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Free Energies of Dilute Bose Gases: Upper Bound

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Abstract We derive an upper bound on the free energy of a Bose gas at density ϱ and temperature T. In combination with the lower bound derived previously by Seiringer (Commun. Math. Phys. 279(3): 595–636, 2008), our result proves that in the low density limit, i.e., when $a^3\varrho \ll 1$, where a denotes the scattering length of the pair-interaction potential, the leading term of Δf, the free energy difference per volume between interacting and ideal Bose gases, is equal to $4\pi a(2\varrho^2 - [\varrho - \varrho_c]_+^2)$. Here, $\varrho_c(T)$ denotes the critical density for Bose–Einstein condensation (for the ideal Bose gas), and $[\cdot]_+ = \max\{\cdot, 0\}$ denotes the positive part.

Keywords Bose gas · Free energy · Variational principle

1 Introduction

The ground state energy and the free energy are the fundamental properties of a quantum system and they have been intensively studied since the invention of the quantum mechanics. The recent progresses in experiments on Bose-Einstein condensation, especially the achievement of Bose-Einstein condensation in dilute gases of alkali atoms in 1995 [1], have inspired re-examination of the theoretic foundation concerning the Bose system, e.g., [3, 4, 6, 9, 11–13, 18] and [17] on ground state energy and [15] on free energy.

In the low density limit, the leading term of the ground state energy per volume was identified rigorously by Dyson (upper bound) [2] and Lieb-Yngvason (lower bound) [13] to be $4\pi a\varrho^2$, where a is the scattering length of the two-body potential and ϱ is the density. We note that $4\pi a\varrho^2$ is also the first leading term of ΔE, the ground state energy difference per volume between interacting and ideal Bose gases. (The ground state energy per volume of the ideal Bose gas is zero.)

On the other hand, the first leading term of Δf, the free energy difference between interacting and ideal Bose gases, is the second leading order term of the free energy per

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volume f. More specifically, if $a^3\varrho \ll 1$, where a denotes the scattering length of the pair-interaction potential, then

$$f(\varrho, T) = f_0(\varrho, T) + 4\pi a(2\varrho^2 - [\varrho - \varrho_c]_+^2) + o(a\varrho^2) \tag{1.1}$$

Here, f is the free energy per volume of the interacting Bose gas, f_0 is the one of the ideal Bose gas, $\varrho_c(T)$ denotes the critical density for Bose-Einstein condensation (for the ideal gas), and $[\cdot]_+ = \max\{\cdot, 0\}$ denotes the positive part. The lower bound on f has been proved in Seiringer's work [15]. In this paper, we prove the upper bound on f and obtain the main result (1.1).

The trial state we use in this proof is of a new type, which was first used in [17]. Let ϕ_0 be the ground state of the ideal Bose gas. In [17], we constructed a trial state (pure state) for interacting Bose gases which is obtained by slightly modifying a state of the following form,

$$\exp\left[\sum_{k\sim 1}\sum_{v\sim\sqrt{\varrho}} 2\sqrt{\lambda_{k+v/2}\lambda_{-k+v/2}}a^\dagger_{k+v/2}a^\dagger_{-k+v/2}a_v a_0 + \sum_k c_k a^\dagger_k a^\dagger_{-k} a_0 a_0\right]|\phi_0\rangle \tag{1.2}$$

(with suitably chosen c and λ). Here the notation $A \sim B$ means that A and B have the same order. The expression of (1.2) is simple but it is hard to use itself for our calculation in [17]. If one tried to write (1.2) with the occupation-number representation as (for calculating interaction energies)

$$\sum_\alpha f_\alpha |\alpha\rangle, \tag{1.3}$$

he will see that it is very hard to calculate f_α's. Therefore in [17], we constructed a trial state $\sum_\alpha \tilde{f}_\alpha|\alpha\rangle$ by defining $\tilde{f}_\alpha$ directly. The $\tilde{f}_\alpha$'s have many properties, which have no physical meaning but can simplify our proof. E.g. if the state $|\alpha\rangle$ contains a particle with extremely high momentum, then $\tilde{f}_\alpha = 0$. Furthermore, the trial state $\sum_\alpha \tilde{f}_\alpha|\alpha\rangle$ is very close to (1.2) i.e., for some $c > 0$,

$$\sum_\alpha |f_\alpha - \tilde{f}_\alpha|^2\langle\alpha|\alpha\rangle \ll \varrho^c. \tag{1.4}$$

This basic idea will be used again in this paper.

This trial state (pure state) in [17] is used to rigorously prove the upper bound of the second order correction to the ground state energy, which was first computed by Lee-Yang [8] (see also Lee-Huang-Yang [7] and the recent paper by Yang [16] for results in other dimensions. Another derivation was later given by Lieb [10] using a self-consistent closure assumption for the hierarchy of correlation functions.)

We can rewrite the pure state (1.2) as follows

$$(1.2) = P_{(0,0)}P_{(0,\sqrt{\varrho})}|\phi_0\rangle \tag{1.5}$$

where

$$\begin{aligned} P_{(0,0)} &= \exp\left[\sum_{k\sim 1} c_k a^\dagger_k a^\dagger_{-k} a_0 a_0\right] \\ P_{(0,\sqrt{\varrho})} &= \exp\left[\sum_{k\sim 1}\sum_{v\sim\sqrt{\varrho}} 2\sqrt{\lambda_{k+v/2}\lambda_{-k+v/2}}a^\dagger_{k+v/2}a^\dagger_{-k+v/2}a_v a_0\right] \end{aligned} \tag{1.6}$$

We note: $P_{(0,0)}$ represents the interactions between condensate and condensate, since in the operator $a_k^\dagger a_{-k}^\dagger a_0 a_0$ two particles with momenta zero are annihilated ($a_0 a_0$) and two particles with high momentum are created ($a_k^\dagger a_{-k}^\dagger$). Similarly $P_{(0,\sqrt{\varrho})}$ represents the interaction between condensate and the particles with momentum of order $\varrho^{1/2}$, since in this operator one particle with momentum zero and one with momentum of order $\varrho^{1/2}$ are annihilated ($a_v a_0$) and two particles with high momenta are created.

In this paper, we construct a trial state of a similar form. More specifically, let Γ_I be Gibbs state of the ideal Bose gas at temperature T. The trial state we are going to use is very close to

$$\Gamma \sim \left(P_{(\varrho^{1/3},\varrho^{1/3})} P_{(0,\varrho^{1/3})} P_{(0,0)}\right) \Gamma_I \left(P_{(\varrho^{1/3},\varrho^{1/3})} P_{(0,\varrho^{1/3})} P_{(0,0)}\right)^\dagger \tag{1.7}$$

where

$$\begin{aligned} P_{(0,0)} &= \exp\left[\sum_{k\sim 1} c_k a_k^\dagger a_{-k}^\dagger a_0 a_0\right] \\ P_{(0,\varrho^{1/3})} &= \exp\left[\sum_{k\sim 1}\sum_{v\sim\varrho^{1/3}} 2\sqrt{\lambda_{k+v/2}\lambda_{-k+v/2}}\, a_{k+v/2}^\dagger a_{-k+v/2}^\dagger a_v a_0\right] \\ P_{(\varrho^{1/3},\varrho^{1/3})} &= \exp\left[\sum_{k\sim 1}\sum_{u\neq v\sim\varrho^{1/3}} \sqrt{\lambda_{k+\frac{v+u}{2}}\lambda_{-k+\frac{v+u}{2}}}\, a_{k+\frac{v+u}{2}}^\dagger a_{-k+\frac{v+u}{2}}^\dagger a_v a_u\right] \end{aligned} \tag{1.8}$$

where the constant 2 comes from the ordering of $a_v a_0$. As one can see, $P_{(0,0)}$ represents the interactions between condensate and condensate, $P_{(0,\varrho^{1/3})}$ represents the interaction between condensate and the particles with momentum of order $\varrho^{1/3}$, and $P_{(\varrho^{1/3},\varrho^{1/3})}$ represents the interaction between the particles with momentum of order $\varrho^{1/3}$.

2 Model and Main Results

2.1 Hamiltonian and Notations

We consider a Bose gas which is composed of N identical bosons confined to a cubic box Λ of side length L. The Hilbert space $\mathcal{H}_{N,\Lambda}$ for the system is the set of symmetric functions in $L^2(\Lambda^N)$. The Hamiltonian is given as

$$H_{N,\Lambda} = -\sum_{i=1}^N \Delta_i + \sum_{1\le i<j\le N} V(x_i - x_j) \tag{2.1}$$

Here $x_i \in \Lambda$ $(1 \le i \le N)$ is the position of ith particle. The two body interaction is given by a spherically symmetric non-negative function V, such that $\|V\|_\infty < \infty$, as in [17] and [3]. In the proof on the lower bound of the free energy, [15], the V is assumed to have a finite range R_0, i.e., $V(r) = 0$ for $r > R_0$. Therefore we will also use this assumption in this paper. In particular, it has a finite scattering length, which we denote by a.

We note that the interaction only depends on the distance between the particles. As usually, we denote by $H^P_{N,\Lambda}$ ($H^D_{N,\Lambda}$) the Hamiltonians with periodic (Dirichlet) boundary conditions. (Here $x_i - x_j$ in (2.1) is really the distance on the torus in the periodic case.)

In periodic case, we can also write Hamiltonian with creation and annihilation operators as follows. The dual space of Λ is $\Lambda^* := (\frac{2\pi}{L}\mathbb{Z})^3$. For a continuous function F on $\mathbb{R}^3$, we have

$$\frac{1}{L^3}\sum_{p\in\Lambda^*}F(p)=\frac{1}{|\Lambda|}\sum_{p\in\Lambda^*}F(p)\overset{|\Lambda|\to\infty}{\longrightarrow}\int_{\mathbb{R}^3}\frac{\mathrm{d}^3p}{(2\pi)^3}F(p) \tag{2.2}$$

The Fourier transform is defined as

$$\widehat{V}_p=\int_\Lambda e^{-ipx}V(x)\mathrm{d}x,\qquad V(x)=\frac{1}{|\Lambda|}\sum_{p\in\Lambda^*}e^{ipx}\widehat{V}_p$$

and then

$$\frac{1}{|\Lambda|}\sum_{p\in\Lambda^*}e^{ipx}=\delta_{\mathbb{R}^3}(x),\qquad \int_\Lambda e^{ipx}\mathrm{d}x=\delta_{\Lambda^*}(p)$$

where $\delta_{\mathbb{R}^3}(x)$ is the usual continuum delta function and the function $\delta_{\Lambda^*}(p)=|\Lambda|=L^3$ if $p=0$ (otherwise it is zero) is the lattice delta-function. We will neglect the subscript; the argument indicates whether it is the momentum or position space delta function. In general we will also neglect the hat in the Fourier transform. To avoid confusion, we follow the convention that the variables x, y, z, etc. denote position space, the variables p, q, k, u, v, etc. denote momentum space. We also simplify the notation

$$\sum_p := \sum_{p\in\Lambda^*}$$

i.e. momentum summation is always over Λ^*. We will use the bosonic operators with the commutator relations

$$[a_p,a_q^\dagger]=a_pa_q^\dagger-a_q^\dagger a_p=\begin{cases}1 & \text{if } p=q\\ 0 & \text{otherwise.}\end{cases}$$

Thus our Hamiltonian in the Fock space $\mathcal{F}_\Lambda=\oplus_N\mathcal{H}_{N,\Lambda}$ is given by

$$H_\Lambda^P=\sum_p p^2a_p^\dagger a_p+\frac{1}{|\Lambda|}\sum_{p,q,u}\frac{\widehat{V}_u}{2}a_p^\dagger a_q^\dagger a_{p-u}a_{q+u} \tag{2.3}$$

2.2 Free Energy

The free energy per unit volume of the system at temperature $T=\beta^{-1}>0$ and density $\varrho=N/|\Lambda|>0$ in the cubic box Λ is defined as

$$f(\varrho,\Lambda,\beta)\equiv-\frac{1}{|\Lambda|\beta}\ln\left(\mathrm{Tr}_{\mathcal{H}_{N,\Lambda}}\mathrm{Exp}(-\beta H_{N,\Lambda})\right) \tag{2.4}$$

Let $f^P(\varrho,\Lambda,\beta)$ and $f^D(\varrho,\Lambda,\beta)$ denote the free energy per unit volume of the system with periodic or Dirichlet boundary conditions. Furthermore, we denote by $f(\varrho,\beta)$ the free energy (per unit volume) in the thermodynamic limit, i.e., $|\Lambda|$, $N\to\infty$ with $\varrho=N/|\Lambda|$ fixed, i.e.,

$$f^{P(D)}(\varrho,\beta)\equiv\lim_{|\Lambda|\to\infty}f^{P(D)}(\varrho,\Lambda,\beta) \tag{2.5}$$

As mentioned in the introduction, in this paper we give an upper bound on the leading order correction of $f(\varrho,\beta)$, compared with an ideal gas, in the case that $a^3\varrho$ is small and $\beta\varrho^{2/3}$ is order one. We note that $a^3\varrho$ and $\beta\varrho^{2/3}$ are dimensionless quantities.

2.3 Ideal Bose Gas in the Thermodynamic Limit

In this section, we review some well known results on ideal Bose gases. In the case of vanishing interaction potential ($V=0$), the free energy per unit volume in the thermodynamic limit can be evaluated explicitly. Let ζ denote the Riemann zeta function. It is well known that when $\varrho^{2/3}\beta \geq (4\pi)^{-1}\zeta(3/2)^{2/3}$, i.e., ϱ is greater than critical density ϱ_c,

$$\varrho \geq \varrho_c \equiv (4\pi\beta)^{-3/2}\zeta(3/2) \tag{2.6}$$

the free energy in the thermodynamic limit is given as

$$f_0^{D(P)}(\varrho,\beta) = \frac{1}{(2\pi)^3\beta}\int_{\mathbb{R}^3}\ln(1-e^{-\beta p^2})d^3p \tag{2.7}$$

On the other hand, when $\varrho \leq \varrho_c$,

$$f_0^{D(P)}(\varrho,\beta) = \varrho\mu + \frac{1}{(2\pi)^3\beta}\int_{\mathbb{R}^3}\ln(1-e^{-\beta(p^2-\mu)})d^3p \tag{2.8}$$

Here $\mu(\varrho,\beta)<0$ is determined by

$$\varrho = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\frac{1}{e^{\beta(p^2-\mu)}-1}d^3p \tag{2.9}$$

Note: when $\varrho \geq \varrho_c$, $\mu(\varrho,\beta)$ is defined as zero.

It is easy to see the scaling relation:

$$f_0^{D(P)}(\varrho,\beta) = \varrho^{5/3} f_0^{D(P)}(1,\varrho^{2/3}\beta)$$

and the ration ϱ_c/ϱ only depends on dimensionless quantity $\varrho^{2/3}\beta$, i.e.,

$$\varrho_c/\varrho = (4\pi)^{-3/2}\zeta(3/2)(\varrho^{2/3}\beta)^{-3/2} \tag{2.10}$$

Let $\beta(\varrho)$ be a function of ϱ, we define $R[\beta]$ as the ratio ϱ_c/ϱ in the limit $\varrho\to 0$, i.e.,

$$R[\beta] \equiv \lim_{\varrho\to 0}\varrho_c(\beta)/\varrho = \lim_{\varrho\to 0}(4\pi)^{-3/2}\zeta(3/2)\left(\varrho^{2/3}\beta(\varrho)\right)^{-3/2} \tag{2.11}$$

2.4 Scattering Length

In this paper, we use the standard definition of scattering length, as in [3, 4, 6, 13, 15, 17, 18]. Let $1-w$ be the zero energy scattering solution, i.e.,

$$-\Delta(1-w) + \frac{1}{2}V(1-w) = 0 \tag{2.12}$$

with $0 \leq w < 1$ and $w(x)\to 0$ as $|x|\to\infty$. Then the scattering length is given by the formula

$$a := \frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{1}{2}V(x)(1-w(x))\mathrm{d}x \tag{2.13}$$

With (2.12), we have, for $p \neq 0$,

$$w_p = \left[\frac{1}{2}V(1-w)\right]_p |p|^{-2}. \tag{2.14}$$

Because $V(1-w) \geq 0$, so for $\forall p$,

$$\left|[V(1-w)]_p\right| \leq \int V(1-w).$$

Then with (2.13), i.e., $\int \frac{1}{2}V(1-w)$ is equal to $4\pi a$, we obtain the following bound on w_p

$$\left|w_p\right| \leq 4\pi a|p|^{-2} \tag{2.15}$$

Furthermore, when V is C^∞ function with compact support, one can easily prove that

$$\left|\frac{dw_p}{dp}\right| \leq \text{const.}\left(|p|^{-3} + |p|^{-2}\right) \tag{2.16}$$

Here the constant only depends on a and R_0.

2.5 Main Results

Theorem 1 *Let $V(x) \geq 0$ be a bounded, piecewise continuous function with compact support. In the temperature region where $\lim_{\varrho\to 0}\varrho^{2/3}\beta(\varrho) \in (0,\infty)$ and in the thermodynamic limit, we have the following upper bound on the free energy difference per volume between the interacting Bose gas $f^D(\varrho,\beta)$ and the ideal Bose gas $f_0^D(\varrho,\beta)$*:

$$\overline{\lim}_{\varrho\to 0}\left(f^D(\varrho,\beta) - f_0^D(\varrho,\beta)\right)\varrho^{-2} \leq 4\pi a(2 - [1 - R[\beta]]_+^2), \tag{2.17}$$

where $R[\beta]$ is defined in (2.11) as the ratio ϱ_c/ϱ in the limit $\varrho \to 0$, and a is the scattering length of V.

It is well known that the effect of boundary conditions for free particles in the thermodynamic limit is negligible, i.e.,

$$f_0(\varrho,\beta) \equiv f_0^D(\varrho,\beta) = f_0^P(\varrho,\beta) = f_0^N(\varrho,\beta) = f_0^R(\varrho,\beta) \tag{2.18}$$

where N denotes Neumann condition and R denotes Robin boundary condition: $\partial u/\partial\nu = -\alpha u$ (for some given constant $\alpha > 0$, with ν denoting the outward normal).

On the other hand, the Propositions 2.3.5 and 2.3.7 of [14] show that

$$f^D(\varrho,\beta) = f^P(\varrho,\beta) = f^N(\varrho,\beta) = f^R(\varrho,\beta). \tag{2.19}$$

Therefore, with the results on lower bound in Seiringer's work [15], we can obtain the following result.

Corollary 1 *Under the assumption of Theorem 1, in Dirichlet, periodic, Neumann and Robin boundary condition, we have*:

$$\lim_{\varrho\to 0}\left(f^{P(N,D,R)}(\varrho,\beta) - f_0(\varrho,\beta)\right)\varrho^{-2} = 4\pi a(2 - [1 - R[\beta]]_+^2), \tag{2.20}$$

3 Basic Strategy

3.1 Reduction to Small Torus with Periodic Boundary Conditions

To obtain the upper bound to the free energy, we can use the variational principle, which states that, for any state $\Gamma^{D(P)}$ $(\mathcal{H}_N \to \mathcal{H}_N)$ in the domain of $H^{D(P)}_{N,\Lambda}$ (we will omit these superscripts of H since it will be clear from the context what they are), the following inequality holds.

$$f^{D(P)}(\varrho, \Lambda, \beta) \le \frac{1}{|\Lambda|} \mathrm{Tr}_{\mathcal{H}_{N,\Lambda}} H_{N,\Lambda} \Gamma^{D(P)} - \frac{1}{|\Lambda|\beta} S(\Gamma^{D(P)}) \tag{3.1}$$

Here, $S(\Gamma) = -\mathrm{Tr}\,\Gamma \ln \Gamma$ denotes the von Neumann entropy. Hence, to prove Theorem 1, one only needs to construct a trial states $\Gamma^D(\varrho, \Lambda, \beta)$ satisfying Dirichlet boundary condition and the following inequality:

$$\begin{aligned}&\overline{\lim}_{\varrho\to 0}\overline{\lim}_{|\Lambda|\to\infty}\left(\frac{1}{|\Lambda|}\mathrm{Tr}\, H_{N,\Lambda}\Gamma^D - \frac{1}{|\Lambda|\beta} S(\Gamma^D) - f_0^D(\varrho,\beta)\right)\varrho^{-2}\\ &\quad\le 4\pi a(2 - [1 - R[\beta]]_+^2)\end{aligned} \tag{3.2}$$

Furthermore, the proper trial states in the thermodynamic limit ($\Lambda \to \infty$) can be constructed by duplicating the proper trial states in the *small* boxes ($|\Lambda| = \varrho^{-c}, c > 2$) with Dirichlet boundary condition. (Let the distance between the adjacent small boxes be R_0. Therefore there is no interaction between different boxes.) Hence, the following Proposition 1 implies our main result, Theorem 1.

