The relation between the Gross–Pitaevskii and Bogoliubov descriptions of a dilute Bose gas

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Abstract. I formulate a ‘pseudo-paradox’ in the theory of a dilute Bose gas with repulsive interactions: the standard expression for the ground state energy within the Gross–Pitaevskii (GP) approximation is lower than that in the Bogoliubov approximation, and hence, by the standard variational argument, the former should prima facie be a better approximation than the latter to the true ground state—a conclusion which is of course opposite to the established wisdom concerning this problem. It is shown that the pseudo-paradox is (unsurprisingly) resolved by a correct transcription of the two-body scattering theory to the many-body case; however, contrary to what appears to be a widespread belief, the resolution has nothing to do with any spurious ultraviolet divergences which result from the replacement of the true interatomic potential by a delta-function pseudopotential. Rather, it relates to an infrared divergence which has the consequence that (a) the most obvious form of the GP ‘approximation’ actually does not correspond to any well-defined ansatz for the many-body wavefunction, and (b) that the ‘best shot’ at such a wavefunction always produces an energy which exceeds, or at best equals, that calculated in the Bogoliubov approximation. In fact, the necessity of the latter may be seen as a consequence of the need to reduce the Fock term in the energy, which is absent in the two-particle problem but dominant in the many-body case; it does this by increasing the density correlations, at distances less than or approximately equal to the correlation length ξ, above the value extrapolated from the two-body case. As a by-product I devise an alternative formulation of the Bogoliubov approximation which does not require the explicit replacement of the true interatomic potential by a delta-function pseudopotential.
1. Introduction

In this paper I will address a very basic question concerning the problem of a dilute Bose gas of spinless particles with repulsive interactions at zero temperature. Interest in this problem goes back more than 50 years [1], but has increased dramatically following the experimental realization in 1995 [2] of Bose–Einstein condensation (BEC) in dilute systems of alkali-gas atoms. In the discussion below I will have in mind such a BEC alkali-gas system, and will assume that all atoms are in the same hyperfine state so that the hyperfine degree of freedom drops out of the problem and it becomes equivalent to that of a gas of spinless atoms. Also, I shall assume that for the atoms in question the two-particle zero-energy s-wave scattering length \(a_s\) is positive. The problem then becomes closely similar to one discussed intensively in the 1950s and 1960s (see e.g. [3]), namely that of a gas of bosonic hard spheres with radius \(a_s\); it is, however, not identical to it, so that one cannot necessarily assume without explicit argument that all results obtained for the hard-sphere model can be taken over verbatim. Thus, even if it should turn out (as it well may) that the question to be discussed here has been resolved, explicitly or implicitly, in the classic papers of the 1950s and 1960s, it may not be entirely pointless to restate and analyse it in the context of the alkali gases. For simplicity I confine myself below to the case of zero temperature.

In the recent alkali-gas literature one frequently finds reference made to two different ‘approximations’ [sic] (cf below) to the ground state of a dilute gas of bosons with repulsive effective interactions (positive \(a_s\) ) in a specified external potential. Those two approximations may be characterized qualitatively as follows (for a more quantitative treatment see, e.g., [4] sections V.A and VIII.B, and below): the first, known as the Gross–Pitaevskii (GP) approximation, is nothing but the special case of the Hartree approximation appropriate to condensed bosons: all atoms occupy the same orbital state (the ‘condensate’ state), which is determined self-consistently. The second is the Bogoliubov approximation, in which the condensate is ‘depleted’ by pairwise scattering of atoms into excited states. The general belief is that the GP and Bogoliubov approximations are respectively the zeroth- and first-order approximations in an expansion in the so-called ‘gas parameter’ \((na_s^3)^{1/2}\) (where \(n\) is a typical value of the particle density) (cf below).

In section 2 I will first amplify and quantify the above considerations, and then raise a question concerning the relation between the GP and Bogoliubov descriptions in the form of a (pseudo-)paradox. My experience in discussing this paradox with colleagues knowledgeable in the BEC area suggests that while it is readily recognized not to be a real or even serious one, its explicit resolution is not common knowledge in the field. I believe that this resolution is in fact implicit in some recent papers on the BEC problem, in particular those of Cherny and...
It may help the reader to appreciate the point of section 3 (indeed of the paper as a whole) if I add the following remarks: the conventional use of the phrase ‘GP approximation’ in the literature is to denote a state of the form (2.6), that is, a Hartree-like state with no nontrivial two-body correlations. On the other hand, in determining the correct form of the condensate wavefunction $\chi_0(r)$ in all but the trivial (uniform) case, an essential role is played by the two-body pseudopotential $U(r) = U_0 \delta(r)$ which enters the GP equation. But whether our original model is one of hard spheres or a realistic short-range interatomic potential, the interaction $U(r)$ is an effective potential, which neglects the presence of strong two-body correlations on the scale of the $s$-wave scattering length $a_s$. Thus the ‘GP approximation’ as usually understood is strictly speaking not self-consistent (see footnote 18 of [4]), and the part of the argument of section 3 which starts below equation (3.9) and ends above equation (3.21) may be viewed as exploring the consequences of an attempt to make it self-consistent.

2. Review of some basic ideas, and a (pseudo-)paradox

In order to set up the paradox and its resolution, I first remind the reader of some basic ideas concerning the physics of a dilute atomic Bose gas (for details see, e.g., [4] sections IV.A–D, V.A and VIII.A–C; however, see section 3 below for a caution regarding the last paragraph of section IV.B).

