Ground-State Energy of a Weakly Interacting Bose Gas: Calculation Without Regularization

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The textbook calculation of the ground-state energy of a dilute gas of Bose particles is examined in detail, and certain mathematical inconsistencies are pointed out. On the basis of this analysis, a refined approach suitable for soft interaction potentials which lend themselves to a low-order Born approximation is developed. This procedure emphasizes the low-density character of the resulting formula for the ground-state energy, and avoids all divergent expressions at intermediate stages of the computation. It is stressed that the standard Bogoliubov approximation, if not augmented by some additional device, leads to an error which manifests itself already in the lowest order of the density. – PACS 03.75.Hh, 05.30.Jp, 03.65.Nk.

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1. Introduction

The calculation of the ground-state energy of a homogeneous, weakly interacting Bose gas constitutes a classic topic of quantum many-body theory [1 – 7]. It is, therefore, remarkable that a mathematically rigorous proof for the leading term in a density expansion of the ground-state energy per particle,

$$E_0/N = \frac{2\pi a\hbar^2}{m} n \,, \tag{1}$$

could be given only recently [8]. In this formula, m denotes the mass of the Bose particles, n is their density, and a is the s-wave scattering length of the repulsive two-body interaction potential.

In view of the mathematical difficulties presented by the subject, it seems somewhat surprising that standard textbook arguments [9 – 11] usually lead one, in the framework of the Bogoliubov approximation [12] and without apparent difficulties, even to the next-to-leading term, and state the result for the ground-state energy per particle in the form

$$E_0/N = \frac{2\pi a\hbar^2}{m} n \left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3}\right] \,, \tag{2}$$

which coincides with an expression derived already in 1957 by Lee and Yang [1] and Lee, Huang and Yang [2] for the particular case of a Bose gas with hard-sphere interaction. One might wonder, therefore, why a proof of (1) has still been necessary, and whether the usual textbook arguments contain some hidden deficiency. Given the enormous recent interest in Bose–Einstein condensates [7, 13 – 15], it appears appropriate to consider this question in some depth.

In this paper, we will first examine in Sect. 2 the calculation of the ground-state energy as presented by Lifshitz and Pitaevskii [9]. As we will discuss in detail, that reasoning actually does not lead to the formula (2) by algebra alone but also, without proof, the validity of the so-called Landau postulate is assumed, which asserts that the properties of a dilute Bose gas at low temperatures are governed solely by the s-wave scattering length a. Hence one simply replaces [9] the actual interaction potential, which usually is difficult to handle because of a strong short-range singularity like that of the Lennard–Jones potential, by a more convenient one, which shares the same value of a. With the help of a delicate regularization procedure, which becomes necessary if one also assumes that all matrix elements of the interaction potential can be replaced by a constant, one then recovers the formula (2). However, as pointed out by Lieb and Yngvason [8], the content of the Landau postulate is not trivial. In the extreme case of a hard-sphere interaction potential, the ground-state energy is entirely kinetic, and the ground-state wave function is highly correlated. For very soft interaction potentials $U(r)$, on the other hand, the Born approxi-

mation yields

$$a \approx (m/\hbar^2) \int_0^\infty \mathrm{d}r\, r^2 U(r),$$

so that the energy (2) is almost all potential, and the ground-state wave function is essentially the noninteracting one [8]. The Landau postulate, if correct, therefore implies that if one continuously deforms the potential from one extreme to the other, while keeping the scattering length fixed, the ground-state energy remains unchanged. Thus it is of interest to see how the Landau postulate can be derived, rather than assumed *a priori*. It is well known that non-universal contributions, which do depend on the shape of the interaction potential, arise in higher orders of a low-density expansion of the ground-state energy [5, 16]. In the present work, however, we are concerned with the two leading terms (2).

When discussing the textbook calculation [9] of the ground-state energy in Sect. 2, we spot some mathematical inconsistencies which render that reasoning problematic. We will then specifically focus on "soft" interaction potentials in Sect. 3, and present an analysis which neither invokes the Landau hypothesis, nor requires any regularisation scheme, and thus by-passes the above mentioned shortcomings. In this way we will obtain an expression for the ground-state energy which coincides with a well-known result due to Brueckner and Sawada [3], and which differs from the hard-sphere formula (2) in that only the lowest terms of the Born series for the scattering length appear. However, that result is not in full accordance with the rigorously established formula (1), so that the standard Bogoliubov method, if not augmented by some additional device such as the Landau postulate, contains a shortcoming which makes itself felt even in the lowest order of the density.

Besides the detailed discussion of this issue, the main content of the present paper consists in the development, presented in Sect. 3, of a systematic method for avoiding the divergent expressions one usually encounters at intermediate stages in the calculation of the ground-state energy. This new method possesses an intrinsic interest of its own, and has already been found useful for the calculation of the ground-state energy and depletion of a two-species condensate [17], and for establishing an improved, mathematically rigorous upper bound on the ground-state energy of a single condensate [18].

2. Investigating the Textbook: Landau Postulate and Regularization

We start by recapitulating the conventional textbook arguments [9–11] for calculating the ground-state energy of a homogeneous, weakly interacting Bose gas. It is assumed that N identical Bose particles of mass m are contained in a cubic volume $V = L^3$. Since eventually the thermodynamic limit will be taken, $N \to \infty$ and $V \to \infty$ such that the density $N/V = n$ remains constant, one imposes the convenient periodic boundary conditions, so that the single-particle states are plane waves with momentum $\hbar\boldsymbol{k} = \hbar(2\pi/L)\boldsymbol{n}$, where $\boldsymbol{n}$ is a vector with integer components.

The repulsive particle-particle interaction potential $U(r)$ is supposed to be spherically symmetric; it should not possess any many-body, negative energy bound state. Such states may exist even when there is no two-body bound state [8, 19]. The gas is considered as "weakly interacting" if the range of $U(r)$ is small in comparison to the mean interparticle distance $(V/N)^{1/3}$. In the limit of slow collisions, as is appropriate for very low temperatures, the particle-particle scattering amplitude tends to the constant $-a$, where the s-wave scattering length a is positive, $a > 0$. Assuming that the potential range is of the order of a, the criterion for the interaction to be regarded as "weak" becomes

$$\left(\frac{N}{V}\, a^3\right)^{1/3} \ll 1\,. \tag{3}$$

Starting from the basis of plane-wave single-particle states, and employing the formalism of second quantization, the Hamiltonian of the gas is given by [9]

$$H = \sum_{\boldsymbol{k}} \frac{\hbar^2\boldsymbol{k}^2}{2m}\, a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{1}{2} \sum \langle \boldsymbol{k}_1' \boldsymbol{k}_2' | U | \boldsymbol{k}_1 \boldsymbol{k}_2 \rangle\, a_{\boldsymbol{k}_1'}^\dagger a_{\boldsymbol{k}_2'}^\dagger a_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1}\,, \tag{4}$$

where $a_{\boldsymbol{k}}^\dagger$ and $a_{\boldsymbol{k}}$ are the creation and annihilation operators for Bose particles with momentum $\hbar\boldsymbol{k}$. The summation in the interaction term extends over all momenta which appear as suffixes, subject to conservation of momentum in the collisions, $\boldsymbol{k}_1' + \boldsymbol{k}_2' = \boldsymbol{k}_1 + \boldsymbol{k}_2$. The nonvanishing matrix elements of the interaction

potential read

$$\langle \boldsymbol{k}_1' \boldsymbol{k}_2' | U | \boldsymbol{k}_1 \boldsymbol{k}_2 \rangle = \frac{1}{V^2} \int \mathrm{d}^3 \boldsymbol{r}_1 \int \mathrm{d}^3 \boldsymbol{r}_2 \, e^{-i(\boldsymbol{k}_2' - \boldsymbol{k}_2)\cdot \boldsymbol{r}_2} \cdot U(|\boldsymbol{r}_1 - \boldsymbol{r}_2|) \, e^{i(\boldsymbol{k}_1 - \boldsymbol{k}_1')\cdot \boldsymbol{r}_1}$$
$$= \frac{1}{V} \int \mathrm{d}^3 \boldsymbol{r} \, e^{i\boldsymbol{q}\cdot\boldsymbol{r}} U(r) , \qquad (5)$$

