Zero temperature correlations in trapped Bose-Einstein condensates

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Abstract

We introduce a family of correlated trial wave functions for the \( N \)-particle ground state of an interacting Bose gas in a harmonic trap. For large \( N \), the correlations lead to a relative energy decrease of a fraction \( \frac{3}{5N} \), compared to mean field Gross-Pitaevskii theory. The kinetic energy in the weakly confining direction turns out to be most sensitive to our correlations and, remarkably, is higher by as much as a few per cent for condensates with atom numbers of a few thousand. Thus, the predicted deviations from Gross-Pitaevskii theory originating from ground state correlations might be observed in momentum distribution measurements of small condensates.

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Initiated by the first realizations of alkali Bose-Einstein condensates in magnetic traps a few years ago \[1\] there is now an ever growing number of experiments with atomic condensates in laboratories all over the world. As a result of these efforts, a more and more detailed understanding of such quantum $N$-body systems is emerging. Properties hitherto measured are successfully described by updated versions of many-body theories established many years ago, see \[2\] for a recent review. Very importantly, the ‘condensate wave function’, the most relevant object well below the transition temperature, is determined by the mean field Gross-Pitaevskii (GP) equation \[3\].

Among future challenges remains experimental access to the detailed nature of the $N$-particle state of these quantum systems well below the critical temperature, exploring new physics beyond the standard mean field description. This paper presents a theoretical backup of this aim, emphasizing non-mean-field effects in trapped condensates with a relatively small number of atoms. Consequences of a correlated ground state are expected to be most prominent in two-body or even higher-order correlation functions. Nevertheless, in this paper we show that correlations may already have a significant effect on experimentally directly accessible quantities like the kinetic energy of the condensate. This holds true, as we will show, whenever the particle number is not too large and the trap is anisotropic.

The harmonic trap potential with frequencies $\omega_x = \omega_y$, and $\omega_z$, provides the scales of the problem. We express energies in units of $\hbar \bar{\omega}$ where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{\frac{1}{3}}$, the corresponding oscillator ground state length scale is $\bar{d} = \sqrt{\frac{\hbar}{m \bar{\omega}}}$, and thus the momentum scale ($\hbar/\bar{d}$). In these units the Hamilton operator, representing the energy of $N$ interacting atoms in an axially symmetric harmonic trap with anisotropy parameter $\lambda = \omega_z/\omega_x$, reads

$$H = \sum_{i=1}^{N} \left\{ \frac{p_i^2}{2} + \frac{1}{2} \left( \lambda^{-\frac{2}{3}} (x_i^2 + y_i^2) + \lambda^{\frac{4}{3}} z_i^2 \right) \right\} + 4 \pi a \sum_{i<j} \delta (\mathbf{r}_i - \mathbf{r}_j).$$

Interactions between atoms are two-body collisions with a strength determined by the $s$–wave scattering length $a$ of the atoms (measured in units of the oscillator length $\bar{d}$). The problem thus depends on the three parameters $N$, $\lambda$, and $a$.

Bose-Einstein condensation occurs when the thermal de-Broglie wave length of the atoms
becomes larger than the mean distance between atoms. Then, loosely speaking, a noticeable fraction of all atoms occupy the same one-particle state. Near zero temperature, i.e. well below the critical temperature, we therefore expect the \(N\)-particle state to be well approximated by a product state \(\Psi\) of one-particle states \(\psi\) \[4\],

\[
\Psi(r_1, \ldots, r_N) = \psi(r_1)\psi(r_2) \cdots \psi(r_N).
\] (2)

In second-quantized language with atom field operator \(\hat{\psi}(r)\), the product state (2) becomes a Fock state with particle number \(N\), resulting in the more common expressions for the manifestation of a Bose condensate, for instance \(\langle \hat{\psi}^\dagger(r) \hat{\psi}(r') \rangle = N\psi^\ast(r)\psi(r')\).

