Ground-state energy of a low-density Bose gas: A second-order upper bound

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Consider N bosons in a finite box $\Lambda = [0,L]^3 \subset \mathbb{R}^3$ interacting via a two-body non-negative soft potential $V = \lambda \widetilde{V}$ with $\widetilde{V}$ fixed and $\lambda > 0$ small. We will take the limit $L, N \to \infty$ by keeping the density $\varrho = N/L^3$ fixed and small. We construct a variational state, which gives an upper bound on the ground-state energy per particle ε, $\varepsilon \leq 4\pi\varrho a[1 + (128/15\sqrt{\pi})(\varrho a^3)^{1/2} S_\lambda] + O(\varrho^2|\ln \varrho|)$, as $\varrho \to 0$, with a constant satisfying $1 \leq S_\lambda \leq 1 + C\lambda$. Here a is the scattering length of V and thus depends on λ. In comparison, the prediction by Lee and Yang [Phys. Rev. **105**, 1119 (1957)] and Lee, Huang, and Yang [Phys. Rev. **106**, 1135 (1957)] asserts that $S_\lambda = 1$ independent of λ.

I. INTRODUCTION

Although Bose-Einstein condensation has been firmly established since the experiments detailed in Refs. [1,2], rigorous understanding of the Bose gas starting from the many-body Schrödinger equation is still in a very rudimentary stage and many theoretical predictions at present are still based on uncontrolled approximations [3]. Notable exceptions are the rigorous derivations of the Gross-Pitaevskii equation in both the stationary and the dynamical settings [4,5]. In particular, in the limit of low density, the leading term of the ground-state energy per particle of an interacting Bose gas was proved by Dyson (upper bound) [6] and Lieb-Yngvason (lower bound) [7] to be $4\pi a\varrho$, where a is the scattering length of the two-body potential and ϱ is the density. The famous second-order correction to this leading term was first computed by Lee-Yang [8] (see also Lee-Huang-Yang [9] and the recent paper by Yang [10] for results in other dimensions). In this paper, we construct a trial function with a second-order term in the energy which, up to a constant factor, is the same as predicted in [8,9]. To present this result, we now introduce our setup rigorously.

Consider N interacting bosons in a finite box $\Lambda = [0,L]^3 \subset \mathbb{R}^3$ with periodic boundary conditions. Let $\widetilde{V}$ be a smooth, radially symmetric, non-negative potential with fast decay. The two-body interaction V is given by $V = \lambda \widetilde{V}$ with λ a small constant. We will first take the limit $L, N \to \infty$ by keeping the density $\varrho = N/L^3$ fixed. In the limit $\varrho \to 0$, the leading term for the ground-state energy per particle of this system is $4\pi\varrho a$, where a is the scattering length of the potential V. Lee-Yang's prediction of the energy per particle up to the second order term is given by

$$\varepsilon = 4\pi\varrho a\left[1 + \frac{128}{15\sqrt{\pi}}(\varrho a^3)^{1/2} + \cdots\right]. \quad (1)$$

The approach by Lee-Yang [8] is based on the pseudopotential approximation [9,11] and the "binary collision expansion method" [9]. One can also obtain Eq. (1) by performing the Bogoliubov [12] approximation and then replacing the integral of the potential by its scattering length [13]. Another derivation of Eq. (1) was later given by Lieb [14] using a

self-consistent closure assumption for the hierarchy of correlation functions. Although these approaches gave the same answer for the second-order term (1), it is nevertheless difficult to extract rigorous results on the energy using these ideas. In fact, the first rigorous upper bound on the energy to the leading order by Dyson [6] was based on a completely different construction. The proof of Lieb-Yngvason [7] on the lower bound of the energy to the leading order was also very different from the earlier approaches.

The trial wave function of Dyson [6] also shows that the next order correction in energy for hard-core bosons is bounded from above by $C(\varrho a^3)^{1/3}$. The same upper bound for soft potentials was obtained in [5]. In this paper, we construct a variational state, which gives a rigorous upper bound on the ground-state energy per particle,

$$\varepsilon \leq 4\pi\varrho a\left[1 + \frac{128}{15\sqrt{\pi}}(\varrho a^3)^{1/2}S_\lambda\right] + O(\varrho^2|\ln \varrho|), \quad (2)$$

with $S_\lambda \leq 1 + C\lambda$. The second-order term in this upper bound (2) is of the same form as the conjectured one (1), up to a *positive* correction in the constant of order λ. This constant C and the constant in the error term in Eq. (2) depends on the details of the interaction potential, in particular, our proof specifies that $\hat{V}$ is a soft potential.

The trial state in this paper consists only of condensate particles and of noncondensate particle pairs with momenta $k, -k$, reminiscent of the original idea of Bogoliubov. In our computation, however, the interactions between noncondensate particle pairs are also relevant. Our trial state does not have a fixed number of particles, but it is a state in the Fock space with an expected number of particles equal to N. It is similar to the trial states used by Solovej [15] to give rigorous upper bounds to the ground-state energies of the one- and two-component charged Bose gases in the high-density limit.

Variational trial states with particle pairs have been used earlier in the context of the low-density Bose gas by Girardeau and Arnowitt [16]. Their state, however, had a fixed number of particles, which slightly complicated the calculation (the details are available only in Ref. [17]). The variational formula we obtain is nevertheless the same as theirs up

to lower-order terms due to the choice of a different ensemble. However, in [16], the solution of the minimization problem was given only implicitly as a solution to a nonlinear integral equation and thus the energy was not evaluated explicitly. In our work, we identify the presumed main term from the calculations of each individual term in the energy. This enables us to find the minimizer for the main terms of the energy. By choosing the minimizer of the main part as our trial state, we *a posteriori* justify that the neglected terms are indeed of lower order and thus give a rigorous upper bound on the energy. We believe that the difference between the energy of our state and that of the true minimizer of the full functional is of lower order.

II. SETUP

We work in a finite box $\Lambda = \Lambda_L = [0,L]^3 \subset \mathbb{R}^3$ with periodic boundary conditions. Its dual space is $\Lambda^* := (\frac{2\pi}{L}\mathbb{Z})^3$. For a continuous function F on $\mathbb{R}^3$, we have

$$\lim_{L\to\infty} \frac{1}{L^3} \sum_{p\in\Lambda^*} F(p) = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{p\in\Lambda^*} F(p) = \int_{\mathbb{R}^3} \frac{d^3p}{(2\pi)^3} F(p).$$

The Fourier transform of an arbitrary function $f(x)$ on Λ is defined as

$$\hat{f}_p = \int_\Lambda e^{-ipx} f(x) dx, \quad f(x) = \frac{1}{|\Lambda|} \sum_{p\in\Lambda^*} e^{ipx} \hat{f}_p.$$

Note that the Fourier transform depends on Λ, a fact that is omitted from the notation. In most cases we will take Fourier transforms of sufficiently decaying functions, so that their Λ dependence is negligible in the limit $L \to \infty$. Since $V(x)$ is real and symmetric, we have that $\hat{V}_u$ is real and

$$\hat{V}_u = \hat{V}_{-u}.$$

We also have

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

where $\delta_{\mathbb{R}^3}(x)$ is the usual continuum delta function and δ_{Λ^*} is the lattice delta function, i.e., $\delta_{\Lambda^*}(p) = |\Lambda| = L^3$ if $p=0$, and $\delta_{\Lambda^*}(p) = 0$ if $p \in \Lambda^* \backslash \{0\}$. We will neglect the subscripts in the delta functions, the argument indicates whether it is the momentum or position space delta function. We also simplify the notation

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

i.e., momentum summation is always on the whole Λ^*.

Notice that the choice of the δ_{Λ^*} ensures that in the $L \to \infty$ limit, this delta function converges to the usual continuum delta function $\delta(p)$ in momentum space with respect to the measure $d^3p/(2\pi)^3$.

$$\lim_{L\to\infty} \frac{1}{|\Lambda|} \sum_{p\in\Lambda^*} F(p)\delta_{\Lambda^*}(p-q) = \int_{\mathbb{R}^3} \frac{d^3p}{(2\pi)^3} F(p)\delta(p-q) = F(q)$$

[where $\delta(p)$ is defined by the last formula].

