Mean-field expansion in Bose-Einstein condensates with finite-range interactions

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We present a formal derivation of the mean-field expansion for dilute Bose-Einstein condensates with two-particle interaction potentials which are weak and finite-range, but otherwise arbitrary. The expansion allows for a controlled investigation of the impact of microscopic interaction details (e.g., the scaling behavior) on the mean-field approach and the induced higher-order corrections beyond the $s$-wave scattering approximation.

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I. INTRODUCTION

The experimental realization of Bose-Einstein condensation in atomic or molecular gases has rekindled interest in the quantum theory of dilute bosonic gases\cite{1,2,3,4}. So far, most investigations were based on the $s$-wave scattering approximation which neglects microscopic details of the two-particle interaction (such as attractive regions of the potential), and replaces the true interaction by a contact interaction pseudopotential. To describe the impact of a possibly complicated microscopic structure of the potential on quantities like the occupation number of the condensate, it is however necessary to go beyond the $s$-wave approximation. On the other hand, the current theoretical description of Bose-Einstein condensates is predominantly based on a mean-field expansion around a macroscopically occupied state representing the condensate. In leading order this expansion yields the Gross-Pitaevskii equation, which forms the basis of most theoretical approaches to Bose-Einstein condensed gases\cite{5}.

The scope of the present article is to investigate consequences of deviations from pure $s$-wave scattering for the applicability of this mean-field expansion, and to derive the general zero-temperature equations governing the condensate and quantum fluctuations above it. To this end, we present an \textit{ab initio} approach, controlled by properties of the bare interaction potential in the microscopic second-quantized equation of motion. While the presented approach is essentially restricted to sufficiently “weak”, that is, integrable potentials, we do not use pseudopotential or T-matrix approaches\cite{6,7,8}, for which the direct connection to microscopic properties of the interaction potential is lost. Our approach can thus be viewed as being complementary to the latter treatments. In particular, if one can separate the potential into a strong ultra-short-range part, assumed to be replaceable by an integrable (pseudo-)potential, and a weaker remaining contribution with longer range, our analysis applies to this latter part as a low-energy, effective description.

II. NUMBER-CONSERVING MEAN-FIELD EXPANSION

We test the validity of the mean-field expansion, which is usually an \textit{ad hoc} assumption, employing well-defined scaling properties of the interaction potential with the number of particles and thus the density of the system, under the prescription that the system always remains dilute. It turns out that the consistency of the mean-field expansion sensitively depends on the scaling exponent of the interaction potential, and thus on the (formal) dependence of the interaction range on the particle number. This formal dependence on the particle number can be made more intuitive by comparing the dilute-gas limit with the thermodynamic limit.