The total energy of the system, \(E = \langle \Psi|H|\Psi \rangle\) with Hamiltonian \([1]\), evaluated with the product state (2) is the Gross-Pitaevskii energy functional

\[
E_{\text{GP}}[\psi] = N \int d^3r \psi^*\psi \left[ -\frac{1}{2}\Delta + \frac{1}{2} \left( \lambda_{\frac{2}{3}}(x^2 + y^2) + \lambda_{\frac{4}{3}} z^2 \right) + 2\pi a(N-1)|\psi(r)|^2 \right] \psi(r). \] (3)

The determination of the approximate \(N\)-particle ground state is thus reduced to finding the minimum energy wave function of the energy functional (3), resulting in the famous Gross-Pitaevskii equation \([3]\) for the condensate wave function \(\psi(r)\) (strictly speaking, in GP theory the factor \((N-1)\) in front of the interaction term is replaced by \(N\); as we are interested in effects for a fixed, finite number of particles \(N\), we stick to \((N-1)\) throughout this paper).

By now it is experimentally established that the one-particle state \(\psi(r)\) so obtained does in fact well describe the properties of the condensate. For these dilute bosonic gases at near-zero temperature, the assumption of a product wave function (2) for the \(N\)-particle state is thus a good approximation. There is now also a rigorous proof available \([5]\) showing that in the limit \(N \to \infty\), keeping the product \(Na\) fixed (dilute), the true \(N\)-particle ground state energy is indeed given by the the minimum of \(E_{\text{GP}}[\psi]\).

Nevertheless, it is clear for finite \(N\) that due to two-body forces a product wave function (4) can only be an approximation for the \(N\)-particle ground state and it is worth thinking about possible observable deviations for not too large atom numbers \(N\).
In particular, as the center-of-mass motion of the $N$-body problem may be separated, we expect the true ground state to be a product wave function of center of mass $r_{cm} = \frac{1}{N} \sum_i r_i$ and relative coordinates, i.e. $\Psi(r_1, \ldots, r_N) = \psi_{cm}(r_{cm}) \cdot \tilde{\psi}$(relative coordinates) with the wave function $\tilde{\psi}$ for the relative motion symmetric in the $r_i$. This form of the wave function is clearly different from the product state (2).

In this paper, we are not going to separate the center-of-mass motion, but instead we introduce new coordinates

$$R_i = r_i + (C - \mathbb{I})r_{cm}, \quad (i = 1, \ldots, N)$$

(4)

that democratically incorporate the center-of-mass degree of freedom. The matrix $C$, without loss of generality, is chosen to be the diagonal matrix

$$C = \begin{pmatrix} c_r & 0 \\ 0 & c_r & 0 \\ 0 & 0 & c_z \end{pmatrix},$$

(5)

where $c_r$ and $c_z$ are two positive parameters; $C$ will play the role of an additional variational variable and will help to lower the total energy. For a totally anisotropic trap one should introduce two parameters $c_x, c_y$ instead of just $c_r$. The Jacobian of transformation (4) is $d^N R = (\det C) d^N r$, and notice that the choice $C = \mathbb{I}$ corresponds to the identity transformation $R_i = r_i$.

Apart from simplicity, transformation (4) is motivated by the fact that a wave function $\Psi(r_1, \ldots, r_N) = \sqrt{\det C} \Phi(R_1, \ldots, R_N)$ is a proper bosonic wave function whenever $\Phi(R_1, \ldots, R_N)$ is a bosonic wave function in $R_i$ coordinates. Crucially, the wave function obtained from a product wave function in $R_i$-coordinates

$$\Psi(r_1, \ldots, r_N) = \sqrt{\det C} \phi(R_1)\phi(R_2) \cdots \phi(R_N)$$

(6)

will be a correlated bosonic wave function in atom coordinates unless $C = \mathbb{I}$, when (6) coincides with the usual product state (2).
The actual values of the transformation parameters $c_r, c_z$ and the shape of the wave function $\phi$ are fixed by the requirement that the total energy $E = \langle \Psi | H | \Psi \rangle$ evaluated in the space of correlated atomic wave functions (6) should be minimal. It is straightforward to express the energy operator (1) of the $N$ atoms in new coordinates $R_i$ and the corresponding momenta. Variation with respect to $C$ determines the parameters $c_r, c_z$ of the transformation (4) with minimum energy, for a given wave function $\phi$ in (6). We find

$$c_r = \lambda^{-\frac{1}{8}} \left( \frac{\langle X^2 + Y^2 \rangle}{\langle P_X^2 + P_Y^2 \rangle} \right)^{\frac{1}{4}}, \quad c_z = \lambda^{\frac{1}{8}} \left( \frac{\langle Z^2 \rangle}{\langle P_Z^2 \rangle} \right)^{\frac{1}{4}},$$

(7)

where $P_X = -i \frac{\partial}{\partial X}$, and, for instance, $\langle Z^2 \rangle = \langle \phi | Z^2 | \phi \rangle$. In deriving (7) we simplified using the fact that in determining the ground state $\Psi$ we may restrict ourselves to wave functions $\phi (R)$ with $\langle R \rangle = \langle P \rangle = 0$.