Note: Late we will choose the volume of the small box as $\varrho^{-2-\varepsilon}$, where ε is a small positive number. As one can see that, when size of the box is too small, the Dirichlet Boundary condition will affect (increase) the (total) free energy. When the volume of the small box is $O(\varrho^{-2})$, we noticed that we can not prove that the effect of Dirichlet Boundary condition is much less than the effect of the interaction. Therefore, to study the effect of the interaction, we have to choose the volume of the small box as $\varrho^{-2-\varepsilon}$.

Proposition 1 *In the temperature region where* $\lim_{\varrho\to 0}\varrho^{2/3}\beta(\varrho) \in (0,\infty)$, *for fixed scattering length* a, *there exist* Λ *with* $|\Lambda| \ge \varrho^{-41/20}$ *and trial states* $\Gamma^D(\varrho,\Lambda,\beta)$ *satisfying the Dirichlet boundary condition and the inequality* (*set* $N = |\Lambda|\varrho$)

$$\begin{aligned}&\overline{\lim}_{\varrho\to 0}\left(\frac{1}{|\Lambda|}\mathrm{Tr}\, H_{N,\Lambda}\Gamma^D - \frac{1}{|\Lambda|\beta} S(\Gamma^D) - f_0^D(\varrho,\beta)\right)\varrho^{-2}\\ &\quad\le 4\pi a(2 - [1 - R(\beta)]_+^2),\end{aligned} \tag{3.3}$$

where $R(\beta)$ *is defined in* (2.11).

Here the number $41/20$ in the assumption can be replaced with any number larger than 2.

On the other hand, the next lemma shows that a Dirichlet boundary condition trial state with correct free energy can be obtained from a periodic trial state in a slightly smaller box.

Lemma 1 *Let the volume* $|\Lambda|$ *be equal to* $\varrho^{-41/20}$. *In the temperature region of Theorem* 1, *if*

$$f^P(\varrho, \Lambda, \beta) \le \text{const. } \varrho^{5/3}, \tag{3.4}$$

then for the revised box Λ^* *and density* ϱ^*, *defined by*

$$|\Lambda^*| \equiv |\Lambda|(1+2\varrho^{41/120})^3, \qquad \varrho^* \equiv \varrho(1+2\varrho^{41/120})^{-3}, \tag{3.5}$$

we have $f^D(\varrho^*, \Lambda^*, \beta)$ *bounded from above as follows*

$$\overline{\lim}_{\varrho\to 0}\left(f^D(\varrho^*, \Lambda^*, \beta) - f^P(\varrho, \Lambda, \beta)\right)\varrho^{-2} \le 0 \tag{3.6}$$

Lemma 1 can be proved with standard methods as in [17] and we postpone the proof to Sect. 12.1.

We note: $|\Lambda^*| \ge (\varrho^*)^{-41/20}$, and satisfies the assumption in Proposition 1. The construction of a periodic trial state yielding the correct free energy upper bound is the core of this paper. We state it as the following theorem, which gives the upper bound on $f^P(\varrho, \Lambda, \beta)$ in (3.4) and (3.6).

Theorem 2 *Assume* $\lim_{\varrho\to 0}\varrho^{2/3}\beta \in (0,\infty)$. *For* $|\Lambda| = \varrho^{-41/20}$ *and* $N = |\Lambda|\varrho$, *there exists a periodic trial state* $\Gamma(\varrho, \Lambda, \beta)$ *satisfying*

$$\overline{\lim}_{\varrho\to 0}\left(\frac{1}{|\Lambda|}\operatorname{Tr} H_N\Gamma - \frac{1}{|\Lambda|\beta}S(\Gamma) - f_0^P(\varrho,\beta)\right)\varrho^{-2} \le 4\pi a(2-[1-R[\beta]]_+^2) \tag{3.7}$$

It implies

$$\overline{\lim}_{\varrho\to 0}\left(f^P(\varrho, \Lambda, \beta) - f_0^P(\varrho,\beta)\right)\varrho^{-2} \le 4\pi a(2-[1-R[\beta]]_+^2) \tag{3.8}$$

3.2 Proof of Proposition 1

To prove Proposition 1, we can directly apply Lemma 1 and Theorem 2. Lemma 1 shows that the upper bound of the free energy (with Dirichlet boundary conditions) is sightly larger than the one (with Periodic boundary conditions) in a slightly smaller box. In the smaller box the density is sightly increased. But the temperature is unchanged. Therefore the relation between temperature and density is different from the one in the initial small box. In this subsection, we will show that this difference will not affect our result(up to the order ϱ^2).

Proof of Proposition 1 Using the temperature function β in the assumption of Proposition 1, we define a new temperature function $\tilde\beta$ as follows

$$\tilde\beta : \tilde\beta(\varrho) = \beta(\varrho^*), \tag{3.9}$$

where $\varrho^* = \varrho(1+2\varrho^{41/120})^{-3}$, as in (3.5).

Insert the result in Theorem 2 into Lemma 1. With the definition of Λ^*, ϱ^* in Lemma 1 (3.5), we obtain at the inverse temperature $\tilde\beta(\varrho)$,

$$\overline{\lim}_{\varrho\to 0}\left(f^D(\varrho^*, \Lambda^*, \tilde\beta) - f_0^P(\varrho,\tilde\beta)\right)\varrho^{-2} \le 4\pi a(2-[1-R[\tilde\beta]]_+^2). \tag{3.10}$$

Since $\varrho^* = \varrho(1+o(\varrho^{1/3}))$, we have the following equalities on the free energies of ideal Bose gases in the thermodynamic limit:

$$f_0^P(\varrho,\tilde\beta) = f_0^D(\varrho,\tilde\beta) = f_0^D(\varrho^*,\tilde\beta)(1+o(\varrho^{1/3})). \tag{3.11}$$

Therefore, we can replace $f_0^P(\varrho, \tilde{\beta})$ in (3.10) with $f_0^D(\varrho^*, \tilde{\beta})$, i.e.,

$$\overline{\lim}_{\varrho\to 0}\left(f^D(\varrho^*, \Lambda^*, \tilde{\beta}) - f_0^D(\varrho^*, \tilde{\beta})\right)\varrho^{-2} \le 4\pi a(2 - [1 - R[\tilde{\beta}]]_+^2). \tag{3.12}$$

Then by the definition of $\tilde{\beta}$ in (3.9), we obtain $R[\beta] = R[\tilde{\beta}]$, so

$$\begin{aligned}\overline{\lim}_{\varrho\to 0}\left(f^D(\varrho^*, \Lambda^*, \beta(\varrho^*)) - f_0^D(\varrho^*, \beta(\varrho^*))\right)\varrho^{-2} &\le 4\pi a(2 - [1 - R[\beta]]_+^2)\\ &= 4\pi a(2 - [1 - R[\tilde{\beta}]]_+^2)\end{aligned}$$

Finally, using that $\Lambda^* \ge (\varrho^*)^{-\frac{41}{20}}$ and the fact that the limit $\varrho \to 0$ is equivalent to the limit $\varrho^* \to 0$, we arrive at the desired result (3.3). □

3.3 Outline of the Proof of Theorem 2: Reduction to Pure States

As we showed in Appendix, for any non-negative, bound, piecewise continuous, spherically symmetric function f supported in unit ball, there exist C^∞ non-negative, spherically symmetric function $f_1, f_2, \dots$ supported in the ball of radius 2, such that for any $i \ge 1$,

$$f_i - f \ge 0 \quad \text{and} \quad \lim_{i\to\infty} \|f_i - f\|_1 \to 0 \tag{3.13}$$

Therefore, for any $\varepsilon > 0$, there exists a C^∞ function V^ε with compact support such that $V^\varepsilon \ge V$ and the scattering length of V^ε is less than $a + \varepsilon$. By the definition of free energy and the variational principle,

$$f(\varrho, \beta, \Lambda) \le f^\varepsilon(\varrho, \beta, \Lambda) \tag{3.14}$$

where f^ε corresponds to the Bose gas with interaction V^ε. Therefore to prove Theorem 2 and (3.7), we only need to focus on the V's that are C^∞-functions and have compact support. Hence in the remainder of this paper we assume that V is C^∞.

In this subsection, we introduce the basic strategy of proving Theorem 2. With the assumption of Theorem 2, we have

$$\Lambda = [0, L]^3, \qquad L = \varrho^{-\frac{41}{60}}, \qquad N = \varrho^{-\frac{21}{20}} \quad \text{and} \quad \lim_{\varrho\to 0} \varrho^{2/3}\beta \in (0, \infty). \tag{3.15}$$

We first identify four regions in the momentum space Λ^* which are relevant to the construction of the trial state: P_0 for the condensate; P_L for the low momenta, which are of the order $\varrho^{1/3}$; P_H for momenta of order one; and P_I the region between P_0 and P_L.

Definition 1 (Definitions of P_0, P_I, P_L and P_H)

Define four subsets of momentum space $\Lambda^* = (2\pi L^{-1}\mathbb{Z})^3$: P_0, P_I, P_L and P_H as follows.

$$\begin{aligned} P_0 &\equiv \{p = 0\}\\ P_I &\equiv \left\{p \in \Lambda^* : 0 < |p| < \varepsilon_L \varrho^{1/3}\right\}\\ P_L &\equiv \left\{p \in \Lambda^* : \varepsilon_L \varrho^{1/3} \le |p| \le \eta_L^{-1} \varrho^{1/3}\right\}\\ P_H &\equiv \left\{p \in \Lambda^* : \varepsilon_H \le |p| \le \eta_H^{-1}\right\}, \end{aligned} \tag{3.16}$$

where the parameters are chosen as follows

$$\varepsilon_L, \eta_L, \varepsilon_H, \eta_H \equiv \varrho^\eta \quad \text{and} \quad \eta \equiv 1/200 \tag{3.17}$$

We remark that the momenta between P_L and P_H are irrelevant to our construction and η can be any positive number less than $1/200$. When $V=0$, most particles have momentum in $P_0\cup P_I\cup P_L$. When we turn on the interaction, pairs of these particles are annihilated and usually pairs of particles with momenta of order one will be created.

Next, as in [17], we define some notations for the states and subsets of the Fock space. Using the occupation number representation, we describe a state in Fock space with a function mapping from momentum space to integers.

Definition 2 (Definitions of P_0, P_I, P_L and P_H)
Let P denote $P_0\cup P_L\cup P_I\cup P_H$. We define $\tilde{M}$ as the set of all functions $\alpha: P\to\mathbb{N}\cup 0$ such that

$$\sum_{k\in P}\alpha(k)=N \tag{3.18}$$

For any $\alpha\in\tilde{M}$, denote by $|\alpha\rangle\in\mathcal{H}_{N,\Lambda}$ the unique state (in this case, an N-particle wave function) defined by the map α

$$|\alpha\rangle=C\prod_{k\in P}(a_k^{\dagger})^{\alpha(k)}|0\rangle,$$

where the positive constant C is chosen so that $|\alpha\rangle$ is L_2-normalized.

Moreover, we define M as the following subset of $\tilde{M}$

$$M\equiv\{\alpha\in\tilde{M}|\mathrm{supp}(\alpha)\subset P_0\cup P_I\cup P_L \text{ and } \alpha(k)\le m_c \text{ for } \forall k\in P_L\}, \tag{3.19}$$

where m_c is defined as

$$m_c\equiv\varrho^{-3\eta}=\varrho^{-3/200} \tag{3.20}$$

Clearly, we have

$$a_k^{\dagger}a_k|\alpha\rangle=\alpha(k)|\alpha\rangle,\quad \forall k\in P \tag{3.21}$$

The states corresponding to the functions in M, (3.19), have no particle with momentum of order one, and there is a restriction on the particle number. But when $V=0$, the total probability of finding the states corresponding to M is almost equal to one.

Furthermore, as follows, we can construct a trial state Γ_0, with α's in M, satisfying (3.7) with $4\pi a$ replaced with $\int_{\mathbb{R}^3}\frac{1}{2}V dx$ in the r.h.s. of (3.7). We postpone the proof of the next lemma to the Sect. 12.2.

Lemma 2 *For* $\Lambda=[0,L]^3$, $L=\varrho^{-\frac{41}{60}}$, $N=\varrho^{-\frac{21}{20}}$ *and* $\lim_{\varrho\to 0}\varrho^{2/3}\beta\in(0,\infty)$. *There exists a state* $\Gamma_0(\varrho,\beta)$ *having the form*: $(g_\alpha(\varrho,\beta)\in\mathbb{R})$

$$\Gamma_0=\sum_{\alpha\in M}g_\alpha(\varrho,\beta)|\alpha\rangle\langle\alpha|,\qquad \sum_{\alpha\in M}g_\alpha(\varrho,\beta)=1, \tag{3.22}$$

and satisfying

$$\overline{\lim}_{\varrho\to 0}\left(\frac{1}{|\Lambda|}\operatorname{Tr}H_N\Gamma_0-\frac{1}{|\Lambda|\beta}S(\Gamma_0)-f_0(\varrho,\beta)\right)\varrho^{-2}\le\frac{1}{2}V_0(2-[1-R[\beta]]_+^2) \tag{3.23}$$

Furthermore, the coefficient function g_α *satisfies*

$$\lim_{\varrho\to 0}\sum_{\alpha\in M} N^{-2}N_\alpha g_\alpha = 2-[1-R(\beta)]_+^2 \tag{3.24}$$

where we defined $N_\alpha \in \mathbb{R}$ $(\alpha\in M)$ *as*

$$N_\alpha \equiv \alpha(0)\alpha(0) + \sum_{u,v\in P_L\cup P_0,\, u\neq \pm v} 2\alpha(u)\alpha(v), \quad \alpha\in M \tag{3.25}$$

We remark: actually Γ_0 is very close to Γ_I, the canonical Gibbs state of ideal Bose gases. The state $\Gamma_0(\varrho,\beta)$ satisfies (3.23), but for all potentials $V\neq 0$, $V_0=\int V(x)dx^3$ is strictly larger than $8\pi a$. So we need to improve Γ_0. To do that, we need to replace the $|\alpha\rangle$'s $(\alpha\in M)$ with some non-product state Ψ_α's. The energy of $|\alpha\rangle$ is higher than what we really want, since in $|\alpha\rangle$ when two particles are close to each other their behavior does not look like $(1-w)$, which is the zero energy scattering solution of V. For this reason, we should construct Ψ_α as follows

$$\begin{aligned}
\Psi_\alpha &\sim C\prod_{i<j}(1-w)(x_i-x_j)|\alpha\rangle \\
&\sim C\Big(1-\sum_{i<j} w(x_i-x_j)+\sum w(x_i-x_j)w(x_k-x_l)\cdots\Big)|\alpha\rangle \\
&\sim C\Big(1-\sum_k \frac{w_k}{|\Lambda|}\sum_{u,v} a^\dagger_{u+k}a^\dagger_{v-k}a_u a_v + \Big(\sum_k \frac{w_k}{|\Lambda|}\sum_{u,v} a^\dagger_{u+k}a^\dagger_{v-k}a_u a_v\Big)^2\cdots\Big)|\alpha\rangle
\end{aligned} \tag{3.26}$$

We give the rigorous definition in the next section. First, we noticed that the operator $\sum_{i<j} w(x_i-x_j)$ annihilates two particles and creates two new particles. In our temperature regime, usually the momenta of the annihilated particles are of order $\varrho^{1/3}$ or zero, belong to $P_L\cup P_0$ and momenta of the two created particles are of order one, i.e., belong to P_H. With this fact, we will construct Ψ_α as the linear combination of α and the states which can be obtained by keeping annihilating 2 particles with momenta in $P_L\cup P_0$ and creating 2 new particles with momentum of order one, i.e.,

$$\begin{aligned}
\Psi_\alpha \sim C\Bigg(1-\sum_k \frac{w_k}{|\Lambda|}\sum_{u,v\in P_0\cup P_L}^{u+k,v-k\in P_H} a^\dagger_{u+k}a^\dagger_{v-k}a_u a_v \\
+\Bigg(\sum_k \frac{w_k}{|\Lambda|}\sum_{u,v\in P_0\cup P_L}^{u+k,v-k\in P_H} a^\dagger_{u+k}a^\dagger_{v-k}a_u a_v\Bigg)^2\cdots\Bigg)|\alpha\rangle
\end{aligned} \tag{3.27}$$

For simplicity, we divide the P_H and P_L, which are subsets of momentum space, into small boxes. When the size of the boxes is small enough, the probability of finding two particles annihilated (created) in same box is extremely low. Therefore to construct Ψ_α, we only use the states in which there is at most one particle annihilated (P_L) or created (P_H) in each small box. Now we define these boxes.

Definition 3 (Definitions of $B_H(u)$, $B_L(u)$)

Let $\varkappa_L, \varkappa_H > 0$. Divide P_L and P_H (3.16) into small *boxes* (could be non-rectangular box) s.t. the sides of the boxes are about $\varrho^{\varkappa_L}$ and $\varrho^{\varkappa_H}$. We denote the box containing u by $B_H(u)$ when $u \in P_H$ ($B_L(u)$ when $u \in P_L$).

Then we define the states which we will use to construct Ψ_α.

Definition 4 (Definition of $\tilde{M}_\alpha$)
For any $\alpha \in M$, we define $\tilde{M}_\alpha$ as the set of the β's in $\tilde{M}$ (Definition 2) such that

1. If $k \in P_0$, then $\beta(k) \le \alpha(k)$. If $k \in P_I$, then $\beta(k) = \alpha(k)$.
2. There is **at most** one k in each B_L or B_H satisfying $\beta(k) \ne \alpha(k)$.
3. If $\beta(k) \ne \alpha(k)$, then

$$\begin{aligned} \beta(k) &= \alpha(k) - 1, \quad \text{for } k \in P_L \\ \beta(k) &= \alpha(k) + 1 = 1, \quad \text{for } k \in P_H \end{aligned} \tag{3.28}$$

As we explained, for each $\alpha \in M$, we construct a normalized pure state Ψ_α, which is a linear combination of $\beta \in \tilde{M}_\alpha$, i.e.,

$$|\Psi_\alpha\rangle = \sum_{\beta \in \tilde{M}_\alpha} f_\alpha(\beta)|\beta\rangle, \qquad \sum_{\beta \in \tilde{M}_\alpha} |f_\alpha(\beta)|^2 = 1 \tag{3.29}$$

To prove Theorem 2, i.e., to improve the Γ_0 in Lemma 2, we choose the correct trial state Γ of following form:

$$\Gamma = \sum_{\alpha \in M} g_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|, \tag{3.30}$$

where we choose g_α in (3.22) and Ψ_α in (3.29).

With proper $\varkappa_L$ and $\varkappa_H$, ΔS the entropy difference between Γ_0 in (3.22) and Γ in (3.30) can be proved to be much less than $|\Lambda|\varrho^2$.

Lemma 3 *Let $\Lambda = \varrho^{-41/20}$, $\varkappa_L \le 5/9$ and $\varkappa_H \le 2/9$. Then for any $\{\Psi_\alpha, \alpha \in M\}$ having the form* (3.29) *and any $g_\alpha > 0$ such that $\sum_{\alpha \in M} g_\alpha = 1$, we have*

$$\overline{\lim}_{\varrho \to 0}\big[-S(\Gamma) - (-S(\Gamma_0))\big](\Lambda\varrho^2)^{-1} = 0 \tag{3.31}$$

with Γ defined in (3.30) *and $\Gamma_0 = \sum_{\alpha \in M} g_\alpha |\alpha\rangle\langle\alpha|$.*

We postpone the proof of this lemma to Sect. 12.3. The assumptions $\varkappa_L \le 5/9$ and $\varkappa_H \le 2/9$ imply

$$\varrho^{1-4\eta-3\varkappa_L} + \varrho^{-4\eta-3\varkappa_H} \ll N\varrho^{1/3}. \tag{3.32}$$

In the next theorem, we show that, for each $\alpha \in M$, there exists a pure state Ψ_α of the form (3.29) such that, comparing with $|\alpha\rangle$, the new pure state $|\Psi_\alpha\rangle$ lowers the total energy by about $(\frac{1}{2}V_0 - 4\pi a)N_\alpha\Lambda^{-1}$, where N_α is defined in (3.25). The construction of the pure state yielding the correct total energy is the core of the proof of Theorem 2.