where $\hbar\boldsymbol{q} = \hbar(\boldsymbol{k}_1 - \boldsymbol{k}_1') = \hbar(\boldsymbol{k}_2' - \boldsymbol{k}_2)$ is the momentum transferred in the collision. Since one is primarily interested in low temperatures, for which the relevant particle momenta are small, it seems tempting to replace [9] all matrix elements by the element which contains zero momentum states only,

$$\langle \boldsymbol{k}_1' \boldsymbol{k}_2' | U | \boldsymbol{k}_1 \boldsymbol{k}_2 \rangle \approx \widehat{U}(\boldsymbol{0}) , \qquad (6)$$

so that

$$\widehat{U}(\boldsymbol{0}) = \frac{1}{V} \int \mathrm{d}^3 \boldsymbol{r} \, U(r) \qquad (7)$$

carries the dimension of energy. Although this "approximation" might appear quite natural, it will be seen shortly that it would lead to an infinite ground-state energy of the system, if the divergence tacitly admitted here were not properly compensated at some other point. One is now left with

$$H = \sum_{\boldsymbol{k}} \frac{\hbar^2 \boldsymbol{k}^2}{2m} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{\widehat{U}(\boldsymbol{0})}{2} \sum a_{\boldsymbol{k}_1'}^\dagger a_{\boldsymbol{k}_2'}^\dagger a_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1} . \qquad (8)$$

The calculation of the low-energy part of the spectrum furnished by this Hamiltonian (8) rests on the following observation [9]: In the ground state of an ideal Bose gas, all particles are in the condensate, that is, in the single-particle state $\boldsymbol{k} = \boldsymbol{0}$, so that the occupation number of that state is $N_0 = N \gg 1$, whereas the occupation numbers of all other single-particle states are zero, $N_{\boldsymbol{k}} = 0$ for $\boldsymbol{k} \neq \boldsymbol{0}$. In the case of a weakly interacting gas, the condensate is partially depleted even when the system is in its many-body ground state $|\Psi_0\rangle$, so that even at zero temperature one finds $N_{\boldsymbol{k}} \neq 0$ for $\boldsymbol{k} \neq \boldsymbol{0}$. However, "weak" interaction implies that these occupation numbers remain small in comparison with N_0. Thus one has

$$a_0^\dagger a_0 = N_0 \approx N , \qquad (9)$$

while the ground-state commutator

$$a_0 a_0^\dagger - a_0^\dagger a_0 = 1 \ll N \qquad (10)$$

is small compared to the magnitudes of the individual operators $a_0^\dagger$ and a_0. Therefore, one can neglect the operator character of these entities, and approximate both $a_0^\dagger$ and a_0 by the square root of the condensate occupation number N_0,

$$a_0 \approx \sqrt{N_0} , \; a_0^\dagger \approx \sqrt{N_0} . \qquad (11)$$

One now makes the decomposition

$$N = \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} = N_0 + \sum_{\boldsymbol{k}\neq\boldsymbol{0}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} , \qquad (12)$$

and treats $a_{\boldsymbol{k}}^\dagger$ and $a_{\boldsymbol{k}}$ for $\boldsymbol{k} \neq \boldsymbol{0}$ as small quantities when expanding the fourfold sum in the Hamiltonian (8), so that essentially one considers an expansion in the number of non-condensed particles.

To zeroth order, one simply has

$$\sum a_{\boldsymbol{k}_1'}^\dagger a_{\boldsymbol{k}_2'}^\dagger a_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1} \approx a_0^\dagger a_0^\dagger a_0 a_0 \approx N^2 . \qquad (13)$$

Since conservation of momentum is impossible when only one of the four indices $\boldsymbol{k}_1$, $\boldsymbol{k}_2$, $\boldsymbol{k}_1'$, and $\boldsymbol{k}_2'$ differs from zero, there are no first-order contributions. To second order, there are $\binom{4}{2} = 6$ possibilities for assigning two condensate labels "0" to the four operators, giving

$$\sum a_{\boldsymbol{k}_1'}^\dagger a_{\boldsymbol{k}_2'}^\dagger a_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1} \approx$$
$$N_0^2 + \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \Big(a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + a_0^\dagger a_{\boldsymbol{k}}^\dagger a_0 a_{\boldsymbol{k}} + a_0^\dagger a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} a_0 + a_{\boldsymbol{k}}^\dagger a_0^\dagger a_0 a_{\boldsymbol{k}} + a_{\boldsymbol{k}}^\dagger a_0^\dagger a_{\boldsymbol{k}} a_0 \Big) . \qquad (14)$$

For consistent second-order analysis, (12) now requires the approximation

$$N_0^2 \approx N^2 - 2N \sum_{\boldsymbol{k}\neq\boldsymbol{0}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \qquad (15)$$

for the first term on the r.h.s. of (14), while one may set $N_0 \approx N$ under the sum. Hence, one is led to the "quadratic" Hamiltonian

$$H = \frac{N^2}{2} \widehat{U}(\boldsymbol{0}) + \sum_{\boldsymbol{k}} \frac{\hbar^2 \boldsymbol{k}^2}{2m} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{N}{2} \widehat{U}(\boldsymbol{0}) \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \Big(a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger + a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + 2 a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \Big) . \qquad (16)$$

Observe that the coefficient "2" multiplying $a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}}$ in the second sum results from "$4-2$", with "4" originating from (14), and "-2" stemming from (15). It should also be pointed out that the reduction of the original Hamiltonian to a quadratic one, *i. e.* the omission of all matrix elements involving three or more non-zero momenta, might appeal to the intuition, but constitutes an uncontrolled approximation at this point.

The Hamiltonian (16) still suffers from the drawback that for quite typical interaction potentials $U(r)$, such as the Lennard–Jones 6–12 potential, the zero-momentum matrix element $\widehat{U}(\boldsymbol{0})$ diverges, because of the rapid increase of $U(r)$ at short distances. In order to circumvent this difficulty, one usually adopts the following renormalization strategy [20]: One first replaces the actual, hard potential $U(r)$ by some auxiliary soft potential $\widetilde{U}(r)$, for which a perturbative treatment in a plane-wave basis (and, hence, the Born approximation) is viable, and which possesses the same s-wave scattering length a as the original $U(r)$. If then the result of the calculations, performed with the auxiliary potential $\widetilde{U}(r)$, can be written entirely in terms of a, it is supposed to coincide with the result corresponding to the true interaction potential $U(r)$. This is where the Landau postulate is invoked: It is taken for granted that the scattering length is all that matters.

To give an example, a repulsive step potential with range r_0 and a height parametrized by a wave number k_0,

$$U(r) = \begin{cases} \hbar^2 k_0^2/m & \text{for } r \le r_0 \\ 0 & \text{for } r > r_0 \,, \end{cases} \tag{17}$$

approximates a hard-sphere potential of diameter r_0 when r_0 is kept fixed and k_0 is made large, so that

$$k_0 r_0 \gg 1 \,; \tag{18}$$

this inequality (18) forbids the application of perturbation theory in the plane-wave basis. Now the s-wave scattering length provided by this potential reads

$$a = \left(1 - \frac{\tanh(k_0 r_0)}{k_0 r_0} \right) r_0 \,, \tag{19}$$

implying $a \to r_0$ for $k_0 \to \infty$. If one is originally given such a hard-sphere potential, it appears natural to choose the required renormalization potential $\widetilde{U}(r)$ again as a step potential of the form (17),

$$\widetilde{U}(r) = \begin{cases} \hbar^2 \widetilde{k}_0^2/m & \text{for } r \le \widetilde{r}_0 \\ 0 & \text{for } r > \widetilde{r}_0 \,, \end{cases} \tag{20}$$

but such that

$$\widetilde{k}_0 \widetilde{r}_0 \ll 1 \,, \tag{21}$$

so that perturbation theory is viable. It then follows from (19) that the corresponding scattering length reduces to

$$a \approx \frac{1}{3} \left(\widetilde{k}_0 \widetilde{r}_0 \right)^2 \widetilde{r}_0 \,, \tag{22}$$

which means that the renormalization condition $\widetilde{a} = a$ demands

$$\widetilde{r}_0 = \frac{3 r_0}{\left(\widetilde{k}_0 \widetilde{r}_0 \right)^2} \,. \tag{23}$$

Since the numerical value of the product $\widetilde{k}_0 \widetilde{r}_0$ has to be fixed in accordance with the inequality (21), it follows that

$$\widetilde{r}_0 \gg r_0 \,. \tag{24}$$

Choosing $\widetilde{k}_0 \widetilde{r}_0 = 1/10$, say, one obtains $\widetilde{r}_0 = 300\, r_0$. Hence, one estimates that the range $\widetilde{r}_0$ of the auxiliary potential should exceed the range r_0 of the actual potential by at least two orders of magnitude.