The structure of the paper is as follows. In the next Section we derive, using a number-conserving mean-field expansion, the equations of motion for the mean field itself (a modified Gross-Pitaevskii equation) and for the single- and multi-particle excitations above mean-field. In the third Section, the consistency of this mean-field expansion is tested with three scaling behaviors of the particle interaction potential. The fourth Section treats, as an explicit example, a dipole-dipole interaction potential. Even though such a potential is on the borderline of applicability of our approach [because it is (just) not integrable in three spatial dimensions], we show that the calculation of certain quantities like the quantum depletion of the condensate is still feasible.
equal to unity, the Heisenberg equation of motion for the field operator reads
\[
\frac{i}{\hbar} \frac{\partial \hat{\Psi}}{\partial t} = \left( -\nabla^2 + V_{\text{ext}}(r) \right) \hat{\Psi}(r) + \int d^3 r' \hat{\Psi}^\dagger(r') V_{\text{int}}(r - r') \hat{\Psi}(r') \hat{\Psi}(r),
\]
with \( V_{\text{ext}}(r) \) denoting the external one-particle potential of the trap. The finite-range two-particle interaction potential \( V_{\text{int}}(r - r') \) is assumed to be sufficiently “weak” in the sense that the Born approximation applies, e.g., \( V_{\text{int}}(r) \) is supposed to be integrable (i.e., to decay more rapidly with distance than \( 1/r^3 \)) such that its Fourier transform \( \tilde{V}_{\text{int}}(k) \) is a well-defined function of \( k \). For large wavelengths, the finite-range two-particle interaction potential \( V_{\text{int}}(r - r') \) yields an effective coupling constant \( g \) determined by the s-wave scattering length \( a_s \) (in three spatial dimensions)
\[
g = 4\pi a_s = \int d^3 r \, V_{\text{int}}(r) = \tilde{V}_{\text{int}}(k = 0) = 0. \tag{2}
\]
The Bogoliubov mean-field approximation \[1\] is based on the assumption that the fluctuations \( \hat{\chi} \), describing single-particle excitations above the ground state are small (compared to the mean field) if the number \( N \) of particles is large. In the following, we present a formal derivation of the mean-field expansion for the system described in Eq. \[1\] in the large-\( N \) limit, i.e., an expansion of \( \hat{\Psi} \) into powers of \( N \). We shall employ a particle-number-conserving mean-field ansatz (satisfying \( \langle \hat{\Psi} \rangle = 0 \)) \[11, 12\]
\[
\hat{\Psi} = \left( \psi_0 + \hat{\chi} + \hat{\zeta} \right) \frac{A}{\sqrt{N}}. \tag{3}
\]
Here, the \textit{order parameter} is \( \psi_0 \). The single-particle excitations are described by \( \hat{\chi} \), where single-particle here means that the Fourier components of \( \hat{\chi} \) are linear superpositions of annihilation and creation operators of quasiparticles \( \hat{a}_k \) and \( \hat{a}_k^\dagger \), cf. Eq. \[5\]. The higher-order corrections \( \hat{\zeta} \) are due to multi-particle excitations and correlations. Here \( N = A^\dagger A \) counts the total number of particles.

The \textit{dilute-gas limit} may formally be defined by placing a very large number \( N \uparrow \infty \) of identical bosons into a finite trap with \( gN \) remaining constant \[12, 13\]. The diluteness parameter of the gas then scales as \( (g^2 \varrho)^{1/2} \propto 1/N \), i.e., the gas becomes rapidly more dilute with increasing particle number in this limit. This limit should be compared and contrasted with the usual thermodynamic limit, in which the density and particle interaction remains constant, while the size of the (trapped) system increases with \( N \to \infty \), adjusting the trapping potential correspondingly (in \( D \) spatial dimensions, the thermodynamic limit corresponds to keeping \( N \omega^D \) constant for \( N \to \infty \), where \( \omega \) is the geometric mean of the trapping frequencies \[3\]). In the presently used dilute-gas limit, on the other hand, the trapping potential remains constant, but the interaction and the density change. The advantage of the limit \( gN \) constant is that in this limit we have a well-defined prescription for checking the mean-field approximation, keeping one power of \( g \) for each factor of \( N \), cf. \[2\].

Given the dilute-gas limit, there arises a question which is central to the applicability of the mean-field expansion: Do the supposedly small multi-particle corrections \( \hat{\zeta} \) actually become small in this limit for a given behavior of the interparticle potential \( V_{\text{int}}(r - r') \)? In order to tackle this question, let us consider the following scenario: Initially, the interaction is completely switched off, \( V_{\text{int}}(r - r') = 0 \), and all \( N \) bosons occupy the same single-particle state (at zero temperature), described by the single-particle wave-function \( \psi_0/\sqrt{N} \). In this case, Eq. \[3\] is trivially satisfied with \( \psi_0 = O(\sqrt{N}), \hat{\chi} = O(N^0), \hat{\zeta} = 0 \), and \( A = \hat{a}_0 \hat{a}_0^\dagger \) corresponds to the macroscopically occupied state, cf. \[11\]. If we now switch on the interaction slowly enough, the system stays in its ground state due to the adiabatic theorem and we may follow the evolution of the field operator \( \hat{\Psi} \) and hence \( \psi_0, \hat{\chi}, \hat{\zeta} \) (with \( A \) remaining constant, i.e., the evolution at given particle number) via insertion of Eq. \[3\] into \[1\].