Using the formalism of the second quantization, we work on the bosonic Fock space $\mathcal{F} = \oplus_{n=0}^\infty \mathcal{H}^{\otimes_s n}$ built upon the single-particle Hilbert space $\mathcal{H} = \ell^2(\Lambda^*)$, where $\mathcal{H}^{\otimes_s n}$ denotes the symmetric tensor product of n copies of $\mathcal{H}$. The vacuum is denoted by $|0\rangle$. We consider bosonic annihilation and creation operators, $\tilde{a}_k, \tilde{a}_k^\dagger$, for any $k \in \Lambda^*$, with the usual canonical commutation relations (CCR)

$$[\tilde{a}_p, \tilde{a}_q^\dagger] = \tilde{a}_p\tilde{a}_q^\dagger - \tilde{a}_q^\dagger\tilde{a}_p = \delta(p-q) = \begin{cases} L^d & \text{if } p = q \\ 0 & \text{otherwise.} \end{cases}$$

The Hamiltonian of the system is given by

$$H = \frac{1}{|\Lambda|} \sum_p p^2 \tilde{a}_p^\dagger \tilde{a}_p + \frac{1}{2|\Lambda|^3} \sum_{p,q,u} \hat{V}_u \tilde{a}_p^\dagger \tilde{a}_q^\dagger \tilde{a}_{p-u} \tilde{a}_{q+u},$$

where the first term is the kinetic energy, and the second term is the interaction energy of the particles in appropriate physical units. It is more convenient to redefine the bosonic operators as

$$a_k = \frac{1}{\sqrt{|\Lambda|}}\tilde{a}_k, \quad a_k^\dagger = \frac{1}{\sqrt{|\Lambda|}}\tilde{a}_k^\dagger,$$

i.e., from now on we assume that

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

Thus the Hamiltonian is given by

$$H = \sum_p p^2 a_p^\dagger a_p + \frac{1}{2|\Lambda|} \sum_{p,q,u} \hat{V}_u a_p^\dagger a_q^\dagger a_{p-u} a_{q+u}. \tag{3}$$

III. TRIAL STATE

Let c_k denote a family of complex numbers parametrized by $k \in \Lambda^* \backslash \{0\}$ with the property that $|c_k| < 1$ and $c_k = c_{-k}$. We define a state

$$\Psi := e^{(1/2)\sum_{k\neq 0} c_k a_k^\dagger a_{-k}^\dagger + \sqrt{N_0} a_0^\dagger} |0\rangle, \tag{4}$$

where N_0 is a positive real number. The parameters c_k and N_0 will be fixed later on.

Fix a small positive number ϱ, which will be the density of the system, and let N denote

$$N := \varrho|\Lambda|.$$

Define the expectation with respect to Ψ by

$$\langle A \rangle_\Psi = \frac{\langle \Psi, A\Psi \rangle}{\langle \Psi, \Psi \rangle},$$

where $\langle \, , \, \rangle$ denote the standard L^2 inner product. We shall fix the parameters in Ψ so that the expected number of particles is given by N,

$$N = \left\langle \sum_{m\in\Lambda^*} a_m^\dagger a_m \right\rangle_\Psi. \tag{5}$$

Let $E = \langle H \rangle_\Psi$ be the energy.

Let $1 - w$ be the zero energy scattering solution to the potential V,

$$-\Delta(1-w)+\frac{1}{2}V(1-w)=0, \tag{6}$$

on $\mathbb{R}^3$ with $0 \leq w < 1$ and $w(x) \to 0$ as $|x| \to \infty$. Then the scattering length is defined by

$$a := \frac{1}{8\pi} \int_{\mathbb{R}^3} V(x)[1-w(x)]dx$$

$$= \frac{1}{8\pi} \lim_{L \to \infty} \int_{\Lambda_L} V(x)[1-w(x)]dx. \tag{7}$$

It is well known that

$$8\pi a < \int_{\mathbb{R}^3} V(x)dx = \lim_{L \to \infty} \int_{\Lambda} V(x)dx = \lim_{L \to \infty} \hat{V}_0, \tag{8}$$

where, in the last step, we recall that the definition of the Fourier transform depends on L.

Define the number h by

$$h = \frac{\hat{V}_0}{8\pi a} - 1. \tag{9}$$

From Eq. (8) it follows that $h > 0$ if L is sufficiently large. Recall that $V = \lambda \widetilde{V}$ with $\widetilde{V}$ being fixed. The scattering length a can be computed via the Born series for small λ. In particular, we will show in Lemma 3 that h is of order λ,

$$h = O(\lambda). \tag{10}$$

Define the function

$$\Phi(h) := \int_0^\infty dy \, y^{1/2}$$

$$\times \left(\sqrt{(y+2h)(y+2+2h)} - (y+1+2h) + \frac{1}{2y} \right). \tag{11}$$

One can check that this integral is convergent for $h \geq 0$. Our main result is the following theorem.

Theorem 1. Let $\widetilde{V}(x) \geq 0$, $\widetilde{V} \not\equiv 0$, be a non-negative radially symmetric smooth function with a decay $\widetilde{V}(x) \leq C(1 + |x|)^{-3-\delta}$ for some $\delta > 0$, and set $V(x) = \lambda \widetilde{V}(x)$. Then for λ small enough, we have, in the limit $\varrho \to 0$, the following estimate:

$$E = 4\pi\varrho N a + Q + O(N\varrho^2 |\ln \varrho|) \tag{12}$$

for the energy of the trial state (4) with an appropriate choice of c_k and N_0, under the constraint (5). Here $Q = Q(h)$ is given by

$$Q(h) = 4\pi a N \varrho \left[\sqrt{\frac{32}{\pi}} \Phi(h)(a^3 \varrho)^{1/2} \right],$$

and the constant in the error term in Eq. (12) depends on λ and $\widetilde{V}$.

The assumptions on $\widetilde{V}$ can certainly be relaxed but we do not aim at identifying the optimal conditions.

A direct calculation gives

$$\Phi(0) = \frac{\sqrt{512}}{15},$$

thus at $h = 0$ we obtain

$$Q(0) = 4\pi a N \varrho \frac{128}{15\sqrt{\pi}} (a^3 \varrho)^{1/2}.$$

Moreover, a simple calculation also shows that

$$0 < \Phi'(0) = \int_0^\infty \frac{2y^{1/2}dy}{(y+1)\sqrt{y(y+2)}} < \infty,$$

thus infinitesimally $\Phi(0) < \Phi(h)$ if $0 < h \ll 1$ and

$$Q(h) = Q(0) + O(h) = Q(0) + O(\lambda)$$

by Eq. (10). In fact, it is also easy to see that

$$\Phi(0) < \Phi(h)$$

holds for any $h > 0$. Thus our trial state delivers a second-order term with an explicit constant that is bigger than the Lee-Yang prediction [7,8] by a factor $[1+O(\lambda)]$ for a small coupling constant λ.

IV. COMPUTATION OF THE ENERGY

We start the proof of the main theorem by the following Lemma. We first define a few quantities as follows:

$$\Omega_2 = -\sum_{p \neq 0} \frac{(\hat{V}_p + \hat{V}_0)}{|\Lambda|} \left(\sum_{m \neq 0} \frac{|c_m|^2}{1-|c_m|^2} \right) \frac{|c_p|^2}{1-|c_p|^2}$$

$$+ \frac{\hat{V}_0}{2|\Lambda|} \left(\sum_{m \neq 0} \frac{|c_m|^2}{1-|c_m|^2} \right)^2, \tag{13}$$

$$\Omega_4 = \sum_{p \neq 0} \left[\frac{1}{2|\Lambda|} \sum_{r \neq 0, \pm p} (\hat{V}_0 + \hat{V}_{p-r}) \frac{|c_p|^2 |c_r|^2}{(1-|c_p|^2)(1-|c_r|^2)} \right.$$

$$\left. + \frac{1}{2|\Lambda|} \frac{\hat{V}_0 |c_p|^2(1+3|c_p|^2) + \hat{V}_{2p}|c_p|^2(1+|c_p|^2)}{(1-|c_p|^2)^2} \right]. \tag{14}$$

Lemma 2. The energy $E = \langle H \rangle_\Psi$ of the state (4) under the constraint (5) is given by $E = E_M + \Omega_2 + \Omega_4$, where

$$E_M := \frac{1}{2|\Lambda|} \hat{V}_0 N^2 + \sum_{p \neq 0} \left[(p^2 + \varrho\hat{V}_p) \frac{|c_p|^2}{1-|c_p|^2} + \varrho\hat{V}_p \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} \right.$$

$$+ \frac{1}{2|\Lambda|} \sum_{r \neq 0, \pm p} \hat{V}_{p-r} \frac{\bar{c}_p c_r}{(1-|c_p|^2)(1-|c_r|^2)}$$

$$\left. - \frac{\hat{V}_p}{|\Lambda|} \sum_{m \neq 0} \frac{|c_m|^2}{1-|c_m|^2} \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} \right]. \tag{15}$$

Remark. We shall see later on that the first four terms in the main term E_M are of order $N\varrho$, the fifth one is of order

$N\varrho^{3/2}$. Each term in the error terms Ω_2 and Ω_4 is at most of order $N\varrho^2|\ln \varrho|$ except the last term in Ω_4, which is nonextensive.