Returning to the general case, one first formally invokes some suitable renormalization potential $\widetilde{U}(r)$ to replace the problematic matrix elements $\widehat{U}(\boldsymbol{0})$ in the Hamiltonian (16) by a well-behaved substitute $\widehat{\widetilde{U}}(\boldsymbol{0})$. Next, one expresses the latter matrix element in terms of the scattering length a which, by construction, is the same for both $\widetilde{U}(r)$ and $U(r)$. Since $\widetilde{U}(r)$ can be chosen as soft as desired, already the first Born approximation

$$a \approx \frac{m}{4\pi\hbar^2} \int \mathrm{d}^3 r \, \widetilde{U}(r) \tag{25}$$

yields an arbitrarily accurate relation between $\widehat{\widetilde{U}}(\boldsymbol{0})$ and a,

$$\widehat{\widetilde{U}}(\boldsymbol{0}) \approx \frac{4\pi a \hbar^2}{mV} \,. \tag{26}$$

Nonetheless, this approximation is used only for the prefactor of the second sum on the r. h. s. of (16). The leading N^2-proportional term is treated in the second approximation [20]

$$\frac{4\pi a \hbar^2}{mV} \approx \widehat{\widetilde{U}}(\boldsymbol{0}) + \sum_{\boldsymbol{k} \neq \boldsymbol{0}} \frac{\widehat{\widetilde{U}}(\boldsymbol{0})^2}{0 + 0 - \dfrac{\hbar^2 \boldsymbol{k}^2}{2m} - \dfrac{\hbar^2 \boldsymbol{k}^2}{2m}} \,, \tag{27}$$

where "$0+0$" in the denominator is meant to indicate that two particles in the condensate interact, so that $\boldsymbol{k}_1 = \boldsymbol{0}$, $\boldsymbol{k}_2 = \boldsymbol{0}$, and $\boldsymbol{k}'_1 = -\boldsymbol{k}'_2 = \boldsymbol{k}$. In proper second-order perturbation theory, the squared matrix elements

$$|\widehat{\widetilde{U}}(\boldsymbol{k})|^2 = \left| \frac{1}{V} \int \mathrm{d}^3 r \, \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}} \widetilde{U}(r) \right|^2 \tag{28}$$

appear under the sum; note that these elements vanish for large $|\boldsymbol{k}|$ in accordance with the Riemann–Lebesgue lemma [21]. Therefore the replacement of these elements by the constant $\widehat{\widetilde{U}}(\boldsymbol{0})^2$ is quite significant: As its consequence, the high-momentum contributions to the sum in (27) are no longer suppressed, so that this sum is linearly divergent. It will be found soon that this artificial divergence is required to cancel another, still hidden divergence arising from the similar replacement (6) which led from the original Hamiltonian (4) to the simplified form (8).

If one now formally regards the divergent sum in (27) as a *small* correction to the leading term $\widehat{\widetilde{U}}(\boldsymbol{0})$, this equation is easily inverted [20]:

$$\begin{aligned} \widehat{\widetilde{U}}(\boldsymbol{0}) &\approx \frac{4\pi a\hbar^2}{mV} + \frac{m}{\hbar^2} \widehat{\widetilde{U}}(\boldsymbol{0})^2 \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{1}{\boldsymbol{k}^2} \\ &\approx \frac{4\pi a\hbar^2}{mV} \left[1 + \frac{4\pi a}{V} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{1}{\boldsymbol{k}^2} \right] . \end{aligned} \tag{29}$$

Substituting this somewhat dubious expression (29) for the first $\widehat{\widetilde{U}}(\boldsymbol{0})$, and the first Born approximation (26) for the second $\widehat{\widetilde{U}}(\boldsymbol{0})$ appearing in (16), the scattering-length form of this Hamiltonian reads

$$\begin{aligned} H = \frac{2\pi a\hbar^2}{m} \frac{N^2}{V} \left[1 + \frac{4\pi a}{V} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{1}{\boldsymbol{k}^2} \right] + \sum_{\boldsymbol{k}} \frac{\hbar^2\boldsymbol{k}^2}{2m} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \\ + \frac{2\pi a\hbar^2}{m} \frac{N}{V} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \left(a^\dagger_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}} + a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + 2 a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \right) . \end{aligned} \tag{30}$$

Naturally, one wonders why the two zero-momentum matrix elements in (16) are treated in such a different manner, since the Hamiltonian (16) itself does not seem to provide a mathematically convincing clue for this asymmetry. The guiding principle enforcing the above procedure will become evident only in the following section, and is discussed in Section 4.

In the next step, this Hamiltonian (30) is diagonalized by means of a Bogoliubov transformation [12]. That is, for each pair $(\boldsymbol{k}, -\boldsymbol{k})$ of momenta $\boldsymbol{k} \neq \boldsymbol{0}$ one considers a "quadratic" operator

$$\begin{aligned} H_{\boldsymbol{k}} = A_{\boldsymbol{k}} + B_{\boldsymbol{k}} \left(a^\dagger_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}} + a_{\boldsymbol{k}} a_{-\boldsymbol{k}} \right) \\ + C_{\boldsymbol{k}} \, a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} + (\boldsymbol{k} \to -\boldsymbol{k}) , \end{aligned} \tag{31}$$

with

$$\begin{aligned} A_{\boldsymbol{k}} &= \frac{1}{2} \left(\frac{4\pi a\hbar^2}{m} \frac{N}{V} \right)^2 \frac{m}{\hbar^2\boldsymbol{k}^2} \\ B_{\boldsymbol{k}} &= \frac{2\pi a\hbar^2}{m} \frac{N}{V} \\ C_{\boldsymbol{k}} &= \frac{4\pi a\hbar^2}{m} \frac{N}{V} + \frac{\hbar^2\boldsymbol{k}^2}{2m} , \end{aligned} \tag{32}$$

so that $A_{\boldsymbol{k}} = A_{-\boldsymbol{k}}$, $B_{\boldsymbol{k}} = B_{-\boldsymbol{k}}$, and $C_{\boldsymbol{k}} = C_{-\boldsymbol{k}}$. This operator (31) shall be brought into the diagonal form

$$H_{\boldsymbol{k}} = \alpha(\boldsymbol{k}) + \varepsilon(\boldsymbol{k}) \, b^\dagger_{\boldsymbol{k}} b_{\boldsymbol{k}} + (\boldsymbol{k} \to -\boldsymbol{k}) , \tag{33}$$

where the new operators $b^\dagger_{\boldsymbol{k}}$, $b_{\boldsymbol{k}}$ are required to obey the Bose commutation rules,

$$[b_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k},\boldsymbol{k}'} . \tag{34}$$

Then $b^\dagger_{\boldsymbol{k}}$ and $b_{\boldsymbol{k}}$ can be interpreted as creation and annihilation operators for noninteracting quasiparticles with energy $\varepsilon(\boldsymbol{k})$, which again obey Bose statistics, while the energy shift $\alpha(\boldsymbol{k})$ defines the ground-state energy of the corresponding harmonic oscillator.