The total energy $E = \langle \Psi | H | \Psi \rangle$ based on the correlated state (6) with the best matrix $C$ from (7) becomes

$$E_{\text{cor}}[\phi] = E_{\text{GP}}[\phi] - \frac{1}{2} \left( \lambda^{-\frac{1}{4}} \sqrt{\langle X^2 + Y^2 \rangle} - \sqrt{\langle P_X^2 + P_Y^2 \rangle} \right)^2 - \frac{1}{2} \left( \lambda^{\frac{1}{4}} \sqrt{\langle Z^2 \rangle} - \sqrt{\langle P_Z^2 \rangle} \right)^2$$

(8)

which is manifestly lower than the uncorrelated Gross-Pitaevskii energy $E_{\text{GP}}[\phi]$ (3) and one of the main results of this paper.

Let us first discuss result (8) for the case of a very large number $N$ of atoms. The difference between $E_{\text{cor}}[\phi]$ and $E_{\text{GP}}[\phi]$ is of the order of expectation values like $\langle X^2 + Y^2 \rangle$ or $\langle P_Z^2 \rangle$, while the dominating term $E_{\text{GP}}[\phi]$ is $N$ times larger. To leading order, therefore, we may evaluate the improved total energy with the state $\phi$ obtained from the minimum of $E_{\text{GP}}[\phi]$ alone, i.e. with the solution of the usual GP equation. Since, for $N \to \infty$, $\langle P^2 \rangle$ (‘kinetic energy’) may be neglected with respect to $\langle R^2 \rangle$ (‘potential energy’), we see from (8) that in this limit, the energy of the correlated state (6) may be written as $E_{\text{cor}}[\phi] = E_{\text{GP}}[\phi] - \frac{1}{N} E_{\text{pot}}^{\text{GP}}[\phi]$, where $\phi$ is the solution of the usual GP equation and $E_{\text{GP}}^{\text{pot}}$ the GP potential energy. Note that this energy decrease is possible due to the existence of the trap potential. Using the asymptotic Thomas-Fermi expressions for the total GP energy $E_{\text{GP}} = \frac{5N}{11} (15(N - 1)a)^{\frac{7}{5}}$ and the GP potential energy $E_{\text{GP}}^{\text{pot}}[\phi] = \frac{3N}{4} (15(N - 1)a)^{\frac{2}{5}}$ [2], we find for the energy of our correlated approximate ground state (6).
\[
E_{\text{cor}} = (1 - \frac{3}{5N})E_{\text{GP}} \quad \text{as } N \to \infty,
\]

a small decrease for the assumed large \(N\).

Far more relevant are effects of the correlated ground state (8) on the properties of small condensates. Let us therefore concentrate on the full expression (8) for the total energy \(E_{\text{cor}}[\phi]\) of the correlated state. As in usual GP theory [2,6], we may proceed analytically and use Gaussian trial wave functions \(\phi(R)\) parameterized by two parameters \(\Sigma_r\) and \(\Sigma_z\) for the radial and axial widths (note that these are widths in \(R\) coordinates and should not be confused with the condensate widths in physical space, the difference being of the order \(N^{-1}\)). The full energy functional (8) becomes a function of \(\Sigma_r\) and \(\Sigma_z\) only, and it is a simple numerical task to find its minimizing values. Results based on this Gaussian approximation are shown in the following Figures.

