Two-body correlations in Bose condensates

O. Sørensen, D.V. Fedorov, A.S. Jensen and E. Nielsen

Institute of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark

March 22, 2022

We formulate a method to study two-body correlations in a condensate of \( N \) identical bosons. We use the adiabatic hyperspherical approach and assume a Faddeev-like decomposition of the wave function. We derive for a fixed hyperradius an integro-differential equation for the angular eigenvalue and wave function. We discuss properties of the solutions and illustrate with numerical results. The interaction energy is for \( N \approx 20 \) five times smaller than that of the Gross-Pitaevskii equation.

PACS number(s): 31.15.-p, 03.75.Fi, 05.30.Jp

Introduction. Few-body correlations often express the distinguishing characteristic features of an \( N \)-body system. Two-body correlations are not only the simplest but in most cases also the most important. Higher order correlations have a tendency to either strongly confine spatially or correlate into clusters of particles effectively reducing the correlations to lower order. Exceptions are the three-body correlations decisive for the stability of Borromean systems known for dripline nuclei.

Non-correlated mean-field computations of nuclei with the free two-body nucleon-nucleon interaction produce disastrously wrong results. Two-body correlations compensating for the short range hard core repulsion are absolutely necessary. For atoms the effective interaction is also strongly repulsive at shorter distances. Furthermore for an atomic Bose condensate a short-range two-body attraction produces diatomic recombination and thereby the atoms decay out of the condensate. For both nuclei and molecules correlations are decisive. For nuclei various methods have been designed to deal with this problem, i.e. Jastrow theory, Bruckner theory, effective interactions in model spaces.

For Bose condensates the Gross-Pitaevskii (non-correlated) mean-field equation has been the starting point since the first observation of the condensate in 1995. The wave function does not include any correlations. The wave function does not include any correlations since the first observation of the condensate in 1995. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations. The wave function does not include any correlations.

For nuclei various methods have been designed to deal with this problem, i.e. Jastrow theory, Bruckner theory, effective interactions in model spaces.

For Bose condensates the Gross-Pitaevskii (non-correlated) mean-field equation has been the starting point since the first observation of the condensate in 1995. The wave function does not include any correlations and the assumed repulsive \( \delta \)-interaction has the immediate consequence that the short range behavior cannot be described even qualitatively correct. Repulsive \( \delta \)-interactions in three dimensions lead to divergences demanding renormalization or a change of boundary conditions. When two-body bound states appear even dimer condensates may be possible.

To include correlations we must necessarily go beyond the mean-field Hartree-Fock-Bogoliubov approximation. Then finite range potentials with realistic features can as well be used as the starting point in the theoretical formulation. The other crucial ingredient is the degrees of freedom or, equivalently, the Hilbert space. An interesting formulation was recently introduced in terms of generalized hyperspherical coordinates and an adiabatic expansion with the hyperradius as the adiabatic coordinate. Still only a zero-range interaction was used with the lowest hyperspherical angular wave function. These are very crude approximations, since the expansion in the hyperspherical basis necessarily must be extremely slowly converging for large \( r \) hyperradii.

The purpose of this letter is to go a step further and establish the optimum equation to determine two-body correlations. We shall derive a practical and realistic equation applicable to a system of \( N \) identical bosons. We shall allow general two-body interactions and in particular both attractive and repulsive finite range potentials. The resulting equation may be considered as an alternative to the Gross-Pitaevskii equation, but allowing two-body correlations.

