Separable Structure of Many-Body Ground-State Wave Function

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Abstract

We have investigated a general structure of the ground-state wave function for the Schrödinger equation for $N$ identical interacting particles (bosons or fermions) confined in a harmonic anisotropic trap in the limit of large $N$. It is shown that the ground-state wave function can be written in a separable form. As an example of its applications, this form is used to obtain the ground-state wave function describing collective dynamics for $N$ trapped bosons interacting via contact forces.
The structure of the ground-state wave function for a many-body system is very important for theoretical understanding of recently observed Bose-Einstein condensation (BEC) [1] (the theoretical aspects of the BEC are discussed in recent reviews [2]) and other many body problems. The Ginzburg-Pitaevskii-Gross (GPG) equation [3] is most widely used to describe the experimental results for the BEC. Recently, an alternative method of equivalent linear two-body (ELTB) equations for many body systems has been developed based on the variational principle [4,5]. In this paper, we consider \( N \) identical particles (bosons or fermions) confined in a harmonic anisotropic trap. We show that in the case of large \( N \) the ground-state wave function can be written in separable form as

\[
\Psi(\vec{r}_1, \vec{r}_2, ... \vec{r}_N) = \phi(x, y, z) \cdot \chi(\Omega, \sigma),
\]

where

\[
x = \sqrt{\sum_{i=1}^{N} x_i^2}, \quad y = \sqrt{\sum_{i=1}^{N} y_i^2}, \quad z = \sqrt{\sum_{i=1}^{N} z_i^2},
\]

\( \Omega \) is a set of \((3N-3)\) angular variables, and \( \sigma \) is a set of spin variables.

We start from a generalization of the hyperspherical expansion of the Hamiltonian

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_i + \frac{1}{2} m \sum_{i=1}^{N} (\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) + \sum_{i<j} V_{int}(r_i - r_j)
\]

in the form [4,6]

\[
\Psi(\vec{r}_1, ... \vec{r}_N) = \sum_{[K]} \Phi_{[K]}(x, y, z) Y_{[K]}(\Omega^N_x, \Omega^N_y, \Omega^N_z, \sigma),
\]

where \( Y_{[K]}(\Omega^N_x, \Omega^N_y, \Omega^N_z, \sigma) = Y_{K_x, K_y, K_z}^{\nu_x, \nu_y, \nu_z}(\Omega^N_x, \Omega^N_y, \Omega^N_z, \sigma) \) is the combination of the hyperspherical harmonics, \( Y_{K_x}^{\nu_x}(\Omega^N_x), Y_{K_y}^{\nu_y}(\Omega^N_y), \) and \( Y_{K_z}^{\nu_z}(\Omega^N_z) \), with functions of spin variables \( \sigma \), which is symmetric or antisymmetric with respect to
permutations of particles for bosons or fermions respectively. $[K]$ represents a set of numbers $[K_x, \nu_x, K_y, \nu_y, K_z, \nu_z]$.

The hyperspherical harmonics $Y^\mu_x(\Omega^N_x), Y^\mu_y(\Omega^N_y), \text{and } Y^\mu_z(\Omega^N_z)$ are eigenfunctions of the hyperspherical angular parts of the Laplace operators $\sum_{i=1}^N \frac{\partial^2}{\partial x_i^2}, \sum_{i=1}^N \frac{\partial^2}{\partial y_i^2}, \text{and } \sum_{i=1}^N \frac{\partial^2}{\partial z_i^2}$, respectively.