In Fig.1 we show the parameters \(c_r\) (Fig. 1a) and \(c_z\) (Fig. 1b) of our transformation on correlated coordinates (4) for the minimum energy correlated state (6) as a function of particle number \(N\), and for two different anisotropies \(\lambda = 0.04\) (cigar), and \(\lambda = 3\) (pancake). The three corresponding different graphs in each figure represent different interaction strengths: \(a = 0.004\) (solid line), \(a = 0.008\) (dashed line), and \(a = 0.012\) (dotted line). Recall that \(c_r = c_z = 1\) would correspond to the usual uncorrelated GP ground state (2). We clearly see that the transformation parameters \(c_r\) and \(c_z\) are larger in the weakly confining direction, and become larger for larger interaction strength \(a\).

Is there any hope to measure effects induced by the correlations of the improved ground state (6)? Among the various contributions to the total energy of the condensate, it turns out that the small kinetic energy in the weakly confining direction is most sensitive to our correlations and exhibits an increase of a few per cent compared to GP theory, for small condensates. This increase is compensated for by a larger decrease of potential energy of the correlated ground state, such that the total energy is indeed lowered.

In Fig.2 we show the kinetic energy in the weakly confining \(z\)-direction \(E_{\text{cor}}^{\text{kin},z}\) of the correlated state (8) as a function of atom number \(N\) for an anisotropy \(\lambda = 0.04\) (cigar). As
in Fig.1, results are shown for three different interaction strengths, \( a = 0.004 \) (solid line), 
\( a = 0.008 \) (dashed line), and \( a = 0.012 \) (dotted line). Recall that energies are measured in
units of \( \hbar \omega \), i.e. the kinetic energy shown in Fig.2 is very small compared to the potential
and internal energy of the condensate.

In Fig.3 we compare the predictions of correlated (6) and uncorrelated (2) ground state
for the kinetic energy \( E_{\text{kin}}^{z} \) in the weakly confining \( z \)-direction, again for a cigar shaped
condensate with \( \lambda = 0.04 \) (both quantities evaluated in a Gaussian approximation). Shown
is the relative energy increase \( \Delta E_{\text{kin}}^{z} = (E_{\text{cor}}^{\text{kin}} - E_{\text{GP}}^{\text{kin}})/E_{\text{GP}}^{\text{kin}} \), compared to GP theory.
We see that the difference may be a few per cent, depending on interaction strength and
atom number. For larger anisotropy, the observed difference is even larger. Similar, yet
less pronounced results are obtained for the change of radial kinetic energy in pancake-type
condensates.

The difference being a few per cent, high precision momentum distribution measurements
might be able to distinguish between the predictions of correlated and uncorrelated ground
state. In principle, the kinetic energy could be measured indirectly via the virial relation
\( E_{\text{kin}}^{z} = E_{\text{rel}} - E_{\text{pot}}^{r} \) from the knowledge of release energy \( E_{\text{rel}} = E_{\text{kin}} + E_{\text{int}} \)
and radial potential energy \( E_{\text{pot}}^{r} \). In this approach, however, the small kinetic energy is
measured as the difference of two very large quantities and it seems doubtful whether the
required precision can be achieved.

Far more promising are direct methods to measure the momentum distribution of the
condensate, as recently established through Bragg spectroscopy [9]. The high precision
achieved in this experiment might be sufficient to confirm the predicted deviations from GP
theory experimentally.

Let us summarize this paper. We found a correlated \( N \)-particle wave function \( \Phi \) for
an interacting Bose gas in a harmonic trap with lower total energy than the mean field GP
product state. The existence of the trap potential is crucial for the correlations; the energy
decrease is roughly the potential energy of \emph{one} atom. We have concentrated on effects on
simple averaged quantities, like kinetic, potential or release energy. Consequences of our
correlations will be most significant for relatively small condensates and a more detailed investigation of further effects is required, focusing on higher-order correlation functions.

Studying the dynamics of the condensate in a correlated state $\Psi$ will also be of interest as excitation frequencies can be measured with fairly high precision. Based on a hydrodynamic approach to superfluids, non-mean field corrections to the frequency of elementary excitations due to a finite gas parameter have been calculated in [10] in the large $N$-limit. Note that for dynamics, we have to replace the correlated energy functional ($\mathcal{S}$) by the more general expression, valid for nonvanishing $\langle R \rangle$, $\langle P \rangle$.

