$ and clearly we have $\mathbb{1}(\mathcal{N} \leq M)\Phi = \Phi$ and $\mathbb{1}\left(\mathcal{N} > \frac{M}{2}\right)\widetilde{\Phi} = \widetilde{\Phi}$. Making use of the algebraic identity

$$H_N = f\left(\frac{\mathcal{N}}{M}\right) H_N f\left(\frac{\mathcal{N}}{M}\right) + g\left(\frac{\mathcal{N}}{M}\right) H_N g\left(\frac{\mathcal{N}}{M}\right) + \mathcal{E}$$

with the residual term

$$\mathcal{E} := \frac{1}{2}\left[f\left(\frac{\mathcal{N}}{M}\right), \left[H_N, f\left(\frac{\mathcal{N}}{M}\right)\right]\right] + \frac{1}{2}\left[g\left(\frac{\mathcal{N}}{M}\right), \left[H_N, g\left(\frac{\mathcal{N}}{M}\right)\right]\right],$$

we obtain

$$m\langle \Phi, H_N \Phi\rangle + (1-m)\langle \widetilde{\Phi}, H_N \widetilde{\Phi}\rangle = E_N + \delta - \langle \Psi, \mathcal{E}\Psi\rangle.$$

In order to estimate $\langle \Psi, \mathcal{E}\Psi\rangle$, let π^0 denote the projection onto the constant function in $L^2(\Lambda)$ and $\pi^1 := 1 - \pi^0$. Then we can rewrite $\mathcal{E}$ as

$$\mathcal{E} = \frac{1}{4M^2}\sum_{I,J\in\{0,1\}^3}\sum_{ijk,\ell mn}(\pi^{I_1}\pi^{I_2}\pi^{I_3}V_N\pi^{J_1}\pi^{J_2}\pi^{J_3})_{ijk,\ell mn}a_k^\dagger a_j^\dagger a_i^\dagger X_{I,J}a_\ell a_m a_n,$$

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with

$$X_{I,J} := M^2\left[f\left(\frac{\mathcal{N}+\#_I}{M}\right)-f\left(\frac{\mathcal{N}+\#_J}{M}\right)\right]^2+M^2\left[g\left(\frac{\mathcal{N}+\#_I}{M}\right)-g\left(\frac{\mathcal{N}+\#_J}{M}\right)\right]^2$$

and $\#_I$ counting the number of indices in I that are equal to 1. Using $0 \leq X_{I,J} \leq X$, where

$$X := \left(\|\nabla f\|^2+\|\nabla g\|^2\right)\mathbb{1}(\mathcal{N} \leq M),$$

we obtain by the Cauchy-Schwarz inequality

$$\pm\mathcal{E} \lesssim \frac{1}{4M^2}\sum_{I\in\{0,1\}^3}\sum_{ijk,\ell mn}(\pi^{I_1}\pi^{I_2}\pi^{I_3}V_N\pi^{I_1}\pi^{I_2}\pi^{I_3})_{ijk,\ell mn}a_k^\dagger a_j^\dagger a_i^\dagger X a_\ell a_m a_n. \tag{57}$$

In the following we want to show that for any $I \in \{0,1\}^3$, the Ψ-expectation value of the corresponding term appearing in the sum on the right side of Eq. (57) is of the order $\sqrt{N}M+N$. For $I=(0,0,0)$ we have

$$(V_N)_{000,000}(a_0^\dagger)^3 X a_0^3 \lesssim N^{-2}\|X\|(a_0^\dagger)^3 a_0^3 \leq \left(\|\nabla f\|^2+\|\nabla g\|^2\right)N.$$

Similarly,

$$\sum_{k\neq 0}(V_N)_{001,001}(a_0^\dagger)^2 a_k^\dagger X a_k a_0^2 \lesssim M \leq N$$

in the case $I=(0,0,1)$. Regarding the case $I=(0,1,1)$, let us first observe that we have the upper bound

$$\sum_{jk,mn\neq 0}(V_N)_{0jk,0mn}a_0^\dagger a_k^\dagger a_j^\dagger X a_m a_n a_0 \leq C_N\sum_k |k|^2 a_k^\dagger\left(\sum_{j\neq 0}a_0^\dagger a_j^\dagger X a_j a_0\right)a_k \tag{58}$$

with the constant C_N being defined as

$$C_N := \sup_{m,n\neq 0}\left\{\sum_{j,k\neq 0}\frac{\left|(V_N)_{0jk,0mn}\right|}{|k|^2}\right\} = \frac{1}{N^2}\left\{\sup_{p,q\neq 0}\sum_{t:p+t\neq 0}\frac{\left|V\left(N^{-\frac{1}{2}}t\right)\right|}{|p+t|^2}\right\}.$$

Due to our regularity assumptions on V we have $\left|V\left(N^{-\frac{1}{2}}t\right)\right| \lesssim \frac{1}{1+N^{-1}|t|^2}$ and therefore

$$\begin{aligned}C_N &\lesssim N^{-2}\sum_{t:p+t\neq 0}\frac{1}{|p+t|^2(1+N^{-1}|t|^2)} \lesssim N^{-2}\int_{\mathbb{R}^3}\frac{\mathrm{d}x}{|p+x|^2(1+N^{-1}|x|^2)}\\ &\leq N^{-2}\int_{\mathbb{R}^3}\frac{\mathrm{d}x}{|x|^2(1+N^{-1}|x|^2)} = N^{-2}4\pi\int_0^\infty\frac{\mathrm{d}r}{1+N^{-1}r^2} = 2\pi^2 N^{-\frac{3}{2}},\end{aligned} \tag{59}$$

where we have used the Hardy-Littlewood inequality in the first estimate of Eq. (59). Since

$$\sum_{j\neq 0}a_0^\dagger a_j^\dagger X a_j a_0 \lesssim MN$$

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we obtain by Eq. (58)

$$\Big\langle \Psi, \sum_{jk,mn\neq 0} (V_N)_{0jk,0mn} a_0^\dagger a_k^\dagger a_j^\dagger X a_m a_n a_0 \Psi \Big\rangle \lesssim N^{-\frac{1}{2}} M \Big\langle \Psi, \sum_k |k|^2 a_k^\dagger a_k \Psi \Big\rangle$$
$$\leq N^{-\frac{1}{2}} M \langle \Psi, H_N \Psi\rangle \leq N^{-\frac{1}{2}} M (E_N + N) \lesssim N^{\frac{1}{2}} M,$$

where we have used the assumption $\delta \leq N$ and the upper bound on E_N derived in Theorem 4. The only distinguished case left is $I = (1, 1, 1)$. We start its analysis by defining

$$\mathbb{V}_{\alpha,\beta} := \frac{1}{4M^2} \sum_{\substack{I,J\in\{0,1\}^3:\\ \#I=\alpha,\#J=\beta}} \sum_{ijk,\ell mn} (\pi^{I_1}\pi^{I_2}\pi^{I_3} V_N \pi^{J_1}\pi^{J_2}\pi^{J_3})_{ijk,\ell mn} a_k^\dagger a_j^\dagger a_i^\dagger X_{I,J} a_\ell a_m a_n,$$

which allows us to estimate, using the Cauchy-Schwarz inequality,

$$\mathbb{V}_{3,3} \leq H_N - \big(\mathbb{V}_{2,3} + \mathbb{V}_{3,2} + \mathbb{V}_{1,3} + \mathbb{V}_{3,1} + \mathbb{V}_{0,3} + \mathbb{V}_{3,0}\big) \leq H_N + \frac{1}{2}\mathbb{V}_{3,3} + 6\big(\mathbb{V}_{0,0} + \mathbb{V}_{1,1} + \mathbb{V}_{2,2}\big).$$

From the previous cases we know that

$$\langle \Psi, (\mathbb{V}_{0,0} + \mathbb{V}_{1,1} + \mathbb{V}_{2,2})\Psi\rangle \lesssim N^{\frac{1}{2}} M + N,$$
$$\langle \Psi, H_N \Psi\rangle \lesssim N,$$

and therefore $\langle \Psi, \mathbb{V}_{3,3}\Psi\rangle \lesssim N^{\frac{1}{2}} M + N$. Summarizing what we have so far yields the inequality

$$m\langle \Phi, H_N \Phi\rangle + (1-m)\langle \widetilde{\Phi}, H_N \widetilde{\Phi}\rangle \leq E_N + \delta + C\left(\frac{\sqrt{N}}{M} + \frac{N}{M^2}\right).$$

Using $\langle \widetilde{\Phi}, H_N \widetilde{\Phi}\rangle \geq E_N$ and the simple observation that $m \geq 1 - \frac{2\langle \Psi, \mathcal{N}\Psi\rangle}{M}$ immediately yields Eq. (55), and using $\langle \Phi, H_N \Phi\rangle \geq E_N$ we obtain for a suitable constant $C > 0$

$$1 - m \leq \frac{C}{\langle \widetilde{\Phi}, H_N \widetilde{\Phi}} - E_N\rangle \left(\frac{\sqrt{N}}{M} + \frac{N}{M^2} + \delta\right).$$

In order to derive Eq. (56), we note that $\mathcal{N} = f\big(\frac{\mathcal{N}}{M}\big)\mathcal{N} f\big(\frac{\mathcal{N}}{M}\big) + g\big(\frac{\mathcal{N}}{M}\big)\mathcal{N} g\big(\frac{\mathcal{N}}{M}\big)$ and therefore

$$\langle \Psi, \mathcal{E}\Psi\rangle = m\langle \Phi, \mathcal{N}\Phi\rangle + (1-m)\langle \widetilde{\Phi}, \mathcal{N}\widetilde{\Phi}\rangle \leq \langle \Phi, \mathcal{N}\Phi\rangle + (1-m)N. \qquad \square$$

Before we come to the lower bound on the ground state energy E_N in the main result of this Section Corollary 2, let us first state the corresponding upper bound in the subsequent Theorem 4, which has essentially been verified in [23]. To be precise, it has been shown in [23] that $E_N \leq \frac{1}{6} b_{\mathcal{M}}(V) N + C N^{\frac{2}{3}}$, and, as is explained in [25], the method in [23] can be improved to yield $E_N \leq \frac{1}{6} b_{\mathcal{M}}(V) N + C N^{\frac{1}{2}}$ as well. However, since the computations in the proof of Theorem 4 are relevant for the proof of the upper bound in Theorem 1, and for the sake of completeness, we are nevertheless going to verify Theorem 4 in detail in the subsequent Section 3.

Theorem 4. *There exists a constant $C > 0$ such that the ground state energy E_N is bounded from above by $E_N \leq \frac{1}{6} b_{\mathcal{M}}(V) N + C\sqrt{N}$.*

Using Bose-Einstein condensation in the spectral sense, Theorem 3 allows us to derive an asymptotically correct lower bound on the ground state energy in Corollary 2 with an error of the order $\sqrt{N}$, see

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Eq. (62). In this context we call Ψ_N an approximate ground state, in case $\|\Psi_N\| = 1$ and there exists a constant $C > 0$ such that

$$\langle \Psi_N, H_N \Psi_N \rangle \leq E_N + C. \tag{60}$$

Note that the assumption in Eq. (60) is more restrictive compared to the one employed in [23], where the authors call Ψ_N an approximate ground state in case $\|\Psi_N\| = 1$ and

$$\lim_{N\to\infty} \frac{1}{N} \langle \Psi_N, H_N \Psi_N \rangle = \frac{1}{6} b_{\mathcal{M}}(V). \tag{61}$$

The fact that Eq. (60) implies Eq. (61) follows immediately from the leading-order asymptotics in Eq. (3), which has been verified in [23], together with the trivial lower bound $\langle \Psi_N, H_N \Psi_N \rangle \geq E_N$.

Corollary 2. *The ground state Ψ_N^{GS} of the operator H_N satisfies for a suitable $C > 0$*

$$\langle \Psi_N^{\mathrm{GS}}, \mathcal{N} \Psi_N^{\mathrm{GS}} \rangle \leq C\sqrt{N},$$

and we have the lower bound

$$E_N \geq \frac{1}{6} b_{\mathcal{M}}(V) N - C\sqrt{N}. \tag{62}$$

Furthermore there exists a constant $C > 0$ and states Φ_N, such that Φ_N is an approximate ground state of H_N satisfying (BEC) in the spectral sense with rate $\frac{1}{\sqrt{N}}$, that is,

$$\langle \Phi_N, H_N \Phi_N \rangle \leq E_N + C,$$
$$\mathbb{1}\left(\mathcal{N} \leq C\sqrt{N}\right) \Phi_N = \Phi_N,$$

and we have the estimate on the kinetic energy $\left\langle \Phi_N, \sum_k |k|^2 c_k^\dagger c_k \Phi_N \right\rangle \leq C\sqrt{N}$.

Proof. From the results in [23] we know that the ground state Ψ_N^{GS} of H_N satisfies

$$\langle \Psi_N^{\mathrm{GS}}, \mathcal{N} \Psi_N^{\mathrm{GS}} \rangle = o_{N\to\infty}(N).$$

Consequently, we know by Lemma 5 that there exist states ξ_N satisfying

$$\langle \xi_N, H_N \xi_N \rangle \leq E_N + C\left(\frac{1}{\epsilon\sqrt{N}} + \frac{1}{\epsilon^2 N} \right) \tag{63}$$

and $\mathbb{1}(\mathcal{N} \leq \epsilon N)\xi_N = \xi_N$, where we choose $\epsilon > 0$ as in Theorem 3. By Theorem 3 and Theorem 4 we therefore obtain for a suitable constant $C > 0$

$$\begin{aligned} \frac{1}{6} b_{\mathcal{M}}(V) N + \delta \left\langle \xi_N, \sum_k |k|^2 c_k^\dagger c_k \xi_N \right\rangle + \delta \langle \xi_N, \mathcal{N} \xi_N \rangle - C\sqrt{N} &\leq \langle \xi_N, H_N \xi_N \rangle \\ \leq E_N + C \leq \frac{1}{6} b_{\mathcal{M}}(V) N + C\sqrt{N}. \end{aligned} \tag{64}$$

This immediately implies $E_N \geq \frac{1}{6} b_{\mathcal{M}}(V) N - C\sqrt{N}$ for a suitable constant $C > 0$ and

$$\langle \xi_N, \mathcal{N} \xi_N \rangle = O_{N\to\infty}\left(\sqrt{N}\right), \tag{65}$$

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as well as $\left\langle \xi_N, \sum_k |k|^2 c_k^\dagger c_k \xi_N \right\rangle = O_{N\to\infty}\left(\sqrt{N}\right)$. Furthermore, there exist by Lemma 5 states $\widetilde{\xi}_N$ satisfying $\mathbb{1}(\mathcal{N} > \frac{\epsilon}{2}N)\widetilde{\xi}_N = \widetilde{\xi}_N$ and

$$\langle \Psi_N^{\mathrm{GS}}, \mathcal{N}\Psi_N^{\mathrm{GS}}\rangle \lesssim \langle \xi_N, \mathcal{N}\xi_N\rangle + \frac{\sqrt{N}}{\langle \widetilde{\xi}_N, H_N \widetilde{\xi}_N} - E_N\rangle \lesssim \sqrt{N} + \frac{\sqrt{N}}{\langle \widetilde{\xi}_N, H_N \widetilde{\xi}_N\rangle - E_N}. \tag{66}$$

In the following we show by a contradiction argument, similar to the one employed in the proof of [4, Theorem 1.1], that

$$\liminf_N \left\{ \langle \widetilde{\xi}_N, H_N \widetilde{\xi}_N\rangle - E_N \right\} = \infty. \tag{67}$$

For this purpose let us assume that Eq. (67) is violated, that is, we assume that there exists a subsequence N_j and a constant $C > 0$ such that $\sup_j \langle \widetilde{\xi}_{N_j}, H_{N_j} \widetilde{\xi}_{N_j}\rangle - E_{N_j} \leq C$. Let us complete this subsequence to a proper sequence by defining $\xi'_N := \widetilde{\xi}_N$ in case $N = N_j$ for some j and $\xi'_N := \Psi_N^{\mathrm{GS}}$ otherwise. Clearly ξ'_N is a sequence of approximate ground states, see Eq. (60), and as such ξ'_N satisfies complete (BEC) by the results in [23], that is, $\langle \xi'_N, \mathcal{N}\xi'_N\rangle = o_{N\to\infty}(N)$. This is, however, a contradiction to

$$\langle \xi'_{N_j}, \mathcal{N}\xi'_{N_j}\rangle = \langle \widetilde{\xi}_{N_j}, \mathcal{N}\widetilde{\xi}_{N_j}\rangle \geq \frac{\epsilon}{2}N,$$

which concludes the proof of Eq. (67). Combining Eq. (66) and Eq. (67) yields

$$\langle \Psi_N^{\mathrm{GS}}, \mathcal{N}\Psi_N^{\mathrm{GS}}\rangle \leq C\sqrt{N},$$

for a suitable constant $C > 0$. Applying again Lemma 5 for the state Ψ_N^{GS} and $M := K\sqrt{N}$, we obtain states Φ_N satisfying $\mathbb{1}(\mathcal{N} \leq K\sqrt{N})\Phi_N = \Phi_N$ and

$$\langle \Phi_N, H_N \Phi_N\rangle \leq E_N + \frac{C}{1 - \frac{2}{K\sqrt{N}}\langle \Psi_N^{\mathrm{GS}}, \mathcal{N}\Psi_N^{\mathrm{GS}}} \rangle \leq E_N + \frac{C}{1 - \frac{2C}{K}},$$

for a large enough $C > 0$. Consequently Φ_N is a sequence of approximate ground states for $K > 2C$. Finally we notice that the states Φ_N satisfy the chain of inequalities in Eq. (64) as well, and therefore

$$\left\langle \Phi_N, \sum_k |k|^2 c_k^\dagger c_k \Phi_N \right\rangle = O_{N\to\infty}\left(\sqrt{N}\right).$$

□

3. First-order upper bound

It is the goal of this section to introduce a trial state Γ, which simultaneously annihilates the variables c_k for $k \neq 0$ and $\psi_{\ell m n}$ in case $(\ell, m, n) \neq 0$, at least in an approximate sense, which allows us to verify the upper bound on the ground state energy E_N in Theorem 4. For the rest of this Section we specify the parameter K introduced above the definition of π_K in Eq. (17) as $K := 0$, which especially means that with $\eta_{ijk} := (T-1)_{ijk,000}$ we have

$$c_k = a_k + \frac{1}{2}\sum_{ij} \eta_{ijk}\, a_i^\dagger a_j^\dagger a_0^3, \tag{68}$$

$$\psi_{ijk} = a_i a_j a_k + \eta_{ijk}\, a_0^3. \tag{69}$$

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In order to find a suitable state Γ, let $\eta_{ijk} := (T-1)_{ijk,000}$ and let us follow the strategy in [23], respectively in the case of Bose gases with two-particle interactions see, for example, [3, 7, 13], by defining the generator

$$\mathcal{G} := \frac{1}{6}\sum_{ijk}\eta_{ijk}\, a_i^\dagger a_j^\dagger a_k^\dagger a_0^3 \tag{70}$$

of a unitary group $U_s := e^{s\mathcal{G}^\dagger - s\mathcal{G}}$ and $U := U_1$. The generator $\mathcal{G}$ is chosen, such that

$$c_k = a_k + [a_k, \mathcal{G}],$$

and in particular, as we show this section, the unitary U has the property $U^{-1}c_k U \approx a_k$ and $U^{-1}\psi_{ijk}U \approx a_i a_j a_k$ in a suitable sense. Denoting with

$$\Gamma_0(x_1, \ldots, x_N) := 1 \tag{71}$$

the constant function in $L^2_{\mathrm{sym}}(\Lambda^N)$, that is, $a_k\Gamma_0 = 0$ for $k \neq 0$, we observe that $\Gamma := U\Gamma_0$ is a suitable trial state for the (approximate) annihilation of c_k, given $k \neq 0$, and $\psi_{\ell mn}$, given $(\ell, m, n) \neq 0$, where the action of the unitary U introduces a three-particle correlation structure on the completely uncorrelated wavefunction Γ_0. We note at this point, that the action of the unitary operator U only creates an $O(1)$ amount of particles, in the sense that

$$U_{-s}\mathcal{N}^m U_s \leq e^{C_m|s|}(\mathcal{N}+1)^m, \tag{72}$$

as is proven in Appendix A, see Lemma A1.

For the purpose of verifying that $U^{-1}\psi_{ijk}U$ is approximately identical to $a_i a_j a_k$, we first apply Duhamel's formula, which yields

$$U^{-1}a_i a_j a_k U = a_i a_j a_k - \int_0^1 U_{-s}\left[a_i a_j a_k, \mathcal{G}\right]U_s\, \mathrm{d}s + \int_0^1 U_{-s}\left[a_i a_j a_k, \mathcal{G}^\dagger\right]U_s\, \mathrm{d}s. \tag{73}$$

Furthermore, note that we can write

$$\left[a_i a_j a_k, \mathcal{G}\right] = \eta_{ijk}a_0^3 + (\delta_1\psi)_{ijk} + (\delta_2\psi)_{ijk}$$

using the definition

$$(\delta_1\psi)_{i_1i_2i_3} := \frac{1}{2}\sum_{\sigma\in S_3}\sum_j \eta_{i_{\sigma_1}i_{\sigma_2}j}\mathbb{1}(i_{\sigma_3}=0)\, a_j^\dagger a_0^4,$$
$$(\delta_2\psi)_{i_1i_2i_3} := \frac{1}{2}\sum_{\sigma\in S_3}\sum_j \eta_{i_{\sigma_1}i_{\sigma_2}j}\mathbb{1}(i_{\sigma_3}\neq 0)\, a_j^\dagger a_{i_{\sigma_3}}a_0^3 + \frac{1}{4}\sum_{\sigma\in S_3}\sum_{jk}\eta_{i_{\sigma_1}jk}\, a_k^\dagger a_j^\dagger a_{i_{\sigma_2}}a_{i_{\sigma_3}}a_0^3.$$

Therefore we can identify the transformed operators $U^{-1}\psi_{ijk}U$ as

$$\begin{aligned} U^{-1}\psi_{ijk}U &= a_i a_j a_k + \int_0^1 U_{-s}\left\{\left[a_i a_j a_k, \mathcal{G}^\dagger\right] - (\delta_1\psi)_{ijk} - (\delta_2\psi)_{ijk} - \eta_{ijk}a_0^3\right\}U_s\mathrm{d}s + \eta_{ijk}U^{-1}a_0^3U \\ &= a_i a_j a_k + \int_0^1 U_{-s}\left[a_i a_j a_k, \mathcal{G}^\dagger\right]U_s\mathrm{d}s - \int_0^1 U_{-s}(\delta_1\psi)_{ijk}U_s\mathrm{d}s - \int_0^1 U_{-s}(\delta_2\psi)_{ijk}U_s\mathrm{d}s \\ &\quad + \int_0^1\int_s^1 U_{-t}\eta_{ijk}\left[a_0^3, \mathcal{G}^\dagger\right]U_t\mathrm{d}t\mathrm{d}s, \end{aligned} \tag{74}$$

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where we have used Duhamel's formula to express $U^{-1}\eta_{ijk}a_0^3U - U_{-s}\eta_{ijk}a_0^3U_s$. The following Lemma 6 demonstrates that we can treat the quantities $\delta_1\psi$ and $\delta_2\psi$ in Eq. (74) as error terms. In order to formulate Lemma 6, recall the set $\mathcal{L}_0 := \{(0,0,0)\}$ from Eq. (16) and let us define

$$A := (2\pi\mathbb{Z})^9 \setminus \mathcal{L}_0 = (2\pi\mathbb{Z})^9 \setminus \{(0,0,0)\},$$

and the potential energy $\mathcal{E}_\mathcal{P}$ of an operator-valued three particle vector $\Theta_{i_1i_2i_3}$ as

$$\mathcal{E}_\mathcal{P}(\Theta) := \sum_{(i_1i_2i_3),(i_1'i_2'i_3')\in A} (V_N)_{i_1i_2i_3,i_1'i_2'i_3'}\Theta^\dagger_{i_1i_2i_3}\Theta_{i_1'i_2'i_3'}. \tag{75}$$

To keep the notation light, we will occasionally write $\mathcal{E}_\mathcal{P}(\Theta_{i_1i_2i_3})$ for $\mathcal{E}_\mathcal{P}(\Theta)$ with dummy indices $i_1i_2i_3$.

Lemma 6. *There exists a constant $C > 0$, such that*

$$\mathcal{E}_\mathcal{P}(\delta_1\psi) \leq CN^{\frac{1}{2}}(\mathcal{N}+1), \tag{76}$$

$$\mathcal{E}_\mathcal{P}(\delta_2\psi) \leq C(\mathcal{N}+1)^4. \tag{77}$$

Furthermore, $\mathcal{E}_P\left(\left[a_{i_1}a_{i_2}a_{i_3},\mathcal{G}^\dagger\right]\right) \leq CN^{-\frac{3}{2}}(\mathcal{N}+1)^5$.