Theorem 3 *Let $1/2 \ge \varkappa_L \ge 4/9$ and $\varkappa_H \ge 1/9$. For any $\alpha \in M$, there exists Ψ_α having the form* (3.29) *and satisfying*

$$\langle\Psi_\alpha|H_N|\Psi_\alpha\rangle - \langle\alpha|H_N|\alpha\rangle + \left(\frac{1}{2}V_0 - 4\pi a\right)N_\alpha\Lambda^{-1} \le \varepsilon_\varrho\varrho^2\Lambda$$

where the ε_ϱ *is independent of* α *and* $\lim_{\varrho\to 0}\varepsilon_\varrho = 0$.

Finally, by choosing the proper size of the small boxes in P_L and P_H, we can prove Theorem 2 with Theorem 3, Lemma 3 and Lemma 2.

Proof of Theorem 2 Let $1/2 \ge \varkappa_L \ge 4/9$ and $2/9 \ge \varkappa_H \ge 1/9$. We choose trial state Γ (3.30) with g_α in Lemma 2 (3.22) and Ψ_α's in Theorem 3. Then combine Theorem 3, Lemma 3 and Lemma 2. □

This paper is organized as follows: In Sect. 4, we rigorously define Ψ_α's and the trial state Γ. In Sect. 5, we outline the lemmas needed to prove Theorem 3. In Sect. 6, we estimate the number of particles in the condensate and various momentum regimes. These estimates are the building blocks for all other estimates later on. The kinetic energy is estimated in Sect. 7 and the potential energy is estimated in Sects. 8–11. Finally in Sect. 12, we prove Lemmas 1, 2, 3.

4 Definition of the Trial Pure States Ψ_α's

In this section, we give a formal definition of the trial pure state Ψ_α's for Theorem 3. For simplicity, we define a special 'state' $|\mathbf{0}\rangle = 0 \in \mathcal{H}_{N,\Lambda}$. As in [17], to construct Ψ_α, we use the following operators $A^{u,v}_{p,q}$:

$$A^{u,v}_{p,q} : \tilde{M} \to \tilde{M} \cup \mathbf{0}, \quad u, v \in P_0 \cup P_L,\ p, q \in P_H \text{ and } u + v = p + q \tag{4.1}$$

With the notation $|\mathbf{0}\rangle$, we have the following simple formula for $A^{u,v}_{p,q}$,

$$|A^{u,v}_{p,q}\beta\rangle = C a^\dagger_p a^\dagger_q a_u a_v |\beta\rangle, \quad \beta \in \tilde{M} \tag{4.2}$$

where C is a positive normalization constant. We can see that, with the notation $\mathbf{0}$, $A^{u,v}_{p,q}\beta$ makes sense when the r.h.s. is 0. We note that here $\mathbf{0}$ is introduced just for simplifying the expression.

The operator $A^{u,v}_{p,q}$ annihilates two particles with momenta in P_L or P_0 and creates two particles with momenta in P_H. We note: the total momentum is conserved.

For simplicity, the pure trial state Ψ_α will be of the form $\sum_{\beta\in M_\alpha} f_\alpha(\beta)|\beta\rangle$ where f_α is supported in $M_\alpha \subset \tilde{M}_\alpha$ (Definition 4) which we now define.

Note that there is no physical mean to construct Ψ_α on M_α and not $\tilde{M}_\alpha$, but the properties of M_α simplify our proof. We can define the coefficient function f_α on M_α with a very clear relation between $f_\alpha(\mathcal{A}^{u_1,u_2}_{k_1,k_2}\beta)$ and $f_\alpha(\beta)$, as in Lemma 5. But we can not do this on $\tilde{M}_\alpha$.

Definition 5 (Definition of nontrivial subset in P_L)

Let A be a subset of P_L, it is called non-trivial when

1. If $u_i \in A$ and $u_i \ne u_j$ $(1 \le i \ne j \le 2)$, then $u_1 + u_2 \ne 0$
2. If $u_i \in A$ and $u_i \ne u_j$ $(1 \le i \ne j \le 3)$, then $u_1 + u_2 \ne u_3$
3. If $u_i \in A$ and $u_i \ne u_j$ $(1 \le i \ne j \le 4)$, then $u_1 + u_2 \ne u_3 + u_4$.

Definition of M_α:

Recall $\tilde{M}_\alpha$ in Definition 4. For $\alpha \in M$, we define the subset $M_\alpha \subset \tilde{M}_\alpha$ as the smallest set with the following properties.

1. For any α and $\gamma \in \tilde{M}_\alpha$, let $P_L(\gamma, \alpha)$ denote the following subset of P_L,

$$P_L(\gamma, \alpha) \equiv \{u \in P_L : \gamma(u) < \alpha(u)\}. \tag{4.3}$$

   Then for any $\gamma \in M_\alpha$, $P_L(\gamma, \alpha)$ is non-trivial subset of P_L.
2. $\alpha \in M_\alpha$
3. If $\beta \in M_\alpha$ and $\gamma = A^{0,0}_{p,-p}\beta \in \tilde{M}_\alpha$, then $\gamma \in M_\alpha$.
4. If $\beta \in M_\alpha$, $\gamma = A^{u,v}_{p,q}\beta \in \tilde{M}_\alpha$ and
   (a) $P_L(\gamma, \alpha)$ is non-trivial
   (b) $\beta(-p) = \beta(-q) = 0$
   then $\gamma \in M_\alpha$.

Note: The set M_α is unique since the intersection of two such sets M_{a1} and $M_{\alpha,2}$ satisfies all four conditions.

We collect a few obvious properties of the elements in M_α into the next lemma.

Lemma 4 *By the definition of M_α, any $\beta \in M_\alpha$ has the following form*:

$$\beta = \prod_{i=1}^{m} \mathcal{A}^{u_{2i-1}, u_{2i}}_{k_{2i-1}, k_{2i}} \prod_{j=1}^{n} \mathcal{A}^{0,0}_{p_j, -p_j} \alpha \tag{4.4}$$

where $u_i \in P_L \cup P_0$, $k_i \in P_H$ for $i = 1, \ldots, 2m$ and $p_j \in P_H$ for $j = 1, \ldots, n$. And

$$p_i \neq \pm p_j, \qquad k_i \neq \pm k_j \quad \text{for } i \neq j \quad \text{and} \quad k_i \neq \pm p_j \quad \text{for } \forall i, j \tag{4.5}$$

On the other hand, if $\{u_i, (i = 1, \ldots, 2m)\} \cap P_L$ is a non-trivial subset of P_L, then any $\beta \in \tilde{M}_\alpha$ with form (4.4) *and* (4.5) *belongs to M_α.*

Furthermore, one can change the order of the $\mathcal{A}$'s in (4.4). *With the fact that the subset of non-trivial subset of P_L is still non-trivial, we can see, if β belongs to M_α and has the form* (4.4) *and* (4.5), *then we have*

$$\prod_{i \in A} \mathcal{A}^{u_{2i-1}, u_{2i}}_{k_{2i-1}, k_{2i}} \prod_{j \in B} \mathcal{A}^{0,0}_{p_j, -p_j} \alpha \in M_\alpha \tag{4.6}$$

Here A, B are any subsets of $\{1, \ldots, m\}$ and $\{1, \ldots, n\}$.

Now, to define $\Psi_\alpha = \sum_{\beta \in M_\alpha} f_\alpha(\beta)|\beta\rangle$, it only remains to define f_α, which is supported on M_α. As suggested in (3.27), for $u, v \in P_0 \cup P_L$, $p, q \in P_H$, and $u + v = p + q$, we have the following relation between $f_\alpha(\alpha)$ and $f_\alpha(\mathcal{A}^{u,v}_{p,q}\alpha)$

$$f_\alpha(\mathcal{A}^{u,v}_{p,q}\alpha) \approx -(1 - \delta_{u,v}/2)\left[w_{(p-u)} + w_{(v-p)}\right]|\Lambda|^{-1}\sqrt{\alpha(u)\alpha(v)}\, f_\alpha(\alpha) \tag{4.7}$$

Furthermore, if $\beta \in M_\alpha$ and $\sum_{k \in P_H} \beta(k)$ is small (like < 5), the approximation (3.27) implies that for most u, v, p, q,

$$f_\alpha(\mathcal{A}^{u,v}_{p,q}\beta) \approx -(1 - \delta_{u,v}/2)\left[w_{(p-u)} + w_{(v-p)}\right]|\Lambda|^{-1}\sqrt{\beta(u)\beta(v)}\, f_\alpha(\beta) \tag{4.8}$$

when $A^{u,v}_{p,q}\beta \in M_\alpha$. Here we have used the fact that when $\beta \in M_\alpha$ and $A^{u,v}_{p,q}\beta \in M_\alpha$, $\beta(p) = \beta(q) = 0$.

We hope that for most $u, v \in P_0 \cup P_L$, $p, q \in P_H$, the approximation (4.8) would hold for most $\beta \in M_\alpha$ such that $A^{u,v}_{p,q}\beta \in M_\alpha$. Here "most β have some property A" means that the probability of finding β with this property in Ψ_α is almost one, i.e.,

$$\sum_{\beta \text{ has property } A} |\langle\beta|\Psi_\alpha\rangle|^2 = \sum_{\beta \text{ has property } A} |f_\alpha(\beta)|^2 \approx 1 \tag{4.9}$$

If the approximation (4.8) holds for some $u, v \in P_0 \cup P_L$, $p, q \in P_H$, then we can easily obtain

$$\begin{aligned}&\langle\Psi_\alpha|a_u a_v a_p^\dagger a_q^\dagger|\Psi_\alpha\rangle\\ &\quad\approx -(1-\delta_{u,v}/2)\left[w_{(p-u)} + w_{(v-p)}\right]|\Lambda|^{-1}\sum_{\beta\in M_\alpha}\sqrt{\beta(u)\beta(v)}|f^2(\beta)|\end{aligned} \tag{4.10}$$

Using the definition of M_α, we may guess that for most $\beta \in M_\alpha$,

$$\begin{aligned}&\beta(u) = \alpha(u), \quad u, \in P_L\\ &\beta(0) \sim \alpha(0)\end{aligned} \tag{4.11}$$

Therefore

$$\langle\Psi_\alpha|a_u a_v a_p^\dagger a_q^\dagger|\Psi_\alpha\rangle \approx -(1-\delta_{u,v}/2)\left[w_{(p-u)} + w_{(v-p)}\right]|\Lambda|^{-1}\sqrt{\alpha(u)\alpha(v)} \tag{4.12}$$

This approximation (4.12) is very useful for calculating $\langle\Psi_\alpha|V|\Psi_\alpha\rangle$.

Now we give the definition of f_α as follows. In Lemma 5 we check that it has this property (4.8).

Definition 6 (The Pure Trial State Ψ_α) Recall that the function $(1-w)$ is the zero energy scattering solution of the potential V, as in (2.12). Define the pure trial state Ψ_α as

$$|\Psi_\alpha\rangle \equiv \sum_{\beta\in M_\alpha} f_\alpha(\beta)|\beta\rangle \tag{4.13}$$

where the coefficient $f_\alpha(\beta)$'s are given by

$$f_\alpha(\beta) = C_\alpha\sqrt{\frac{|\Lambda|^{\beta(0)}}{\beta(0)!}}\left(\prod_{k\in P_H}^{\beta(k)>0}\sqrt{-w_k}\right)\left(\prod_{k\in P_H}^{\beta(k)>\beta(-k)}\sqrt{2}\right)\left(\prod_{u\in P_L(\beta,\alpha)}\sqrt{\frac{\alpha(u)}{|\Lambda|}}\right) \tag{4.14}$$

Here we follow the convention $\sqrt{x} = \sqrt{|x|}i$ for $x < 0$. For convenience, we define $f(\beta) = 0$ for $\beta \notin M_\alpha$. The constant C_α is chosen so that Ψ_α is L_2 normalized, i.e.,

$$\langle\Psi_\alpha|\Psi_\alpha\rangle = 1, \quad \text{i.e.,} \sum_{\beta\in M_\alpha}|f_\alpha(\beta)|^2 = 1$$

In next Lemma, with the f_α chosen above, we show that (4.8) holds for most u, v, p, q, β such that $\beta \in M_\alpha$ and $A^{u,v}_{p,q}\beta \in M_\alpha$.

Lemma 5

1. *If* $k \in P_H$ *and* $\beta \in M_\alpha$, $\mathcal{A}^{0,0}_{k,-k}\beta \in M_\alpha$, *then*

$$f_\alpha(\mathcal{A}^{0,0}_{k,-k}\beta) = (-w_k)\sqrt{\frac{\beta(0)}{|\Lambda|}}\sqrt{\frac{\beta(0)-1}{|\Lambda|}} f_\alpha(\beta) \tag{4.15}$$

2. *If* $u_1, u_2 \in P_L$, $u_2 = \pm u_1$ *or* $u_2 \in B_L(u_1)$, $k_1, k_2 \in P_H$ *and* $\beta \in M_\alpha$, *then* $\gamma = \mathcal{A}^{u_1,u_2}_{k_1,k_2}\beta \notin M_\alpha$, *i.e.*, $f_\alpha(\gamma) = 0$.
3. *If* $u_1, u_2 \in P_L \cup P_0$ *and* $u_2 \neq \pm u_1$, $k_1, k_2 \in P_H$, $\beta \in M_\alpha$ *and* $\mathcal{A}^{u_1,u_2}_{k_1,k_2}\beta \in M_\alpha$, *then when* $\beta(-p) = \beta(-q) = 0$, *we have*

$$f_\alpha(\mathcal{A}^{u_1,u_2}_{k_1,k_2}\beta) = 2\sqrt{-w_{k_1}}\sqrt{-w_{k_2}}\sqrt{\frac{\beta(u_1)}{|\Lambda|}}\sqrt{\frac{\beta(u_2)}{|\Lambda|}} f_\alpha(\beta) \tag{4.16}$$

when $\beta(-p) \neq 0$ *or* $\beta(-q) \neq 0$, *we have*

$$\left|f_\alpha(\mathcal{A}^{u_1,u_2}_{k_1,k_2}\beta)\right| \le \left|\sqrt{w_{k_1}}\sqrt{w_{k_2}}\sqrt{\frac{\beta(u_1)}{|\Lambda|}}\sqrt{\frac{\beta(u_2)}{|\Lambda|}} f_\alpha(\beta)\right| \tag{4.17}$$

Again the result 2 in Lemma 5 has no physical meaning, but it can simplify our proof.

In next section, we can see that, for fixed $p \in P_H$ and most $\beta \in M_\alpha$, $\beta(-p) = 0$. Hence the identity (4.15) or (4.16) hold for most $\beta \in M_\alpha$. Since k_1, k_2 are order one and $u_1, u_2 \in P_0 \cup P_L$, we have

$$w_{k_1} \approx w_{k_2} \approx w_{k_1-u_1} \approx w_{k_1-u_2} = w_{u_2-k_1} \tag{4.18}$$

which implies that f_α satisfies the property (4.8) in most case.

5 Proof of Theorem 3

Proof Our goal is to prove

$$\langle\Psi_\alpha|H_N|\Psi_\alpha\rangle - \langle\alpha|H_N|\alpha\rangle + \left(\frac{1}{2}V_0 - 4\pi a\right)N_\alpha\Lambda^{-1} \le \varepsilon_\varrho\varrho^2\Lambda \tag{5.1}$$

First we decompose the Hamiltonian H_N as in [17]. By the rule 1 of the definition of $\tilde{M}_\alpha$, if $\beta \in M_\alpha \subset \tilde{M}_\alpha$ then $\beta(k)$ is equal to $\alpha(k)$ for any $k \in P_I$. Hence if $k_1 \in P_I$, $\beta, \gamma \in M_\alpha$ and $\langle\beta|a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}|\gamma\rangle \neq 0$, then one of k_3 and k_4 must be equal to k_1.

On the other hand, since the particles with momenta in P_H are created in pairs, the total number of the particles with momenta in P_H is always even. With these two results and momentum conservation, we can decompose the expectation value $\langle\Psi_\alpha|H_N|\Psi_\alpha\rangle$ as follows:

$$\langle H_N\rangle_{\Psi_\alpha} = \left\langle\sum_{i=1}^N -\Delta_i\right\rangle_{\Psi_\alpha} + \langle H_{abab}\rangle_{\Psi_\alpha} + \langle H_{\tilde{L}\tilde{L}}\rangle_{\Psi_\alpha} + \langle H_{\tilde{L}H}\rangle_{\Psi_\alpha} + \langle H_{HH}\rangle_{\Psi_\alpha}, \tag{5.2}$$

where

1. H_{abab} is the part of interaction that annihilates two particles and creates the same two particles, i.e.,

$$H_{abab}=|2\Lambda|^{-1}\sum_{u}V_0a_u^\dagger a_u^\dagger a_u a_u+|2\Lambda|^{-1}\sum_{u\neq v}(V_{u-v}+V_0)a_u^\dagger a_v^\dagger a_u a_v \tag{5.3}$$

2. $H_{\tilde{L}\tilde{L}}$ is the interaction between four particles with momenta in $P_{\tilde{L}}$:

$$P_{\tilde{L}}\equiv P_0\cup P_L \tag{5.4}$$

and

$$H_{\tilde{L}\tilde{L}}=|2\Lambda|^{-1}\sum_{u_i\in P_{\tilde{L}}}V_{u_3-u_1}a_{u_1}^\dagger a_{u_2}^\dagger a_{u_3}a_{u_4}, \tag{5.5}$$

where $u_1\neq u_3$ or u_4.

3. $H_{\tilde{L}H}$ is the part of interaction that involves two particles with momenta in $P_{\tilde{L}}$ and two particles with momenta in P_H i.e.,

$$\begin{aligned}H_{\tilde{L}H}&=|2\Lambda|^{-1}\sum_{u_1,u_2\in P_{\tilde{L}},k_1,k_2\in P_H}V_{u_1-k_1}a_{u_1}^\dagger a_{u_2}^\dagger a_{k_1}a_{k_2}+H.C.\\&\quad+|2\Lambda|^{-1}\sum_{u_1,u_2\in P_{\tilde{L}},k_1,k_2\in P_H}2(V_{u_1-u_2}+V_{u_1-k_2})a_{u_1}^\dagger a_{k_1}^\dagger a_{u_2}a_{k_2},\end{aligned} \tag{5.6}$$

where $u_1\neq u_2$ and $H.C.$ denotes the hermitian conjugate of the first term.

4. H_{HH} is the part of interaction between 4 particles with momenta in P_H,

$$H_{HH}=|2\Lambda|^{-1}\sum_{k_i\in P_H}V_{k_3-k_1}a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}a_{k_4}, \tag{5.7}$$

where $k_1\neq k_3$ or k_4.

With these definitions, since there is no high momentum particle in $|\alpha\rangle$ ($\alpha\in M$), the total energy of $|\alpha\rangle$ is:

$$\langle\alpha|H_N|\alpha\rangle=\langle\alpha|\sum_{i=1}^{N}-\Delta_i|\alpha\rangle+\langle\alpha|H_{abab}|\alpha\rangle \tag{5.8}$$

Recall the definition of N_α for $\alpha\in M$ in (3.25). The estimates for the energies of these components in (5.2) are stated as the following lemmas, which will be proved in later sections with different methods.

Lemma 6 *The total kinetic energy is bounded from above by*

$$\left\langle\sum_{i=1}^{N}-\Delta_i\right\rangle_{\Psi_\alpha}-\left\langle\sum_{i=1}^{N}-\Delta_i\right\rangle_{\alpha}-\|\nabla w\|_2^2N_\alpha|\Lambda|^{-1}\leq\varepsilon_1\varrho^2\Lambda, \tag{5.9}$$

where ε_1 *is independent of* α *and* $\lim_{\varrho\to0}\varepsilon_1=0$.

Lemma 7 *The expectation value of* H_{abab} *is bounded above by,*

$$\langle H_{abab}\rangle_{\Psi_\alpha}-\langle H_{abab}\rangle_\alpha\leq\varrho^{11/4}\Lambda \tag{5.10}$$

Lemma 8 *The expectation value of $H_{\tilde{L}\tilde{L}}$ is bounded above by,*

$$\left\langle H_{\tilde{L}\tilde{L}} \right\rangle_{\Psi_\alpha} \le \varrho^{11/4} \Lambda \tag{5.11}$$

Lemma 9 *The expectation value of $H_{\tilde{L}H}$ is bounded above by,*

$$\left\langle H_{\tilde{L}H} \right\rangle_{\Psi_\alpha} + N_\alpha |\Lambda|^{-1} \|Vw\|_1 \le \varepsilon_2 \varrho^2 \Lambda \tag{5.12}$$

where ε_2 is independent of α and $\lim_{\varrho \to 0} \varepsilon_2 = 0$.