Proof. We collect a few elementary facts from direct calculations. Similar formulas in an abstract setup applicable in general, not only for the translation invariant case, were presented in [15].

$$\langle 0|e^{\bar{c}_k a_k a_{-k}}e^{c_k a_k^\dagger a_{-k}^\dagger}|0\rangle = \frac{1}{1-|c_k|^2} \quad \text{for } k \neq 0,$$

$$\langle \Psi, \Psi \rangle = e^{N_0}\prod_{k\neq 0}\frac{1}{(1-|c_k|^2)^{1/2}},$$

$$\langle a_0^\dagger a_0 \rangle_\Psi = N_0,$$

$$\langle a_0^\dagger a_0^\dagger a_0 a_0 \rangle_\Psi = N_0^2,$$

and for $m\neq 0$,

$$\langle a_m^\dagger a_m \rangle_\Psi = \frac{|c_m|^2}{1-|c_m|^2},$$

$$\overline{\langle a_m^\dagger a_{-m}^\dagger \rangle_\Psi} = \langle a_m a_{-m} \rangle_\Psi = \frac{c_m}{1-|c_m|^2},$$

$$\langle a_m^\dagger a_m^\dagger a_{-m} a_{-m} \rangle_\Psi = 0,$$

$$\langle a_m^\dagger a_{-m}^\dagger a_m a_{-m} \rangle_\Psi = \frac{|c_m|^2(1+|c_m|^2)}{(1-|c_m|^2)^2},$$

$$\langle a_m^\dagger a_m^\dagger a_m a_m \rangle_\Psi = \frac{2|c_m|^4}{(1-|c_m|^2)^2}.$$

Moreover,

$$\langle A a_m B \rangle_\Psi = 0, \quad m \neq 0, \tag{16}$$

where A and B are any operator not containing $a_m^\dagger$ or a_{-m}. In fact, for an appropriate operator C commuting with $a_m, a_{-m}, a_m^\dagger, a_{-m}^\dagger$, we have

$$\langle A a_m B \rangle_\Psi = \langle 0|C^* e^{\bar{c}_m a_m a_{-m}} A a_m B e^{c_m a_m^\dagger a_{-m}^\dagger} C|0\rangle$$

$$= \sum_{n,k\geqslant 0}\frac{\bar{c}_m^n c_m^k}{n!k!}\langle 0|C^*(a_m a_{-m})^n A a_m B(a_m^\dagger a_{-m}^\dagger)^k C|0\rangle$$

$$= \sum_{n,k\geqslant 0}\frac{\bar{c}_m^n c_m^k}{n!k!}$$

$$\times \langle 0|(a_{-m})^n(a_{-m}^\dagger)^k C^* A B C(a_m)^{n+1}(a_m^\dagger)^k|0\rangle.$$

Equation (16) follows because, on the one hand, $(a_m)^{n+1}(a_m^\dagger)^k|0\rangle=0$ if $n+1>k$ and, on the other hand $\langle 0|(a_{-m})^n(a_{-m}^\dagger)^k=0$ if $k>n$.

The total particle number is computed as

$$\left\langle \sum_m a_m^\dagger a_m \right\rangle_\Psi = \langle a_0^\dagger a_0 \rangle_\Psi + \sum_{m\neq 0}\langle a_m^\dagger a_m \rangle_\Psi = N_0 + \sum_{m\neq 0}\frac{|c_m|^2}{1-|c_m|^2},$$

so the constraint (5) is equivalent to

$$N = N_0 + \sum_{m\neq 0}\frac{|c_m|^2}{1-|c_m|^2}. \tag{17}$$

We shall see after Eq. (56) that with our choice of parameters c_m and N_0, we have

$$\frac{N-N_0}{N} \sim C\lambda^{3/2}\varrho^{1/2} + O(\lambda^2\varrho), \tag{18}$$

with a positive constant C that depends only on the unscaled potential $\hat{V}_0$. In particular, the depletion rate of the condensate is of order $\lambda^{3/2}\varrho^{1/2}$.

We classify the interaction terms in the Hamiltonian (3) according to their number of zero-momentum operators, $a_0^\dagger$ or a_0. It will turn out that only an even number of zero-momentum operators give nonzero contribution. We will thus write

$$\left\langle \frac{1}{2|\Lambda|}\sum_{p,q,u}\hat{V}_u a_p^\dagger a_q^\dagger a_{p-u} a_{q+u} \right\rangle_\Psi = E_0 + E_2 + E_4,$$

where E_k, $k=0,2,4$, defined below, denote the contributions of terms with exactly k zero-momentum operators.

Case 1. All four operators are with zero momentum, i.e., $p=q=u=0$, and the contribution of this part is

$$E_0 = \frac{1}{2|\Lambda|}\hat{V}_0 N_0^2. \tag{19}$$

Case 2. By momentum conservation in the interaction term, it is impossible to have exactly three zero-momentum operators. The terms containing exactly two zero-momentum operators are

$$\frac{1}{2|\Lambda|}\sum_{u\neq 0}(\hat{V}_u a_0^\dagger a_0^\dagger a_u a_{-u} + \hat{V}_u a_u^\dagger a_{-u}^\dagger a_0 a_0 + 2(\hat{V}_u + \hat{V}_0)a_u^\dagger a_0^\dagger a_0 a_u).$$

$$\tag{20}$$

The contribution of this term to the potential energy of Ψ is

$$E_2 = \sum_{p\neq 0}\left[\frac{N_0\hat{V}_p}{2|\Lambda|}\frac{c_p+\bar{c}_p}{1-|c_p|^2} + \frac{2(\hat{V}_p+\hat{V}_0)N_0}{2|\Lambda|}\frac{|c_p|^2}{1-|c_p|^2}\right]. \tag{21}$$

Suppose that among the four momenta $p,q,p-u,q+u$, exactly one is zero, say $p-u$ (other cases are analogous). Then the remaining three operators are $a_p^\dagger a_q^\dagger a_{p+q}$. Since $p,q,p+q$ are nonzero, either $p,q,p+q,-p,-q,-(p+q)$ are all different, or $p=q$, in which case a_{p+q} stands alone without any other operator $a_{\pm(p+q)}^\dagger$ or $a_{\pm(p+q)}$. From Eq. (16), the expectation of this term with respect to Ψ vanishes. This proves that there is no contribution for the case of exactly one zero-momentum operator.