The desired transformation from the original form (31) to the quasiparticle form (33) is achieved by a linear combination of the operators referring to the bare particles, such that the annihilation operator $a_{\boldsymbol{k}}$ for a particle with momentum $\boldsymbol{k}$ is combined with the creation operator $a^\dagger_{-\boldsymbol{k}}$ for a particle with reverse momentum $-\boldsymbol{k}$:

$$b_{\boldsymbol{k}} = u_{\boldsymbol{k}} a_{\boldsymbol{k}} + v_{\boldsymbol{k}} a^\dagger_{-\boldsymbol{k}}, \; b^\dagger_{\boldsymbol{k}} = u_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} + v_{\boldsymbol{k}} a_{-\boldsymbol{k}} ; \tag{35}$$

the real coefficients $u_{\boldsymbol{k}} = u_{-\boldsymbol{k}}$ and $v_{\boldsymbol{k}} = v_{-\boldsymbol{k}}$ still have to be determined. Since (35) implies

$$[b_{\boldsymbol{k}}, b^\dagger_{\boldsymbol{k}}] = u^2_{\boldsymbol{k}} - v^2_{\boldsymbol{k}} , \tag{36}$$

the requirement (34) gives

$$u^2_{\boldsymbol{k}} - v^2_{\boldsymbol{k}} = 1 , \tag{37}$$

so that there is only one independent transformation parameter. Thus, instead of the parameters $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ one can introduce a single parameter $L_{\boldsymbol{k}}$ through

$$u_{\boldsymbol{k}} = \frac{1}{\sqrt{1-L_{\boldsymbol{k}}^2}} \,,\; v_{\boldsymbol{k}} = \frac{L_{\boldsymbol{k}}}{\sqrt{1-L_{\boldsymbol{k}}^2}} \,. \tag{38}$$

Then

$$L_{\boldsymbol{k}} = \frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}} \,, \tag{39}$$

and (37) is satisfied automatically.

Inserting the ansatz (35) for the quasiparticle operators into the desired form (33), and rearranging terms with indices $\boldsymbol{k}$ and $-\boldsymbol{k}$ as required, one obtains

$$\begin{aligned} H_{\boldsymbol{k}} &= \alpha(\boldsymbol{k}) + \varepsilon(\boldsymbol{k})\, v_{\boldsymbol{k}}^2 + \varepsilon(\boldsymbol{k})\, u_{\boldsymbol{k}} v_{\boldsymbol{k}} \left(a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger + a_{\boldsymbol{k}} a_{-\boldsymbol{k}} \right) \\ &\quad + \varepsilon(\boldsymbol{k})(u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2)\, a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + (\boldsymbol{k} \to -\boldsymbol{k}) \,, \end{aligned} \tag{40}$$

and comparison with the original form (31) reveals

$$\begin{aligned} A_{\boldsymbol{k}} &= \alpha(\boldsymbol{k}) + \varepsilon(\boldsymbol{k}) v_{\boldsymbol{k}}^2 , \\ B_{\boldsymbol{k}} &= \varepsilon(\boldsymbol{k}) u_{\boldsymbol{k}} v_{\boldsymbol{k}} , \\ C_{\boldsymbol{k}} &= \varepsilon(\boldsymbol{k})(u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2) \,. \end{aligned} \tag{41}$$

Inversion of these latter equations with the help of the relation (37) immediately yields

$$\begin{aligned} \varepsilon(\boldsymbol{k})^2 &= C_{\boldsymbol{k}}^2 - 4B_{\boldsymbol{k}}^2 , \\ \varepsilon(\boldsymbol{k}) - 2\alpha(\boldsymbol{k}) &= C_{\boldsymbol{k}} - 2A_{\boldsymbol{k}} \,. \end{aligned} \tag{42}$$

Moreover, the transformation parameter $L_{\boldsymbol{k}} = v_{\boldsymbol{k}}/u_{\boldsymbol{k}}$ is expressed, with the help of the first and second of the equations (41), as

$$L_{\boldsymbol{k}} = \frac{\varepsilon(\boldsymbol{k})\, v_{\boldsymbol{k}}^2}{\varepsilon(\boldsymbol{k})\, u_{\boldsymbol{k}} v_{\boldsymbol{k}}} = \frac{C_{\boldsymbol{k}} - \varepsilon(\boldsymbol{k})}{2B_{\boldsymbol{k}}} \,. \tag{43}$$

In essence, the Bogoliubov transformation thus converts the information contained in the coefficients $A_{\boldsymbol{k}}$, $B_{\boldsymbol{k}}$, and $C_{\boldsymbol{k}}$ of the original form (31) into the quasiparticle energy $\varepsilon(\boldsymbol{k})$, the energy shift $\alpha(\boldsymbol{k})$, and the transformation parameter $L_{\boldsymbol{k}}$. For our purposes it is of interest to observe that the coefficients $A_{\boldsymbol{k}}$, which embody the formally divergent second-order contributions to the expression (27), enter only into the energy shifts $\alpha(\boldsymbol{k})$, whereas both $\varepsilon(\boldsymbol{k})$ and $L_{\boldsymbol{k}}$ are independent of $A_{\boldsymbol{k}}$.

When applying this transformation scheme to the particular Hamiltonian (30) describing the low-energy dynamics of the Bose gas, insertion of the parameters (32) into the first of the Eqs. (42) yields the celebrated Bogoliubov quasiparticle spectrum

$$\varepsilon(\boldsymbol{k}) = \left[\left(\frac{\hbar^2 \boldsymbol{k}^2}{2m} \right)^2 + \frac{4\pi a \hbar^2}{m} \frac{N}{V} \frac{\hbar^2 \boldsymbol{k}^2}{m} \right]^{1/2} \,. \tag{44}$$

The second of the Eqs. (42) then gives the quasiparticle energy shift

$$\begin{aligned} \alpha(\boldsymbol{k}) &= \frac{1}{2} \left(\varepsilon(\boldsymbol{k}) - C_{\boldsymbol{k}} + 2A_{\boldsymbol{k}} \right) \\ &= \frac{1}{2} \Big[\varepsilon(\boldsymbol{k}) - \frac{\hbar^2 \boldsymbol{k}^2}{2m} - \frac{4\pi a \hbar^2}{m} \frac{N}{V} \\ &\qquad + \Big(\frac{4\pi a \hbar^2}{m} \frac{N}{V} \Big)^2 \frac{m}{\hbar^2 \boldsymbol{k}^2} \Big] \,, \end{aligned} \tag{45}$$

while the transformation parameter $L_{\boldsymbol{k}}$ is obtained from (43) in the form

$$L_{\boldsymbol{k}} = 1 + \left(\frac{4\pi a \hbar^2}{m} \frac{N}{V} \right)^{-1} \left(\frac{\hbar^2 \boldsymbol{k}^2}{2m} - \varepsilon(\boldsymbol{k}) \right) \,. \tag{46}$$

Taking all things together, the Bogoliubov transformation (35) brings the Hamiltonian (30) into the quasiparticle form

$$H = \frac{2\pi a \hbar^2}{m} \frac{N^2}{V} + \sum_{\boldsymbol{k} \neq \boldsymbol{0}} H_{\boldsymbol{k}} = E_0 + \sum_{\boldsymbol{k} \neq \boldsymbol{0}} \varepsilon(\boldsymbol{k})\, b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}} \,, \tag{47}$$

where the ground-state energy E_0 is given by the momentum-independent term in (30), as corresponding to the first Born approximation (26), plus the sum of all energy shifts $\alpha(\boldsymbol{k})$:

$$\begin{aligned} E_0 &= \frac{2\pi a \hbar^2}{m} \frac{N^2}{V} + \sum_{\boldsymbol{k} \neq \boldsymbol{0}} \alpha(\boldsymbol{k}) \\ &= \frac{2\pi a \hbar^2}{m} \frac{N^2}{V} + \frac{1}{2} \sum_{\boldsymbol{k} \neq \boldsymbol{0}} \Big[\varepsilon(\boldsymbol{k}) - \frac{\hbar^2 \boldsymbol{k}^2}{2m} - \frac{4\pi a \hbar^2}{m} \frac{N}{V} \\ &\qquad + \Big(\frac{4\pi a \hbar^2}{m} \frac{N}{V} \Big)^2 \frac{m}{\hbar^2 \boldsymbol{k}^2} \Big] \,. \end{aligned} \tag{48}$$

