Ground-state energy and depletions for a dilute binary Bose gas

André Eckardt, Christoph Weiss, and Martin Holthaus
Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany
(Dated: March 23, 2022)

When calculating the ground-state energy of a weakly interacting Bose gas with the help of the customary contact pseudopotential, one meets an artificial ultraviolet divergence which is caused by the incorrect treatment of the true interparticle interactions at small distances. We argue that this problem can be avoided by retaining the actual, momentum-dependent interaction matrix elements, and use this insight for computing both the ground-state energy and the depletions of a binary Bose gas mixture. Even when considering the experimentally relevant case of equal masses of both species, the resulting expressions are quite involved, and no straightforward generalizations of the known single-species formulas. On the other hand, we demonstrate in detail how these latter formulas are recovered from our two-species results in the limit of vanishing interspecies interaction.

PACS numbers: 03.75.Mn, 03.75.Hh, 05.30.Jp
Keywords: Bose-Einstein condensation (BEC), binary Bose gas, ground-state energy, depletion, Bogoliubov approximation

I. INTRODUCTION

Recently, the experimental investigation of multicomponent Bose–Einstein condensates has made substantial progress [1,2,3,4,5,6,7]. A considerable amount of theoretical work has been devoted to such systems, focusing, among others, on mean-field descriptions of trapped binary mixtures [8,9,10,11,12,13,14], stability properties and phase segregation [14,15,16,17], collective excitations [15,16,17], spiner condensates [18,19], and multicomponent condensates in optical lattices [20,21,22].

In this paper we determine the ground-state energy and the depletions for a homogeneous binary condensate within the Bogoliubov approximation [22]. The calculation of the ground-state energy beyond the mean-field approximation, and of the depletion, of a single-species condensate is a major achievement of the theory of weakly interacting Bose gases designed in the late fifties [23,24,25,26,27,28]. Recent significant developments include the first mathematically rigorous proof of the leading term of the commonly accepted expression for the ground-state energy per particle [29], the explicit calculation of nonuniversal contributions due to three-body scattering within the framework of effective field theory [30,31,32], and the clarification of the relation between the Gross–Pitaevskii and Bogoliubov descriptions of a dilute Bose gas [32]. One of the technical difficulties presented by the subject stems from the fact that typical atomic interaction potentials exhibit a strong increase at short distances, so that their Fourier transforms diverge for vanishing momentum transfer. Hence, one customarily replaces the true interaction potential by the contact pseudopotential

\[ U_p(r) = \frac{4\pi a^2 \hbar^2}{m} \delta(r) , \quad (1) \]

where \( m \) denotes the atomic mass, and \( a \) is the \( s \)-wave scattering length for collisions among the cold atoms. Thus, one relies on the knowledge that the low-temperature properties of dilute Bose gases are governed solely by the scattering lengths, an assertion commonly referred to as the “Landau postulate” [33]. Indeed, the leading terms of an expansion of the energy density for the ground state of a dilute homogeneous single-species gas of Bose particles interacting via some potential with scattering length \( a \) can be written as [32]

\[ \frac{E_0}{V} = \frac{2\pi a^2 \hbar^2}{m} n^2 \left[ 1 + \frac{128}{15\sqrt{\pi}} \sqrt{na^3} \right] , \quad (2) \]

first derived by Lee and Yang for the particular case of hard-sphere Bosons with diameter \( a \) [23,24]. Nonuniversal, i.e. potential-dependent contributions figure only as higher-order corrections, due to the effective range for \( s \)-wave scattering, and three-body interaction [30,31].

While the standard contact pseudopotential [1] is sufficient for determining the quasiparticle energy dispersion for a weakly interacting Bose gas, problems arise in the calculation of its ground-state energy. Namely, when coupling bare-particles states with opposite momenta \( \hbar k \) and \(-\hbar k\) for setting up the harmonic oscillator-like states corresponding to the phonon quasiparticles, one also has to account for the “vacuum” energies of these oscillators. The energy of the ground state of the weakly interacting gas, defined by the absence of phonons for all \( k \), then acquires a contribution from the sum over all these vacuum energies. However, if one naively uses the pseudopotential [1], all interaction matrix elements are replaced by a constant, instead of being properly suppressed at high momentum transfer, so that this sum becomes ultraviolet divergent. It is understood that this divergence is not a fundamental physical problem, but rather a consequence of the incorrect handling of the true interparticle interaction at short distances through the delta-function pseudopotential [1]. Actually, the proper pseudopotential op-
erator derived by Huang and Yang is given by
\[ U_p(r) = \frac{4\pi a\hbar^2}{m} \delta(r) \frac{\partial}{\partial r} r ; \] (3)
when operating on wave functions with a 1/r-type singularity, this operator yields results quite different from those given by its simplification \[ \text{Huang and Yang} \] \cite{34}. The modern solution to the problem is based on local effective field theory and renormalization theory, as reviewed recently in Ref. \[ \text{35} \].

A possible strategy for avoiding such complications has been suggested by Lifshitz and Pitaevskii \[ \text{36} \]: If one accepts the Landau postulate, one may replace the true, singular interparticle interaction potential by a smooth, well-behaved one, with the requirement that the substitute shares the same value of the scattering length \[ a \]. If then the result of the calculations, performed with the auxiliary potential, can be expressed entirely in terms of \[ a \], this result is the same as the one provided by the original interaction.

In the following sections, we exploit this idea for computing the ground-state energy and the depletions of a binary condensate mixture by considering soft, nonsingular interaction potentials. Contrary to standard textbook approaches \[ \text{36, 37} \], we do not replace the interaction matrix elements by constants, but keep track of their actual momentum dependence, so that the spurious ultraviolet divergence is avoided altogether. Only at the end of the calculation, we identify the various contributions to the ground-state energy of the binary gas with certain terms of the Born series for the three scattering lengths involved. This allows us to cast our results into the desired form, enabling a comparison with the known single-species results. Thus, we do neither invoke the pseudopotential nor its refined form, but work directly with nonsingular interaction potentials.

We proceed as follows: In Sec. II the quadratic low-temperature approximation to the full Hamiltonian of the binary gas is obtained by adapting the reasoning customarily applied in the single-species case. In Sec. III this approximate Hamiltonian is then diagonalized exactly, relying on a method used by Hopfield in 1958 when studying the interaction of the radiation field with a polarization field \[ \text{38} \]. In this way, we necessarily recover the already known results for the quasiparticle excitation spectra \[ \text{8, 13} \], but we also identify an energy shift associated, for each wavevector \( \mathbf{k} \), with the transformation to the quasiparticle form of the Hamiltonian. In order to obtain the ground-state energy of the system, the sum over all these shifts has to be evaluated; this is achieved in Sec. IV with the help of a density expansion which yields only finite quantities at each intermediate step of the calculation \[ \text{34} \]. The depletions for a binary condensate are determined by the coefficients of the quasiparticle transformation, and calculated at the end of Sec. IV. In Sec. V we briefly discuss our main findings.