The correlations reported in this paper depend on the finite number of atoms and the existence of the trap; both conditions are met by current experiments. They are thus of very different nature than zero-temperature non-mean field effects described by Bogoliubov theory ($\textit{quantum depletion}$) [2,11]. In our approach, Bogoliubov theory in $R$-coordinates may be introduced on top of the correlated ground state (6). We conclude that there is no obvious relation between the correlations described by our wave function (6) and the usual Bogoliubov quantum depletion corrections.

Last but not least, recent progress in high precision spectroscopy of the momentum distribution of the condensate [9] might lead to an experimental confirmation of our results.

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REFERENCES

[1] M. H. Anderson, J. R. Esher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science*, 269, 198 (1995); C. C. Bradley, C. A. Sacket, J. J. Tollett, and R. G. Hulet, *Phys. Rev. Lett.* 75, 1687 (1995); K. B. Davis, M.-O. Mewes, M. R. Andrews, H. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* 75, 3969 (1995).

[2] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* 71, 463 (1999).

[3] E. P. Gross, Nuovo Cimento 20, 454 (1961); L. P. Pitaevskii, Sov. Phys. JETP 13, 451 (1961); E. P. Gross, J. Math. Phys. 4, 195 (1963).

[4] J.-P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems*, (Cambridge, MA: MIT Press) (1986).

[5] E. H. Lieb and J. Yngvason, *Phys. Rev. Lett.* 80, 2504 (1998); E. H. Lieb, R. Seiringer, and J. Yngvason, [math-ph/9908027](http://arxiv.org/abs/math-ph/9908027) and [math-ph/9911026](http://arxiv.org/abs/math-ph/9911026).

[6] G. Baym and C. J. Pethik, *Phys. Rev. Lett.* 77, 6, (1996); V. M. Perez-Garcia, H Michinel, J. I. Cirac, M. Lewenstein, and P. Zoller *Phys. Rev. Lett.* 77, 5320 (1996); M. Ueda and J. Leggett, *Phys. Rev. Lett.* 80, 1576 (1998).

[7] F. Dalfovo and S. Stringari, *Phys. Rev. A* 53, 2477 (1996).

[8] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, *Phys. Rev. Lett.* 77, 416 (1997); M. J. Holland, D. S. Jin, M. L. Chiofalo, and J. Cooper, *Phys. Rev. Lett.* 78, 3801 (1997).

[9] J. Stenger, S. Inouye, A. P. Chikkatur, D. M. Stamper-Kurn, D. E. Pritchard, and W. Ketterle, *Phys. Rev. Lett.* 82, 4569 (1999); see also A. B. Kuklov and B. V. Svistunov, *Phys. Rev. A* 60, R769 (1999).

[10] L. Pitaevskii and S. Stringari, *Phys. Rev. Lett.* 81, 4541 (1998).
[11] J. O. Andersen and E. Braaten, *Phys. Rev. A* **60**, 2330 (1999).
Fig. 1. Parameters $c_r$ (Fig. 1a) and $c_z$ (Fig. 1b) of our transformation on correlated coordinates for the minimum energy state $\Psi$ as a function of particle number $N$ for two different anisotropies $\lambda = 0.04$ (cigar), and $\lambda = 3$ (pancake). The three corresponding different graphs in each figure represent different interaction strengths: $a = 0.004$ (solid line), $a = 0.008$ (dashed line), and $a = 0.012$ (dotted line). The uncorrelated case is $c_r = c_z = 1$. 
Fig. 2. Kinetic energy $E_{\text{kin}, z}^{\text{cor}}$ of the correlated state in the weakly confining $z$-direction as a function of atom number $N$ for an anisotropy $\lambda = 0.04$ (cigar). As in Fig.1 we show results for three different interaction strengths, $a = 0.004$ (solid line), $a = 0.008$ (dashed line), and $a = 0.012$ (dotted line).
Fig. 3. Relative difference between the predictions for the kinetic energy $E^{\text{kin},z}$ in the weakly confining $z$-direction based on the correlated state and the uncorrelated GP state as a function of atom number $N$ for an anisotropy $\lambda = 0.04$ (cigar). As in Fig. 1 and 2, we show results for three different interaction strengths, $a = 0.004$ (solid line), $a = 0.008$ (dashed line), and $a = 0.012$ (dotted line).