In order to evaluate this approximation to the ground-state energy explicitly, one takes the thermodynamic limit and utilizes the density of states $\rho(k)$ in momentum space,

$$\rho(k)\, \mathrm{d}k = \frac{V k^2\, \mathrm{d}k}{2\pi^2} \,. \tag{49}$$

Since the natural energy scale of the weakly interacting Bose gas is set by the quantity $4\pi a\bar{h}^2 N/(mV)$, roughly equal to two times the ground-state energy per particle, it is convenient to define a dimensionless momentum x through the relation

$$\frac{\bar{h}^2\boldsymbol{k}^2}{2m} = \frac{4\pi a\bar{h}^2}{m}\frac{N}{V}x^2 \,, \tag{50}$$

so that

$$\varepsilon(\boldsymbol{k}) = \frac{4\pi a\bar{h}^2}{m}\frac{N}{V}x\sqrt{x^2+2}\,. \tag{51}$$

According to (48) one then has

$$E_0 = \frac{2\pi a\bar{h}^2}{m}\frac{N^2}{V}\left[1+\sqrt{\frac{128}{\pi}}\left(\frac{N}{V}a^3\right)^{1/2} I\right] \,, \tag{52}$$

where the number

$$I = \int_0^\infty \mathrm{d}x\, x^2\left(x\sqrt{x^2+2}-x^2-1+\frac{1}{2x^2}\right) \tag{53}$$

results from converting the sum over $\boldsymbol{k}\neq\boldsymbol{0}$ into an integral over x with the help of the density (49). The integrand $f(x) = x^3\sqrt{x^2+2}-x^4-x^2+1/2$ is a positive, monotonously decreasing function with $f(0)=1/2$ and $f(x)\sim 1/(2x^2)$ for large arguments. Therefore the integral I converges; it collects its main contributions (roughly) for $0\leq x\leq 2$. Elementary calculation yields

$$\begin{aligned} I &= \lim_{\ell\to\infty}\left(\int_0^\ell \mathrm{d}x\, x^3\sqrt{x^2+2}-\frac{1}{5}\ell^5-\frac{1}{3}\ell^3+\frac{1}{2}\ell\right) \\ &= \frac{\sqrt{128}}{15} \,, \end{aligned} \tag{54}$$

so that one finally recovers the Lee-Yang result (2) for the ground-state energy.

Only at this point can one appreciate the significance of the second Born approximation (27). The linearly divergent "correction" to the leading term in (29), which results from the replacement of $|\widetilde{U}(\boldsymbol{k})|^2$ by the constant $\widetilde{U}(\boldsymbol{0})^2$ in (27), is the reason why there are non-vanishing coefficients $A_{\boldsymbol{k}}$ in the operators (31). These coefficients, in their turn, do affect neither the quasiparticle energies $\varepsilon(\boldsymbol{k})$ nor the Bogoliubov transformation parameters $L_{\boldsymbol{k}}$, but they do result in a contribution to the integral I which renders this integral convergent. Without this contribution, which is represented by the last term in the integrand in (53), the remaining integral would be linearly divergent, and negative. It thus appears that the second Born approximation in the peculiar form of (29) is necessary to compensate the high-momentum error committed already in (8) by ignoring the fact that the actual matrix elements (5) vanish for high momentum transfer: Since the ground-state energy (48) results from summing the energy shifts $\alpha(\boldsymbol{k})$ for *all* $\boldsymbol{k}$, their behavior for high momenta *does* matter.

One still has to evaluate the depletion of the condensate at zero temperature, that is, the extent to which single-particle states other than the single-particle ground state are occupied when the weakly interacting gas is in its many-particle ground state $|\Psi_0\rangle$, in order to make sure that the "classical" approximation (11) and the expansion (14) are justified. To do so, it is convenient to invert the transformation formulas (35) with the help of (37), which gives

$$a_{\boldsymbol{k}} = u_{\boldsymbol{k}}b_{\boldsymbol{k}} - v_{\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}}, \quad a^\dagger_{\boldsymbol{k}} = u_{\boldsymbol{k}}b^\dagger_{\boldsymbol{k}} - v_{\boldsymbol{k}}b_{-\boldsymbol{k}} \tag{55}$$

or

$$a_{\boldsymbol{k}} = \frac{b_{\boldsymbol{k}} - L_{\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}}}{\sqrt{1-L_{\boldsymbol{k}}^2}}, \quad a^\dagger_{\boldsymbol{k}} = \frac{b^\dagger_{\boldsymbol{k}} - L_{\boldsymbol{k}}b_{-\boldsymbol{k}}}{\sqrt{1-L_{\boldsymbol{k}}^2}} \,. \tag{56}$$

Since the many-particle ground state $|\Psi_0\rangle$ constitutes the vacuum for the quasiparticle operators, so that $b_{\boldsymbol{k}}|\Psi_0\rangle = 0$ for $\boldsymbol{k}\neq 0$, one then has

$$a_{\boldsymbol{k}}|\Psi_0\rangle = \frac{-L_{\boldsymbol{k}}}{\sqrt{1-L_{\boldsymbol{k}}}}\,b^\dagger_{-\boldsymbol{k}}|\Psi_0\rangle \,, \tag{57}$$

implying

$$\begin{aligned} \langle\Psi_0|a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}|\Psi_0\rangle &= \frac{L_{\boldsymbol{k}}^2}{1-L_{\boldsymbol{k}}^2}\,\langle\Psi_0|b_{-\boldsymbol{k}}b^\dagger_{-\boldsymbol{k}}|\Psi_0\rangle \\ &= \frac{L_{\boldsymbol{k}}^2}{1-L_{\boldsymbol{k}}^2} \,. \end{aligned} \tag{58}$$

Again, invoking the dimensionless magnitude x of the momentum defined in (50), the transformation parameter (46) becomes

$$L_{\boldsymbol{k}} = 1+x^2-x\sqrt{x^2+2} \,, \tag{59}$$

giving

$$\langle\Psi_0|a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}|\Psi_0\rangle = \frac{1}{2}\,\frac{1+x^2}{x\sqrt{x^2+2}} - \frac{1}{2} \,. \tag{60}$$

In the thermodynamic limit, the total depletion of the condensate is then expressed, with the help of the density of states (49), as

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \langle\Psi_0|a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}|\Psi_0\rangle = 2N\left(\frac{32}{\pi}\frac{N}{V}a^3\right)^{1/2} \cdot \int_0^\infty \frac{\mathrm{d}x}{2}\left(\frac{x+x^3}{\sqrt{x^2+2}}-x^2\right). \quad (61)$$

The integral emerging here has the value

$$\lim_{\ell\to\infty}\int_0^\ell \frac{\mathrm{d}x}{2}\left(\frac{x+x^3}{\sqrt{x^2+2}}-x^2\right) = \frac{\sqrt{2}}{6}\,, \quad (62)$$

so that the depletion takes the final form

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \langle\Psi_0|a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}|\Psi_0\rangle = N\frac{8}{3\sqrt{\pi}}\left(\frac{N}{V}a^3\right)^{1/2}. \quad (63)$$

Accordingly, the expectation value for the number of particles occupying the single-particle ground state at zero temperature reads [2]

$$\langle\Psi_0|a_0^\dagger a_0|\Psi_0\rangle = N\left[1-\frac{8}{3\sqrt{\pi}}\left(\frac{N}{V}a^3\right)^{1/2}\right]. \quad (64)$$

Thus, the relative depletion of the condensate is of the order $\mathcal{O}\big((na^3)^{1/2}\big)$, which, according to the proposition (3), is small compared to unity. Therefore the result (63) also constitutes an *a posteriori* justification for the decisive approximations (11) and (14), which required a large occupation of the single-particle ground state, and a relatively small number of non-condensed particles.