As is well known, for any physically reasonable interatomic potential the scattering of two identical spin-zero atoms at sufficiently low energies can be expressed in terms of the $s$-wave scattering length $a_s$; in particular, in the centre-of-mass (COM) frame the $s$-wave zero-energy solution to the time-independent Schrödinger equation (TISE) as a function of relative coordinates $r$ has the form

$$\psi_0(r) = A(1 - a_s/r) \quad (A = \text{constant}) \tag{2.1}$$

provided $r$ is much greater than the effective range $r_0$ of the potential. For $a_s > 0$ (the case of interest here) this form is identical, for $r > a_s$, to that for two hard spheres of radius $a_s/2$ (i.e. ‘exclusion radius’ $a_s$); however, we see that if $a_s > r_0$ (a condition which I will assume below without explicit comment) there is a region where the expression (2.1) is negative, and this has no direct analogue in the hard sphere problem. Given the expression (2.1), it is a well-known result that the effective interaction energy of the two atoms has the form

$$\langle E_{\text{int}} \rangle = (4\pi a_s \hbar^2/m) |A|^2. \tag{2.2}$$

For the two-particle problem the simplest way of establishing the result (2.2) is probably to constrain the relative coordinate $r$ to lie within a large (radius $R \gg a_s, r_0$) sphere with hard-wall boundary conditions and solve the TISE explicitly subject to the asymptotic ($r \ll R$) behaviour specified by (2.1). The generalization of (2.2) to the dilute many-particle problem can be obtained, for example, by the heuristic argument given in [4] section IV.C (or in many other ways): it is

$$\langle E_{\text{int}} \rangle = \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \sum_{ij} |\Psi(r_{ij} \sim 0)|^2 \tag{2.3}$$
where the notation \( r_{ij} \to 0 \), as explained in the cited reference, means that the distance \( r_{ij} \) between atoms \( i \) and \( j \) is large compared to \( a_s \) but small compared to all other characteristic lengths such as the mean interparticle separation \( n^{-1/3} \). In the literature, the result (2.3) is often expressed by saying that the true interatomic potential \( V(r) \) (which may in general be very complicated and contain both attractive and repulsive terms) may be replaced by an effective ‘contact’ potential (pseudopotential) of the form
\[
V_{ps}(r) = \left(4\pi a_s \hbar^2 / m\right) \delta(r) \equiv U_0 \delta(r)
\]  
(2.4)
so that
\[
\langle E_{\text{int}} \rangle = \frac{1}{2} \sum_{ij} \langle V_{ps}(r_i - r_j) \rangle
\]  
(2.5)
with, however, the stipulation that when evaluating the effects of this potential we must not double-count terms which are already taken into account in the transition from \( V \) to \( V_{ps} \).

The GP ansatz may now be defined as follows: we consider an arbitrary normalized single-particle wavefunction \( \chi_0(r) \), and define the associated creation operator to be \( a_0^+ \). We then make for the many-body wavefunction \( \Psi(r_1, r_2, \cdots, r_N) \) the ansatz
\[
\Psi(r_1, r_2, \cdots, r_N) = N \prod_{i=1}^{N} \chi_0(r_i) \equiv (N!)^{-1/2} (a_0^+)^N |\text{vac}\rangle
\]  
(2.6)
where \( N \) is the total number of particles and \( |\text{vac}\rangle \) denotes the vacuum; in words, all particles are assumed to be condensed into the same one-particle state \( \chi_0(r) \). The expectation value (2.5) of the interaction energy is then seen, from (2.4), to be given by
\[
\langle E_{\text{int}} \rangle = \frac{1}{2} \int d^3r |\chi_0(r)|^4.
\]  
(2.7)
We now combine (2.7) with the expressions for the expectation values of the kinetic and external-potential energies, and minimize the resulting expression with respect to the choice of the ‘condensate wavefunction’ \( \chi_0(r) \); this gives the well-known GP equation (nonlinear Schrödinger equation), and on substituting the lowest-energy solution into (2.6) we obtain the GP ansatz for the ground state, which then leads, via (2.7), to an expression for the total ground state energy (GSE). In the general case the latter may have to be evaluated numerically. However, for the simple (‘translation invariant’) case of a system in zero external potential with periodic boundary conditions (to which I will confine myself from now on) it is rather obvious (and follows from explicit implementation of the above procedure) that the condensate wavefunction \( \chi_0(r) \) is simply the single-particle ground state, \( \chi_0(r) = \Omega^{-1/2} \) where \( \Omega \) is the volume. Substituting this into (2.7) and noting that the kinetic energy associated with \( \chi_0 \) is in this case zero, we immediately obtain for the total GSE \( E_{\text{GP}}^{(0)} \) in the GP approximation
\[
E_{\text{GP}}^{(0)} = \frac{1}{2} \frac{N^2}{\Omega} \frac{4\pi \hbar^2 a_s}{m} \equiv \frac{1}{2} \frac{N^2}{\Omega} U_0.
\]  
(2.8)
It is worth noting that this expression leads to a nonzero bulk modulus of the system and thus to a speed of sound \( c_s \) given by
\[
c_s = (n U_0 / m)^{1/2} \quad (n \equiv N / \Omega).
\]  
(2.9)
I also note for future reference that there is a characteristic length associated with the GP ansatz, namely the ‘healing length’ $\xi$ defined by

$$\xi \equiv (8\pi na_s)^{-1/2}. \tag{2.10}$$

It is well known that in an inhomogeneous situation (for example near a wall) $\xi$ is the characteristic length over which the condensate wavefunction (order parameter) ‘heals’ to its bulk value; we shall see below that it is also in some sense a measure of the length required to ‘heal’ internally, from the effect of interatomic interactions. A very important role in the subsequent discussion is played by the fact that in the ‘dilute’ limit, namely $na_s^3 \ll 1$, $\xi$ is large compared to both the s-wave scattering length $a_s$ and the interparticle spacing $n^{-1/3}$.

