The kinetic and interaction energies of a trapped Bose gas: Beyond the mean field

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The kinetic and interaction energies of a three-dimensional (3D) dilute ground-state Bose gas confined in a trap are calculated beyond a mean-field treatment. They are found to depend on the pairwise interaction through two characteristic lengths: the first, \(a\), is the well-known scattering length and the second, \(b\), is related to the latter by \(b = a - \lambda \partial a / \partial \lambda\) with \(\lambda\) being the coupling constant. Numerical estimations show that the pairwise interaction energy of a dilute gas of alkali atoms in a trap is negative (in spite of the positive scattering length); its absolute value is found by about the order of magnitude larger than that of the mean-field interaction energy that corresponds to the last term in the Gross-Pitaevskii (GP) functional.

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It is known that the total energy \(E\) of a dilute 3D Bose gas confined in a trap can be represented at \(T \ll T_c\) (\(T_c\) is the temperature of the Bose-Einstein condensation) as the functional of the order parameter \(\phi = \phi(r) = \langle \hat{\psi}(r) \rangle\) (here \(\hat{\psi}(r)\) is the Bose field operator)

\[
E = \int d^3r \left[ \frac{\hbar^2}{2m} \nabla \phi^2 + V_{\text{ext}}(r) |\phi|^2 + \frac{2\pi \hbar^2 a}{m} |\phi|^4 \right],
\]

called the Gross-Pitaevskii functional. In Eq. (1) \(V_{\text{ext}}(r)\) denotes an external trapping field with the characteristic length \(L\), typical for the spatial variation of this field [for a harmonic trap, \(L \approx a_{ho} = \sqrt{\hbar/(m \omega_{ho})}\)], and \(|a| \ll L\) stands for the scattering length in a gas considered. From the definition it follows that the order parameter satisfies the normalization condition \(\int d^3r |\phi|^2 = N\), where the number of bosons \(N_0\) in the Bose-Einstein condensate is replaced by their total number \(N\) due to a small condensate depletion. The stationary solution corresponding to the minimum of the functional (1) obeys the relations

\[
\delta(E - \mu N)/\delta \phi^*(r) = \delta(E - \mu N)/\delta \phi(r) = 0,
\]

which give the GP equation

\[
\mu \phi = -\frac{\hbar^2 \nabla^2 \phi}{2m} + V_{\text{ext}}(r) \phi + \frac{4\pi \hbar^2 a}{m} |\phi|^2 \phi.
\]

The term \(\mu N\) appears in Eq. (2) due to the normalization condition, and the Lagrange multiplier \(\mu\) is nothing but the chemical potential. In this paper we address the problem of interpretation of different terms in the GP functional; namely, the kinetic \(E_{\text{kin}}\) and pairwise interaction \(E_{\text{int}}\) energies are under investigation below. Note that this is of actual interest because analysis of the experiments with magnetically trapped Bose gases is carried out usually in terms of \(E_{\text{kin}}\) and \(E_{\text{int}}\). Moreover, the problem of that interpretation is rather ambiguous due to just opposite points of view on this subject found in the literature. Indeed, in the paper \(E_{\text{int}}\) the third term of the GP functional is treated as the energy of the pairwise boson interaction. While according to another point of view \(E_{\text{int}}\), in the homogeneous case \(V_{\text{ext}} = 0\) this term makes contribution only to the kinetic energy if the boson-boson interaction potential \(V(r)\) is of the hard-sphere form: \(V(r) = +\infty\) at \(r < a\), and \(V(r) = 0\) at \(r \geq a\).