The Laplace operators are defined by

\[ \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} = \frac{1}{x^{N-1}} \frac{\partial}{\partial x} (x^{N-1} \frac{\partial}{\partial x}) + \frac{1}{x^2} \Delta_{\Omega^N_x}, \]
\[ \sum_{i=1}^N \frac{\partial^2}{\partial y_i^2} = \frac{1}{y^{N-1}} \frac{\partial}{\partial y} (y^{N-1} \frac{\partial}{\partial y}) + \frac{1}{y^2} \Delta_{\Omega^N_y}, \tag{5} \]
\[ \text{and} \]
\[ \sum_{i=1}^N \frac{\partial^2}{\partial z_i^2} = \frac{1}{z^{N-1}} \frac{\partial}{\partial z} (z^{N-1} \frac{\partial}{\partial z}) + \frac{1}{z^2} \Delta_{\Omega^N_z}. \]

The hyperspherical angles $\theta^x_1, \theta^x_2, \ldots, \theta^x_{N-1}, \theta^y_1, \theta^y_2, \ldots, \theta^y_{N-1}, \theta^z_1, \theta^z_2, \ldots, \theta^z_{N-1}$ can be chosen in such a way that the hyperspherical angular parts of the Laplace operators $\Delta_{\Omega^N_u}$ satisfy the recursion relation [7]

\[ \Delta_{\Omega^N_u} = \frac{1}{\sin^{N-2} \theta^u_{N-1}} \frac{\partial}{\partial \theta^u_N} (\sin^{N-2} \theta^u_{N-1} \frac{\partial}{\partial \theta^u_{N-1}}) + \frac{1}{\sin^2 \theta^u_{N-1}} \Delta_{\Omega^{N-1}_u} \tag{6} \]

with $u = x, y, \text{or } z$.

Functions $\Phi_{[K]}(x, y, z)$ satisfy equations

\[ \sum_{[K']} h_{[K],[K']} \Phi_{[K']}(x, y, z) = \Phi_{[K]}(x, y, z), \tag{7} \]
where
\[ h_{[K][K']} = \delta_{K_x,K'_x} \delta_{K_y,K'_y} \delta_{K_z,K'_z} \delta_{\nu_x,\nu'_x} \delta_{\nu_y,\nu'_y} \delta_{\nu_z,\nu'_z} \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \right] \]
\[ + \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right) + \frac{\hbar^2}{2m} \frac{(N - 1 + 2K_x)(N - 3 + 2K_x)}{4x^2} \]
\[ + \frac{(N - 1 + 2K_y)(N - 3 + 2K_y)}{4y^2} + \frac{(N - 1 + 2K_z)(N - 3 + 2K_z)}{4z^2} \]
\[ + V_{[K][K']}(x, y, z), \]  
with  
\[ V_{[K][K']}(x, y, z) = < K_x, \nu_x, K_y, \nu_y, K_z, \nu_z | \sum_{i<j} V_{\text{int}}(r_i - r_j) | K'_x, \nu'_x, K'_y, \nu'_y, K'_z, \nu'_z >. \]  
(8)

We write \( \Phi_{[K]}(x, y, z) \) in the form of a Laplace integral  
\[ \Phi_{[K]}(x, y, z) = \int f_{[K]}(\alpha_x, \alpha_y, \alpha_z) \phi_x(x, \alpha_x) \phi_y(y, \alpha_y) \phi_z(z, \alpha_z) d\alpha_x d\alpha_y d\alpha_z, \]  
(10)

where  
\[ \phi_t(t, \alpha_t) = \sqrt{\frac{2}{\Gamma(N/2)}} \left( \frac{m\tilde{\omega}}{\alpha_t^2 \hbar} \right)^{N/4} \exp \left[ -m\tilde{\omega} \left( \frac{t}{\alpha_t} \right)^2 / (2\hbar) \right] t^{(N-1)/2}, \]  
(11)

and \( \tilde{\omega} = (\omega_x \omega_y \omega_z)^{1/3} \).