Proof. Let us define A_j as the set of all s such that $(-s, j-s, 0) \in A$ and

$$\alpha_j := 9\sum_{s,t\in A_j}\eta_{-s(s-j)j}\overline{\eta_{-t(t-j)j}}(V_N)_{-s(j-s)0,-t(j-t)0}.$$

Making use of the fact that $V_N \geq 0$, we obtain by the Cauchy-Schwarz inequality

$$\sum_{(i_1i_2i_3),(i_1'i_2'i_3')\in A}(V_N)_{i_1i_2i_3,i_1'i_2'i_3'}(\delta_1\psi)^\dagger_{i_1i_2i_3}(\delta_1\psi)_{i_1'i_2'i_3'} \leq (a_0^\dagger)^4a_0^4\sum_j\alpha_j\,a_ja_j^\dagger \leq N^4\left(\sum_j\alpha_j\right)(\mathcal{N}+1).$$

By Lemma 15 and the fact that $|(V_N)_{-s(j-s)0,-t(j-t)0}| \lesssim \frac{1}{N^2}$, we have $N^4\sum_j\alpha_j \lesssim CN^{\frac{1}{2}}$, which concludes the proof of Eq. (76). In order to verify Eq. (77), let us first define

$$(\widetilde{\delta}_{2,\sigma}\psi)_{i_1i_2i_3} := \sum_{jk}\eta_{i_{\sigma_1}jk}\,a_k^\dagger a_j^\dagger a_{i_{\sigma_2}}a_{i_{\sigma_3}}a_0^3.$$

Then we obtain, using the sign $V_N \geq 0$ and a Cauchy-Schwarz estimate,

$$\mathcal{E}_\mathcal{P}(\delta_2\psi) \lesssim \sum_{\sigma\in S_3}\mathcal{E}_\mathcal{P}\left(\widetilde{\delta}_{2,\sigma}\psi\right) + \mathcal{E}_\mathcal{P}\left(\delta_2\psi - \frac{1}{4}\sum_{\sigma\in S_3}\widetilde{\delta}_{2,\sigma}\psi\right) = 6\mathcal{E}_\mathcal{P}\left(\widetilde{\delta}_{2,\mathrm{id}}\psi\right) + \mathcal{E}_\mathcal{P}\left(\delta_2\psi - \frac{1}{4}\sum_{\sigma\in S_3}\widetilde{\delta}_{2,\sigma}\psi\right).$$

Proceeding as in the proof of Eq. (76), we obtain

$$\mathcal{E}_\mathcal{P}\left(\delta_2\psi - \frac{1}{4}\sum_{\sigma\in S_3}\widetilde{\delta}_{2,\sigma}\psi\right) \lesssim N^{-\frac{1}{2}}(\mathcal{N}+1)^2.$$

Regarding the term $\mathcal{E}_\mathcal{P}\left(\widetilde{\delta}_{2,\mathrm{id}}\psi\right)$, let us define

$$(G)_{i_1..i_4,j_1..j_4} := (V_N)_{i_1i_2(-j_3-j_4),j_1j_2(-i_3-i_4)}\eta_{i_3i_4(-i_3-i_4)}\overline{\eta_{j_3j_4(-j_3-j_4)}}$$

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for $(i_1, i_2, -j_3 - j_4) \in A$ and $(j_1, j_2, -i_3 - i_4) \in A$, and $(G)_{i_1..i_4,j_1..j_4} := 0$ otherwise. Then

$$\begin{aligned}\mathcal{E}_{\mathcal{P}}\left(\widetilde{\delta}_{2,\mathrm{id}}\psi\right) &= \sum_{i_1..i_4,j_1..j_4} (G)_{i_1..i_4,j_1..j_4} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{j_3} a_{j_4} a_{i_3}^\dagger a_{i_4}^\dagger a_{j_1} a_{j_2} a_0^3 \\ &= \sum_{i_1..i_4,j_1..j_4} (G)_{i_1..i_4,j_1..j_4} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{i_3}^\dagger a_{i_4}^\dagger a_{j_3} a_{j_4} a_{j_1} a_{j_2} a_0^3 + 2 \\ &\quad \times \sum_{i_1..i_3,j_1..j_3,k} (G')_{i_1..i_3,j_1..j_3} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{i_3}^\dagger a_{j_3} a_{j_1} a_{j_2} a_0^3 \\ &\quad + \sum_{i_1 i_2, j_1 j_2} (G'')_{i_1 i_2, j_1 j_2} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{j_1} a_{j_2} a_0^3, \end{aligned} \tag{78}$$

with $(G')_{i_1..i_3,j_1..j_3} := \sum_k G_{i_1..i_3 k, j_1..j_3 k}$ and $(G'')_{i_1 i_2, j_1 j_2} := \sum_{k_1 k_2} G_{i_1 i_2 k_1 k_2, j_1 j_2 k_1 k_2}$. In the following let us study the term involving G'', which is responsible for the largest contribution. Since $(V_N)_{i_1 i_2 (-k_1-k_2), j_1 j_2 (-k_1-k_2)} = (V_N)_{i_1 i_2 0, j_1 j_2 0}$, see Eq. (24), we obtain

$$\begin{aligned}&\sum_{i_1 i_2, j_1 j_2} (G'')_{i_1 i_2, j_1 j_2} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{j_1} a_{j_2} a_0^3 = \left(\sum_{k_1 k_2} |\eta_{k_1 k_2 (-k_1-k_2)}|^2\right) \sum_{i_1 i_2, j_1 j_2} (V_N)_{i_1 i_2 0, j_1 j_2 0} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{j_1} a_{j_2} a_0^3 \\ &\quad \lesssim N^{-3} \sum_{i_1 i_2, j_1 j_2} (V_N)_{i_1 i_2 0, j_1 j_2 0} (a_0^\dagger)^3 a_{i_1}^\dagger a_{i_2}^\dagger a_{j_1} a_{j_2} a_0^3 \lesssim N^{-3} (a_0^\dagger)^3 (\mathcal{N}+1)^2 a_0^3 \leq (\mathcal{N}+1)^2,\end{aligned}$$

where we have used

$$\begin{aligned}&\sum_{i_1 i_2, j_1 j_2} (V_N)_{i_1 i_2 0, j_1 j_2 0} a_{i_1}^\dagger a_{i_2}^\dagger a_{j_1} a_{j_2} \lesssim (\mathcal{N}+1)^2, \\ &\sum_{k_1 k_2} |\eta_{k_1 k_2 (-k_1-k_2)}|^2 \lesssim N^{-3},\end{aligned}$$

see Lemma 15. Proceeding similarly for the other terms in Eq. (78), concludes the proof of Eq. (77). Regarding the bound on $\mathcal{E}_P\left(\left[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}^\dagger\right]\right)$, let us identify

$$\begin{aligned}\left[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}^\dagger\right] = \bigg\{ &\frac{3}{2} \mathbb{1}(i_1 = 0) (a_0^\dagger)^2 a_{i_2} a_{i_3}\, \mathbb{A} + 3\mathbb{1}(i_1 = i_2 = 0) a_0^\dagger a_{i_3}\, \mathbb{A} \\ &+ \mathbb{1}(i_1 = i_2 = i_3 = 0)\, \mathbb{A} \bigg\} + \{\text{Permutations}\},\end{aligned}$$

where $\mathbb{A} := \frac{1}{6} \sum_{ijk} \eta_{ijk} a_i a_j a_k$. Due to the sign $V_N \geq 0$ and the permutations symmetry of V_N, as well as to the fact that there are 6 permutations of the set $\{1, 2, 3\}$, we can bound the operator $\mathcal{E}_P\left(\left[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}^\dagger\right]\right)$ from above by

$$\begin{aligned}&6\, \mathcal{E}_P\left(\frac{3}{2} \mathbb{1}(i_1 = 0) (a_0^\dagger)^2 a_{i_2} a_{i_3}\, \mathbb{A} + 3\mathbb{1}(i_1 = i_2 = 0) a_0^\dagger a_{i_3}\, \mathbb{A} + \mathbb{1}(i_1 = i_2 = i_3 = 0)\, \mathbb{A}\right) \\ &\quad \leq 18\, \mathcal{E}_P\left(\frac{3}{2} \mathbb{1}(i_1 = 0) (a_0^\dagger)^2 a_{i_2} a_{i_3}\, \mathbb{A}\right) + 18\, \mathcal{E}_P\left(3\mathbb{1}(i_1 = i_2 = 0) a_0^\dagger a_{i_3}\, \mathbb{A}\right) \\ &\qquad + 18\, \mathcal{E}_P(\mathbb{1}(i_1 = i_2 = i_3 = 0)\, \mathbb{A}).\end{aligned}$$

In the following we focus on $\mathcal{E}_P\left(\mathbb{1}(i_1 = 0) (a_0^\dagger)^2 a_{i_2} a_{i_3}\, \mathbb{A}\right)$, the other terms can be treated in a similar fashion. By Lemma 15 we have $\mathbb{A}^\dagger \mathbb{A} \lesssim N^{-3} (\mathcal{N}+1)^3$, and therefore

$$\mathcal{E}_P\Big(\mathbb{1}(i_1=0)(a_0^\dagger)^2 a_{i_2}a_{i_3}\,\mathbb{A}\Big) = \mathbb{A}^\dagger \sum_{(ij),(\ell m)\in A^0} (V_N)_{0jk,0mn} a_k^\dagger a_j^\dagger a_0^2 (a_0^\dagger)^2 a_m a_n \mathbb{A}$$
$$\lesssim a_0^2(a_0^\dagger)^2\mathbb{A}^\dagger(\mathcal{N}+1)^2\mathbb{A} = a_0^2(a_0^\dagger)^2(\mathcal{N}+4)\mathbb{A}^\dagger\mathbb{A}(\mathcal{N}+4) \lesssim a_0^2(a_0^\dagger)^2 N^{-3}(\mathcal{N}+1)^5 \le N^{-1}(\mathcal{N}+1)^5,$$

where A^0 contains all pairs (jk) such that $(0jk)\in A$. □

As a consequence of Lemma 6, we obtain that the trial state Γ defined below Eq. (71) has a potential energy $\mathcal{E}_\mathcal{P}(\psi)$ of the order $O_{N\to\infty}\left(\sqrt{N}\right)$, see the following Corollary 3.

Corollary 3. *There exists a constant $C>0$, such that $\langle\Gamma,\mathcal{E}_\mathcal{P}(\psi+\delta_1\psi)\Gamma\rangle\le C$ and*

$$\langle\Gamma,\mathcal{E}_\mathcal{P}(\psi)\Gamma\rangle \le C\sqrt{N}.$$

Proof. Recall that we can express the transformed quantity $U^{-1}\psi_{ijk}U$ by Eq. (74) as

$$U^{-1}\psi_{ijk}U = a_ia_ja_k + \int_0^1 U_{-s}\left[a_ia_ja_k,\mathcal{G}^\dagger\right]U_s\mathrm{d}s - \int_0^1 U_{-s}(\delta_1\psi)_{ijk}U_s\mathrm{d}s - \int_0^1 U_{-s}(\delta_2\psi)_{ijk}U_s\mathrm{d}s$$
$$+\int_0^1\int_s^1 U_{-t}\eta_{ijk}\left[a_0^3,\mathcal{G}^\dagger\right]U_t\mathrm{d}t\mathrm{d}s,$$

where we have used Duhamel's formula to express $U^{-1}\eta_{ijk}a_0^3U - U_{-s}\eta_{ijk}a_0^3U_s$. Using the sign $V_N\ge 0$ and Lemma 6, we estimate using the Cauchy-Schwarz inequality

$$\mathcal{E}_\mathcal{P}\left(\int_0^1 U_{-s}(\delta_1\psi)_{ijk}U_s\mathrm{d}s\right) \le \int_0^1 U_{-s}\mathcal{E}_\mathcal{P}(\delta_1\psi)U_s\,\mathrm{d}s \le CN^{\frac{1}{2}}\int_0^1 U_{-s}(\mathcal{N}+1)^4U_s\mathrm{d}s \le C'N^{\frac{1}{2}}(\mathcal{N}+1),$$
$$\mathcal{E}_\mathcal{P}\left(\int_0^1 U_{-s}(\delta_2\psi)_{ijk}U_s\mathrm{d}s\right) \le \int_0^1 U_{-s}\mathcal{E}_\mathcal{P}(\delta_2\psi)U_s\,\mathrm{d}s \le CN^{\frac{1}{2}}\int_0^1 U_{-s}(\mathcal{N}+1)^4U_s\mathrm{d}s \le C'(\mathcal{N}+1)^4. \tag{79}$$

for suitable C, C', where we utilize Eq. (72) in order to estimate $U_{-s}(\mathcal{N}+1)^4U_s$. Similarly

$$\mathcal{E}_\mathcal{P}\left(\int_0^1 U_{-s}\left[a_ia_ja_k,\mathcal{G}^\dagger\right]U_s\mathrm{d}s\right) \le C'N^{-\frac{3}{2}}(\mathcal{N}+1)^5 \tag{80}$$

follows from Lemma 6. Regarding the term in the last line of Eq. (74), we note that

$$\left[a_0^3,\mathcal{G}^\dagger\right]^\dagger\left[a_0^3,\mathcal{G}^\dagger\right] \lesssim N(\mathcal{N}+1)^3$$

follows from an analogous argument as we have seen in the proof of Lemma 6 and

$$\sum_{(ijk),(\ell mn)\in A} (V_N)_{ijk,\ell mn}\overline{\eta_{ijk}}\eta_{\ell mn} \lesssim N^{-2}$$

by Eq. (36). Therefore

$$\mathcal{E}_\mathcal{P}\left(\int_0^1\int_s^1 U_{-t}\eta_{ijk}\left[a_0^3,\mathcal{G}^\dagger\right]U_t\mathrm{d}t\mathrm{d}s\right) \le \frac{1}{2}\int_0^1\int_s^1 U_{-t}\mathcal{E}_\mathcal{P}\left(\eta_{ijk}\left[a_0^3,\mathcal{G}^\dagger\right]\right)U_t\,\mathrm{d}t\mathrm{d}s \lesssim N^{-1}(\mathcal{N}+1)^3, \tag{81}$$

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where we have used Eq. (72) again. Using $a_i a_j a_k \Gamma_0 = 0$ in case $(ijk) \in A$, we obtain by Eq. (74) together with Eq. (79), Eq. (80) and Eq. (81) for a suitable constant C

$$\langle \Gamma, \mathcal{E}_{\mathcal{P}}(\psi)\Gamma\rangle = \left\langle \Gamma_0, \mathcal{E}_{\mathcal{P}}\left(U^{-1}\psi U\right)\Gamma_0\right\rangle \leq CN^{\frac{1}{2}}\left\langle \Gamma_0, (\mathcal{N}+1)^5\Gamma_0\right\rangle = CN^{\frac{1}{2}}.$$

Analogously we obtain $\langle \Gamma, \mathcal{E}_{\mathcal{P}}(\psi + \delta_1\psi)\Gamma\rangle \leq C$. □

Regarding the variable $c_k = a_k + [a_k, \mathcal{G}]$ from Eq. (68), let us apply Duahmel's formula

$$U^{-1}c_k U = a_k - \int_0^1 U_{-s}[a_k, \mathcal{G}]U_s \, \mathrm{d}s + U^{-1}[a_k, \mathcal{G}]U = a_k + \int_0^1 \int_s^1 U_{-t}\left[[a_k, \mathcal{G}], \mathcal{G}^\dagger\right]U_t \, \mathrm{d}t\mathrm{d}s, \quad (82)$$

where we have used $\left[a_k, \mathcal{G}^\dagger\right] = 0$ for $k \neq 0$ and $[[a_k, \mathcal{G}], \mathcal{G}] = 0$, which follows from the observation that $\eta_{ijk} = 0$ in case one of the indices in $\{i, j, k\}$ is zero. The following Lemma 7 provides useful estimates on the quantity $\left[[a_k, \mathcal{G}], \mathcal{G}^\dagger\right]$. In order to formulate Lemma 7 let us define the kinetic energy of an operator-valued one-particle vector Θ_k, written as $\mathcal{E}_{\mathcal{K}}(\Theta)$ or $\mathcal{E}_{\mathcal{K}}(\Theta_k)$ with k being a dummy index, as

$$\mathcal{E}_{\mathcal{K}}(\Theta) := \sum_k |k|^2 \Theta_k^\dagger \Theta_k. \quad (83)$$

Lemma 7. *For $m \geq 0$ there exists a constant $C_m > 0$, such that*

$$\mathcal{E}_{\mathcal{K}}\left(\mathcal{N}^m\left[[a_k, \mathcal{G}], \mathcal{G}^\dagger\right]\right) \leq C_m N^{-1}(\mathcal{N}+1)^{5+2m}.$$

Proof. Let us write the double commutator as $\left[[a_k, \mathcal{G}], \mathcal{G}^\dagger\right] = (\delta_1 c)_k + (\delta_2 c)_k + (\delta_3 c)_k$, where

$$(\delta_1 c)_k := (a_0^\dagger)^3 a_0^3 \sum_{ij} |\eta_{ijk}|^2 a_k,$$

$$(\delta_2 c)_k := (a_0^\dagger)^3 a_0^3 \sum_{ij, j'k'} \overline{\eta_{ij'k'}}\eta_{ijk} a_j^\dagger a_{j'} a_{k'},$$

$$(\delta_3 c)_k := \left[a_0^3, (a_0^\dagger)^3\right]\left(\sum_{ij} \eta_{ijk} a_j^\dagger a_k^\dagger\right)\left(\sum_{i'j'k'} \overline{\eta_{i'j'k'}} a_{i'} a_{j'} a_{k'}\right).$$

By Eq. (36) it is clear that

$$\sum_{ij} |\eta_{ijk}|^2 \lesssim \frac{1}{N^4}\sum_t \frac{1}{(|k|^2+|t|^2)^2} \lesssim \frac{1}{N^4|k|},$$

and therefore

$$\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m \delta_1 c) = \sum_k |k|^2 (\delta_1 c)_k^\dagger \mathcal{N}^{2m}(\delta_1 c)_k \lesssim \frac{1}{N^8}\sum_{k\neq 0} a_k^\dagger \left((a_0^\dagger)^3 a_0^3\right)^2 \mathcal{N}^{2m} a_k \leq \frac{1}{N^2}\mathcal{N}^{2m+1}.$$

Using $J_{p_1p_2p_3, p_1'p_2'p_3'} := \sum_{qq'k} |k|^2 \overline{\eta_{q'p_2'p_3'}\eta_{qp_1'k}}\eta_{q'p_1k}\eta_{qp_2p_3}$ and $\widetilde{J}_{p_2p_3, p_2'p_3'} := \sum_{p_1} J_{p_1p_2p_3, p_1p_2'p_3'}$

$$\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m \delta_2 c) = \left((a_0^\dagger)^3 a_0^3\right)^2 \sum_{jp'n', pj'k'} J_{jp'n', pj'k'} \, a_j^\dagger a_{p'}^\dagger a_{n'}^\dagger (\mathcal{N}+2)^{2m} a_p a_{j'} a_{k'}$$
$$+ \left((a_0^\dagger)^3 a_0^3\right)^2 \sum_{p'n', j'k'} \widetilde{J}_{p'n', j'k'} \, a_{p'}^\dagger a_{n'}^\dagger (\mathcal{N}+1)^{2m} a_{j'} a_{k'}.$$

Utilizing the operator $X_{jk,j'k'} := \sum_q |k|\eta_{qjk}\overline{\eta_{qj'k'}}$ acting on $L^2(\Lambda)^{\otimes 2}$ and the permutation operator $(S\Psi)(x_1,x_2,x_3) := \Psi(x_2,x_1,x_3)$ acting on $L^2(\Lambda)^{\otimes 3}$, we can write

$$J = (1 \otimes X^\dagger)S(1 \otimes X),$$

and $\widetilde{J} = X^\dagger X$. Consequently

$$\|J\| \leq \|S\|\,\|1 \otimes X\|^2 = \|X\|^2 = \|\widetilde{J}\|.$$

By Eq. (36) we have $\|\widetilde{J}\| \leq CN^{-\frac{15}{2}}$ for a suitable constant C. Consequently

$$\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m\delta_2 c) \leq CN^{-\frac{15}{2}}\left((a_0^\dagger)^3 a_0^3\right)^2(\mathcal{N}+2)^{3+2m} \leq CN^{-\frac{3}{2}}(\mathcal{N}+2)^{3+2m}.$$

Similarly one can show that $\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m\delta_3 c) \lesssim N^{-1}(\mathcal{N}+1)^{5+2m}$, and therefore

$$\begin{aligned}\mathcal{E}_{\mathcal{K}}\left(\mathcal{N}^m\left[[a_k,\mathcal{G}],\mathcal{G}^\dagger\right]\right) &= \mathcal{E}_{\mathcal{K}}(\mathcal{N}^m\delta_1 + \mathcal{N}^m\delta_2 + \mathcal{N}^m\delta_3)\\ &\leq 3\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m\delta_1) + 3\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m\delta_2) + 3\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m\delta_3) \lesssim C_m N^{-1}(\mathcal{N}+1)^{5+2m}.\end{aligned}$$

□

As a consequence of Lemma 7, we obtain that the trial state Γ defined below Eq. (71) has a kinetic energy $\mathcal{E}_{\mathcal{K}}(c)$ of the order $O_{N\to\infty}(1)$ in the subsequent Corollary 4. Since in the residual term $\mathcal{E}$ defined in Lemma 1 the term $\mathcal{E}_{\mathcal{K}}\left(\sqrt{\mathcal{N}}c\right) \leq \frac{1}{2}\mathcal{E}_{\mathcal{K}}(c) + \frac{1}{2}\mathcal{E}_{\mathcal{K}}(\mathcal{N}c)$ appears, it will be convenient to estimate the expectation value in the state Γ of $\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c)$ for $m \geq 1$ as well.

Corollary 4. *Let Γ be the state defined below Eq. (71) and $m \geq 0$. Then there exists a constant $C > 0$, such that $\langle\Gamma, \mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c)\Gamma\rangle \leq \frac{C_m}{N}$.*

Proof. By Eq. (72) we have

$$U^{-1}\mathcal{N}^{2m}U = (U^{-1}\mathcal{N}^m U)^\dagger U^{-1}\mathcal{N}^m U \lesssim (\mathcal{N}^m+1)^2$$

and hence

$$U^{-1}\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c)U = \mathcal{E}_{\mathcal{K}}\left(U^{-1}\mathcal{N}^m U\, U^{-1}c\, U\right) \lesssim \mathcal{E}_{\mathcal{K}}\left((\mathcal{N}^m+1)U^{-1}c\, U\right),$$

where we have used that for operators f_k and A, B satisfying $A^\dagger A \leq CB^\dagger B$ we have

$$\mathcal{E}_{\mathcal{K}}(Af_k) \leq C\mathcal{E}_{\mathcal{K}}(Bf_k).$$

Proceeding as in the proof of Corollary 3, we obtain by Eq. (82) and Lemma 7

$$\begin{aligned}\mathcal{E}_{\mathcal{K}}\left((\mathcal{N}^m+1)U^{-1}c\, U\right) &\lesssim \mathcal{E}_{\mathcal{K}}((\mathcal{N}^m+1)a) + \int_0^1 \mathcal{E}_{\mathcal{K}}\left((\mathcal{N}^m+1)U_{-t}\left[[a_k,\mathcal{G}],\mathcal{G}^\dagger\right]U_t\right)\mathrm{d}t\\ &= \mathcal{E}_{\mathcal{K}}((\mathcal{N}^m+1)a) + \int_0^1 U_{-t}\mathcal{E}_{\mathcal{K}}\left(U_t(\mathcal{N}^m+1)U_t\left[[a_k,\mathcal{G}],\mathcal{G}^\dagger\right]\right)U_t\mathrm{d}t\\ &\lesssim \mathcal{E}_{\mathcal{K}}((\mathcal{N}^m+1)a) + \int_0^1 U_{-t}\mathcal{E}_{\mathcal{K}}\left((\mathcal{N}^m+1)\left[[a_k,\mathcal{G}],\mathcal{G}^\dagger\right]\right)U_t\mathrm{d}t\\ &\lesssim \mathcal{E}_{\mathcal{K}}((\mathcal{N}^m+1)a) + N^{-1}\int_0^1 U_{-t}(\mathcal{N}+1)^{5+2m}U_t\mathrm{d}t\\ &\lesssim \mathcal{E}_{\mathcal{K}}((\mathcal{N}^m+1)a) + N^{-1}(\mathcal{N}+1)^{5+2m}.\end{aligned}$$

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where we have made use of Eq. (36) again. Using $a_k\Gamma_0 = 0$ for $k \neq 0$, therefore yields

$$\begin{aligned}\langle\Gamma, \mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c)\Gamma\rangle &= \left\langle\Gamma_0, U^{-1}\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c)U\Gamma_0\right\rangle \\ &\lesssim \langle\Gamma_0, \mathcal{E}_{\mathcal{K}}((\mathcal{N}^m+1)a)\Gamma_0\rangle + N^{-1}\left\langle\Gamma_0, (\mathcal{N}+1)^{5+2m}\Gamma_0\right\rangle = \frac{1}{N}. \qquad \square\end{aligned}$$

Having Corollary 3 and Corollary 4 at hand, we are in a position to verify the upper bound on the ground state energy E_N in Theorem 4.

Proof of Theorem 4. Let $A := (2\pi\mathbb{Z})^9 \setminus \{(0,0,0)\}$, and let Γ be the state defined below Eq. (71). Using Eq. (27) and Eq. (21), and the fact that $\left(\widetilde{V}_N\right)_{ijk,\ell mn} = (V_N)_{ijk,\ell mn}$ for index triples $(ijk), (\ell mn) \in A$, we obtain

$$\begin{aligned}H_N &= \sum_k |k|^2 c_k^\dagger c_k + \lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \frac{1}{6}\sum_{(ijk),(\ell mn)\in A}(V_N)_{ijk,\ell mn}\psi_{ijk}^\dagger\psi_{\ell mn} \\ &\quad + \left(3a_0^\dagger a_0^3 \sum_{\ell\neq 0}\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger + \text{H.c.}\right) - \mathcal{E} \\ &= \lambda_{0,0}(a_0^\dagger)^3 a_0^3 + \mathcal{E}_{\mathcal{K}}(c) + \mathcal{E}_{\mathcal{P}}(\psi) + \left(3a_0^\dagger a_0^3\sum_{\ell\neq 0}\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger + \text{H.c.}\right) - \mathcal{E}.\end{aligned}$$

By a symmetry argument it is clear that $\langle\Gamma, a_0^\dagger a_0^3 a_\ell^\dagger a_{-\ell}^\dagger\Gamma\rangle = 0$. Applying Corollary 3 as well as Corollary 4, with $m = 0$, yields for suitable constants $C > 0$

$$\langle\Gamma, \mathcal{E}_{\mathcal{P}}(\psi)\Gamma\rangle \leq C\sqrt{N}, \qquad \langle\Gamma, \mathcal{E}_{\mathcal{K}}(c)\Gamma\rangle \leq \frac{C}{N}.$$

Furthermore, observe that $N^3\lambda_{0,0} \leq \frac{1}{6}b_{\mathcal{M}}(V)N + C'$ by Eq. (37) for a suitable C'. In order to estimate the final term $\langle\Psi, \mathcal{E}\Psi\rangle$, note that we have by Eq. (72) for $m \in \mathbb{N}$

$$\langle\Gamma, \mathcal{N}^m\Gamma\rangle = \langle\Gamma_0, U^{-1}\mathcal{N}^m U\Gamma_0\rangle \lesssim \langle\Gamma_0, (\mathcal{N}+1)^m\Gamma_0\rangle = 1. \tag{84}$$

Using Lemma 3 together with the estimate from Corollary 4 for $m = 0$ and $m = 1$, we therefore obtain $|\langle\Psi, \mathcal{E}\Psi\rangle| \lesssim N^{-\frac{1}{3}}$. $\square$

4. Refined correlation structure

Utilizing the set of operators defined in Eq. (25) and Eq. (26), we were able to identify the ground state energy E_N up to errors of the magnitude $O_{N\to\infty}(\sqrt{N})$ in the previous Sections 2 and 3. It is the purpose of this Section to obtain a higher resolution of the energy, which especially captures the subleading term proportional to $\sqrt{N}$ in the asymptotic expansion of E_N, using a more refined correlation structure compared to the one introduced in Subsection 1.1. On a technical level, the new correlation structure is implemented by the new set of operators d_k and ξ_{ijk} defined below in Eq. (89) and Eq. (90), which constitute a refined version of the operators c_k and ψ_{ijk} respectively. Writing the operator H_N in terms of d_k and ξ_{ijk} will then allow us to verify the lower bound from Theorem 1 in Subsection 4.2 and the corresponding upper bound in Section 5.

The approach presented in Sections 2 and 3 fails to capture the correct term of order $\sqrt{N}$ for two reasons: (I) The following expression appearing in Eq. (32)

$$3\sum_{|\ell|>K} N^2\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger \frac{a_0^\dagger a_0^3}{N^2} \tag{85}$$

is expected to lower the ground state energy by an amount proportional to $\sqrt{N}$, to be precise naive perturbation theory suggests that the term in Eq. (85) is giving rise to an energy correction proportional to

$$\sum_{|\ell|>K} \frac{|N^2 \lambda_{0,\ell}|^2}{|\ell|^2} = O(\sqrt{N}), \tag{86}$$

see Eq. (35), and therefore consistent with our estimate in Lemma 4. (II) In the pursue of an upper bound on E_N we expressed the unitary conjugated variables $U^{-1}\psi_{ijk}U$ as a sum of $a_i a_j a_k$ and various error terms according to Eq. (74) as

$$U^{-1}\psi_{ijk}U = a_i a_j a_k + \int_0^1 U_{-s}\left[a_i a_j a_k, \mathcal{G}^\dagger\right]U_s \mathrm{d}s - \int_0^1 U_{-s}(\delta_1\psi)_{ijk}U_s \mathrm{d}s - \int_0^1 U_{-s}(\delta_2\psi)_{ijk}U_s \mathrm{d}s \\ + \int_0^1 \int_s^1 U_{-t}\eta_{ijk}\left[a_0^3, \mathcal{G}^\dagger\right]U_t \mathrm{d}t\mathrm{d}s. \tag{87}$$

While most of the terms appearing in Eq. (87) give a contribution of the order $o_{N\to}\left(\sqrt{N}\right)$, the term $\delta_1\psi$ is expected to increase the ground state energy by an amount proportional to $\sqrt{N}$, which is consistent with our estimate in Eq. (76). In order to extract the energy shift due to the expression in Eq. (85), we follow the strategy in Subsection 1.1 and introduce an additional two-particle correlation structure via a map acting on the two-particle space

$$T_2 : L^2(\Lambda^2) \longrightarrow L^2(\Lambda^2)$$

in Eq. (88), which will give rise to the negative energy correction $-\mu(V)\sqrt{N}$ from Theorem 1. To be precise, we define the map T_2 via its matrix elements as

$$(T_2 - 1)_{\ell(-\ell),00} := (T_2 - 1)_{00,\ell(-\ell)} := 3N\frac{\lambda_{0,\ell}}{|\ell|^2}, \tag{88}$$

for $|\ell| > K$ and $(T_2 - 1)_{jk,mn} := 0$ otherwise, where $\lambda_{k,\ell}$ is defined below Eq. (32). Regarding the energy shift associated with $\delta_1\psi$, it is a natural idea to include this term in the definition of our new operators ξ_{ijk}, giving rise to the positive energy correction $\gamma(V)\sqrt{N}$ from Theorem 1. However, a computation in Eq. (93) demonstrates that the presence of $\delta_1\psi$ produces new four-particle correlation terms of the form

$$\sum_{uijk} \theta_{uijk} a_u^\dagger a_i^\dagger a_j^\dagger a_k^\dagger \frac{a_0^4}{N^2} + \mathrm{H.c.},$$

with coefficients θ_{uijk} proportional to $N^2 \sum_{mn}(V_N)_{ijk,0mn}\eta_{mnu}$, which behave like

$$N^{-\frac{3}{2}}\mathbb{1}(i + j + k + u = 0)$$

for momenta of the order $\sqrt{N}$, and decay fast for higher momenta. Therefore, the four-particle correlation terms are expected to lower the ground state energy, similar to Eq. (86), by an amount of the order

$$\sum_{|u|,|i|,|j|,|k|\le\sqrt{N}} \frac{|N^{-\frac{3}{2}}\mathbb{1}(i + j + k + u = 0)|^2}{|i|^2 + |j|^2 + |k|^2 + |u|^2} = O(\sqrt{N}).$$

Again we extract the correlation energy by introducing a map, acting this time on the four-particle space

$$T_4 : L^2(\Lambda^4) \longrightarrow L^2(\Lambda^4)$$

in Eq. (95), which gives rise to the negative energy correction $-\sigma(V)\sqrt{N}$ from Theorem 1.