Lemma 10 *The expectation value of H_{HH} is bounded above by,*

$$\langle H_{HH} \rangle_{\Psi_\alpha} - N_\alpha |\Lambda|^{-1} \left\| \frac{1}{2} V w^2 \right\|_1 \le \varepsilon_3 \varrho^2 \Lambda \tag{5.13}$$

where ε_3 is independent of α and $\lim_{\varrho \to 0} \varepsilon_3 = 0$.

On the other hand, by definition of w in (2.12) and (2.13), we have

$$\|\nabla w\|_2^2 - \left\| \frac{1}{2} V w \right\|_1 + \left\| \frac{1}{2} V w^2 \right\|_1 = 0, \qquad \frac{1}{2} V_0 - \left\| \frac{1}{2} V w \right\|_1 = 4\pi a \tag{5.14}$$

Together with (5.8) and (5.9)–(5.13), we arrive at the desired result (5.1). □

6 Estimates on the Numbers of Particles

As in [17], the first step to prove the Lemma 6 to Lemma 10 is to estimate the particle number of Ψ_α in the condensate, P_L, P_I, and P_H. This is the main task of this section and we start with the following notations.

Definition 7 Suppose $u_i \in P = P_0 \cup P_I \cup P_L \cup P_H$ for $i = 1, \dots, s$. The expectation of the product of particle numbers with momenta $u_1, \dots, u_s$:

$$Q_\alpha(u_1, u_2, \dots, u_s) \equiv \left\langle \prod_{i=1}^{s} a_{u_i}^\dagger a_{u_i} \right\rangle_{\Psi_\alpha} = \sum_{\beta \in M_\alpha} \prod_{i=1}^{s} \beta(u_i) |f_\alpha(\beta)|^2 \tag{6.1}$$

Definition 8 (The definition of $M_\alpha(u)$ and $M_\alpha^B(u)$)

We denote by $M_\alpha(u)$ the set of $\beta \in M_\alpha$'s satisfying $\beta(u) = \alpha(u)$, i.e.

$$M_\alpha(u) \equiv \{\beta \in M_\alpha : \beta(u) = \alpha(u)\} \tag{6.2}$$

Furthermore, with the definition of $B_L(u)$ (when $u \in P_L$) and $B_H(u)$ (when $u \in P_H$), we define $M_\alpha^B(u) \subset M_\alpha(u)$ as the intersection of $M_\alpha(v)$'s of all $v \in B_L(u)$ (when $u \in P_L$) or $B_H(u)$(when $u \in P_H$), i.e.,

$$M_\alpha^B(u) \equiv \bigcap_{v \in B_{L(H)}(u)} M_\alpha(v) \tag{6.3}$$

We can see

$$\beta \in M_\alpha^B(u) \quad \Leftrightarrow \quad \beta(v) = \alpha(v) \quad \text{for } \forall v \in B_{L(H)}(u) \tag{6.4}$$

The coefficient function f_α is supported on $M_\alpha \subset \tilde{M}_\alpha$. Using (3.28), if $\beta \in M_\alpha$ and $u \in P_L$, either $\beta(u) = \alpha(u)$, i.e., $\beta \in M_\alpha(u)$ or $\beta(u) = \alpha(u) - 1$, i.e., $\beta \notin M_\alpha(u)$. Therefore the average number of the particles with momentum u, for $u \in P_L$, can be written as follows

$$Q_\alpha(u) = \langle a_u^\dagger a_u \rangle_{\Psi_\alpha} = \alpha(u) - \sum_{\beta \notin M_\alpha(u)} |f_\alpha(\beta)|^2. \tag{6.5}$$

For any $k \in P_H$, we have

$$Q_\alpha(k) = \sum_{\beta \notin M_\alpha(u)} |f_\alpha(\beta)|^2. \tag{6.6}$$

The following theorem provides the main estimates on $Q_\alpha(u)$ and $Q_\alpha(k)$.

Lemma 11 *For small enough ϱ, $Q_\alpha(u)$ and $Q_\alpha(k)$ can be estimated as follows* ($u, u_1, u_2 \in P_L$ *and* $k \in P_H$)

$$Q_\alpha(k) = \sum_{\beta \notin M_\alpha(k)} |f_\alpha(\beta)|^2 \le \text{const. } \varrho^{2-4\eta}, \quad \textit{for } k \in P_H \tag{6.7}$$

$$0 \le \alpha(u) - Q_\alpha(u) = \sum_{\beta \notin M_\alpha(u)} |f_\alpha(\beta)|^2 \le \text{const. } \varrho^{1-4\eta}, \quad \textit{for } u \in P_L \tag{6.8}$$

Furthermore, the probabilities of the combined cases are bounded as follows: ($u, u_1, u_2 \in P_L$ *and* $k \in P_H$)

$$\sum_{\beta \notin M_\alpha(u_1) \cup M_\alpha(u_2)} |f_\alpha(\beta)|^2 \le \text{const. } \varrho^{2-8\eta} \quad \textit{when } u_1 \ne u_2 \tag{6.9}$$

$$\sum_{\beta \notin M_\alpha(u) \cup M_\alpha(k)} |f_\alpha(\beta)|^2 \le \text{const. } \varrho^{3-7\eta} |w_k| \tag{6.10}$$

Proof of Lemma 11 First, we prove (6.7) concerning $k \in P_H$. With Lemma 4 ((4.4)–(4.6)), when $\beta(k) > 0$, there exist some $\gamma \in M_\alpha$ and $u, v \in P_L \cup P_0$, $p \in P_H$ such that

$$\mathcal{A}_{k,p}^{u,v} \gamma = \beta \quad \text{and} \quad p = u + v - k \tag{6.11}$$

With the properties of f_α in Lemma 5 ((4.15)–(4.17)), $f_\alpha(\beta)$ is bounded as

$$|f_\alpha(\beta)|^2 \le 4\gamma(u)\gamma(v)\Lambda^{-2} \left| w_k w_p \right| |f_\alpha(\gamma)|^2. \tag{6.12}$$

Then sum up $\beta \notin M_\alpha(k)$, i.e., $\beta(k) > 0$, by summing up u, v and γ, we obtain:

$$\begin{aligned} \sum_{\beta \notin M_\alpha(k)} |f_\alpha(\beta)|^2 &\le 4 \sum_{u,v \in P_L \cup P_0} \sum_{\gamma \in M_\alpha} \gamma(u)\gamma(v)\Lambda^{-2} |w_k w_{u+v-k}| \, |f_\alpha(\gamma)|^2 \\ &\le 4\varrho^2 |w_k| \max_{p \in P_H} \{|w_p|\} \end{aligned} \tag{6.13}$$

The upper bound of $|w_p|$ is derived in (2.15): $\left| w_p \right| \le 4\pi a |p|^{-2}$, therefore

$$Q_\alpha(k) = \sum_{\beta \notin M_\alpha(k)} |f_\alpha(\beta)|^2 \le \text{const. } \varrho^{2-2\eta} |w_k|, \quad k \in P_H \tag{6.14}$$

Using (2.15) again, we obtain (6.7).

Then, we prove (6.8) concerning $u \in P_L$. Similarly, with Lemma 4, for any $\beta \notin M_\alpha(u)$, i.e., $\beta(u) = \alpha(u) - 1$, there exist some $\gamma \in M_\alpha$ and $v \in P_L \cup P_0$, $p, k \in P_H$ such that (6.11) holds. This implies (6.12). Using (2.15) and $|k + p| = |u + v| \ll |k|$, we have

$$|w_p w_k| \le \text{const. } |k|^{-4}, \quad \text{when } p, k \in P_H \text{ and } |p + k| \ll |k| \tag{6.15}$$

Inserting (6.15) and the bounds $\gamma(u) \le \alpha(u) \le m_c = \varrho^{-3\eta}$ into (6.12), we obtain:

$$|f_\alpha(\beta)|^2 \le \text{const. } \varrho^{-3\eta}|k|^{-4}\gamma(v)\Lambda^{-2}|f_\alpha(\gamma)|^2 \tag{6.16}$$

Again, summing up β (by summing up γ, v, p and k), with $\sum_v \gamma(v) \le N$, we obtain (6.8) as follows

$$\sum_{\beta \notin M_\alpha(u)} |f_\alpha(\beta)|^2 \le \sum_{v \in P_L \cup P_0}^{k \in P_H} \sum_{\gamma \in M_\alpha} \text{const. } \varrho^{-3\eta}|k|^{-4}\gamma(v)\Lambda^{-2}|f_\alpha(\gamma)|^2 \le \varrho^{1-4\eta} \tag{6.17}$$

Next, we prove (6.9) concerning $u_1, u_2 \in P_L$. For any $\beta \notin M_\alpha(u_1) \cup M_\alpha(u_2)$, i.e.,

$$\beta(u_1) = \alpha(u_1) - 1, \qquad \beta(u_2) = \alpha(u_2) - 1 \tag{6.18}$$

using Lemma 4, we can see that there are only two cases:

1. there exist one $\gamma \in M_\alpha$, p_1, $p_2 \in P_H$ and $\mathcal{A}^{u_1,u_2}_{p_1,p_2}\gamma = \beta$
2. there exist one $\gamma \notin M_\alpha(u_2)$, $v \in P_L \cup P_0$, $v \ne u_2$, p_1, $p_2 \in P_H$ and $\mathcal{A}^{u_1,v}_{p_1,p_2}\gamma = \beta$

As before, with the properties of f_α in Lemma 5, the bounds on $\alpha(u)$'s ($u \in P_L$) and (6.15), we have

$$\begin{aligned}\sum_{\beta \notin M_\alpha(u_1) \cup M_\alpha(u_2)} |f_\alpha(\beta)|^2 \le{}& \text{const. } \sum_{\gamma \in M_\alpha} \varrho^{-7\eta}|\Lambda|^{-1}|f_\alpha(\gamma)|^2 \\ &+ \text{const. } \sum_{v \in P_L \cup P_0, \gamma \notin M_\alpha(u_2)} \varrho^{-4\eta}\gamma(v)|\Lambda|^{-1}|f_\alpha(\gamma)|^2\end{aligned} \tag{6.19}$$

Using $\sum_v \gamma(v) \le N$ and (6.8), we obtain (6.9).

At last, we prove (6.10) concerning $u \in P_L$ and $k \in P_k$. For any $\beta \notin M_\alpha(u) \cup M_\alpha(k)$. Using Lemma 4, we can see that there are only two cases:

1. there exist $\gamma \in M_\alpha$, $v \in P_L \cup P_0$, $p \in P_H$ and $\mathcal{A}^{u,v}_{p,k}\gamma = \beta$
2. there exist $\gamma \notin M_\alpha(u)$, v_1, $v_2 \in P_L \cup P_0$, $p \in P_H$ and $\mathcal{A}^{v_1,v_2}_{p,k}\gamma = \beta$

Summing up v, p or v_1, v_2, p, we obtain

$$\begin{aligned}\sum_{\beta \notin M_\alpha(k) \cup M_\alpha(u)} |f_\alpha(\beta)|^2 \le{}& \text{const. } \sum_{v \in P_L \cup P_0} \sum_{\gamma} \gamma(u)\gamma(v)\Lambda^{-2}|w_k w_{u+v-k}||f_\alpha(\gamma)|^2 \\ &+ \sum_{\gamma \notin M_\alpha(u)} 4\varrho^2|w_k| \max_{p \in P_H}\{|w_p|\}|f_\alpha(\gamma)|^2\end{aligned} \tag{6.20}$$

With the result in (2.15): $\left|w_p\right| \le 4\pi a|p|^{-2}$ and $\sum_v \gamma(v) \le N$, we have:

$$\sum_{\beta \notin M_\alpha(k) \cup M_\alpha(u)} |f_\alpha(\beta)|^2 \le \text{const. } \gamma(u)\varrho^{1-2\eta}\Lambda^{-1}|w_k| + \sum_{\gamma \notin M_\alpha(u)} 4\varrho^{2-2\eta}|w_k||f_\alpha(\gamma)|^2 \tag{6.21}$$

At last using (6.8) and the fact $\gamma(u)\le\alpha(u)\le\varrho^{-3\eta}$ and $\Lambda=\varrho^{-41/20}$, we obtain the desired result (6.10) □

Moreover $Q_\alpha(k)(k\in P_H)$, has a more precise upper bound as follows.

Lemma 12 *For $k\in P_H$, and $Q_\alpha(k)$ is bounded above by*:

$$Q_\alpha(k)\le N_\alpha\Lambda^{-2}|w_k|^2+\varrho^{7/3-7\eta} \tag{6.22}$$

Proof First using Lemma 4, we have that, for any $\beta\notin M_\alpha(k)$, there are two cases:

1. there exists $\gamma\in M_\alpha$, such that, $\mathcal{A}^{0,0}_{-k,k}\gamma=\beta$
2. there exist $\gamma\in M_\alpha$, $u\ne\pm v\in P_L\cup P_0$, $p\in P_H$, s.t., $\mathcal{A}^{u,v}_{p,k}\gamma=\beta$.

Then with the identities and bound of f_α in Lemma 5 (4.15), (4.16) and (4.17), $Q_\alpha(k)$ is bounded above by

$$Q_\alpha(k)=\sum_{\beta\notin M_\alpha(k)}|f_\alpha(\beta)|^2\le\alpha(0)^2\Lambda^{-2}w_k^2+\sum_{u,v\in P_L\cup P_0,u\ne\pm v}2\alpha(u)\alpha(v)\Lambda^{-2}|w_kw_p| \tag{6.23}$$

where $p=u+v-k$. Since $w_p=w_{-p}$ and $|p+k|\le 2(\varrho^{1/3-\eta})$, with (2.16), we have

$$\big||w_k|-|w_p|\big|\le\text{const. }\varrho^{1/3-4\eta} \tag{6.24}$$

Inserting this into (6.23), we obtain

$$Q_\alpha(k)\le N_\alpha\Lambda^{-2}w_k^2+\varrho^{7/4-4\eta}|w_k| \tag{6.25}$$

Then using $|w_k|\le\text{const. }\varrho^{-2\eta}$, we obtain the desired result (6.22). □

At last, with Lemmas 11, 12 and the definition of M_α, one can easily obtain the following inequalities on f_α.

Lemma 13 *Recall the definition of $M^B_\alpha(k)$ or $M^B_\alpha(u)$ in Definition 8 (6.3), the upper bounds on f_α in (6.8) and (6.7) imply*:

$$\sum_{\beta\notin M^B_\alpha(k)}|f_\alpha(\beta)|^2\le\varrho^{2-4\eta}\Lambda\varrho^{3\varkappa_H}\le\varrho^{1/6}\quad \textit{for } k\in P_H \tag{6.26}$$

and

$$\sum_{\beta\notin M^B_\alpha(u)}|f_\alpha(\beta)|^2\le\varrho^{1-4\eta}\Lambda\varrho^{3\varkappa_L}\le\varrho^{1/6}\quad \textit{for } u\in P_L \tag{6.27}$$

Recall B_L and B_H in Definition 3. Suppose $u_1,u_2\in P_L\cup P_0$, $k_1,k_2\in P_H$, $u_1+u_2=k_1+k_2$, $u_1+u_2\ne 0$ and $u_1\notin B_L(u_2)$. Then using (6.8), (6.9) and the definition of M_α, we have

$$\sum_{\beta\in M_\alpha,\mathcal{A}^{u_1,u_2}_{k_1,k_2}\beta\notin M_\alpha}|f(\beta)|^2\le\varrho^{1/2} \tag{6.28}$$

At last, with (6.7) and the fact

$$0\le\alpha(0)-\beta(0)\le\sum_{k\in P_H}\beta(k),$$

we have $Q_\alpha(0)$ *and* $Q_\alpha(0,0)$ *bounded as follows*

$$\alpha(0) \geq Q_\alpha(0) \geq \alpha(0) - \varrho^{5/6} N \tag{6.29}$$

and

$$\left[\alpha(0)\right]^2 \geq Q_\alpha(0,0) \geq \left[\alpha(0)\right]^2 - N^2 \varrho^{5/6} \tag{6.30}$$

7 Proof of Lemma 6

In this section, with the bounds on $Q_\alpha(u)(u \in P_L)$ and $Q_\alpha(k)(k \in P_H)$, we estimate the kinetic energy of Ψ_α by proving Lemma 6.

Proof By the definition,

$$\left\langle \sum_{i=1}^N -\Delta_i \right\rangle_{\Psi_\alpha} = \sum_{u \in P_L \cup P_I \cup P_H} u^2 Q_\alpha(u) \quad \text{and} \quad \left\langle \sum_{i=1}^N -\Delta_i \right\rangle_{\alpha} = \sum_{u \in P_L \cup P_I} u^2 \alpha(u) \tag{7.1}$$

With the definition of M_α and $\tilde{M}_\alpha$, we have $Q_\alpha(u) \leq \alpha(u)$, for $u \in P_I \cup P_L$. Then the l.h.s. of (5.9) bounded above by

$$\begin{aligned} &\left\langle \sum_{i=1}^N -\Delta_i \right\rangle_{\Psi_\alpha} - \left\langle \sum_{i=1}^N -\Delta_i \right\rangle_{\alpha} - \|\nabla w\|_2^2 N_\alpha |\Lambda|^{-1} \\ &\quad \leq \sum_{k \in P_H} k^2 Q_\alpha(k) - \|\nabla w\|_2^2 N_\alpha |\Lambda|^{-1} \end{aligned} \tag{7.2}$$

With the upper bound on $Q_\alpha(k)$ in (6.22), we have

$$(7.2) \leq N_\alpha |\Lambda|^{-1} \left| \|\nabla w\|_2^2 - \sum_{k \in P_H} |\Lambda|^{-1} k^2 |w_k|^2 \right| + \varrho^{13/6} \Lambda \tag{7.3}$$

Together with $\lim_{\varrho \to 0} \left| \|\nabla w\|_2^2 - \sum_{k \in P_H} |\Lambda|^{-1} k^2 |w_k|^2 \right| = 0$, we complete the proof of Lemma 6. □

8 Proof of Lemma 7

Proof First we rewrite the expectation value of H_{abab} as

$$\begin{aligned} &\langle H_{abab} \rangle_{\Psi_\alpha} \\ &\quad = |2\Lambda|^{-1} \sum_{\beta \in M_\alpha} \left(V_0 \sum_u \left(\beta(u)^2 - \beta(u) \right) + \sum_{u \neq v} (V_0 + V_{u-v}) \beta(u) \beta(v) \right) |f_\alpha(\beta)|^2 \\ &\quad = |2\Lambda|^{-1} \sum_{\beta \in M_\alpha} \left(V_0 (N^2 - N) + \sum_{u \neq v} V_{u-v} \beta(u) \beta(v) \right) |f_\alpha(\beta)|^2 \end{aligned} \tag{8.1}$$

On the other hand,

$$\langle H_{abab}\rangle_\alpha = |2\Lambda|^{-1}\left(V_0(N^2-N)+\sum_{u\neq v} V_{u-v}\alpha(u)\alpha(v)\right) \tag{8.2}$$

By the assumptions, V_v is positive when $|v|\ll 1$. For any $\beta\in M_\alpha$, $\beta(u)\le\alpha(u)$ for $u\in P_0\cup P_I\cup P_L$, therefore we have

$$V_{u-v}\beta(u)\beta(v)\le V_{u-v}\alpha(u)\alpha(v),\quad \text{when } u,v\in P_0\cup P_I\cup P_L \tag{8.3}$$

Using this inequality and the fact $\alpha(k)=0$ for $k\in P_H$, we have

$$\begin{aligned}&\langle H_{abab}\rangle_{\Psi_\alpha}-\langle H_{abab}\rangle_\alpha\\ &\le |2\Lambda|^{-1}\left(\sum_{u\notin P_H, v\in P_H} 2V_{u-v}Q_\alpha(u,v)+\sum_{u,v\in P_H} V_{u-v}Q_\alpha(u,v)\right)\end{aligned}$$

For any $u\in P$, $|V_u|$ is no more than $|V_0|$, with (6.7), we obtain:

$$\langle H_{abab}\rangle_{\Psi_\alpha}-\langle H_{abab}\rangle_\alpha\le V_0\varrho\sum_{v\in P_H}Q_\alpha(v)\le\varrho^{11/4}\Lambda \tag{8.4}$$

□

9 Proof of Lemma 8

As in [17], to calculate $\langle a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}\rangle_{\Psi_\alpha}$, we start with the following identity.