I now turn to the Bogoliubov ansatz, confining myself as above to the translation-invariant case. In the literature, this ansatz is most commonly expressed, following the original paper [1], by relaxing the constraint of particle number conservation; however, since we wish to compare the result with that of the (particle-conserving) GP ansatz, it is necessary to write the Bogoliubov ansatz as the following explicitly particle-conserving ansatz for the ground state (cf [4], section VIII):

$$\Psi_N = N^{-1/2} \left( a_0^+ a_0^+ - \sum_q c_q a_q^+ a_{-q}^+ \right)^{N/2} \left| \text{vac} \right> \tag{2.11}$$

where for simplicity I have assumed that $N$ is even, and where $c_q$ is a variational parameter; $N$ is a normalization constant, which is of course a function of the $c_q$s. We now proceed as in the GP case, by evaluating the expectation value (2.5) of the interaction energy, adding that of the kinetic energy and minimizing the total energy so obtained as a function of the parameters $c_q$; the lowest energy so obtained is the GSE in the Bogoliubov approximation, and the corresponding values of the $c_q$s, when substituted in (2.11), give the Bogoliubov ansatz for the particle-conserving many-body ground state. The details of the procedure are sketched in [4], section VIII.B. It is necessary to note one point explicitly: as a result of the variational procedure, we find that in the limit of large $q$ the quantity $c_q$ is equal to $nU_0/2\epsilon_q$, leading (in three dimensions) to a divergent expression for the GSE (here and subsequently $\epsilon_q \equiv \hbar^2 q^2 / 2m$). This difficulty arises of course equally in alternative (particle-nonconserving) approaches, and is routinely resolved by noting that the terms in question have already been implicitly taken into account in the transition from $V$ to $V_{ps}$ and should therefore not be counted again. (An alternative and equivalent technique (see [3]) is to replace the $\delta$-function in equation (2.4) by the operator $\delta(r) \partial_\mathbf{r} (r \cdots)$.) Thus, one subtracts from the formally divergent GSE the appropriate term $-(nU_0)^2/2\epsilon_q$, and thereby obtains the following result for the GSE $E_{\text{Bog}}^{(0)}$ calculated in the Bogoliubov approximation:

$$E_{\text{Bog}}^{(0)} = \frac{1}{2} \frac{N^2}{\Omega} U_0 [1 + \alpha (na_s^3)^{1/2}] \tag{2.12}$$

where the positive numerical constant $\alpha$ is equal to $128/(15\sqrt{\pi})$. The result (2.12), with the given value of $\alpha$, was first obtained by Lee and Yang [6] in the context of the hard-sphere problem; it is re-derived and reproduced in many standard texts such as [7]. I note in parenthesis that the expression (2.12) may be regarded as the leading terms in a (nonanalytic) expansion of the GSE of a dilute repulsive Bose gas in the small parameter $\lambda \equiv (na_s^3)^{1/2}$, and that while it has long been known that the next term is proportional to $\lambda^2 \ln \lambda$, the calculational difficulties are sufficiently formidable that it has been only recently [8] that the complete expression to this order has been obtained (cf also [9], for the $\lambda^2$ term).
With the possible exception of the use of the particle-conserving form of the Bogoliubov approximation, (on which, however, see e.g. section 3 of [3]) the above results, and in particular equations (2.8) and (2.12), are entirely standard. We can now see the (pseudo-)paradox in stark form: we have two ansätze for the ground state of the \( N \)-particle system, namely the GP ansatz (2.6) and the Bogoliubov ansatz (2.11), and the general belief is that the latter is a more accurate description. However, if we compare the respective GSEs, namely the expressions (2.8) and (2.12), we see that \( E_{\text{GP}}^{(0)} < E_{\text{Bog}}^{(0)} \). Consequently, the GP description should \textit{prima facie} be a better description than the Bogoliubov one, contrary to the universally established wisdom.

I have deliberately set up, above, the background for the pseudo-paradox in such a way that the reader’s immediate reaction should be that it has to do with the fact that the two-body correlations embodied in equation (2.1) are not carried over into the GP ansatz (2.6) (cf [4], footnote 18). This is correct; however, in discussing the problem with colleagues it has been my experience that most believe that the reduction has something to do with the problem, mentioned above, of ‘double counting’ of the high-energy terms. In fact, as we shall see in the next section, this question is entirely irrelevant; the real issue relates not to an ultraviolet but to an infrared divergence.

Before proceeding to the resolution of the paradox, I would like to note a second question which turns out to be closely related to it, namely: do the corrections to the GP picture embodied in the Bogoliubov approximation increase or decrease the probability of finding two atoms close together in space? Intuitively, one might think that since the interaction is of the repulsive contact type, an improved approximation should decrease this probability (cf the remarks in [4], section VIII.A). However, we shall see in the next section that the question needs careful definition before we can give a sensible answer.

3. Resolution of the paradox

Let us consider an even number \( N \) of spinless atoms obeying Bose statistics and moving in a large volume \( \Omega \) subject to the standard periodic boundary conditions. The interatomic potential, \( V(r) \), is taken to be spherically symmetric, to possess a Fourier transform \( V_q \) and to be characterized by some effective range \( r_0 \), so that \( V_q \) tends to a constant for \( qr_0 \ll 1 \). The potential \( V(r) \) (which may in general be very complicated) is characterized by a positive low-energy s-wave scattering length \( a_s \) which I take to be \( \gtrsim r_0 \), and when we come to consider the many-body problem we shall assume the ‘dilute-gas’ condition \( na_s^2 \ll 1 \), where \( n \equiv N/\Omega \). In the following, the operator \( a_q^+(a_q) \) creates (destroys) a particle in the normalized plane-wave state \( \frac{1}{\sqrt{\Omega}} e^{iq \cdot r} \). I first consider the case \( N = 2, \Omega \to \infty \), set the centre-of-mass momentum equal to zero and seek the solution of the time-dependent Schrödinger equation for relative motion corresponding to zero-energy scattering, i.e. with an energy of order \( \Omega^{-1/2} \exp iq \cdot r \). The general form of the two-body wavefunction is

\[
\psi_2 = 2^{-1/2} \left( c_0^{(2)} a_0^+ a_0^+ - \sum_{q \neq 0} c_q^{(2)} a_q^+ a_{-q}^+ \right) |\text{vac}\rangle \tag{3.1}
\]

where the explicit separation out of the \( q = 0 \) state, and the minus sign, are introduced for subsequent convenience. We will see below that the ‘depletion’ of the \( q = 0 \) state, that is the quantity \( \sum_{q \neq 0} |c_q^{(2)}|^2 \), is proportional to a negative power of \( \Omega \), so in the limit \( \Omega \to \infty \) we may consistently take \( c_0^{(2)} \) to be equal to 1. Moreover, it is easy to establish that the energy is
minimized by choosing the coefficients $c_q^{(2)}$ to be real. Thus the expectation value of the two-body Hamiltonian, $(H)_2$, may be written in the form

$$
(H)_2 = \sum_{q \neq 0} 2\epsilon_q |c_q^{(2)}|^2 + \Omega^{-1} \left( V_0 - 2 \sum_{q \neq 0} V_q c_q^{(2)} + \sum_{q, q' \neq 0} V_{q-q'} c_q^{(2)} c_{q'}^{(2)} \right)
$$

(3.2)

where $\epsilon_q \equiv \hbar^2 q^2 / 2m$. Variation of the expression (3.2) with respect to the set of parameters $c_q^{(2)}$ yields the standard TISE, with an eigenvalue (at this stage unknown) of order $\Omega^{-1}$.