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In the following let $T : L^2(\Lambda^3) \longrightarrow L^2(\Lambda^3)$ be the map constructed in Eq. (19), and for now let us think of $T_2 : L^2(\Lambda^2) \longrightarrow L^2(\Lambda^2)$ and $T_4 : L^2(\Lambda^4) \longrightarrow L^2(\Lambda^4)$ as generic bounded permutation-symmetric operators modeling the two-particle and four-particle correlation structure respectively. Following the approach in Section 2, we are implementing many-particle counterparts to the transformations T, T_2, and T_4 as

$$d_k := a_k + \sum_{j,mn} (T_2 - 1)_{jk,mn}\, a_j^\dagger a_m a_n + \frac{1}{2} \sum_{ij,\ell mn} (T-1)_{ijk,\ell mn}\, a_i^\dagger a_j^\dagger a_\ell a_m a_n \tag{89}$$
$$+ \frac{1}{6} \sum_{uij,v\ell mn} (T_4 - 1)_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_v a_\ell a_m a_n,$$

$$\xi_{ijk} := \sum_{\ell mn} (T)_{ijk,\ell mn}\, a_\ell a_m a_n + (\delta_1 \psi)_{ijk} + \sum_{u,v\ell mn} (T_4 - 1)_{uijk,v\ell mn}\, a_u^\dagger a_v a_\ell a_m a_n. \tag{90}$$

Note that T_2 is not included in the definition of ξ_{ijk}, as it would only give contributions of the order $O_{N\to\infty}(1)$. Using the Laplace operator Δ_s acting on the space $L^2(\Lambda)^{\otimes s}$ and the coefficients

$$(\chi)_{i_1..i_4,j_1..j_4} := \frac{1}{2} \sum_{\sigma \in S_3} \mathbb{1}(j_1 = .. = j_4 = i_{\sigma_3} = 0)\eta_{i_{\sigma_1} i_{\sigma_2} i_4}, \tag{91}$$

let us furthermore define the operators $X_2 := T_2^\dagger(-\Delta_2)T_2 + \Delta_2$ and

$$X_4 := \left(\left\{(-\Delta_4 + 4(\widetilde{V}_N \otimes 1))(T_4 - 1) + 4(\widetilde{V}_N \otimes 1)\chi\right\} + \text{H.c.}\right) \tag{92}$$
$$+ (T_4 - 1)^\dagger(-\Delta_4)(T_4 - 1) + \left((T \otimes 1 - 1)^\dagger 4(\widetilde{V}_N \otimes 1)(T_4 - 1 + \chi) + \text{H.c.}\right)$$
$$+ (T_4 - 1 + \chi)^\dagger 4(\widetilde{V}_N \otimes 1)(T_4 - 1 + \chi).$$

A straightforward computation, similar to the one in Eq. (27), reveals that up to excess terms involving X_2, X_4 and an error term $\widetilde{\mathcal{E}}$, we can write the operator H_N as a sum of squares in the variables d_k and ξ_{ijk} according to

$$\sum_k |k|^2 d_k^\dagger d_k + \frac{1}{6} \sum_{ijk,\ell mn} \left(\widetilde{V}_N\right)_{ijk,\ell mn} \xi_{ijk}^\dagger \xi_{\ell mn}$$
$$= H_N + \frac{1}{2} \sum_{jk,mn} (X_2)_{jk,mn}\, a_j^\dagger a_k^\dagger a_m a_n + \frac{1}{24} \sum_{uijk,v\ell mn} (X_4)_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_k^\dagger a_v a_\ell a_m a_n + \widetilde{\mathcal{E}}, \tag{93}$$

where the error $\widetilde{\mathcal{E}}$ contains all the non-fully contracted products appearing in the squares

$$\sum_k |k|^2 (d_k - a_k)^\dagger (d_k - a_k),\ \frac{1}{6} \sum_{ijk,\ell mn} \left(\widetilde{V}_N\right)_{ijk,\ell mn} (\xi_{ijk} - \psi_{ijk})^\dagger (\xi_{\ell mn} - \psi_{ijk}). \tag{94}$$

In this context we define the fully contracted part of a product of monomials

$$\left(a_{i_1}^\dagger \dots a_{i_r}^\dagger a_{j_1} \dots a_{j_t}\right)\left(a_{i'_1}^\dagger \dots a_{i'_{r'}}^\dagger a_{j'_1} \dots a_{j'_{t'}}\right)$$

as $C_{j_1\dots j_t, i'_1 \dots i'_{r'}} a_{i_1}^\dagger \dots a_{i_r}^\dagger a_{j'_1} \dots a_{j'_{t'}}$ with $C_{j_1\dots j_t, i'_1\dots i'_{r'}}$ being the expectation of $a_{j_1} \dots a_{j_t} a_{i'_1}^\dagger \dots a_{i'_{r'}}^\dagger$ in the vacuum. For a term by term definition of $\widetilde{\mathcal{E}}$ see Eq. (111) in Subsection 4.1.

In the following we want to choose T_4, such that the term $4(\widetilde{V}_N \otimes 1)\chi$ is cancelled in the expression $\{..\}$ from Eq. (92), at least after symmetrization and projection onto the range of $Q^{\otimes 4}$, that is, we define

$$T_4 := 1 - R_4 \Pi_{\mathrm{sym}} Q^{\otimes 4} 4(\widetilde{V}_N \otimes 1)\chi = 1 - R_4 \Pi_{\mathrm{sym}} Q^{\otimes 4} 4(V_N \otimes 1)\chi, \tag{95}$$

where Π_{sym} is the orthogonal projection onto the subspace $L^2_{\mathrm{sym}}(\Lambda^4) \subseteq L^2(\Lambda^4)$ and R_4 is the pseudoinverse of

$$Q^{\otimes 4}\left(-\Delta_4 + 4(\widetilde{V}_N \otimes 1)\right)Q^{\otimes 4} = Q^{\otimes 4}(-\Delta_4 + 4(V_N \otimes 1))Q^{\otimes 4}. \tag{96}$$

In order to obtain an improved representation of the operator X_4 defined in Eq. (92), let us introduce the constants

$$\begin{aligned} \sigma_N &:= \frac{N^4}{6}\langle(\widetilde{V}_N \otimes 1)\chi u_0^{\otimes 4}, (1 - T_4)u_0^{\otimes 4}\rangle, \\ &= \frac{N^4}{24}\left\langle (T_4 - 1)u_0^{\otimes 4}, (-\Delta_4 + 4V_N \otimes 1)(T_4 - 1)u_0^{\otimes 4}\right\rangle, \end{aligned} \tag{97}$$

$$\gamma_N := \frac{N^4}{6}\langle(\widetilde{V}_N \otimes 1)\chi u_0^{\otimes 4}, \chi u_0^{\otimes 4}\rangle = \frac{N^4}{6}\langle(V_N \otimes 1)\chi u_0^{\otimes 4}, \chi u_0^{\otimes 4}\rangle, \tag{98}$$

which allow us to write $\gamma_N - \sigma_N = \frac{N^4}{24}(X_4)_{0000,0000}$. Furthermore, we define the three-particle state Θ as

$$\begin{aligned} (\Theta)_{ijk} &:= 4\left(\Pi_{\mathrm{sym}} \frac{X_4}{24} \Pi_{\mathrm{sym}}\right)_{0ijk,000}, \\ (\Theta)_{0jk} &:= 6\left(\Pi_{\mathrm{sym}} \frac{X_4}{24} \Pi_{\mathrm{sym}}\right)_{00jk,000} \end{aligned} \tag{99}$$

for $\{i, j, k\}$ all different from zero and $(\Theta)_{ijk} := 0$ otherwise. According to the definition of T_4 we have $Q^{\otimes 4}\Pi_{\mathrm{sym}} X_4 \Pi_{\mathrm{sym}} P^{\otimes 4} = 0$, and therefore

$$\begin{aligned} &\frac{1}{24}\sum_{uijk,v\ell mn} (X_4)_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_k^\dagger a_v a_\ell a_m a_n \\ &\quad = \frac{1}{24}\sum_{uijk,v\ell mn} (\Pi_{\mathrm{sym}} X_4 \Pi_{\mathrm{sym}})_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_k^\dagger a_v a_\ell a_m a_n \\ &\quad = (a_0^\dagger)^4 a_0^4\, N^{-4}(\gamma_N - \sigma_N) + \left(\sum_{ijk,\ell mn} (\Theta)_{ijk}\, a_i^\dagger a_j^\dagger a_k^\dagger\, a_0^\dagger a_0^4 + \mathrm{H.c.}\right). \end{aligned} \tag{100}$$

In order to understand the size of the term in Eq. (100) better, we are going to rewrite it in terms of the variables ψ_{ijk} defined in Eq. (26), respectively the variables

$$\widetilde{\psi}_{ijk} = a_i a_j a_k + \eta_{ijk}\, a_0^3 \tag{101}$$

defined in Eq. (26) for the concrete choice $K := 0$, see Eq. (69), with the corresponding operator $T_{K=0} := 1 + R V_N \pi_0$, see Eq. (17). Note that

$$(T_{K=0}^{-1})^\dagger \Theta = \Theta + 2(\sigma_N - \gamma_N)u_0^{\otimes 3},$$

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and therefore

$$\frac{1}{24}\sum_{uijk,v\ell mn}(X_4)_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_k^\dagger a_v a_\ell a_m a_n = N^{-4}(a_0^\dagger)^4 a_0^4\,(\sigma_N-\gamma_N)$$
$$+\left(\sum_{ijk,\ell mn}(\Theta)_{ijk}\,\widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4+\mathrm{H.c.}\right).$$

In order to address the correlation term in Eq. (85), we use the concrete choice for T_2 from Eq. (88). With

$$\mu_N := \frac{N^2}{2}(X_2)_{00,00}, \tag{102}$$

this choice for a transformation T_2 yields

$$\frac{1}{2}\sum_{jk,mn}(X_2)_{jk,mn}\, a_j^\dagger a_k^\dagger a_m a_n = N^{-2}(a_0^\dagger)^2 a_0^2\,\mu_N+\left(3Na_0^2\sum_{|\ell|>K}\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger+\mathrm{H.c.}\right).$$

Summarizing what we have so far allows us to write the operator H_N in terms of the new variables d_k and ξ_{ijk} as

$$H_N=\sum_k |k|^2 d_k^\dagger d_k+\frac{1}{6}\sum_{ijk,\ell mn}\left(\widetilde{V}_N\right)_{ijk,\ell mn}\xi_{ijk}^\dagger\xi_{\ell mn}+N^{-4}(a_0^\dagger)^4 a_0^4\,(\gamma_N-\sigma_N)-N^{-2}(a_0^\dagger)^2 a_0^2\,\mu_N$$
$$-\left(3Na_0^2\sum_{|\ell|>K}\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger+\mathrm{H.c.}\right)-\left(\sum_{ijk,\ell mn}(\Theta)_{ijk}\,\widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4+\mathrm{H.c.}\right)-\widetilde{\mathcal{E}}. \tag{103}$$

Defining the error term

$$\mathcal{E}_* := 3\left(a_0^\dagger a_0-N\right)a_0^2\sum_{|\ell|>K}\lambda_{0,\ell}\, a_\ell^\dagger a_{-\ell}^\dagger+9a_0^\dagger a_0^2\sum_{\ell,0<|k|\le K}\lambda_{k,\ell}a_\ell^\dagger a_{k-\ell}^\dagger a_k, \tag{104}$$

we obtain as a consequence of Eq. (103) the following Corollary 5.

Corollary 5. *Let d_k and ξ_{ijk} be as in Eq. (89) and Eq. (90), with T_2 defined in Eq. (88) and T_4 defined in Eq. (95), γ_N, σ_N, and μ_N as in Eq. (98), Eq. (97) and Eq. (102), and let $\mathcal{E}_*$ be as in Eq. (104), Θ as in Eq. (99) and $\widetilde{\psi}_{ijk}$ as in Eq. (101). Furthermore, recall the definition of $\lambda_{0,0}$ in Eq. (29) and $\mathbb{Q}_K$ in Eq. (33). Then*

$$H_N\ge (a_0^\dagger)^3 a_0^3\lambda_{0,0}+N^{-4}(a_0^\dagger)^4 a_0^4\,(\gamma_N-\sigma_N)-N^{-2}(a_0^\dagger)^2 a_0^2\,\mu_N+\sum_k |k|^2 d_k^\dagger d_k+\mathbb{Q}_K$$
$$-\left(\sum_{ijk,\ell mn}(\Theta)_{ijk}\,\widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4+\mathrm{H.c.}\right)+\left(\mathcal{E}_*+\mathcal{E}_*^\dagger\right)-\widetilde{\mathcal{E}}. \tag{105}$$

Making use of the notation $\mathcal{E}_\mathcal{K}(d)$ from Eq. (83) and $\mathcal{E}_\mathcal{P}(\xi)$ from Eq. (75), we obtain in the case $K=0$ the identity

$$H_N=\lambda_{0,0}(a_0^\dagger)^3 a_0^3+(\gamma_N-\sigma_N)N^{-4}(a_0^\dagger)^4 a_0^4-\mu_N N^{-2}(a_0^\dagger)^2 a_0^2+\mathcal{E}_\mathcal{K}(d)+\mathcal{E}_\mathcal{P}(\xi)$$
$$-\left(\sum_{ijk,\ell mn}(\Theta)_{ijk}\,\widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4+\mathrm{H.c.}\right)+\left(\mathcal{E}_*+\mathcal{E}_*^\dagger\right)-\widetilde{\mathcal{E}}. \tag{106}$$

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Proof. Using Eq. (103) and the definition of $\widetilde{V}_N$ in Eq. (21), as well as the identities in Eq. (30) and Eq. (31), we obtain

$$\begin{aligned} H_N &= \lambda_{0,0}(a_0^\dagger)^3 a_0^3 + (\gamma_N - \sigma_N)N^{-4}(a_0^\dagger)^4 a_0^4 - \mu_N N^{-2}(a_0^\dagger)^2 a_0^2 + \sum_k |k|^2 d_k^\dagger d_k + \mathbb{Q}_K \\ &\quad + \frac{1}{6}\sum_{ijk,\ell mn} ((1-\pi_K)V_N(1-\pi_K))_{ijk,\ell mn}\xi_{ijk}^\dagger \xi_{\ell mn} \\ &\quad - \left(\sum_{ijk,\ell mn} (\Theta)_{ijk}\, \widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4 + \mathrm{H.c.}\right) + \left(\mathcal{E}_* + \mathcal{E}_*^\dagger\right) - \widetilde{\mathcal{E}}. \end{aligned}$$

Since $\mathbb{Q}_0 = 0$ and

$$\begin{aligned} &\frac{1}{6}\sum_{ijk,\ell mn} ((1-\pi_K)V_N(1-\pi_K))_{ijk,\ell mn}\xi_{ijk}^\dagger \xi_{\ell mn} \geq 0, \\ &\frac{1}{6}\sum_{ijk,\ell mn} ((1-\pi_0)V_N(1-\pi_0))_{ijk,\ell mn}\xi_{ijk}^\dagger \xi_{\ell mn} = \mathcal{E}_{\mathcal{P}}(\xi), \end{aligned}$$

we immediately obtain Eq. (105), respectively Eq. (106). □

4.1. Analysis of the error terms

In the following we are providing an explicit representation of the error term $\widetilde{\mathcal{E}}$ introduced in Eq. (93), which we subsequently use in Lemma 8 in order to control $\widetilde{\mathcal{E}}$. For this purpose, we are going to utilize the following estimates on the matrix elements of T, T_2 and T_4

$$\left|(T-1)_{ijk,\ell 00}\right| \leq \frac{C\,\mathbb{1}(i+j+k=\ell)}{N^2(|i|^2+|j|^2+|k|^2)}\left(1+\frac{|i|^2+|j|^2+|k|^2}{N+|\ell|^2}\right)^{-2}, \tag{107}$$

$$|(T_2-1)_{jk,00}| \leq CN^{-1}\frac{\mathbb{1}(j+k=0)}{|j|^2+|k|^2}\left(1+\frac{|j|^2+|k|^2}{N}\right)^{-1}, \tag{108}$$

$$|(T_4-1)_{\ell ijk,0000}| \leq CN^{-\frac{7}{2}}\frac{\mathbb{1}(\ell+i+j+k=0)}{|\ell|^2+|i|^2+|j|^2+|k|^2}\left(1+\frac{|\ell|^2+|i|^2+|j|^2+|k|^2}{N}\right)^{-3}, \tag{109}$$

which are verified in Lemma 15 and Lemma 18 respectively. Furthermore, it is useful to introduce the two-particle state $(\varphi_2^0)_{jk} := N(T_2-1)_{jk,00}$, the three-particle states $(\varphi_3^0)_{ijk} := \frac{N^{\frac{3}{2}}}{2}(T-1)_{ijk,000}$ and for $m \in (2\pi\mathbb{Z})^3 \setminus \{0\}$

$$(\varphi_3^m)_{ijk} := \frac{N^{\frac{3}{2}}}{2}(T-1)_{ijk,m00} + \frac{N^{\frac{3}{2}}}{2}(T-1)_{ijk,0m0} + \frac{N^{\frac{3}{2}}}{2}(T-1)_{ijk,00m},$$

and the four particle state $(\varphi_4^0)_{uijk} := \frac{N^2}{6}(T_4-1)_{uijk,0000}$ as well as

$$(\varphi_4)_{uijk} := N^2(T_4 - 1 + \chi)_{uijk,0000}.$$

Additionally, let us introduce for $\varphi \in L^2(\Lambda^s)$ and $\psi \in L^2(\Lambda^t)$ with $s,t \geq 0$, and $\ell \leq \min\{s,t\}$, the operator

$$G_\ell(\varphi,\psi) := \mathrm{Tr}_{1\to\ell}\left[(-\Delta)_{x_1}\varphi\psi^\dagger\right] \tag{110}$$

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acting on $L^2(\Lambda^{t-\ell}) \longrightarrow L^2(\Lambda^{s-\ell})$. In coordinates, the operator is given by

$$\Big(G_\ell(\varphi,\psi)\Big)_{i_1\dots i_{s-\ell},j_1\dots j_{t-\ell}} := \sum_{k_1\dots k_\ell} |k_1|^2 \varphi_{k_1\dots k_\ell i_1\dots i_{s-\ell}} \overline{\psi}_{k_1\dots k_\ell j_1\dots j_{t-\ell}}.$$

Finally let $\widetilde{G} := \mathrm{Tr}_{1\to 3}\Big[\widetilde{V}_N \otimes 1\varphi_4\varphi_4^\dagger\Big]$. With this at hand we can write

$$\widetilde{\mathcal{E}} = \sum_{(s,t,\ell,m,n)\in\mathcal{S}} C_{s,t,\ell} \sum_{\substack{i_1\dots i_{s-\ell}\\ j_1\dots j_{t-\ell}}} \Big(G_\ell(\varphi_s^m,\varphi_t^n)\Big)_{i_1\dots i_{s-\ell},j_1\dots j_{t-\ell}} a^\dagger_{i_{s-\ell}}\dots a^\dagger_{i_1} \frac{a_m^\dagger (a_0^\dagger)^{s-1} a_0^{t-1} a_n}{N^{\frac{s+t}{2}}} a_{j_1}\dots a_{j_{t-\ell}}$$
$$+ \sum_{i,j} \Big(\widetilde{G}\Big)_{i,j} a_i^\dagger \frac{(a_0^\dagger)^4 a_0^4}{N^4} a_j, \tag{111}$$

where $C_{s,t,\ell} := \frac{(s-1)!(t-1)!}{(\ell-1)!(s-\ell)!(t-\ell)!}$ and the set of allowed configurations $(s,t,\ell,m,n)\in\mathcal{S}$ is defined by the rules $\ell \le \min\{s,t\}$ and $\ell < \max\{s,t\}$, where $2 \le s,t \le 4$ and $|n|,|m| \le K$ with $m = 0$, respectively $n = 0$, in case $s \ne 3$, respectively $t \ne 3$. Note that the criterion $\ell < \max\{s,t\}$ makes sure that we only include non-fully contracted parts of the first product in Eq. (94) and $\widetilde{G}$ is the kernel associated with the non-fully contracted part of the second product in Eq. (94). Furthermore, $C_{s,t,\ell}$ counts the various different ways to have an $\ell - 1$ fold contraction between $s - 1$ many annihilation operators and $t - 1$ many creation operators, that is, $C_{s,t,\ell}$ counts the number of partially defined injective functions

$$f : \{1,\dots,s-1\} \longrightarrow \{1,\dots,t-1\}$$

with $\#\mathrm{dom} f = \ell - 1$. Let us illustrate the derivation of Eq. (94), looking at the term

$$\sum_k |k|^2 (d_k - a_k)^\dagger (d_k - a_k),$$

from Eq. (94). According to the definition of d_k in Eq. (89), the term $d_k - a_k$ decomposes into three terms, and in the following we focus only on the last one involving $T_4 - 1$

$$\sum_k |k|^2 \Bigg(\frac{1}{6}\sum_{uij,v\ell mn} (T_4-1)_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_v a_\ell a_m a_n\Bigg)^\dagger \Bigg(\frac{1}{6}\sum_{uij,v\ell mn} (T_4-1)_{uijk,v\ell mn}\, a_u^\dagger a_i^\dagger a_j^\dagger a_v a_\ell a_m a_n\Bigg)$$
$$= N^{-4} \sum_{k,uij,u'i'j'} |k|^2 \overline{(\varphi_0^4)_{uijk}} (\varphi_0^4)_{u'i'j'k} (a_0^\dagger)^4 a_u a_i a_j a_{u'}^\dagger a_{i'}^\dagger a_{j'}^\dagger a_0^4$$
$$= N^{-4} \sum_{k,uij,u'i'j'} |k|^2 \overline{(\varphi_0^4)_{uijk}} (\varphi_0^4)_{u'i'j'k} a_{u'}^\dagger a_{i'}^\dagger a_{j'}^\dagger (a_0^\dagger)^4 a_0^4 a_u a_i a_j$$
$$+ 9N^{-4} \sum_{jk,ui,u'i'} |k|^2 \overline{(\varphi_0^4)_{uijk}} (\varphi_0^4)_{u'i'jk} a_{u'}^\dagger a_{i'}^\dagger (a_0^\dagger)^4 a_0^4 a_u a_i$$
$$+ 18N^{-4} \sum_{ijk,u,u'} |k|^2 \overline{(\varphi_0^4)_{uijk}} (\varphi_0^4)_{u'i'j'k} a_{u'}^\dagger (a_0^\dagger)^4 a_0^4 a_u$$
$$+ 6N^{-4} \sum_{uijk} |k|^2 \overline{(\varphi_0^4)_{uijk}} (\varphi_0^4)_{u'i'j'k} (a_0^\dagger)^4 a_0^4$$
$$= \sum_{\ell=1}^{3} C_{4,4,\ell} \sum_{\substack{i_1\dots i_{4-\ell}\\ j_1\dots j_{4-\ell}}} \Big(G_\ell(\varphi_4^0,\varphi_4^0)\Big)_{i_1\dots i_{4-\ell},j_1\dots j_{4-\ell}} a^\dagger_{i_{4-\ell}}\dots a^\dagger_{i_1} \frac{(a_0^\dagger)^4 a_0^4}{N^4} a_{j_1}\dots a_{j_{4-\ell}}$$
$$+ 6N^{-4} \sum_{uijk} |k|^2 \overline{(\varphi_0^4)_{uijk}} (\varphi_0^4)_{u'i'j'k} (a_0^\dagger)^4 a_0^4. \tag{112}$$

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Notably, the final term in Eq. (112) is a fully contracted contribution and therefore part of the operator X_4 defined in Eq. (92) and not of the error term $\widetilde{\mathcal{E}}$.

Estimating the various terms appearing in Eq. (111) individually allows us to prove the following Lemma 8.