Assuming that the corrections \( \hat{\zeta} \) indeed become small for \( N \uparrow \infty \), the leading order \( (N^0) \) yields, in the dilute-gas limit, the Gross-Pitaevskii (GP) equation \[9\] for the order parameter \( \psi_0 \)
\[
i \frac{\partial \psi_0}{\partial t} = \left( -\nabla^2 + V_{\text{ext}} + g|\psi_0|^2 \right) \psi_0. \tag{4}
\]
The next-to-leading order \( (N^0) \) terms govern the evolution of the fluctuations \( \hat{\chi} \) via the nonlocal analogue of the Bogoliubov-de Gennes equations \[10\]
\[
i \frac{\partial \hat{\chi}}{\partial t} = \int d^3 r' V_{\text{int}}(r - r') \left[ |\psi_0|^2 \hat{\chi}(r') + \psi_0^2 \hat{\chi}^\dagger(r') \right] + \left( -\nabla^2 + V_{\text{ext}} + g|\psi_0|^2 \right) \hat{\chi}. \tag{5}
\]
The remaining equation of motion for \( \hat{\zeta} \) takes for a general nonlocal potential the rather complicated form
\[
i \frac{\partial \hat{\zeta}}{\partial t} = \left( -\nabla^2 + V_{\text{ext}} + |\psi_0|^2 \left[ \frac{g}{\hat{V}_{\text{int}}} \right] \right) \hat{\zeta} + \psi_0^2 \hat{V}_{\text{int}} \hat{\chi}^\dagger \hat{\chi} + \psi_0 \hat{V}_{\text{int}} \hat{\chi} + \psi_0 \hat{V}_{\text{int}} \hat{\chi} \hat{\chi} + \hat{V}_{\text{int}} \hat{\chi} \hat{\chi} + O \left( \frac{\hat{\zeta}}{\sqrt{N}} \right), \tag{6}
\]
where \( \hat{V}_{\text{int}} \) is an abbreviation for the convolution with the quantity right from the “\( a \)” as in Eq. \[8\], and \( O(\zeta/\sqrt{N}) \) denote formally sub-leading terms containing \( \hat{\zeta} \) or \( \hat{\zeta}^\dagger \) or both. Observe that the commutation relations \( \{ \hat{\chi}, \hat{\chi}^\dagger \} = \{ \hat{\zeta}, \hat{\zeta}^\dagger \} = 0 \) valid initially are
preserved under the evolution given by the equations above, i.e., the excitations $\hat{\chi}$ and $\zeta$ are always particle-number-conserving, cf. [11, 12].

If we start with free particles, and switch on the interaction by following the evolution in Eqs. (4), (5), and (6), we observe a mixing of $\hat{\chi}$ and $\hat{\chi}^\dagger$ due to Eq. (7), and $\zeta$ does not vanish anymore due to the four source terms $\hat{V}_{\text{int}} \hat{\chi}^\dagger$, $(\hat{V}_{\text{int}} \hat{\chi})^\dagger$, $\hat{V}_{\text{int}} (\hat{\chi}^\dagger \hat{\chi})$, and $[\hat{V}_{\text{int}} (\hat{\chi}^\dagger \hat{\chi})].$ The viability of mean-field theory depends on the scaling of the induced terms in $\zeta$ with particle number, i.e., if and to which extent they decrease for $N \uparrow \infty.$ Naive power counting would imply $\zeta = O(1/\sqrt{N}),$ but the non-linearity due to the product of two or more field operators (such as in the above source terms) and the associated mode sum(s) may compensate the smallness of $1/\sqrt{N}.$

As an example, let us consider the expectation values of the remaining terms do not vanish, and affect $\zeta(N)).$