Case 3. No zero-momentum operator is present in the interaction term in Eq. (3). Let $r:=p-u$ and $s:=q+u$. Based upon Eq. (16), only the following cases yield a nonzero contribution:

(1) $p=-q$ and $r\notin\{p,-p\}$, but since r must be $\pm s$ and we have momentum conservation, $r=-s$. The energy contribution is the main term in this case.

$$\tilde{E}_4 := \frac{1}{2|\Lambda|} \sum_{p\neq 0} \sum_{r\neq 0, \pm p} \hat{V}_{p-r} \langle a_p^\dagger a_{-p}^\dagger a_r a_{-r} \rangle_\Psi$$

$$= \frac{1}{2|\Lambda|} \sum_{p\neq 0} \sum_{r\neq 0, \pm p} \hat{V}_{p-r} \frac{\bar{c}_p c_r}{(1-|c_p|^2)(1-|c_r|^2)}.$$

(2) $p = -q = r = -s$.

$$\frac{1}{2|\Lambda|} \hat{V}_0 \sum_{p\neq 0} \langle a_p^\dagger a_{-p}^\dagger a_p a_{-p} \rangle_\Psi = \frac{\hat{V}_0}{2|\Lambda|} \sum_{p\neq 0} \frac{|c_p|^2(1+|c_p|^2)}{(1-|c_p|^2)^2}.$$

(3) $p = -q = -r = s$.

$$\frac{1}{2|\Lambda|} \sum_{p\neq 0} \hat{V}_{2p} \langle a_p^\dagger a_{-p}^\dagger a_{-p} a_p \rangle_\Psi = \frac{1}{2|\Lambda|} \sum_{p\neq 0} \hat{V}_{2p} \frac{|c_p|^2(1+|c_p|^2)}{(1-|c_p|^2)^2}.$$

(4) $p = q$, then $r + s = 2p$ and $r = \pm s$ implies $r = s = p$ and we have

$$\frac{1}{2|\Lambda|} \sum_{p\neq 0} \hat{V}_0 \langle a_p^\dagger a_p^\dagger a_p a_p \rangle_\Psi = \frac{\hat{V}_0}{2|\Lambda|} \sum_{p\neq 0} \frac{2|c_p|^4}{(1-|c_p|^2)^2}.$$

(5) $p = r$, $q = s$ and $p = s$, $q = r$ but $p \neq \pm q$.

$$\frac{1}{2|\Lambda|} \sum_{p\neq 0} \sum_{q\neq 0, \pm p} \hat{V}_0 \langle a_p^\dagger a_q^\dagger a_p a_q \rangle_\Psi$$

$$+ \frac{1}{2|\Lambda|} \sum_{p\neq 0} \sum_{q\neq 0, \pm p} \hat{V}_{p-q} \langle a_p^\dagger a_q^\dagger a_q a_p \rangle_\Psi$$

$$= \frac{1}{2|\Lambda|} \sum_{p\neq 0} \sum_{q\neq 0, \pm p} (\hat{V}_0 + \hat{V}_{p-q}) \frac{|c_p|^2|c_q|^2}{(1-|c_p|^2)(1-|c_q|^2)}.$$

Collecting all these terms, the contribution of case 3 to the potential energy is

$$E_4 = \tilde{E}_4 + \Omega_4, \tag{22}$$

where Ω_4 was defined in Eq. (14).

We now combine the contribution to the potential energy from case 1 and case 2 and we use the relation between N and N_0 given by Eq. (17) as follows:

$$E_0 + E_2 = \frac{1}{2|\Lambda|} \hat{V}_0 N_0^2 + \sum_{p\neq 0} \left[\frac{N_0 \hat{V}_p}{|\Lambda|} \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} \right.$$

$$\left. + \frac{2(\hat{V}_p + \hat{V}_0)N_0}{2|\Lambda|} \frac{|c_p|^2}{1-|c_p|^2} \right]$$

$$= \frac{1}{2|\Lambda|} \hat{V}_0 N^2 - \frac{N}{|\Lambda|} \hat{V}_0 \sum_{m\neq 0} \frac{|c_m|^2}{1-|c_m|^2}$$

$$+ \frac{\hat{V}_0}{2|\Lambda|} \left(\sum_{m\neq 0} \frac{|c_m|^2}{1-|c_m|^2} \right)^2$$

$$+ \sum_{p\neq 0} \left[\frac{N\hat{V}_p}{|\Lambda|} \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} + \frac{(\hat{V}_p + \hat{V}_0)N}{|\Lambda|} \frac{|c_p|^2}{1-|c_p|^2} \right]$$

$$- \sum_{p\neq 0} \left[\frac{\hat{V}_p}{|\Lambda|} \left(\sum_{m\neq 0} \frac{|c_m|^2}{1-|c_m|^2} \right) \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} \right.$$

$$\left. + \frac{(\hat{V}_p + \hat{V}_0)}{|\Lambda|} \left(\sum_{m\neq 0} \frac{|c_m|^2}{1-|c_m|^2} \right) \frac{|c_p|^2}{1-|c_p|^2} \right]. \tag{23}$$

Notice that there are two terms of the form $-\frac{N}{|\Lambda|} \hat{V}_0 \sum_{m\neq 0} \frac{|c_m|^2}{1-|c_m|^2}$, which cancel each other. So we can rewrite Eq. (23) as

$$E_0 + E_2 = \tilde{E}_0 + \tilde{E}_2 + \Omega_2, \tag{24}$$

where

$$\tilde{E}_0 = \frac{1}{2|\Lambda|} \hat{V}_0 N^2, \tag{25}$$

$$\tilde{E}_2 = \sum_{p\neq 0} \left[\varrho \hat{V}_p \frac{|c_p|^2}{1-|c_p|^2} + \varrho \hat{V}_p \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} \right.$$

$$\left. - \frac{\hat{V}_p}{|\Lambda|} \left(\sum_{m\neq 0} \frac{|c_m|^2}{1-|c_m|^2} \right) \frac{\mathrm{Re}\, c_p}{1-|c_p|^2} \right], \tag{26}$$

and Ω_2 is given in Eq. (13). The first term in Eq. (26), when combined with the kinetic energy contribution

$$\sum_{p\neq 0} p^2 \frac{|c_p|^2}{1-|c_p|^2},$$

is the second term in Eq. (15). The remaining main terms in Eq. (15) come from the rest of $\tilde{E}_2$, $\tilde{E}_0$, and $\tilde{E}_4$, i.e.,

$$E_M = \sum_{p\neq 0} p^2 \frac{|c_p|^2}{1-|c_p|^2} + \tilde{E}_0 + \tilde{E}_2 + \tilde{E}_4. \tag{27}$$

This completes the proof of Lemma 2. ∎

Notice that the main terms in the potential energy come from the following channels:

$$\frac{1}{2|\Lambda|} a_0^\dagger a_0^\dagger a_0 a_0 + \frac{1}{2|\Lambda|} \sum_{u\neq 0} (\hat{V}_u a_0^\dagger a_0^\dagger a_u a_{-u} + \hat{V}_u a_u^\dagger a_{-u}^\dagger a_0 a_0$$

$$+ 2(\hat{V}_u + \hat{V}_0) a_u^\dagger a_0^\dagger a_0 a_u) + \frac{1}{2|\Lambda|} \sum_{p\neq 0} \sum_{r\neq 0, \pm p} \hat{V}_{p-r} a_p^\dagger a_{-p}^\dagger a_r a_{-r}. \tag{28}$$

The main energy contribution from these terms are all of order $N\varrho$. In the last term, the interaction between two large momenta $(|p|, |r| \sim 1)$ pairs contribute with order $N\varrho$. The order $N\varrho^{3/2}$ term comes partly from substituting N_0, the expected value of $a_0^\dagger a_0$, with N (using that $N - N_0 \sim CN\varrho^{1/2}$) and partly from the interaction between a low-momentum pair, $|p| \ll 1$, and a large-momentum pair, $|r| \sim 1$.

V. ONE-PARTICLE SCATTERING PROBLEM

Recall that $1 - w$ was the solution to the zero energy scattering equation (6) and $\hat{w}_p$ denotes the Fourier transform of w. If V is smooth and it decays sufficiently fast at infinity, then $w(x)$ is smooth and $w(x) \leq C|x|^{-1}$ for large $|x|$. Its Fourier transform on $\mathbb{R}^3$, $\int_{\mathbb{R}^3} e^{-ipx} w(x) dx$, has a $|p|^{-2}$ singularity at

the origin. The lattice Fourier transform satisfies the regularized bound

$$|\hat{w}_p| \leq \hat{w}_0 = \int_\Lambda w(x)dx \leq CL^2, \quad p \in \Lambda^*.$$

This bound guarantees that for any function $\varphi \in L^1(\mathbb{R}^3)$, the lattice Fourier transform of φw can be computed as

$$\widehat{(\varphi w)}_p = (\hat{\varphi} * \hat{w})_p = \frac{1}{|\Lambda|} \sum_{r \in \Lambda^*} \hat{\varphi}_{p-r} \hat{w}_r = \frac{1}{|\Lambda|} \sum_{r \neq 0} \hat{\varphi}_{p-r} \hat{w}_r + O\left(\frac{1}{L}\right).$$

Thus, modulo an error that is negligible in the thermodynamic limit, we can restrict the momentum summations involving $\hat{w}_r$ to $r \neq 0$.