Theory. The system of \( N \) identical interacting bosons of mass \( m \) may be described by the coordinates \( \vec{r}_i \) or CM \((\vec{R})\) and the \( k = 1, 2, \ldots, N - 1 \) Jacobi coordinates.

\[
\tilde{\eta}_k = \sqrt{\frac{N-k}{N-k+1}} \left( \vec{r}_{N-k+1} - \frac{1}{N-k} \sum_{j=1}^{N-k} \vec{r}_j \right).
\]

(1)

The hyperspherical coordinates are given by the hyper-radius \( \rho \) and the hyperangles \( \alpha_k \in [0, \pi/2] \).

\[
\rho^2 = \sum_{k=1}^N \tilde{\eta}_k^2, \quad \rho^2 = \sum_{k=1}^{N} r_{ij}^2, \quad \eta_k = \rho_k \sin \alpha_k,
\]

(2)

where \( r_{ij} = |\vec{r}_i - \vec{r}_j| = \sqrt{2} \rho \sin \alpha_{ij} \), and we distinguish between one and two indices on \( \alpha \). The remaining \( 2(N-1) \) angles are the directions of the \( N - 1 \) \( \tilde{\eta}_k \)-vectors. All the angles together, including the \( \alpha \)'s, are denoted \( \Omega \).

Removing the center of mass motion the intrinsic hamiltonian \( \hat{H} \) for a trap of angular frequency \( \omega \) becomes

\[
\hat{H} = \hat{T} + \sum_{i<j=1}^{N} \frac{m \omega^2}{N} r_{ij}^2 + V_{ij},
\]

(3)

where \( V_{ij} = V(r_{ij}) \) is the two-body interaction and the internal kinetic energy \( \hat{T} \) is of the form.

\[
\hat{T} = -\frac{\hbar^2}{2m} \left[ \frac{1}{\rho^{N-4}} \frac{\partial}{\partial \rho} \rho^4 \frac{\partial}{\partial \rho} - \frac{1}{\rho^2} \hat{\Lambda}^2 \right],
\]

(4)

\[
\hat{\Lambda}^2 = \frac{\partial^2}{\partial \alpha^2} + \frac{3N - 9 - (3N - 5) \cos 2\alpha}{\sin 2\alpha} \frac{\partial}{\partial \alpha} + D,
\]

(5)
where $D$ only contains derivatives with respect to angles different from $\alpha \equiv \alpha_{12}$. The Hamiltonian is then

$$
\hat{H} = \hat{H}_p + \frac{\hbar^2}{2m\rho^2} \hat{\rho}_\Omega , \quad \hat{\rho}_\Omega = \hat{\Lambda}^2 + \sum_{i<j=1}^N v_{ij} ,
$$

where $v_{ij} = V_{ij}2m\rho^2/\hbar^2$ is a dimensionless potential.

The total wave function $\Psi$, obeying $\hat{H}\Psi = E\Psi$, is for each $\rho$ expanded as

$$
\Psi = \rho^{-\frac{(3N-4)}{2}} \sum_n f_n(\rho) \Phi_n(\rho, \Omega) ,
$$

where $f_n(\rho)$ are the expansion coefficients on the solutions $\Phi_n(\rho, \Omega)$ to the angular eigenvalue equation

$$
(\hat{\rho}_\Omega - \lambda_n) \Phi_n(\rho, \Omega) = 0 .
$$

The coupled set of radial equations are then

$$
\left( - \frac{d^2}{d\rho^2} + \frac{\lambda_n(\rho)}{\rho^2} + \frac{2m(U(\rho) - E)}{\hbar^2} \right) f_n = \sum_{n'} \left( 2Q_{nn'}(\rho) \frac{d}{d\rho} + Q_{nn'}(\rho) \right) f_{n'} ,
$$

where $U(\rho)$ from the external trap and centrifugal barrier

$$
U(\rho) = \frac{1}{2} m\omega^2\rho^2 + \frac{\hbar^2}{8m\rho^2} (3N - 4)(3N - 6) .
$$