Lemma 8. *There exists a constant $C > 0$ and a function $\epsilon : [0, \infty) \longrightarrow (0, C)$ satisfying $\lim_{K\to\infty} \epsilon(K) = 0$, such that we have for K as in the definition of π_K below Eq. (17)*

$$\pm\widetilde{\mathcal{E}} \leq CN^{-\frac{1}{4}} \sum_k |k|^2 c_k^\dagger \left(\frac{\mathcal{N}}{\sqrt{N}} + 1\right)^2 c_k + CN^{-\frac{1}{4}} \left(\frac{\mathcal{N}}{\sqrt{N}} + 1\right)^2 \left(\mathcal{N} + \sqrt{N}\right) + \epsilon(K)\mathcal{N}.$$

Proof. In the following let $\tau \leq \frac{1}{2}$. Using the fact that $\| \frac{a_m^\dagger (a_0^\dagger)^{s-1} a_0^{t-1} a_n}{N^{\frac{s+t}{2}}} \| \leq 1$, there exists by Corollary 1 a constant $C > 0$ such that for $\delta > 0$ and $s, t \geq \ell + 1$

$$\begin{aligned} &\pm\left(\sum_{\substack{i_1\ldots i_{s-\ell}\\ j_1\ldots j_{t-\ell}}} \left(G_{\ell,\sigma,\tau}(\varphi_s^m, \varphi_t^n)\right)_{i_1\ldots i_{s-\ell}, j_1\ldots j_{t-\ell}} (\Phi_{\sigma,s})^\dagger_{i_1\ldots i_{s-\ell}} \frac{a_m^\dagger (a_0^\dagger)^{s-1} a_0^{t-1} a_n}{N^{\frac{s+t}{2}}} (\Phi_{\tau,t})_{j_1\ldots j_{t-\ell}} + \mathrm{H.c.}\right) \\ &\leq C\left\|\mathcal{K}_{\tau,s-\ell}^{-\frac{1}{2}} G_\ell(\varphi_s^m, \varphi_t^n) \mathcal{K}_{\tau,t-\ell}^{-\frac{1}{2}}\right\| \left(\sum_k |k|^2 c_k^\dagger \left(\delta\mathcal{N}^{s-\ell-1} + \delta^{-1}\mathcal{N}^{t-\ell-1}\right) c_k \right. \\ &\quad \left. + \left(\mathcal{N} + \sqrt{N}\right)\left(\delta\mathcal{N}^{s-\ell-1} + \delta^{-1}\mathcal{N}^{t-\ell-1}\right)\right). \end{aligned} \tag{113}$$

For $\tau = \sigma = 0$, we have the improved bound on the left-hand side of Eq. (113)

$$C\left\|G_\ell(\varphi_s^m, \varphi_t^n)\right\|\left(\delta\mathcal{N}^{s-\ell} + \delta^{-1}\mathcal{N}^{t-\ell}\right). \tag{114}$$

In the case that either s or t is equal to ℓ, for example, $t = \ell$ we obtain by Corollary 1

$$\begin{aligned} &\pm\left(\sum_{i_1\ldots i_{s-\ell}} \left(G_{\ell,\sigma,\tau}(\varphi_s^m, \varphi_t^n)\right)_{i_1\ldots i_{s-\ell}} (\Phi_{\sigma,s})^\dagger_{i_1\ldots i_{s-\ell}} \frac{a_m^\dagger (a_0^\dagger)^{s-1} a_0^{t-1} a_n}{N^{\frac{s+t}{2}}} + \mathrm{H.c.}\right) \\ &\quad \leq C\left\|\mathcal{K}_{\tau,s-\ell}^{-\frac{1}{2}} G_\ell(\varphi_s^m, \varphi_t^n)\right\|\left(\delta^{-1} + \delta\sum_k |k|^2 c_k^\dagger \mathcal{N}^{s-\ell-1} c_k + \delta\left(\mathcal{N} + \sqrt{N}\right)\mathcal{N}^{s-\ell-1}\right). \end{aligned} \tag{115}$$

In order to obtain good estimates on the operator norms $\left\|\mathcal{K}_{\sigma,s-\ell}^{-\frac{1}{2}} G_\ell(\varphi_s^m, \varphi_t^n) \mathcal{K}_{\tau,t-\ell}^{-\frac{1}{2}}\right\|$, observe that we obtain by a Cauchy-Schwarz argument

$$\left\|\mathcal{K}_{\sigma,s-\ell}^{-\frac{1}{2}} G_\ell(\varphi_s^m, \varphi_t^n) \mathcal{K}_{\tau,t-\ell}^{-\frac{1}{2}}\right\| \leq \sqrt{\left\|\mathcal{K}_{\sigma,s-\ell}^{-\frac{1}{2}} G_\ell(\varphi_s^m, \varphi_s^m) \mathcal{K}_{\sigma,s-\ell}^{-\frac{1}{2}}\right\| \left\|\mathcal{K}_{\tau,t-\ell}^{-\frac{1}{2}} G_\ell(\varphi_t^n, \varphi_t^n) \mathcal{K}_{\tau,t-\ell}^{-\frac{1}{2}}\right\|},$$

that is, it is enough to control the norm of the symmetric ones. In the following we choose $\sigma = \tau = \frac{1}{2}$, except for the case $s = t = 2$ where we choose $\sigma = \tau = 0$. By Eq. (107) and Eq. (109) we obtain for a suitable $C > 0$

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$$\left\|\mathcal{K}_{\frac{1}{2},3}^{-\frac{1}{2}} G_1(\varphi_4^0,\varphi_4^0)\mathcal{K}_{\frac{1}{2},3}^{-\frac{1}{2}}\right\| \leq CN^{-\frac{3}{2}}, \qquad \left\|\mathcal{K}_{\frac{1}{2},2}^{-\frac{1}{2}} G_1(\varphi_3^m,\varphi_3^m)\mathcal{K}_{\frac{1}{2},2}^{-\frac{1}{2}}\right\| \leq CN^{-1},$$
$$\left\|\mathcal{K}_{\frac{1}{2},2}^{-\frac{1}{2}} G_2(\varphi_4^0,\varphi_4^0)\mathcal{K}_{\frac{1}{2},2}^{-\frac{1}{2}}\right\| \leq CN^{-\frac{3}{2}}, \qquad \left\|\mathcal{K}_{\frac{1}{2},1}^{-\frac{1}{2}} G_2(\varphi_3^m,\varphi_3^m)\mathcal{K}_{\frac{1}{2},1}^{-\frac{1}{2}}\right\| \leq CN^{-\frac{1}{2}},$$
$$\left\|\mathcal{K}_{\frac{1}{2},1}^{-\frac{1}{2}} G_3(\varphi_4^0,\varphi_4^0)\mathcal{K}_{\frac{1}{2},1}^{-\frac{1}{2}}\right\| \leq CN^{-1}, \qquad \left\|G_3(\varphi_3^m,\varphi_3^m)\right\| \leq CN.$$

Furthermore by Eq. (108), $\|G_1(\varphi_2^0,\varphi_2^0)\| \leq \epsilon$ in case K is large enough and $\|G_2(\varphi_2^0,\varphi_2^0)\| \leq C\sqrt{N}$, as well as $\left\|\widetilde{G}\right\| \leq CN^{-1}$ by Eq. (109). Choosing $\delta := N^{\frac{t-s}{4}}$, and combining the estimates on the operator norms with Eq. (113), respectively Eq. (114), and Eq. (115) concludes the proof by Eq. (111). □

Following the ideas in the proof of Lemma 8, we can furthermore compare the operator $\sum_k |k|^{2\tau} a_k^\dagger a_k$ with the corresponding operator $\sum_k |k|^{2\tau} d_k^\dagger d_k$ in the variables d_k defined in Eq. (89). This is the content of the subsequent Lemma 9.

Lemma 9. *Let $0 \leq \tau < \frac{1}{4}$. Then there exists $K_0, C > 0$ such that for $K \geq K_0$, with K as in the definition of π_K below Eq. (17),*

$$\sum_k |k|^{2\tau} a_k^\dagger a_k \leq C\sum_k |k|^2 d_k^\dagger d_k + CN^{-\frac{3}{2}}\mathcal{N}^3 + CN^\tau.$$

Proof. By Eq. (40), there exists a constant $C > 0$ such that

$$\sum_k |k|^{2\tau} a_k^\dagger a_k \leq C\sum_k |k|^{2\tau} c_k^\dagger c_k + CN^{-1}\mathcal{N}^2 + CN^\tau.$$

Furthermore, we have by Cauchy-Schwarz the estimate

$$\sum_k |k|^{2\tau} c_k^\dagger c_k \leq 2\sum_k |k|^{2\tau} d_k^\dagger d_k + 2\sum_k |k|^{2\tau}(d_k - c_k)^\dagger(d_k - c_k).$$

Similar to the definition of G_ℓ in Eq. (110) let us introduce

$$G'_\ell := \mathrm{Tr}_{1\to\ell}\left[(-\Delta)_{x_1}\varphi_2^0(\varphi_2^0)^\dagger\right],$$
$$G''_\ell := \mathrm{Tr}_{1\to\ell}\left[(-\Delta)_{x_1}\varphi_4^0(\varphi_4^0)^\dagger\right].$$

A similar computation as in Eq. (111) together with a Cauchy-Schwarz estimate yields

$$\sum_k |k|^{2\tau}(d_k - c_k)^\dagger(d_k - c_k) \leq CG'_2\frac{(a_0^\dagger)^2 a_0^2}{N^2} + C\sum_{i,j}(G'_1)_{i,j} a_i^\dagger \frac{(a_0^\dagger)^2 a_0^2}{N^2} a_j$$
$$+ C\sum_{\ell=1}^4 \sum_{\substack{i_1\dots i_{4-\ell}\\ j_1\dots j_{4-\ell}}} \left(G''_\ell\right)_{i_1\dots i_{4-\ell}, j_1\dots j_{4-\ell}} a_{i_{4-\ell}}^\dagger \dots a_{i_1}^\dagger \frac{(a_0^\dagger)^4 a_0^4}{N^4} a_{j_1}\dots a_{j_{4-\ell}},$$

for a suitable constant $C > 0$. Utilizing the estimates in Eq. (108) and Eq. (109) we obtain that $|G'_2| \lesssim 1$, $\|G'_2\| \lesssim \frac{1}{K^2}$, $|G''_4| \lesssim N^{\tau-\frac{1}{2}} \leq 1$ and $\|G''_\ell\| \lesssim N^{\tau-2} \leq N^{-\frac{3}{2}}$ for $\ell \leq 3$. Consequently there exists a $C > 0$ such that

$$\sum_k |k|^{2\tau}(d_k - c_k)^\dagger(d_k - c_k) \leq C + \frac{C}{K^2}\mathcal{N} + CN^{-\frac{3}{2}}(\mathcal{N}+1)^3.$$

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Using $\mathcal{N} \leq \sum_k |k|^{2\tau} a_k^\dagger a_k$ and $\sum_k |k|^{2\tau} d_k^\dagger d_k \leq \sum_k |k|^2 d_k^\dagger d_k$ we therefore obtain

$$\sum_k |k|^{2\tau} a_k^\dagger a_k \leq \frac{C}{K^2} \sum_k |k|^{2\tau} a_k^\dagger a_k + C \sum_k |k|^2 d_k^\dagger d_k + CN^{-\frac{3}{2}} \mathcal{N}^3 + CN^\tau + CN^{-1}\mathcal{N}^2$$
$$\leq \frac{C}{K^2} \sum_k |k|^{2\tau} a_k^\dagger a_k + C \sum_k |k|^2 d_k^\dagger d_k + 2CN^{-\frac{3}{2}} \mathcal{N}^3 + 2CN^\tau.$$

Choosing K large enough such that $\frac{C}{K^2} < 1$ concludes the proof. □

Before we come to the proof of the lower bound in Theorem 1 in the following Subsection 4.2, we are going to derive sufficient estimates on

$$\sum_{ijk,\ell mn} (\Theta)_{ijk}\, \widetilde{\psi}^\dagger_{ijk}\, a_0^\dagger a_0^4 + \text{H.c.}$$

in the following Lemma 10. In order to verify Lemma 10, we require the estimate

$$\sum_k |k|^2 \tilde{c}_k^\dagger \tilde{c}_k \leq C\left(\sum_k |k|^2 c_k^\dagger c_k + \mathcal{N} + 1\right) \tag{116}$$

for $\tilde{c}_k := a_k + \frac{1}{2}\sum_{ij}(T-1)_{ijk,000} a_i^\dagger a_j^\dagger a_0^3$, which is verified in Appendix A, see Lemma A3.

Lemma 10. *Let* $0 \leq \gamma < \frac{1}{4}$. *Then there exists a* $C > 0$ *such that*

$$\pm\left(\sum_{ijk,\ell mn} (\Theta)_{ijk}\, \widetilde{\psi}^\dagger_{ijk}\, a_0^\dagger a_0^4 + \text{H.c.}\right) \leq N^{-\frac{1}{4}} \sum_k |k|^2 c_k^\dagger c_k + N^{-\frac{1}{4}}\mathcal{N} + CN^{\frac{1}{4}}.$$

Proof. Let us define for $ijk \neq 0$

$$\zeta_{ijk} := \frac{1}{24}\Big(\Pi_{\text{sym}} 4(\widetilde{V}_N \otimes 1)(T_4 - 1 + \chi)\Big)_{0ijk,0000} = \frac{1}{24}\Big(\Pi_{\text{sym}} 4(V_N \otimes 1)(T_4 - 1 + \chi)\Big)_{0ijk,0000}, \tag{117}$$
$$\zeta_k := \frac{1}{24}\Big(\Pi_{\text{sym}} 4(T^\dagger \widetilde{V}_N \otimes 1)(T_4 - 1 + \chi)\Big)_{00k(-k),0000},$$

where χ is defined in Eq. (91). Then we have the decomposition

$$\left(\sum_{ijk,\ell mn} (\Theta)_{ijk}\, \widetilde{\psi}^\dagger_{ijk}\, a_0^\dagger a_0^4 + \text{H.c.}\right)$$
$$= 4\left(\sum_{ijk\neq 0} \overline{\zeta_{ijk}} (a_0^\dagger)^4 a_0\, \widetilde{\psi}_{ijk} + \text{H.c.}\right) + 6\left(\sum_{k\neq 0} \overline{\zeta_k} (a_0^\dagger)^4 a_0^2\, a_k a_{-k} + \text{H.c.}\right). \tag{118}$$

Note that $\zeta_k = \frac{1}{24}\Big(\Pi_{\text{sym}} 4(V_N \otimes 1)(T_4 - 1 + \chi)\Big)_{00k(-k),0000}$ for $|k| > K$. Using the regularity of V and the bounds derived in Eq. (107) and Eq. (109), we observe that we have $|N^3 \zeta_k| \lesssim N^{-\frac{1}{2}}\left(1 + \frac{|k|^2}{N}\right)^{-1}$, and therefore

$$\pm\left(\sum_{k\neq 0} \overline{\zeta_k} (a_0^\dagger)^4 a_0^2 a_k a_{-k} + \text{H.c.}\right) \lesssim \epsilon \sum_{k\neq 0} |k|^{2\tau} a_k^\dagger a_k + \epsilon^{-1} N^{\frac{1}{2}-\tau} \lesssim \epsilon \sum_{k\neq 0} |k|^{2\tau} c_k^\dagger c_k + \epsilon\mathcal{N} + \epsilon N^\tau + \epsilon^{-1} N^{\frac{1}{2}-\tau},$$

where we have used Eq. (40). Choosing ϵ of the order $N^{-\frac{1}{4}}$ and $\tau = \frac{1}{2}$ concludes the analysis of the second term in Eq. (118). Regarding the first term, we use the definition of $\tilde{c}_k$ below Eq. (116), in order to identify $\sum_{ijk}\overline{\zeta_{ijk}}(a_0^\dagger)^4\widetilde{\psi}_{ijk}a_0$ as

$$\begin{aligned}
&\sum_{ijk}\overline{\zeta_{ijk}}(a_0^\dagger)^4 a_i a_j \tilde{c}_k a_0 - \sum_{ijk}\overline{\zeta_{ijk}}(a_0^\dagger)^4 a_i a_j(\tilde{c}_k - a_k)a_0 + \sum_{ijk}\zeta_{ijk}(a_0^\dagger)^4 a_0^4 (T-1)_{ijk,000}\\
&\quad = \sum_{ijk}\overline{\zeta_{ijk}}(a_0^\dagger)^4 a_i a_j \tilde{c}_k a_0 - \frac{1}{2}\sum_{ijk,i'j'}\overline{\zeta_{ijk}}(T-1)_{i'j'k,000}a_{i'}^\dagger a_{j'}^\dagger a_0^{4\dagger}a_0^4 a_i a_j\\
&\qquad - 2\sum_{ijk,i'}\overline{\zeta_{ijk}}(T-1)_{i'jk,000}a_{i'}^\dagger a_0^{4\dagger}a_0^4 a_i. \qquad (119)
\end{aligned}$$

In the following we are going to verify that the most significant term $\sum_{ijk}\overline{\zeta_{ijk}}(a_0^\dagger)^4 a_i a_j \tilde{c}_k a_0$ in Eq. (119) satisfies the desired bound. By Cauchy-Schwarz, we have for $\epsilon > 0$

$$\begin{aligned}
&\left(\sum_{ijk}\overline{\zeta_{ijk}}(a_0^\dagger)^4 a_i a_j \tilde{c}_k a_0 + \text{H.c.}\right) \leq \epsilon\sum_k |k|^2 \tilde{c}_k^\dagger \tilde{c}_k + \epsilon^{-1}\sum_k \frac{1}{|k|^2}\left|\sum_{ij}\zeta_{ijk}a_0^\dagger a_0^4 a_i^\dagger a_j^\dagger\right|^2\\
&\quad = \epsilon\sum_k |k|^2\tilde{c}_k^\dagger\tilde{c}_k + \epsilon^{-1}G^{(0)}X + \epsilon^{-1}\sum_{i,i'}(G^{(1)})_{i,i'}a_i^\dagger a_{i'}X + \epsilon^{-1}\sum_{ij,i'j'}(G^{(2)})_{ij,i'j'}a_i^\dagger a_j^\dagger X a_{j'}a_{i'}
\end{aligned}$$

with $G^{(0)} := N^5\sum_{ijk}\frac{|\zeta_{ijk}|^2}{|k|^2}$, $G^{(1)}_{i,i'} := N^5\delta_{i,i'}\sum_{jk}\frac{|\zeta_{ijk}|^2+\overline{\zeta_{ijk}}\zeta_{jik}}{|k|^2}$ and $G^{(2)}_{ij,i'j'} := N^5\sum_k\frac{\zeta_{ijk}\zeta_{i'j'k}}{|k|^2}$, and $X := N^{-5}a_0^{4\dagger}a_0 a_0^\dagger a_0^4$. Using again the regularity of V and Eq. (107), as well as the bounds on T_4 in Eq. (109), yields

$$|\zeta_{ijk}| \leq CN^{-\frac{7}{2}}\delta_{i+j+k=0}\left(1+\frac{|i|^2+|j|^2+|k|^2}{N}\right)^{-3},$$

and therefore $|G^{(0)}| \lesssim 1$ and $\|G^{(1)}\| \lesssim N^{-\frac{3}{2}}$. The choice $\epsilon := N-\frac{1}{4}$ then yields

$$\epsilon^{-1}G^{(0)}X + \epsilon^{-1}\sum_{i,i'}G^{(1)}_{i,i'}a_i^\dagger a_{i'}X \lesssim N^{\frac{1}{4}} + N^{-\frac{5}{4}}\mathcal{N}.$$

Finally $\|G^{(2)}\| \leq N^{-\frac{3}{2}}$, and therefore

$$\sum_{ij,i'j'}G^{(2)}_{ij,i'j'}a_i^\dagger a_j^\dagger X a_{j'}a_{i'} \lesssim N^{-\frac{3}{2}}\mathcal{N}^2 \leq N^{-\frac{1}{2}}\mathcal{N}.$$

This concludes the proof together with Eq. (116). □

4.2. *Proof of the lower bound in Theorem 1*

In this subsection, we are going to verify the lower bound in Theorem 1 making use of the sequence of states Φ_N constructed in Corollary 2, which simultaneously satisfies

$$\begin{aligned}
&\mathbb{1}\left(\mathcal{N} \leq C\sqrt{N}\right)\Phi_N = \Phi_N,\\
&\langle\Phi_N, H_N\Phi_N\rangle \leq E_N + C,\\
&\left\langle\Phi_N, \sum_k |k|^2 c_k^\dagger c_k\Phi_N\right\rangle \leq C\sqrt{N}.
\end{aligned}$$

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Starting point for our investigations is then the lower bound

$$H_N \geq \sum_k |k|^2 d_k^\dagger d_k + (a_0^\dagger)^3 a_0^3 \lambda_{0,0} + N^{-4}(a_0^\dagger)^4 a_0^4 (\gamma_N - \sigma_N) - N^{-2}(a_0^\dagger)^2 a_0^2 \mu_N + \mathbb{Q}_K$$
$$- \left(\sum_{ijk,\ell mn} (\Theta)_{ijk} \widetilde{\psi}^\dagger_{ijk} a_0^\dagger a_0^4 + \text{H.c.} \right) + \left(\mathcal{E}_* + \mathcal{E}_*^\dagger \right) - \widetilde{\mathcal{E}},$$

see Eq. (105). As is proven in Section 7, the coefficients γ_N, μ_N and σ_N converge to the corresponding constants $\gamma(V)$, $\mu(V)$ and $\sigma(V)$ introduced in Eq. (10), Eq. (5) and Eq. (9)

$$\gamma_N = \gamma(V)\sqrt{N} + O_{N\to\infty}\left(N^{-\frac{1}{4}}\right), \tag{120}$$
$$\mu_N = \mu(V)\sqrt{N} + O_{N\to\infty}(1), \tag{121}$$
$$\sigma_N = \sigma(V)\sqrt{N} + O_{N\to\infty}\left(N^{\frac{1}{4}}\right), \tag{122}$$

see Lemma 17. Given $\epsilon > 0$, assume that K is large enough such that the function $\epsilon(K)$ from Lemma 8 satisfies $\epsilon(K) \leq \epsilon$. Making use of the fact that

$$\mathbb{1}\left(\mathcal{N} \leq C\sqrt{N}\right)\Phi_N = \Phi_N,$$
$$\left\langle \Phi_N, \sum_k |k|^2 c_k^\dagger c_k \Phi_N \right\rangle \lesssim \sqrt{N},$$

we immediately obtain for C and $\widetilde{C}$ large enough

$$|\langle \Phi_N, \widetilde{\mathcal{E}}\Phi_N\rangle| \leq CN^{-\frac{1}{4}}\left\langle \Phi_N, \sum_k |k|^2 c_k^\dagger c_k \Phi_N \right\rangle + \epsilon\langle \Phi_N, \mathcal{N}\Phi_N\rangle + CN^{\frac{1}{4}} \leq \widetilde{C}N^{\frac{1}{4}} + \epsilon\langle \Phi_N, \mathcal{N}\Phi_N\rangle.$$

Similarly we obtain by Lemma 10 and Lemma 4 for suitable $C, \widetilde{C} > 0$

$$\left| \langle \Phi_N, \left(\sum_{ijk,\ell mn} (\Theta)_{ijk} \widetilde{\psi}^\dagger_{ijk} a_0^\dagger a_0^4 + \text{H.c.} \right) \Phi_N \rangle \right|$$
$$\leq CN^{-\frac{1}{4}}\left(\left\langle \Phi_N, \sum_k |k|^2 c_k^\dagger c_k \Phi_N \right\rangle + \sqrt{N} \right) + CN^{\frac{1}{4}} \leq \widetilde{C}N^{\frac{1}{4}},$$
$$\left| \langle \Phi_N, \left(\mathcal{E}_* + \mathcal{E}_*^\dagger \right) \Phi_N \rangle \right| \leq CN^{\frac{1}{4}}.$$

By Lemma 2 we furthermore obtain for $\tau, \epsilon > 0$ and K large enough, and a suitable $C > 0$,

$$\langle \Phi_N, \left((a_0^\dagger)^3 a_0^3 \lambda_{0,0} + \mathbb{Q}_K \right) \Phi_N \rangle \geq \frac{1}{6} b_{\mathcal{M}}(V) N - \epsilon \left\langle \Phi_N, \sum_k |k|^{2\tau} a_k^\dagger a_k \Phi_N \right\rangle - C.$$

Moreover we note that we have by Eq. (120)-(122)

$$\langle \Phi_N, N^{-4}(a_0^\dagger)^4 a_0^4 (\sigma_N - \gamma_N)\Phi_N\rangle \leq (\sigma_N - \gamma_N) + |\sigma_N - \gamma_N| \langle \Phi_N, \left(1 - N^{-4}(a_0^\dagger)^4 a_0^4\right)\Phi_N\rangle$$
$$\leq \sigma_N - \gamma_N + |\sigma_N - \gamma_N| \left\langle \Phi_N, \frac{\mathcal{N}}{N}\Phi_N \right\rangle \leq (\sigma(V) - \gamma(V))\sqrt{N} + o_{N\to\infty}\left(N^{\frac{1}{4}}\right),$$

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and similarly $\langle \Phi_N, N^{-2}(a_0^\dagger)^2 a_0^2 \mu_N \Phi_N \rangle \leq \mu(V)\sqrt{N} + o_{N\to\infty}(1)$. Finally by Lemma 9

$$\langle \Phi_N, \mathcal{N}\Phi_N \rangle \leq \left\langle \Phi_N, \sum_k |k|^{2\tau} a_k^\dagger a_k \Phi_N \right\rangle \leq C\left\langle \Phi_N, \sum_k |k|^2 d_k^\dagger d_k \Phi_N \right\rangle + CN^\tau. \tag{123}$$

Choosing $\tau < \frac{1}{4}$ and $\epsilon < \frac{1}{2C}$ concludes the proof, since

$$\begin{aligned} E_N + C \geq \langle \Phi_N, H_N \Phi_N \rangle \geq \frac{1}{6} b_{\mathcal{M}}(V) N + (\gamma - \sigma - \mu)\sqrt{N} \\ - CN^{\frac{1}{4}} + (1 - 2C\epsilon)\left\langle \Phi_N, \sum_k |k|^2 d_k^\dagger d_k \Phi_N \right\rangle. \end{aligned}$$

5. Second-order upper bound

It is the goal of this Section to introduce a trial state Φ, which simultaneously annihilates the variables d_k for $k \neq 0$ and $\xi_{\ell mn}$ in case $(\ell, m, m) \neq 0$, at least in an approximate sense. We are then going to use this trial state Φ to verify the upper bound in Theorem 1. For the rest of this Section we specify the parameter K introduced above the definition of π_K in Eq. (17) as $K := 0$. In order to find Φ, we define $\alpha_{jk} := (T_2 - 1)_{jk,00}$ and $\beta_{uijk} := (T_4 - 1)_{uijk,0000}$, and the generator

$$\begin{aligned} \mathcal{G}_2 &:= \frac{1}{2} \sum_{jk} \alpha_{jk} a_j^\dagger a_k^\dagger a_0^2, \\ \mathcal{G}_4 &:= \frac{1}{24} \sum_{uijk} \beta_{uijk} a_u^\dagger a_i^\dagger a_j^\dagger a_k^\dagger a_0^4 \end{aligned} \tag{124}$$

of a unitary group $W_s := e^{s(\mathcal{G}_2+\mathcal{G}_4)^\dagger - s(\mathcal{G}_2+\mathcal{G}_4)}$ and $W := W_1$. We note at this point, that the action of the unitary operator W only creates an $O(1)$ amount of particles, in the sense that

$$W_{-s}\mathcal{N}^m W_s \leq e^{C_m|s|}(\mathcal{N}+1)^m, \tag{125}$$

as is proven in Appendix A, see Lemma A1. Applying Duhamel's formula, we can express $W^{-1} a_{i_1} a_{i_2} a_{i_3} W$ as

$$W^{-1} a_{i_1} a_{i_2} a_{i_3} W = a_{i_1} a_{i_2} a_{i_3} - \int_0^1 W_{-s}[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}_4] W_s \mathrm{d}s + \int_0^1 W_{-s}[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2] W_s \mathrm{d}s. \tag{126}$$

Furthermore, note that we can write

$$[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}_4] = \sum_u \beta_{u i_1 i_2 i_3} a_u^\dagger a_0^4 + (\delta\xi)_{i_1 i_2 i_3}, \tag{127}$$

where we define the error term

$$(\delta\xi)_{i_1 i_2 i_3} := \frac{1}{4} \sum_{\sigma\in S_3} \sum_{jk} \beta_{i_{\sigma_2} i_{\sigma_3} jk} a_j^\dagger a_k^\dagger a_{i_{\sigma_1}} a_0^4 + \frac{1}{12} \sum_{\sigma\in S_3} \sum_{ijk} \beta_{i_{\sigma_3} ijk} a_i^\dagger a_j^\dagger a_k^\dagger a_{i_{\sigma_1}} a_{i_{\sigma_2}} a_0^4.$$

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Therefore we can write the transformed operators $W^{-1}\xi_{i_1i_2i_3}W$ as

$$W^{-1}\xi_{i_1i_2i_3}W = (\psi + \delta_1\psi)_{i_1i_2i_3} - \int_0^1 W_s^{-1}(\delta\xi)_{i_1i_2i_3}W_s\,\mathrm{d}s + \int_0^1 W_{-s}[a_ia_ja_k, \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2]W_s\mathrm{d}s$$
$$+ \int_0^1\int_0^s W_t^{-1}\left[\sum_u \beta_{ui_1i_2i_3}a_u^\dagger a_0^4,\ \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2 - \mathcal{G}_4\right]W_t\,\mathrm{d}t\mathrm{d}s$$
$$+ \int_0^1 W_{-s}[\xi_{i_1i_2i_3} - a_{i_1}a_{i_2}a_{i_3},\ \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2 - \mathcal{G}_4]W_s\,\mathrm{d}s. \tag{128}$$

Recall the definition of $\mathcal{E}_\mathcal{P}$ defined in Eq. (75). The following Lemma 11 provides sufficient bounds on the various error terms appearing in Eq. (128).