We now carry out a standard renormalization procedure to eliminate the ‘bare’ potential $V_q$ in favour of the scattering length $a_q$ or a related quantity. We choose a ‘cut-off’ value $q_c$ of $q$ which is small compared to $r_0^{-1}$; it is also convenient, though not essential, to choose it smaller than $(\pi/2)a_s^{-1}$. We then introduce a projector ($\hat{P}_2$) which projects on to the states $q > q_c$ and define the quantity (a matrix with constant elements $U_{qq'} \equiv U(q_c)$ for $q, q' < q_c$)

$$
U(q_c) = (1 + \hat{V}_2 \hat{H}_0)^{-1} \hat{V}
$$

(3.3)

where $\hat{V}$ is treated as a matrix with elements $\hat{V}_{qq'} \equiv V_{q-q'}$. Then, taking into account the fact that the eigenvalue of the TISE derived from (3.2) is of order $\Omega^{-1}$ and hence small compared to all the $\epsilon_q$ for $q \neq 0$, we find that $(H)_2$ can be rewritten in the form

$$
(H)_2 = \sum_{q \neq 0} 2\epsilon_q |c_q^{(2)}|^2 + (U(q_c) / \Omega) \left( 1 - 2 \sum_{q \neq 0} c_q^{(2)} + \sum_{q, q' \neq 0} c_q^{(2)} c_{q'}^{(2)} \right)
$$

(3.4)

when the sum now runs only up to the cut-off $q_c$. The associated TISE is easily solved, and we find that the GSE $E_0$ is given by the expression (where the notation anticipates the identification of $U_0$ below)

$$
E_0 = U_0 / \Omega
$$

(3.5)

where the quantity

$$
U_0 \equiv \frac{U(q_c)}{1 + U(q_c) \sum_{q < q_c} (2\epsilon_q)^{-1}} = \frac{U(q_c)}{1 + (m/2\pi^2\hbar^2)q_c U(q_c)}
$$

(3.6)

may be explicitly verified (by a further renormalization procedure) to be independent of $q_c$ (so that it may be taken as $\lim_{q_c \to 0} U(q_c)$). We may further verify that the coefficients $c_q$ are given, for $q < q_c$, by the expression

$$
c_q^{(2)} = (U_0 / \Omega)(2\epsilon_q)^{-1}.
$$

(3.7)

By comparing the resulting form of the relative wavefunction with the standard expression $\Omega^{-1/2}(1 - a_s/r)$, we see that $U_0$ is related to $a_s$ by the familiar formula (cf (2.4))

$$
U_0 = 4\pi \hbar^2 a_s / m
$$

(3.8)

so that (2.5) just reproduces the usual result for the two-body energy shift. The above argument is of course entirely standard except perhaps for the explicit introduction of a finite cut-off wavevector $q_c$, which we shall see below plays a useful role in the many-body calculation.
To conclude the discussion of the two-body problem, I note that the ‘depletion’ $\delta$ of the zero-momentum state is given by the expression (here I am interested only in possible low-energy divergences, so approximate the $c^{(2)}_q$ by their $q \to 0$ form)

$$\delta \equiv \sum_{q \neq 0} |c^{(2)}_q|^2 = (U_0^2/\Omega^2) \sum_{q \neq 0} (2\epsilon_q)^{-2} \sim \Omega^{-1} \int_{q_{\text{min}}} \text{d}^3 q/q^4$$

(3.9)

where $q_{\text{min}} \sim \Omega^{-1/3}$ is the smallest nonzero $q$-vector allowed by the boundary conditions. This expression is proportional to $\Omega^{-1} q_{\text{min}}^{-1} \sim 2^{-2/3}$, so the depletion indeed vanishes in the limit $\Omega \to \infty$, as we should intuitively expect (since in this limit the atoms never ‘see’ one another).

I now turn to the many-body case and consider the limit $N (= \text{even}) \to \infty, \Omega \to \infty, N/\Omega \equiv n = \text{constant}$. Let us first enquire how we might try to implement the GP ansatz for the many-body ground state while explicitly taking into account the two-particle effects considered above (cf the last paragraph of the introduction). It is clear that the naive ansatz (2.6) (with $\chi_0(r) = \Omega^{-1/2}$) is inadequate; the most obvious way of generalizing the two-particle wavefunction (3.1) to the many-body case is to allow the atoms to interact pairwise, i.e. to write

$$\Psi_N = \psi_2(r_1 - r_2)\psi_2(r_3 - r_4) \cdots \psi_2(r_{n-1} - r_n)$$

(3.10)

where $\psi_2(r)$ is the relative wavefunction of the two-particle problem, and then to symmetrize with respect to interchange of any pair, $r_i \equiv r_j$. Note that (3.10) is not of the form of a Jastrow function, $\prod_{i<j} \psi(r_i - r_j)$. In second-quantized notation the result of this procedure is the ansatz

$$\Psi_N = \text{constant}\left((a_0^+a_0^- - (N/2) \sum_{q \neq 0} c^{(2)}_q a_0^+ a_{-q}^+) \right)^{N/2} \left| \text{vac} \right>$$

(3.11)

The necessity for the odd-looking factor of $N/2$ multiplying the two-body coefficients $c^{(2)}_q$ may be seen by writing down the first few terms in an expression of the symmetrized version of (3.10) in powers of the deviation of $\psi_2(r_1 - r_2)$ from $\Omega^{-1/2}$. It is tempting to treat (3.11) as the ‘best guess’ at an explicit many-body implementation of the GP description.