Lemma 14 *For any fixed momenta $u_{1,2,3,4}$ and $\beta\in M_\alpha$, define $T(\beta)$ to be the state*

$$|T(\beta)\rangle\equiv C a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}|\beta\rangle, \tag{9.1}$$

where C is the positive normalization constant when $|T(\beta)\rangle\neq 0$. Then we have

$$\langle a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}\rangle_{\Psi_\alpha}=\sum_{\beta\in M_\alpha} f_\alpha(\beta)\overline{f_\alpha(T(\beta))}\sqrt{\langle\beta|a^\dagger_{u_4}a^\dagger_{u_3}a_{u_2}a_{u_1}|a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}|\beta\rangle} \tag{9.2}$$

The map T depends on $u_{1,2,3,4}$ and in principle it has to carry them as subscripts. We omit these subscripts since it will be clear from the context what they are.

Proof For any fixed $u_{1,2,3,4}$, by the definition of Ψ_α, we have

$$\langle\Psi_\alpha|a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}|\Psi_\alpha\rangle=\sum_{\gamma,\beta\in M} f_\alpha(\beta)\overline{f_\alpha(\gamma)}\langle\gamma|a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}|\beta\rangle \tag{9.3}$$

By definition of M_α, one can see

$$\langle\gamma|a^\dagger_{u_1}a^\dagger_{u_2}a_{u_3}a_{u_4}|\beta\rangle\neq 0\quad\Rightarrow\quad\gamma=T(\beta) \tag{9.4}$$

Since $|T(\beta)\rangle$ is normalized, the identity in Lemma 14 is obvious. □

9.1 Proof of Lemma 8

Proof Using the fact $|V_u| \le V_0$ for any $u \in \mathbb{R}^3$, we can see

$$\left|\left\langle H_{\tilde{L}\tilde{L}}\right\rangle_{\Psi_\alpha}\right| \le V_0|2\Lambda|^{-1} \sum_{u_i\in P_{\tilde{L}}, u_1\neq u_3,u_4} \left|\left\langle a^\dagger_{u_1} a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right|, \tag{9.5}$$

We are going to prove:

$$\sum_{u\in P_L} \left|\left\langle a^\dagger_0 a^\dagger_0 a_u a_{-u}\right\rangle_{\Psi_\alpha}\right| = 0 \tag{9.6}$$

$$\sum_{u_2,u_3,u_4\in P_L} \left|\left\langle a^\dagger_0 a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right| \le \Lambda^2 \varrho^{3-5\eta} \tag{9.7}$$

$$\sum_{u_i\in P_L \text{ and } u_1\neq u_3,u_4} \left|\left\langle a^\dagger_{u_1} a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right| \le \Lambda^3 \varrho^{5-9\eta} \tag{9.8}$$

First we note (9.6) is trivial. Because if $\beta \in M_\alpha$, then $P_L(\beta,\alpha)$ is non-trivial subset of P_L, which tells if $\beta(u) < \alpha(u)$ then $\beta(-u) = \alpha(-u)$.

Then we prove (9.7) concerning $u_{2,3,4} \in P_L$. By definition of M_α,

$$\langle \beta | a^\dagger_0 a^\dagger_{u_2} a_{u_3} a_{u_4} |\gamma\rangle \neq 0$$

implies $u_3 \neq u_4$ and $\gamma \notin M_\alpha(u_2)$, i.e., $\gamma(u_2) < \alpha(u_2)$. Furthermore, with the definition of f_α (2.4), we have

$$f_\alpha(\beta) = \sqrt{\frac{\alpha(u_3)\alpha(u_4)}{\beta(0)\alpha(u_2)}}\, f_\alpha(\gamma) \tag{9.9}$$

Combining with Lemma 14, we obtain

$$\left|\left\langle a^\dagger_0 a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right| \le \alpha(u_3)\alpha(u_4) \sum_{\gamma\notin M_\alpha(u_2)} |f_\alpha(\gamma)^2| \tag{9.10}$$

Using (6.8) in Lemma 11, we obtain

$$\left|\left\langle a^\dagger_0 a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right| \le \text{const. } \alpha(u_3)\alpha(u_4)\varrho^{1-4\eta}, \tag{9.11}$$

which implies (9.7).

Next, we prove (9.8). Similarly, we have

$$\left|\left\langle a^\dagger_{u_1} a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right| \le \alpha(u_3)\alpha(u_4) \sum_{\gamma\notin M_\alpha(u_1)\cup M_\alpha(u_2)} |f_\alpha(\gamma)^2| \tag{9.12}$$

Again, using Lemma 11, we obtain

$$\left|\left\langle a^\dagger_{u_1} a^\dagger_{u_2} a_{u_3} a_{u_4}\right\rangle_{\Psi_\alpha}\right| \le \text{const. } \alpha(u_3)\alpha(u_4)\varrho^{2-8\eta}, \tag{9.13}$$

which implies (9.8). At last, combine (9.6)–(9.8) and we obtain

$$\left|\left\langle H_{\tilde{L}\tilde{L}}\right\rangle_{\Psi_\alpha}\right| \le \varrho^{11/4}\Lambda \tag{9.14}$$

□

10 Proof of Lemma 9

We start the proof with estimating $\langle a^\dagger_{u_1} a^\dagger_{u_2} a_{k_1} a_{k_2}\rangle_{\Psi_\alpha}$ in the special case: $u_1 = \pm u_2 \in P_L$. By the definition of M_α, if $\beta \in M_\alpha$, $u \in P_L$ and $\beta(u) < \alpha(u)$, then $\beta(u) = \alpha(u) - 1$ and $\beta(-u) = \alpha(-u)$. Since f_α is supported on M_α, we have:

$$\langle a^\dagger_{u_1} a^\dagger_{u_2} a_{k_1} a_{k_2}\rangle_{\Psi_\alpha} = 0, \quad \text{for } \forall k_1, k_2 \in P_H,\ u_1 = \pm u_2 \in P_L \tag{10.1}$$

For the other cases, we leave the bounds in the following lemma. As explained before, with the f_α we chose, the approximation (4.12) should hold for most $u, v \in P_L \cup P_0$, $p, q \in P_H$. In the proof of Lemma 15, one can see that the approximation (4.12) implies the main results (10.2) and (10.3).

Lemma 15 *Recall $P_{\tilde L} = P_0 \cup P_L$. For $u, u_1, u_2 \in P_{\tilde L}$ and $k, k_1, k_2 \in P_H$, we have*

$$\left| \sum V_{u-k} \langle a^\dagger_u a^\dagger_{-u} a_k a_{-k}\rangle_{\Psi_\alpha} + \alpha(0)^2 \|Vw\|_1 \right| \le \varepsilon_4 N^2 \tag{10.2}$$

$$\left| \sum_{u_1 \ne \pm u_2} V_{u_1-k_1} \langle a^\dagger_{u_1} a^\dagger_{u_2} a_{k_1} a_{k_2}\rangle_{\Psi_\alpha} + \sum_{u_1 \ne \pm u_2} 2\alpha(u_1)\alpha(u_2) \|Vw\|_1 \right| \le \varepsilon_5 N^2 \tag{10.3}$$

and

$$\sum_{u_1 \ne u_2} \left| \langle a^\dagger_{u_1} a^\dagger_{k_1} a_{u_2} a_{k_2}\rangle_{\Psi_\alpha} \right| \le \varepsilon_6 N^2 \tag{10.4}$$

where we omitted $u, u_1, u_2 \in P_{\tilde L}$, $k, k_1, k_2 \in P_H$ and momentum conservation equality in $\sum$. The small numbers $\varepsilon_4, \varepsilon_5, \varepsilon_6$ are independent of α and $\lim_{\varrho \to 0} \varepsilon_i = 0$ for $i = 4, 5, 6$.

Proof of Lemma 9 Combine the bounds in (10.1), (10.2), (10.3) and (10.4). □

10.1 Proof of Lemma 15

Proof First we prove (10.2) concerning $u \in P_{\tilde L}$ and $k \in P_H$. By (10.1), if $\langle a^\dagger_u a^\dagger_{-u} a_k a_{-k}\rangle_{\Psi_\alpha} \ne 0$, then u must be zero. The property of f_α in Lemma 5 (4.15) implies

$$\langle \beta | a^\dagger_0 a^\dagger_{-0} a_k a_{-k} | \gamma\rangle \ne 0 \quad \Rightarrow \quad \frac{f_\alpha(\gamma)}{f_\alpha(\beta)} = -\frac{w_k}{|\Lambda|}\sqrt{\gamma(0)^2 - \gamma(0)} \tag{10.5}$$

Together with Lemma 14, we have

$$\langle a^\dagger_0 a^\dagger_0 a_k a_{-k}\rangle_{\Psi_\alpha} = -w_k \sum_{\beta:\beta\in M_\alpha, \mathcal{A}^{0,0}_{k,-k}\beta \in M_\alpha} \big(\beta(0)^2 - \beta(0)\big)\, \Lambda^{-1} |f_\alpha(\beta)|^2, \tag{10.6}$$

Recall the definitions of M^B_α's in Definition 4. One can see if $\beta(0) > 1$, then $\beta \in M_\alpha$ and $\mathcal{A}^{0,0}_{k,-k}\beta \in M_\alpha$ is equivalent to $\beta \in M^B_\alpha(k) \cap M^B_\alpha(-k)$. Therefore, we have the following identity,

$$\langle a^\dagger_0 a^\dagger_0 a_k a_{-k}\rangle_{\Psi_\alpha} = -w_k \sum_{\beta \in M^B_\alpha(k) \cap M^B_\alpha(-k)} \big(\beta(0)^2 - \beta(0)\big)\, \Lambda^{-1} |f_\alpha(\beta)|^2, \tag{10.7}$$

Using the bound on $\sum_{\beta\notin M_\alpha^B(k)}|f_\alpha(\beta)|^2$ (6.26) and the bounds on $Q_\alpha(0)$, $Q_\alpha(0,0)$ in (6.29) and (6.30). We obtain that

$$\left|\sum_{\beta\in M_\alpha^B(k)\cap M_\alpha^B(-k)}\big(\beta(0)^2-\beta(0)\big)|f_\alpha(\beta)|^2-\alpha(0)^2\right|\le O(\varrho^{1/6}N^2) \tag{10.8}$$

Insert (10.8) into (10.7). Then summing up $k\in P_H$, with $u=0$, we obtain

$$\begin{aligned}&\left|\sum V_{u-k}\langle a_u^\dagger a_{-u}^\dagger a_k a_{-k}\rangle_{\Psi_\alpha}+\alpha(0)^2\|Vw\|_1\right|\\&\quad\le\alpha(0)^2\left|\sum_{k\in P_H}-V_k w_k\Lambda^{-1}+\|Vw\|_1\right|+O(\varrho^{1/6-3\eta}N^2)\end{aligned} \tag{10.9}$$

Combining with the fact $\lim_{\varrho\to0}|\sum_{k\in P_H}-V_k w_k\Lambda^{-1}+\|Vw\|_1|=0$, we obtain the desired result (10.2).

Next, we prove (10.3) concerning $u_1,u_2\in P_{\tilde L}$, $u_1\ne\pm u_2$ and $k_1,k_2\in P_H$. Using the result 2 in Lemma 5, one can see

$$\langle a_{u_1}^\dagger a_{u_2}^\dagger a_{k_1}a_{k_2}\rangle_{\Psi_\alpha}=0\quad\text{when } u_2\in B_L(u_1) \tag{10.10}$$

Then from now on, we assume $u_2\notin B_L(u_1)$. The property of f_α in Lemma 5 implies, when $\langle\beta|a_{u_1}^\dagger a_{u_2}^\dagger a_{k_1}a_{k_2}|\gamma\rangle\ne0$ and $\beta,\gamma\in M_\alpha$,

$$f(\gamma)=C_\beta\sqrt{-w_{k_1}}\sqrt{-w_{k_2}}\sqrt{\beta(u_1)\beta(u_2)}f(\beta) \tag{10.11}$$

Here C_β depends on β and $|C_\beta|\le2$. Especially, when $\beta\in M_\alpha(-k_1)\cap M_\alpha(-k_2)$, $C_\beta=2$. Again with Lemma 14, for fixed u_1, $u_2\notin B_L(u_1)$, k_1 and k_2, we have

$$\langle a_{u_1}^\dagger a_{u_2}^\dagger a_{k_1}a_{k_2}\rangle_{\Psi_\alpha}=\sqrt{-w_{k_1}}\sqrt{-w_{k_2}}\sum_{\beta\in M_\alpha,\mathcal{A}_{k_1,k_2}^{u_1,u_2}\beta\in M_\alpha}C_\beta\beta(u_1)\beta(u_2)|f(\beta)|^2, \tag{10.12}$$

First, using the facts $|k_1+k_2|\le2\varrho^{1/3}\eta_L^{-1}$ and the bound on dw_p/dp (2.16), we obtain $|w_{k_1}-w_{k_2}|\le\varrho^{1/4}$, therefore

$$\left|\left(\sqrt{-w_{k_1}}\sqrt{-w_{k_2}}\right)+w_{k_1}\right|\le\varrho^{1/4} \tag{10.13}$$

Insert (10.13) into (10.12), we have

$$\langle a_{u_1}^\dagger a_{u_2}^\dagger a_{k_1}a_{k_2}\rangle_{\Psi_\alpha}=(-w_{k_1}+O(\varrho^{1/4}))\sum_{\beta\in M_\alpha,\mathcal{A}_{k_1,k_2}^{u_1,u_2}\beta\in M_\alpha}C_\beta\beta(u_1)\beta(u_2)|f_\alpha(\beta)|^2. \tag{10.14}$$

Now we bound

$$\sum_{\beta\in M_\alpha,\mathcal{A}_{k_1,k_2}^{u_1,u_2}\beta\in M_\alpha}C_\beta\beta(u_1)\beta(u_2)|f_\alpha(\beta)|^2.$$

In the case $\beta\notin M_\alpha(-k_1)\cap M_\alpha(-k_2)$, using the result in (6.7) and $|C_\beta|\le2$, we have

$$\left|\sum_{\beta\notin M_\alpha(k_1)\cap M_\alpha(k_2)}C_\beta\beta(u_1)\beta(u_2)|f_\alpha(\beta)|^2\right|\le\varrho\alpha(u_1)\alpha(u_2) \tag{10.15}$$

In the case $\beta \in M_\alpha(-k_1) \cap M_\alpha(-k_2)$, we have $C_\beta = 2$. Using the results in Lemma 11 and Lemma 13 ((6.7), (6.26), (6.27), (6.28) and $\alpha(u) \le m_c = \varrho^{-3\eta}$ for $u \in P_L$), we obtain that if $u_1, u_2 \in P_L$

$$\left| \sum_{A^{u_1,u_2}_{k_1,k_2} \beta \in M_\alpha}^{\beta \in M_\alpha(-k_1) \cap M_\alpha(-k_2)} \beta(u_1)\beta(u_2)|f_\alpha(\beta)|^2 - \alpha(u_1)\alpha(u_2) \right| \le O(\varrho^{1/6-6\eta}) \tag{10.16}$$

and if $u_1 = 0, u_2 \in P_L$, we have

$$\left| \sum_{A^{u_1,u_2}_{k_1,k_2} \beta \in M_\alpha}^{\beta \in M_\alpha(-k_1) \cap M_\alpha(-k_2)} \beta(u_1)\beta(u_2)|f_\alpha(\beta)|^2 - \alpha(u_1)\alpha(u_2) \right| \le O(\varrho^{1/6-3\eta} N) \tag{10.17}$$

Inserting (10.15), (10.16) and (10.17) into (10.14), with the fact $|w_p| \le 4\pi a|p|^{-2}$, we obtain that for $u_1, u_2 \in P_L$:

$$\left| \langle a^\dagger_{u_1} a^\dagger_{u_2} a_{k_1} a_{k_2} \rangle_{\Psi_\alpha} + 2 w_{k_1} \alpha(u_1)\alpha(u_2) \right| \le O(\varrho^{1/6-8\eta}) \tag{10.18}$$

and for $u_1 = 0, u_2 \in P_L$,

$$\left| \langle a^\dagger_{u_1} a^\dagger_{u_2} a_{k_1} a_{k_2} \rangle_{\Psi_\alpha} + 2 w_{k_1} \alpha(u_1)\alpha(u_2) \right| \le O(\varrho^{1/6-5\eta} N). \tag{10.19}$$

Furthermore, the smoothness and symmetry of V implies

$$|V_{u_1-k_1} - V_{k_1}| \le \varrho^{1/4}.$$

Then summing up $u_1, u_2 : u_2 \notin B_L(u_1)$ and k_1, k_2, we obtain

$$\begin{aligned} &\left| \sum_{u_1 \ne \pm u_2} V_{u_1-k_1} \langle a^\dagger_{u_1} a^\dagger_{u_2} a_{k_1} a_{k_2} \rangle_{\Psi_\alpha} + 2 \sum_{u_1 \ne \pm u_2} \alpha(u_1)\alpha(u_2) \|V w\|_1 \right| \\ &\quad \le 2 \sum_{u_1 \ne \pm u_2} \left(\alpha(u_1)\alpha(u_2) \left| \sum |V_{k_1} w_{k_1}| \Lambda^{-1} - \|V w\|_1 \right| \right) + O(\varrho^{1/6-17\eta} N^2) \\ &\qquad + \sum_{\{u_1, u_2 : u_2 \in B_L(u_1)\}} 2\alpha(u_1)\alpha(u_2) \|V w\|_1 \end{aligned} \tag{10.20}$$

One can see the first line of the r.h.s. is less than $\varepsilon_5 N^2/2$. Here ε_5 is independent of α and $\lim_{\varrho \to 0} \varepsilon_5 = 0$. With the bound $\alpha(u) \le m_c$ for $u \in P_L$, we can obtain that the second line of the right side is also $o(N^2)$. Therefore we arrive at the desired result (10.3).

At last, we prove (10.4) concerning $u_{1,2} \in P_L$, $u_1 \ne u_2$ and $k_{1,2} \in P_H$. The definitions of M_α and f_α imply that, when $\langle \beta | a^\dagger_{u_1} a^\dagger_{k_1} a_{u_2} a_{k_2} | \gamma \rangle \ne 0$ and $\beta, \gamma \in M_\alpha$,

$$\gamma \notin M_\alpha(u_1) \cup M_\alpha(k_2), \qquad \beta \notin M_\alpha(u_2) \cup M_\alpha(k_1)$$

and

$$|f_\alpha(\gamma)| \le \text{const.} \left| \sqrt{\frac{\alpha(u_1)}{\alpha(u_2)}} \sqrt{\frac{w_{k_2}}{w_{k_1}}} \right| |f_\alpha(\beta)| \tag{10.21}$$

This implies

$$\left| f_\alpha(\beta) f_\alpha(\gamma) \langle\beta| a^\dagger_{u_1} a^\dagger_{k_1} a_{u_2} a_{k_2} |\gamma\rangle \right| \le \text{const.}\ \alpha(u_1) \left| \sqrt{\frac{w_{k_2}}{w_{k_1}}} \right| |f_\alpha(\beta)|^2 \tag{10.22}$$

Summing up $\beta \notin M_\alpha(u_2) \cup M_\alpha(k_1)$, with the upper bound on $\sum_\beta |f_\alpha(\beta)|^2$ (6.10), we have

$$\begin{aligned} \left| \langle a^\dagger_{u_1} a^\dagger_{k_1} a_{u_2} a_{k_2} \rangle_{\Psi_\alpha} \right| &\le \text{const.}\ \alpha(u_1) \left| \sqrt{\frac{w_{k_2}}{w_{k_1}}} \right| \sum_{\beta \notin M_\alpha(u_2) \cup M_\alpha(k_1)} |f_\alpha(\beta)|^2 \\ &\le \alpha(u_1) |\sqrt{w_{k_1} w_{k_2}}| \varrho^{3-8\eta} \end{aligned} \tag{10.23}$$

At last, using $|w_p| \le 4\pi a |p|^{-2}$ and $|k_1| \sim |k_2|$, we have

$$\begin{aligned} \sum_{u_1 \ne u_2} \left| \langle a^\dagger_{u_1} a^\dagger_{k_1} a_{u_2} a_{k_2} \rangle_{\Psi_\alpha} \right| &\le \sum_{u_1, u_2, k_1, k_2} \alpha(u_1) \varrho^{3-10\eta} \\ &\le \Lambda^3 \varrho^{5-13\eta} = o(\Lambda^2 \varrho^{5/2}) \end{aligned} \tag{10.24}$$

□

11 Proof of Lemma 10

In this section, we will prove Lemma 10 involving interaction energy between particles with momenta in P_H. We will show that the only contribution to the accuracy we need comes from four high momentum particles, to be computed in Lemma 16 (11.4). We start with separating $\langle H_{HH} \rangle_{\Psi_\alpha}$ into the main terms and the error terms.