This problem is usually considered to be trivial \(E_{\text{int}}\). Indeed, in the mean-field interpretation \(E_{\text{int}}\), the terms in Eq. (2) are associated with the kinetic energy, the energy of interaction with the external field, and the pairwise interaction energy, respectively. However, in the particular case \(V_{\text{ext}} = 0\), this interpretation contradicts both the results of Lieb and Yngvason \(E_{\text{int}}\) and ours \(E_{\text{int}}\). To have an understanding of the situation, let us calculate the kinetic and interaction energies of a trapped Bose gas on a solid theoretical basis beyond the mean-field interpretation of the terms of the GP functional. This can be realized with the help of the well-known variational theorem for the grand canonical potential at zero temperature \(\delta \Omega = \delta(E - \mu N) = \delta(H - \mu \bar{N})\), where \(\bar{\cdots}\) stands for the statistical average over the grand canonical ensemble. To calculate the pairwise interaction energy \(E_{\text{int}} = \langle \sum_{i\neq j} V(|r_i - r_j|)/2 \rangle\), it is useful to introduce the coupling constant \(\lambda [V(r) \rightarrow \lambda V(r)\), and \(\lambda = 1\) in final formulas]. Then the thermodynamic variational theorem leads to \(E_{\text{int}} = \partial \langle E - \mu N \rangle / \partial \lambda\), which, in conjunction with Eqs. (1) and (2), yields

\[
E_{\text{int}} = \frac{1}{2} \left\langle \sum_{i\neq j} V(|r_i - r_j|) \right\rangle = \frac{2\pi \hbar^2 \partial a}{m} \int d^3r |\phi|^4.
\]

where \(\phi\) is the stationary order parameter obeying the GP equation (3). Being the characteristic of the two-body problem, the derivative \(\partial a / \partial \lambda\) is obtained from the other variational theorem proved in the papers \(E_{\text{int}}\) for the short-range pairwise interaction potentials that go to zero at \(r \rightarrow \infty\) as \(V(r) \rightarrow 1/r^m\) \((m > 3)\), or even faster. The particular variant of this theorem allows for connecting the infinitesimal change of the scattering length \(\delta a\) with that of the potential \(\delta V(r)\):
\[ \delta a = \frac{m}{4\pi \hbar^2} \int d^3r \left[ \varphi^{(0)}(r) \right]^2 \delta V(r), \]

where \( \varphi^{(0)}(r) \) is the s-wave solution of the two-body Schrödinger equation in the center-of-mass system

\[ -(\hbar^2/m) \nabla^2 \varphi^{(0)}(r) + V(r) \varphi^{(0)}(r) = 0. \]

Equation (5) corresponds to the scattering state with the momentum \( p = 0 \), and its solution \( \varphi^{(0)}(r) \) is chosen to be real due to the real boundary condition \( \varphi^{(0)}(r) \rightarrow 1 - a/r \) at \( r \rightarrow \infty \). This boundary condition and Eq. (6) yield the following relation:

\[ \frac{4\pi \hbar^2 a}{m} = \int d^3r V(r) \varphi^{(0)}(r). \]

Equations (5) and (6) lead to

\[ \lambda \frac{\partial a}{\partial \lambda} = \frac{m}{4\pi \hbar^2} \int d^3r \lambda V(r) \left[ \varphi^{(0)}(r) \right]^2 = a - b, \]

where we put by definition

\[ b = \frac{1}{4\pi} \int d^3r \left| \nabla \varphi^{(0)}(r) \right|^2. \]

From Eq. (7) it follows that \( b \) is a positive quantity and can be considered as a new characteristic length, which is not expressed in terms of \( a \) and depends on a particular shape of the interaction potential \( V(r) \). For example, for the hard spheres \( V(r) = +\infty \) at \( r < a \), and \( V(r) = 0 \) at \( r \geq a \) we have \( b = a \). While for \( V(r) \) close to zero, in the weak-coupling regime, we obtain \( b \ll |a| \).

Thus, Eq. (7), taken together with Eq. (8), gives

\[ E_{\text{int}} = \frac{2\pi \hbar^2}{m} (a - b) \int d^3r \left| \phi \right|^4. \]

In the same manner, using the thermodynamic variational theorem with respect to \( \lambda V_{\text{ext}}(r) \), one obtains for the energy of interaction with the external field

\[ E_{\text{ext}} = \left\langle \sum_i V_{\text{ext}}(r_i) \right\rangle = \int d^3r V_{\text{ext}}(r) \left| \phi \right|^2. \]

In turn, the kinetic energy can be calculated by using Eqs. (9), (10) and (11) with the result

\[ E_{\text{kin}} = \left\langle \sum_i \frac{p_i^2}{2m} \right\rangle = \int d^3r \left[ \frac{\hbar^2}{2m} \left| \nabla \phi \right|^2 + \frac{2\pi \hbar^2 b}{m} \left| \phi \right|^4 \right]. \]