The Hill-Wheeler type equations [8,9] are obtained by requiring that energy of the system is stationary with respect to the functions \( f_{[K]}(\alpha_x, \alpha_y, \alpha_z) \).
\[
\sum_{[K]} \int d\alpha_x d\alpha_y d\alpha_z f_{[K]}(\alpha_x, \alpha_y, \alpha_z) [H_{[K]'}[K'](\alpha_x \alpha_y \alpha_z, \alpha_x' \alpha_y' \alpha_z') \nonumber \\
- \delta_{[K]'[K]}S(\alpha_x \alpha_y \alpha_z, \alpha_x' \alpha_y' \alpha_z') E] = 0,
\]

where
\[
H_{[K]'}[K'](\alpha_x \alpha_y \alpha_z, \alpha_x' \alpha_y' \alpha_z') = \langle \phi_x(x, \alpha_x) \phi_y(y, \alpha_y) \phi_z(z, \alpha_z) Y_{[K]} \nonumber \\
\times | H | \phi_x(x, \alpha_x') \phi_y(y, \alpha_y') \phi_z(z, \alpha_z') Y_{[K']} >,
\]

and
\[
S(\alpha_x \alpha_y \alpha_z, \alpha_x' \alpha_y' \alpha_z') = \langle \phi_x(x, \alpha_x) \phi_y(y, \alpha_y) \phi_z(z, \alpha_z) | \phi_x(x, \alpha_x') \phi_y(y, \alpha_y') \phi_z(z, \alpha_z') >.
\]

In order to solve the Hill-Wheeler type equations (12), we assume that the integral in Eq. (10) can be replaced by sum
\[
\Phi_{[K]}(x, y, z) = \sum_{i,j,k=1}^{\infty} c_{ijk}^{[K]} \phi_x(x, \alpha_x) \phi_y(y, \alpha_y) \phi_z(z, \alpha_z),
\]

where \( c_{ijk}^{[K]} \) are solutions of the following equations
\[
\sum_{i'j'k'} [H_{[K]}'[K']'(\alpha_x' \alpha_y' \alpha_z', \alpha_x' \alpha_y' \alpha_z')] - \delta_{[K]'[K]}S(\alpha_x' \alpha_y' \alpha_z', \alpha_x' \alpha_y' \alpha_z') E] c_{i'j'k'}^{[K']} = 0.
\]

For the case of large \( N \), the overlap, Eq. (14),
\[
S(\alpha_x \alpha_y \alpha_z, \alpha_x' \alpha_y' \alpha_z') = \left[ \frac{8\alpha_x \alpha_y \alpha_x' \alpha_y' \alpha_z \alpha_z'}{((\alpha_x)^2 + (\alpha_x')^2)((\alpha_y)^2 + (\alpha_y')^2)((\alpha_z)^2 + (\alpha_z')^2)} \right]^{N/2}
\]

where
\[
\sum_{i,j,k=1}^{\infty} [H_{[K]}'[K']'(\alpha_x' \alpha_y' \alpha_z', \alpha_x' \alpha_y' \alpha_z')] - \delta_{[K]'[K]}S(\alpha_x' \alpha_y' \alpha_z', \alpha_x' \alpha_y' \alpha_z') E] c_{i'j'k'}^{[K']} = 0.
\]
reduces to the Kronecker deltas

\[ S(\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x^i \alpha_y^j \alpha_z^k) = \delta_{ii'} \delta_{jj'} \delta_{kk'} \]  

(18)

Since the ratio

\[ \frac{H_{[K][K']} (\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x^i \alpha_y^j \alpha_z^k)}{S(\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x^i \alpha_y^j \alpha_z^k)} \]

is a much more slowly varying function of \( \alpha \) compared to \( S(\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x^i \alpha_y^j \alpha_z^k) \) in almost all cases [10], we have for the case of large \( N \)

\[ H_{[K][K']} (\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x^i \alpha_y^j \alpha_z^k) = \tilde{H}_{[K][K']} (\tilde{\alpha}_x, \tilde{\alpha}_y, \tilde{\alpha}_z) \delta_{ii'} \delta_{jj'} \delta_{kk'}, \]  

(19)

(see Appendix for the case of \( N \) identical particles interacting via contact repulsive force).