For the sake of notational convenience, we consider in what follows a homogeneous condensate $\psi_0 = \sqrt{g_0} = \text{const}$ in a constant “trapping” potential $V_{\text{ext}} = -g_0 \rho$, so that the two last terms in the round brackets on the right-hand side of the Bogoliubov-de Gennes equations (5) cancel. A normal-mode expansion for the fluctuation operators then yields in Fourier space

$$i \frac{\partial \hat{\chi}_k}{\partial t} = \left( \frac{k^2}{2} + g_0 \hat{V}_{\text{int}}(k) \right) \hat{\chi}_k + g_0 \hat{V}_{\text{int}}(k) \hat{\chi}^\dagger_k ,$$

so that the annihilation operators $\hat{\chi}_k$ of the original bosons have the following Bogoliubov transformation form in terms of the quasiparticle operators $\hat{a}_k, \hat{a}^\dagger_k$:

$$\hat{\chi}_k = \sqrt{\frac{k^2}{2 \omega_k}} \left[ \left( \frac{1}{2} - \frac{\omega_k}{k^2} \right) \hat{a}_k + \left( \frac{1}{2} + \frac{\omega_k}{k^2} \right) \hat{a}^\dagger_k \right].$$

The generalized Bogoliubov dispersion relation reads

$$\omega_k^2 = k^2 g_0 \hat{V}_{\text{int}}(k) + \frac{k^4}{4}.$$  

This faster-than-polynomial decrease renders all relevant expectation values finite. For example, the expectation value of the so-called “anomalous” term reads

$$\langle \hat{\chi} \hat{V}_{\text{int}} \hat{\chi} \rangle = -\frac{\psi_0^2}{2\pi^2} \int \frac{dk}{2\omega_k},$$

where we have assumed a spherically symmetric potential $V_{\text{int}}(r)$ and hence $\hat{V}_{\text{int}} = \hat{V}_{\text{int}}(k).$ The expectation value is taken in the ground state of the quasiparticles (remember the adiabatic switching process) which is annihilated by $\hat{a}_k$ (but not by $\hat{\chi}_k$, of course). For a sufficiently regular $\hat{V}_{\text{int}}(k),$ an expansion into powers of $1/(\xi k_{\text{cut}})$ yields

$$\langle \hat{\chi} \hat{V}_{\text{int}} \hat{\chi} \rangle = -\frac{\psi_0^2}{2\pi^2} \int \frac{dk}{2\omega_k} + \frac{g^2 \psi_0^2}{\xi \pi^2} + O\left( \frac{g^3 \psi_0^2}{\xi k_{\text{cut}}} \right).$$

The $1/(\xi k_{\text{cut}})$-corrections depend on the explicit form of $V_{\text{int}}(r)$ and hence $\hat{V}_{\text{int}}(k),$ e.g., for $\hat{V}_{\text{int}}(k) = g\hat{0}(k_{\text{cut}} - k),$ the integral in Eq. (10) yields $g^2 (\sqrt{\xi^2 k_{\text{cut}}^2 + 4} - 2)/\xi.$

In contrast to the so-called “anomalous” term $\langle \hat{\chi} \hat{V}_{\text{int}} \hat{\chi} \rangle$, the expectation value of the quantum depletion terms $\hat{V}_{\text{int}} \hat{\chi} \hat{\chi}^\dagger$ and $(\hat{\chi} \hat{V}_{\text{int}} \hat{\chi}^\dagger)$ occurring as source terms in Eq. (6) do not have a contribution linear in $k_{\text{cut}}.$ Hence their (for $\xi k_{\text{cut}} \gg 1$) dominant terms independent of $k_{\text{cut}}$ and both give $g(\xi^2 \chi) \approx \sqrt{g^2 \psi_0^2 / (3\pi^2)}.$ The higher-order $1/(\xi k_{\text{cut}})$-corrections, however, again depend on the shape of $\hat{V}_{\text{int}}(k)$ and can be calculated analogously.

III. CONSISTENCY OF MEAN-FIELD EXPANSION

To explicitly address our principal question of whether the higher-order corrections $\zeta$ in the mean-field expansion (5) indeed become small in the large-$N$ limit (in which one would naively expect mean-field to become more and more accurate), we now discuss three concrete examples for the formal scaling behavior of the interaction $\hat{V}_{\text{int}}$ with the number of particles $N.$ To this end, the particle-number-dependent potential $V^{(N)}_{\text{int}}$ is always chosen such that it reproduces the $g \propto 1/N$ dilute-gas limit prescription for the behavior of the coupling constant in the large-$N$ limit.