Lemma 11. *There exists a constant* $C > 0$*, such that*

$$\mathcal{E}_\mathcal{P}(\delta\xi) \le C(\mathcal{N}+1)^6. \tag{129}$$

Furthermore, we have $\mathcal{E}_\mathcal{P}\Big([a_{i_1}a_{i_2}a_{i_3}, \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2]\Big) \le C(\mathcal{N}+1)^6$ *and*

$$\mathcal{E}_\mathcal{P}\Big([\xi_{i_1i_2i_3} - a_{i_1}a_{i_2}a_{i_3},\ \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2 - \mathcal{G}_4]\Big) \le C(\mathcal{N}+1)^6, \tag{130}$$

$$\mathcal{E}_\mathcal{P}\left(\left[\sum_u \beta_{ui_1i_2i_3}a_u^\dagger a_0^4,\ \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2 - \mathcal{G}_4\right]\right) \le C(\mathcal{N}+1)^6. \tag{131}$$

Proof. Let us define

$$(\delta_1\xi)_{i_1i_2i_3} := \frac{1}{4}\sum_{jk}\beta_{i_2i_3jk}a_j^\dagger a_k^\dagger a_{i_1}a_0^4,$$
$$C_N := \sup_{i_1}\sum_{jk,i_2i_3,i_1'i_2'i_3'}\left|(V_N)_{i_1i_2i_3,i_1'i_2'i_3'}\beta_{i_2i_3jk}\beta_{i_2'i_3'jk}\right| \lesssim N^{-5},$$

where we have used Eq. (109) to estimate C_N. Applying Cauchy-Schwarz yields

$$\sum_{(i_1i_2i_3),(i_1'i_2'i_3')\in A}(V_N)_{i_1i_2i_3,i_1'i_2'i_3'}(\delta_1\xi)^\dagger_{i_1i_2i_3}(\delta_1\xi)_{i_1'i_2'i_3'} \le C_N(a_0^\dagger)^4a_0^4\left(\sum_{i_1}a_{i_1}^\dagger a_{i_1}\right)(\mathcal{N}+1)^2. \tag{132}$$

Using the fact that $C_N(a_0^\dagger)^4a_0^4\Big(\sum_{i_1}a_{i_1}^\dagger a_{i_1}\Big) \le C_NN^5 \lesssim 1$, we observe that the quantity in Eq. (132) is bounded by the right-hand side of Eq. (129). Let us furthermore define

$$(\delta_2\xi)_{i_1i_2i_3} := \frac{1}{12}\sum_{ijk}\beta_{i_3ijk}a_i^\dagger a_j^\dagger a_k^\dagger a_{i_1}a_{i_2}a_0^4.$$

In the following we want to distinguish between the cases $A' := \{(i_1i_2i_3) \in A : i_1, i_2 \neq 0\}$ and $A'' := A \setminus A'$, leading to the definition

$$C_N' := \sup_{i_1i_2}\sum_{ijk,i_3,i_1'i_2'i_3'}\mathbb{1}\big((i_1,i_2,i_3),(i_1'i_2'i_3') \in A'\big)\left|(V_N)_{i_1i_2i_3,i_1'i_2'i_3'}\beta_{i_3ijk}\beta_{i_3'ijk}\right| \lesssim N^{-5},$$
$$C_N'' := \sup_{i_1i_2}\sum_{ijk,i_3,i_1'i_2'i_3'}\mathbb{1}\big((i_1,i_2,i_3),(i_1'i_2'i_3') \in A''\big)\left|(V_N)_{i_1i_2i_3,i_1'i_2'i_3'}\beta_{i_3ijk}\beta_{i_3'ijk}\right| \lesssim N^{-\frac{13}{2}},$$

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where we have again used Eq. (109). Applying Cauchy-Schwarz leads to the estimate

$$\sum_{(i_1 i_2 i_3),(i_1' i_2' i_3')\in A} (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} (\delta_2 \xi)^\dagger_{i_1 i_2 i_3} (\delta_2 \xi)_{i_1' i_2' i_3'} \leq C_N' N^4 (\mathcal{N}+1)^5 + C_N'' N^6 (\mathcal{N}+1)^3,$$

which is bounded by the right-hand side of Eq. (129). Finally we use that V_N is permutation-symmetric and non-negative, and therefore the left-hand side of Eq. (129) is bounded by

$$6 \sum_{(i_1 i_2 i_3),(i_1' i_2' i_3')\in A} (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} (\delta_1 \xi + \delta_2 \xi)^\dagger_{i_1 i_2 i_3} (\delta_1 \xi + \delta_2 \xi)_{i_1' i_2' i_3'}$$
$$\leq 12 \sum_{(i_1 i_2 i_3),(i_1' i_2' i_3')\in A} (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} (\delta_1 \xi)^\dagger_{i_1 i_2 i_3} (\delta_1 \xi)_{i_1' i_2' i_3'} + 12 \sum_{(i_1 i_2 i_3),(i_1' i_2' i_3')\in A} (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} (\delta_2 \xi)^\dagger_{i_1 i_2 i_3} (\delta_2 \xi)_{i_1' i_2' i_3'}.$$

Regarding the term $\mathcal{E}_\mathcal{P}\left([a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2]\right)$, let us analyze the term involving the commutator with $\mathcal{G}_2$, the terms involving $\mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger$ can be analyzed in a similar fashion as has been done in Lemma 6. We compute

$$[a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}_2] = \alpha_{i_2 i_3} a_{i_1} a_0^2 + \sum_u \alpha_{u i_3} a_u^\dagger a_{i_2} a_{i_3} + \{\text{Permutations}\}. \tag{133}$$

In order to analyze the first term on the right-hand side of Eq. (133), let us define $D_N := \sup_{i_1} \sum_{i_2 i_3, i_1' i_2' i_3'} \left| (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} \alpha_{i_2 i_3} \alpha_{i_2' i_3'} \right|$ and note that $D_N \lesssim N^{-3}$ by Eq. (108). Hence

$$\sum_{(i_1 i_2 i_3),(i_1' i_2' i_3')\in A} (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} \left(\alpha_{i_2 i_3} a_{i_1} a_0^2\right)^\dagger \alpha_{i_2' i_3'} a_{i_1'} a_0^2 \leq D_N N^3 \lesssim 1.$$

Regarding the second term on the right-hand side of Eq. (133), we use again the split $A = A' \cup A''$ and define

$$D_N' := \sup_{i_1 i_2} \sum_{u, i_3, i_1' i_2' i_3'} \mathbb{1}\left((i_1, i_2, i_3), (i_1' i_2' i_3') \in A'\right) \left| (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} \alpha_{u i_3} \alpha_{u i_3'} \right| \lesssim N^{-\frac{5}{2}},$$
$$D_N' := \sup_{i_1 i_2} \sum_{u, i_3, i_1' i_2' i_3'} \mathbb{1}\left((i_1, i_2, i_3), (i_1' i_2' i_3') \in A''\right) \left| (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} \alpha_{u i_3} \alpha_{u i_3'} \right| \lesssim N^{-4},$$

where we have used Eq. (108). Consequently

$$\sum_{(i_1 i_2 i_3),(i_1' i_2' i_3')\in A} (V_N)_{i_1 i_2 i_3, i_1' i_2' i_3'} \left(\sum_u \alpha_{u i_3} a_u^\dagger a_{i_2} a_{i_3}\right)^\dagger \left(\sum_u \alpha_{u i_3} a_u^\dagger a_{i_2} a_{i_3}\right) \lesssim N^{-\frac{1}{2}} (\mathcal{N}+1)^3 + 1,$$

and therefore $\mathcal{E}_\mathcal{P}\left([a_{i_1} a_{i_2} a_{i_3}, \mathcal{G}_2]\right) \leq 12 \mathcal{E}_\mathcal{P}\left(\alpha_{i_2 i_3} a_{i_1} a_0^2\right) + 12 \mathcal{E}_\mathcal{P}\left(\sum_u \alpha_{u i_3} a_u^\dagger a_{i_2} a_{i_3}\right) \lesssim (\mathcal{N}+1)^3$. The inequalities in Eq. (130) and Eq. (131) can be verified similarly. □

With Lemma 11 at hand, we show in the subsequent Corollary 6 that after conjugation with the unitary W, the potential energy of the operators ξ_{ijk} is comparable to the potential energy of $(\psi + \delta_1)_{ijk}$.

Corollary 6. *There exists a constant $C > 0$, such that*

$$W^{-1} \mathcal{E}_\mathcal{P}(\xi) W \leq C\, \mathcal{E}_\mathcal{P}(\psi + \delta_1 \psi) + C\, (\mathcal{N}+1)^6.$$

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Proof. Using the sign $V_N \geq 0$, we obtain by the Cauchy-Schwarz inequality and the representation of $W^{-1}\xi_{i_1i_2i_3}W$ in Eq. (128) the estimate

$$\begin{aligned}
W^{-1}\mathcal{E}_{\mathcal{P}}(\xi)W &= \mathcal{E}_{\mathcal{P}}\left(W^{-1}\xi W\right) \leq 5\mathcal{E}_{\mathcal{P}}(\psi+\delta_1) + 5\int_0^1 W_s^{-1}\mathcal{E}_{\mathcal{P}}(\delta\xi)W_s\mathrm{d}s \\
&+ 5\int_0^1 W_{-s}\mathcal{E}_{\mathcal{P}}\left([a_ia_ja_k, \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2]\right)\mathrm{d}sW_s \\
&+ \frac{5}{2}\int_0^1\int_0^s W_t^{-1}\mathcal{E}_{\mathcal{P}}\left(\left[\sum_u \beta_{ui_1i_2i_3}a_u^\dagger a_0^4,\ \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2 - \mathcal{G}_4\right]\right)W_t\mathrm{d}t\mathrm{d}s \\
&+ 5\int_0^1 W_{-s}\mathcal{E}_{\mathcal{P}}\left([\xi_{i_1i_2i_3} - a_{i_1}a_{i_2}a_{i_3},\ \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger - \mathcal{G}_2 - \mathcal{G}_4]\right)W_s\mathrm{d}s \\
&\lesssim \mathcal{E}_{\mathcal{P}}(\psi+\delta_1) + \int_0^1 W_{-s}(\mathcal{N}+1)^6W_s\,\mathrm{d}s + \int_0^1\int_0^s W_{-t}(\mathcal{N}+1)^6W_t\,\mathrm{d}t\mathrm{d}s \lesssim \mathcal{E}_{\mathcal{P}}(\psi+\delta_1) + (\mathcal{N}+1)^6,
\end{aligned}$$

where we have first used Lemma 11 and subsequently Eq. (125) in the last line. □

Regarding the variable d_k, Duhamel's formula yields for $k \neq 0$

$$W^{-1}d_kW = c_k + \int_0^1\int_0^s W_{-t}\left[[a_k, G_2+G_4], \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger\right]W_t\mathrm{d}t\mathrm{d}s + \int_0^1 W_{-s}\left[d_k - a_k, G_2^\dagger + G_4^\dagger\right]W_s\mathrm{d}s. \tag{134}$$

Recall the kinetic energy of an operator-valued one-particle vector Θ_k defined in Eq. (83). Then the following Lemma 12 provides sufficient bounds on the various error terms appearing in Eq. (134).

Lemma 12. *There exists a constant $C > 0$, such that for $m \in \mathbb{N}$*

$$\begin{aligned}
\mathcal{E}_{\mathcal{K}}\left(\mathcal{N}^m\left[d_k - a_k, G_2^\dagger + G_4^\dagger\right]\right) &\leq \frac{C}{N}(\mathcal{N}+1)^{5+2m}, \\
\mathcal{E}_{\mathcal{K}}\left(\mathcal{N}^m\left[[a_k, G_2+G_4], \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger\right]\right) &\leq \frac{C}{N}(\mathcal{N}+1)^{5+2m}.
\end{aligned}$$

Proof. Let us compute as an example for $k \neq 0$

$$\begin{aligned}
\left[[a_k, G_4], \mathcal{G}_4^\dagger\right] &= \frac{1}{24}\sum_{i_1i_2i_3}\beta_{ki_1i_2i_3}\left[a_{i_1}^\dagger a_{i_2}^\dagger a_{i_3}^\dagger a_0^4, \mathcal{G}_4^\dagger\right] \\
&= \frac{1}{24}\sum_{i_1i_2i_3}\beta_{ki_1i_2i_3}a_{i_1}^\dagger a_{i_2}^\dagger\left[a_{i_3}^\dagger, \mathcal{G}_4^\dagger\right]a_0^4 + \frac{1}{24}\sum_{i_1i_2i_3}\beta_{ki_1i_2i_3}a_{i_1}^\dagger\left[a_{i_2}^\dagger, \mathcal{G}_4^\dagger\right]a_{i_3}^\dagger a_0^4 \\
&\quad + \frac{1}{24}\sum_{i_1i_2i_3}\beta_{ki_1i_2i_3}\left[a_{i_1}^\dagger, \mathcal{G}_4^\dagger\right]a_{i_2}^\dagger a_{i_3}^\dagger a_0^4 + \frac{1}{24}\sum_{i_1i_2i_3}\beta_{ki_1i_2i_3}a_{i_1}^\dagger a_{i_2}^\dagger a_{i_3}^\dagger\left[a_0^4, \mathcal{G}_4^\dagger\right],
\end{aligned}$$

and let us focus on the term

$$\sum_{i_1i_2i_3}\beta_{ki_1i_2i_3}a_{i_1}^\dagger a_{i_2}^\dagger\left[a_{i_3}^\dagger, \mathcal{G}_4^\dagger\right]a_0^4 = \frac{1}{6}\sum_{i_1i_2i_3,j_1j_2j_3}\beta_{ki_1i_2i_3}\overline{\beta_{i_3j_1j_2j_3}}(a_0^\dagger)^4a_0^4a_{i_1}^\dagger a_{i_2}^\dagger a_{j_1}a_{j_2}a_{j_3}.$$

Defining

$$C_N := \sum_{k,i_1i_2,j_1j_2j_3}|k|^2\left|\sum_{i_3}\beta_{ki_1i_2i_3}\overline{\beta_{i_3j_1j_2j_3}}\right|^2 \lesssim N^{-\frac{19}{2}},$$

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where we have used Eq. (109), we obtain

$$\mathcal{E}_{\mathcal{K}}\Bigg(\sum_{i_1 i_2 i_3} \beta_{k i_1 i_2 i_3} \mathcal{N}^m a_{i_1}^\dagger a_{i_2}^\dagger \Big[a_{i_3}^\dagger, \mathcal{G}_4^\dagger\Big] a_0^4\Bigg) \lesssim N^{-\frac{19}{2}} \Big((a_0^\dagger)^4 a_0^4\Big)^2 (\mathcal{N}+1)^{5+2m} \leq N^{-\frac{3}{2}} (\mathcal{N}+1)^{5+2m}.$$

The other estimates in Lemma 12 can be verified similarly. □

Similar to Corollary 6, we show in the following Corollary 7 that, after conjugation with the unitary W, the kinetic energy of the operators d_k is comparable to the one of c_k.

Corollary 7. *There exists a constant $C > 0$, such that for $m \in \mathbb{N}$*

$$W^{-1}\mathcal{E}_K(\mathcal{N}^m d)W \leq C\mathcal{E}_K(c) + C\mathcal{E}_K(\mathcal{N}^m c) + \frac{C}{N}(\mathcal{N}+1)^{5+2m}.$$

Proof. By Eq. (125) we have $(W^{-1}\mathcal{N}^m W)^* W^{-1}\mathcal{N}^m W = W^{-1}\mathcal{N}^{2m} W \lesssim \mathcal{N}^{2m} + 1$, hence

$$W^{-1}\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m d)W = \mathcal{E}_{\mathcal{K}}\Big(W^{-1}\mathcal{N}^m W\, W^{-1} d\, W\Big) \lesssim \mathcal{E}_{\mathcal{K}}\Big(W^{-1} d\, W\Big) + \mathcal{E}_{\mathcal{K}}\Big(\mathcal{N}^m W^{-1} d\, W\Big).$$

Following the ideas in Corollary 6, we estimate using Eq. (134)

$$\begin{aligned}
\mathcal{E}_{\mathcal{K}}\Big(\mathcal{N}^m W^{-1} d\, W\Big) &\leq 3\,\mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c) \\
&\quad + \frac{3}{2}\int_0^1 \int_0^s W_{-t}\mathcal{E}_{\mathcal{K}}\Big(\mathcal{N}^m\Big[[a_k, G_2 + G_4], \mathcal{G}_2^\dagger + \mathcal{G}_4^\dagger\Big]\Big) W_t \mathrm{d}s \\
&\quad + 3\int_0^1 W_{-s}\mathcal{E}_{\mathcal{K}}\Big(\mathcal{N}^m\Big[d_k - a_k, G_2^\dagger + G_4^\dagger\Big]\Big) W_s \mathrm{d}s \\
&\lesssim \mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c) + \frac{1}{N}\int_0^1 \int_0^s W_{-t}(\mathcal{N}+1)^{5+2m} W_t \mathrm{d}s + \frac{1}{N}\int_0^1 W_{-s}(\mathcal{N}+1)^5 W_s \mathrm{d}s \\
&\lesssim \mathcal{E}_{\mathcal{K}}(\mathcal{N}^m c) + \frac{1}{N}(\mathcal{N}+1)^{5+2m},
\end{aligned}$$

where we have first used Lemma 12 and subsequently Eq. (125) in the last line. □

Before we come to the proof of the upper bound in Theorem 1, we are showing in the following Lemma 13 that even without a unitary conjugation, the kinetic energy of c_k is comparable with the one of d_k. The price for dropping the unitary W is that we obtain an order $O_{N\to\infty}\big(\sqrt{N}\big)$ prefactor in front of the excess term $(\mathcal{N}+3)^{3+2m}$, instead of a prefactor of the order $O_{N\to\infty}(1)$.

Lemma 13. *There exists a constant $C > 0$, such that for $m \in \mathbb{N}$*

$$\mathcal{E}_K(\mathcal{N}^m c) \leq C\mathcal{E}_K(\mathcal{N}^m d) + C\sqrt{N}(\mathcal{N}+1)^{3+2m}.$$

Proof. Note that we can write c_k as

$$c_k = d_k - 2\sum_j \alpha_{jk}\alpha_{jk} a_j^\dagger a_0^2 - 4\sum_{uij} \beta_{uijk} a_u^\dagger a_i^\dagger a_j^\dagger a_0^4,$$

and therefore

$$\mathcal{E}_K(\mathcal{N}^m c) \leq 3\,\mathcal{E}_K(\mathcal{N}^m d) + 12\,\mathcal{E}_K\Bigg(\sum_j \alpha_{jk}\,\mathcal{N}^m a_j^\dagger a_0^2\Bigg) + 48\,\mathcal{E}_K\Bigg(\sum_{uij} \beta_{uijk}\,\mathcal{N}^m a_u^\dagger a_i^\dagger a_j^\dagger a_0^4\Bigg).$$

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Defining the constant $C_N := \sum_{jk} |k|^2|\alpha_{jk}|^2 \lesssim N^{-\frac{3}{2}}$, which follows from Eq. (108), we obtain

$$\mathcal{E}_K\left(\sum_j \alpha_{jk}\mathcal{N}^m a_j^\dagger a_0^2\right) \leq C_N (a_0^\dagger)^2 a_0^2 (\mathcal{N}+1)^{m+1} \lesssim \sqrt{N}(\mathcal{N}+1)^{m+1}.$$

Similarly we obtain

$$\mathcal{E}_K\left(\sum_{uij} \beta_{uijk}\mathcal{N}^m a_u^\dagger a_i^\dagger a_j^\dagger a_0^4\right) \lesssim \sqrt{N}(\mathcal{N}+3)^3 \lesssim \sqrt{N}(\mathcal{N}+1)^3. \qquad \square$$

Proof of the upper bound in Theorem 1. Let us define the trial state $\Phi := W\Gamma$, where Γ is the state defined below Eq. (71), and recall the representation of H_N in Eq. (106)

$$\begin{aligned}\langle \Phi, H_N \Phi\rangle &= \lambda_{0,0}N^3\langle \Phi, N^{-3}(a_0^\dagger)^3 a_0^3\Phi\rangle + (\gamma_N - \sigma_N)\langle \Phi, N^{-4}(a_0^\dagger)^4 a_0^4\Phi\rangle - \mu_N\langle \Phi, N^{-2}(a_0^\dagger)^2 a_0^2\Phi\rangle \\ &\quad + \langle \Phi, \mathcal{E}_{\mathcal{K}}(d)\Phi\rangle + \langle \Phi, \mathcal{E}_{\mathcal{P}}(\xi)\Phi\rangle + 2\mathfrak{Re}\langle \Phi, \mathcal{E}_*\Phi\rangle - \left\langle \Phi, \widetilde{\mathcal{E}}\Phi\right\rangle \\ &\quad - \left\langle \Phi, \left(\sum_{ijk,\ell mn} (\Theta)_{ijk}\, \widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4 + \text{H.c.}\right)\Phi\right\rangle.\end{aligned}$$

By Eq. (125) and the fact that $\pm\left(N^{-m}(a_0^\dagger)^m a_0^m - 1\right) \lesssim N^{-1}\mathcal{N}$, we obtain that

$$\left|\langle \Phi, N^{-3}(a_0^\dagger)^3 a_0^3\Phi\rangle - 1\right| \lesssim N^{-1}\langle \Phi, \mathcal{N}\Phi\rangle = N^{-1}\langle \Gamma, W^{-1}\mathcal{N}W\Gamma\rangle \lesssim N^{-1}\langle \Gamma, (\mathcal{N}+1)\Gamma\rangle \lesssim N^{-1},$$

see Eq. (84) for the last estimate. Making use of Lemma 8, Lemma 4 and Lemma 10 yields

$$\begin{aligned}&|\langle \Phi, \mathcal{E}_*\Phi\rangle| \lesssim N^{-\frac{1}{4}}\langle \Phi, \mathcal{E}_{\mathcal{K}}(c)\Phi\rangle + N^{\frac{1}{4}}\langle \Phi, \mathcal{N}\Phi\rangle, \\ &\left|\left\langle \Phi, \left(\sum_{ijk,\ell mn} (\Theta)_{ijk}\, \widetilde{\psi}_{ijk}^\dagger\, a_0^\dagger a_0^4 + \text{H.c.}\right)\Phi\right\rangle\right| \lesssim N^{-\frac{1}{4}}\langle \Phi, \mathcal{E}_{\mathcal{K}}(c)\Phi\rangle + N^{-\frac{1}{4}}\langle \Phi, \mathcal{N}\Phi\rangle + N^{\frac{1}{4}}, \\ &\left|\left\langle \Phi, \widetilde{\mathcal{E}}\Phi\right\rangle\right| \lesssim N^{-\frac{1}{4}}\left\langle \Phi, \mathcal{E}_{\mathcal{K}}\left(\left(\frac{\mathcal{N}}{\sqrt{N}}+1\right)c\right)\Phi\right\rangle + N^{\frac{1}{4}}\left\langle \Phi, \left(\frac{\mathcal{N}}{\sqrt{N}}+1\right)^2\left(\mathcal{N}+\sqrt{N}\right)\Phi\right\rangle + \langle \Phi, \mathcal{N}\Phi\rangle.\end{aligned}$$

Observe that $\langle \Phi, \mathcal{N}^m\Phi\rangle \lesssim 1$ and furthermore we have by Lemma 13 and Corollary 7

$$\begin{aligned}\langle \Phi, \mathcal{E}_K(\mathcal{N}^m c)\Phi\rangle &\lesssim \langle \Phi, \mathcal{E}_K(\mathcal{N}^m d)\Phi\rangle + \sqrt{N} = \left\langle \Gamma, W^{-1}\mathcal{E}_K(\mathcal{N}^m d)W\Gamma\right\rangle + \sqrt{N} \\ &\lesssim \langle \Gamma, \mathcal{E}_K(c)\Gamma\rangle + \langle \Gamma, \mathcal{E}_K(\mathcal{N}^m c)\Gamma\rangle + \sqrt{N} \lesssim \sqrt{N},\end{aligned}$$

where we used Corollary 4 in the last estimate. Putting together what we have so far, and utilizing Eq. (120)-(122) again, yields

$$\langle \Phi, H_N\Phi\rangle = \frac{1}{6}b_{\mathcal{M}}(V)N + \left(\gamma(V) - \sigma(V) - \mu(V)\right)\sqrt{N} + \langle \Phi, \mathcal{E}_{\mathcal{K}}(d)\Phi\rangle + \langle \Phi, \mathcal{E}_{\mathcal{P}}(\xi)\Phi\rangle + O_{N\to\infty}\left(N^{\frac{1}{4}}\right).$$

Using Corollary 6, Corollary 7, Corollary 3 and Corollary 4, we further have

$$\begin{aligned}&0 \leq \langle \Phi, \mathcal{E}_{\mathcal{P}}(\xi)\Phi\rangle = \langle \Gamma, W^{-1}\mathcal{E}_{\mathcal{P}}(\xi)W\Gamma\rangle \lesssim \langle \Gamma, \mathcal{E}_{\mathcal{P}}(\psi+\delta_1\psi)\Gamma\rangle + 1 \lesssim 1, \\ &0 \leq \langle \Phi, \mathcal{E}_{\mathcal{K}}(d)\Phi\rangle = \langle \Gamma, W^{-1}\mathcal{E}_{\mathcal{K}}(d)W\Gamma\rangle \lesssim \langle \Gamma, \mathcal{E}_{\mathcal{K}}(c)\Gamma\rangle + \frac{1}{N} \lesssim \frac{1}{N}. \qquad \square\end{aligned}$$

6. Proof of Theorem 2

In the following, we want to verify Theorem 2, claiming that any sequence of states Ψ_N with

$$\langle \Psi_N, H_N \Psi \rangle \le E_N + O_{N\to\infty}\left(N^{\frac{1}{4}}\right),$$

satisfies complete Bose-Einstein condensation with a rate of the order $N^{-\frac{3}{4}}$. Together with Theorem 1, the statement follows immediately once we can show that

$$H_N(\alpha) := H_N - \alpha\mathcal{N} \ge \frac{1}{6} b_{\mathcal{M}}(V) N + \Big(\gamma(V) - \mu(V) - \sigma(V)\Big)\sqrt{N} - C N^{\frac{1}{4}}, \tag{135}$$

for some constant C. In order to prove Eq. (135), we observe that by the results in [23, Section 7], see also the comment below [25, Theorem 4], the modified operators $H_N(2\alpha)$ satisfy the asymptotic identity

$$\lim_{N\to\infty} \frac{1}{N} \inf \sigma\big(H_N(2\alpha)\big) = \inf_{u \in L^2(\Lambda): \|u\|=1} \mathcal{E}^{\alpha}_{\mathrm{GP}}(u),$$

where the modified Gross-Pitaevskii functional is defined as

$$\mathcal{E}^{\alpha}_{\mathrm{GP}}(u) := \langle u, (-\Delta) u \rangle + \frac{b_{\mathcal{M}}(V)}{6} \int_{\Lambda} |u(x)|^6 \mathrm{d}x + 2\alpha \|Pu\|^2 - 2\alpha$$

using the projection $P = 1 - Q$, with Q being introduced in Eq. (18). Note that in the notation of [25] the operator $H_N(2\alpha)$ reads

$$H_N(2\alpha) = H_N + 2\alpha \sum_{j=1}^{N} P_{x_j} - 2\alpha N.$$

Furthermore, for $\alpha < 2\pi^2$, we have that

$$\langle u, (-\Delta) u \rangle \ge 4\pi^2 \|Qu\|^2 \ge 2\alpha \|u\|^2 - 2\alpha \|Pu\|^2,$$

and by Hölder's inequality we have

$$1 = \left(\int |u|^2 \mathrm{d}x\right)^3 \le \left(\int_{\Lambda} 1 \mathrm{d}x\right)^2 \int |u|^6 \mathrm{d}x = \int |u|^6 \mathrm{d}x$$

for any $u \in L^2(\Lambda)$ with $\|u\| = 1$, leading to the lower bound

$$\lim_{N\to\infty} \frac{1}{N} \inf \sigma\big(H_N(2\alpha)\big) \ge \frac{b_{\mathcal{M}}(V)}{6}.$$

Therefore, the ground state $\Psi_{N,\alpha}$ of $H_N(\alpha)$ satisfies

$$\begin{aligned}\langle \Psi_{N,\alpha}, H_N(\alpha) \Psi_{N,\alpha} \rangle &= \langle \Psi_{N,\alpha}, H_N(2\alpha) \Psi_{N,\alpha} \rangle + \alpha \langle \Psi_{N,\alpha}, \mathcal{N} \Psi_{N,\alpha} \rangle \\ &\ge \frac{b_{\mathcal{M}}(V)}{6} N + \alpha \langle \Psi_{N,\alpha}, \mathcal{N} \Psi_{N,\alpha} \rangle - o_{N\to\infty}(N),\end{aligned}$$

and by Theorem 1 we obtain the matching upper bound

$$\langle \Psi_{N,\alpha}, H_N(\alpha) \Psi_{N,\alpha} \rangle = \inf \sigma\big(H_N(\alpha)\big) \le \inf \sigma\big(H_N\big) \le \frac{b_{\mathcal{M}}(V)}{6} N + o_{N\to\infty}(N).$$

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As a consequence, the states $\Psi_{N,\alpha}$ satisfy complete Bose-Einstein condensation

$$\langle \Psi_{N,\alpha}, \mathcal{N}\Psi_{N,\alpha}\rangle = o_{N\to\infty}(N),$$

and we can proceed exactly as in Corollary 2, as long as the additional condition $\alpha < \delta$ holds with δ being the constant in Eq. (64). In particular, there exist states $\Phi_{N,\alpha}$ such that

$$\langle \Phi_{N,\alpha}, H_N(\alpha)\Phi_{N,\alpha}\rangle \leq \inf \sigma\big(H_N(\alpha)\big) + C,$$
$$\mathbb{1}\Big(\mathcal{N} \leq C\sqrt{N}\Big)\Phi_{N,\alpha} = \Phi_{N,\alpha},$$

and we have the estimate on the kinetic energy $\Big\langle \Phi_{N,\alpha}, \sum_k |k|^2 c_k^\dagger c_k \Phi_{N,\alpha}\Big\rangle \leq C\sqrt{N}$. Note that the localization results in Lemma 5 hold without any modification for the operator $H_N(\alpha)$, since $\mathcal{N}$ commutes with the localization functions $\mathbb{1}(\mathcal{N} \leq M)$. Following Subsection 4.2, we therefore arrive at the lower bound

$$\begin{aligned}\inf \sigma\big(H_N(\alpha)\big) + C \geq \langle \Phi_{N,\alpha}, H_N(\alpha)\Phi_{N,\alpha}\rangle &\geq \frac{1}{6} b_{\mathcal{M}}(V)N + (\gamma - \sigma - \mu)\sqrt{N}\\ &- \alpha\langle \Phi_{N,\alpha}, \mathcal{N}\Phi_{N,\alpha}\rangle - CN^{\frac{1}{4}} + (1-2C\epsilon)\Big\langle \Phi_N, \sum_k |k|^2 d_k^\dagger d_k \Phi_N\Big\rangle.\end{aligned}$$

Using again Eq. (123), for $\tau < \frac{1}{4}$, we obtain for a large enough constant C

$$\begin{aligned}\inf \sigma\big(H_N(\alpha)\big) \geq\ & \frac{1}{6} b_{\mathcal{M}}(V)N + (\gamma - \sigma - \mu)\sqrt{N} - CN^{\frac{1}{4}}\\ &+ (1 - 2C\epsilon - C\alpha)\Big\langle \Phi_N, \sum_k |k|^2 d_k^\dagger d_k \Phi_N\Big\rangle.\end{aligned}$$

Choosing α and ϵ small enough such that $2\epsilon + \alpha < \frac{1}{C}$ concludes the proof of Eq. (135).