However, such an assumption immediately leads to a contradiction: it is clear that since for small enough $q$ ($n U_0/4\epsilon_q > 1$, or equivalently $q < 1/(2\xi)$) the coefficient of $a_0^+a_0^+$ is greater than that of $a_0^+a_0^+$, and there are many such values of $q$, the state (3.11) does not correspond to $N_0 \equiv \langle a_0^+ a_0^- \rangle \sim N$, i.e. it is not Bose condensed, contrary to the basic assumption of the GP description! One might perhaps attempt to get around this difficulty by deleting, in (3.11), all the $c^{(2)}_q$’s for which (say) $q\xi < 1$. However, I will now show that such an ansatz, while corresponding to a nonzero degree of Bose condensation, is not the ground state. The proof simply consists in showing that the ansatz corresponding to the standard Bogoliubov approximation does better. Needless to say, this does not establish that the latter ansatz is the true ground state, even in the limit $na_3^3 \to 0$ (indeed, it would seem to be highly nontrivial to do this); however, it is adequate for the purposes of resolving the paradox which was stated in section 2. The argument below follows that of [4], section VIII.B.2, but treats explicitly (as that reference does not) the question of potential renormalization in the many-body case.

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1 I take this opportunity to note that the discussion in the last paragraph (only) of section IV.B of [4] is completely wrong and misleading (see erratum, submitted); in particular, there is no justification for equations (4.2) or (4.3) (for the correct result, see below). Fortunately, no subsequent results of [4] are affected.

2 Note that in [4, (8.9)] the sum should run over all nonzero $q$, and that some equations are misreferenced (see erratum, submitted).
We write down an ansatz for the many-body wavefunction which is a generalization of (3.11)

\[ \Psi_N = \text{constant} \left( a_0^+ a_0^+ - \sum_{q \neq 0} c_q a_q^+ a_{-q}^+ \right)^{N/2} |\text{vac}\rangle \]  

where we make the explicit assumption that all coefficients \( c_q \) are real and have magnitude less than unity. (Note that a value of \( c_0 \) different from 1 can be absorbed in the normalization constant.) For a wavefunction of the form (3.12), only a few terms in the Hamiltonian have nonzero expectation value; analogously to the terms kept in [4], section VIII.B, these are

(a) the kinetic energy terms

\[ \sum_{q \neq 0} \epsilon_q a_q^+ a_q \]  

(b) the Hartree terms,

\[ \frac{1}{2} \frac{V_0}{\Omega} \sum_{qq'} a_q^+ a_{q'}^+ a_q a_{q'} \equiv \hat{H}_F \]  

(c) the Fock terms,

\[ \frac{1}{2\Omega} \sum_{q \neq q'} V_{q-q'} a_q^+ a_{q'}^+ a_{-q} a_{-q'} \equiv \hat{H}_F \]  

(d) the pairing terms,

\[ \frac{1}{2\Omega} \sum_{q \neq q'} V_{q-q'} a_q^+ a_{q'}^+ a_{-q} a_{-q'} \equiv \hat{H}_P. \]

In writing (3.13), we have neglected terms of relative order \( N^{-1} \). Note in particular that in the two-particle case the Fock term simply adds (negligible) terms to \( \frac{3.13}{d} \) corresponding to \( q = -q' \).

We now use the fact that for a wavefunction of the form (3.12) a generalized ‘Hartree–Fock’ decoupling is valid to order \( N^{-1} \); that is, this order we can set \( \langle a_q^+ a_q a_{q'} a_{q'}^+ \rangle = n_q n_{q'} \), \( \langle a_q^+ a_{-q} a_{-q'} a_{q'}^+ \rangle \equiv x_q x_{-q} \), where \( n_q \equiv \langle a_q^+ a_q \rangle \) and \( x_q \equiv \langle a_{-q} a_q N \rangle \). Moreover, as argued in [4], section VIII.B, to calculate \( n_q \) and \( x_q \) for a specified value of \( q \) it is adequate to write the relevant factor in the many-body wavefunction in the form

\[ \Psi(q) = (N!)^{-1/2} \left( 1 - |c_q|^2 \right)^{1/2} (a_0^+ a_0^+ - c_q a_q^+ a_{-q}^+)^{N/2} |\text{vac}\rangle. \]

The expectation values are then explicitly

\[ n_q = \frac{|c_q|^2}{(1 - |c_q|^2)}, \quad x_q = \frac{c_q}{(1 - |c_q|^2)}. \]

Note that equation (3.15) uniquely determines the condensate number \( N_0 \equiv N - \sum_{q \neq 0} n_q \). Although this is of course a function of the \( c_q \)s, it is easily verified that it is consistent to neglect the term in \( \partial N_0 / \partial c_q \) when carrying out the variational calculation below.

Expressing \( n_q \) in terms of \( x_q \) by equation (3.15), and inserting in equations (3.13), we find for the expectation value of the Hamiltonian in the many-body state (3.12) the expression
\[
\langle H \rangle = \frac{1}{2} \frac{N^2}{\Omega} V_0 + \sum_{q \neq 0} \tilde{\epsilon}_q \left( \sqrt{x_q^2 + 1/4} - 1/2 \right) - n_0 \sum_{q \neq 0} V_q x_q + \frac{1}{2} \frac{1}{\Omega} \sum_{qq' \neq 0} V_{q-q'} x_q x_{q'} (n_0 \equiv (N_0 / \Omega))
\] (3.16)

where
\[
\tilde{\epsilon}_q \equiv \epsilon_q + n_0 V_q + \frac{1}{2} \sum_q V_{q-q} \left( \sqrt{x_q^2 + 1/4} - 1/2 \right) (\epsilon_q \equiv \hbar^2 q^2 / 2m)
\] (3.17)

(the factor of 1/2 is introduced to avoid double counting the Fock terms). The last term in equation (3.17) is clearly of order \( \delta \sim (n a_s^3)^{1/2} \) relative to the second term, and for simplicity I shall therefore omit it in what follows.