In the first example, we assume $k_{\text{cut}}$ to be (formally) independent of $N$

$$V^{(N)}_{\text{int}}(r) = \frac{1}{N} V^{(1)}_{\text{int}}(r).$$

Since $k_{\text{cut}}$ remains constant for $N \uparrow \infty$, the mode sums due to the nonlinear terms in Eq. (4) cannot compensate the smallness of the pre-factors such as $1/\sqrt{N}$ and thus we obtain

$$\zeta = O\left( \frac{1}{\sqrt{N}} \right).$$
However, this decrease is not sufficient yet for ensuring the usual split of the total density
\[ \rho = \langle \hat{\Psi}^\dagger \hat{\Psi} \rangle = \lvert \psi_0 \rvert^2 + \langle \hat{\chi}^\dagger \hat{\chi} \rangle + \mathcal{O} \left( \frac{1}{\sqrt{N}} \right), \tag{14} \]

since \( \psi_0 (\hat{\zeta}) \) could be of the same order as \( \langle \hat{\chi}^\dagger \hat{\chi} \rangle \). For the above split, we need \( \langle \hat{\zeta} \rangle = \mathcal{O}(1/N) \) instead of \( \mathcal{O}(1/\sqrt{N}) \), which requires absorbing the expectation values of the source terms into a modified GP equation
\[ \frac{i}{\hbar} \frac{\partial \psi_0}{\partial t} = \left( -\nabla^2/2 + V_{\text{ext}} + g \lvert \psi_0 \rvert^2 + g \langle \hat{\chi}^\dagger \hat{\chi} \rangle \right) \psi_0 \]
\[ + \langle \hat{\chi} \hat{V}_{\text{int}} * \hat{\chi} \rangle \psi_0^* + \langle \hat{\chi} \hat{V}_{\text{int}} * \hat{\chi} \rangle \psi_0. \tag{15} \]
Inserting Eq. (11), we see that the dominant (for \( k_{\text{cut}} \gg 1 \)) and density-independent fluctuation contribution \( \langle \hat{\chi} \hat{V}_{\text{int}} * \hat{\chi} \rangle \) proportional to \( k_{\text{cut}} \) can be absorbed by a renormalization of the coupling constant
\[ g_{\text{ren}} = g - \frac{1}{2\pi^2} \int dk \hat{V}_{\text{int}}^2 \]
\[ = g + \int d^3 r \ V_{\text{int}} \nabla^{-2} V_{\text{int}}, \tag{16} \]
where the second line is due to Parseval’s theorem, using the formal inverse of the Laplace operator \( \nabla^2 \). Since \( -\nabla^{-2}/2 \) and \( V_{\text{int}}/2 \) are the kernels of the Schrödinger Hamiltonian \( \hat{H}_0 \) and the interaction Hamiltonian \( \hat{H}_1 \), respectively, this just corresponds to the usual one-loop renormalization of the interaction potential. Note that in three spatial dimensions, sub-dominant contributions like \( \langle \hat{\chi}^\dagger \hat{\chi} \rangle \) cannot be absorbed by such a renormalization procedure.

The physical significance of the renormalized coupling \( g_{\text{ren}} \) can be demonstrated further by calculating the \( k_{\text{cut}} \) corrections to the total energy of a homogeneous gas
\[ E = \langle \hat{H} \rangle \approx NV_{\text{ext}} + \frac{N}{2} g \rho - \frac{N}{4\pi^2} \int dk \hat{V}_{\text{int}}^2, \tag{17} \]
which gives \( E = NV_{\text{ext}} + Ng_{\text{ren}} \rho/2 \) plus higher-order corrections (cf. [2]).