From the definition of the scattering length (7), we have

$$8\pi a = \hat{V}_0 - \int \hat{V}_p \hat{w}_p \frac{d^3p}{(2\pi)^3} = \hat{V}_0 - \frac{1}{|\Lambda|} \sum_{p \neq 0} \hat{V}_p \hat{w}_p + O\left(\frac{1}{L}\right). \tag{29}$$

From the scattering equation we get

$$-p^2 \hat{w}_p + \frac{1}{2}\hat{V}_p - \frac{1}{2|\Lambda|} \sum_{r \neq 0} \hat{V}_{p-r} \hat{w}_r = O\left(\frac{1}{L}\right) \quad \forall \ p \neq 0. \tag{30}$$

Define

$$f(x) := V(x)w(x), \quad g(x) := V(x) - f(x), \tag{31}$$

then in Fourier space we have

$$\hat{f}_p = (\hat{V} * \hat{w})_p = \frac{1}{|\Lambda|} \sum_{r \neq 0} \hat{V}_{p-r} \hat{w}_r + O\left(\frac{1}{L}\right).$$

In particular, from Eq. (29),

$$8\pi a = \hat{g}_0 + O\left(\frac{1}{L}\right). \tag{32}$$

In the sequel we will not carry the negligible error term $O(1/L)$ in the formulas.

Lemma 3. Let $\tilde{V}(x) \geq 0$, $\tilde{V} \not\equiv 0$, be a radially symmetric smooth function with a sufficiently fast decay as $|x| \to \infty$ and let $V = \lambda \tilde{V}$. Then, for a sufficiently small λ,

$$\hat{V}_p, \hat{f}_p, \hat{g}_p \text{ are real and have a fast decay as } |p| \to \infty, \tag{33}$$

$$0 < \hat{f}_0, \hat{g}_0 < \hat{V}_0. \tag{34}$$

Moreover,

$$0 < \frac{\hat{V}_0}{8\pi a} - 1 = \frac{\hat{f}_0}{\hat{g}_0} = O(\lambda). \tag{35}$$

Furthermore, $\hat{f}_p, \hat{g}_p, \hat{V}_p$ are uniformly Lipschitz continuous, i.e.,

$$\sup_p (|\hat{g}_p - \hat{g}_{p-r}| + |\hat{V}_p - \hat{V}_{p-r}|) \leq C\lambda|r|,$$

$$\sup_p |\hat{f}_p - \hat{f}_{p-r}| \leq C\lambda^2 |r|, \tag{36}$$

with a constant C depending only on $\tilde{V}$. All statements hold uniformly in the thermodynamic limit, i.e., for all L sufficiently large.

Proof. The reality of $\hat{V}_p, \hat{f}_p, \hat{g}_p$ follows from the radial symmetry. From the scattering equation (30),

$$-2p^2 \hat{w}_p + \hat{V}_p - \hat{f}_p = 0, \quad \hat{g}_p = 2p^2 \hat{w}_p \quad \forall \ p \neq 0. \tag{37}$$

By iteration, we obtain the Born series for the scattering wave function ($p \neq 0$)

$$\hat{w}_p = \frac{\hat{V}_p}{2p^2} - \frac{1}{2p^2} \sum_{r \neq 0} \frac{\hat{V}_{p-r} \hat{V}_r}{2r^2} + \frac{1}{2p^2} \sum_{r,u \neq 0} \frac{\hat{V}_{p-r} \hat{V}_{r-u} \hat{V}_u}{4r^2 u^2} - \cdots. \tag{38}$$

It is easy to see from the expansion (38) that Eq. (33) is satisfied if $\hat{V}_p$ is sufficiently small and decaying. Furthermore, $\hat{f}_0 = |\Lambda|^{-1} \Sigma_{p \neq 0} \hat{V}_p \hat{w}_p = O(\lambda^2)$, while $\hat{V}_0 = c\lambda$ with a positive constant $c = \int \tilde{V}$, thus $\hat{g}_0 = \hat{V}_0 - \hat{f}_0 \geq c\lambda/2$ if λ is sufficiently small and Eq. (35) follows. The rest of the statements of the Lemma also easily follow from Eq. (38). ∎

VI. MINIMIZATION

From now on we assume that c_p are real; it is most likely that a complex choice does not lower the energy of our trial state. We introduce new variables

$$e_p := \frac{c_p}{1 + c_p}, \quad c_p = \frac{e_p}{1 - e_p}.$$

From $|c_p| < 1$ we have $e_p \in (-\infty, \frac{1}{2})$. We also have the relations

$$\frac{c_p^2}{1 - c_p^2} = \frac{e_p^2}{1 - 2e_p}, \quad \frac{c_p}{1 - c_p^2} = \frac{e_p(1 - e_p)}{1 - 2e_p}. \tag{39}$$

We shall choose e_p via the following Lemma. This choice will become clear later on.

Lemma 4. For any sufficiently small $\varrho \leq \varrho_0(\lambda)$ let $-\infty < e_p < 1/2$ be the minimizer of

$$m_p := \min_{e_p} \left[p^2 \frac{e_p^2}{1 - 2e_p} + \varrho \hat{V}_p \frac{e_p}{1 - 2e_p} - \varrho \hat{f}_p e_p \right]. \tag{40}$$

Then

$$e_p = \frac{1}{2} \left[1 - \left(1 + 2 \frac{\varrho \hat{g}_p}{p^2 + 2\varrho \hat{f}_p} \right)^{1/2} \right], \tag{41}$$

and the minimal value is given by

$$m_p = \frac{1}{2} \{ \sqrt{(p^2 + 2\varrho \hat{V}_p)(p^2 + \varrho \hat{f}_p)} - [p^2 + \varrho(\hat{V}_p + \hat{f}_p)] \}. \tag{42}$$

Proof. Consider the minimization problem

$$\min_{e<1/2}\left[a\frac{e^2}{1-2e}+b\frac{e}{1-2e}-ce\right],$$

where the parameters satisfy $a+2c>0$ and $a+2b>0$. After differentiating in e, the minimizers satisfy the equation

$$\frac{2(a+2c)(e-e^2)+b-c}{(1-2e)^2}=0.$$

Solving the quadratic equation, we get

$$e=\frac{1}{2}\left[1\pm\left(1+2\frac{b-c}{a+2c}\right)^{1/2}\right],\qquad(43)$$

and by the conditions on a,b,c we have $1+2(b-c)/(a+2c)\geq 0$. In our case, since $e<\frac{1}{2}$, only the negative sign can be correct. With this choice, the minimum value is

$$\left[a\frac{e^2}{1-2e}+b\frac{e}{1-2e}-ce\right]=\frac{1}{2}[\sqrt{(a+2b)(a+2c)}$$
$$-(a+b+c)].$$

In our application, the conditions $a+2c>0$, $a+2b>0$ are equivalent to

$$p^2+2\varrho\hat{f}_p>0,\quad p^2+2\varrho\hat{V}_p>0,\qquad(44)$$

and they are always satisfied if ϱ is sufficiently small. In the regime $|p|\geq 4(\varrho\hat{V}_0)^{1/2}$, these inequalities follow from the bounds $|\hat{V}_p|\leq V_0$ and $|\hat{f}_p|\leq\hat{f}_0\leq\hat{V}_0$ [see Eq. (34)]. For $|p|\leq 4(\varrho\hat{V}_0)^{1/2}$ we have $p^2+2\varrho\hat{f}_p=p^2+2\varrho\hat{f}_0+O(\varrho^{3/2})\geq p^2+\varrho\hat{f}_0>0$ by the Lipschitz continuity of $\hat{f}_p$ [Eq. (36)] and the lower bound $\hat{f}_0>0$. The other inequality in Eq. (44) is proven analogously. Actually, these calculations also show that $p^2+2\varrho\hat{f}_p$ and $p^2+2\varrho\hat{V}_p$ have a positive lower bound uniformly in p, if ϱ is sufficiently small as follows:

$$\inf_p(p^2+2\varrho\hat{f}_p)>0,\quad \inf_p(p^2+2\varrho\hat{V}_p)>0.\qquad(45)$$