Then $\Phi_n$ is decomposed in Faddeev components $\phi_{ij}$ as

$$
\Phi_n(\rho, \Omega) = \sum_{i<j=1}^N \phi_{ij}^{(n)}(\rho, \Omega) .
$$

where $\alpha$ different from $\Omega$ to the angular eigenvalue equation

$$
(\hat{\rho}_\Omega - \lambda_n) \Phi_n(\rho, \Omega) = 0 .
$$

The coupled set of radial equations are then

$$
\left( - \frac{d^2}{d\rho^2} + \frac{\lambda_n(\rho)}{\rho^2} + \frac{2m(U(\rho) - E)}{\hbar^2} \right) f_n = \sum_{n'} \left( 2Q_{nn'}(\rho) \frac{d}{d\rho} + Q_{nn'}(\rho) \right) f_{n'} ,
$$

The integrals in eq.\[13\] involve at most six particle coordinates. By appropriate choices\[13\] of Jacobi system these can be expressed in terms of the five vectors $\vec{\eta}_{N-1}, \ldots, \vec{\eta}_{N-5}$. One variable ($\alpha \equiv \alpha_{12}$) is the argument of the variational function $\phi_{12}$ and not an integration variable. Furthermore 7 variables only enter in the phase space and can be integrated analytically leaving at most five-dimensional integrals. With $v(\alpha) \equiv v_{12}(\sqrt{2}\rho \sin \alpha)$ we rewrite eq.\[13\]

$$
\left( \hat{\Lambda}^2 + v(\alpha) - \lambda \right) \phi(\alpha) = \int d\tau G(\tau, \alpha) = 0 ,
$$

where $\tau$ denotes the remaining 5 variables and $G$ is a definite homogeneous linear combination of $\phi(\alpha\beta(\tau, \alpha))$.

The integrals in eq.\[16\] reduce to at most two dimensions when the two-body interaction-range $b$ is much less than the characteristic length $\rho$ of the system. To illustrate we use a gaussian potential $V(r_{ij}) = V_0 \exp(-r_{ij}^2/\ell^2)$, but the results depend mainly on $a_p \equiv \sqrt{\pi}mbV_0/4\hbar^2$, i.e. the Born-approximation of the scattering length $a_s$. When $mbV_0 \ll \hbar^2$ we have $a_p \approx a_s$. For $b \ll \rho$ we get, almost independent of the potential,

$$
\int d\tau G(\tau, \alpha) \approx \frac{3}{\sqrt{\pi}} \Theta(\tan \alpha < \sqrt{3}) \cos^{3N-11} \beta N - 3 .
$$

Here $\Gamma$ is the gamma function, $\sin \beta = \tan \alpha/\sqrt{3}$, $\Theta$ is the truth function, and $R$, a functional of $v$ and $\phi$ and a function of $\alpha$, arises from rotations of interaction and wave function from one set of Jacobi coordinates to another.

The $\delta$-interaction with a constant wave function, labeled $K = 0$, leads to the eigenvalue\[12\]

$$
\lambda_{K=0} = \sqrt{\frac{2}{\pi}} \frac{\Gamma\left(\frac{3(N-2)}{2}\right) a_p}{\Gamma\left(\frac{3(N-2)}{2}\right)} N(N-1) \frac{a_p}{\rho} ,
$$

which for large $N$ coincides with the term $\tilde{v}(\alpha = 0)$ in eq.\[17\]. The interaction dependent part of the strength is collected in the parameter $a_p$.

The limit of $\lambda_{K=0}$ is not, even for large $N$, obtained by solving eqs.\[13\] and \[14\], since the highest power of $N$ is found in one of the rotated terms in $R$ proportional to $N^2\tilde{v}(\alpha)$. In the zero-range approximation the two non-local terms in eq.\[17\] proportional to $\phi(0)$ are very sensitive to the initial two-body potential $v(\alpha)$ which is very large and of very short range already for moderate values of $\rho$. These terms are therefore crucial for the development of correlations.
**Quantitative behavior.** We now solve numerically eq. (14) using eq. (17) with the realistic parameter set in [12] for the condensate of \(^{87}\text{Rb}-\)atoms. For numerical illustration we choose \(N = 10, 20, 30\).