A potential complication which arises from the prescription [12] is that the range of the two-particle interaction potential in Eq. (12) will exceed the inter-particle distance \( d_i \) for large \( N \) since \( g_0 \sim N \) and thus \( d_i \sim 1/N^{1/3} \) (in three spatial dimensions). If the two-particle interaction potential is mainly caused by direct collisions, this might lead to a conflict with the point-particle approximation used in writing down the starting point of the analysis, Eq. (11). Therefore, as a second example, consider the support of \( V_{\text{int}}(r) \) to be decreasing in proportion to the inter-particle distance \( d_i \),
\[ V_{\text{int}}^{(N)}(r) = V_{\text{int}}^{(1)}(N^{1/3}r). \tag{18} \]
As a consequence, the cut-off scales as \( k_{\text{cut}} \sim N^{1/3} \), and thus \( \langle \hat{\chi} \hat{V}_{\text{int}} * \hat{\chi} \rangle \sim N^{-2/3} \), which ensures that the remaining \( \zeta \) corrections are still small, though decreasing with a smaller power in \( N \) than in the first example Eq. (13):
\[ \zeta = \mathcal{O} \left( \frac{1}{N^{1/6}} \right). \tag{19} \]
The above scaling with particle number is due to the fact that for each additional operator in Eq. (16), which might contribute a factor \( k_{\text{cut}} \sim N^{1/3} \) after the mode summation, there is a pre-factor of order \( 1/\sqrt{N} \). In this case, the split in Eq. (14) is still possible provided the modification of the GP equation (16) is employed, but the estimate of the accuracy is now the rather slow decrease of \( \mathcal{O}(1/N^{1/6}) \) instead of \( \mathcal{O}(1/N^{1/2}) \).

Finally, as a third example, we investigate a scaling employed by Lieb et al. [13 14], used in a proof of the asymptotic exactness of the Gross-Pitaevskii energy functional in three spatial dimensions, and in a analysis of one-dimensional systems of bosons in 3D traps, respectively. This scaling reads
\[ V_{\text{int}}^{(N)}(r) = N^2 V_{\text{int}}^{(1)}(N^2 r), \tag{20} \]
and implies that the cut-off increases linearly with particle number, \( k_{\text{cut}} \sim N \), and thus \( \langle \hat{\chi} \hat{V}_{\text{int}} * \hat{\chi} \rangle \sim N^0 \), so that the anomalous term becomes of the same order as other terms in the GP equation, for example as large as the mean-field interaction term \( g \lvert \psi_0 \rvert^2 \). The “correction” operator then behaves as
\[ \zeta = \mathcal{O} \left( \frac{1}{\sqrt{N}} \right), \tag{21} \]
and we have no true control over the corrections in the mean-field expansion which ought to be negligible. The mean-field approximation can only be consistent (if at all) with a modified GP equation (16) inducing a renormalization of the coupling according to Eq. (11). However, even given these modifications, the applicability of the mean-field expansion is not obvious since higher-order operator products can yield \( \mathcal{O}(N) \) contributions after the \( k \)-summation/integration and thus the hierarchy \( \zeta \ll \hat{\chi} \) is not evident. Similarly, the first-order correction in Eq. (11) is comparable to the zeroth order (i.e., of the same order in \( N \)), which hints at the fact that all orders must be taken into account in a suitable way.

It is illuminating to compare the employed dilute-gas limit \( N \uparrow \infty \) particles in a fixed volume with \( gN \) remaining constant) with the thermodynamic limit \( (N \uparrow \infty) \) particles in an increasing volume \( V \) with \( g \) and \( N/V \) remaining constant): Translation of the scaling in Eq. (12) to the thermodynamic limit yields an interaction potential whose range increases proportional to the system size \( V \) whereas its strength decreases accordingly. It is not very surprising that the mean-field expansion is very good in this case. The analogue of Eq. (16) in the thermodynamic limit is an interaction potential with constant strength and range (where the applicability of the mean-field expansion is less obvious). Finally, Eq. (20) corresponds to a potential with decreasing range and increasing strength.
IV. DIPOLE-DIPOLE INTERACTION

As an example for interactions with a finite range, let us consider a dipole-dipole force \( \propto g_d \) in addition to the usual contact repulsion \( \propto g \). Dipole-dipole interactions between atoms can either be induced by an external electric field or be due to an intrinsic magnetic dipole moment. E.g., for magnetic dipoles, \( g_d = \mu_0 d_m^2 / 3 \); Bose-Einstein condensation of chromium, which has a ground state moment of \( d_m = 6 \mu_B \), has been achieved recently.