■

We now rewrite the error terms $\Omega_2+\Omega_4$ in terms of e_p as follows:

$$\Omega_2+\Omega_4=\sum_{p\neq 0}\left[\frac{1}{2|\Lambda|}\sum_{r\neq 0,\pm p}(\hat{V}_0+\hat{V}_{p-r})\frac{e_p^2 e_r^2}{(1-2e_p)(1-2e_r)}\right.$$
$$+\frac{1}{2|\Lambda|}\left(\frac{e_p(1-e_p)}{1-2e_p}\right)^2\left(\hat{V}_0\frac{1-2e_p+4e_p^2}{(1-e_p)^2}\right.$$
$$\left.+\hat{V}_{2p}\frac{1-2e_p+2e_p^2}{(1-e_p)^2}\right)$$
$$-\frac{\hat{V}_p+\hat{V}_0}{|\Lambda|}\left(\sum_{r\neq 0}\frac{e_r^2}{1-2e_r}\right)\frac{e_p^2}{1-2e_p}\right]$$
$$+\frac{\hat{V}_0}{2|\Lambda|}\left(\sum_{p\neq 0}\frac{e_p^2}{1-2e_p}\right)^2.\qquad(46)$$

For the main term (15), we replace $\hat{V}_0$ with $8\pi a$

$+|\Lambda|^{-1}\Sigma_{p\neq 0}\hat{V}_p\hat{w}_p$ in $\tilde{E}_0$ [see Eqs. (25) and (27)] by using Eq. (29) at the expense of a term of order $1/L$ that is negligible in the thermodynamic limit. Thus, neglecting this error term, we have

$$E_M=4\pi aN\varrho+\frac{\varrho^2}{2}\sum_{p\neq 0}\hat{V}_p\hat{w}_p+\sum_{p\neq 0}\left[(p^2+\varrho\hat{V}_p)\frac{e_p^2}{1-2e_p}\right.$$
$$+\varrho\hat{V}_p\frac{e_p(1-e_p)}{1-2e_p}+\frac{1}{2|\Lambda|}\sum_{r\neq 0,\pm p}\hat{V}_{p-r}\frac{e_p(1-e_p)e_r(1-e_r)}{(1-2e_p)(1-2e_r)}$$
$$\left.-\frac{\hat{V}_p}{|\Lambda|}\left(\sum_{r\neq 0}\frac{e_r^2}{1-2e_r}\right)\frac{e_p(1-e_p)}{1-2e_p}\right].\qquad(47)$$

By using Eqs. (34) and (36) we have that for a sufficiently small but fixed δ (depending on V),

$$\frac{\hat{V}_0}{2}\leq\hat{V}_p\leq\hat{V}_0,\quad\frac{\hat{f}_0}{2}\leq\hat{f}_p\leq\hat{f}_0,\quad\frac{\hat{g}_0}{2}\leq\hat{g}_p\leq\hat{g}_0,$$

for all $|p|\leq\delta$. In particular, we have

$$\frac{\hat{g}_0}{4p^2}\leq\hat{w}_p\leq\frac{\hat{g}_0}{2p^2}\quad\text{for }|p|\leq\delta.\qquad(48)$$

Using the lower bounds (45) and the approximation (36) of $\hat{g}_p,\hat{f}_p$ for small p, we obtain the following estimate on e_p defined in Eq. (41):

$$|e_p|\leq C\quad\text{for }\forall\ p,$$

$$e_p\sim-\frac{\varrho\hat{g}_0}{2(p^2+\varrho\hat{f}_0)}\quad\text{for }\delta^{-1}\varrho\lambda^2\leq|p|\leq\delta,$$

$$|e_p|\sim\frac{\varrho|\hat{g}_p|}{2p^2}\quad\text{for }|p|\geq\delta,\qquad(49)$$

where C is a constant depending on V and the notation $A\sim B$ indicates that A and B have the same sign and $\frac{1}{2}|A|\leq|B|\leq|A|$. Here we have used the fact that $0<\hat{f}_0,\hat{g}_0<\hat{V}_0$ and that $\hat{f}_0$ is of order $\hat{V}^2$ while $\hat{g}_0=\hat{V}_0-\hat{f}_0$. Similarly, we have

$$\left|\frac{e_p}{1-2e_p}\right|\lesssim\begin{cases}\dfrac{\varrho\hat{g}_0}{p^2+\varrho\hat{V}_0}&\text{for }|p|\leq\delta\\[2mm]\dfrac{\varrho|\hat{g}_p|}{p^2}&\text{for }|p|\geq\delta,\end{cases}\qquad(50)$$

and

$$\left|\frac{e_p(1-e_p)}{1-2e_p}\right|\lesssim\begin{cases}\dfrac{\varrho\hat{g}_0}{p^2+\varrho\hat{f}_0}&\text{for }|p|\leq\delta\\[2mm]\dfrac{\varrho|\hat{g}_p|}{p^2}&\text{for }|p|\geq\delta,\end{cases}\qquad(51)$$

where for positive quantities $A\lesssim B$ indicates that $A\leq CB$ with a constant C depending only on V.

Lemma 5. Suppose e_p is given by Eq. (41). Then the energy $E = \langle H \rangle_\Psi$ of the state (4) satisfies

$$E = 4\pi a N \varrho + \sum_{p \neq 0} \left(p^2 \frac{e_p^2}{1 - 2e_p} + \varrho \hat{V}_p \frac{e_p}{1 - 2e_p} \right.$$
$$\left. + \frac{1}{2|\Lambda|} \sum_{r \neq 0} \hat{V}_{p-r} e_p e_r + \frac{\varrho^2}{2} \hat{V}_p \hat{w}_p \right) + O(N\varrho^2 |\ln \varrho|)$$
$$(52)$$

as $\varrho \to 0$.

Proof. We first prove that $\Omega_2 + \Omega_4$ is negligible. Note that, using $|\hat{g}_p| \leq \hat{g}_0 \leq \hat{V}_0$, and the bounds (49) and (50), we have

$$\frac{1}{|\Lambda|} \sum_{p \neq 0} \frac{e_p^2}{1 - 2e_p} \leq \frac{C}{|\Lambda|} \sum_{0 \neq |p| \leq \delta} \frac{(\varrho \hat{V}_0)^2}{p^2(p^2 + \varrho \hat{V}_0)} + \frac{C}{|\Lambda|} \sum_{|p| \geq \delta} \frac{(\varrho \hat{g}_p)^2}{p^4}$$
$$\leq C\varrho^{3/2}. \tag{53}$$

Similarly, we find

$$\frac{1}{|\Lambda|} \sum_{p \neq 0} \frac{|e_p(1 - e_p)|}{1 - 2e_p} \leq \frac{C}{|\Lambda|} \sum_{0 \neq |p| \leq \delta} \frac{\varrho \hat{g}_0}{p^2 + \varrho \hat{f}_0} + \frac{C}{|\Lambda|} \sum_{|p| \geq \delta} \frac{\varrho \hat{g}_p}{p^2}$$
$$\leq C\varrho, \tag{54}$$

and

$$\frac{1}{|\Lambda|} \sum_{p \neq 0} \left| \frac{e_p(1 - e_p)}{1 - 2e_p} \right|^2 \leq \frac{C}{|\Lambda|} \sum_{0 \neq |p| \leq \delta} \left(\frac{\varrho \hat{g}_0}{p^2 + \varrho \hat{f}_0} \right)^2$$
$$+ \frac{C}{|\Lambda|} \sum_{|p| \geq \delta} \frac{(\varrho \hat{g}_p)^2}{p^4} \leq C\varrho^{3/2}, \tag{55}$$

with constants depending on V. In terms of c_p's, we have, by Eq. (39),

$$\sum_{p \neq 0} \frac{|c_p|^2}{1 - |c_p|^2} \leq C N \varrho^{1/2}, \quad \sum_{p \neq 0} \frac{|c_p|}{1 - |c_p|^2} \leq C N. \tag{56}$$

The lower bounds in Eqs. (49) and (50) also imply that

$$\frac{1}{|\Lambda|} \sum_{p \neq 0} \frac{|c_p|^2}{1 - |c_p|^2} \sim C \lambda^{3/2} \varrho^{3/2} [1 + O(\lambda \varrho)^{1/2}]. \tag{57}$$

In particular, we have proved Eq. (18) after recalling Eq. (17).