The lowest angular eigenvalues for \(N = 20\) are shown in Fig. 1 in the relevant range of hyperradii selected by the external trap. The minimum of \(U(\rho)\) is located near \(\rho \approx b_{\text{r}} \sqrt{3N}/2\) where \(b_{\text{r}} = \sqrt{\hbar/(m\omega)}\) is the trap length. Inclusion of the interaction terms, expressed in eq. (10) by \(\lambda\) through the effective radial potential \(U(\rho) + \hbar^2 \lambda^2/2m\rho^2\), push the minimum outwards. For the repulsive interaction the angular eigenvalues decrease with \(\rho\) due to an increasing average two-body distance.

We first only include the local terms \((\propto \phi(\alpha))\) in eq. (17). The angular energy in Fig. 1 is then larger than the \(\lambda_{K=0}\) value, because these terms are repulsive. Including also the \(\hat{R}\)-terms in eq. (17) leads to rather similar results, where however, the correlations are exploited giving a lower energy. Finally, inclusion of all terms reduces the angular energy to only 19\% of the \(\lambda_{K=0}\) value.

The almost discontinuous behavior at this point of the full and rotated angular wave function is caused by the very short range of the initial repulsive two-body potential \(\nu(\alpha)\). The \(K = 0\) wave function has no nodes and the local terms maintain this structure but marginally shifted to larger \(\alpha\)-values by the repulsive potential. The rotated terms introduce one node indicating the substantial restructuring due to correlations. The higher kinetic energy is more than compensated by the correlations build up to avoid the repulsion at short distance. The full solution maintains qualitatively this behavior, but now the probability is shifted to larger \(\alpha\) or equivalently to larger distances between each pair of particles.

The terms proportional to \(\phi(0)\) decreases the angular energy drastically. This is consistent with the node in the wave function which lowers the angular energy because then large \(|\phi(0)|\) results in smaller \(\lambda\). More oscillations allow constructive interference which in turn substantially lowers the potential energy. The result is the increasing deviation of \(\lambda\) from \(\lambda_{K=0}\) for decreasing \(\rho\), see Fig. 1.

The \(N\) and \(\rho\) dependences of the angular wave functions are shown in Fig. 2. The \(\sqrt{N}\) scaling follow the \(N\) dependence of the potential minimum of \(U(\rho)\), see Fig. 1. The strong variation for small \(\alpha\) for \(N = 30\) disappears with increasing \(\rho\). The same tendency, but less pronounced, is found for \(N = 10\). The size of the angular wave functions for \(\alpha = 0\) decreases with increasing \(\rho\). In the relevant parameter interval defined by the trap the \(\rho\)-dependence of the angular wave function is weak except at small \(\alpha\) corresponding to distances inside the two-body potential. The corresponding angular eigenvalue \(\lambda\) relative to \(\lambda_{K=0}\) is essentially independent of \(\rho\), i.e. 0.33, 0.19 and 0.16 for \(N = 10, 20\) and 30, respectively. This confirms numerically our conjecture that the \(K = 0\) behavior obtained in [12] with a \(\delta\)-interaction is not approached with increasing \(N\) at large distances.

The total energies obtained by solving the radial equation in eq. (14) reflect the relative sizes of the angular eigenvalues in Fig. 1. The radial wave functions \(f_{n}(\rho)\) resemble the \(K = 0\) solutions. However, it is essential to understand that even if the effective radial potential only deviates insignificantly from the \(K = 0\) potential the corresponding angular wave functions may differ enormously, i.e. none versus many oscillations. Thus effects of correlations may easily be strong without showing up
in the total energy and perhaps also not even significantly in the interaction energy.

The Gross-Pitaevskii mean-field solution does not remove the (small) spurious contribution from the center of mass motion. Still we compare directly and find that our total energy only is slightly smaller than this total mean-field energy. However, our interaction energy, excluding the external trap energy, is about 3, 5, and 7 times smaller for \( N = 10, 20, \) and 30, respectively. This reflects the huge difference in structure between the mean-field and correlated solutions.