Define $M_\alpha(k_1, k_2, k_3, k_4, u_1, u_2) \subset M_\alpha \otimes M_\alpha$ as the set of (β, γ)'s where β and γ can be created from the same $\tilde{\alpha} \in M_\alpha$ as follows,

$$\begin{aligned} &M_\alpha(k_1, k_2, k_3, k_4, u_1, u_2) \\ &\quad \equiv \{(\beta, \gamma) \in M_\alpha \otimes M_\alpha : \exists \tilde{\alpha} \in M_\alpha \text{s.}t.\mathcal{A}^{u_1, u_2}_{k_1, k_2} \tilde{\alpha} = \beta \text{ and } A^{u_1, u_2}_{k_3, k_4} \tilde{\alpha} = \gamma\}, \end{aligned} \tag{11.1}$$

where $k_1, k_2, k_3, k_4 \in P_H$ and $u_1, u_2 \in P_{\tilde{L}}$. We define $A_{u_1, u_2, k_1, k_2, k_3, k_4}$ as

$$A_{u_1, u_2, k_1, k_2, k_3, k_4} \equiv \sum_{(\beta, \gamma) \in M_\alpha(k_1, k_2, k_3, k_4, u_1, u_2)} \overline{f_\alpha(\beta)} f_\alpha(\gamma) \left\langle \beta | a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} | \gamma \right\rangle \tag{11.2}$$

We note:

$$\left\langle a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} \right\rangle_{\Psi_\alpha} = \sum_{\beta, \gamma \in M_\alpha} \overline{f_\alpha(\beta)} f_\alpha(\gamma) \left\langle \beta | a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} | \gamma \right\rangle \tag{11.3}$$

With (11.2), we can separate the expectation value of H_{HH} into two parts, main term (Lemma 16) and error term (Lemma 17).

Lemma 16 *Summing up $k_1, k_2, k_3, k_4 \in P_H$, $k_i \ne k_j$ for $i \ne j$, $u_1, u_2 \in P_{\tilde{L}}$, we have*

$$\left| \sum_{u_i, k_i} V_{k_1 - k_3} \Lambda^{-1} A_{u_1, u_2, k_1, k_2, k_3, k_4} - N_\alpha |\Lambda|^{-1} \| V w^2 \|_1 \right| \le \frac{\varepsilon_3}{2} \varrho^2 \Lambda, \tag{11.4}$$

where ε_3 is independent of α and $\lim_{\varrho \to 0} \varepsilon_3 = 0$.

Lemma 17 *Let $M_\alpha(k_1,k_2,k_3,k_4)$ be the union of $M_\alpha(k_1,k_2,k_3,k_4,u_1,u_2)$, i.e.,*

$$M_\alpha(k_1,k_2,k_3,k_4)\equiv\bigcup_{u_1,u_2\in P_{\tilde L}} M_\alpha(k_1,k_2,k_3,k_4,u_1,u_2). \tag{11.5}$$

Then we have

$$\sum_{k_i\in P_H}\sum_{(\beta,\gamma)\notin M_\alpha(k_1,k_2,k_3,k_4)} V_0\Lambda^{-1}\left|\overline{f_\alpha(\beta)}f_\alpha(\gamma)\langle\beta|a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}|\gamma\rangle\right|\le\frac{\varepsilon_3}{2}\varrho^2\Lambda \tag{11.6}$$

Here $k_i\neq k_j$ for $i\neq j$ and ε_3 is independent of α, $\lim_{\varrho\to0}\varepsilon_3=0$.

11.1 Proof of Lemma 10

Proof Definition of M_α implies that when $k\in P_H$ and $\beta\in M_\alpha$,

$$\beta(k)\in\{0,1\}$$

Then the expectation value of $a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}$ must be zero when $k_1=k_2$ or $k_3=k_4$. Together with the definition of H_{HH}, we can rewrite $\langle H_{HH}\rangle_{\Psi_\alpha}$ as

$$\langle H_{HH}\rangle_{\Psi_\alpha}=\sum_{k_i\in P_H}^{k_i\neq k_j}\sum_{\beta,\gamma\in M_\alpha}\frac12 V_{k_1-k_3}\Lambda^{-1}\overline{f_\alpha(\beta)}f_\alpha(\gamma)\langle\beta|a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}|\gamma\rangle \tag{11.7}$$

On the other hand, if $\beta,\gamma\in M_\alpha$ and $\langle\beta|a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}|\gamma\rangle\neq0$ for some $k_{1,2,3,4}\in P_H$, then by the fact $P_L(\beta,\alpha)=P_L(\gamma,\alpha)$ is non-trivial subset of P_L (Definition 5), there exists **at most** one pair of $\{u_1,u_2\}$ such that

$$(\beta,\gamma)\in M_\alpha(k_1,k_2,k_3,k_4,u_1,u_2) \tag{11.8}$$

Therefore combining (11.4) and (11.6), with $|V_{k_1-k_3}|\le V_0$, we obtain the desired result (5.13). □

11.2 Proof of Lemma 16

Proof We start with bounding $A_{u_1,u_2,k_1,k_2,k_3,k_4}$.

Lemma 18 *When $u_1,u_2\in P_L$ and $u_1=\pm u_2$ or $u_2\in B_L(u_1)$, for any $k_i\in P_H$, we have*

$$A_{u_1,u_2,k_1,k_2,k_3,k_4}=0 \tag{11.9}$$

In other cases, $A_{u_1,u_2,k_1,k_2,k_3,k_4}$ is bounded by (recall $P_0=\{0\}$)

$$\begin{aligned}&\left|A_{u_1,u_2,k_1,k_2,k_3,k_4}-\alpha(u_1)\alpha(u_2)F_a(u_1,u_2)^2w_{k_1}w_{k_3}\Lambda^{-2}\right|\\&\le\varrho^{1/8}\Lambda^{-2}\times\begin{cases}\alpha(u_1)\alpha(u_2), & u_1,u_2\in P_L\\ N\alpha(u_2), & u_1\in P_0,u_2\in P_L\\ N^2, & u_1=u_2\in P_0,\end{cases}\end{aligned} \tag{11.10}$$

where $F_a(u_1,u_2)=1$ when $u_1=u_2=0$, otherwise $F_a(u_1,u_2)=2$.

Proof of Lemma 18 First we prove (11.9). One can see that it follows the definition of $A_{u_1,u_2,k_1,k_2,k_3,k_4}$ and the result 2 in Lemma 5.

Then we prove (11.10) when $u_1, u_2 \in P_L$. When (11.8) holds, by the definition of M_α $(k_1, k_2, k_3, k_4, u_1, u_2)$ in (11.1), there exists $\tilde{\alpha} \in M_\alpha$ such that

$$\mathcal{A}^{u_1,u_2}_{k_1,k_2}\tilde{\alpha} = \beta, \qquad \mathcal{A}^{u_1,u_2}_{k_3,k_4}\tilde{\alpha} = \gamma. \tag{11.11}$$

With definition of f_α, when $\tilde{\alpha} \in \bigcap_{i=1}^4 M_\alpha(-k_i)$, we have

$$\begin{aligned} f_\alpha(\beta) &= -F_a(u_1, u_2)\sqrt{\alpha(u_1)\alpha(u_2)}\Lambda^{-1}\sqrt{-w_{k_1}}\sqrt{-w_{k_2}}\, f_\alpha(\tilde{\alpha}) \\ f_\alpha(\gamma) &= -F_a(u_1, u_2)\sqrt{\alpha(u_1)\alpha(u_2)}\Lambda^{-1}\sqrt{-w_{k_1}}\sqrt{-w_{k_2}}\, f_\alpha(\tilde{\alpha}). \end{aligned} \tag{11.12}$$

And when $\tilde{\alpha} \notin \bigcap_{i=1}^4 M_\alpha(-k_i)$, we have the following bound on $|f_\alpha(\beta) f_\alpha(\gamma)|$,

$$|f_\alpha(\beta) f_\alpha(\gamma)| \le 4\alpha(u_1)\alpha(u_2)\Lambda^{-2}\prod_{i=1}^4 |\sqrt{w_{k_i}}||f_\alpha(\tilde{\alpha})|^2 \tag{11.13}$$

On the other hand, if $k_i \in P_H$ for $1 \le i \le 4$ and

$$\beta, \gamma \in M_\alpha \quad \text{and} \quad \langle \beta | a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} | \gamma \rangle \neq 0, \tag{11.14}$$

then by the definition of M_α, we have $\beta(k_1) = \beta(k_2) = 1$ and $\gamma(k_3) = \gamma(k_4) = 1$. This implies

$$\langle \beta | a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} | \gamma \rangle = 1 \tag{11.15}$$

Combining (11.12), (11.13) and (11.15), we obtain that when (11.11) holds and $\tilde{\alpha} \in \bigcap_{i=1}^4 M_\alpha(-k_i)$,

$$f_\alpha(\beta)\overline{f_\alpha(\gamma)}\langle \beta | a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} | \gamma \rangle = F_a(u_1, u_2)^2\tilde{\alpha}(u_1)\tilde{\alpha}(u_2)\Lambda^{-2}\prod_{i=1}^4\sqrt{-w_{k_i}}|f_\alpha(\tilde{\alpha})|^2 \tag{11.16}$$

When $\tilde{\alpha} \notin \bigcap_{i=1}^4 M_\alpha(-k_i)$, using (6.7), we have

$$\sum_{\tilde{\alpha}\notin\cap_{i=1}^4 M_\alpha(-k_i)} \left| f_\alpha(\beta)\overline{f_\alpha(\gamma)}\langle \beta | a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4} | \gamma \rangle \right| \le \text{const.}\ \varrho^{3/2}\alpha(u_1)\alpha(u_2)\Lambda^{-2} \tag{11.17}$$

Combining (11.16) and (11.17), we can see

$$\begin{aligned} &A_{u_1,u_2,k_1,k_2,k_3,k_4} + O(\varrho^{3/2})\alpha(u_1)\alpha(u_2)\Lambda^{-2} \\ &\quad = F_a(u_1, u_2)^2\Lambda^{-2}\prod_{i=1}^4\sqrt{-w_{k_i}}\sum_{\tilde{\alpha}\in A}\tilde{\alpha}(u_1)\tilde{\alpha}(u_2)|f(\tilde{\alpha})|^2 \end{aligned} \tag{11.18}$$

Where A is defined as the set

$$A \equiv \{\tilde{\alpha} \in M_\alpha : \mathcal{A}^{u_1,u_2}_{k_1,k_2}\tilde{\alpha} = \beta \in M_\alpha,\ \mathcal{A}^{u_1,u_2}_{k_3,k_4}\tilde{\alpha} = \gamma \in M_\alpha,\ \tilde{\alpha} \in \bigcap_{i=1}^4 M_\alpha(-k_i)\}$$

Since $u_1, u_2 \in P_L$, when $\tilde{\alpha} \in A$,

$$\tilde{\alpha}(u_i) = \alpha(u_i) \quad (i = 1, 2). \tag{11.19}$$

Furthermore, using the results in Lemma 13, we have that $\sum_{\tilde{\alpha}\in A} |f(\tilde{\alpha})|^2$ bounded by

$$1 \le \sum_{\tilde{\alpha}\in A} |f(\tilde{\alpha})|^2 \le 1 - O(\varrho^{1/6}) \tag{11.20}$$

On the other hand, using (10.13), with the fact $|k_1 + k_2| = |k_3 + k_4| \le \varrho^{1/3}\varrho^{-\eta}$, one can bound the $\prod_{i=1}^4 \sqrt{-w_{k_i}}$ in (11.18) as follows

$$\left| \prod_{i=1}^4 \sqrt{-w_{k_i}} - w_{k_1} w_{k_3} \right| \le O(\varrho^{1/4-\eta}) \tag{11.21}$$

Inserting (11.19), (11.21) and (11.20) into (11.18), we arrive at the desired result (11.10).

Similarly, using the bounds on $Q_\alpha(0)$ and $Q_\alpha(0,0)$ in (6.29) and (6.30), one can prove (11.10) when one of u_i belongs to P_0 or both of them belong to P_0. □

With (11.10), summing up k_1, k_3, u_1, u_2, one can easily obtain the desired result (11.4). □

11.3 Proof of Lemma 17

Proof As in [17], to estimate the error term of the interaction of particles with high momenta, we need to use a new tool. We start with defining the set $M_\alpha(\tilde{\alpha}, s, \{v_1, \ldots, v_t\})$. Let $v_1, \ldots, v_t \in P_L$ and being in different small boxes B_L, i.e.,

$$B_L(v_i) \ne B_L(v_j), \quad \text{for } i \ne j. \tag{11.22}$$

For non-negative integers s, t satisfying $s + t \in 2\mathbb{N}$ and $\tilde{\alpha} \in M_\alpha$, define

$$M(\tilde{\alpha}, s, \{v_1, \ldots, v_t\}) \equiv \bigcup_m \left\{ \beta \in M_\alpha : \beta = \prod_{i=m+1}^{(s+t)/2} \mathcal{A}^{u_{2i-1}, u_{2i}}_{p_{2i-1}, p_{2i}} \prod_{i=1}^{m} \mathcal{A}^{u_{2i-1}, u_{2i}}_{p_{2i-1}, p_{2i}} \tilde{\alpha} \right\} \tag{11.23}$$

where the u_i's $\in P_{\tilde{L}}$ and p_i's $\in P_H$ such that

1. $u_i = 0$ for $i \le 2m$.
2. $\{u_i, 2m + 1 \le i \le s + t\}$ is a permutation of $s - 2m$ zeros and $\{v_1, \ldots, v_t\}$.
3. for any fixed $2m + 1 \le j \le s + t$, $\tilde{\alpha} \in M_\alpha(-p_j)$, i.e., $\tilde{\alpha}(-p_j) = \alpha(-p_j)$.
4. $p_j \ne -p_i$ for any $2m + 1 \le j \le s + t$ and $1 \le i \le s + t$.

We note: for any u_i's and p_i's satisfying these four conditions, one can easily check that

$$\prod_{i\in A} \mathcal{A}^{u_{2i-1}, u_{2i}}_{p_{2i-1}, p_{2i}} \tilde{\alpha} \in M_\alpha. \tag{11.24}$$

holds for any $A \subset \{1, \ldots, (s + t)/2\}$.

By this definition, if (11.14) holds, then $\beta(u) = \gamma(u)$ for any $u \in P_{\tilde{L}}$, then there at least exists one $M_\alpha(\tilde{\alpha}, s, \{v_i, 1 \le i \le t\})$ such that

$$\beta \text{ and } \gamma \in M_\alpha(\tilde{\alpha}, s, \{v_1, \cdots, v_t\}) \tag{11.25}$$

E.g. using Lemma 4, we can see (11.25) holds when we choose $\tilde{\alpha}=\alpha$, $\{v_1,\dots,v_t\}=P_L(\beta,\alpha)=P_L(\gamma,\alpha)$.

Furthermore, with $M_\alpha(\tilde{\alpha},s,\{v_1,\cdots,v_t\})$, we define $N(\tilde{\alpha},s,\{v_1,\dots,v_t\})$ as the set of the pairs (β,γ) such that

1. $\beta,\gamma\in M_\alpha(\tilde{\alpha},s,\{v_1,\dots,v_t\})$
2. there exist k_i, $1\le i\le 4$ satisfying (11.14) but

$$(\beta,\gamma)\notin M_\alpha(k_1,k_2,k_3,k_4). \tag{11.26}$$

Here $M_\alpha(k_1,k_2,k_3,k_4)$ is defined in (11.5)

3. for any other $\tilde{\alpha}'$, s', $\{v_1',\dots,v_{t'}'\}$, if $\beta,\gamma\in M_\alpha(\tilde{\alpha}',s',\{v_1',\dots,v_{t'}'\})$, then

$$s+t\le s'+t' \tag{11.27}$$

We assume (11.25) and (11.14) holds. Clearly, $s+t=2$ or $t=0$ implies that $(\beta,\gamma)\in M_\alpha(k_1,k_2,k_3,k_4)$. Hence if $N(\tilde{\alpha},s,\{v_1,\dots,v_t\})$ is not an empty set then

$$s+t\ge 4,\quad \text{and}\quad t\ge 1 \tag{11.28}$$

By definition of $N(\tilde{\alpha},s,\{v_1,\dots,v_t\})$ and (11.15), we can bound the left side of (11.6) as follows ($k_i\ne k_j$ for $i\ne j$)

$$\begin{aligned}\sum_{k_i\in P_H}\ \sum_{\beta,\gamma\notin M_\alpha(k_1,k_2,k_3,k_4)} & V_0\Lambda^{-1}\left|\overline{f_\alpha(\beta)}f_\alpha(\gamma)\langle\beta|a^\dagger_{k_1}a^\dagger_{k_2}a_{k_3}a_{k_4}|\gamma\rangle\right|\\ &\le\sum_{\tilde{\alpha},s,\{v_1\dots v_t\}}V_0\Lambda^{-1}\,|N(\tilde{\alpha},s,\{v_1,\dots,v_t\})|\max_{\beta,\gamma\in M_\alpha(\tilde{\alpha},s,\{v_1,\dots,v_t\})}\left|\overline{f_\alpha(\beta)}f_\alpha(\gamma)\right|,\end{aligned} \tag{11.29}$$

where $|N(\tilde{\alpha},s,\{v_1,\dots,v_t\})|$ is the number of the elements in this set. When (11.25) holds, the definition of f_α implies,

$$|\overline{f_\alpha(\beta)}f_\alpha(\gamma)|\le\text{const.}^{t+s}\left|\frac{\alpha(0)}{|\Lambda|}\right|^s\left|\frac{\varrho^{-3\eta}}{|\Lambda|}\right|^t\max_{k\in P_H}\{|w_k|\}^{s+t}|f_\alpha(\tilde{\alpha})|^2$$

Here we used $m_c\le\varrho^{-3\eta}$. Again with the facts $|w_p|\le 4\pi a|p|^{-2}$ and $\alpha(0)\le N$, we obtain

$$|\overline{f_\alpha(\beta)}f_\alpha(\gamma)|\le\text{const.}^{t+s}(\varrho^{1-2\eta})^s(\varrho^{-5\eta})^t|\Lambda|^{-t}|f_\alpha(\tilde{\alpha})|^2 \tag{11.30}$$

Therefore, the r.h.s. of (11.29) is bounded by

$$(11.29)\le\sum_{\tilde{\alpha},s,\{v_1\dots v_t\}}|N(\tilde{\alpha},s,\{v_1,\dots,v_t\})|\,\varrho^s(\varrho^{-6\eta})^{t+s}|\Lambda|^{-t-1}|f(\tilde{\alpha})|^2 \tag{11.31}$$

Define $N(\tilde{\alpha},s,t)$ and $N(s,t)$ by

$$N(\tilde{\alpha},s,t)\equiv\max_{\{v_1,\dots,v_t\}}\{|N(\tilde{\alpha},s,\{v_1,\dots,v_t\})|\} \tag{11.32}$$

$$N(s,t)\equiv\max_{\tilde{\alpha}}\{N(\tilde{\alpha},s,t)\} \tag{11.33}$$

With the notations $N(\tilde{\alpha}, s, t)$ and $N(s, t)$, we can bound (11.31) by

$$(11.29) \le (11.31) \le \sum_{\tilde{\alpha},s,t} |f(\tilde{\alpha})|^2 \sum_{\{v_1 \dots v_t\}} N(\tilde{\alpha}, s, t)\varrho^s (\varrho^{-6\eta})^{t+s} |\Lambda|^{-t-1}$$

$$\le \sum_{s,t} \sum_{\{v_1 \dots v_t\}} N(s, t)\varrho^s (\varrho^{-6\eta})^{t+s} |\Lambda|^{-t-1} \tag{11.34}$$

For fixed t, the total number of sets $\{v_1 \cdots v_t, v_i \in P_L\}$ is bounded by

$$\sum_{\{v_1 \cdots v_t\}} 1 \le (\Lambda \varrho \eta_L^{-3})^t (t!)^{-1} \le (\varrho^{1-3\eta})^t |\Lambda|^t (t!)^{-1}$$

On the other hand, t is bounded above by the total number of B_L's (the sides of B_L's are about $\varrho^{3\varkappa_L}$) in P_L, i.e.,

$$t \le |P_L| / \max_i \{|B_L^i|\} \le \text{const. } \varrho^{1-3\eta-3\varkappa_L} \tag{11.35}$$

where $|P_L|$ and $|B_L^i|$ are the volumes of P_L and the small box B_L^i's. Together with (11.28), we bound the r.h.s. of (11.29) as follows,

$$(11.29) \le \sum_{t=1}^{\varrho^{1-4\eta-3\varkappa_L}} \sum_{s:s+t \ge 4} N(s, t)(\varrho^{1-9\eta})^{s+t} |\Lambda|^{-1} (t!)^{-1} \tag{11.36}$$

We claim that $N(s, t)$ is bounded with the following lemma, which will be proved in next subsection.