Thus, the thermodynamic variational theorem and mean-field treatment [the latter leads to Eqs. (10) and (12) but with \( b = 0 \)] yield in general different results for the kinetic and pairwise interaction energies of a trapped Bose gas. Here one should not be confused by the fact that the GP equation is usually considered to be a product of the mean-field approach. Though it has originally been derived by means of this approach, there exists the rigorous derivation of the GP functional beyond the mean-field approximation. Worth mentioning that this approximation has recently been demonstrated to face significant problems in the strong-coupling regime. The point is that the mean-field approach yields the correct result for the total energy of a Bose gas of strongly interacting particles (strictly speaking, after removing the ultraviolet divergence). However, it fails to give any information about nature of the kinetic and interaction energies. We stress that this only concerns the strong-coupling case. There is no problem with the mean-field theory in the weak-coupling regime, when \( b/|a| \ll 1 \), and, hence, one can approximately put \( b = 0 \) in Eqs. (10) and (12). Note that in the uniform case \( V_{\text{ext}} = 0 \) the GP equation gives \( \phi = \text{const} = \sqrt{n} \) (here \( n = N/V \) is the density of bosons), and Eqs. (10) and (12) are reduced to the results

\[ E_{\text{int}}/N = 2\pi \hbar^2 n(a - b)/m, \quad E_{\text{kin}}/N = 2\pi \hbar^2 nb/m, \]

derived earlier by the present authors.

Mathematically rigorous, the derivation of the GP functional does not give any information about nature of the third term in Eq. (12). This nature becomes, of course, clear from Eqs. (10) and (12), but the method of obtaining them is also rather formal. For a more deep insight, let us find out what approximations for the reduced density matrices result in Eqs. (10) and (12). Introducing the one-body (1-matrix) \( F_1(r, r') = \langle \psi^\dagger(r) \psi(r') \rangle \) and two-body (2-matrix) \( F_2(r_1, r_2; r'_1, r'_2) = \langle \psi^\dagger(r_1) \psi^\dagger(r_2) \psi(r'_2) \psi(r'_1) \rangle \) density matrices, one writes

\[ E_{\text{ext}} = \int d^3r V_{\text{ext}}(r) F_1(r, r), \]

\[ E_{\text{int}} = \frac{1}{2} \int d^3r d^3r' V(|r - r'|) F_2(r, r'; r, r'). \]

The 1-matrix can be expanded in the orthonormal set of its eigenprojectors as

\[ F_1(r, r') = N_0 \phi_0^\dagger(r) \phi_0(r') + \sum_{i \neq 0} n_i \phi_i^\dagger(r) \phi_i(r'). \]

Here \( \phi_0(r) = \phi(r)/\sqrt{N_0} = \langle \hat{\psi}(r) \rangle/\sqrt{N_0} \) is the eigenfunction corresponding to the macroscopic eigenvalue \( N_0 \), \( \int d^3r' F_1(r', r) \phi_0(r') = N_0 \phi_0(r), \int d^3r |\phi_0(r)|^2 = 1 \), see, e.g., Ref. [2]. By definition, the one-body matrix is normalized as \( \int d^3r F_1(r, r) = N \); therefore, in the case of a small condensate depletion \((N - N_0)/N \ll 1\) one can put

\[ F_1(r, r') \approx \langle \hat{\psi}^\dagger(r) \rangle/\langle \hat{\psi}(r') \rangle, \]

which, taken together with Eq. (13), results immediately in Eq. (11). Note that the calculation of the second term of the kinetic energy involves the 1-matrix requires knowledge of the other eigenvalues and eigenfunctions of \( F_1(r, r') \). However, this calculation is not
really needed because, when treating a trapped Bose gas on the basis of the microscopical information concerning the one-body and two-body matrices, we are able to restrict ourselves only to derivation of Eqs. (11) and (11). As to Eq. (12), it can be determined from the relation $E = E_{\text{kin}} + E_{\text{ext}} + E_{\text{int}}$ with the help of Eqs. (9), (10), and (12). Let us repeat one more that the second term in Eq. (12) is exactly due to the second term in Eq. (15). For this reason, the approximation for the momentum distribution $n_\mathbf{p} \approx \vert \phi (\mathbf{p}) \vert^2$ (where $\phi (\mathbf{p})$ is the Fourier transform of the order parameter) is able to produce only the first term in Eq. (12).