In the following I shall repeatedly use the assumption, which will be shown to be self-consistent, that \( x_q \) is small compared to 1 except when \( q \lesssim \xi^{-1} \ll a_s^{-1}, r_0^{-1} \). Let us first carry out a renormalization similar to that done for the two-particle case by introducing a cut-off \( q_c \) which we take to be large compared to \( \xi^{-1} \) but small compared to \( a_s^{-1}, r_0^{-1} \). We differentiate \( \langle H \rangle \) with respect to those \( x_q \) for which \( q > q_c \), and use the result to eliminate these variables in favour of a renormalized potential \( U(q_c) \) which, as in the two-particle case has constant matrix elements \( U_{qq'} \) for \( q < q_c \); since in the range \( q > q_c \), \( \tilde{\epsilon}_q \) is equal to \( \epsilon_q \) up to terms of relative order \( (q_s^2 \xi^2)^{-1} \sim n a_s^3 \) (cf below for the replacement of \( V_q \) by \( a_s \) in this estimate), the quantity \( U(q_c) \) is equal to its value for the two-particle problem to this order. The resulting expression is up to this order
\[
\langle H \rangle = \frac{1}{2} \frac{N^2}{\Omega} U(q_c) + \sum_{q \neq 0} \tilde{\epsilon}_q \left( \sqrt{x_q^2 + 1/4} - 1/2 \right) - n_0 U(q_c) \sum_{q \neq 0} x_q + \frac{1}{2} \frac{1}{\Omega} \sum_{q,q' \neq 0} x_q x_{q'}
\] (3.18)

when the sums over \( q \) now run only up to \( q_c \).

There is one thing that is a little disturbing about equation (3.18): namely, the expression for \( \tilde{\epsilon}_q \) still contains the bare potential \( V_q \) rather than the renormalized one \( U(q_c) \). This is actually a defect of the simple ‘pairing’ ansatz (3.10) for the many-body wavefunction, in fact, it is intuitively clear that the multiple-scattering processes which renormalize the \( q \to 0 \) form of \( V_q \) to \( U(q_c) \) must act equally on the Fock term in \( \tilde{\epsilon}_q \). Formally, this may be achieved by making in (3.11) the replacement (cf [5])
\[
a_q^+ a_0 \to a_q^+ a_0 + \sum_k c_k a_{k+q/2}^+ a_{k-q/2}
\] (3.19)

which may be regarded as the next step, after (3.10) itself, in a systematic approximation to the Jastrow form of the many-body wavefunction. Since this point is not the main focus of attention in this paper, I shall not discuss it further here, but will assume the result, namely that we may replace the Fock terms in the expression (3.17) by \( n_0 U_0 \), where \( U_0 \) is given by (3.6) and is related to \( a_s \) by (3.8). (It is clear that replacement of \( U_0 \) by \( U(q_c) \) would not change the results to the order we consider.) The expectation value (3.18) is then
Equation (3.20) will form the basis of our discussion.

We now compare the expression (3.20) with the corresponding expression in the two-particle case, namely (3.4), with the correspondence \(x_q \leftrightarrow c_q\). There is one rather trivial difference and two more significant ones.

1. The ‘driving’ term is \(N_0\) times what it is for the two-particle case (and the ‘Hartree’ term is \(\frac{1}{2}N^2\) times).

2. For large values of \(x_q\) the first term is proportional to \(|x_q|\) rather than to \(x_q^2\).

3. The first term contains, as well as the kinetic-energy contribution \(\epsilon_q\), the Fock contribution \(n_0U_0\), which remains finite for \(q \to 0\) (see section 4 for a discussion of the physical significance of this term).

Minimization of the expression (3.20) with respect to the parameters \(x_q\), leads, as we shall verify below, to the standard results of the Bogoliubov approximation. We anticipate at this point the result that the last term in (3.20) can be deleted at the expense of replacing \(U(q)\) by \(U_0\). To verify explicitly that the approximation (3.11), even if truncated so that the \(c_q^{(2)}\) are identically zero for \(q\xi < 1\), gives a higher energy, let us consider a value of \(q\) such that \(q\xi \gg 1\); in this limit it is consistent to assume that \(x_q\) is small compared to 1 and hence can be identified with the \(c_q\) parameter in (3.12). The ‘kinetic’ energy is just \((\epsilon_q + n_0U_0)|x_q|^2\). The choice of \(c_q\) corresponding to the truncated ansatz (3.11) is then simply \(n_0U_0/2\epsilon_q\). However, it is clear that the total energy associated with the pair state \(q\) which is so obtained is greater than that obtained from the correct value of \(x_q\), namely \((n_0U_0)^2/2(\epsilon_q + n_0U_0)\). Qualitatively similar considerations hold when \(q\xi\) is comparable to (but larger than) 1, though the situation is more complicated because now \(x_q\) is not small compared to 1; we note that if we were to neglect the nonlinear dependence of the Fock term on \(x_q^2\) and to substitute the ‘two-particle’ form \(x_q = n_0U_0/2\epsilon_q\) even for \(q\xi < 1\), the expectation value (3.20) would actually diverge because of the contribution of the low-\(q\) states.

The qualitative upshot of the above considerations is that the resolution of our original paradox has nothing to do with the ultraviolet processes which replace \(V_q\) by \(U(q)\) and (eventually) by \(U_0\), but is rather associated with the very low-energy pair states, \(q\xi \lesssim 1\), and is in some sense a consequence of the Fock term which is absent in the two-particle case but crucial in the many-particle one. For a physical interpretation of this result, see section 4.

The treatment given in this section differs from the one which is more or less standard in the literature, and is briefly referred to in section 2, in that it never introduces explicitly any \(\delta\)-function pseudopotential. It remains to show that it nevertheless reproduces the results of the standard treatment, in particular the expression (2.12) for the GSE up to the required order in \(\lambda \equiv (n\alpha_q^3)^{1/2}\), namely to order \(\lambda \cdot \frac{1}{2}N^2U_0/\Omega\) in the GSE (below we shall routinely abbreviate this as ‘to order \(\lambda\)’).