II. THE HAMILTONIAN IN QUADRATIC APPROXIMATION

The Hamiltonian of a homogeneous gas consisting of a mixture of \( N_i \) Bose particles of species labeled by \( i \) (with \( i = 1, 2, \ldots \)) in a cubic volume \( V \) reads
\[ H = \sum_i \int_V d\mathbf{r} \Psi_i^\dagger(\mathbf{r})h_i(\mathbf{r})\Psi_i(\mathbf{r}) \]
\[ + \frac{1}{2} \sum_{ij} \int_V d\mathbf{r}_1 d\mathbf{r}_2 \Psi_i^\dagger(\mathbf{r}_1)\Psi_j^\dagger(\mathbf{r}_2) \times U_{ij}(\mathbf{r}_1 - \mathbf{r}_2)\Psi_j(\mathbf{r}_2)\Psi_i(\mathbf{r}_1) , \] (4)
where \( U_{ij}(\mathbf{r}) = U_{ji}(\mathbf{r}) \) denotes the real, isotropic interaction potential between particles of the type \( i \) and those of type \( j \). We assume that the intraspecies potentials \( U_{ii}(\mathbf{r}) \) are repulsive; none of the potentials should admit any many-body bound state. The single-particle Hamiltonian \( h_i(\mathbf{r}) \) is given by the kinetic energy operator for free particles of mass \( m_i \), \( h_i(\mathbf{r}) = -(\hbar^2/2m_i)\Delta_r \). The thermodynamic limit will be taken at a later stage, \( N_i \rightarrow \infty \) and \( V \rightarrow \infty \) such that the density \( n_i = N_i/V \) of each species remains constant. The \( \Psi_i(\mathbf{r}) \) are the usual Bose field operators, obeying the commutation relations
\[ [\Psi_i(\mathbf{r}), \Psi_j^\dagger(\mathbf{r}')] = \delta_{ij} \delta(\mathbf{r} - \mathbf{r}') , \]
\[ [\Psi_i(\mathbf{r}), \Psi_j(\mathbf{r}')] = [\Psi_i^\dagger(\mathbf{r}), \Psi_j^\dagger(\mathbf{r}')] = 0 . \] (5)

Imposing periodic boundary conditions, the single-particle eigenfunctions of \( h_i(\mathbf{r}) \) are given by plane waves, \( \varphi_k(\mathbf{r}) = V^{-1/2} \exp(ik\mathbf{r}) \), labeled by wavevectors \( \mathbf{k} = 2\pi V^{-1/3} \mathbf{n} \), where \( \mathbf{n} \) is a vector with integer components. The field operators then are expanded in this basis,
\[ \Psi_i(\mathbf{r}) = \sum_k a_{i\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{r}). \] (6)
The coefficients \( a_{i\mathbf{k}} \) and their adjoints \( a_{i\mathbf{k}}^\dagger \) are the familiar Bose annihilation and creation operators for particles of species \( i \) in the single-particle state \( \mathbf{k} \). As a consequence of Eq. (5), they satisfy the commutation relations
\[ [a_{i\mathbf{k}}, a_{j\mathbf{k}'}^\dagger] = \delta_{ij} \delta_{\mathbf{kk}'} , \]
\[ [a_{i\mathbf{k}}, a_{j\mathbf{k}'}] = [a_{i\mathbf{k}}^\dagger, a_{j\mathbf{k}'}^\dagger] = 0 . \] (7)

Introducing the Fourier transforms of the interaction potentials,
\[ u_{ij}(\mathbf{q}) \equiv \int_V d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} U_{ij}(\mathbf{r}) , \] (8)
and inserting the expansion \[ \text{(6)} \] into the Hamiltonian \[ \text{(4)} \], one obtains
\[ H = \sum_i \sum_k \frac{\hbar^2 k^2}{2m_i} a_{i\mathbf{k}}^\dagger a_{i\mathbf{k}} + \sum_{i,j} u_{ij}(\mathbf{k}_1 - \mathbf{k}_1') a_{i\mathbf{k}_1}^\dagger a_{j\mathbf{k}_2}^\dagger a_{i\mathbf{k}_1'} a_{j\mathbf{k}_2'} , \] (9)
where the prime at the summation sign indicates restriction to those terms which comply with momentum conservation, $k_1 + k_2 = k'_1 + k'_2$. Note that $u_{ij}(q)$ carries the dimension of energy times volume; moreover, we have $u_{ij}(-q) = u_{ij}(q)$.

For interaction potentials with a strong short-range singularity, such as Lennard-Jones or hard-sphere potentials, the Fourier components diverge for $q \to 0$; this divergence can be seen as a consequence of the use of a single-particle basis $\varphi_k(r)$. Therefore, keeping in mind the remarks made in the introduction, we perform the following analysis with “soft” interactions for which the Fourier transforms remain finite, while stipulating that their scattering lengths be the same as those of typical atomic potentials.

Under the assumption that there exists a condensate for each particle species, such that the single-particle ground state is occupied by macroscopically large numbers of particles of both types, we employ the conventional quadratic approximation for the description of the low-energy dynamics. Firstly, the interaction terms of the Hamiltonian are categorized with respect to the number of ground-state operators $a_{i0}$ or $a_{i0}^\dagger$ they contain. The relevant matrix elements of these operators should be roughly on the order of $N_i^{1/2}$, and thus large compared to the corresponding matrix elements of the operators $a_{i1}$ or $a_{i1}^\dagger$ referring to excited states, and to sums over such elements. However, it will become obvious in the following that this handwaving reasoning requires some caution. Secondly, the “off-diagonal” operators $a_{i0}$ and $a_{i0}^\dagger$ are replaced by the square roots $N_i^{1/2}$ of the single-particle ground-state occupation numbers. This is acceptable as long as the probability distributions for finding $N_{i0}$ particles in the ground state are broad compared to 1, so that shifts by one particle do not essentially change the many-particle ground state. Neglecting supposedly small contributions to the Hamiltonian with three or more nonzero wavenumber indices, note that this handwaving reasoning again neglecting terms which are considered as small within the above categorization scheme, this leads to the cancelation of contributions with zero momentum transfer:

$$\sum_{\{k\}}' u_{ij}(k_1 - k'_1) a_{i1}^\dagger a_{j1}^\dagger a_{j2} a_{j2}^\dagger a_{i1} a_{i1}^\dagger N_{i0} N_{j0}$$

$$\simeq u_{ij}(0) N_{i0} N_{j0} + \sum_{k \neq 0} \left[ u_{ij}(k) a_{i1}^\dagger a_{j1}\right] a_{j2} a_{j2}^\dagger a_{i1} a_{i1}^\dagger N_{i0} N_{j0}$$

$$+ u_{ij}(k) a_{i1}^\dagger a_{j2} a_{j2}^\dagger a_{i1} a_{i1}^\dagger N_{i0} N_{j0}$$

$$+ u_{ij}(k) a_{i1}^\dagger a_{j1} a_{j1}^\dagger N_{i0} N_{j0}$$

$$+ u_{ij}(0) a_{i1}^\dagger a_{j1} a_{j1}^\dagger N_{i0} N_{j0}$$

$$+ u_{ij}(0) a_{i1}^\dagger a_{j2} a_{j2}^\dagger N_{i0} N_{j0}$$

$$+ u_{ij}(0) a_{i1}^\dagger a_{j2} a_{j2}^\dagger N_{i0} N_{j0}$$

$$\simeq u_{ij}(0) N_{i0} N_{j0} + \sum_{k \neq 0} u_{ij}(k) \sqrt{N_{i0} N_{j0}}$$

$$\times \left[ a_{i1}^\dagger a_{j1}^\dagger a_{j2} a_{j2}^\dagger a_{i1} a_{i1}^\dagger a_{i1} a_{i1}^\dagger \right] + \sum_{k \neq 0} u_{ij}(k) \sqrt{N_{i0} N_{j0}}$$

Restricting ourselves from here on to only two particle species 1 and 2, within the quadratic approximation the low-energy Hamiltonian takes the form:

$$H_{QA} = H_k + N_k + N_{k-}$$

where the superscript $2\pi$ at the summation sign is meant to indicate restriction of the sum to one $k$-halfspace, and

$$H_k = \sum_{i=1}^{2} \left[ B_{i,k} \left( a_{i1}^\dagger a_{i1}^\dagger a_{i2} - a_{i2} a_{i2}^\dagger a_{i1} a_{i1}^\dagger \right) + C_{i,k} \left( a_{i1}^\dagger a_{i2}^\dagger a_{i2} - a_{i2} a_{i1}^\dagger a_{i1} a_{i2}^\dagger \right) \right] + \sum_{i=1}^{2} D_{i,k} \left( a_{i1}^\dagger a_{i2} a_{i2} - a_{i2} a_{i1} a_{i2}^\dagger + a_{i1}^\dagger a_{i2} a_{i2}^\dagger \right)$$

$$+ ( k \rightarrow -k )$$

The symbol $(k \rightarrow -k)$ denotes contributions of the same kind as appearing in the first two lines of this definition, with $k$ replaced by $-k$. Moreover, we have introduced the abbreviations

$$A_0 = \frac{1}{2} v_{11}(0) N_1 + \frac{1}{2} v_{22}(0) N_2$$

$$+ \frac{1}{2} v_{12}(0) \sqrt{N_1 N_2}$$

$$B_{i,k} = B_{i,-k} = \frac{1}{2} v_{ii}(k)$$

$$C_{i,k} = C_{i,-k} = t_{i}(k) + v_{ii}(k)$$

$$D_{i,k} = D_{i,-k} = v_{12}(k)$$

with

$$t_{i}(k) = \frac{\hbar^2 \vec{k}^2}{2m_i}$$

$$v_{ij}(k) = \sqrt{m_i m_j} u_{ij}(k)$$

which will be used extensively in the following. Thus, within the quadratic approximation the Hamiltonian of the Bose gas mixture is given by a sum of commuting parts $H_k$, quadratic in the $a$-operators, which can be diagonalized separately; the interactions couple particles of both types with momenta $\hbar \vec{k}$ and $-\hbar \vec{k}$.