3. Soft Potentials: Avoiding Divergencies

The previous line of reasoning [9] contains several steps that deserve to be investigated in more detail. In particular, the admission of an intermediate divergence into the ground-state energy through the replacement (6) and its subsequent cancellation by means of the second Born approximation (27), together with the asymmetric treatment of the zero-momentum matrix elements in (16), might appear questionable. In this section, we therefore provide a different derivation of the ground-state energy which avoids these manipulations at least for soft interaction potentials. We start again from the Hamiltonian (4), but now we do *not* replace the matrix elements

$$\langle\boldsymbol{k}_1'\boldsymbol{k}_2'|U|\boldsymbol{k}_1\boldsymbol{k}_2\rangle = \frac{1}{V}\int \mathrm{d}^3\boldsymbol{r}\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}}U(r) = \widehat{U}(\boldsymbol{q}) \quad (65)$$

by the constant $\widehat{U}(\boldsymbol{0})$. As is clear from the discussion in Sect. 2, the error committed at high momenta through that replacement would lead, even when the interaction potential $U(r)$ is well-behaved, to an infinite (negative) ground-state energy E_0, if it were not compensated by the second Born approximation in the peculiar form of (29). While that device actually does cancel the linear divergence and indeed leads to the finite Lee-Yang ground-state energy (2), it does not seem obvious that this procedure necessarily is correct.

Therefore, we again assume the depletion of the condensate to be small and invoke the "classical" approximation (11) for the ground-state operators a_0 and $a_0^\dagger$, but keep the exact matrix elements in the quadratic expansion of the interaction term of the Hamiltonian (4). Proceeding as in (14), this gives

$$\begin{aligned} H = {} & \sum_{\boldsymbol{k}} \frac{\hbar^2\boldsymbol{k}^2}{2m}a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{1}{2}\langle\boldsymbol{0}\,\boldsymbol{0}|U|\boldsymbol{0}\,\boldsymbol{0}\rangle\, a_0^\dagger a_0^\dagger a_0 a_0 \\ & + \frac{1}{2}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\Big[\langle\boldsymbol{k}\,-\boldsymbol{k}|U|\boldsymbol{0}\,\boldsymbol{0}\rangle\, a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger a_0 a_0 \\ & \qquad + \langle\boldsymbol{0}\,\boldsymbol{0}|U|-\boldsymbol{k}\,\boldsymbol{k}\rangle\, a_0^\dagger a_0^\dagger a_{\boldsymbol{k}} a_{-\boldsymbol{k}} \\ & \qquad + \langle\boldsymbol{0}\,\boldsymbol{k}|U|\boldsymbol{k}\,\boldsymbol{0}\rangle\, a_0^\dagger a_{\boldsymbol{k}}^\dagger a_0 a_{\boldsymbol{k}} \\ & \qquad + \langle\boldsymbol{0}\,\boldsymbol{k}|U|\boldsymbol{0}\,\boldsymbol{k}\rangle\, a_0^\dagger a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} a_0 \\ & \qquad + \langle\boldsymbol{k}\,\boldsymbol{0}|U|\boldsymbol{k}\,\boldsymbol{0}\rangle\, a_{\boldsymbol{k}}^\dagger a_0^\dagger a_0 a_{\boldsymbol{k}} \\ & \qquad + \langle\boldsymbol{k}\,\boldsymbol{0}|U|\boldsymbol{0}\,\boldsymbol{k}\rangle\, a_{\boldsymbol{k}}^\dagger a_0^\dagger a_{\boldsymbol{k}} a_0\Big]. \end{aligned} \quad (66)$$

Again using the approximation (15) in the zero-order term, we then find

$$\begin{aligned} H = {} & \sum_{\boldsymbol{k}} \frac{\hbar^2\boldsymbol{k}^2}{2m}a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} + \frac{1}{2}\widehat{U}(\boldsymbol{0})\Big[N^2 - 2N\sum_{\boldsymbol{k}\neq\boldsymbol{0}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}\Big] \\ & + \frac{1}{2}N\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\Big[\widehat{U}(-\boldsymbol{k})\, a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger + \widehat{U}(-\boldsymbol{k})\, a_{\boldsymbol{k}} a_{-\boldsymbol{k}} \end{aligned}$$

$$+\widehat{U}(\boldsymbol{k})\,a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}+\widehat{U}(\boldsymbol{0})\,a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}$$

$$+\widehat{U}(\boldsymbol{0})\,a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}+\widehat{U}(-\boldsymbol{k})\,a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}\Big]. \quad (67)$$

It is important to observe that the second-order terms proportional to $\widehat{U}(\boldsymbol{0})$, corresponding to processes with zero momentum transfer, drop out at this point. Since $U(r)$ is a real function, we also have $\widehat{U}(-\boldsymbol{k})=\widehat{U}(\boldsymbol{k})$, so that the analogue of the previous Eq. (16) now takes the simple form

$$H=\frac{N^2}{2}\widehat{U}(\boldsymbol{0})+\sum_{\boldsymbol{k}}\frac{\hbar\boldsymbol{k}^2}{2m}a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}$$

$$+\frac{N}{2}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\widehat{U}(\boldsymbol{k})\Big(a_{\boldsymbol{k}}^\dagger a_{-\boldsymbol{k}}^\dagger+a_{\boldsymbol{k}}a_{-\boldsymbol{k}}+2a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}\Big). \quad (68)$$

Still, the leading term is ill-defined for a hard potential with a strong short-range singularity. We will discuss Bose gases with such a hard interaction potential in a subsequent work and restrict ourselves here to soft potentials, for which $\widehat{U}(\boldsymbol{0})$ exists. However, we do not attempt to express the matrix elements in terms of the scattering length at this stage. Consequently, there is no need to invoke the Born approximations (26) or (27); instead we apply the Bogoliubov transformation directly to the Hamiltonian (68). That is, we again consider a set of operators of the form (31), but now with coefficients

$$A_{\boldsymbol{k}}=0,\; B_{\boldsymbol{k}}=\frac{N}{2}\widehat{U}(\boldsymbol{k}),C_{\boldsymbol{k}}=N\widehat{U}(\boldsymbol{k})+\frac{\hbar^2\boldsymbol{k}^2}{2m}. \quad (69)$$

The transformation procedure then is exactly the same as in the preceding section; in particular (42) and (43) can be taken over. Thus, we find the quasiparticle energies

$$\varepsilon(\boldsymbol{k})=\left[\left(\frac{\hbar^2\boldsymbol{k}^2}{2m}\right)^2+N\widehat{U}(\boldsymbol{k})\frac{\hbar^2\boldsymbol{k}^2}{m}\right]^{1/2}, \quad (70)$$

the energy shifts

$$\alpha(\boldsymbol{k})=\frac{1}{2}\big(\varepsilon(\boldsymbol{k})-C_{\boldsymbol{k}}\big)$$

$$=\frac{1}{2}\left[\varepsilon(\boldsymbol{k})-\frac{\hbar^2\boldsymbol{k}^2}{2m}-N\widehat{U}(\boldsymbol{k})\right], \quad (71)$$

and the transformation parameters

$$L_{\boldsymbol{k}}=1+\frac{\frac{\hbar^2\boldsymbol{k}^2}{2m}-\varepsilon(\boldsymbol{k})}{N\widehat{U}(\boldsymbol{k})}\,. \quad (72)$$

The principal difference between these expressions and the corresponding Eqs. (44), (45), and (46) lies in the fact that $A_{\boldsymbol{k}}=0$ here, so that the shifts $\alpha(\boldsymbol{k})$ remain regular for $\boldsymbol{k}\to\boldsymbol{0}$. As before, a necessary consistency condition is that the total depletion $N-N_0$ be small in comparison with the particle number N.