If the dipole moments of all atoms/molecules are aligned along the z-axis, the dipole-dipole interaction potential reads (in three spatial dimensions)

\[
V_{dd}(r) = \frac{3g_d}{4\pi} \frac{1 - 3z^2/|r|^2}{|r|^3}.
\]

In addition to this long-range interaction, the particles are subject to a short-range repulsion whose impact can be represented by a contact potential \( \propto \delta^3(r) \). Consequently, the Fourier transformed potential reads for intermediate momenta

\[
\tilde{V}_{\text{int}}(k) = g + g_d \left( \frac{3k^2}{k^2} - 1 \right).
\]

The (ideal) dipole-dipole interaction potential behaves as \( 1/r^3 \) which is not integrable and, strictly speaking, is therefore just at the limit of applicability of our analysis – for example, \( \tilde{V}_{\text{int}} \) is not well-defined at \( k = 0 \), which complicates the introduction of an effective coupling \( g \) (finite-size effects etc.). Nevertheless, we may regard the non-integrable dipole-dipole interaction potential as a limit of integrable potentials and calculate the corresponding corrections beyond the s-wave scattering approximation. For example, the quantum depletion is modified from the pure contact case via

\[
\langle \hat{\chi} \rangle = \frac{g_0^{3/2}}{24\pi^2} \sqrt{2g_d + g} (g_d + 5g) \\
- \frac{g_0^{3/2}}{16\pi^2} \frac{(g - g_d)^2}{\sqrt{3g_d}} \ln \left( \frac{g_d + g}{\sqrt{3g_d + 2g_d + g}} \right) \\
= \frac{g_0^{3/2}}{3\pi^2} \left[ 1 + \frac{3}{10} \frac{g_0^2}{g^2} + O \left( \frac{g_0^2}{g^2} \right) \right].
\]

This expression is valid for \( g \geq g_d \) only, since otherwise the excitation spectrum (for a homogeneous condensate) and hence also \( \langle \hat{\chi} \rangle \) contain imaginary parts indicating an instability, cf. \cite{17}. Further expectation values such as the total energy \( E = \langle \hat{H} \rangle \) can be calculated analogously \cite{18}.

V. CONCLUSION

Based on the point-particle approximation of Eq. \( \text{11} \), we derived the mean-field expansion Eq. \( \text{3} \) for dilute Bose-Einstein condensates with arbitrary weak finite-range two-particle interaction potentials, obeying suitable scaling behavior in the large-\( N \) limit. It turns out that, although the gas rapidly becomes ever more dilute in the large \( N \) limit (the gas parameter \( (g^3/\varrho)^{1/2} \propto 1/N \)), the validity of the mean-field approximation strongly depends on the detailed scaling behavior of the particle interaction potential. Therefore, care needs to be exercised in applying the mean-field approximation – if one does not take the detailed structure of the bare interaction potential into account, one possibly encounters inconsistencies with the basic assumptions the mean-field expansion is built on.

Apart from exploring limits of the mean-field approximation, our derivation facilitates the calculation of the impact of microscopic details of the interaction beyond the s-wave scattering approximation \cite{19}. Another advantage of the presented approach is the natural emergence and \textit{ab initio} derivation of the cut-off \( k_{\text{cut}} \) as a microscopic property of the interaction potential – instead of a cut-off \( k_{\text{cut}} \) introduced \textit{ad hoc} for the regularization of pseudo-potentials \( \propto \delta^3(r - r') \), see, e.g., \cite{20}. However, one should bear in mind that the presented method requires weak potentials – if nonperturbative effects such as bound states or total reflection at a finite radius become important, the direct mean-field ansatz \cite{21} cannot be applied in this way. Instead of homogeneous plane waves, one has to start from atomic/molecular eigenfunctions in this case and the ansatz \cite{21} can only work as a low-energy effective description. Nevertheless, if it is possible to divide a nonperturbative \( V_{\text{int}}(r - r') \) into a strong ultra-short-range part and a comparably weak remaining contribution which is more spread out, the presented analysis should be applicable to the latter part, provided the ultra-short-range part can be replaced in an adequate manner by an integrable (pseudo-)potential. An example for the application of our analysis to the longer-range contribution we gave in the last Section, using a dipole-dipole interaction potential.

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