Explicit expressions for a number of eigenvalues and eigenfunctions of the two-body matrix have been obtained for a homogeneous system of bosons in the paper [10] and were then successfully employed in the papers [11]. In particular, the anomalous two-operator (quasi-) average \( \langle \hat{\psi} (\mathbf{r}_1) \hat{\psi} (\mathbf{r}_2) \rangle / \sqrt{N_0 (N_0 - 1)} \) was shown to be the eigenfunction (pair wave function) of the 2-matrix, corresponding to the maximum macroscopic eigenvalue $N_0 (N_0 - 1) \approx N_0^2$, which is nothing else but the number of pairs of bosons in the Bose-Einstein condensate. This result is also valid for a non-uniform (trapped) Bose system. In the homogeneous case, this average, contrary to the situation for the Fermi systems [11], describes the scattering (not bound) state of a pair of the condensed bosons. From this interpretation it follows that at small separations the pair wave function $\langle \hat{\psi} (\mathbf{r}_1) \hat{\psi} (\mathbf{r}_2) \rangle / \sqrt{N_0 (N_0 - 1)}$ should be proportional to the two-body wave function $\varphi^{(0)} (r)$ obeying the Schrödinger equation (11). On the other hand, the Bogoliubov principle of the correlation weakening [11] yields $\langle \hat{\psi} (\mathbf{r}_1) \hat{\psi} (\mathbf{r}_2) \rangle \rightarrow \langle \hat{\psi} (\mathbf{r}_1) \rangle \langle \hat{\psi} (\mathbf{r}_2) \rangle$ when $|r_1 - r_2| \rightarrow \infty$. From the physical point of view, the latter limit implies $|r_1 - r_2| \gg l_{\text{coh}}$, where the length of coherence $l_{\text{coh}} = 1/\sqrt{\pi m a}$ (here $n \approx |\varphi (\mathbf{r}_1)|^2 \approx |\varphi (\mathbf{r}_2)|^2$ is the local density) is assumed to obey the inequalities $|a| \leq l_{\text{coh}} \ll L$. Therefore, we arrive at the following approximation:

$$\langle \hat{\psi} (\mathbf{r}_1) \hat{\psi} (\mathbf{r}_2) \rangle \approx \varphi (\mathbf{r}_1) \varphi (\mathbf{r}_2) \varphi^{(0)} (|\mathbf{r}_1 - \mathbf{r}_2|).$$

(16)

Remind that $\varphi^{(0)} (r)$ is the solution of Eq. (11) with the asymptotics $\varphi^{(0)} (r) \rightarrow 1 - a/r$ for $r \rightarrow \infty$. We stress that the approximation (14) works well at $|r_1 - r_2| \leq l_{\text{coh}}$. By analogy with the 1-matrix, the small condensate depletion leads to the representation

$$F_2 (\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1', \mathbf{r}_2') \approx \langle \hat{\psi} (\mathbf{r}_1) \hat{\psi} (\mathbf{r}_2) \rangle \langle \hat{\psi} (\mathbf{r}_2') \hat{\psi} (\mathbf{r}_1') \rangle,$$

(17)

which, with the help of Eqs. (14) and (15), yields

$$E_{\text{int}} = \frac{1}{2} \int d^3r d^3r' V (|\mathbf{r} - \mathbf{r}'|) \varphi^{(0)} (|\mathbf{r} - \mathbf{r}'|)^2 \times \| \varphi (\mathbf{r}) \|^2 \| \varphi (\mathbf{r}') \|^2.$$  

(18)

Finally, using the inequality $L \gg a$ valid in the GP approximation and the theorem (13) at $\lambda = 1$, we arrive at Eq. (14).