7. Analysis of the scattering coefficients

This Section is devoted to the study of the variational problems in the definition of $b_{\mathcal{M}}(V)$ in Eq. (4) and the definition of $\sigma(V)$ in Eq. (9) as well as the study of their corresponding minimizers ω and η. Especially we want to compare $\gamma(V), \mu(V)$, and $\sigma(V)$ defined in Eq. (10), Eq. (5) and Eq. (9) with γ_N, μ_N, and σ_N defined in Eq. (97), Eq. (102) and Eq. (98), see Lemma 17. The proof will be based on the observation that the N-dependent quantities can be seen as a counterpart on the three-dimensional torus Λ to the N-independent quantities defined in terms of variational problems on the full space $\mathbb{R}^3$. Similarly we will compare in Lemma 16 the modified scattering length $b_{\mathcal{M}}(V)$, which can be expressed in terms of the minimizer ω as

$$b_{\mathcal{M}}(V) = \int_{\mathbb{R}^6} (1-\omega)V \,\mathrm{d}x,$$

see [23], with its counterpart on the torus Λ defined in Eq. (29) as

$$6\lambda_{0,0} = \langle u_0u_0u_0, (V_N - V_N R V_N)u_0u_0u_0\rangle = (V_N - V_N R V_N)_{000,000}.$$

The proof of Lemma 16 is based on the observation that $(1-\omega)V = V - \omega V$ is the full space counterpart to the renormalized potential $V_N - V_N R V_N$.

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In the following Lemma 14 we want to derive properties of $\mathcal{Q}$ defined in Eq. (8) as

$$\mathcal{Q}(\varphi) = \int_{\mathbb{R}^9} \left\{ 2\left|\mathcal{M}_* \nabla \varphi(x)\right|^2 + \mathbb{V}(x) \left| \frac{f(x)}{\mathbb{V}(x)} - \varphi(x) \right|^2 \right\} \mathrm{d}x$$

and its minimizers. For this purpose it will be useful to introduce for a given cut-off parameter ℓ and a smooth function $\chi : \mathbb{R}^6 \longrightarrow \mathbb{R}$ function with $\chi(x) = 1$ for $|x|_\infty \leq \frac{1}{3}$ and $\chi(x) = 0$ for $|x|_\infty > \frac{1}{2}$, the modified function

$$f_\ell(x_1, x_2, x_3) := V(x_1, x_2)\chi(\ell^{-1}x_2, \ell^{-1}x_3)\omega(x_2, x_3).$$

Furthermore, we define the corresponding functional, acting on $\dot{H}^1(\mathbb{R}^9)$, as

$$\mathcal{Q}_\ell(\varphi) := \int_{\mathbb{R}^9} \left\{ 2\left|\mathcal{M}_* \nabla \varphi(x)\right|^2 + \mathbb{V}(x) \left| \frac{f_\ell(x)}{\mathbb{V}(x)} - \varphi(x) \right|^2 \right\} \mathrm{d}x,$$

and $\sigma_\ell(V) := \mathcal{Q}_\ell(0) - \inf_{\varphi \in \dot{H}^1(\mathbb{R}^9)} \mathcal{Q}_\ell(\varphi)$.

Lemma 14. *There exists a unique minimizer η of the functional $\mathcal{Q}$ in $\dot{H}^1(\mathbb{R}^9)$, and η satisfies the pointwise bounds $0 \leq \eta \leq \frac{1}{-2\Delta_{\mathcal{M}_*}} f$ and $\sigma(V) = \int_{\mathbb{R}^9} f(x)\eta(x)\mathrm{d}x$, as well as*

$$(-2\Delta_{\mathcal{M}_*} + \mathbb{V})\eta = f$$

in the sense of distributions. Furthermore, $\mathcal{Q}_\ell$ has a unique minimizer η_ℓ, and η_ℓ satisfyies $0 \leq \eta_\ell \leq \frac{1}{-2\Delta_{\mathcal{M}_*}} f_\ell$ and $\sigma_\ell(V) = \int_{\mathbb{R}^9} f_\ell(x)\eta_\ell(x)\mathrm{d}x$, as well as $(-2\Delta_{\mathcal{M}_*} + \mathbb{V})\eta_\ell = f_\ell$ and

$$\sigma(V) = \lim_{\ell \to \infty} \sigma_\ell(V).$$

Proof. Following the proof of [23], we observe that since $\mathcal{Q}(0) < \infty$, there exists a minimizing sequence $\varphi_n \in \dot{H}^1(\mathbb{R}^9)$ for $\mathcal{Q}$ with $\sup_n \|\nabla \varphi_n\| < \infty$ and $\sup_n \left\| \sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \varphi_n \right) \right\| < \infty$, and therefore there exists by Banach-Alaoglu a subsequence φ_n and elements $X, Y \in L^2(\mathbb{R}^9)$ such that $\nabla \varphi_n \rightharpoonup X$ and $\sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \varphi_n \right) \rightharpoonup Y$ converge weakly in $L^2(\mathbb{R}^9)$. By [17, Theorem 8.6], we obtain that there exists an element $\eta \in \dot{H}^1(\mathbb{R}^9)$ such that $X = \nabla \eta$ and $\varphi_n|_A$ converges (strongly) to $\eta|_A$ in $L^2(A)$ for any set $A \subseteq \mathbb{R}^9$ of finite measure. Since $\sqrt{\mathbb{V}}$ is a bounded function, we further have the convergence of $\sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \varphi_n \right)|_A$ to $\sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \eta \right)|_A$, and in particular $Y = \sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \eta \right)$. In summary we have

$$\nabla \varphi_n \rightharpoonup \nabla \eta,$$
$$\sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \varphi_n \right) \rightharpoonup \sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \eta \right)$$

weakly in $L^2(\mathbb{R}^9)$, and therefore we observe that η is a minimizer of $\mathcal{Q}$

$$\mathcal{Q}(\eta) = 2\|\mathcal{M}_* \nabla \eta\|^2 + \left\| \sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \eta \right) \right\|^2 \leq \liminf_n \left\{ 2\|\mathcal{M}_* \nabla \varphi_n\|^2 + \left\| \sqrt{\mathbb{V}} \left(\frac{f}{\mathbb{V}} - \varphi_n \right) \right\|^2 \right\} = \liminf_n \mathcal{Q}(\varphi_n).$$

Computing $0 = \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{Q}(\eta + t\varphi)$ for $\varphi \in C_0^\infty(\mathbb{R}^9)$ immediately gives in the sense of distributions

$$(-2\Delta_{\mathcal{M}_*} + \mathbb{V})\eta = f,$$

and computing $0 = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}(\eta + t\eta)$ yields $\sigma(V) = \int_{\mathbb{R}^9} f(x)\eta(x)\mathrm{d}x$. Regarding the uniqueness, we note that $\varphi \mapsto \|\mathcal{M}_*\nabla\varphi\|^2$ is strictly convex on $\dot{H}^1(\mathbb{R}^9)$, and therefore $\mathcal{Q}$ is strictly convex too. Consequently the minimizer η is unique. Using that $\frac{f}{\mathbb{V}} \geq 0$, we have

$$\left|\frac{f(x)}{\mathbb{V}(x)} - |\varphi(x)|\right| = \left|\left|\frac{f(x)}{\mathbb{V}(x)}\right| - |\varphi(x)|\right| \leq \left|\frac{f(x)}{\mathbb{V}(x)} - \varphi(x)\right|,$$

and using furthermore the fact that $\varphi \mapsto \int_{\mathbb{R}^9} |\nabla\varphi(x)|^2\mathrm{d}x$ is a Dirichlet form yields

$$\begin{aligned}\int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla|\varphi(x)|\right|^2\mathrm{d}x = |\mathrm{det}\mathcal{M}_*| \int_{\mathbb{R}^9} \left|\nabla_x|\varphi(\mathcal{M}_*x)|\right|^2\mathrm{d}x \leq |\mathrm{det}\mathcal{M}_*| \int_{\mathbb{R}^9} \left|\nabla_x\varphi(\mathcal{M}_*x)\right|^2\mathrm{d}x \\ = \int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla\varphi(x)\right|^2\mathrm{d}x.\end{aligned}$$

Therefore, $\mathcal{Q}(|\varphi|) \leq \mathcal{Q}(\varphi)$ for all $\varphi \in \dot{H}^1(\mathbb{R}^9)$ and by the uniqueness of the minimizer we obtain $\eta = |\eta| \geq 0$. For the purpose of obtaining an upper bound on η, we observe that $\frac{1}{\mathcal{M}_*\nabla} f \in L^2(\mathbb{R}^9)$ and define the functional

$$\widetilde{\mathcal{Q}}(\varphi) := \int_{\mathbb{R}^9} \left\{2\left|\mathcal{M}_*\nabla\varphi(x) + \frac{1}{2\mathcal{M}_*\nabla} f(x)\right|^2 + \mathbb{V}(x)|\varphi(x)|^2\right\}\mathrm{d}x.$$

Since $\widetilde{\mathcal{Q}}(\varphi) = \mathcal{Q}(\varphi) + \widetilde{\mathcal{Q}}(0) - \mathcal{Q}(0)$, we observe that η is the unique minimizer of $\widetilde{\mathcal{Q}}$. It is furthermore clear that

$$\int_{\mathbb{R}^9} \mathbb{V}(x)\left|\min\{\varphi, \frac{1}{-2\Delta_{\mathcal{M}_*}} f\}\right|^2 \mathrm{d}x \leq \int_{\mathbb{R}^9} \mathbb{V}(x)|\varphi(x)|^2\mathrm{d}x,$$

and utilizing again that $\varphi \mapsto \int_{\mathbb{R}^9} |\nabla\varphi(x)|^2\mathrm{d}x$ is a Dirichlet form yields

$$\begin{aligned}&\int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla \min\{\varphi, \frac{1}{-2\Delta_{\mathcal{M}_*}} f\} + \frac{1}{2\mathcal{M}_*\nabla} f(x)\right|^2 \mathrm{d}x \\ &\quad = \int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla\left(\min\{\varphi, \frac{1}{-2\Delta_{\mathcal{M}_*}} f\} + \frac{1}{2\Delta_{\mathcal{M}_*}} f(x)\right)\right|^2 \mathrm{d}x \\ &\quad = \int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla\left(\min\{\varphi + \frac{1}{2\Delta_{\mathcal{M}_*}} f(x), 0\}\right)\right|^2 \mathrm{d}x \\ &\quad \leq \int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla\left(\varphi + \frac{1}{2\Delta_{\mathcal{M}_*}} f(x)\right)\right|^2 \mathrm{d}x \\ &\quad = \int_{\mathbb{R}^9} \left|\mathcal{M}_*\nabla\varphi(x) + \frac{1}{2\mathcal{M}_*\nabla} f(x)\right|^2 \mathrm{d}x.\end{aligned}$$

In particular, $\widetilde{\mathcal{Q}}(\min\{\varphi, \frac{1}{-2\Delta_{\mathcal{M}_*}} f\}) \leq \widetilde{\mathcal{Q}}(\varphi)$, and therefore we obtain by the uniqueness of minimizer for $\widetilde{\mathcal{Q}}$

$$\eta = \min\left\{\eta, \frac{1}{-2\Delta_{\mathcal{M}_*}} f\right\} \leq \frac{1}{-2\Delta_{\mathcal{M}_*}} f.$$

The properties of $\mathcal{Q}_\ell$ can be verified analogously.

In order to compare $\sigma(V)$ with $\sigma_\ell(V)$, let us first verify the point-wise bounds

$$\eta_\ell \leq \eta \leq \eta_\ell + \frac{1}{-2\Delta_{\mathcal{M}_*}}(f - f_\ell). \tag{136}$$

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For this purpose we introduce the additional functionals $\mathcal{Q}'_\ell$ and $\mathcal{Q}''_\ell$ as

$$\mathcal{Q}'_\ell(\varphi) := \int_{\mathbb{R}^9} \left\{ 2\left|\mathcal{M}_* \nabla \varphi - \mathcal{M}_* \nabla \eta\right|^2 + \mathbb{V}\left|\varphi - \eta + \frac{f - f_\ell}{\mathbb{V}}\right|^2 \right\} \mathrm{d}x,$$

$$\mathcal{Q}''_\ell(\varphi) := \int_{\mathbb{R}^9} \left\{ 2\left|\mathcal{M}_* \nabla \varphi - \mathcal{M}_* \nabla \eta_\ell + \frac{1}{2\mathcal{M}_* \nabla} f - \frac{1}{2\mathcal{M}_* \nabla} f_\ell\right|^2 + \mathbb{V}|\varphi - \eta_\ell|^2 \right\} \mathrm{d}x.$$

By a straightforward computation, we observe that $\mathcal{Q}'_\ell(\varphi) = \mathcal{Q}_\ell(\varphi) + \mathcal{Q}'_\ell(0) - \mathcal{Q}_\ell(0)$ and similarly $\mathcal{Q}''_\ell(\varphi) = \mathcal{Q}(\varphi) + \mathcal{Q}''_\ell(0) - \mathcal{Q}(0)$. Therefore η_ℓ is the unique minimizer of $\mathcal{Q}'_\ell$, and since $f(x) \geq f_\ell(x)$ we further have

$$\mathcal{Q}'_\ell(\min\{\varphi, \eta\}) \leq \mathcal{Q}'_\ell(\varphi).$$

Consequently $\eta_\ell \leq \eta$. The second inequality in Eq. (136) follows analogously, utilizing that η is the unique minimizer of $\mathcal{Q}''_\ell$ and that

$$\mathcal{Q}''_\ell\left(\min\left\{\varphi, \eta_\ell + \frac{1}{-2\Delta_{\mathcal{M}_*}}(f - f_\ell)\right\}\right) \leq \mathcal{Q}''_\ell(\varphi).$$

Using the fact that $|f(x) - f_\ell(x)| \lesssim \frac{\mathbb{1}(|x| > \frac{\ell}{3})}{|x|^4}$, see [23], the fundamental solution

$$\frac{\Gamma\left(\frac{9}{2}\right)}{28\pi^{\frac{9}{2}} \det[M_*]} \frac{1}{|\mathcal{M}_*^{-1}(x - y)|^7}$$

for the differential operator $-2\Delta_{\mathcal{M}_*}$ and the observation $\frac{1}{|\mathcal{M}_*^{-1} v|} \leq \frac{\|\mathcal{M}_*\|}{|v|}$, we obtain

$$\frac{1}{-2\Delta_{\mathcal{M}_*}}(f - f_\ell)(x) = \frac{\Gamma\left(\frac{9}{2}\right)}{28\pi^{\frac{9}{2}} \det[M_*]} \int_{\mathbb{R}^9} \frac{f(y) - f_\ell(y)}{|\mathcal{M}_*^{-1}(x - y)|^7} \mathrm{d}y \lesssim \int_{|y| \geq \frac{\ell}{3}} \frac{1}{|y|^4 |x - y|^7} \mathrm{d}y$$
$$\lesssim \int_{\mathbb{R}^9} \frac{1}{(\ell + |y|)^4 |x - y|^7} \mathrm{d}y \leq \int_{\mathbb{R}^9} \frac{1}{(\ell + |y|)^4 |y|^7} \mathrm{d}y = \ell^{-2} \int_{\mathbb{R}^9} \frac{1}{(1 + |y|)^4 |y|^7} \mathrm{d}y,$$

where we have used symmetric rearrangement. Since $\int_{\mathbb{R}^9} \frac{1}{(1+|y|)^4 |y|^7} \mathrm{d}y < \infty$ is finite, we obtain that $\frac{1}{-2\Delta_{\mathcal{M}_*}}(f - f_\ell)$ converges point-wise to zero and consequently η_ℓ converges point-wise to η by Eq. (136). Using Fatou's Lemma and $f_\ell(x)\eta_\ell(x) \geq 0$, as well as the fact that f_ℓ converges point-wise to f, therefore yields

$$\sigma(V) = \int_{\mathbb{R}^9} f(x)\eta(x) \mathrm{d}x \leq \liminf_{\ell \to \infty} \int_{\mathbb{R}^9} f_\ell(x)\eta_\ell(x) \mathrm{d}x = \liminf_{\ell \to \infty} \sigma_\ell(V) \leq \limsup_{\ell \to \infty} \sigma_\ell(V) \leq \sigma(V),$$

where we have used in the last inequality that $f_\ell \eta_\ell \leq f\eta$ by Eq. (136). □

Before we can compare the modified scattering length $b_{\mathcal{M}}(V)$ with its counterpart on the torus in Lemma 16, we need the following auxiliary result Lemma 15.

Lemma 15. *Recall the definition of the coefficients $\lambda_{k,\ell}$ in Eq. (29) and the definition of T in Eq. (19). Then there exists a constant $C > 0$ such that $|\lambda_{k,\ell}| \leq \frac{C}{N^2}\left(1 + \frac{|\ell|^2}{N}\right)^{-1}$ and*

$$\left|(T - 1)_{ijk,\ell 00}\right| \leq \frac{C\,\mathbb{1}(i + j + k = \ell)}{N^2(|i|^2 + |j|^2 + |k|^2)} \left(1 + \frac{|i|^2 + |j|^2 + |k|^2}{N + |\ell|^2}\right)^{-2}. \tag{137}$$

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Proof. In order to verify Eq. (137), we observe that for $|\ell| \leq K$ and $n \geq 2$

$$\nabla^n (T-1) e^{i\ell x} = \nabla^n R V_N e^{i\ell x}$$

can be written as the sum of terms of the form

$$Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3}\, \nabla^a R^{1-b} Q^{\otimes 3} V_N e^{i\ell x}, \tag{138}$$

where the coefficients satisfy $k_1 + \cdots + k_m + 2m + a + 2b = n$ and either (I) that $b = 1$, (II) that $b = 0$ and $a = 1$ or (III) that $b = 0$, $a = 0$ and $m \geq 1$. We are going to verify Eq. (138) by induction, using the resolvent identity

$$-\Delta R = Q^{\otimes 3} - Q^{\otimes 3} V_N Q^{\otimes 3} R.$$

We start with the case $n = 2$

$$\nabla^2 R V_N e^{i\ell x} = -(-\Delta) R V_N e^{i\ell x} = Q^{\otimes 3} V_N Q^{\otimes 3} R V_N e^{i\ell x} - Q^{\otimes 3} V_N e^{i\ell x}, \tag{139}$$

and observe that the first term in Eq. (139) is of the type (III) and the second one is of type (I). For the inductive argument, let

$$T = Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3}\, \nabla^a R^{1-b} Q^{\otimes 3} V_N e^{i\ell x}$$

be of type X with X being (I), (II) or (III), and let us compute

$$\begin{aligned}
\nabla T = \Big(& Q^{\otimes 3} \nabla^{k_1+1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3} + \cdots + Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m+1}(V_N) Q^{\otimes 3} \Big) \\
& \times (V_N) Q^{\otimes 3}\, \nabla^a R^{1-b} Q^{\otimes 3} V_N e^{i\ell x} && (140) \\
& + Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3}\, \nabla^{a+1} R^{1-b} Q^{\otimes 3} V_N e^{i\ell x}. && (141)
\end{aligned}$$

The terms in the first two lines, see Eq. (140), are clearly of type X again. Regarding the term in the third line, see Eq. (141), we obtain that ∇T is type I in case T itself is type I. In case T is type III we obtain that ∇T is type II, and finally in case T is type II, we have $a = 1$ and use Eq. (139) again

$$\begin{aligned}
& Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3}\, \nabla^{a+1} R^{1-b} Q^{\otimes 3} V_N e^{i\ell x} \\
& \quad = Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3} V_N Q^{\otimes 3} R V_N e^{i\ell x} && (142) \\
& \quad\quad + Q^{\otimes 3} \nabla^{k_1}(V_N) Q^{\otimes 3} \dots Q^{\otimes 3} \nabla^{k_m}(V_N) Q^{\otimes 3} V_N e^{i\ell x}. && (143)
\end{aligned}$$

The right-hand side of Eq. (143) is clearly a sum of a type I and type III term, which concludes the inductive proof of Eq. (138).

In the following we are going to verify individually for the three cases (I)–(III) that the Fourier transform of the expression in Eq. (138) has an L^∞ bound of the order $N^{-2}(\sqrt{N} + |\ell|)^{n-2}$ for $n \geq 2$, which immediately implies Eq. (137). Let us first of all state the useful bounds

$$\left\| \sqrt{Q^{\otimes 3} \nabla^k (V_N) Q^{\otimes 3}} \right\| \leq \sqrt{\| Q^{\otimes 3} \nabla^k (V_N) Q^{\otimes 3} \|} \lesssim \sqrt{N}^{\frac{k}{2}+1}, \tag{144}$$

$$\left\| \frac{1}{\nabla} Q^{\otimes 3} \nabla^k (V_N) Q^{\otimes 3} \frac{1}{\nabla} \right\| \lesssim \sqrt{N}^k, \tag{145}$$

$$\left\| \sqrt{Q^{\otimes 3} \nabla^k (V_N) Q^{\otimes 3}} e^{iK\cdot X} \right\| \leq \sqrt{\langle e^{iK\cdot X}, \nabla^k (V_N) e^{iK\cdot X} \rangle} \lesssim \sqrt{N}^{\frac{k}{2}-2} \tag{146}$$

for $k \geq 0$. Regarding the case (I), we obtain immediately by Eq. (144) and Eq. (146)

$$\left|\left\langle e^{iK\cdot X}, Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_m}(V_N)Q^{\otimes 3}\,\nabla^a V_N e^{i\ell x}\right\rangle\right| \lesssim \sqrt{N}^{k_1+\dots+k_m+2m-4}\left(\sqrt{N}+|\ell|\right)^a \leq N^{-2}(\sqrt{N}+|\ell|)^{n-2}.$$

Since the case (II) is similar to the case (III), let us directly have a look at the case (III), where we use the fact that by Eq. (145)

$$\begin{aligned}&\|\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}R\nabla\|^2 = \|\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}R\nabla^2 R\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}\|\\ &\leq \|\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}R\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}\| \leq \|\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}\frac{1}{-\Delta}\sqrt{Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}}\|\\ &= \|\frac{1}{\nabla}Q^{\otimes 3}\nabla^k(V_N)Q^{\otimes 3}\frac{1}{\nabla}\| \lesssim \sqrt{N}^k,\end{aligned}$$

to obtain

$$\begin{aligned}&\left|\left\langle e^{iK\cdot X}, Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_{m-1}}(V_N)Q^{\otimes 3}\,Q^{\otimes 3}V_N Q^{\otimes 3}\,RV_N e^{i\ell x}\right\rangle\right| \\ &\lesssim \sqrt{N}^{\frac{k_m}{2}}\left\|\sqrt{Q^{\otimes 3}\nabla^{k_m}(V_N)Q^{\otimes 3}}\,Q^{\otimes 3}\nabla^{k_{m-1}}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\,e^{iK\cdot X}\right\|\left\|\frac{1}{\nabla}Q^{\otimes 3}V_N e^{i\ell x}\right\|.\end{aligned} \tag{147}$$

As a consequence of Eq. (144) and Eq. (146) we have

$$\left\|\sqrt{Q^{\otimes 3}V_N Q^{\otimes 3}}\,Q^{\otimes 3}\nabla^{k_{m-1}}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\,e^{iK\cdot X}\right\| \lesssim \sqrt{N}^{k_1+\dots+k_m+2(m-1)-2}. \tag{148}$$

This yields the desired estimate for the term in Eq. (147), since $\left\|\frac{1}{\nabla}Q^{\otimes 3}V_N e^{i\ell x}\right\| \lesssim \sqrt{N}^{-2}$. The bounds on $\lambda_{k,\ell}$ can be verified similarly. □

In the following Lemma 16, we show that the renormalized potential $N^2(V_N - V_N R V_N)$ converges to $b_{\mathcal{M}}(V)\delta(x-y, x-z)$ in a suitable sense. The analogous result for Bose gases with two-particle interactions has been verified in [8, Lemma 1].

Lemma 16. *Let $b_{\mathcal{M}}(V)$ be the modified scattering length introduced in Eq. (4). Then*

$$\left|N^2(V_N - V_N R V_N)_{000,000} - b_{\mathcal{M}}(V)\right| \leq \frac{1}{N}$$

Furthermore, $(V_N - V_N R V_N)_{ijk,\ell mn} = 0$ in case $i+j+k \neq \ell+m+n$ and otherwise

$$\left|N^2(V_N - V_N R V_N)_{ijk,\ell mn} - b_{\mathcal{M}}(V)\right| \leq \frac{C_{ijk,\ell mn}}{\sqrt{N}}$$

for suitable constants $C_{ijk,\ell mn}$.