Lemma 19 *For any $N(\alpha, s, \{v_1, \dots, v_t\})$, $s + t \ge 4$ and $t \ge 1$, we have*

$$|N(\alpha, s, \{v_1, \dots, v_t\})| \le t! t^{(\frac{3t}{4})} |\Lambda|^{\frac{s+t}{4}+1} (\varrho^{-\eta})^{t+s} \tag{11.37}$$

Combining this Lemma with (11.36), we obtain

$$\text{r.h.s. of } (11.29) \le \sum_{t=1}^{\varrho^{1-4\eta-3\varkappa_L}} \sum_{s:s+t \ge 4} (\varrho^{1-10\eta})^{s+t} t^{(\frac{3t}{4})} |\Lambda|^{\frac{s+t}{4}}$$

$$= \sum_{t=1}^{\varrho^{1-4\eta-3\varkappa_L}} \sum_{s:s+t \ge 4} (\varrho^{1-10\eta} \Lambda^{1/4})^s (\varrho^{1-10\eta} t^{3/4} \Lambda^{1/4})^t \tag{11.38}$$

With the Λ we chose, $\varrho^{1-10\eta}\Lambda^{1/4}$ is much less than one. Using the assumption $\varkappa_L \le 1/2$, we have $\varrho^{1-10\eta} t^{3/4} \Lambda^{1/4} \ll 1$. Therefore, we arrive at the desired result:

$$(11.29) \le O(1) \ll \varrho^2 \Lambda \tag{11.39}$$

□

11.4 Proof of Lemma 19

We now prove Lemma 19.

Proof Since $(\beta,\gamma)\in N(\tilde\alpha, s,\{v_1,\dots,v_t\})$, we can express them as in the r.h.s. of (11.23),

$$\beta=\prod_{i=1}^{(s+t)/2}\mathcal{A}^{u_{2i-1},u_{2i}}_{q_{2i-1},q_{2i}}\tilde\alpha,\qquad \gamma=\prod_{i=1}^{(s+t)/2}\mathcal{A}^{\tilde u_{2i-1},\tilde u_{2i}}_{\tilde q_{2i-1},\tilde q_{2i}}\tilde\alpha \tag{11.40}$$

Here $u,\tilde u$'s belong to $P_{\tilde L}$ and $q,\tilde q$'s belong to P_H. We note that for any $1\le i\le (s+t)/2$, we have

$$\{q_{2i-1},q_{2i}\}\ne\{k_1,k_2\}\quad\text{and}\quad\{\tilde q_{2i-1},\tilde q_{2i}\}\ne\{k_3,k_4\}, \tag{11.41}$$

otherwise $(\beta,\gamma)\in M_\alpha(k_1,k_2,k_3,k_4)$, which contradicts with the assumption that $(\beta,\gamma)\in N(\tilde\alpha,s,\{v_1,\dots,v_t\})$.

From (11.14), one can see that the sets $\{q_1,\dots,q_{2s+2t}\}$ is very close to $\{\tilde q_1,\dots,\tilde q_{2s+2t}\}$, i.e.,

$$\{q_1,\dots,q_{2s+2t}\}-\{k_1,k_2\}=\{\tilde q_1,\dots,\tilde q_{2s+2t}\}-\{k_3,k_4\} \tag{11.42}$$

Denote the common elements in sets $\{q_i\}$ and $\{\tilde q_i\}$ by p_1, p_2, …, p_{s+t-2}. Then we have

$$\{q_i\}=\{k_1,k_2,p_1,p_2,\dots,p_{s+t-2}\} \tag{11.43}$$

$$\{\tilde q_i\}=\{k_3,k_4,p_1,p_2,\dots,p_{s+t-2}\} \tag{11.44}$$

We now construct a graph with vertices $\{k_1,k_2,k_3,k_4,p_i,1\le i\le s+t-2\}$. The edges of the graphs are β edges (q_{2i-1},q_{2i}), $1\le i\le (s+t)/2$ and γ edges $(\tilde q_{2j-1},\tilde q_{2j})$, $1\le i\le (s+t)/2$. From (11.14), we know each k_i $(1\le i\le 4)$ touches one edge and each p_i $(1\le i\le s+t-2)$ touches two edges. Hence the graph can be decomposed into two chains and loops. Thus there exist $l, m_i\in\mathbb{Z}$ and $0<m_1<m_2<\dots<m_l=s+t$ such that

$$\begin{aligned}&\text{chains}\begin{cases}k_1\longleftrightarrow p_1\longleftrightarrow p_2\longleftrightarrow p_3\cdots p_{2m_1-1}\longleftrightarrow k_4\ (\text{or }k_2)\\ k_3\longleftrightarrow p_{2m_1}\longleftrightarrow p_{2m_1+1}\cdots p_{2m_2-2}\longleftrightarrow k_2\ (\text{or }k_4)\end{cases}\\ &\text{loops}\begin{cases}p_{2m_2-1}\longleftrightarrow p_{2m_2}\longleftrightarrow p_{2m_2+1}\cdots p_{2(m_3)-2}\longleftrightarrow p_{2m_2-1}\\ \vdots\\ p_{2m_{l-1}-1}\longleftrightarrow p_{2m_{l-1}}\longleftrightarrow p_{2m_{l-1}+1}\cdots p_{2(m_l)-2}\longleftrightarrow p_{2m_{l-1}-1}\end{cases}\end{aligned} \tag{11.45}$$

Here we have relabeled the indices of p and do not distinguish β edges and γ edges. We also disregard the obvious symmetry $k_1\to k_2$ and $k_3\to k_4$. Due to the condition (11.27) and the facts $P_L(\beta,\alpha)=P_L(\gamma,\alpha)$ is non-trivial (Definition 5), the length of the loop must be 4 or more, i.e., each loop has at least 4 edges and 4 vertices, i.e,

$$m_{i-1}+2\le m_i\quad\text{for }3\le i\le l \tag{11.46}$$

The inequality (11.41) implies $m_2\ge 2$. Together with $m_l=(s+t)/2$ and (11.46), we obtain

$$l\le (s+t)/4+1,\qquad t\ge 1. \tag{11.47}$$

Without loss of generality, we assume $m_i - m_{i-1}$ is creasing with $i \geq 3$, i.e., for $3 \leq i < j \leq l$

$$m_i - m_{i-1} \leq m_j - m_{j-1} \tag{11.48}$$

Denote by $N(\alpha, s, \{v_1, \ldots, v_t\}, l, \{m_1, \ldots, m_l\})$ the set of all pairs (β, γ) having the graph above and we now estimate the number of elements of this set.

Using the notions $W_i = (w_{2i-1}, w_{2i})$ and $\tilde{W}_i = (\tilde{w}_{2i-1}, \tilde{w}_{2i})$, we can add the information between k_i's and p_i's into the graph as follows

$$\begin{aligned}
&k_1 \overset{W_1}{\longleftrightarrow} p_1 \overset{\tilde{W}_1}{\longleftrightarrow} p_2 \overset{W_2}{\longleftrightarrow} p_3 \cdots p_{2m_1-1} \overset{\tilde{W}_{m_1}}{\longleftrightarrow} k_4(\text{or } k_2)\\
&k_3 \overset{\tilde{W}_{m_1+1}}{\longleftrightarrow} p_{2m_1} \overset{W_{m_1+1}}{\longleftrightarrow} p_{2m_1+1} \cdots p_{2m_2-2} \overset{W_{m_2}}{\longleftrightarrow} k_2(\text{or } k_4)\\
&p_{2m_2-1} \overset{W_{m_2+1}}{\longleftrightarrow} p_{2m_2} \overset{\tilde{W}_{m_2+1}}{\longleftrightarrow} p_{2m_2+1} \cdots p_{2(m_3)-2} \overset{\tilde{W}_{m_3}}{\longleftrightarrow} p_{2m_2-1}\\
&\vdots\\
&p_{2m_{l-1}-1} \overset{W_{m_{l-1}+1}}{\longleftrightarrow} p_{2m_{l-1}} \overset{\tilde{W}_{m_{l-1}+1}}{\longleftrightarrow} p_{2m_{l-1}+1} \cdots p_{2(m_l)-2} \overset{\tilde{W}_{m_l}}{\longleftrightarrow} p_{2m_{l-1}-1},
\end{aligned} \tag{11.49}$$

where w_i's are the union of s zero's and $\{v_1, \ldots, v_t\}$, so are $\tilde{w}$'s. More specifically, if $A \overset{W}{\longleftrightarrow} B$ appears in the graph and $W = (C, D)$, then the operator $\mathcal{A}_{A,B}^{C,D}$ appears in (11.40). Since the momentum is conserved, we have

$$A \overset{W_i}{\longleftrightarrow} B \quad \Leftrightarrow \quad A + B = w_{2i-1} + w_{2i}$$

so as $\tilde{W}$'s. With this relation, we can see that β and γ is uniquely determined by the structure of the graph, w_i's, $\tilde{w}_i$'s and one k_i or p_i for each loop or chain.

To bound $|N(\tilde{\alpha}, s, \{v_1, \ldots, v_t\}, l, \{m_1, \ldots, m_l\})|$, we note that the sum of momentum (p_i's) in each loop is zero. Thus we can count the number of graphs as follows.

1. choose the positions of zeros in β edges. The total number of choices is less than 2^{t+s}.
2. choose the positions of $v_1 \cdots v_t$ in β edges. The total number of choices is $t!$.
3. choose the positions of zeros in γ edges. The total number of choices is less than 2^{t+s} again.
4. choose the positions of $v_1 \cdots v_t$ in γ edges. We call a loop trivial if all the momenta associated with γ edges are zero. The number of trivial loops is at most $s/4$ since there are at least two γ edges(4 zero's) per loop. Hence the number of non-trivial loops is at least $l - s/4$. Thus we only have to fix v in at most $t - (l - s/4)$ edges and the number of choices is at most $t^{t-l+s/4}$.

Thus, with the bound on ℓ in (11.47), we obtain

$$\begin{aligned}
&|N(\alpha, s, \{v_1, \ldots, v_t\}, l, \{m_1, \ldots, m_l\})|\\
&\quad \leq (\text{const.})^{t+s} t! t^{(t-l+s/4)} \left(\varrho^{-3\eta}\Lambda\right)^l\\
&\quad \leq (\text{const.})^{t+s} t! t^{(3t/4)} \left(\varrho^{-3\eta}\Lambda\right)^{t/4+s/4+1}
\end{aligned} \tag{11.50}$$

At last, with

$$|N(\alpha, s, \{v_1, \ldots, v_t\})| = \sum_{l} \sum_{\{m_1, \ldots, m_l\}} |N(\alpha, s, \{v_1, \ldots, v_t\}, l, \{m_1, \ldots, m_l\})|$$

and

$$\sum_{l} \sum_{\{m_1,\ldots,m_l\}} 1 \le \text{const.}^{s+t}, \tag{11.51}$$

we complete the proof of (11.37). □

12 Proofs of Lemmas 1, 2, 3

12.1 Proof of Lemma 1

The proof of Lemma 1 is standard and only a sketch will be given. We first construct an isometry between functions with periodic boundary condition in $\Lambda = [0, L]^3$ and functions with Dirichlet boundary condition in $\Lambda^* = [-\ell, L+\ell]^3$, where $L = \varrho^{-41/60}$ and $\ell = \varrho^{-41/120}$. We note, by the definition of ϱ^* in (3.5),

$$|\Lambda|\varrho = |\Lambda^*|\varrho^* \tag{12.1}$$

Denote the coordinates of x by $\mathrm{x} = (x^{(1)}, x^{(2)}, x^{(3)})$. Let $h(\mathrm{x})$ supported on $[-\ell, L+\ell]^3$ be the function $h(\mathrm{x}) = q(x^{(1)})q(x^{(2)})q(x^{(3)})$ where

$$q(x) = \begin{cases} \cos[(x-\ell)\pi/4\ell], & |x| \le \ell \\ 1, & \ell < x < L-\ell \\ \cos[(x-(L-\ell))\pi/4\ell], & |x-L| \le \ell \\ 0, & \text{otherwise} \end{cases} \tag{12.2}$$

The function $q(x)$ is symmetric w.r.t. $x = L/2$. Due to the property of cosine, for any function ϕ with the period L we have

$$\int_{\mathrm{x}\in[-\ell,L+\ell]^3} |h\phi(\mathrm{x})|^2 d\mathrm{x} = \int_{\mathrm{x}\in[0,L]^3} |\phi(\mathrm{x})|^2 d\mathrm{x} \tag{12.3}$$

Thus the map $\phi \longrightarrow h\phi$ is an isometry:

$$L^2_{\text{Periodic}}\left([0,L]^3\right) \to L^2_{\text{Dirichlet}}\left([-\ell, L+\ell]^3\right).$$

Let $\chi(\mathrm{x})$ be the characteristic function of the ℓ-boundary of $[-\ell, L+\ell]^3$, i.e., $\chi(\mathrm{x}) = 1$ if $|x^{(\alpha)}| \le \ell$ for some $\alpha = 1, 2$ or 3 where $|x^{(\alpha)}|$ is the distance on the torus $[-\ell, L+\ell]^3$. Then standard methods yield the following estimate on the kinetic energy of $h\phi$

$$\int_{\mathrm{x}\in[-\ell,L+\ell]^3} |\nabla(h\phi)(\mathrm{x})|^2 \le \int_{\mathrm{x}\in[0,L]^3} |\nabla\phi(\mathrm{x})|^2 + \text{const. } \ell^{-2} \int \chi(\mathrm{x})|\phi(\mathrm{x})|^2 \tag{12.4}$$

The generalization of this isometry to higher dimensions is straightforward. Suppose $\Psi(\mathrm{x}_1, \ldots, \mathrm{x}_N)$ is a function with period L. Here

$$N = |\Lambda|\varrho = |\Lambda^*|\varrho^* \tag{12.5}$$

Then for any $u \in \mathbb{R}^3$, the map

$$\mathcal{F}^u(\Psi) := \Psi(\mathrm{x}_1, \ldots, \mathrm{x}_N) \prod_{i=1}^{N} h(\mathrm{x}_i + u) \tag{12.6}$$

is an isometry from $L^2_{\text{Periodic}}([0, L]^{3N})$ to $L^2_{\text{Dirichlet}}([-\ell - u, L + \ell - u]^{3N})$. Clearly, $\mathcal{F}^u$ has the property (12.4).

The potential V can be extended to be periodic by defining $V^P(x-y) = V([x-y]_P)$ where $[x-y]_P$ is the difference of x and y as elements on the torus $[0, L]$. Since V is nonnegative and has fast decay in the position space, we have $V(x-y) \le V^P(x-y)$. From the definition of $\mathcal{F}^u$, we conclude that

$$\int_{[-\ell-u, L+\ell-u]^{3N}} |\mathcal{F}^u(\Psi)|^2 V(\mathrm{x}_1 - \mathrm{x}_2) \prod_{i=1}^{N} d\mathrm{x}_i \le \int_{[0,L]^{3N}} |\Psi|^2 V^P(\mathrm{x}_1 - \mathrm{x}_2) \prod_{i=1}^{N} d\mathrm{x}_i$$

Therefore, the total energies of $\mathcal{F}^u(\Psi)$ and Ψ are related by

$$\langle H_N \rangle_{\mathcal{F}^u(\Psi)} \le \langle H_N \rangle_{\Psi} + \text{const.}\, \ell^{-2} \sum_{i=1}^{N} \langle \chi(\mathrm{x}_i + u) \rangle_{\Psi} \tag{12.7}$$

We note $\mathcal{F}^u$ is operator on *pure* states. It can be generalized to operator $\mathcal{G}^u$ on states as follows. For any state Γ^P of N particles in $[0, L]^3$ with periodic boundary condition, we define

$$\mathcal{G}^u(\Gamma^P) := \mathcal{F}^u \Gamma^P (\mathcal{F}^u)^\dagger \tag{12.8}$$

So $\Gamma^D = \mathcal{G}^u(\Gamma^P)$ is a state of N particles in $[-\ell - u, L + \ell - u]^3$ with Dirichlet boundary condition. With (12.1), one can see

$$\mathcal{G}^u : \Gamma^P(\varrho, \Lambda, \beta) \to \Gamma^D\left(\varrho^*, \Lambda^*, \beta\right) \tag{12.9}$$

Using (12.7), we have:

$$\operatorname{Tr} H_N \mathcal{G}^u(\Gamma^P) \le \operatorname{Tr} H_N \Gamma^P + \text{const.}\, \ell^{-2} \sum_{i=1}^{N} \operatorname{Tr} \chi(\mathrm{x}_i + u) \Gamma^P \tag{12.10}$$

Averaging over $u \in [0, L]^3$, we have

$$L^{-3} \int \left(\operatorname{Tr} H_N \mathcal{G}^u(\Gamma^P)\right) du \le \operatorname{Tr} H_N \Gamma^P + \text{const.}\, \ell^{-1} L^{-1} N \tag{12.11}$$

So for any Γ^P there exists at least one u such that

$$\operatorname{Tr} H_N \mathcal{G}^u(\Gamma^P) \le \operatorname{Tr} H_N \Gamma^P + \text{const.}\, N\left(\frac{1}{\ell L}\right) \tag{12.12}$$

On the other hand, the fact $\mathcal{F}^u$((12.6)) is a isometry implies that $\mathcal{G}^u(\Gamma^P)$ and Γ^P have the same von-Neumann entropy, i.e.,

$$S(\mathcal{G}^u(\Gamma^P)) = S(\Gamma^P) \tag{12.13}$$

Combine (12.12) and (12.13), we obtain Δf the free energy difference between $\mathcal{G}^u(\Gamma^P)$ and Γ^P is less than const. $N(\ell L)^{-1}$. With the choice $L = \varrho^{-41/60}$ and $\ell = \varrho^{-41/120}$, the error term is negligible to the accuracy we need in proving Lemma 1. This concludes the proof of Lemma 1.

12.2 Proof of Lemma 2

It is not easy to define (construct) Γ_0 (the state of N particles) directly. We start with constructing a state $\Gamma_{\mathcal{F}}$ in Fock space. Then pick up the useful component of $\Gamma_{\mathcal{F}}$ and revise it to Γ_0.

First, let $B_{\mathcal{F}}$ be the standard basis of the Fock space $\mathcal{F}(\Lambda)$ as follows

$$B_{\mathcal{F}} \equiv \left\{ |\alpha\rangle : |\alpha\rangle = C_\alpha \prod_{k \in (\frac{2\pi\mathbb{Z}}{L})^3} (a_k^\dagger)^{\alpha(k)} |0\rangle, \alpha(k) \in \mathbb{N} \cup \{0\} \right\}, \tag{12.14}$$

where C_α is a positive normalization constant. We define a revised 'Bose' statistics, i.e.,

1. The number of the particles in single particle state $|k\rangle$ is nonzero only when $k \in P_I \cup P_L$.
2. The number of the particles in single particle state $|k\rangle$, $k \in P_L \cup P_I$, must be no more than C_k, which will be chosen later.