Using Eqs. (53) and (55), the following terms are negligible from Eq. (46):

$$\frac{1}{2|\Lambda|} \sum_{p \neq 0} \sum_{r \neq 0, \pm p} (\hat{V}_0 + \hat{V}_{p-r}) \frac{e_p^2 e_r^2}{(1 - 2e_p)(1 - 2e_r)} \leq C N \varrho^2, \tag{58}$$

$$\frac{\hat{V}_0}{2|\Lambda|} \left(\sum_{p \neq 0} \frac{e_p^2}{1 - 2e_p} \right)^2 \leq C N \varrho^2 \tag{59}$$

$$\sum_{p \neq 0} \frac{\hat{V}_p + \hat{V}_0}{|\Lambda|} \left(\sum_{r \neq 0} \frac{e_r^2}{1 - 2e_r} \right) \frac{e_p^2}{1 - 2e_p} \leq C N \varrho^2, \tag{60}$$

$$\sum_{p \neq 0} \frac{\hat{V}_0}{|\Lambda|} \left(\frac{e_p(1 - e_p)}{1 - 2e_p} \right)^2 \frac{1 - 2e_p + 4e_p^2}{(1 - e_p)^2} \leq C \varrho^{3/2}, \tag{61}$$

where we used

$$\frac{1 - 2e_p + 4e_p^2}{(1 - e_p)^2} = 1 + 3c_p^2 \leq 4,$$

and similarly

$$\sum_{p \neq 0} \frac{\hat{V}_{2p}}{|\Lambda|} \left(\frac{e_p(1 - e_p)}{1 - 2e_p} \right)^2 \frac{1 - 2e_p + 2e_p^2}{(1 - e_p)^2} \leq C \varrho^{3/2}. \tag{62}$$

Notice that the terms (61) and (62) are not extensive. All constants depend on V. We have thus proved that $\Omega_2 + \Omega_4$ is bounded by $N\varrho^2$.

We now replace $\hat{V}_p$ by $\hat{V}_{p-r}$ in the last term of the main term E_M (47). The difference can be estimated by using Eqs. (36) and (54) as

$$\left| \sum_{p \neq 0} \frac{1}{|\Lambda|} \left(\sum_{r \neq 0} (\hat{V}_p - \hat{V}_{p-r}) \frac{e_r^2}{1 - 2e_r} \right) \frac{e_p(1 - e_p)}{1 - 2e_p} \right|$$
$$\leq \frac{C}{|\Lambda|} \left(\sum_{0 \neq |r| \leq \delta} \frac{(\varrho \hat{V}_0)^2 |r|}{(r^2 + \varrho \hat{f}_0)(r^2 + \varrho \hat{V}_0)} + \sum_{|r| \geq \delta} \frac{(\varrho \hat{g}_r)^2 |r|}{r^4} \right)$$
$$\times \sum_{p \neq 0} \frac{|e_p(1 - e_p)|}{1 - 2e_p} \leq C N \varrho^2 |\ln \varrho|. \tag{63}$$

We remark that this is the only term of size $N\varrho^2 |\ln \varrho|$ and is the candidate for the third-order term.

After this change, we can combine the two terms in the last two lines of Eq. (47) as

$$\sum_{p \neq 0} \frac{1}{2|\Lambda|} \sum_{r \neq 0, \pm p} \hat{V}_{p-r} \frac{e_p(1 - e_p)e_r(1 - e_r)}{(1 - 2e_p)(1 - 2e_r)}$$
$$- \sum_{p \neq 0} \frac{1}{|\Lambda|} \left(\sum_{r \neq 0} \hat{V}_{p-r} \frac{e_r^2}{1 - 2e_r} \right) \frac{e_p(1 - e_p)}{1 - 2e_p}$$
$$= \frac{1}{2|\Lambda|} \sum_{p, r \neq 0} \hat{V}_{p-r} \left(\frac{e_p(1 - e_p)}{1 - 2e_p} - \frac{e_p^2}{1 - 2e_p} \right)$$
$$\times \left(\frac{e_r(1 - e_r)}{1 - 2e_r} - \frac{e_r^2}{1 - 2e_r} \right)$$
$$- \frac{1}{2|\Lambda|} \sum_{p, r \neq 0} \hat{V}_{p-r} \frac{e_p^2}{1 - 2e_p} \frac{e_r^2}{1 - 2e_r}$$
$$- \frac{1}{2|\Lambda|} \sum_{p \neq 0} (\hat{V}_0 + \hat{V}_{2p}) \left(\frac{e_p(1 - e_p)}{(1 - 2e_p)} \right)^2.$$

The last term comes from compensating for removing the restriction $p \neq \pm r$. Similar to Eq. (61), it is not extensive and is thus negligible. The second term is estimated exactly as

Eq. (59) after estimating $|\hat{V}_{p-r}| \leq \hat{V}_0$; it is $O(N\varrho^2)$ and thus is negligible.

Since

$$\frac{e_p(1-e_p)}{1-2e_p} - \frac{e_p^2}{1-2e_p} = e_p.$$

This concludes the proof of Lemma 5. ∎

Proof of Theorem 1. Our goal is to minimize the energy given in Eq. (52) in the parameters e_p. This can be done either directly or via the following observation, which converts the nonlocal term involving both e_p and e_r to a local term. For two functions φ, ψ defined in Λ^*, we denote

$$(\varphi, \hat{V} * \psi) = \frac{1}{|\Lambda|} \sum_{p \neq 0} \frac{1}{|\Lambda|} \sum_{r \neq 0} \hat{V}_{p-r} \varphi_p \psi_r.$$

Hence,

$$\frac{1}{|\Lambda|} \sum_{p \neq 0} \frac{1}{|\Lambda|} \sum_{r \neq 0} \hat{V}_{p-r} e_p e_r = (e, \hat{V} * e).$$

We use the identity

$$\frac{1}{2}(e, \hat{V} * e) = \frac{1}{2}[e + \varrho\hat{w}, \hat{V} * (e + \varrho\hat{w})] - \varrho(e, \hat{V} * \hat{w})$$

$$- \frac{\varrho^2}{2}(\hat{w}, \hat{V} * \hat{w})$$

and $\hat{g} = \hat{V} - \hat{V} * \hat{w}$ [see Eq. (31)]. We can combine the last term with the last term in Eq. (52) to obtain

$$-\frac{|\Lambda|\varrho^2}{2}(\hat{w}, \hat{V} * \hat{w}) + \frac{\varrho^2}{2} \sum_{p \neq 0} \hat{V}_p \hat{w}_p = \frac{1}{4}|\Lambda|\varrho^2(\hat{g}, p^{-2}\hat{g}),$$

(64)

where we have used $\hat{g}_p = 2p^2 \hat{w}_p$. Thus we have

$$E = 4\pi a N\varrho + \sum_{p \neq 0} \left(p^2 \frac{e_p^2}{1-2e_p} + \varrho\hat{V}_p \frac{e_p}{1-2e_p} - \varrho(\hat{V} * \hat{w})_p e_p \right.$$

$$\left. + \frac{\varrho^2 \hat{g}_p^2}{4p^2} \right) + \frac{1}{2|\Lambda|} \sum_{p,r \neq 0} \hat{V}_{p-r}(e_p + \varrho\hat{w}_p)(e_r + \varrho\hat{w}_r)$$

$$+ O(N\varrho^2|\ln \varrho|).$$

(65)

From the definition of e_p in Eq. (41), we have for $p^2 \geq \delta^{-1}\varrho$,

$$e_p = -\frac{\varrho\hat{g}_p}{2(p^2 + 2\varrho\hat{f}_p)} + \varrho^2 O\left(\frac{\hat{g}_p^2}{p^4}\right).$$

(66)

Therefore, for $p^2 \geq \delta^{-1}\varrho$, we have

$$e_p + \varrho\hat{w}_p = -\frac{\varrho\hat{g}_p}{2(p^2 + 2\varrho\hat{f}_p)} + \frac{\varrho\hat{g}_p}{2p^2} + \varrho^2 O\left(\frac{\hat{g}_p^2}{p^4}\right)$$

$$= \varrho^2 O\left(\frac{\hat{g}_p^2 + |\hat{g}_p \hat{f}_p|}{p^4}\right).$$

(67)