Proof. Let ω be the unique minimizer to the variational problem in Eq. (4), which exists according to [23] and satisfies in the sense of distributions

$$(-2\Delta_{\mathcal{M}} + V)\omega = V.$$

Furthermore, let χ be a smooth function with $\chi(x) = 1$ for $|x|_\infty \leq \frac{1}{3}$ and $\chi(x) = 0$ for $|x|_\infty > \frac{1}{2}$, and let us denote for a function f the rescaled version with $f^L(x) := f(Lx)$. Then we define for $n = (n_1, n_2, n_3) \in (2\pi\mathbb{Z})^{3\times 3}$ and $0 < \ell < \sqrt{N}$

$$\psi_n(x,y,z) := e^{in_1 x}e^{in_2 y}e^{in_3 z}\chi^{\frac{\sqrt{N}}{\ell}}(x-y, x-z)\,\omega^{\sqrt{N}}(x-y, x-z). \tag{149}$$

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In the following we want to show that ψ_n is an approximation of $RV_N e^{in_1x}e^{in_2y}e^{in_3z}$. For this purpose we observe that the function ψ_n satisfies the differential equation

$$(-\Delta+V_N)\psi_n = e^{in_1x}e^{in_2y}e^{in_3z}\Big(V_N - \xi_n(x-y,x-z)\Big), \tag{150}$$

where we define $\xi_n : \mathbb{T}^2 \longrightarrow \mathbb{R}$ as

$$\begin{aligned}
\xi_n &:= e^{-in_1x}e^{-in_2y}e^{-in_3z}\Big[\Delta, e^{in_1x}e^{in_2y}e^{in_3z}\chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\Big]\omega^{\sqrt{N}}(x-y,x-z) \qquad (151)\\
&= \Big((\nabla+in)^2\chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z) - \chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\Delta\Big)\omega^{\sqrt{N}}(x-y,x-z)\\
&= \Big(\Delta\Big(\chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\Big) + 2\nabla\Big(\chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\Big)\nabla - (n_1^2+n_2^2+n_3^2)\chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\\
&\quad + 2in\Big(\nabla\Big(\chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\Big) + \chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\nabla\Big)\Big)\omega^{\sqrt{N}}(x-y,x-z)\\
&= 2\Delta_{\mathcal{M}}(\chi^{\frac{\sqrt{N}}{\ell}})\omega^{\sqrt{N}} + 4\mathcal{M}^2\nabla(\chi^{\frac{\sqrt{N}}{\ell}})\nabla\omega^{\sqrt{N}} - (n_1^2+n_2^2+n_3^2)\chi^{\frac{\sqrt{N}}{\ell}}\omega^{\sqrt{N}} \qquad (152)\\
&\quad + 4i(n_1-n_2)\Big(\nabla_{x_1}(\chi^{\frac{\sqrt{N}}{\ell}})\omega^{\sqrt{N}} + \chi^{\frac{\sqrt{N}}{\ell}}\nabla_{x_1}(\omega^{\sqrt{N}})\Big) + 4i(n_1-n_3)\Big(\nabla_{x_2}(\chi^{\frac{\sqrt{N}}{\ell}})\omega^{\sqrt{N}} + \chi^{\frac{\sqrt{N}}{\ell}}\nabla_{x_2}(\omega^{\sqrt{N}})\Big).
\end{aligned}$$

In order to verify that ξ_n can be treated as an error term, we first note that we have

$$\begin{aligned}
\widehat{\Delta_{\mathcal{M}}\chi^{\frac{\sqrt{N}}{\ell}}} &= \Big(\sqrt{N}^{-1}\ell\Big)^4\widehat{\Delta_{\mathcal{M}}\chi^{\frac{\ell}{\sqrt{N}}}},\\
\widehat{\mathcal{M}^2\nabla\chi^{\frac{\sqrt{N}}{\ell}}} &= \Big(\sqrt{N}^{-1}\ell\Big)^5\widehat{\mathcal{M}^2\nabla\chi^{\frac{\ell}{\sqrt{N}}}},
\end{aligned}$$

and utilizing the density $\rho := -2\Delta_{\mathcal{M}}\omega$ we obtain

$$\begin{aligned}
\widehat{\omega^{\sqrt{N}}}(K) &= \sqrt{N}^{-6}\widehat{\omega}^{\frac{1}{\sqrt{N}}}(K) = \sqrt{N}^{-6}\frac{\widehat{\rho}(\sqrt{N}^{-1}K)}{|\sqrt{N}^{-1}K|^2} = \sqrt{N}^{-4}\frac{\widehat{\rho}(\sqrt{N}^{-1}K)}{|K|^2},\\
\widehat{\nabla\omega^{\sqrt{N}}}(K) &= \sqrt{N}^{-4}\frac{\widehat{\rho}(\sqrt{N}^{-1}K)K}{|K|^2},
\end{aligned}$$

Furthermore, we observe that we can write the Fourier transform of ξ_n as

$$\begin{aligned}
\widehat{\xi}_n = \widehat{\Delta_{\mathcal{M}}\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\omega^{\sqrt{N}}} &+ 2\widehat{\mathcal{M}^2\nabla\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\nabla\omega^{\sqrt{N}}} - (n_1^2+n_2^2+n_3^2)\widehat{\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\omega^{\sqrt{N}}}\\
&+ 4i(n_1-n_2)\Big(\widehat{\nabla_{x_1}(\chi^{\frac{\sqrt{N}}{\ell}})} * \widehat{\omega^{\sqrt{N}}} + \widehat{\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\nabla_{x_1}(\omega^{\sqrt{N}})}\Big)\\
&+ 4i(n_1-n_3)\Big(\widehat{\nabla_{x_2}(\chi^{\frac{\sqrt{N}}{\ell}})} * \widehat{\omega^{\sqrt{N}}} + \widehat{\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\nabla_{x_2}(\omega^{\sqrt{N}})}\Big).
\end{aligned}$$

Since $\rho \in L^1(\mathbb{R}^6)$, see [23], we have $\widehat{\rho} \in L^\infty(\mathbb{R}^6)$, and distinguishing between the cases $|K| \lesssim \frac{\sqrt{N}}{\ell}$ and $|K| \gg \frac{\sqrt{N}}{\ell}$, yields the estimate

$$\Big|\widehat{\Delta_{\mathcal{M}}\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\omega^{\sqrt{N}}}(K)\Big| \lesssim \sqrt{N}^{-4}\Big(\sqrt{N}^{-1}\ell\Big)^4\int_{\mathbb{R}^6}\frac{|\widehat{\Delta_{\mathcal{M}}\chi}(\sqrt{N}^{-1}\ell P)|}{|K+P|^2}\mathrm{d}P \lesssim \sqrt{N}^{-4}\min\left\{\left(\frac{\sqrt{N}}{\ell|K|}\right)^2, 1\right\}. \tag{153}$$

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Using that ρ has compact support as a consequence of the scattering equation, we obtain that $x\nabla\rho(x) \in L^1(\mathbb{R}^6)$ and therefore

$$\left|K_1\widehat{\rho}(\sqrt{N}^{-1}K_1) - K_2\widehat{\rho}(\sqrt{N}^{-1}K_2)\right| \lesssim |K_1 - K_2|.$$

Since $\widehat{\mathcal{M}^2\nabla\chi}$ is reflection antisymmetric, we furthermore have

$$\begin{aligned}
\left|\widehat{\mathcal{M}^2\nabla\chi^{\frac{\sqrt{N}}{\ell}}} * \widehat{\nabla\omega^{\sqrt{N}}}\right| &\lesssim \sqrt{N}^{-4}\left(\sqrt{N}^{-1}\ell\right)^5 \int_{\mathbb{R}^6} \frac{|\widehat{\mathcal{M}^2\nabla\chi}(\sqrt{N}^{-1}\ell P)|}{|K+P|^2} |(K+P) - (K-P)| \mathrm{d}P \\
&\quad + \sqrt{N}^{-4}\left(\sqrt{N}^{-1}\ell\right)^5 \int_{\mathbb{R}^6} \left|\widehat{\mathcal{M}^2\nabla\chi}(\sqrt{N}^{-1}\ell P)\right| \left|(K-P)\widehat{\rho}\left(\sqrt{N}^{-1}(K-P)\right)\right| \left|\frac{1}{|K+P|^2} - \frac{1}{|K-P|^2}\right| \\
&\lesssim \sqrt{N}^{-4} \min\left\{\left(\frac{\sqrt{N}}{\ell|K|}\right)^2, 1\right\}.
\end{aligned}$$

Summarizing what we have so far, we can estimate the Fourier coefficients of ξ_0 by

$$|\widehat{\xi}_0(K)| \lesssim N^{-2} \min\left\{\left(\frac{\sqrt{N}}{\ell|K|}\right)^2, 1\right\}. \tag{154}$$

Proceeding similarly for general $n \neq 0$ we observe the slightly weaker estimate

$$|\widehat{\xi}_n(K)| \lesssim N^{-2} \min\left\{\frac{\sqrt{N}}{\ell|K|}, 1\right\}. \tag{155}$$

In the following let R denote the resolvent of the operator $Q^{\otimes 3}(-\Delta + V_N)Q^{\otimes 3}$ on the torus, and note that we obtain as a consequence of the differential equation Eq. (150)

$$RV_N e^{in_1x}e^{in_2y}e^{in_3z} = \psi_n + R\xi_n(x-y, x-z)e^{in_1x}e^{in_2y}e^{in_3z} + (RV_N - 1)(1 - Q^{\otimes 3})\psi_n. \tag{156}$$

Using the fact that V has compact support, there exists a $\ell_0 > 0$ such that $\chi^{\frac{1}{\ell}}(x) = 1$ for $x \in \mathrm{supp}(V)$ and $\ell \geq \ell_0$, and therefore we obtain for $n = (n_1, n_2, n_3)$ and $m = (m_1, m_2, m_3)$

$$\begin{aligned}
(V_N)_{m,n} - \langle V_N e^{im_1x}e^{im_2y}e^{im_3z}, \psi_n\rangle &= \frac{\delta_{\overline{n}=\overline{m}}}{N^2} \int_{\mathbb{R}^6} e^{i\frac{m_2-n_2}{\sqrt{N}}x} e^{i\frac{m_3-n_3}{\sqrt{N}}y} V(x,y)\left(1 - \omega(x,y)\right)\mathrm{d}x\mathrm{d}y \\
&= \frac{\delta_{\overline{n}=\overline{m}}}{N^2} b_{\mathcal{M}}(V) + O_{N\to\infty}\left(N^{-\frac{5}{2}}\right),
\end{aligned} \tag{157}$$

where $\overline{n} := n_1 + n_2 + n_3$ and we have used that we can express the minimum in Eq. (4) according to [23] as

$$b_{\mathcal{M}}(V) = \int_{\mathbb{R}^6} V(x,y)\left(1 - \omega(x,y)\right)\mathrm{d}x\mathrm{d}y.$$

We observe that in the case $m = 0$ and $n = 0$, we even have the exact identity

$$N^2(V_N)_{000,000} - N^2\langle V_N, \psi_0\rangle = b_{\mathcal{M}}(V).$$

Consequently we obtain

$$N^2(V_N - V_N R V_N)_{000,000} = b_{\mathcal{M}}(V) - N^2\langle RV_N, \xi_0\rangle - 3N^2\sum_k \langle V_N, (RV_N - 1)e^{ik(x-y)}\rangle\langle e^{ik(x-y)}, \psi_0\rangle.$$

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Using Lemma 15 and the fact that $(RV)_{ijk,000} = (T-1)_{ijk,000} = 0$ in case $i \neq -(j+k)$, we can estimate

$$\begin{aligned} N^2|\langle RV_N, \xi_0\rangle| &= N^2\left|\sum_{jk} \overline{(RV_N)_{-(j+k)jk}}\,\widehat{\xi}_0(-(j+k),j,k)\right| \\ &\lesssim N^{-2}\sum_{jk}\frac{\left(1+\frac{|j|^2+|k|^2}{N}\right)^{-2}}{|j|^2+|k|^2}\min\left\{\left(\frac{\sqrt{N}}{\ell(|j|+|k|)}\right)^2,1\right\} \\ &\leq N^{-2}\sum_{jk}\frac{\left(1+\frac{|j|^2+|k|^2}{N}\right)^{-\frac{3}{2}}\left(\frac{\sqrt{N}}{\ell(|j|+|k|)}\right)^2}{|j|^2+|k|^2} \lesssim \frac{1}{\ell^2}. \end{aligned}$$

Again by Lemma 15 we have that

$$\left|\langle V_N, (RV_N-1)e^{ik(x-y)}\rangle\right| \lesssim N^{-2}\left(1+\frac{|k|^2}{N}\right)^{-1},$$

and following the proof of Eq. (153) we obtain that $|\langle e^{ik(x-y)},\psi_0\rangle| \lesssim N^{-2}\frac{1}{1+|k|^2}$. Therefore

$$N^2\sum_k\left|\langle V_N,(RV_N-1)e^{ik(x-y)}\rangle\langle e^{ik(x-y)},\psi_0\rangle\right| \lesssim N^{-2}\sum_k\frac{\left(1+\frac{|k|^2}{N}\right)^{-1}}{1+|k|^2} \lesssim N^{-\frac{3}{2}}.$$

Choosing ℓ of the order $\sqrt{N}$ yields

$$\left|N^2(V_N - V_N RV_N)_{000,000} - b_{\mathcal{M}}(V)\right| \lesssim \frac{1}{N}. \tag{158}$$

For general $n=(n_1,n_2,n_3)$ and $m=(m_1,m_2,m_3)$ with $n_1+n_2+n_3 = m_1+m_2+m_3$ the estimates in Eq. (155) and Eq. (157) yield in a similar fashion the desired estimate. □

In Eq. (156) we saw that RV_N, an object defined on the torus Λ, is approximated by

$$\psi_n(x,y,z) := \chi^{\frac{\sqrt{N}}{\ell}}(x-y,x-z)\omega^{\sqrt{N}}(x-y,x-z),$$

which involves the corresponding object ω defined on the full space. In the following Lemma 17 we make use of this correspondence again, to compare γ_N,μ_N and σ_N with γ,μ and σ.

Lemma 17. *Let γ_N,μ_N and σ_N be as in Eq. (97), Eq. (102) and Eq. (98), and $\sigma(V)$, $\mu(V)$ and $\gamma(V)$ as in Eq. (10), Eq. (5) and Eq. (9). Then*

$$\begin{aligned} \gamma_N &= \gamma(V)\sqrt{N} + O_{N\to\infty}\left(N^{-\frac{1}{4}}\right), \\ \mu_N &= \mu(V)\sqrt{N} + O_{N\to\infty}(1), \\ \sigma_N &= \sigma(V)\sqrt{N} + O_{N\to\infty}\left(N^{\frac{1}{4}}\right), \end{aligned}$$

and there exists a constant $\lambda(V) > 0$ such that for $0<\lambda\leq\lambda(V)$

$$\gamma(\lambda V) - \mu(\lambda V) - \sigma(\lambda V) < 0. \tag{159}$$

Furthermore, σ_N and γ_N are independent of the parameter K from the definition of π_K below Eq. (17), and the limit $\mu(V) = \lim_N \frac{\mu_N}{\sqrt{N}}$ is independent of K as well.

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Proof. In order to analyze γ_N, let us denote with $L_i : L^2(\Lambda^4) \longrightarrow L^2(\Lambda^4)$ the linear map that exchanges the fist factor in the tensor product $L^2(\Lambda^4) \cong L^2(\Lambda)^{\otimes 4}$ with the i-th factor and observe that

$$\sqrt{N}^{-1}\gamma_N = \frac{N^{\frac{7}{2}}}{6}\sum_{i=1}^{3}\langle L_i\, 1 \otimes (RV_N), (V_N \otimes 1)L_j\, 1 \otimes (RV_N)\rangle.$$

Furthermore, recall the definition of ψ_0 from Eq. (149) in the proof of Lemma 16 and define

$$\begin{aligned}\gamma^{(\ell)} &:= \int_{\mathbb{R}^9} V(x,y)\left(\chi^{\frac{1}{\ell}}(x,z)\omega(x,z)\chi^{\frac{1}{\ell}}(y,z)\omega(y,z) + \frac{1}{2}\left|\chi^{\frac{1}{\ell}}(y,z)\omega(y,z)\right|^2\right)\mathrm{d}x\mathrm{d}y\mathrm{d}z\\ &= \frac{N^{\frac{7}{2}}}{6}\sum_{i,j=1}^{3}\langle L_i\, 1 \otimes \psi_0, (V_N \otimes 1)L_j\, 1 \otimes \psi_0\rangle,\end{aligned}$$

where the second identity holds by a scaling argument for all $0 < \ell < N$. We observe that by the permutation symmetry of V_N we have $L_i V_N \otimes 1 L_i = V_N \otimes 1$ and therefore

$$\begin{aligned}N^{\frac{7}{2}}\left|\langle L_i\, 1 \otimes \psi_0, (V_N \otimes 1)L_j\, 1 \otimes \psi_0\rangle\right| &\leq \sup_{i\in\{1,2,3\}} \langle L_i\, 1 \otimes \psi_0, (V_N \otimes 1)L_i\, 1 \otimes \psi_0\rangle\\ = N^{\frac{7}{2}}\langle 1 \otimes \psi_0, (V_N \otimes 1)1 \otimes \psi_0\rangle &= \int_{\mathbb{R}^9} V(x,y)\left|\chi^{\frac{1}{\ell}}(y,z)\omega(y,z)\right|^2\mathrm{d}x\mathrm{d}y\mathrm{d}z \lesssim 1.\end{aligned}$$

Using $L_i V_N \otimes 1 L_i = V_N \otimes 1$ again, together with the identity in Eq. (156) and the Cauchy-Schwarz inequality yields

$$\begin{aligned}\left|\sqrt{N}^{-1}\gamma_N - \gamma^{(\ell)}\right| &\lesssim N^{\frac{7}{2}}\sqrt{\langle 1 \otimes (R\xi_0(x-y,x-z)), (V_N \otimes 1)1 \otimes (R\xi_0(x-y,x-z))\rangle}\\ &\quad + N^{\frac{7}{2}}\sqrt{\left\langle 1 \otimes (RV_N - 1)(1-Q^{\otimes 3}), (V_N \otimes 1)1 \otimes (RV_N - 1)(1-Q^{\otimes 3})\right\rangle}.\end{aligned} \tag{160}$$

Regarding the analysis of the term on the right side of Eq. (160), we observe that

$$\rho := -2\Delta_{\mathcal{M}}\omega = V(1-\omega)$$

satisfies $\nabla^k \rho \in L^1$ due to the regularity assumptions on V. Proceeding as in Eq. (153) we obtain the improved version of Eq. (154)

$$\left|\widehat{\xi_0}(K)\right| \lesssim N^{-2}\min\left\{\left(\frac{\sqrt{N}}{\ell|K|}\right)^2, 1\right\}\left(1 + \frac{|K|^2}{N}\right)^{-m}, \tag{161}$$

Similar to Eq. (138) we can write $\nabla^n R\xi_0$, where ξ_0 is introduced in Eq. (151), as the sum of terms of the form

$$Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_m}(V_N)Q^{\otimes 3}\,\nabla^a R^{1-b}\xi_0, \tag{162}$$

where the coefficients satisfy $k_1 + \dots + k_m + 2m + a + 2b = n$ and either (I) that $b = 1$, (II) that $b = 0$ and $a = 1$ or (III) that $b = 0$, $a = 0$ and $m \geq 1$ as well as $k_m = 0$. In the following we are going to verify individually for the three cases (I)–(III) that the Fourier transform of the expression in Eq. (162) has an L^∞ bound of the order $\frac{\sqrt{N}^n}{N^3\ell^2}$ for $n \geq 4$, and consequently

$$\left|\widehat{R\xi_0}(K)\right| \lesssim \frac{1}{\ell^2 N^2|K|^2}\,\frac{N}{|K|^2}\left(1 + \frac{|K|^2}{N}\right)^{-m}. \tag{163}$$

Regarding the case (I), we obtain using Eq. (161) and our regularity assumptions on V by a direct computation in Fourier space, for $n \geq 4$

$$\left|\left\langle e^{iK\cdot X}, Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_m}(V_N)Q^{\otimes 3}\,\nabla^a\xi_0\right\rangle\right| \lesssim \frac{\sqrt{N}^{k_1+\dots+k_m+a+2m}}{N^2\ell^2} = \frac{\sqrt{N}^n}{N^3\ell^2}.$$

Since the case (II) is similar to the case (III), let us directly have a look at the case (III), where we use the fact that $\|\sqrt{Q^{\otimes 3}V_N Q^{\otimes 3}}R\nabla\| \lesssim 1$ to obtain

$$\begin{aligned}&\left|\left\langle e^{iK\cdot X}, Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_{m-1}}(V_N)Q^{\otimes 3}\,Q^{\otimes 3}V_N Q^{\otimes 3}\,R\xi_0\right\rangle\right| \\ &\quad\lesssim \left\|\sqrt{Q^{\otimes 3}V_N Q^{\otimes 3}}\,Q^{\otimes 3}\nabla^{k_{m-1}}(V_N)Q^{\otimes 3}\dots Q^{\otimes 3}\nabla^{k_1}(V_N)Q^{\otimes 3}\,e^{iK\cdot X}\right\|\left\|\frac{1}{\nabla}Q^{\otimes 3}\xi_0\right\|.\end{aligned} \tag{164}$$

Since we have $\left\|\frac{1}{\nabla}Q^{\otimes 3}\xi_0\right\| \lesssim \frac{1}{N\ell^2}$, we obtain together with Eq. (148) that the term in Eq. (164) is bounded by $\frac{\sqrt{N}^{k_1+\dots+k_m+2(m-1)-2}}{N\ell^2} = \frac{\sqrt{N}^n}{N^3\ell^2}$, which concludes the proof of Eq. (163). Consequently

$$N^{\frac{7}{2}}\langle 1\otimes(R\xi_0(x-y,x-z)),(V_N\otimes 1)1\otimes(R\xi_0(x-y,x-z))\rangle \lesssim \frac{1}{\ell^4}. \tag{165}$$

Using $N^{\frac{7}{2}}\langle 1\otimes(RV_N-1)e^{ik(x_i-x_j)},(V_N\otimes 1)1\otimes(RV_N-1)e^{ik'(x_i-x_j)}\rangle \lesssim N^{\frac{3}{2}}\left(1+\frac{|k-k'|^2}{N}\right)^{-2}$ by Lemma 15 for $i \neq j$, we further have

$$\begin{aligned}&N^{\frac{7}{2}}\langle 1\otimes(RV_N-1)(1-Q^{\otimes 3})\psi_0,(V_N\otimes 1)1\otimes(RV_N-1)(1-Q^{\otimes 3})\psi_0\rangle \\ &\quad\lesssim \sum_{k,k'}N^{\frac{3}{2}}\left(1+\frac{|k-k'|^2}{N}\right)^{-2}\left|\langle e^{ik(x-y)},\psi_0\rangle\right|\left|\langle e^{ik'(x-y)},\psi_0\rangle\right| \\ &\quad\lesssim N^{-\frac{5}{2}}\sum_{k,k'}\left(1+\frac{|k-k'|^2}{N}\right)^{-2}\frac{1}{1+|k|^2}\frac{1}{1+|k'|^2} \lesssim N^{-\frac{3}{2}}.\end{aligned} \tag{166}$$

By Eq. (160) we consequently obtain $\left|\sqrt{N}^{-1}\gamma_N - \gamma^{(\ell)}\right| \lesssim \ell^{-\frac{3}{2}}$ for $\ell \leq \sqrt{N}$. Note that for $\ell_1,\ell_2 > 0$ we can always pick an arbitrary $N \geq \max\{\ell_1,\ell_2\}^2$ yielding

$$\left|\gamma^{(\ell_1)} - \gamma^{(\ell_2)}\right| \lesssim \frac{1}{\min\{\ell_1,\ell_2\}^{\frac{3}{2}}},$$

that is, $\gamma^{(\ell)}$ is convergent with rate $\frac{1}{\ell^{\frac{3}{2}}}$, and by monotone convergence the limit is given by $\gamma(V)$.

In order to establish the convergence of σ_N, let us define $f_{N,\ell} := (V_N\otimes 1)1\otimes\psi_0$, where we keep track of the N and ℓ dependence in our notation, and

$$\sigma_{N,\ell} := N^{\frac{7}{2}}\langle f_{N,\ell}, R_4 f_{N,\ell}\rangle,$$

for $\ell < \sqrt{N}$ and let R_4 be defined above Eq. (96). As a consequence of the operator inequality

$$(V_N\otimes 1)R_4^{(N)}(V_N\otimes 1) \leq (V_N\otimes 1)\frac{1}{-\Delta}(V_N\otimes 1) \lesssim V_N\otimes 1,$$

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we obtain by Eq. (165) and Eq. (166)

$$N^{\frac{7}{2}}\left\langle 1\otimes R\xi_0,(V_N\otimes 1)R_4^{(N)}(V_N\otimes 1)1\otimes R\xi_0\right\rangle \lesssim N^{\frac{7}{2}}\langle 1\otimes R\xi_0,(V_N\otimes 1)1\otimes R\xi_0\rangle \lesssim \frac{1}{\ell^2},$$
$$N^{\frac{7}{2}}\langle 1\otimes (RV_N-1)(1-Q^{\otimes 3})\psi_0,(V_N\otimes 1)R_4^{(N)}(V_N\otimes 1)1\otimes (RV_N-1)(1-Q^{\otimes 3})\psi_0\rangle$$
$$\lesssim N^{\frac{7}{2}}\langle 1\otimes (RV_N-1)(1-Q^{\otimes 3})\psi_0,(V_N\otimes 1)1\otimes (RV_N-1)(1-Q^{\otimes 3})\psi_0\rangle \lesssim N^{-\frac{3}{2}}.$$

Using the identity Eq. (156), this immediately implies for $\ell<\sqrt{N}$

$$\left|\sqrt{N}^{-1}\sigma_N-\sigma_{N,\ell}\right|\lesssim \ell^{-\frac{3}{4}}. \tag{167}$$

To understand the dependence of $\sigma_{N,\ell}$ on the parameter N, recall the function

$$f_\ell(x_1,x_2,x_3):=V(x_1,x_2)\chi^{\frac{1}{\ell}}(x_2,x_3)\omega(x_2,x_3)$$

and $\eta_\ell:\mathbb{R}^9\longrightarrow\mathbb{R}$ from Lemma 14, which solves in the sense of distributions

$$\left(-2\Delta_{\mathcal{M}_*}+\mathbb{V}\right)\eta_\ell=f_\ell. \tag{168}$$

By Lemma 14 we have the point-wise bound $0\leq\eta_\ell\leq\eta_\ell^*$ with

$$\eta_\ell^*(x):=\frac{1}{-2\Delta_{\mathcal{M}_*}}f_\ell(x)=\frac{\Gamma\left(\frac{9}{2}\right)}{28\pi^{\frac{9}{2}}\det[M_*]}\int_{\mathbb{R}^9}\frac{f_\ell(y)\mathrm{d}y}{|\mathcal{M}_*^{-1}(x-y)|^7}.$$

In the following let us write $x_1 g$ for the function $x\mapsto x_1 g(x)$. By Eq. (168) we obtain that $\rho_\ell:=-2\Delta_{\mathcal{M}_*}\eta_\ell$ satisfies the (uniform in ℓ) bounds

$$\|\rho_\ell\|_{L^1(\mathbb{R}^9)}\leq\|f_\ell\|_{L^1(\mathbb{R}^9)}+\|\mathbb{V}\eta_\ell^*\|_{L^1(\mathbb{R}^9)}\lesssim 1, \tag{169}$$

$$\|x_1\rho_\ell\|_{L^1(\mathbb{R}^9)}\leq\|x_1 f_\ell\|_{L^1(\mathbb{R}^9)}+\|\mathbb{V}x_1\eta_\ell^*\|_{L^1(\mathbb{R}^9)}\lesssim 1, \tag{170}$$

where we have used in the second estimates that $f_\ell(x)$ is compactly supported in the variables x_1 and x_2, and satisfies $\sup_{x_1,x_2} f_\ell(x)\lesssim\frac{1}{1+|x_3|^4}$, see the estimates on ω in [23], and therefore $\|(1+|x_1|)f_\ell\|_{L^1(\mathbb{R}^9)}\lesssim 1$, as well as the fact that $x\mapsto\frac{1}{|x|^4}\mathbb{V}(x)\in L^1(\mathbb{R}^9)$ and hence

$$\|\mathbb{V}x\eta_\ell^*\|_{L^1(\mathbb{R}^9)}\lesssim\||x|^5\eta_\ell^*\|_\infty\lesssim\sup_x|x|^5\int_{\mathbb{R}^9}\frac{\mathrm{d}y}{|x-y|^7(|y_1|+|y_2|)^5|y_3|^2}\lesssim 1,$$

and similarly we obtain $\|\mathbb{V}\eta_\ell^*\|_{L^1(\mathbb{R}^9)}\lesssim 1$. Using Eq. (168), we obtain the analogue estimates on the derivatives of ρ_ℓ

$$\left\|\nabla^k\rho_\ell\right\|_{L^1(\mathbb{R}^9)}+\left\|x_1\nabla^k\rho_\ell\right\|_{L^1(\mathbb{R}^9)}\lesssim 1. \tag{171}$$

Having η_ℓ at hand, we use a smooth function χ_* with $\chi_*(x)=1$ for $|x|_\infty\leq\frac{1}{2}$ and $\chi_*(x)=0$ for $|x|_\infty>\frac{2}{3}$, in order to define

$$\Psi:=\chi_*(x_1-x_2,x_1-x_3,x_1-x_4)\,\eta_\ell^{\sqrt{N}}(x_1-x_2,x_1-x_3,x_1-x_4).$$

Notably, the state Ψ allows us to express

$$R_4 f_{N,\ell}=\Psi+R_4\zeta+(R_4\mathbb{V}_N-1)(1-Q^{\otimes 4})\Psi, \tag{172}$$

with $\zeta := [2\Delta_{\mathcal{M}_*}, \chi_*]\eta_\ell^{\sqrt{N}} = 2\Delta_{\mathcal{M}_*}(\chi_*)\eta_\ell^{\sqrt{N}} + 4\mathcal{M}_*^2\nabla(\chi_*)\nabla\eta_\ell^{\sqrt{N}}$ and

$$\mathbb{V}_N(x_1,x_2,x_3,x_4) := N\mathbb{V}\Big(\sqrt{N}(x_1-x_2), \sqrt{N}(x_1-x_3), \sqrt{N}(x_1-x_4)\Big).$$