In order to estimate the ratio $b/a$ typical for the alkali atoms, we make use of the model potential

$$V (r) = \begin{cases} +\infty, & r \leq r_0, \\ -\hbar^2 a^4 / (m r^6), & r > r_0. \end{cases}$$

(19)

It is usually considered (see, e.g., [13]) to be relevant in the situation of interest. This model interaction leads [13] to the scattering length

$$a/r_c = \Gamma (3/4) J_{-1/4} (x_0) / [2 \Gamma (5/4) J_{1/4} (x_0)].$$

(20)

Here $x_0 = r_c^2 / (2r_0^2)$; $J_{\nu} (x)$ and $\Gamma (z)$ denote the Bessel function and the Euler gamma-function, respectively. Further, calculating $\partial a / \partial \lambda$ with Eq. (20) ($r_c \rightarrow \lambda^{1/4} r_c$ in Eq. (17)) and, then, using Eqs. (6) and (21) at $\lambda = 1$, we arrive at

$$b/a = 3/4 + 1 / [\pi \sqrt{2} J_{1/4} (x_0) J_{-1/4} (x_0)].$$

(21)

For the potential (19), the parameter $x_0$ is connected with the number of the bound states for the two-body problem: larger the number, larger $x_0$. It is well-known that this number is equal to that of the nodes of the wave function $\varphi^{(0)} (r)$ obeying Eq. (11). The pairwise interaction of alkali atoms is characterized by large amount of possible bound pair states, which, however, kinetically inaccessible in the trapped systems [14]. So, we are interested in the regime when $x_0 \gg 1$. According to Eq. (21), $b/a \gg 1$ at $x_0 \gg 1$. The same situation ($b/a \gg 1$) takes place also at any $x_0$ provided the denominator in Eq. (20) is close to zero (as in the case of the Feshbach resonance). The large value of $b/a$ means that the second term in Eq. (12) is positive and much larger than the absolute value of the third term in the GP functional, while the pairwise interaction energy (14) is negative and close, in absolute value, to the second term of Eq. (12).

In other words, for a homogeneous dilute Bose gas of alkali atoms [when the first term in Eq. (12) equals to zero] we can expect $E_{\text{kin}} \approx | E_{\text{int}} | \gg | E |$. In order to obtain numerical estimations for sodium atoms, we utilize the data of Ref. [14] $r_c = 88.1 a_0$ and $a = 52 a_0$ ($a_0$ is the Bohr radius). Note that, at any $r_c$ and $a$, solutions of Eq. (20) for the core radius $r_0$ form an infinite sequence, approaching zero; each of the solutions for $r_0$ corresponds to a certain number $N_{\text{node}}$ of the nodes of $\varphi^{(0)} (r)$. Numerical results for $b/a$ versus $N_{\text{node}}$ are shown in Fig. 1(a). A typical solution of the Schrödinger equation (11) with the potential (19) corresponding to $N_{\text{node}} = 12$ [and, hence, $r_0 = 10.0 a_0$] is given in Fig. 1(b). Now, the Na-Na interaction is expected [14] to provide more than 15 possible bound states, and, thus, we have the estimation $b/a \gtrsim 20$ [see Fig. 1(a)]. We remark that the visible linear dependence of $b/a$ on the number of the nodes is a specific feature of the attractive interatomic potential proportional to $1/r^6$ but not a general relation between $b$ and $a$. We also stress that the pair distribution function of sodium atoms given in Fig. 1(c) is equal to zero
interacting via the potential (19) with $N_g r_{\text{at}}$. The pairwise interaction energy has been derived beyond the mean-field interpretation (12) of a 3D dilute ground-state Bose gas confined in a trap (10) involves the positive parameter $r_c = 88.1 a_0$. This ratio is equal to $E_{\text{kin}}/E$ for a homogeneous dilute Bose gas of sodium atoms. (b) The wave function $\varphi^{(0)}(r)$ for the model potential (19) with $N_{\text{node}} = 12$. (c) The pair distribution function $g(r_1 - r_2) = F_2(r_1, r_2; r_1, r_2)/[|\varphi(r_1)|^2|\varphi(r_2)|^2] \approx [\varphi^{(0)}(r_1 - r_2)]^2$ [see Eqs. (10) and (19)] in a trapped sodium atom, interacting via the potential (19) with $N_{\text{node}} = 5$. Intensive oscillations occur when $r \lesssim a = 52 a_0$.

at $r = 0$, contrary to the expectations [3] inspired by the mean-field treatment.