We now prove that the term in the last but one line of Eq. (65) is negligible. By Eqs. (48) and (49) we have

$$\frac{1}{2|\Lambda|} \sum_{p,r \neq 0} \hat{V}_{p-r}(e_p + \varrho\hat{w}_p)(e_r + \varrho\hat{w}_r)$$

$$\leq C|\Lambda| \left(\int_{p^2 \leq \delta^{-1}\varrho} \frac{\varrho\hat{g}_0}{p^2} + \int_{p^2 \geq \delta^{-1}\varrho} \varrho^2 \frac{\hat{g}_p^2 + |\hat{g}_p \hat{f}_p|}{p^4} \right)^2$$

$$\leq CN\varrho^2.$$

The minimization of the first three terms in the summation over $p \neq 0$ in Eq. (65) is exactly given by Lemma 4. With the choice (41) for e_p, we have proved that the energy satisfies the following estimate:

$$E = 4\pi\varrho Na + Q + O(N\varrho^2|\ln \varrho|),$$

(68)

where

$$Q = \frac{\varrho}{2} \sum_{p \neq 0} \left[\sqrt{\left(\frac{p^2}{\varrho} + 2\hat{f}_p\right)\left(\frac{p^2}{\varrho} + 2\hat{V}_p\right)} \right.$$

$$\left. - \left(\frac{p^2}{\varrho} + \hat{V}_p + \hat{f}_p\right) + \frac{\varrho\hat{g}_p^2}{2p^2} \right].$$

(69)

We now take the limit $L \to \infty$ and change the summation to integration. Changing variables, $x = p^2/\varrho$, $d^3p = 2\pi\varrho^{3/2}x^{1/2}dx$ for $x \in (0, \infty)$, then Q is given by

$$Q = \frac{\pi N\varrho^{3/2}}{(2\pi)^3} \int_0^\infty F(x, \sqrt{x\varrho})dx,$$

(70)

where

$$F(x,p) = \left(\sqrt{(x + 2\hat{f}_p)(x + 2\hat{V}_p)} - (x + \hat{f}_p + \hat{V}_p) + \frac{\hat{g}_p^2}{2x} \right) x^{1/2}.$$

It should be noted that in our formulas, x and p are always related via the relation $x = p^2/\varrho$.

With the notation $\alpha = 2\hat{f}_p/x$, $\beta = 2\hat{V}_p/x$ and recalling $\hat{g}_p = \hat{V}_p - \hat{f}_p$ from Eq. (37) we can write

$$F(x,p) = \left(\sqrt{(1+\alpha)(1+\beta)} - \left[1 + \frac{\alpha+\beta}{2} + \frac{(\alpha-\beta)^2}{8} \right] \right) x^{3/2}.$$

We divide the integration (70) into $x \geq c\varrho^{-1}$ and $x \leq c\varrho^{-1}$ regimes for some small constant c. Since $|\hat{V}_p| + |\hat{f}_p|$ is bounded for all p, in the region $x \geq c\varrho^{-1}$, we have $|\alpha| + |\beta| \ll 1$ for c independent of ϱ and if ϱ is small enough, a condition we assume from now on. We can thus expand α and β in the Taylor series and it turns out that the leading contribution is the third-order term $(\alpha+\beta)(\alpha-\beta)^2/16$. Hence, we have $F(x, \sqrt{\varrho x}) \geq 0$ for $x \geq c\varrho^{-1}$ and ϱ small. Furthermore, we have the following estimate:

$$\int_{c\varrho^{-1}}^\infty F(x, \sqrt{x\varrho})dx \leq \int_{c\varrho^{-1}}^\infty x^{-3/2}dx \leq C\sqrt{\varrho}.$$

(71)

Similarly, the following inequalities, which will be useful later on, also hold:

$$\int_{c\varrho^{-1}}^\infty F(x,0)dx \leq C\sqrt{\varrho}, \quad F(x,0) \geq 0 \quad \text{for } x \geq c\varrho^{-1}.$$

(72)

For $x \leq c\varrho^{-1}$, we again use $\hat{g}_p = \hat{V}_p - \hat{f}_p$ and rewrite $F(x,p) = x^{-1/2}G(x,p)$, where

$$
\begin{aligned}
G(x,p) &= \frac{\hat{g}_p^2[\sqrt{(x+2\hat{f}_p)(x+2\hat{V}_p)} + \hat{f}_p + \hat{V}_p - x]}{2[\sqrt{(x+2\hat{f}_p)(x+2\hat{V}_p)} + (x+\hat{f}_p+\hat{V}_p)]} \\
&= \frac{\hat{g}_p^2[4(\hat{f}_p+\hat{V}_p)x - \hat{g}_p^2]}{2[\sqrt{(x+2\hat{f}_p)(x+2\hat{V}_p)} + (x+\hat{f}_p+\hat{V}_p)]} \\
&\quad \times \frac{1}{\sqrt{(x+2\hat{f}_p)(x+2\hat{V}_p)} + x - \hat{f}_p - \hat{V}_p}.
\end{aligned}
\tag{73}
$$

The numerator in Eq. (73) may vanish only when

$$
\sqrt{(x+2\hat{f}_p)(x+2\hat{V}_p)} = x - \hat{f}_p - \hat{V}_p.
\tag{74}
$$

Solving for x, we have

$$
x = \frac{(\hat{f}_p - \hat{V}_p)^2}{4(\hat{f}_p + \hat{V}_p)}.
\tag{75}
$$

In the regime $x \leq c\varrho^{-1}$, $|p| \leq \sqrt{c}$ and from the continuity of $\hat{f}_p, \hat{V}_p$ (36), the leading contribution of $\hat{f}_p, \hat{V}_p$ is given by $\hat{f}_0, \hat{V}_0 > 0$. Hence, for c small enough (depending on λ, but not on ϱ), the solution (75) satisfies that

$$
x = \frac{(\hat{f}_p - \hat{V}_p)^2}{4(\hat{f}_p + \hat{V}_p)} < \hat{f}_p + \hat{V}_p.
\tag{76}
$$

Therefore, the numerator in Eq. (73) is positive in the neighborhood of the solution (75) and is thus also positive for all $x \leq c\varrho^{-1}$. As a side remark, when combined with the previous argument for $x \geq c\varrho^{-1}$, this proves that $G(x, \sqrt{\varrho x})$ and $F(x, \sqrt{\varrho x})$ are positive everywhere.

From Eq. (73), G depends smoothly on x, $\hat{f}_p$, and $\hat{V}_p$ in the regime $x \leq c\varrho^{-1}$. Using the uniformly Lipschitz continuity of $\hat{f}_p$ and $\hat{V}_p$ (36), we thus have

$$
|G(x,p) - G(x,0)| \leq C|p|(1+x)^{-1}.
$$

Here we have used the second line of Eq. (73) to obtain the decay in x for x large. Therefore, we have the error estimate

$$
\begin{aligned}
\int_0^{c\varrho^{-1}} |F(x,\sqrt{x\varrho}) - F(x,0)|dx &\leq C\sqrt{\varrho} \int_0^{c\varrho^{-1}} \frac{dx}{1+x} \\
&\leq C\sqrt{\varrho}|\ln \varrho|.
\end{aligned}
$$

Together with Eqs. (71) and (72), the same estimate holds if the integration domain is extended to the whole $\mathbb{R}^+$.

From Eqs. (9), (31), and (32) we see that $h = \hat{f}_0 / \hat{g}_0$. With this notation we have

$$
\begin{aligned}
Q &= \frac{\pi N\varrho^{3/2}}{(2\pi)^3} \int_0^\infty dx\, x^{1/2} \Bigg(\sqrt{(x+2\hat{f}_0)(x+2\hat{f}_0+2\hat{g}_0)} \\
&\quad - (x+2\hat{f}_0+\hat{g}_0) + \frac{\hat{g}_0^2}{2x} \Bigg) + O(N\varrho^2|\ln \varrho|) \\
&= \frac{\pi N\varrho^{3/2}\hat{g}_0^{5/2}}{(2\pi)^3} \int_0^\infty dy\, y^{1/2} \Bigg(\sqrt{(y+2h)(y+2+2h)} \\
&\quad - (y+1+2h) + \frac{1}{2y} \Bigg) + O(N\varrho^2|\ln \varrho|).
\end{aligned}
$$

Recall $\hat{g}_0 = 8\pi a$ from Eq. (32) and the definition of $\Phi(h)$ from Eq. (11). We can thus write Q as

$$
Q = 4\pi a N\varrho \left[\sqrt{\frac{32}{\pi}} \Phi(h)(a^3\varrho)^{1/2} \right] + O(N\varrho^2|\ln \varrho|).
$$

Together with Eq. (68), this proves the main theorem. ∎

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