### III. Quasiparticle Form of the Hamiltonian

In order to convert $H_k$ into a form which corresponds to noninteracting quasiparticles, we consider excitations...
characterized by a wavevector $k \neq 0$. Such excitations are described by linear combinations of annihilation operators for particles with momentum $\hbar k$ and creation operators for particles with reverse momentum $-\hbar k$, 

$$
\tilde{b}_{i,k} = u_{i,k}a_{1_k} + v_{i,k}a_{1_{-k}} + \mu_{i,k}a_{2_k} + v_{i,k}a_{2_{-k}},
$$

(16)

so that $u_{i,k}$ and $v_{i,k}$ quantify the contributions of species 1 to the $i$th quasiparticle excitation, and $\mu_{i,k}$ and $v_{i,k}$ those of species 2. As a consequence of the symmetry of the eigenvalue problem (18), we also have $u_{i,k} = v_{i,-k}$, etc. We then require the commutation relations 

$$
\left[\tilde{b}_{i,k}, H_k\right] = \varepsilon_i(k)\tilde{b}_{i,k},
$$

(17)

in analogy to the relation fulfilled by the Hamiltonian and the annihilation operator of the simple harmonic oscillator. Inserting the ansatz (14) and the expression (13) for $H_k$ into these relations, utilizing the symmetry of the coefficients under interchange of $k$ and $-k$, and comparing coefficients of identical operators, leads us to the eigenvalue problem 

$$
Q_kv_i = \varepsilon_i(k)v_i,
$$

(18)

where the $4 \times 4$ matrix $Q_k$ is given by

$$
Q_k = \begin{pmatrix}
C_{1,k} & -2B_{1,k} & D_k & -D_k \\
2B_{1,k} & -C_{1,k} & -D_k & D_k \\
D_k & -D_k & C_{2,k} & -2B_{2,k} \\
D_k & -D_k & 2B_{2,k} & -C_{2,k}
\end{pmatrix},
$$

(19)

and

$$
v_i = (u_{i,k} \ v_{i,k} \ \mu_{i,k} \ \nu_{i,k})^T.
$$

(20)

Since $Q_k$ is not hermitian, the eigenvalues $\varepsilon_i(k)$ are not necessarily real. For continuing the analysis, we first assume that only real eigenvalues occur, so that also the components of the eigenvectors $v_i$ can be chosen as real numbers, and will state the physical condition for the reality of the eigenvalues later (cf. Eqs. (56) and (57)).

The specific structure of $Q_k$ can be exploited with the help of the matrix

$$
h = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0
\end{pmatrix}.
$$

(21)

Since $h^2 = 1$, and $hQ_kh = -Q_k$, multiplying the eigenvalue problem (18) from the left by $h$ leads to

$$
Q_khv_i = -\varepsilon_i(k)hv_i.
$$

(22)

Hence, if $v_k = (u_k \ v_k \ \mu_k \ \nu_k)^T$ is an eigenvector with eigenvalue $+\varepsilon(k)$, then $hv_k = (v_k \ u_k \ \nu_k \ \mu_k)^T$ is an eigenvector with eigenvalue $-\varepsilon(k)$. Therefore, the eigenvalues occur in pairs of opposite sign: We may fix the indices such that

$$
\varepsilon_1(k) = -\varepsilon_1(k),
$$

(23)

while stipulating that $\varepsilon_1(k)$ and $\varepsilon_2(k)$ be positive.

Introducing the further matrix

$$
g \equiv \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & -1
\end{pmatrix},
$$

(24)

which obeys $g = g^t = g^{-1}$, it is easy to see that $gQ_k$ is hermitian. Hence, two eigenvectors belonging to different eigenvalues of the problem (18) are orthogonal with respect to the bilinear form mediated by $g$:

$$
[\tilde{b}_i, \tilde{b}_j] = v_i^g v_{j,k} = 0 \quad \text{for } i \neq j,
$$

(25)

where the first equality is an immediate consequence of the definitions (14) and the commutation relations (17) obeyed by the bare particle operators. In addition, some lines of elementary algebra reveal that the eigenvalues $\varepsilon_i(k)$ of the matrix $Q_k$ are real — which we do assume here — if and only if the matrix $gQ_k$ is positive semidefinite. Hence, we also have

$$
\varepsilon_i(k) v_i^g v_{j,k} = v_i^g Q_k v_{j,k} \geq 0.
$$

(26)

Therefore, normalizing the eigenvectors $v_i$ such that $|v_i^g v_{j,k}| = 1$ (note that it is not possible to change the sign of $v_i^g v_{j,k}$ by normalization), we thus find that the sign of $v_i^g v_{j,k}$ is fixed by the sign of the corresponding eigenvalue:

$$
[\tilde{b}_i, \tilde{b}_j] = v_i^g v_{j,k} = \text{sign}(\varepsilon_i(k)) \delta_{ij}.
$$

(27)

Multiplying the basic commutation relation (17) from the left by $\tilde{b}_i^k$, then multiplying its adjoint relation from the right by $\tilde{b}_j^k$, and subtracting, immediately gives

$$
[\tilde{b}_i^k, \tilde{b}_j^k, H_k] = 0,
$$

(28)

again relying on the proposition that $\varepsilon_i(k)$ be real. Since $H_k$ depends quadratically on creation and annihilation operators for the bare particles, and the transformation (16) is linear, this operator therefore has to have the form

$$
H_k = \sum_{i=1}^{4} f_{i,k} \tilde{b}_i^k \tilde{b}_i^k + g_k
$$

(29)

when expressed in terms of $\tilde{b}$-operators, where $f_{i,k}$ and $g_k$ are real numbers. Once again invoking the relation (17) then yields the identities

$$
f_{i,k} [\tilde{b}_i^k, \tilde{b}_j^k] \tilde{b}_i^k = \varepsilon_i(k) \tilde{b}_i^k,
$$

(30)
which, in the light of the commutators \( \{ \), allows us to identify \( f_{i,k} \) with the absolute value of \( \varepsilon_i(k) \):

\[
H_k = \sum_{i=1}^{4} |\varepsilon_i(k)| \tilde{b}_{i,k}^\dagger \tilde{b}_{i,k} + g_k .
\]  \( \tag{31} \)

In order to exploit these algebraic deliberations for the construction of proper quasiparticle annihilation and creation operators \( \tilde{b}_{i,k} \) and \( \tilde{b}_{i,k}^\dagger \) pertaining to the two-species Bose gas, we now have to make sure that these latter operators satisfy the Bose commutation relations

\[
[\tilde{b}_{i,k}, \tilde{b}_{j,k'}^\dagger] = \delta_{i,j} \delta_{k,k'} ,
\]

\[
[\tilde{b}_{i,k}, \tilde{b}_{j,k'}] = [\tilde{b}_{i,k}^\dagger, \tilde{b}_{j,k'}^\dagger] = 0 .
\]  \( \tag{32} \)