In conclusion, the kinetic and interaction energies (10)- (12) of a 3D dilute ground-state Bose gas confined in a trap have been derived beyond the mean-field interpretation. The pairwise interaction energy $E_{\text{int}}$ is found to be controlled by the two characteristic lengths: in addition to the well-known scattering length $a$ [Eq. (3)], the expression (10) involves the positive parameter $b$ [Eq. (3)]. Whereas the kinetic energy (12) depends on the pairwise interaction only through the characteristic length $b$. The derived estimations suggest that in the experimentally interesting case of a dilute Bose gas of alkali atoms the part of the kinetic energy coming from the pairwise interaction is much larger than the absolute value of the third term in the GP functional (1).

Note that experimental observation of $E_{\text{kin}}$ and $E_{\text{int}}$ is quite possible provided the diagonal element of the 2-matrix $F_2(r, r'; r, r')$ (the familiar pair distribution function) and the momentum occupation number $n_p = \langle a_p^\dagger a_p \rangle$ are experimentally determined. Indeed, the pairwise interaction energy is then calculated by means of Eq. (14) with the pairwise potential $V(r)$ that can be found numerically (see, e.g., Ref. [14]). The kinetic energy per particle can be represented as

$$E_{\text{kin}}/N = \int \frac{d^3 p}{(2\pi)^3} \frac{\hbar^2 p^2}{2m} n_p/\pi^2 \approx 52 a_0.$$  (22)

The quantities $F_2$ and $n_p$ are the well-known subjects of experimental investigations in the condensed matter physics, and there is technique of measuring these quantities (see, e.g., discussion in Ref. [15]). However, in the situation of interest, the trouble point is that, in order to calculate $E_{\text{kin}}$, one needs to know $n_p$ beyond the phonon regime for $p \gtrsim h/a$ because the contribution of the phonon region is small in the integral in Eq. (22).

Moreover, measurements with sufficiently small step in the momentum direction are of importance here to integrate properly in Eq. (22). The same is related to Eq. (14), where the short-range behaviour $|r - r'| \lesssim a$ of the pair distribution function $F_2(r, r'; r, r')$ is of importance. For this reason, accurate data are needed for the static structure factor at $p \gtrsim h/a$. Moreover, one again needs to make fine step-by-step measurements. To the best of our knowledge, so far there are only several experimental points for the static structure factor [16].

The situation concerning $n_p$ is now even worse. Thus, additional experiments are needed to make final conclusions about the failure of the mean-field approach.

It is also worth noting that, in experiments on the expansion of a condensate, one observes a kinetic energy of the freely expanding condensate, which is equal to a sum of the pairwise potential (10) and kinetic (12) energies of the trapped one, in effect proportional to the scattering length.

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FIG. 1. (a) The ratio $b/a$ versus the number $N_{\text{node}}$ of the nodes of $\varphi^{(0)}(r)$ $[\varphi^{(0)}(r)$ is the s-wave solution of the Schrödinger equation (3) with $V(r)$ given by Eq. (5)] for the given values of the scattering length $a = 52 a_0$ and the model parameter $r_c = 88.1 a_0$. This ratio is equal to $E_{\text{kin}}/E$ for a homogeneous dilute Bose gas of sodium atoms. (b) The wave function $\varphi^{(0)}(r)$ for the model potential (19) with $N_{\text{node}} = 12$. (c) The pair distribution function $g(r_1 - r_2) = F_2(r_1, r_2; r_1, r_2)/[|\varphi(r_1)|^2|\varphi(r_2)|^2] \approx [\varphi^{(0)}(r_1 - r_2)]^2$ [see Eqs. (10) and (19)] in a trapped sodium atom, interacting via the potential (19) with $N_{\text{node}} = 5$. Intensive oscillations occur when $r \lesssim a = 52 a_0$. 

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the potential is of a weak-coupling type \[9\]. The extension to the strong-coupling case is usually carried out by the pseudopotential replacement: 

$$V(r) \rightarrow \delta(r)4\pi\hbar^2\alpha/m.$$ 

However, such a replacement faces serious troubles upon treating the short-range correlations [see discussion after Eq. (12)].

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