Proceeding as in the proof of Eq. (154), we have by Eq. (171)

$$\left|\widehat{\zeta}(K)\right| \lesssim N^{-\frac{7}{2}} \min\left\{\frac{1}{|K|^2}, 1\right\}\left(1+\frac{|K|^2}{N}\right)^{-m}. \tag{173}$$

Using the fact that $\|\sqrt{Q^{\otimes 4}\mathbb{V}_N Q^{\otimes 4}} R_4 \nabla\| \leq 1$ we furthermore obtain

$$\left|\widehat{R_4\zeta}(K)\right| = \frac{\left|\widehat{\zeta}(K) - \langle K, \mathbb{V}_N R_4\zeta\rangle\right|}{|K|^2} \leq \frac{\left|\widehat{\zeta}(K)\right| + \sqrt{\langle K, \mathbb{V}_N K\rangle\langle\zeta, \frac{1}{-\Delta}\zeta\rangle}}{|K|^2} \lesssim \frac{\max\{N^{-\frac{1}{4}}, |K|^{-2}\}}{N^{\frac{7}{2}}|K|^2}.$$

Using furthermore Eq. (162), we can utilize Eq. (173) to improve this result to

$$\left|\widehat{R_4\zeta}(K)\right| \lesssim \frac{\max\{N^{-\frac{1}{4}}, |K|^{-1}\}}{N^{\frac{7}{2}}|K|^2}\left(1+\frac{|K|^2}{N}\right)^{-m}. \tag{174}$$

In analogy to Eq. (161), one can show that $\left|\widehat{\chi^{\frac{\sqrt{N}}{\ell}}\omega^{\sqrt{N}}}(k)\right| \lesssim N^{-2}\frac{1}{1+|k|^2}\left(1+\frac{|k|^2}{N}\right)^{-m}$, and therefore we have $\left|\widehat{f}_{N,\ell}(K)\right| \lesssim N^{-\frac{7}{2}}\left(1+\frac{|K|^2}{N}\right)^{-m}$, which yields together with Eq. (174)

$$N^{\frac{7}{2}}\left|\langle f_{N,\ell}, R_4\zeta\rangle\right| \lesssim N^{-\frac{1}{4}}. \tag{175}$$

Furthermore, in analogy to Eq. (174), we have the estimate

$$\left|\widehat{\Psi}(K)\right| \lesssim \frac{1}{N^{\frac{7}{2}}|K|^2}\left(1+\frac{|K|^2}{N}\right)^{-m}.$$

Denoting with $\mathbb{I}$ the set of all indices $K = (k_1, \ldots, k_4)$ such that $k_1 + \cdots + k_4 = 0$ and at least one of the indices satisfies $k_\alpha = 0$, we obtain

$$\begin{aligned} N^{\frac{7}{2}}\left|\langle f_{N,\ell}, (R_4\mathbb{V}_N - 1)(1-Q^{\otimes 4})\Psi\rangle\right| &= N^{\frac{7}{2}}\left|\sum_{K\in\mathbb{I}}\widehat{\Psi}(K)\langle(\mathbb{V}_N R_4 - 1)f_{N,\ell}, e^{iK\cdot X}\rangle\right| \\ &\lesssim N^{-\frac{7}{2}}\sum_{K\in\mathbb{I}}\frac{N^{\frac{3}{4}}}{|K|^2}\left(1+\frac{|K|^2}{N}\right)^{-3} \lesssim N^{-\frac{3}{4}}, \end{aligned} \tag{176}$$

where we used

$$|\langle\mathbb{V}_N R_4 f_{N,\ell}, e^{iK\cdot X}\rangle| \leq \langle e^{iK\cdot X}, \mathbb{V}_N e^{iK\cdot X}\rangle^{\frac{1}{2}}\langle f_{N,\ell}, \frac{1}{-\Delta}f_{N,\ell}\rangle^{\frac{1}{2}} \lesssim N^{-\frac{7}{2}}N^{\frac{3}{4}}.$$

Applying Eq. (172), Eq. (175) and Eq. (176) therefore yields for $\ell < \frac{\sqrt{N}}{2}$

$$\begin{aligned} \sigma_{N,\ell} &= N^{\frac{7}{2}}\langle f_{N,\ell}, R_4 f_{N,\ell}\rangle = N^{\frac{7}{2}}\langle f_{N,\ell}, \Psi\rangle + O_{N\to\infty}\Big(N^{-\frac{1}{4}}\Big) = \langle f_\ell, \eta_\ell\rangle + O_{N\to\infty}\Big(N^{-\frac{1}{4}}\Big) \\ &= \sigma_\ell(V) + O_{N\to\infty}\Big(N^{-\frac{1}{4}}\Big). \end{aligned}$$

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In combination with Eq. (167) and the fact that $\sigma(V) = \lim_\ell \sigma_\ell(V)$, see Lemma 14, we obtain that $|\sigma_\ell(V) - \sigma(V)| \lesssim \frac{1}{\sqrt{\ell}}$ and conclude

$$\left|\sqrt{N}^{-1}\sigma_N - \sigma(V)\right| \lesssim N^{-\frac{1}{4}}.$$

To establish the convergence of $\sqrt{N}^{-1}\mu_N$, let us recall the effective potential

$$V_{\text{eff}} : \begin{cases} \mathbb{R}^3 \longrightarrow \mathbb{R}, \\ x \mapsto \int_{\mathbb{R}^3} V(x,y)(1-\omega(x,y))\,\mathrm{d}y, \end{cases}$$

and let θ solve $-2\Delta\theta = V_{\text{eff}}$ with $\theta(x) \underset{|x|\to\infty}{\longrightarrow} 0$. Then

$$\mu(V) = \int_{\mathbb{R}^3} V_{\text{eff}}(x)\theta(x)\,\mathrm{d}x.$$

Applying the techniques developed in this proof so far, yields furthermore

$$|\sqrt{N}^{-1}\mu_N - \mu(V)| \lesssim \frac{1}{\sqrt{N}}.$$

Finally, in order to establish Eq. (159) let us denote with ω_λ the minimizer in Eq. (4) for the rescaled potential λV, which satisfies $0 \le \omega_\lambda \le 1$ and $\omega_\lambda(x,y) \le \frac{\lambda C(V)}{1+|x|^4+|y|^4}$, for a V dependent, constant $C(V) > 0$. Consequently $\lim_{\lambda\to 0}(1-\omega_\lambda) = 1$, and hence we obtain by dominated convergence

$$\begin{aligned}\lim_{\lambda\to 0}\frac{1}{\lambda^2}\mu(\lambda V) &= \lim_{\lambda\to 0}\int_{\mathbb{R}^{12}} \frac{V(x,u)V(y,v)(1-\omega_\lambda(x,u))(1-\omega_\lambda(y,v))}{8\pi|x-y|}\mathrm{d}u\mathrm{d}v\mathrm{d}x\mathrm{d}y \\ &= \int_{\mathbb{R}^{12}} \frac{V(x,u)V(y,v)}{8\pi|x-y|}\mathrm{d}u\mathrm{d}v\mathrm{d}x\mathrm{d}y \in (0,\infty).\end{aligned}$$

This concludes the proof, since $\sigma(V) \ge 0$ and

$$\frac{1}{\lambda^3}\gamma(\lambda V) \le \frac{3C(V)^2}{2}\int_{\mathbb{R}^9} \frac{V(x,y)}{(1+|y|^4+|z|^4)^2}\mathrm{d}x\mathrm{d}y\mathrm{d}z < \infty. \qquad \square$$

Making use of Eq. (172) again, we can furthermore verify decay properties for the matrix entries of $T_4 - 1$ in momentum space in the subsequent Lemma 18.

Lemma 18. *Recall the definition of the linear map T_2 in Eq. (88) and T_4 in Eq. (95). Then there exists a constant $C > 0$ such that* $|(T_2-1)_{jk,00}| \le CN^{-1}\frac{\mathbb{1}(j+k=0)}{|j|^2+|k|^2}\left(1+\frac{|j|^2+|k|^2}{N}\right)^{-1}$,

$$|(T_4-1)_{\ell ijk,0000}| \le CN^{-\frac{7}{2}}\frac{\mathbb{1}(\ell+i+j+k=0)}{|\ell|^2+|i|^2+|j|^2+|k|^2}\left(1+\frac{|\ell|^2+|i|^2+|j|^2+|k|^2}{N}\right)^{-3}.$$

Proof. For the purpose of verifying the bound on

$$(T_4-1)_{uijk,0000} = \langle e^{iK\cdot X}, R_4(V_N\otimes 1)1\otimes RV_N\rangle$$

with $K = (uijk)$, let us choose $\ell := \frac{\sqrt{N}}{3}$ and recall the elements ζ and Ψ from Eq. (172), and the set $\mathbb{I}$ above Eq. (176), in the proof of Lemma 17. With these elements at hand, we can write

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$$\langle e^{iK\cdot X}, R_4(V_N\otimes 1)1\otimes RV_N\rangle = \langle e^{iK\cdot X}, R_4\zeta\rangle + \langle e^{iK\cdot X}, \Psi\rangle + \sum_{K'\in\mathbb{I}}\langle \mathbb{V}_N R_4 e^{iK\cdot X}, e^{iK'\cdot X}\rangle\langle e^{iK'\cdot X}, \Psi\rangle + \left\langle e^{iK\cdot X}, R_4(V_N\otimes 1)1\otimes\left\{RV_N-\psi\right\}\right\rangle. \tag{177}$$

In the proof of Lemma 17 we have established

$$|\langle e^{iK\cdot X}, R_4\zeta\rangle| = |\widehat{R_4\zeta}(K)| \lesssim \frac{1}{N^{\frac{7}{2}}|K|^2}\left(1+\frac{|K|^2}{N}\right)^{-m},$$
$$|\langle e^{iK\cdot X}, \Psi\rangle| \lesssim \frac{1}{N^{\frac{7}{2}}|K|^2}\left(1+\frac{|K|^2}{N}\right)^{-m}.$$

Regarding the sum over $\mathbb{I}$ we have

$$\left|\sum_{K'\in\mathbb{I}}\langle \mathbb{V}_N R_4 e^{iK\cdot X}, e^{iK'\cdot X}\rangle\langle e^{iK'\cdot X}, \Psi\rangle\right| = \frac{1}{|K|^2}\left|\sum_{K'\in\mathbb{I}}\langle (\mathbb{V}_N-\mathbb{V}_N R_4\mathbb{V}_N) e^{iK\cdot X}, e^{iK'\cdot X}\rangle\langle e^{iK'\cdot X}, \Psi\rangle\right|$$
$$\lesssim \frac{1}{N^{\frac{7}{2}}|K|^2}\sum_{K'\in\mathbb{I}}\frac{\left|\langle (\mathbb{V}_N-\mathbb{V}_N R_4\mathbb{V}_N) e^{iK\cdot X}, e^{iK'\cdot X}\right|\rangle}{|K'|^2}\left(1+\frac{|K'|^2}{N}\right)^{-3} \lesssim \frac{1}{N^{\frac{7}{2}}|K|^2}.$$

Regarding the final term in Eq. (177), we observe that we have the estimate

$$\left|\left\langle e^{iK\cdot X}, R_4(V_N\otimes 1)1\otimes\left\{RV_N-\psi\right\}\right\rangle\right| = \frac{1}{|K|^2}\left|\left\langle (1-R_4\mathbb{V}_N)e^{iK\cdot X}, (V_N\otimes 1)1\otimes\left\{RV_N-\psi\right\}\right\rangle\right|$$
$$\leq \frac{\sqrt{\left\langle 1\otimes\left\{RV_N-\psi\right\}, (V_N\otimes 1)1\otimes\left\{RV_N-\psi\right\}\right\rangle}}{|K|^2}\sqrt{\left\langle (1-R_4\mathbb{V}_N)e^{iK\cdot X}, V_N\otimes 1(1-R_4\mathbb{V}_N)e^{iK\cdot X}\right\rangle}.$$

By Eq. (165) and Eq. (166) we know that $\left\langle 1\otimes\left\{RV_N-\psi\right\}, (V_N\otimes 1)1\otimes\left\{RV_N-\psi\right\}\right\rangle \lesssim N^{-5}$,

$$\left\langle (1-R_4\mathbb{V}_N)e^{iK\cdot X}, V_N\otimes 1(1-R_4\mathbb{V}_N)e^{iK\cdot X}\right\rangle \leq 2\left\langle e^{iK\cdot X}, V_N\otimes 1 e^{iK\cdot X}\right\rangle$$
$$+2\left\langle R_4\mathbb{V}_N e^{iK\cdot X}, V_N\otimes 1 R_4\mathbb{V}_N e^{iK\cdot X}\right\rangle \lesssim \frac{1}{N^2} + \left\langle \mathbb{V}_N e^{iK\cdot X}, R_4\mathbb{V}_N e^{iK\cdot X}\right\rangle$$
$$\lesssim \frac{1}{N^2} + \left\langle e^{iK\cdot X}, \mathbb{V}_N e^{iK\cdot X}\right\rangle \lesssim \frac{1}{N^2}.$$

Finally we note that the bound on T_2 is an immediate consequence of the regularity of V and the bounds on RV_N established in Lemma 15. □

A. Appendix A

In the following we establish comparability results between transformed and nontransformed quantities. The first result in this direction, Lemma A1, establishes that the unitarily transformed powers of the particle number operator $\mathcal{N}$, w.r.t. the transformations U_s and W_s, are again of the same order as the bare powers in $\mathcal{N}$.

Lemma A1. *Let U_s be the unitary map defined below Eq. (70) and W_s the one defined below Eq. (124). Then there exists for all $m\in\mathbb{N}$ constants $C_m>0$, such that*

$$U_{-s}\mathcal{N}^m U_s \leq e^{C_m|s|}(\mathcal{N}+1)^m, \tag{A.1}$$

$$W_{-s}\mathcal{N}^m W_s \leq e^{C_m|s|}(\mathcal{N}+1)^m. \tag{A.2}$$

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Proof. Let us recall the definition of the generator $\mathcal{G}^\dagger - \mathcal{G}$ with

$$\mathcal{G} = \frac{1}{6}\sum_{ijk} \eta_{ijk}\, a_i^\dagger a_j^\dagger a_k^\dagger a_0^3,$$
$$\eta_{ijk} = (T-1)_{ijk,000}$$

of the unitary group U_t from Eq. (70). As a consequence of the bounds on T from Lemma 15, we have

$$\pm\left(\mathcal{G}+\mathcal{G}^\dagger\right) \leq \frac{1}{6}\sum_i\left(a_i^\dagger a_i + \left(\sum_{jk}\eta_{ijk}\, a_j^\dagger a_k^\dagger a_0^3\right)^\dagger\left(\sum_{jk}\eta_{ijk}\, a_j^\dagger a_k^\dagger a_0^3\right)\right) \lesssim \mathcal{N} + \frac{\mathcal{N}^2}{N} \lesssim \mathcal{N}+1.$$

Together with $0 \leq (x+n+3)^k - (x+n)^k \leq C_{n,k}(x+3)^{k-1}$ for a suitable $C_{n,k} > 0$, we obtain

$$\begin{aligned}[\mathcal{G},(\mathcal{N}+3)^m] + \text{H.c.} &= -((\mathcal{N}+3)^m - \mathcal{N}^m)\mathcal{G} + \text{H.c.}\\ &= -\sqrt{(\mathcal{N}+3)^m - \mathcal{N}^m}\left(\mathcal{G}+\mathcal{G}^\dagger\right)\sqrt{(\mathcal{N}+6)^m - (\mathcal{N}+3)^m} + \text{H.c.} \lesssim (\mathcal{N}+3)^m.\end{aligned}$$

Applying Duhamel's formula then yields

$$U_{-t}\,(\mathcal{N}+3)^m U_t - (\mathcal{N}+3)^m = \int_0^t U_{-s}[\mathcal{G},(\mathcal{N}+3)^m]U_s\,\mathrm{d}s + \text{H.c.} \lesssim \int_0^1 U_{-s}(\mathcal{N}+3)^m U_s\,\mathrm{d}s.$$

Consequently Grönwall's inequality gives us

$$U_{-t}\,(\mathcal{N}+3)^m U_t \leq e^{C|t|}(\mathcal{N}+3)^m$$

for a suitable constant $C > 0$, which concludes the proof of Eq. (A.1). The proof of Eq. (A.2) follows analogously from $\pm\left(\mathcal{G}_2+\mathcal{G}_2^\dagger\right) \lesssim \mathcal{N}+1$ and

$$\pm\left(\mathcal{G}_4+\mathcal{G}_4^\dagger\right) \lesssim N^{-3}\left(N(\mathcal{N}+1)^3 + \mathcal{N}^{\frac{5}{2}}\right) \lesssim \mathcal{N}+1,$$

where we have used Lemma 18 in order to control the coefficients of T_2 and T_4. □

In the subsequent Lemma A2 we are going to compare the kinetic energy $\sum_k |k|^{2\tau} a_k^\dagger a_k$ in the operators a_k with a fractional Laplace $(-\Delta)^\tau$, with the corresponding expression in the variables c_k.

Lemma A2. *Let $0 \leq \tau \leq 1$ and $0 \leq \sigma < \frac{1}{2}$. Then $\sum_k |k|^{2\sigma}(c_k - a_k)(c_k - a_k)^\dagger \lesssim \frac{1}{N}\mathcal{N}^2$, and furthermore we have for integers $s \geq 0$*

$$\sum_k |k|^{2\tau} a_k^\dagger \mathcal{N}^s a_k \lesssim \sum_k |k|^{2\tau} c_k^\dagger \mathcal{N}^s c_k + \frac{1}{N}\mathcal{N}^{s+2} + N^\tau(\mathcal{N}+1)^s. \tag{A.3}$$

Proof. Let us define $\left(G_\tau^{(I,I')}\right)_{ij,i'j'} := \frac{1}{4}\sum_k |k|^{2\tau}\overline{(T-1)_{i'j'k,I'}}(T-1)_{ijk,I}$ for

$$I, I' \in \mathcal{I} := \{(0,0,0)\} \cup \bigcup_{0<|\ell|\leq K}\{(\ell,0,0),(0,\ell,0),(0,0,\ell)\}$$

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as well as for $0 \le \gamma \le 1$ the operator-valued vector and matrix

$$(\Phi_\tau)_{jk} := \left(|j|^{2\tau} + |k|^{2\tau}\right)^{\frac{1}{2}} a_j a_k,$$
$$\left(\Upsilon^{(I,I')}_{\gamma,\tau}\right)_{jk,j'k'} := \left(\mathcal{K}^{-\frac{1}{2}}_{\gamma,2} G^{(I,I')}_\tau \mathcal{K}^{-\frac{1}{2}}_{\gamma,2}\right)_{j'k',jk} a_{I_1'} a_{I_2'} a_{I_3'} \mathcal{N}^s a^\dagger_{I_1} a^\dagger_{I_2} a^\dagger_{I_3},$$

with $\mathcal{K}_{\gamma,2} := (-\Delta_x)^\gamma + (-\Delta_y)^\gamma$. With these definitions at hand we obtain

$$\sum_k |k|^{2\tau} (c_k - a_k) \mathcal{N}^s (c_k - a_k)^\dagger = \frac{1}{2} \sum_{I,I'} \Phi^\dagger_\gamma \left(\Upsilon^{(I,I')}_{\gamma,\tau} + \text{H.c.}\right) \Phi_\gamma.$$

For $\gamma > \tau - \frac{1}{2}$ we have by the estimates from Lemma 15 that

$$\|\mathcal{K}^{-\frac{1}{2}}_{\gamma,2} G^{(I,I')}_\tau \mathcal{K}^{-\frac{1}{2}}_{\gamma,2}\| \lesssim N^{-4}.$$

Together with

$$\left\|(\mathcal{N}+1)^{-\frac{s}{2}} a_{I_1'} a_{I_2'} a_{I_3'} \mathcal{N}^s a^\dagger_{I_1} a^\dagger_{I_2} a^\dagger_{I_3} (\mathcal{N}+1)^{-\frac{s}{2}}\right\| \lesssim N^3$$

on the N particle sector, we obtain $\left(\Upsilon^{(I,I')}_{\gamma,\tau} + \text{H.c.}\right) \le \frac{C}{N}(\mathcal{N}+1)^s$ for $\gamma > \tau - \frac{1}{2}$ and a suitable constant C. Using Cauchy-Schwarz we therefore have

$$\sum_k |k|^{2\tau} (c_k - a_k) \mathcal{N}^s (c_k - a_k)^\dagger \lesssim \frac{1}{N} \Phi^\dagger_\gamma (\mathcal{N}+1)^s \Phi_\gamma = 2C \sum_k |k|^{2\gamma} a^\dagger_k \frac{\mathcal{N}^{s+1}}{N} a_k.$$

Applying this result for $\tau' := \sigma$, $\gamma' := 0$ and $s' := 0$, yields the first claim of the Lemma

$$\sum_k |k|^{2\sigma} (c_k - a_k)(c_k - a_k)^\dagger \le \frac{1}{N} \mathcal{N}^2.$$

Concerning Eq. (A.3), we have

$$\sum_k |k|^{2\tau} a^\dagger_k \mathcal{N}^s a_k \le 2 \sum_k |k|^{2\tau} c^\dagger_k \mathcal{N}^s c_k + 2 \sum_k |k|^{2\tau} (c_k - a_k)^\dagger \mathcal{N}^s (c_k - a_k),$$

and furthermore we can express

$$\sum_k |k|^{2\tau} (c_k - a_k)^\dagger \mathcal{N}^s (c_k - a_k) = \sum_{I,I'} \left(f^{I,I'} X^{I,I'}_0 + \sum_{k \neq 0} g^{I,I'}_k a^\dagger_k X^{I,I'}_1 a_k + \frac{1}{2} \Phi^\dagger_\gamma \left(\widetilde{\Upsilon}^{(I,I')}_{\gamma,\tau} + \text{H.c.}\right) \Phi_\gamma \right) \tag{A.4}$$

with

$$X^{I,I'}_0 := a^\dagger_{I_1} a^\dagger_{I_2} a^\dagger_{I_3} \left(\mathcal{N}^s + 2s\mathcal{N}^{s-1} + s(s-1)\mathcal{N}^{s-2}\right) a_{I_1'} a_{I_2'} a_{I_3'},$$
$$X^{I,I'}_1 := a^\dagger_{I_1} a^\dagger_{I_2} a^\dagger_{I_3} \left(2\mathcal{N}^s + 4s\mathcal{N}^{s-1} + 4s(s-1)\mathcal{N}^{s-2} + 2s(s-1)(s-2)\mathcal{N}^{s-3}\right) a_{I_1'} a_{I_2'} a_{I_3'},$$
$$X_2 := a^\dagger_{I_1} a^\dagger_{I_2} a^\dagger_{I_3} \Big(\mathcal{N}^s + 4s\mathcal{N}^{s-1} + 6s(s-1)\mathcal{N}^{s-2} + 4s(s-1)(s-2)\mathcal{N}^{s-3}$$
$$+ s(s-1)(s-2)(s-3)\mathcal{N}^{s-4}\Big) a_{I_1'} a_{I_2'} a_{I_3'},$$

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$$f^{I,I'} := \sum_{ij}\left[\left(G_\tau^{I,I'}\right)_{ij,ij} + \left(G_\tau^{I,I'}\right)_{ij,ji}\right],$$

$$g_j^{I,I'} := \sum_{i}\left[\left(G_\tau^{I,I'}\right)_{ij,ij} + \left(G_\tau^{I,I'}\right)_{ij,ji}\right],$$

$$\widetilde{\Upsilon}_{\gamma,\tau}^{(I,I')} := \left(\mathcal{K}_{\gamma,2}^{-\frac{1}{2}} G_\tau^{(I,I')} \mathcal{K}_{\gamma,2}^{-\frac{1}{2}}\right)_{j'k',jk} X_2.$$

Following the proof of the first part of the Lemma, we obtain for $\gamma > \tau - \frac{1}{2}$

$$\frac{1}{2}\sum_{I,I'} \Phi_\gamma^\dagger\left(\widetilde{\Upsilon}_{\gamma,\tau}^{(I,I')} + \text{H.c.}\right)\Phi_\gamma \lesssim \sum_k |k|^{2\gamma} a_k^\dagger \frac{\mathcal{N}^{s+1}}{N} a_k.$$

Using Lemma 15 again, yields $|f| \lesssim N^{\tau-3}$ and $|g_j| \lesssim N^{\max\{\tau-\frac{1}{2},0\}} - 4$, and consequently

$$f^{I,I'} X_0^{I,I'} + \sum_{k\neq 0} g_k^{I,I'} a_k^\dagger X_1^{I,I'} a_k \lesssim N^\tau \mathcal{N}^s + N^{\max\{\tau-\frac{1}{2},0\}} \frac{\mathcal{N}^{s+1}}{N} \lesssim N^\tau \mathcal{N}^s.$$

Summarizing what we have so far we obtain for $\gamma > \tau - \frac{1}{2}$

$$\sum_k |k|^{2\tau} a_k^\dagger \mathcal{N}^s a_k \lesssim \sum_k |k|^{2\tau} c_k^\dagger \mathcal{N}^s c_k + \frac{1}{N}\sum_k |k|^{2\gamma} a_k^\dagger \mathcal{N}^{s+1} a_k + N^\tau (\mathcal{N}+1)^s.$$

Choosing $\gamma := \max\{\tau - \frac{1}{3}, 0\}$ and iterating this equation at most two times with $\tau' := \max\{\tau - \frac{1}{3}, 0\}$ and $\gamma' := \max\{\gamma - \frac{1}{3}, 0\}$, and using $\mathcal{N} \leq N$, yields the desired statement. □

Similar to Lemma A2, the following Lemma A3 allows us to compare the operators

$$\tilde{c}_k := a_k + \frac{1}{2}\sum_{ij} (T-1)_{ijk,000} a_i^\dagger a_j^\dagger a_0^3$$

with the operators c_k.

Lemma A3. *Then there exists a $C > 0$, such that*

$$\sum_k |k|^2 \tilde{c}_k^\dagger \tilde{c}_k \leq C\left(\sum_k |k|^2 c_k^\dagger c_k + \mathcal{N} + 1\right).$$

Proof. Similar to Eq. (A.4), we can write

$$\sum_k |k|^2 (c_k - \tilde{c}_k)^\dagger (c_k - \tilde{c}_k) = \sum_{I,I'\neq 0}\left(f^{I,I'} X_0^{I,I'} + \sum_{k\neq 0} g_k^{I,I'} a_k^\dagger X_1^{I,I'} a_k + \frac{1}{2}\Phi_1^\dagger\left(\widetilde{\Upsilon}_{1,1}^{(I,I')} + \text{H.c.}\right)\Phi_1\right),$$

where $f^{I,I'}, g_k^{I,I'}, \widetilde{\Upsilon}_{1,1}^{(I,I')}, X_0^{I,I'}$ and $X_1^{I,I'}$ are defined below Eq. (A.4) for the concrete choice $s := 0$ and

$$(\Phi_1)_{jk} := \left(|j|^2 + |k|^2\right)^{\frac{1}{2}} a_j a_k.$$

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Using $I, I' \neq 0$, we obtain the improved estimates $\pm X_0^{I,I'} \lesssim N^2\mathcal{N}$ and $\pm X_1^{I,I'} \lesssim N^2\mathcal{N}$. Consequently

$$\pm (f^{I,I'} X_0^{I,I'} + \text{H.c.}) \lesssim \mathcal{N},$$
$$(\sum_{k\neq 0} g_k^{I,I'} a_k^\dagger X_1^{I,I'} a_k + \text{H.c.}) \lesssim N^{-\frac{3}{2}}\mathcal{N}^2 \leq \mathcal{N}.$$

Furthermore,

$$\pm\frac{1}{2}\Phi_1^\dagger\Big(\widetilde{\Upsilon}_{1,1}^{(I,I')} + \text{H.c.}\Big)\Phi_1 \lesssim \sum_k |k|^2 a_k^\dagger \frac{\mathcal{N}}{N} a_k \lesssim \sum_k |k|^2 c_k^\dagger c_k + \mathcal{N} + 1,$$

where we have used Eq. (40) in the last estimate. □

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Competing interest. The authors have no competing interest to declare.

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