In view of the orthonormality-type relations (27), this is easy to achieve: The two eigenvectors \( v_{1,k} \) and \( v_{2,k} \) associated with positive eigenvalues \( \varepsilon_1(k) \) and \( \varepsilon_2(k) \) already provide a commutator with the required magnitude and sign, and therefore directly give rise, by means of Eq. (16), to quasiparticle annihilation operators,

\[
\tilde{b}_{i,k} = v_{i,k} \quad \text{for } i = 1, 2 ;
\]  \( \tag{33} \)

we also write

\[
\varepsilon_i(k) = \varepsilon_i(-k) \quad \text{for } i = 1, 2 .
\]  \( \tag{34} \)

Next, inspecting \( i = j = 3 \) and \( i = j = 4 \), the other two eigenvectors \( v_{3,k} \) and \( v_{4,k} \) produce a negative sign on the r.h.s. of Eq. (27). Therefore, these eigenvectors are associated with quasiparticle creation operators; evidently, we have

\[
\tilde{b}_{3,k} = b_{1,-k}^\dagger , \quad \tilde{b}_{4,k} = b_{2,-k}^\dagger
\]  \( \tag{35} \)

with positive quasiparticle energies

\[
|\varepsilon_3(k)| = \varepsilon_1(k) , \quad |\varepsilon_4(k)| = \varepsilon_2(k) .
\]  \( \tag{36} \)

Note that \( \varepsilon_i(k) = \varepsilon_i(-k) \) for \( i = 1, 2 \), as a consequence of the symmetry of the coefficients (14). Finally, relabeling the operators in Eq. (31) according to these prescriptions, rearranging, and combining all emerging \( c \)-numbers into energy shifts \( \alpha(k) \), allows us to cast the operators \( H_k \) into the standard forms

\[
H_k = \alpha(k) + \varepsilon_1(k) b_{1,k}^\dagger b_{1,k} + \varepsilon_2(k) b_{2,k}^\dagger b_{2,k} + (k \rightarrow -k) .
\]  \( \tag{37} \)

In this way, the above construction directly leads to the desired oscillator Hamiltonian for noninteracting quasiparticles, provided we restrict ourselves to conditions such that the eigenvalues of the problem (15) are real (or, equivalently, those of the matrix \( gQ_k \) are non-negative), and we select the two positive eigenvalues \( \varepsilon_1(k) \) and \( \varepsilon_2(k) \): Although the eigenvalues of the problem (15) occur with both signs, negative quasiparticle energies are strictly excluded by the algebra.

Of particular significance for our purposes are the constants \( \alpha(k) \) occurring in the quasiparticle Hamiltonians \( H_k \): For each \( k \), transformation of the original operator (13) to the normal form (37) necessarily involves such an energy shift. Since the ground state of the gas mixture is characterized by the absence of all quasiparticle excitations, the ground-state energy \( E_0 \) is then given by the sum over all these shifts, plus the constant \( A_0 \) already appearing in the quadratic approximation (12),

\[
E_0 = A_0 + \sum_{k \neq 0} \alpha(k) ,
\]  \( \tag{38} \)

with \( A_0 \) as stated in Eq. (14a). In order to determine the individual shifts \( \alpha(k) \), we substitute in Eq. (37) the original \( a \)-operators for the \( b \)-operators. Comparison with Eq. (13) then yields

\[
\alpha(k) = -\varepsilon_1(k) (v_{1,k}^2 + \varepsilon_2(k)) (v_{2,k}^2 + \varepsilon_2(k)) ,
\]  \( \tag{39} \)

Together with

\[
C_{1,k} = \varepsilon_1(k) (u_{1,k}^2 + \varepsilon_2(k)) (u_{2,k}^2 + \varepsilon_2(k)) , \quad C_{2,k} = \varepsilon_1(k) (\mu_{1,k}^2 + \varepsilon_2(k)) (\mu_{2,k}^2 + \varepsilon_2(k)) \]  \( \tag{40} \)

Finally, utilizing Eqs. (27) in the form \( u_{i,k}^2 - v_{i,k}^2 = \mu_{i,k}^2 \) and \( \mu_{i,k}^2 = \varepsilon_2(k) = 1 \), we obtain the desired relation

\[
\alpha(k) = \frac{1}{2} (\varepsilon_1(k) + \varepsilon_2(k) - C_{1,k} - C_{2,k})
\]

\[
= \frac{1}{2} (\varepsilon_1 + \varepsilon_2 - t_1 - v_{11} - t_2 - v_{22}) .
\]  \( \tag{41} \)

The expression on the right-hand side does no longer contain the transformation coefficients. Thus, for computing the ground-state energy according to Eq. (38), the knowledge of these coefficients is not required.

Before computing the depletions of the single-particle ground state, we have to invert the previous ansatz (16), and to express the bare \( a \)-operators through the quasiparticle \( b \)-operators. Writing

\[
b_k \equiv \begin{pmatrix} b_{1,k} \\ b_{1,-k}^\dagger \\ b_{2,k} \\ b_{2,-k}^\dagger \end{pmatrix} , \quad a_k \equiv \begin{pmatrix} a_{1,k} \\ a_{1,-k}^\dagger \\ a_{2,k} \\ a_{2,-k}^\dagger \end{pmatrix} ,
\]  \( \tag{42} \)

the result of the above construction takes the form

\[
b_k = V_k a_k ,
\]  \( \tag{43} \)

with the transformation matrix

\[
V_k \equiv \begin{pmatrix} u_{1,k} & v_{1,k} & \mu_{1,k} & \nu_{1,k} \\ v_{1,k}^\dagger & u_{1,k}^\dagger & \mu_{1,k}^\dagger & \nu_{1,k}^\dagger \\ u_{2,k} & v_{2,k} & \mu_{2,k} & \nu_{2,k} \\ v_{2,k}^\dagger & u_{2,k}^\dagger & \mu_{2,k}^\dagger & \nu_{2,k}^\dagger \end{pmatrix} .
\]  \( \tag{44} \)

The commutation relations (27) are then written as

\[
V_k g V_k^\dagger = g ,
\]  \( \tag{45} \)
which implies $V_k g V_k^1 g = 1$, or
\[
V_k^{-1} = g V_k^1 g = \begin{pmatrix}
\varepsilon_{11} & -\varepsilon_{12} & \varepsilon_{12} & -\varepsilon_{22} \\
-\varepsilon_{11} & \varepsilon_{12} & -\varepsilon_{22} & \varepsilon_{22} \\
\mu_{11} & -\mu_{12} & -\mu_{22} & \mu_{22} \\
-\mu_{11} & \mu_{12} & -\mu_{22} & \mu_{22}
\end{pmatrix}.
\]

This inverse transformation now allows us to state a convenient expression for the depletions: Since the many-particle ground state $|gs\rangle$ of the two-species gas is the quasiparticle vacuum,
\[
b_{1k}|gs\rangle = 0 \quad \text{for } k \neq 0,
\]
the occupation numbers $N_{1k}$ of the single-particle state with wavevector $k$ for the real particles of species $i$, when the system is in its ground state, are given by
\[
\langle N_{1k} \rangle = \langle gs|a_{1k}^\dagger a_{1k}|gs\rangle = (u_{1k} b_{1k}^\dagger - v_{1k} b_{1k} - u_{2k} b_{2k}^\dagger - v_{2k} b_{2k})
\]
\[
\times (u_{1k} b_{1k}^\dagger - v_{1k} b_{1k} - u_{2k} b_{2k}^\dagger - v_{2k} b_{2k})|gs\rangle
\]
\[
= \varepsilon_{11}^2 |k|^2 + \varepsilon_{22}^2 |k|^2,
\]
\[
\langle N_{2k} \rangle = \langle gs|v_{1k} a_{1k} |gs\rangle = (u_{1k} b_{1k}^\dagger - v_{1k} b_{1k} - u_{2k} b_{2k}^\dagger - v_{2k} b_{2k})
\]
\[
\times (u_{1k} b_{1k}^\dagger - v_{1k} b_{1k} - u_{2k} b_{2k}^\dagger - v_{2k} b_{2k})|gs\rangle
\]
\[
= \varepsilon_{11}^2 |k|^2 + \varepsilon_{22}^2 |k|^2.
\]

Therefore, the depletions are obtained from the sums
\[
N_1 - N_{10} = \sum_{k \neq 0} (\varepsilon_{11}^2 |k|^2 + \varepsilon_{22}^2 |k|^2),
\]
\[
N_2 - N_{20} = \sum_{k \neq 0} (\varepsilon_{11}^2 |k|^2 + \varepsilon_{22}^2 |k|^2),
\]
which will be evaluated in the following section. Contrary to the energy shifts \[13\] the depletions do depend explicitly on the transformation coefficients.