With the definition of μ in (2.9), we define $\Gamma_{\mathcal{F}}$ as the grand-canonical Gibbs state in this revised 'Bose' statistics with the chemical potential $\mu(\tilde{\varrho}, \beta) \le 0$ and temperature $T = \beta^{-1}$, where

$$\tilde{\varrho} \equiv \varrho(1 - L^{-1/2}) = \varrho(1 - o(\varrho^{1/3})) \tag{12.15}$$

and C_k is chosen as follows (Recall $m_c = \varrho^{-3\eta}$)

$$C_k = \begin{cases} \frac{(m_c)^{1/3}}{\beta E_{k,\mu}} & k \in P_I \\ m_c & k \in P_L, \end{cases} \tag{12.16}$$

where $E_{k,\mu}$ is defined as $k^2 - \mu(\tilde{\varrho}, \beta)$. We note that $\beta = O(\varrho^{-2/3})$ implies,

$$\beta E_{k,\mu} C_k \ge O(\varrho^{-\eta}).$$

With these notations, we can write $\Gamma_{\mathcal{F}}$ as

$$\Gamma_{\mathcal{F}} = C \sum_{\alpha \in B_{\mathcal{F}}} f_\alpha |\alpha\rangle\langle\alpha| \tag{12.17}$$

where C is a constant and f_α is non-zero only when $\alpha(k)$ is supported on $P_I \cup P_L$ and

$$\alpha(k) \le C_k, \quad k \in P_I \cup P_L. \tag{12.18}$$

If f_α is non-zero,

$$f_\alpha \equiv \exp\left(-\sum_k \left(k^2 - \mu(\tilde{\varrho}, \beta)\right) \beta\alpha(k) \right) = \exp\left(-\sum_k E_{k,\mu} \beta\alpha(k) \right) \tag{12.19}$$

We claim that the state $\Gamma_{\mathcal{F}}$ in Fock space has the following properties:

Lemma 20 *The free energy per volume of* $\Gamma_{\mathcal{F}}$ *is bounded above by*

$$f(\Gamma_{\mathcal{F}}) \le f_0(\varrho, \beta)(1 - o(\varrho^{1/3})) \tag{12.20}$$

In most cases, the total particle number of $\Gamma_{\mathcal{F}}$ *is less than* $N = \varrho\Lambda$, *i.e.*,

$$\sum_{m=1}^{N} \mathrm{Tr}_{\mathcal{H}_m} \Gamma_{\mathcal{F}}^m \ge 1 - \varrho \tag{12.21}$$

Here $\Gamma_{\mathcal{F}}^m$ *is the component of* $\Gamma_{\mathcal{F}}$ *on* $\mathcal{H}_m$, *i.e.*,

$$\Gamma_{\mathcal{F}} = \sum_{m=0}^{\infty} \oplus \Gamma_{\mathcal{F}}^m, \qquad \Gamma_{\mathcal{F}}^m : \mathcal{H}_m \to \mathcal{H}_m \tag{12.22}$$

Similarly, in most cases, the total particle number of $\Gamma_{\mathcal{F}}$ *is very close to* $\min\{\varrho, \varrho_c\}\Lambda$, *i.e.*, *we have*

$$\sum_{|m - \min\{\varrho, \varrho_c\}\Lambda| \le N\varrho^{1/3}} \mathrm{Tr}_{\mathcal{H}_m} \Gamma_{\mathcal{F}}^m \ge 1 - \varrho \tag{12.23}$$

Proof of Lemma 20 First, we prove (12.20), by the definition, the free energy of $\Gamma_{\mathcal{F}}$ is

$$\frac{-1}{\beta}\left[\sum_{k\in P_L\cup P_I} \log\left(\frac{e^{\beta E_{k,\mu}} - e^{-\beta E_{k,\mu} C_k}}{e^{\beta E_{k,\mu}} - 1}\right)\right]$$
$$+ \sum_{k\in P_L\cup P_I} \mu(\tilde{\varrho}, \beta)\left(\frac{1}{e^{\beta E_{k,\mu}} - 1} - \sum_{k\in P_L\cup P_I} \frac{1 + C_k}{e^{\beta E_{k,\mu}(C_k+1)} - 1}\right). \tag{12.24}$$

With the definition of P_I and P_L, adding the $k \notin P_I \cup P_L$ terms and bounding the C_k terms, one can easily check that (12.24) is equal to

$$\left(\frac{-1}{\beta} \sum_{k\in(\frac{2\pi\mathbb{Z}}{L})^3, k\ne 0} \log\left(\frac{e^{\beta E_{k,\mu}}}{e^{\beta E_{k,\mu}} - 1}\right) + \sum_{k\in(\frac{2\pi\mathbb{Z}}{L})^3, k\ne 0} \mu(\tilde{\varrho}, \beta)\frac{1}{e^{\beta E_{k,\mu}} - 1}\right)(1 + o(\varrho^{1/3})). \tag{12.25}$$

Then with the choice $L = \varrho^{-41/60}$ and the definition of free energy f_0 in (2.7) and (2.8), we have

$$(12.25) = f_0(\tilde{\varrho}, \beta)\Lambda(1 + o(\varrho^{1/3})) \tag{12.26}$$

Combining this with $\tilde{\varrho} = \varrho(1 + o(\varrho^{1/3}))$, we obtain the desired result (12.20).

Then we prove (12.21). Let $n(k)$ denote the number of the particles in one-particle-state $|k\rangle$. Then $\overline{n(k)}$ the average of $n(k)$ is equal to $\mathrm{Tr}\, a_k^\dagger a_k \Gamma_{\mathcal{F}}$. By the definition, the average total number of particles of $\Gamma_{\mathcal{F}}$ is equal to

$$\sum_{k\in P_I\cup P_L} \overline{n(k)} = \sum_{k\in P_I\cup P_L} \frac{1}{e^{\beta E_{k,\mu}} - 1} - \sum_{k\in P_L\cup P_I} \frac{1 + C_k}{e^{\beta E_{k,\mu}(C_k+1)} - 1} \tag{12.27}$$

Similarly, with $L = \varrho^{-41/60}$ and $\beta E_{k,\mu} C_k \gg |\log \varrho|$, one can easily prove:

$$\begin{aligned}(12.27) &= \min\{\tilde{\varrho}, \varrho_c(\beta)\}\Lambda(1 + O(\varrho^{-1/3} L^{-1} \log \varrho)) \\ &= \min\{\tilde{\varrho}, \varrho_c\}\Lambda + o(N\varrho^{41/120})\end{aligned} \tag{12.28}$$

On the other hand, we are going to use Hoeffding's inequality to estimate $\sum_k n(k)$. Hoeffding's inequality said, for independent X_i's, if they are bounded as

$$a_i \le X_i - \mathbb{E}(X_i) \le b_i \tag{12.29}$$

where $\mathbb{E}(X_i)$ is the expected value of X_i, then

$$P\left(\left|\sum_i X_i - \mathbb{E}\left(\sum_i X_i\right)\right| > t\right) \le 2\exp\left(-\frac{2t^2}{\sum_i (b_i - a_i)^2}\right) \tag{12.30}$$

Since $n(k)$'s are independent random variables for different k's and they are bounded in (12.16), we can use Hoeffding's inequality [5] to estimate the distribution of the total particle number of $\Gamma_{\mathcal{F}}$. With $n(k) \le C_k$ and Hoeffding's inequality [5], we obtain that the probability of finding more than N particles in $\Gamma_{\mathcal{F}}$ is bounded above by

$$P\left(\sum_k n(k) > N\right) \le 2\exp\left\{-\frac{2[N - \sum_k \overline{n(k)}]^2}{\sum_{k\in P_I\cup P_L} C_k^2}\right\} \tag{12.31}$$

By the definition of C_k (12.16), the denominator of the r.h.s. of (12.31) is bounded as:

$$\sum_{k\in P_I\cup P_L} C_k^2 = O(\varrho^{4/3}\Lambda L m_c^{2/3}) \tag{12.32}$$

On the other hand, with the fact $\varrho - \tilde{\varrho} = \varrho L^{-1/2}$ and (12.28), the numerator of the r.h.s. of (12.31) is bounded below by

$$\left[N - \sum_k \overline{n(k)}\right]^2 \ge O(\varrho^2 L^5) \tag{12.33}$$

Inserting $L = \varrho^{-41/60}$, (12.32) and (12.33) into (12.31), we obtain the desired result (12.21). And (12.23) can proved similarly with (12.28) and (12.32). □

By Lemma 20, there exists $m_0 \le N$ such that

$$m_0 \le N, \quad |m_0 - \min\{\varrho, \varrho_c\}\Lambda| \le \varrho^{1/3} N \tag{12.34}$$

and the free energy of $\Gamma_{\mathcal{F}}^{m_0}$ is less than $f_0(\varrho,\beta)\Lambda(1 - o(\varrho^{1/3}))$.

Then adding $N - m_0$ ($N = \varrho\Lambda$) particles with momentum zero into the system described by $\Gamma_{\mathcal{F}}^{m_0}$, we obtain a new state Γ_0 of N particles. The state Γ_0 always has $N - m_0$ particles with momentum zero. The free energy of Γ_0 is also less than $f_0(\varrho,\beta)\Lambda(1 - o(\varrho^{1/3}))$, i.e.,

$$\left|\mathrm{Tr}(-\Delta\Gamma_0) + \frac{1}{\beta}S(\Gamma_0) - f_0(\varrho,\beta)\right|\Lambda^{-1} \le o(\varrho^2) \tag{12.35}$$

Furthermore, by the definition of $\Gamma_{\mathcal{F}}$, Γ_0 has the form:

$$\Gamma_0 = \sum_{\alpha\in M} g_\alpha(\varrho,\beta)|\alpha\rangle\langle\alpha|, \qquad \alpha(0) = N - m_0 \quad \text{and} \quad \sum_{\alpha\in M} g_\alpha = 1 \tag{12.36}$$

We note: if $\alpha(k) > C_k$ for some $k \in P_I \cup P_L$, then $g_\alpha(\varrho, \beta) = 0$. This property implies that the total number of the particles with momentum in P_I is $o(N)$. So we have

$$\sum_{\alpha\in M}\sum_{k\in P_I} g_\alpha(\varrho,\beta)\alpha(k) \ll N. \tag{12.37}$$

Together with the facts $\alpha(0) = N - m_0$, (12.34) and $\alpha(k) \le m_c$ for $\alpha \in P_L$, we obtain (3.24).

At last we prove (3.23). First with the structure of Γ_0, we have

$$\begin{aligned}\mathrm{Tr}_{\mathcal{H}_{N,\Lambda}} \frac{1}{2} V\Gamma_0 &= \sum_{\alpha\in M} g_\alpha(\varrho,\beta)\langle\alpha|\frac{1}{2}V|\alpha\rangle \\ &= \sum_{\alpha\in M} g_\alpha(\varrho,\beta)\Bigg(\sum_{k\in P_0\cup P_I\cup P_L} \frac{1}{2} V_0\Lambda^{-1}(\alpha(k)^2-\alpha(k)) \\ &\quad + \sum_{k,k'\in P_0\cup P_I\cup P_L}^{k\neq k'} (V_0+V_{k-k'})\Lambda^{-1}\alpha(k)\alpha(k')\Bigg)\end{aligned} \tag{12.38}$$

Using the smoothness of V and $|k|, |k'| \ll 1$, we can replace $V_{k-k'}$ with V_0 without changing the leading term. Then with the cutoff C_k's, the fact $\alpha(0) = N - m$ and (12.34), we have

$$\lim_{\varrho\to 0}\left|\mathrm{Tr}\,\frac{1}{2}V\Gamma_0\right|\varrho^{-2}\Lambda^{-1} = \frac{1}{2}V_0(2-[1-R[\beta]]_+^2) \tag{12.39}$$

Combine with (12.35), we obtain (3.23).

12.3 Proof of Lemma 3

Proof Since the states $|\alpha\rangle$'s $\in M$ are orthonormal, we can rewrite the entropy of Γ_0 in Lemma 2 as

$$S(\Gamma_0) = -\sum_{\alpha\in M} g_\alpha \log g_\alpha \tag{12.40}$$

For $S(\Gamma)$, we define A_∞ as

$$A_\infty \equiv \left\|\sum_{\alpha\in M}|\Psi_\alpha\rangle\langle\Psi_\alpha|\right\|_\infty$$

and rewrite Γ as

$$\Gamma = A_\infty \sum_{\alpha\in M} g_\alpha \frac{|\Psi_\alpha\rangle}{\sqrt{A_\infty}}\frac{\langle\Psi_\alpha|}{\sqrt{A_\infty}} \tag{12.41}$$

With the fact $\mathrm{Tr}\,\Gamma = 1$, i.e., $\sum g_\alpha = 1$, we have

$$S(\Gamma) = -\log A_\infty - A_\infty\,\mathrm{Tr}\left[\sum_{\alpha\in M} g_\alpha \frac{|\Psi_\alpha\rangle}{\sqrt{A_\infty}}\frac{\langle\Psi_\alpha|}{\sqrt{A_\infty}}\log\left(\sum_{\alpha\in M} g_\alpha \frac{|\Psi_\alpha\rangle}{\sqrt{A_\infty}}\frac{\langle\Psi_\alpha|}{\sqrt{A_\infty}}\right)\right] \tag{12.42}$$

With the concavity of the logarithm, one can easily obtain

$$S(\Gamma) \ge -\log A_\infty - \sum_{\alpha\in M} g_\alpha \log g_\alpha = -\log A_\infty + S(\Gamma_0) \tag{12.43}$$

We claim the following lemma

Lemma 21

$$\lim_{\varrho\to 0}\left(\log\left\|\sum_{\alpha\in M}|\Psi_\alpha\rangle\langle\Psi_\alpha|\right\|_\infty\right)\frac{1}{N\varrho^{1/3}}=0 \tag{12.44}$$

Insert this lemma into (12.43), we arrive at the desired result (3.31). □

12.3.1 Proof of Lemma 21

Proof With the fact: for any hermitian matrix $M=M_{ij}$,

$$\|M\|_\infty\le\max_i\left\{\sum_j|M_{ij}|\right\}$$

we can bound $\|\sum_{\alpha\in M}|\Psi_\alpha\rangle\langle\Psi_\alpha|\|_\infty$ as follows (recall $\tilde{M}$ in Definition 2)

$$\begin{aligned}\left\|\sum_{\alpha\in M}|\Psi_\alpha\rangle\langle\Psi_\alpha|\right\|_\infty &\le\max_{\beta\in\tilde{M}}\left\{\sum_{\alpha\in M}\sum_{\gamma\in\tilde{M}}|\langle\beta|\Psi_\alpha\rangle\langle\Psi_\alpha|\gamma\rangle|\right\}\\ &\le\max_{\beta\in\tilde{M}}\left\{\sum_{\alpha\in M}|\langle\beta|\Psi_\alpha\rangle|\right\}\cdot\max_{\alpha\in M}\left\{\sum_{\gamma\in\tilde{M}}|\langle\gamma|\Psi_\alpha\rangle|\right\},\end{aligned} \tag{12.45}$$

With the fact Ψ_α is the linear combination of states in $M_\alpha\subset\tilde{M}_\alpha$ and $|\beta\rangle$, $|\Psi_\alpha\rangle$ are normalized, we claim

$$\log\left(\max_{\beta\in\tilde{M}}\left\{\sum_{\alpha\in M}|\langle\beta|\Psi_\alpha\rangle|\right\}\right)\le\varrho^{1-4\eta-3\varkappa_L} \tag{12.46}$$

$$\log\left(\max_{\alpha\in M}\left\{\sum_{\gamma\in\tilde{M}}|\langle\gamma|\Psi_\alpha\rangle|\right\}\right)\le\varrho^{1-4\eta-3\varkappa_L}+\varrho^{-4\eta-3\varkappa_H} \tag{12.47}$$

First, we prove (12.46). For any $\alpha\in M$ and $\beta\in\tilde{M}_\alpha$, $|\langle\beta|\Psi_\alpha\rangle|\neq 0$ implies $|\langle\beta|\Psi_\alpha\rangle|\le 1$. Then with the definition of M and $\tilde{M}_\alpha$, if $\alpha\in M$, $\beta\in\tilde{M}_\alpha$, we have

$$\begin{aligned}&\beta(u)=\alpha(u)\quad\text{for } u\in P_I\\ &\beta(u)\le\alpha(u)\quad\text{for } u\in P_L\\ &\alpha(u)=0\quad\text{for } u\in P_H\end{aligned} \tag{12.48}$$

and for any fixed small box $B_L^i(i=1,2,\ldots)$ in P_L, $\beta(u)$ is very close to $\alpha(u)$, i.e.,

$$\sum_{u\in B_L^i}|\beta(u)-\alpha(u)|\le 1 \tag{12.49}$$

Now let's count, for fixed β, how many $\alpha\in M$ satisfy $\beta\in\tilde{M}_\alpha$. This number must be less than the α's satisfying (12.48) and (12.49). By the definition of B_L's, the total number of

B_L's is less than const. $\varrho^{1-3\eta-3\varkappa_L}$. And for any B_L^i, $|B_L^i|$ the number of the elements in B_L^i is less than const.$\varrho^{3\varkappa_L}\Lambda$. Therefore, for fix $\beta \in \tilde{M}$, the total number of $\alpha \in M$ satisfying $\beta \in \tilde{M}_\alpha$ is less than

$$\left(\text{const.}\,\varrho^{3\varkappa_L}\Lambda\right)^{\text{const.}\,\varrho^{1-3\eta-3\varkappa_L}} \tag{12.50}$$

Together with the fact $|\langle\beta|\Psi_\alpha\rangle| \le 1$, we proved (12.46).

Then we prove (12.47). Similarly, using the rule 2 of Definition 3, we can count, for fix $\alpha \in M$, the total number of $\gamma \in \tilde{M}$, s.t. $|\langle\gamma|\Psi_\alpha\rangle| \neq 0$ is less than

$$\left(\text{const.}\,\varrho^{3\varkappa_L}\Lambda\right)^{\text{const.}\,\varrho^{1-3\eta-3\varkappa_L}}\left(\text{const.}\,\varrho^{3\varkappa_H}\Lambda\right)^{\text{const.}\,\varrho^{-3\eta-3\varkappa_H}} \tag{12.51}$$

which implies (12.47). Inserting (12.46) and (12.47) into (12.45), we obtain the desired result (12.44). □

Appendix

Lemma 22 *For any bound, non-negative, piecewise continuous function, spherically symmetric f supported in unit ball, there exist C^∞, non-negative spherically symmetric function $f_1, f_2, \ldots$ supported in the ball of radius 2 such that for any $n \ge 1$,*

$$f_n - f \ge 0 \quad \textit{and} \quad \lim_{n\to\infty} \|f_n - f\|_1 = 0 \tag{13.1}$$

Proof First, we note, for any bound, non-negative, piecewise continuous function f supported in unit ball, there exist non-negative, continuous functions $\tilde{f}_1, \tilde{f}_2, \ldots$ supported in the ball of radius 1.5, such that

$$\tilde{f}_n \ge f \quad \text{and} \quad \lim_{n\to\infty} \|\tilde{f}_n - f\|_1 \to 0 \tag{13.2}$$

Then we claim that for any $\tilde{f}_n$, there exist C^∞, non-negative spherically symmetric function $\tilde{f}_{nm}$ $(m = 1, 2, \ldots)$ supported in the ball of radius 2, such that

$$\tilde{f}_{nm} \ge \tilde{f}_n \quad \text{and} \quad \lim_{n\to\infty} \|\tilde{f}_n - \tilde{f}_{nm}\|_1 \to 0 \tag{13.3}$$

To prove Lemma 22, we can choose f_n as $\tilde{f}_{nm_n}$, where m_n is defined as

$$m_n = \min\left\{m : \|\tilde{f}_n - \tilde{f}_{nm}\|_1 \le \|\tilde{f}_n - f\|_1\right\} \tag{13.4}$$

It only remains to prove (13.3). Let g be a bound C^∞ spherically symmetric function support in the ball of radius 2 such that

$$g \ge 0, \qquad \|g\|_1 = 1 \quad \text{and} \quad g(x) = g(0) > 0 \quad \text{for } |x| \le 1.5 \tag{13.5}$$

And we define g_m as

$$g_m(x) = m^3 g(mx) \tag{13.6}$$

Then $\|g_m\|_1 = 1$. Furthermore, for fixed n

$$\lim_{m\to\infty} \|\tilde{f}_n * g_m - \tilde{f}_n\|_\infty = 0 \quad \text{and} \quad \lim_{m\to\infty} \|\tilde{f}_n * g_m - \tilde{f}_n\|_1 = 0 \tag{13.7}$$

and $\tilde{f}_n * g_m$ are non-negative, C^∞ spherically symmetric functions. Since $\tilde{f}_n$ is supported on the ball of radius 1.5, we can choose $\tilde{f}_{nm}$ as

$$\tilde{f}_{nm} \equiv \tilde{f}_n * g_m + \frac{1}{g(0)} \|\tilde{f}_n * g_m - \tilde{f}_n\|_\infty g \tag{13.8}$$

and complete the proof. □

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