Setting the derivative of the expression (3.20) equal to zero gives

\[
\langle H \rangle = \sum_{q \neq 0}(\epsilon_q + n_0U_0)\left(\sqrt{x_q^2 + 1/4} - \frac{1}{2}\right) + U(q_c)\left\{\frac{1}{2}\frac{N^2}{\Omega} - n_0\sum_{q \neq 0}x_q + \frac{1}{2\Omega}\sum_{qq'}x_qx_{q'}\right\}.
\]

Equation (3.20)
where
\[ \lambda_q \equiv \frac{U(q_c)(N_0 - \eta)}{\tilde{\epsilon}_q} \]  
(3.22a)
\[ \eta = \sum_{q \neq 0} x_q \]  
(3.22b)
\[ \tilde{\epsilon}_q \equiv \epsilon_q + n_0 U(q_c) \rightarrow \epsilon_q + n_0 \tilde{U}_0 \]  
(3.22c)
(for the definition of \( \tilde{U}_0 \), and the second step in (3.22c), see below). Equation (3.22a) gives a self-consistent equation for \( \eta \):
\[ \eta = \frac{1}{2} \left( N_0 - \eta \right) U(q_c) \sum_{q \neq 0, q < q_c} \tilde{E}^{-1}_q(\eta) \]  
(3.23)
where
\[ \tilde{E}_q \equiv \left( \frac{\tilde{\epsilon}_q^2 - U^2(q_c)(N_0 - \eta)^2}{\Omega q} \right)^{1/2} \]  
(3.24)
From (3.23) we obtain
\[ U(q_c)(N_0 - \eta) = \frac{N_0 U(q_c)}{1 + U(q_c) \sum_{q < q_c} (2\tilde{E}_q)^{-1}} \equiv N_0 \tilde{U}_0. \]  
(3.25)
From (3.25) and (3.6) we see that the quantity \( \tilde{U}_0 \), which may be regarded intuitively as the ‘potential renormalized in the medium’, is related to \( U_0 \), the ‘potential renormalized in vacuum’ by the formula
\[ \tilde{U}_0 = \frac{U_0}{1 + \frac{1}{2}(U_0/\Omega) \sum_{q < q_c} (\tilde{E}^{-1}_q - \epsilon^{-1}_q)} \]  
(> \( U_0 \)).
(3.26)
Since the difference between \( \tilde{E}_q \) and \( \epsilon_q \) is of relative order \( (q_c \xi_0)^{-2} \sim n a^3 \) for \( q \sim q_c \), the value of \( \tilde{U}_0 \) is independent of \( q_c \) up to order \( \lambda \), and the difference between \( \tilde{U}_0 \) and \( U_0 \) (which we evaluate explicitly below) is itself of order \( \lambda \). The replacement of \( U(q_c) \) in (3.22c) by \( \tilde{U}_0 \) is not justified by the consideration that the relative difference is small (it is actually of order \( q_c a_n \), which need not be \( \ll 1 \)) but rather by an extension of the ‘self-consistency’ argument already used in connection with the Fock term in (3.18): see the last paragraph of this section. With this replacement we can write
\[ \tilde{E}_q \equiv (\tilde{\epsilon}_q^2 - n_0^2 \tilde{U}_0^2)^{1/2} = (\epsilon_q(\epsilon_q + 2n_0 \tilde{U}_0))^{1/2}. \]  
(3.27)
This is an implicit definition, since by (3.25) \( \tilde{U}_0 \) is itself a function of \( \tilde{E}_q \). Since it is straightforward to show (we shall not pause to do it here) that \( \tilde{E}_q \) is the energy of an excitation of wavevector \( q \), equation (3.23) ensures that the excitation spectrum has no gap, as required by the sum rules and the Hugenholtz–Pines theorem [10]. Moreover we can write the quantity \( n_q \) in the form (cf equations (3.21), (3.22a))
\[ n_q = \frac{1}{2} \left( \frac{\tilde{\epsilon}_q}{\tilde{E}_q} - 1 \right). \]  
(3.28)
We now return to the expectation value (3.20) of the Hamiltonian in the state (3.12), and rewrite it in the form

\[ \langle \hat{H} \rangle = H_1 + H_2 \]  

(3.29a)

\[ H_1 \equiv \frac{1}{2} \frac{U(q_0)}{\Omega} (N^2 - N_0^2) \]  

(3.29b)

\[ H_2 \equiv \frac{1}{2} \sum_{q \neq 0} \left( \frac{\tilde{E}_q}{E_q} - 1 \right) \frac{1}{2} \frac{U(q_0)}{\Omega} (N_0 - \eta)^2. \]  

(3.29c)

We first consider the expression \( H_2 \). Using equation (3.25), subtracting a term \( \frac{1}{2} n_0^2 \tilde{U}_0^2 \sum_q \tilde{E}_q^{-1} \) from the first (‘kinetic’) term in (3.29c) and adding it to the ‘potential’ term, we obtain the result

\[ H_2 = \frac{1}{2} \frac{N_0^2}{\Omega} \tilde{U}_0 + \frac{1}{2} \sum_{q \neq 0} \left( \tilde{E}_q - \tilde{E}_q + n_0^2 \tilde{U}_0^2 / 2 \tilde{E}_q \right). \]  

(3.30)

Now we turn to \( H_1 \). This expresses the part of the Hartree term arising from (a) condensate–noncondensate and (b) noncondensate–noncondensate interactions (the second is actually of order \( \lambda^2 \), but we keep it for completeness). Since we have already argued that in the Fock terms a consistent calculation (which implicitly goes beyond the ansatz (3.12)) should result in the replacement of \( U(q_0) \) by \( \tilde{U}_0 \), we make the same replacement in \( H_1 \). Thus our final result is

\[ \langle H \rangle = \frac{1}{2} \frac{N^2}{\Omega} \tilde{U}_0 + \frac{1}{2} \sum_{q \neq 0} (\tilde{E}_q - \tilde{E}_q + n_0^2 \tilde{U}_0^2 / 2 \tilde{E}_q) \]  

(3.31)

where we recall that

\[ \tilde{E}_q \equiv \epsilon_q + n_0 \tilde{U}_0, \quad \tilde{E}_q \equiv (\tilde{E}_q^2 - n_0^2 \tilde{U}_0^2)^{1/2}. \]  

(3.32)

Note that the expression in curly brackets tends to zero as \( q^{-6} \) for \( q \xi_0 \gg 1 \); thus not only is no counter-term necessary but the value of the sum is independent of the upper cut-off \( q_c \).