The solution of the eigenvalue problem \[13\] is elementary: Straightforward algebra leads to the eigenvalues
\[
\varepsilon_{11}^2(k) = \frac{1}{2} \left[ \varepsilon_{11}^2(k) + \varepsilon_{22}^2(k) \right]
\]
\[
\pm \sqrt{\left(\varepsilon_{11}^2(k) - \varepsilon_{22}^2(k)\right)^2 + 16t_2(k)t_{12}(k)v_{12}^2(k)},
\]
where here and in the following we write $\varepsilon_{\pm}(k)$ for the larger of the two eigenvalues $\varepsilon_1(k)$ and $\varepsilon_2(k)$, and $\varepsilon_{-}(k)$ for the smaller; moreover, $\varepsilon_{\sigma}(k)$ denotes the familiar quasiparticle energies of a single-species Bose gas,
\[
\varepsilon_{\sigma}^2(k) = t_\sigma(k) |t_\sigma(k) + 2v_\sigma(k)|.
\]

As anticipated, with each eigenvalue of the problem \[13\] also its negative appears; however, we only have to consider the positive ones. This spectrum \[30\] has already been obtained through different reasoning in Refs. \[3\] \[13\]. In the limit of vanishing interaction between the two species, $v_{12}(k) = 0$, one sees that $\varepsilon_{+}(k)$ and $\varepsilon_{-}(k)$ become equal to the larger and the smaller of the single-species eigenvalues $\varepsilon_{11}(k)$ and $\varepsilon_{22}(k)$, respectively. Thus, without interspecies interaction the single-species solutions are recovered. “Switching on” $v_{12}(k)$ makes the upper and lower spectral branch repel each other: If the single-species spectra cross for some finite $k_0 \neq 0$, so that $\varepsilon_{\pm}(k_0) = \varepsilon_{\sigma}(k_0) \equiv \varepsilon_0$, one finds $\varepsilon_{\pm}(k_0) = \varepsilon_0^2 \pm 2|t_1(k_0)t_{22}(k_0)v_{12}^2(k_0)|^{1/2}$, so that the crossing of $\varepsilon_+(k)$ and $\varepsilon_-(k)$ is avoided as a consequence of the interspecies interaction.

For $k \to 0$, both spectral branches become phononlike, i.e. proportional to $\hbar |k| \varepsilon_\pm(k)$
\[
\varepsilon_{\pm}^2(k) \to c_{\pm}^2 \hbar^2 k^2,
\]
with sound velocities $c_{+}$ and $c_{-}$ given by
\[
c_{\pm}^2 = \frac{1}{2} \left[ c_{11}^2 + c_{22}^2 \pm \sqrt{(c_{11}^2 - c_{22}^2)^2 + 4c_{12}^4} \right].
\]

Here,
\[
c_{\sigma}^2 = \frac{v_{\sigma}(0)}{m_\sigma} = \frac{u_{\sigma}(0)n_\sigma}{m_\sigma}
\]
denote the squares of the well-known sound velocities for the single-species gases; in addition, we have introduced
\[
c_{12}^2 = \frac{v_{12}(0)}{m_1 m_2} = \frac{v_{12}(0)n_1 n_2}{m_1 m_2}.
\]

It is remarkable that the sign of $U_{12}(r)$, and thus the answer to the question whether the interspecies interaction is attractive or repulsive, does not enter into the spectrum \[30\]. In contrast, the intraspecies interaction has to be repulsive in order to guarantee the existence of a homogeneous single-species condensate.

While the existence of a homogeneous binary condensate requires that both $\varepsilon_{+}(k)$ and $\varepsilon_{-}(k)$ be real, the smaller eigenvalue $\varepsilon_{-}(k)$ actually is real only as long as the interspecies interaction is sufficiently weak, that is, under the condition that both
\[
\varepsilon_{\sigma}(k) > 0, \quad \varepsilon_{\sigma}(k) > 0
\]
and
\[
4v_{12}^2(k) < [t_1(k) + 2v_{11}(k)][t_2(k) + 2v_{22}(k)]
\]
be satisfied. Otherwise, our stationary approach does not have a physically meaningful solution. The formal appearance of complex eigenvalues is related to an instability leading to phase segregation: When $\varepsilon_{-}(k)$ touches the $|k|$-axis at some $k_0$, the corresponding mode can grow without cost of energy; the slightest excitation then makes the system collapse into inhomogeneous structures. The condition \[57\] implies that it is not possible to stabilize an unstable single-species condensate by adding particles of another species. Since the kinetic energy contributions $t_\sigma(k)$ grow like $k^2$, while the potential contributions vanish for large $|k|$, the stability condition \[57\] is most likely to be violated for small momenta, or large.
wavelength-excitations. Invoking the lowest-order Born approximations
\[ a_{ij}^{(0)} = \frac{m_{ij}}{2\pi\hbar^2} u_{ij}(0) \]  
(58)
to the s-wave scattering lengths \( a_{ij} \) for scattering events between particles of species \( i \) and \( j \), where
\[ m_{ij} \equiv m_i m_j/(m_i + m_j) \]  
(59)
denotes the respective reduced mass, this stability condition \( \| \) reduces for \( k \to 0 \) to
\[ \left( \frac{a_{12}^{(0)}}{a_{12}} \right)^2 < \frac{a_{11}^{(0)} a_{22}^{(0)}}{m_{11} m_{22}} . \]  
(60)
This inequality parallels the one known from mean-field studies of binary condensates \[ \text{[11 12].} \]
The transformation coefficients determining the quasiparticle operators \( b_{-\mathbf{k}} \) and \( b_{\mathbf{k}} \) follow from
\[ u_{\pm}^2 = (\varepsilon_\pm + t_2)^2 \left( \varepsilon_\pm^2 - \varepsilon_{\pm}^2 \right) t_2 x^2_\pm , \]
\[ v_{\pm}^2 = (\varepsilon_\pm - t_2)^2 \left( \varepsilon_\pm^2 - \varepsilon_{\pm}^2 \right) t_2 x^2_\pm , \]
\[ \mu_{\pm}^2 = (\varepsilon_\pm + t_2)^2 \left( \varepsilon_\pm + \varepsilon_{\pm} \right) t_1 x^2_\pm , \]
\[ \nu_{\pm}^2 = (\varepsilon_\pm - t_2)^2 \left( \varepsilon_\pm - \varepsilon_{\pm} \right) t_1 x^2_\pm , \]  
(61)
where we have omitted the index \( \mathbf{k} \) for clarity, and the normalization factors \( x_+ \) and \( x_- \) are given by
\[ 1 \over x^2_\pm = 4t_1 t_2 \varepsilon_\pm \left( 2 \varepsilon_\pm^2 - \varepsilon_{\pm}^2 \right) , \]  
(62)
so that the proper commutation relations \([b_\pm, b_{\mp}^\dagger]\) = 1 are satisfied. The explicit knowledge of the coefficients \( v_{\pm} \) and \( \nu_{\pm} \) will be required in the following section for evaluating the depletions according to Eqs. \( \text{[67]} \).