The distance between two particles is \( r_{ij} = \sqrt{2}\rho \sin \alpha_{ij} \) and therefore, the mean square “radius” \( \langle \phi(\alpha) | \sin^2 \alpha | \phi(\alpha) \rangle \) obtained with normalized \( \phi \), quantifies this distance for each \( \rho \). For the \( \rho \)-independent \( K = 0 \) wave function we find \( 1/(N - 1) \) analytically whereas our full wave function with the correlations for \( N = 20 \) gives the much larger distance of about \( 2.4/(N - 1) \) roughly independent of \( N \) and \( \rho \). See Figs. 3 and 4. The full mean square radius is now obtained by multiplying \( | \sin^2 \alpha | \) with \( 2\rho^2 \approx 3(N - 1)b_1^2 \) found as the minimum of \( U \) in Fig. 5 or as the harmonic oscillator expectation value. Thus by increasing \( N \) the decreasing two-particle average distance for fixed \( \rho \) is precisely compensated by the increasing position of the minimum of the potential.

The result is \( \langle r_{ij}^2/b_1^2 \rangle = 3 \) for \( K = 0 \) and 6.83, 7.30 and 7.31 for the full wave function for \( N = 10, 20, 30 \), respectively. These values can be compared to the Gross-Pitaevskii results through the harmonic oscillator relation \( (N - 1)\langle r_{ij}^2 \rangle = 2N\langle r_i^2 \rangle - \langle R^2 \rangle \), where \( N\langle R^2 \rangle = 3b_1^2/2 \) is the center of mass expectation value for the mean square radius. With the mean-field result numerically computed we obtain \( \langle r_{ij}^2/b_1^2 \rangle = 3.1 \) almost independent of \( N \), i.e. almost equal to the \( K = 0 \) result but much smaller than for the correlated solution. Thus the \( K = 0 \) assumption do not even approximately describe two-body correlations. In the mean-field approximation these correlations are by definition completely absent and the average distance between pairs of particles is therefore very small. The accurate detailed behavior can only be obtained by explicit inclusion of correlations.

**Perspectives.** In conclusion, we have variationally derived a linear one-dimensional integro-differential equation describing \( N \) identical bosons in a trap. The equation involves five-dimensional integrals, a tremendous simplification from the original \( N \)-body problem. We assume the Faddeev angular decomposition of the wave function and use the hyperradius as the adiabatic coordinate. A further reduction to at most two-dimensional integrals is achieved for short range interactions for the non-local parts of the equation. The interaction may be attractive and of finite range with bound states and with both signs of the scattering length. This opens the possibility of realistic computation of the diatomic recombination rate which in the present terminology is a process originating from the first excited adiabatic state (condensate) ending in the lowest adiabatic (diatomic bound) state. This process is essential for the stability of atomic Bose condensates. Our equation is an alternative to the Gross-Pitaevskii equation, but apparently both features of mean-field and few-body correlations are now included in a unified approach. Other interesting perspectives are extensions to three-body correlations, to one and two space dimensions, to non-identical bosons, to fermion systems and to systems of mixed symmetry.

![Graph showing \( \rho \) and \( \phi \) values for different \( N \) and \( \rho \) values](image)

**FIG. 3.** The same as Fig. 2 with full solutions for hyper-\( \rho = \rho \sqrt{N} = 100 \text{ nm}, 400 \text{ nm}, 6400 \text{ nm} \) and \( N = 10, 30 \).

\[ \rho_1 = 100 \text{ nm} \]
\[ \rho_2 = 400 \text{ nm} \]
\[ \rho_3 = 6400 \text{ nm} \]

\( N = 10, 20, 30 \) gives the much larger distance of about 2.4/(\( N - 1 \)) roughly independent of \( N \) and \( \rho \). See Figs. 3 and 4.