We now compare the expression (3.31) for the GSE with that routinely derived and quoted in the literature using the pseudopotential approach (see, e.g., [11], equation (25.13), though beware of differences in notation) namely

\[ \langle H \rangle = \frac{1}{2} \frac{N^2}{\Omega} U_0 + \frac{1}{2} \sum_{q \neq 0} (E_q - \epsilon_q + n_0^2 U_0^2 / 2 \epsilon_q) = \frac{1}{2} \frac{N^2}{\Omega} U_0 \left( 1 + \frac{128}{15 \sqrt{\pi} \lambda} \right) \]  

(3.33)

where

\[ \epsilon_q \equiv \epsilon_q + n_0 U_0, \quad E_q \equiv (E_q^2 - n_0^2 U_0^2)^{1/2}. \]  

(3.34)

The expressions (3.31) and (3.33) are not equal term by term; in fact, as already noted, the ‘Hartree’ term (that simply proportional to \( N^2 \)) differs by an amount of relative order \( \lambda \). However, an explicit evaluation of the second term in (3.31) leads to the expression \( \langle H \rangle = \frac{1}{2} \frac{N^2}{\Omega} \tilde{U}_0 \left( 1 + \frac{8}{10 \sqrt{\pi} \lambda} \right) \), where \( \tilde{\lambda} \equiv (n_0^2 \tilde{U}_0^2)^{1/2} \) and \( \tilde{a}_s \equiv m \tilde{U}_0 / 4 \pi \hbar^2 \). Further, explicit evaluation of the sum in the denominator of (3.25) yields
\[ \tilde{U}_0 = U_0 \left( 1 - \frac{8}{\sqrt{\pi}} \lambda \right). \]  

(3.35)

Since the difference between \( \tilde{\lambda} \) and \( \lambda \) is itself of relative order \( \lambda \), we may therefore write (3.31) in the form, valid to order \( \lambda \),

\[ \langle H \rangle = \frac{1}{2} \frac{N^2}{\Omega} U_0 \left( 1 + \frac{8}{\sqrt{\pi}} \lambda \right) \left( 1 + \frac{8}{15 \sqrt{\pi}} \lambda \right) \approx \frac{1}{2} \frac{N^2}{\Omega} U_0 \left( 1 + \frac{128}{15 \sqrt{\pi}} \lambda \right) \]  

(3.36)

in agreement with (3.33). Thus, the method used in this section correctly reproduces the lowest-order ‘Bogoliubov’ corrections to the GP expression for the GSE.

One remark needs to be added concerning our treatment above, of the Hartree and Fock terms, which may seem a little cavalier and arbitrary. Of course, in the general case (\( \lambda \equiv (na_s^3) \frac{1}{2} \) perhaps comparable to 1) we have no guarantee that (for example) the correct renormalization of the Fock term will be independent of \( q \) and equal to the quantity we have called \( \tilde{U}_0 \). However, in the case \( \lambda \ll 1 \) we know on rather general grounds that the values of \( q \) excited (and thus contributing to the Fock term) will be at most of order \( \xi^{-1} \), and it is then relatively easy to see that any corrections due to this consideration will be of higher order in \( \lambda \) than the ones kept. Whether the extension of the method used here into the regime \( \lambda \gtrsim 1 \) might form a useful jumping-off point for a more accurate treatment of this regime is a question I shall not attempt to discuss here.

4. Discussion

In effect, the solution of the pseudo-paradox raised in this paper is that once the two-particle scattering is properly accounted for, the GP ‘approximation’ is actually not a well-defined approximation for the many-body wavefunction at all; any attempt to define such an approximation ends up either simply reproducing the Bogoliubov results or yielding an energy larger than the Bogoliubov one. Needless to say, this in no way invalidates the use, very common in the literature for spatially nonuniform situations, of the GP expression for the GSE as an approximation (to lowest order in \( \lambda \equiv (na_s^3)^{1/2} \)) to the Bogoliubov value.

It may be instructive to look at the original paradox and its resolution from a ‘coordinate-space’ point of view. We recall the well-known result that the effective interactions between two identical spinless bosons which are in different plane-wave states is twice as strong as when they are in the same state (this effect is just what is represented by the ‘Fock term’ in the Hamiltonian). Consider now the mutual scattering of two condensate particles. The unperturbed wavefunction has no Fock term. However, if we substitute the ‘two-particle’ result \( \psi(r) \sim \text{constant}(1 - a_s/r)(r \equiv |r_1 - r_2|) \), then the probability of one of the particles having finite wavevector \( q \) is proportional to \( q^{-4} \). When this particle then interacts with a third particle, the Fock term comes into play and gives a large (actually divergent) repulsive energy. Thus, it is essential to modify the two-particle correlation function so that it falls off faster than \( 1/r \) at large distances. In fact, the many-body effects which are embodied in the Bogoliubov approximation do just that; the relevant expressions were given long ago, in the context of the hard-sphere problem, by Lee et al [3] (their equations (43)–(48)), and we see that while for \( r \ll \xi (\equiv r_0 \) in the notation of [3]) the two-particle density–density correlation function is indeed proportional to \( (1 - a_s/r)^2 \), for \( r \gtrsim \xi \) the correction to unity falls off much faster. In the light of the above it is not entirely clear that a unique meaning can be given to the question ‘does the Bogoliubov
approximation increase or decrease the probability of finding two atoms close together relative to the GP approximation? If by ‘GP approximation’ we simply mean literally \( \Psi = \text{constant} \) then of course the probability is decreased (for all \( r \)); if on the other hand we mean something like the Jastrow-type function \( \prod_{i<j} (1 - a_i/r_{ij}) \), then it is increased at long distances (\( r \gtrsim \xi \)); one can regard this as an ‘internal healing’ effect (cf the remarks of Lee et al [3] on this point).

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