**IV. GROUND-STATE ENERGY AND DEPLETION**

From the definition \( \text{[68]} \) and the Born approximations \( \text{[58]} \), we infer that the first contribution to the ground-state energy \( \text{[68]} \) can be written as
\[ A_0 = 2\pi\hbar^2 \left[ \frac{a_{11}^{(0)} n_1}{2 m_{11}} N_1 + \frac{a_{22}^{(0)} n_2}{2 m_{22}} N_2 \right. \]
\[ \left. + \frac{a_{12}^{(0)} \sqrt{n_1 n_2}}{m_{12}} \sqrt{N_1 N_2} \right] . \]  
(63)
As already emphasized, when performing the transformation from the Hamiltonian \( \text{[63]} \) to the quasiparticle form \( \text{[58]} \), each wavevector \( \mathbf{k} \) furnishes the additional contribution \( \text{[61]} \), namely,
\[ \alpha(\mathbf{k}) = \left. \frac{\varepsilon_k(\mathbf{k}) + \varepsilon_{-\mathbf{k}}(\mathbf{k})}{2} \right|_{\mathbf{k}=0} - \sum_{i=1}^2 \left[ t_i(\mathbf{k}) + v_i(\mathbf{k}) \right] . \]  
(64)
The evaluation of the sum over these shifts \( \alpha(\mathbf{k}) \) is notoriously difficult even in the case of a single-species condensate. If one replaces the \( k \)-dependent interaction matrix elements by a constant, the sum becomes ultraviolet divergent and requires careful regularization \( \text{[40]} \); in the context of the pseudopotential method, this regularization is achieved by the derivative operator appearing in the proper pseudopotential \( \text{[33]} \). In standard textbook treatments some delicate technical details of this procedure are tacitly swept under the carpet through the identification of the full scattering length with only its first Born approximation \( \text{[36 37]} \). However, the artificial divergence, and the subsequent need for regularization, can be avoided altogether if the actual \( k \)-dependence of the interaction matrix elements is kept. Here we follow an approach recently developed in Ref. \( \text{[34]} \), and employ a density expansion for computing the sum in the low-density limit: Starting from Eq. \( \text{[61]} \) with the abbreviations \( \text{[105]} \), somewhat tedious but straightforward calculations yield
\[ \sum_{k \neq 0} \frac{\partial \alpha(\mathbf{k})}{\partial n_i} \bigg|_{n_{1,2}=0} = 0 , \]  
(65)
\[ \sum_{k \neq 0} \frac{\partial^2 \alpha(\mathbf{k})}{\partial n_i \partial n_j} \bigg|_{n_{1,2}=0} = - \frac{1}{2} \sum_{k \neq 0} \frac{u_{ij}(\mathbf{k})}{\hbar^2 k^2/4m_{ij}} . \]  
(66)
Now we observe that the next-to-leading term \( a_{ij}^{(1)} \) of the Born series
\[ a_{ij} = a_{ij}^{(0)} + a_{ij}^{(1)} + \ldots \]  
(68)
for the various s-wave scattering lengths is given, in the limit of large volume \( V \), by \( \text{[32 34]} \)
\[ a_{ij}^{(1)} = - \left( \frac{m_{ij}}{2\pi\hbar^2} \right)^2 \frac{4\pi}{V} \sum_{k \neq 0} \frac{u_{ij}^2(\mathbf{k})}{k^2} , \]  
(69)
which implies
\[ \sum_{k \neq 0} \frac{\partial^2 \alpha(\mathbf{k})}{\partial n_i \partial n_j} \bigg|_{n_{1,2}=0} = \frac{2\pi\hbar^2}{m_{ij}} a_{ij}^{(1)} V . \]  
(70)
Therefore, to second order in the densities the sum over the energy shifts is given by
\[ \sum_{k \neq 0} \alpha(\mathbf{k}) \approx 2\pi\hbar^2 \left[ \frac{a_{11}^{(1)} n_1}{2 m_{11}} N_1 + \frac{a_{22}^{(1)} n_2}{2 m_{22}} N_2 \right. \]
\[ \left. + \frac{a_{12}^{(1)} \sqrt{n_1 n_2}}{m_{12}} \sqrt{N_1 N_2} \right] . \]  
(71)
Adding Eqs. \( \text{[63]} \) and \( \text{[71]} \), we thus find the approximate energy density for the ground state of the binary conden-
At this point, a major weakness of the quadratic approximation employed for the reduction of the original Hamiltonian becomes apparent: Although the contribution arises from the interaction term with all four wavevector-indices equal to the condensate index, and the contribution stems from terms supposed to be “quadratically small”, they are of the same order in the densities. The intuitive categorization of the interaction terms in the original Hamiltonian with respect to the number of ground-state operators they contain thus does not reflect a systematic ordering. The “quadratic” contributions to the Hamiltonian are small compared to the leading one.\( A_0 \) only if the Born series for the scattering lengths converge rapidly, so that

\[
|a_{ij}^{(1)}| \ll |a_{ij}^{(0)}|,
\]

implying that the first terms already provide good approximations to the full scattering lengths \( a_{ij} \).

If one accepts the approximation, one can derive a criterion for phase segregation by comparing the ground-state energy of a homogeneous mixture of \( N_1 \) and \( N_2 \) Bose particles in a volume \( V \) with that of two single-species condensates occupying separate volumes \( V_1 \) and \( V_2 \) with \( N_1 \) and \( N_2 \) particles, respectively, while maintaining a constant total volume \( V = V_1 + V_2 \). Neglecting surface effects, the mixture is stable as long as its ground-state energy is less than the lowest possible value the sum of two separate ground-state energies can attain for any partition \( V_1 + V_2 = V \). Performing the minimization, this stability requirement is translated into the condition

\[
\frac{\left( a_{12}^{(0)} + a_{12}^{(1)} \right)^2}{m_{12}^2} < \frac{\left( a_{11}^{(0)} + a_{11}^{(1)} \right) \left( a_{22}^{(0)} + a_{22}^{(1)} \right)}{m_{11}m_{22}}.
\]

Since we require the inequalities for consistency, this stability condition is practically the same as the condition deduced from the requirement of real quasiparticle energies.

Continuing with the density expansion of the ground-state energy, the next-order contribution turns out to be of intriguing complexity. While our general scheme is fully capable of treating the general case, and one may use this scheme to generate the corresponding terms with the help of symbolic algebraic manipulation software, we restrict ourselves here to the experimentally relevant case of equal masses, \( m_1 = m_2 = m \) or \( t_1 = t_2 = t \), as corresponding, \( e.g.\), to a binary condensate consisting of atoms of a single isotope in two different spin states \( \downarrow \downarrow, \uparrow \downarrow, \downarrow \uparrow, \uparrow \uparrow \). The resulting expressions then simplify considerably: The quasiparticle energies \( \varepsilon_\pm(k) \) acquire a form which is strongly reminiscent of the single-species expressions,

\[
\varepsilon_\pm(k) = t(k)[t(k) + 2u_\pm(k)n] \]

Here we have introduced the auxiliary functions

\[
u_\pm(k) = \frac{1}{2} \left[ c_1u_{11}(k) + c_2u_{22}(k) \right] \pm \sqrt{c_1u_{11}(k) - c_2u_{22}(k))^2 + 4c_1c_2u_{12}^2(k)}
\]

which depend not only on the three interaction potentials, but also on the concentrations \( c_1 \) and \( c_2 \) of the individual species. We also write \( n = n_1 + n_2 \) for the total density, implying both \( n_1 = c_1n \) and \( c_1 + c_2 = 1 \). For vanishing interspecies interaction, \( u_{12}(k) = 0 \), one finds that \( u_+(k) \) and \( u_-(k) \) become equal to the maximum and the minimum of \( c_1u_{11}(k) + c_2u_{22}(k) \), respectively. The explicit appearance of the total density \( n \) in Eq. (76) greatly facilitates the following calculations.