It it now possible to evaluate the ground-state energy for an arbitrary soft potential in the limit of low density $n=N/V$. To this end we write $\widehat{U}(\boldsymbol{k})=u(\boldsymbol{k})/V$, or $N\widehat{U}(\boldsymbol{k})=nu(\boldsymbol{k})$, so that

$$E_0/N=\frac{1}{2}u(\boldsymbol{0})n+\frac{1}{nV}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\alpha(\boldsymbol{k})\,. \quad (73)$$

We proceed by expanding the sum in powers of the density: Obviously

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\alpha(\boldsymbol{k})\bigg|_{n=0}=0\,. \quad (74)$$

Next, we have

$$\frac{\partial\alpha(\boldsymbol{k})}{\partial n}=\frac{1}{4}\frac{2u(\boldsymbol{k})\frac{\hbar^2\boldsymbol{k}^2}{2m}}{\left[\left(\frac{\hbar^2\boldsymbol{k}^2}{2m}\right)^2+2nu(\boldsymbol{k})\frac{\hbar^2\boldsymbol{k}^2}{2m}\right]^{1/2}}-\frac{1}{2}u(\boldsymbol{k}), \quad (75)$$

giving

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\frac{\partial\alpha(\boldsymbol{k})}{\partial n}\bigg|_{n=0}=0\,; \quad (76)$$

moreover

$$\frac{\partial^2\alpha(\boldsymbol{k})}{\partial n^2}=-\frac{1}{8}\frac{\left(2u(\boldsymbol{k})\frac{\hbar^2\boldsymbol{k}^2}{2m}\right)^2}{\left[\left(\frac{\hbar^2\boldsymbol{k}^2}{2m}\right)^2+2nu(\boldsymbol{k})\frac{\hbar^2\boldsymbol{k}^2}{2m}\right]^{3/2}}, \quad (77)$$

resulting in

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\frac{\partial^2\alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0}=-\frac{1}{2}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\frac{u^2(\boldsymbol{k})}{\hbar^2\boldsymbol{k}^2/2m}\,. \quad (78)$$

Considering now the Born series for the scattering length [22],

$$a = \sum_{n=0}^{\infty} a_n \,, \tag{79}$$

its leading term is given by the familiar expression

$$a_0 = \frac{m}{4\pi\hbar^2}\, u(\boldsymbol{0}) \,. \tag{80}$$

This relation had already been employed in (25) for the auxiliary potential $\widetilde{U}(r)$, which could be taken so soft that $a_0 \approx a$ could be assumed. Here we merely use it to write the first contribution to the ground-state energy (73) in the form

$$\frac{1}{2} u(\boldsymbol{0}) n = \frac{2\pi a_0 \hbar^2}{m} n \,, \tag{81}$$

without implying that the series (79) is already exhausted by its first term a_0. The second-order term of the Born series (79) then reads [22]

$$a_1 = -\left(\frac{m}{4\pi\hbar^2}\right)^2 \int \mathrm{d}^3\boldsymbol{r} \int \mathrm{d}^3\boldsymbol{r}'\, U(r) \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} U(r') \,. \tag{82}$$

Anticipating the thermodynamic limit and using

$$\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{4\pi}{V} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{\boldsymbol{k}^2} \,, \tag{83}$$

this expression (82) can be written as

$$a_1 = -\frac{m}{4\pi\hbar^2} \frac{1}{V} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{u^2(\boldsymbol{k})}{\hbar^2\boldsymbol{k}^2/m} \,, \tag{84}$$

from which it follows that (78) reduces to

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\partial^2 \alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0} = \frac{4\pi a_1 \hbar^2}{m} V \,. \tag{85}$$

Combining then (74), (76), and (85), we find the second contribution to the ground-state energy (73),

$$\frac{1}{nV} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \alpha(\boldsymbol{k}) \approx \frac{1}{nV} \frac{4\pi a_1 \hbar^2}{m} V \frac{n^2}{2} \tag{86}$$

for low density n; interestingly, both contributions (81) and (86) are of the same order in n. Adding up, we thus obtain

$$\lim_{n\to 0} \frac{E_0/N}{n} = \frac{2\pi(a_0+a_1)\hbar^2}{m} \,. \tag{87}$$

The scattering length is represented here by only the first two terms of the expansion (79); as a consequence of the quadratic approximation (68) to the full Hamiltonian, the higher-order terms do not come into play within the present scheme.

Proceeding with the density expansion, the naive attempt to consider

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\partial^3 \alpha(\boldsymbol{k})}{\partial n^3}\bigg|_{n=0}$$

appears fruitless, since this sum is converted into an infrared-divergent integral in the thermodynamic limit. However, stipulating that $u(\boldsymbol{k})$ be bounded, the expression

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\partial}{\partial\sqrt{n}} \frac{\partial^2 \alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0} = \tag{88}$$

$$\lim_{n\to 0} \frac{V}{(2\pi)^3} \int \mathrm{d}^3\boldsymbol{k}\, \frac{3\left(u(\boldsymbol{k})\dfrac{\hbar^2\boldsymbol{k}^2}{2m}\right)^3 \sqrt{n}}{\left[\left(\dfrac{\hbar^2\boldsymbol{k}^2}{2m}\right)^2 + 2nu(\boldsymbol{k})\dfrac{\hbar^2\boldsymbol{k}^2}{2m}\right]^{5/2}}$$

converges: Introducing for a given wave vector $\boldsymbol{k}$ and density n a dimensionless variable y by means of the relation (cf. (50))

$$\frac{\hbar^2\boldsymbol{k}^2}{2m} = u(\boldsymbol{0}) n y^2 \,, \tag{89}$$

so that

$$|\boldsymbol{k}| = \frac{1}{\hbar}\sqrt{2mu(\boldsymbol{0})y^2}\sqrt{n} \,, \tag{90}$$

we find

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\partial}{\partial\sqrt{n}} \frac{\partial^2 \alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0} = \tag{91}$$

$$\frac{3V}{2\pi^2} \frac{(2m)^{3/2} u(\boldsymbol{0})^{5/2}}{\hbar^3} \lim_{n\to 0} \int_0^\infty \mathrm{d}y\, \frac{\left(y\dfrac{u(\boldsymbol{k})}{u(\boldsymbol{0})}\right)^3}{\left[y^2 + 2\dfrac{u(\boldsymbol{k})}{u(\boldsymbol{0})}\right]^{5/2}} \,.$$

For bounded $u(\boldsymbol{k})$, the limit $n \to 0$ can now be taken under the integral: Since, by virtue of (90), that limit implies

$$\lim_{n\to 0} \frac{u(\boldsymbol{k})}{u(\boldsymbol{0})} \to 1 \,, \tag{92}$$

we are left with

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\partial}{\partial\sqrt{n}} \frac{\partial^2\alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0}$$
$$= \frac{3V}{2\pi^2} \frac{(2m)^{3/2}u(\boldsymbol{0})^{5/2}}{\bar{h}^3} \int_0^\infty \mathrm{d}y \frac{y^3}{(y^2+2)^{5/2}}$$
$$= \frac{64\sqrt{\pi}a_0^{5/2}\bar{h}^2}{m} V. \qquad (93)$$

Here we have made use of (80) once more, and computed

$$\lim_{\ell\to\infty} \int_0^\ell \mathrm{d}y \frac{y^3}{(y^2+2)^{5/2}} = \frac{\sqrt{2}}{3}\,. \qquad (94)$$

Hence, within the density expansion the next contribution to the ground-state energy per particle is given by

$$\frac{1}{nV} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\partial}{\partial\sqrt{n}} \frac{\partial^2\alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0} \frac{2}{5}\frac{2}{3} n^{5/2}$$
$$= \frac{2\pi a_0\bar{h}^2}{m} \frac{128}{15\sqrt{\pi}} n \left(na_0^3\right)^{1/2}\,, \qquad (95)$$

finally resulting in

$$E_0/N = \frac{2\pi a_0\bar{h}^2}{m} n \left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{na_0^3}\right] + \frac{2\pi a_1\bar{h}^2}{m} n \qquad (96)$$

in the low-density regime. Although the calculation here is substantially different from the one in Sect. 2, this expression (96) differs only slightly from the hard-sphere formula (2): To leading order in the density, the full scattering length a has been replaced by a_0+a_1; in the next-order term, a_0 appears instead of a. This finding coincides with a result obtained by other means by Brueckner and Sawada already in 1957 [3]; it has recently also been derived in [23].