\[ \langle r_{ij}^2/b_1^2 \rangle = 3 \] for \( K = 0 \) and 6.83, 7.30 and 7.31 for the full wave function for \( N = 10, 20, 30 \), respectively.

\[ N\langle R^2 \rangle = 3b_1^2/2 \] is the center of mass expectation value for the mean square radius. With the mean-field result numerically computed we obtain \( \langle r_{ij}^2/b_1^2 \rangle = 3.1 \) almost independent of \( N \), i.e. almost equal to the \( K = 0 \) result but much smaller than for the correlated solution.

\[ \langle r_{ij}^2/b_1^2 \rangle = 3 \] for \( K = 0 \) and 6.83, 7.30 and 7.31 for the full wave function for \( N = 10, 20, 30 \), respectively.

\[ N\langle R^2 \rangle = 3b_1^2/2 \] is the center of mass expectation value for the mean square radius. With the mean-field result numerically computed we obtain \( \langle r_{ij}^2/b_1^2 \rangle = 3.1 \) almost independent of \( N \), i.e. almost equal to the \( K = 0 \) result but much smaller than for the correlated solution. Thus the \( K = 0 \) assumption do not even approximately describe two-body correlations. In the mean-field approximation these correlations are by definition completely absent and the average distance between pairs of particles is therefore very small. The accurate detailed behavior can only be obtained by explicit inclusion of correlations.

**Perspectives.** In conclusion, we have variationally derived a linear one-dimensional integro-differential equation describing \( N \) identical bosons in a trap. The equation involves five-dimensional integrals, a tremendous simplification from the original \( N \)-body problem. We assume the Faddeev angular decomposition of the wave function and use the hyperradius as the adiabatic coordinate. A further reduction to at most two-dimensional integrals is achieved for short range interactions for the non-local parts of the equation. The interaction may be attractive and of finite range with bound states and with both signs of the scattering length. This opens the possibility of realistic computation of the diatomic recombination rate which in the present terminology is a process originating from the first excited adiabatic state (condensate) ending in the lowest adiabatic (diatomic bound) state. This process is essential for the stability of atomic Bose condensates. Our equation is an alternative to the Gross-Pitaevskii equation, but apparently both features of mean-field and few-body correlations are now included in a unified approach. Other interesting perspectives are extensions to three-body correlations, to one and two space dimensions, to non-identical bosons, to fermion systems and to systems of mixed symmetry.

**References:**

[1] J. Carlson and R. Schiavilla, Rev. Mod. Phys. 70, 743 (1998).
[2] K. Riisager, Rev. Mod. Phys. 66, 1105 (1994).
[3] J.E. Amaro et al., Phys. Rev. C 57, 3473 (1998).
[4] E. Nielsen and J. Macek, Phys. Rev. Lett. 83, 1566 (1999).
[5] F.J. Siemens and A.S. Jensen, Elements of Nuclei, Addison-Wesley, 1987.
[6] F. Dalfovo et al., Rev. Mod. Phys. 71, 463 (1999).
[7] D.R. Phillips and T.D. Cohen, Phys. Lett. B 390, 7 (1997).
[8] D. Fedorov and A.S. Jensen, Phys. Rev. A 63, 063608 (2001).
[9] M. Olshanii and L. Pricoupenko, arXiv: cond-mat/0101273.
[10] Yu.N. Demkov and V.N. Ostrovskii, Zero-range potentials and their applications in Atomic Physics (Plenum, New York, 1988).
[11] L. Pricoupenko, arXiv: cond-mat/0006263.
[12] J.L. Bohn et al., Phys. Rev. A 58, 584 (1998).
[13] N. Barnea, Phys. Lett. B 446, 185 (1999); Phys. Rev. A 59, 1135 (1999).
[14] A.S. Jensen et al., Few-Body Systems 22, 193 (1997).
[15] Yu. F. Smirnov et al., Sov. J. Part. Nucl. 8(4), 344 (1977).