It seems to be tempting now to go on with the Taylor expansion in powers of the density, and to compute

\[
\sum_{k \neq 0} \frac{\partial^3 \alpha(k)}{\partial n^3} \bigg|_{n=0} = \frac{3}{2} \sum_{k \neq 0} \frac{u_2^2(k) + u_3^2(k)}{t^2(k)},
\]

but this expression obviously becomes infrared divergent in the thermodynamic limit, and therefore is of no use here. This finding reflects the fact that, analogous to the single-species case, the proper expansion parameters for the ground-state energy of a dilute binary Bose gas are not the parameters \( n \) themselves, but their square roots. Correspondingly, the expression

\[
\lim_{n \to 0} \frac{V}{(2\pi)^3} \int \frac{3(tu_+)^3 \sqrt{n}}{(t^2 + 2tu_+)^{5/2}} + \frac{3(tu_-)^3 \sqrt{n}}{(t^2 + 2tu_-)^{5/2}}
\]

remains finite. For evaluating these integrals, we introduce a dimensionless momentum variable \( x \) by demanding

\[
t = \hbar^2 k^2 / 2m = ux^2,
\]

with a constant \( u \) carrying the same dimension as \( u_\pm(k) \), energy times volume. The limit \( n \to 0 \) can then be taken under the integral, implying \( u_\pm(k) \to u_\pm(0) \) there, and thus leading to

\[
\sum_{k \neq 0} \frac{\partial^2 \alpha(k)}{\partial n^2} \bigg|_{n=0} = \frac{4\pi V}{(2\pi)^3} \left[ (2mu)^{3/2} \right] 3u \int_0^\infty dx \sum_{+, -} \frac{(u_\pm(0)/u)^2 x^3}{(x^2 + 2u_\pm(0)/u)^{5/2}}.
\]
With the help of the identity
\[ \int_0^\infty dx \frac{x^3}{(x^2 + c)^{5/2}} = \frac{2}{3\sqrt{c}} \]  
(81)
one finds
\[ \sum_{k \neq 0} \frac{\partial}{\partial n} \frac{\partial^2 \alpha(k)}{\partial n^2} \bigg|_{n=0} = \frac{2m^3/2V}{\pi^2 \hbar^3} \sum_{+, -} n_\pm(0)^{5/2} . \]  
(82)
Introducing the scattering length-like quantities
\[ a_\pm(0) = \frac{m}{4\pi\hbar^2} n_\pm(0) \]  
(83)
\[ = \frac{1}{2} \left[ c_1 a_{11}^{(0)} + c_2 a_{22}^{(0)} \right] \]
\[ \pm \sqrt{\left[ c_1 a_{11}^{(0)} - c_2 a_{22}^{(0)} \right]^2 + 4c_1 c_2 a_{12}^{(0)}} , \]
which, however, again depend explicitly on the concentrations \( c_1 \) and \( c_2 \) of the individual species, the next contribution to the ground-state energy acquires the form
\[ \sum_{k \neq 0} \frac{\partial}{\partial n} \frac{\partial^2 \alpha(k)}{\partial n^2} \bigg|_{n=0} = \frac{2\pi\hbar^2}{m} n^2 V \frac{128}{15\sqrt{\pi}} \sum_{+, -} a_\pm(0) \sqrt{n a_\pm(0)^3} . \]  
(84)
Hence, adding this result to the previous contribution \[72\], we obtain for the ground-state energy density of a homogeneous binary condensate, consisting of two types of Bosons with equal masses, the expression
\[ E_0 = \frac{2\pi\hbar^2}{m} n^2 \left[ c_1 \left( a_{11}^{(0)} + a_{11}^{(1)} \right) + c_2 \left( a_{22}^{(0)} + a_{22}^{(1)} \right) \right] \]
\[ + 2c_1 c_2 \left( a_{12}^{(0)} + a_{12}^{(1)} \right) \]
\[ + \frac{128}{15\sqrt{\pi}} \sum_{+, -} a_\pm(0) \sqrt{n a_\pm(0)^3} . \]  
(85)
In the limiting case of vanishing interspecies interaction one has
\[ a_+^{(0)} \rightarrow \max \{ c_1 a_{11}^{(0)}, c_2 a_{22}^{(0)} \} , \]
\[ a_-^{(0)} \rightarrow \min \{ c_1 a_{11}^{(0)}, c_2 a_{22}^{(0)} \} , \]  
(86)
giving
\[ E_0 = \frac{2\pi\hbar^2}{m} n^2 \left[ a_{11}^{(0)} + a_{11}^{(1)} + a_{22}^{(0)} + a_{22}^{(1)} \right] \frac{128}{15\sqrt{\pi}} \sqrt{n a_{11}^{(0)} a_{22}^{(0)}} . \]  
(87)
Since we are relying on the assumption that the Born series for the scattering lengths converge rapidly, so that \( a \simeq a_{11}^{(0)} + a_{11}^{(1)} \simeq a_{11}^{(0)} \), this formula \[87\] reduces properly to the expected sum of two Lee-Yang-type expressions \[4\].

Finally, the calculation of the depletions according to Eqs. \[19\] proceeds along similar lines. For species 1 we have to evaluate
\[ N_1 - N_{10} = \sum_{k \neq 0} (v_+^2 k + v_-^2 k) , \]  
(88)
with the transformation coefficients \( v_+^2 k \) read off from Eqs. \[61\]. Restricting ourselves again to the case of equal masses, and employing once more the continuous dimensionless variable \( x \) introduced in Eq. \[76\] for converting the sum over the discrete wavevectors \( k \) in the thermodynamic limit into an integral, we find
\[ v_+^2 k = \frac{(\varepsilon_+ - t)^2 (\varepsilon_+ - \varepsilon_{s1})}{4\varepsilon_+ t} \frac{(2\varepsilon_+ - 2\varepsilon_s - \varepsilon_s)}{2\varepsilon_+ - \varepsilon_s} \]
\[ = \frac{1}{2} \frac{u_+ - c_2 u_{22}}{2a_{11}^{(0)} - c_1 a_{11}^{(0)} - c_2 a_{22}^{(0)}} \sqrt{x^2 + u_+ + 1} \]  
(89)
Taking the limit \( n \rightarrow 0 \) in the same manner as above under the integral, we obtain after some manipulations the desired depletion
\[ \frac{N_1 - N_{10}}{V} \simeq \frac{8}{3\sqrt{\pi}} n \]  
(90a)
\[ \times \sum_{+, -} \frac{a_+^{(0)} - c_2 a_{22}^{(0)}}{2a_+^{(0)} - c_1 a_{11}^{(0)} - c_2 a_{22}^{(0)}} \sqrt{n a_+^{(0)} a_-^{(0)}} . \]  
(90b)

Analogously,
\[ \frac{N_2 - N_{20}}{V} \simeq \frac{8}{3\sqrt{\pi}} n \]  
(90b)
\[ \times \sum_{+, -} \frac{a_+^{(0)} - c_1 a_{11}^{(0)} - c_2 a_{22}^{(0)}}{2a_+^{(0)} - c_1 a_{11}^{(0)} - c_2 a_{22}^{(0)}} \sqrt{n a_+^{(0)} a_-^{(0)}} . \]  
(90b)
The well-known single-species expression is easily recovered in the limit of vanishing interspecies interaction, as it should: Utilizing Eqs. \[76\], the above sums reduce to a single term, and we are left with
\[ \frac{N_i - N_{i0}}{V} \simeq \frac{8}{3\sqrt{\pi}} n a_i^{(0)} \sqrt{n a_i^{(0)} a_i^{(0)}} . \]  
(91)

V. CONCLUSION

The preceding calculations explicitly refer to soft interaction potentials \( U_{ij}(r) \) with a well-behaved Fourier transform, possessing a rapidly converging Born series for the respective scattering length, as is the case for wide and shallow potentials. In that case the first Born approximations \( a_{ij}^{(0)} \) practically exhaust the full Born series. Since the functional dependence of at least the leading terms of the density expansion of the ground-state energy on the scattering lengths is the same for both soft interactions and hard ones with a short-range singularity \[36\] (see also Ref. \[33\] for a recent discussion of

\[ \frac{N_i - N_{i0}}{V} \simeq \frac{8}{3\sqrt{\pi}} n a_i^{(0)} \sqrt{n a_i^{(0)} a_i^{(0)}} . \]  
(91)
with scattering lengths $a$, the ground-state energy density is then given by

$$a_\pm \equiv \frac{1}{2} \left[ c_1 a_{11} + c_2 a_{22} \pm \sqrt{(c_1 a_{11} - c_2 a_{22})^2 + 4 c_1 c_2 a_{12}^2} \right].$$

If the mixture is sufficiently dilute, such that

$$\sqrt{na_+^3} \ll 1,$$

the ground-state energy density is then given by

$$E_0 \equiv \frac{2\pi \hbar^2}{m} n^2 \left[ c_1^2 a_{11} + c_2^2 a_{22} + 2 c_1 c_2 a_{12} + \frac{128}{15\sqrt{\pi}} \left( a_+ \sqrt{na_+^3} + a_- \sqrt{na_-^3} \right) \right],$$

while the depletion can be written as

$$\frac{N_1 - N_10}{V} = \frac{8}{3\sqrt{\pi}} n \left[ \frac{a_+ - c_2 a_{22}}{2a_+ - c_1 a_{11} - c_2 a_{22}} \sqrt{na_+^3} \right. \left. + \frac{a_- - c_2 a_{22}}{2a_- - c_1 a_{11} - c_2 a_{22}} \sqrt{na_-^3} \right].$$

for species $1$; for the other species the depletion is obtained by interchanging the indices $1$ and $2$.