In order to determine the depletion associated with a soft potential,

$$N - N_0 = \frac{V}{(2\pi)^3} \int \mathrm{d}^3\boldsymbol{k} \frac{L_{\boldsymbol{k}}^2}{1-L_{\boldsymbol{k}}^2}\,, \qquad (97)$$

we now consider the transformation parameters (72) and again make the substitution (89), which leads to

$$L_{\boldsymbol{k}} = 1 + \frac{u(\boldsymbol{0})}{u(\boldsymbol{k})}y^2 - \left[\left(\frac{u(\boldsymbol{0})}{u(\boldsymbol{k})}y^2\right)^2 + 2\frac{u(\boldsymbol{0})}{u(\boldsymbol{k})}y^2\right]^{1/2}. \qquad (98)$$

Taking the limit $n\to 0$ as in (92), and comparing with the previous representation (59), one obviously arrives at an integral similar to that which had appeared in (61), namely,

$$\lim_{n\to 0} \frac{n-n_0}{n^{3/2}} = \frac{(2mu(\boldsymbol{0}))^{3/2}}{2\pi^2\bar{h}^3} \int_0^\infty \frac{\mathrm{d}y}{2} \left(\frac{y+y^3}{\sqrt{y^2+2}} - y^2\right)$$
$$= \frac{8}{3\sqrt{\pi}} a_0^{3/2}\,. \qquad (99)$$

Thus, to leading order in the density the depletion is again given by (63), with the first Born approximation a_0 here replacing the full scattering length a there.

4. Discussion

The considerations outlined in the previous section answer the technical questions which emerged when discussing the textbook material [9] in Section 2. To begin with, the reason why the two zero-momentum matrix elements $\widehat{U}(\boldsymbol{0})$ in the Hamiltonian (16) were treated in a substantially different manner when producing the scattering-length form (30) lies in the fact that only one of these elements is genuine: If one keeps carefully track of the actual momentum transfer, as done in (66) and (67), one obtains the more accurate Hamiltonian (68), with $\widehat{U}(\boldsymbol{0})$ appearing only in the leading, N^2-proportional term. Equation (67) shows that it is the approximation (15) which effectuates the removal of $\widehat{U}(\boldsymbol{0})$ from the second-order terms. The Hamiltonian (16), therefore, is an oversimplification which cannot serve as a starting point for a consistent calculation of the ground-state energy; instead, knowledge of the proper Hamiltonian (68) is required.

Next, the debatable relation (29) can be given a mathematically sound meaning: Adding up the first two terms of the Born series for the scattering length, as given by (80) and (84), one has

$$a_0 + a_1 = \frac{mV}{4\pi\bar{h}^2}\widehat{U}(\boldsymbol{0}) - \frac{mV}{4\pi\bar{h}^2} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\widehat{U}(\boldsymbol{k})^2}{\bar{h}^2\boldsymbol{k}^2/m}\,, \qquad (100)$$

which yields

$$\widehat{U}(\boldsymbol{0}) = \frac{4\pi(a_0+a_1)\bar{h}^2}{mV} + \frac{m}{\bar{h}^2} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \frac{\widehat{U}(\boldsymbol{k})^2}{\boldsymbol{k}^2} \qquad (101)$$

instead of the ill-defined Eq. (27). Of course, the r.h.s. of (101) equals just $4\pi a_0\bar{h}^2/(mV)$, with the remaining

terms adding up to zero. Inserting this expression for $\widehat{U}(\boldsymbol{0})$ into the quadratic Hamiltonian (68), one finds a more trustworthy analogue of (30), namely,

$$H = \frac{2\pi(a_0+a_1)\hbar^2}{m}\frac{N^2}{V} + \frac{mN^2}{2\hbar^2}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\frac{\widehat{U}(\boldsymbol{k})^2}{\boldsymbol{k}^2} + \sum_{\boldsymbol{k}}\frac{\hbar^2\boldsymbol{k}^2}{2m}a^\dagger_{s\boldsymbol{k}}a_{\boldsymbol{k}} + \frac{N}{2}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\widehat{U}(\boldsymbol{k})\Big(a^\dagger_{\boldsymbol{k}}a^\dagger_{-\boldsymbol{k}} + a_{\boldsymbol{k}}a_{-\boldsymbol{k}} + 2a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}}\Big). \quad (102)$$

Again writing $N\widehat{U}(\boldsymbol{k}) = nu(\boldsymbol{k})$, and applying the Bogoliubov scheme, one now has

$$A_{\boldsymbol{k}} = \frac{n^2}{2}\frac{u(\boldsymbol{k})^2}{\hbar^2\boldsymbol{k}^2/m}, \quad (103)$$

while $B_{\boldsymbol{k}}$ and $C_{\boldsymbol{k}}$ are still given by (69). Consequently, the quasiparticle energies $\varepsilon(\boldsymbol{k})$ and the transformation parameters $L_{\boldsymbol{k}}$ remain as stated in (70) and (72), respectively, while the corresponding energy shifts now take the form

$$\alpha(\boldsymbol{k}) = \frac{1}{2}\left[\varepsilon(\boldsymbol{k}) - \frac{\hbar^2\boldsymbol{k}^2}{2m} - nu(\boldsymbol{k})\right] + \frac{n^2}{2}\frac{u(\boldsymbol{k})^2}{\hbar^2\boldsymbol{k}^2/m}. \quad (104)$$

Then

$$\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\frac{\partial^2\alpha(\boldsymbol{k})}{\partial n^2}\bigg|_{n=0} = 0 \quad (105)$$

instead of (85), so that now the leading-order term (87) of the energy per particle corresponds precisely to the first term of the Hamiltonian (102), while only the next-to-leading contribution (95) is extracted in the low-density limit from the sum over the energy shifts. Needless to say, the sketch given here is equivalent to the reasoning in Sect. 3, with the slight cosmetic advantage that the contributions (87) and (95) to the ground-state energy are disentangled in a more transparent manner, as a consequence of the fore-sighted use of (101) with its "fat zero" on the r.h.s.

It is also worthwhile to point out that the refined analysis in Sect. 3 directly takes recourse to the low-density limit, as witnessed by the density expansion of the expression (73) for E_0/N and the way the integrals (93) and (99) have been evaluated; this limit had remained somewhat hidden in Section 2. The key insight provided by the comparison of Sects. 2 and 3, however, consists in the fact that if one does *not* take the Landau postulate for granted, the standard textbook arguments, if applied carefully, actually do lead to the Brueckner-Sawada result (96), instead of the Lee-Yang formula (52). Indeed, it is now easy to see that the expression (52) contains the full scattering length a, rather than merely the leading terms of the Born series, only as a consequence of the careless Eq. (25), where a is used as an approximation for a_0, and of the even more sloppy Eq. (27), where a on the l.h.s. should actually be interpreted as a_0+a_1, as revealed by comparison with (101).

It is striking to observe that the formula (96) for the ground-state energy, obtained here by avoiding all unnecessary approximations and thereby retaining only finite, well-defined expressions at all intermediate stages of the calculation, is not fully in accordance with the rigorous result (1), even if one assumes interaction potentials such that the Born series for a converges fast. We are thus forced to conclude that the difference is due to the still uncontrolled "quadratic" approximation (68): Omitting the matrix elements which embody three or more non-zero momenta from the Hamiltonian gives rise to an error, even in the lowest order of the density, of the ground-state energy, amounting to the difference between a_0 and the full scattering length a.

The regularization-free technique for computing the ground-state energy of a Bose gas detailed in Sect. 3 sheds further light on this problem: As will be shown in a forthcoming paper, use of this technique allows one to systematically recover the higher-order terms of the Born series when taking into account the contributions to the Hamiltonian which are neglected in the usual Bogoliubov scheme [18].

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