The particular case $a_{12}^2 = c_{11} a_{22}$ implies $a_- = 0$, so that, according to Eq. (84), one also has $\epsilon_-(k) = t(k)$, independent of the densities. Hence, the lower branch of the spectrum then is collisionless; this phenomenon is of particular interest in atom interferometry [10]. If one disregards the contributions to the ground-state energy obtained in Eq. (81), an argument analogous to the one which led to the stability criterion requires $a_{12}^2 < a_{11} a_{22}$ for a homogeneous binary condensate of particles with equal masses, and thus places a system with $a_- = 0$ right on the borderline between the regime of the homogeneous mixture and that of two segregated phases. However, inclusion of these contributions into the mean-field approach tends to stabilize a homogeneous binary condensate with a collisionless branch of the quasiparticle spectrum.

Even though derived under the restriction of equal masses of both species, both the result [9] for the ground-state energy and, in particular, the expression [10] for the depletion is surprisingly involved and could not have been guessed on the basis of the known single-species formulas. The corresponding expressions for the general case, which are substantially more cumbersome, are obtained by following exactly the steps explained above.

Our reasoning clearly indicates that the elementary Bogoliubov theory, which works directly with the interparticle potentials, gets worse the deeper the potentials are [28], as the missing terms of the Born series become increasingly more important. In the case of a single-species condensate, the emergence of the full scattering length $a$ instead of its first Born approximation in the expression [6] for the ground-state energy density is justified by means of a summation of ladder diagrams [42], or by employing effective field theory with the exact two-point scattering amplitude [52]; these devices may also be used in the binary case. It should be kept in mind, however, that so far only the leading term in Eq. (2) could be established with full mathematical rigor [29], whereas a corresponding rigorous proof for the next-to-leading term is still lacking. It would, therefore, be of considerable conceptual value to demonstrate in explicit detail how the missing terms of the Born series are recovered if one systematically takes into account those contributions to the full Hamiltonian which have been neglected in the quadratic Bogoliubov approximation, thus showing the consistency of the various approaches. We will present such a calculation in a subsequent paper [43].

[1] C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. 78, 586 (1997).
[2] D. M. Stamper-Kurn, M. R. Andrews, A. P. Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, and W. Ketterle, Phys. Rev. Lett. 80, 2027 (1998).
[3] D. S. Hall, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 81, 1539 (1998).
[4] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 83, 2498 (1999).
[5] P. Maddaloni, M. Modugno, C. Fort, F. Minardi, and M. Inguscio, Phys. Rev. Lett. 85, 2413 (2000).
[6] T.-L. Ho and V. B. Shenoy, Phys. Rev. Lett. 77, 3276 (1996).
[7] B. D. Esry, C. H. Greene, J. P. Burke, Jr., and J. L. Bohn, Phys. Rev. Lett. 78, 3504 (1997).
[8] E. V. Goldstein and P. Meystre, Phys. Rev. A 55, 2935 (1997).
[9] C. K. Law, H. Pu, N. P. Bigelow, and J. H. Eberly, Phys. Rev. Lett. 79, 3105 (1997).
[10] E. V. Goldstein, M. G. Moore, H. Pu, and P. Meystre, Phys. Rev. Lett. 85, 5030 (2000).
[11] P. Ao and S. T. Chui, Phys. Rev. A 58, 4836 (1998).
[12] P. Ao and S. T. Chui, J. Phys. B 33, 535 (2000).
[13] A. S. Alexandrov and V. V. Kabanov, J. Phys.: Condens. Matter 14, L327 (2002).
[14] V. I. Yukalov and E. P. Yukalova, Laser Phys. Lett. 1, 50 (2004).
[15] Th. Busch, J. I. Cirac, V. M. Pérez-García, and P. Zoller, Phys. Rev. A 56, 2978 (1997).
[16] R. Graham and D. Walls, Phys. Rev. A 57, 484 (1998).
[17] H. Pu and N. P. Bigelow, Phys. Rev. Lett. 80, 1134 (1998).
[18] T.-L. Ho, Phys. Rev. Lett. 81, 742 (1998).
[19] C. K. Law, H. Pu, and N. P. Bigelow, Phys. Rev. Lett. 81, 5257 (1998).
[20] G.-H. Chen, and Y.-S. Wu, Phys. Rev. A 67, 013606 (2003).
[21] K. V. Krutitsky and R. Graham, Phys. Rev. Lett. 91, 240406 (2003).
[22] N. N. Bogoliubov, J. Phys. (USSR) 11, 23 (1947). Translated and reprinted in D. Pines (ed.), The many-body problem (Benjamin, New York, 1968).
[23] T. D. Lee and C. N. Yang, Phys. Rev. 105, 1119 (1957).
[24] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. 106, 1135 (1957).
[25] K. A. Brueckner and K. Sawada, Phys. Rev. 106, 1117 (1957).
[26] S. T. Beliaev, Zh. Éksp. Teor. Fiz. 34, 433 (1958) [Sov. Phys. JETP 7, 299 (1958)].
[27] N. M. Hugenholtz and D. Pines, Phys. Rev. 116, 489 (1959).
[28] E. H. Lieb, Phys. Rev. 130, 2518 (1963).
[29] E. H. Lieb and J. Yngvason, Phys. Rev. Lett. 80, 2504 (1998).
[30] E. Braaten and A. Nieto, Eur. Phys. J. B 11, 143 (1999).
[31] E. Braaten, H.-W. Hammer, and S. Hermans, Phys. Rev. A 63, 063609 (2001).
[32] A. J. Leggett, New J. Phys. 5, 103 (2003).
[33] A. Yu. Cherny and A. A. Shanenko, Phys. Rev. E 62, 1646 (2000).
[34] K. Huang and C. N. Yang, Phys. Rev. 105, 767 (1957).
[35] J. O. Andersen, Rev. Mod. Phys. 76, 599 (2004).
[36] E. M. Lifshitz and L. P. Pitaevskii, Landau and Lifshitz – Course of Theoretical Physics. Volume 9: Statistical Physics, Part 2 (Butterworth and Heinemann, Oxford, 1998).
[37] R. K. Pathria, Statistical Mechanics (Pergamon Press, Oxford, 1985).
[38] J. J. Hopfield, Phys. Rev. 112, 1555 (1958).
[39] C. Weiss, M. Block, D. Boers, A. Eckardt, and M. Holthaus, Z. Naturforsch. 59a, 1 (2004).
[40] C. J. Pethick and H. Smith, Bose-Einstein Condensation in Dilute Gases (University Press, Cambridge, 2002).
[41] C. Cohen-Tannoudji, B. Diu, and F. Laloë, Quantum Mechanics: Volume 2 (John Wiley, New York, 1977).
[42] A. L. Fetter and J. D. Walecka, Quantum Theory of Many-Particle Systems (Dover, New York, 2003).
[43] C. Weiss and A. Eckardt, Europhys. Lett., in press (2004).