Substitution of Eq. (19) into Eq. (16) gives

\[ \Phi_{[K]} (x, y, z) = \tilde{c}_{[K]} \phi_x (x, \tilde{\alpha}_x) \phi_y (y, \tilde{\alpha}_y) \phi_z (z, \tilde{\alpha}_z), \]  

(20)

where \( \tilde{c}_{[K]} \) are solutions of the following equations

\[ \sum_{[K']} [\tilde{H}_{[K][K']} (\tilde{\alpha}_x, \tilde{\alpha}_y, \tilde{\alpha}_z) - \delta_{[K][K']} E] \tilde{c}_{[K']} = 0, \]  

(21)

and parameters \( \tilde{\alpha}_x, \tilde{\alpha}_y, \) and \( \tilde{\alpha}_z \) are solutions of

\[ \frac{\partial E}{\partial \tilde{\alpha}_x} = \frac{\partial E}{\partial \tilde{\alpha}_y} = \frac{\partial E}{\partial \tilde{\alpha}_z} = 0. \]

Substitution of Eq. (20) into Eq. (4) yields \( \Psi(\vec{r}_1, \vec{r}_2, ... \vec{r}_N) \) given by Eq. (1) with

\[ \phi(x, y, z) = \phi_x (x, \tilde{\alpha}_x) \phi_y (y, \tilde{\alpha}_y) \phi_z (z, \tilde{\alpha}_z), \]
and

\[
\chi(\Omega, \sigma) = \sum_{[K]} \tilde{c}^{[K]} Y_{[K]}(\Omega_x^N, \Omega_y^N, \Omega_z^N, \sigma).
\]

We now consider \(N\) identical particles confined in an anisotropic harmonic trap and interacting via contact force

\[
V_{\text{int}}(\vec{r}_i - \vec{r}_j) = \frac{4\pi \hbar^2 a}{m} \delta(\vec{r}_i - \vec{r}_j),
\]

with positive scattering length \(a > 0\). Using factorization (1) we have

\[
\begin{align*}
&\left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) - \frac{\hbar^2}{2m} (c_x^2 + c_y^2 + c_z^2) \\
&\quad + \frac{\hbar^2}{2m} \frac{(N-1)(N-3)}{4} \left( \frac{1}{x^2} + \frac{1}{y^2} + \frac{1}{z^2} \right) + \frac{c_{xy}}{xyz} \right] \phi(x, y, z) = E \phi(x, y, z),
\end{align*}
\]

where \(c_t = \langle \chi | \Delta_{\Omega_t^N} | \chi \rangle / \langle \chi | \chi \rangle \) with \(t = (x, y, z)\) and

\[
c = \frac{ah^2 N(N-1)}{\sqrt{2\pi m}} \left( \frac{\Gamma(N/2)}{\Gamma((N-1)/2)} \right)^3 \tilde{c}.
\]

In the large \(N\) limit, parameters \(c_x, c_y, c_z\), and \(\tilde{c}\) are expected to be slowly varying functions of \(N\). For \(N\) identical bosonic atoms with large \(N\), an essentially exact expression for the ground state energy can be obtained by neglecting the kinetic energy term in the GPG equation [2,3] (this is called “Thomas-Fermi approximation” [11]). From comparison of the ground state solution of Eq. (24) with the Thomas-Fermi approximation [11], we can fix unknown parameters and find the ground-state solution of Eq. (24) as

\[
\phi(x, y, z) = \psi_x(x) \psi_y(y) \psi_z(z),
\]

\[
E = \frac{5N \hbar \bar{\omega}}{4} \bar{n}^{2/5},
\]

7
with

\[ \psi_x(x) = A x^{(N-1)/2} \exp[-m\tilde{\omega}(x/\alpha)^2/(2\hbar)], \]
\[ \psi_y(y) = A y^{(N-1)/2} \exp[-m\tilde{\omega}(y/\beta)^2/(2\hbar)], \]
\[ \psi_z(z) = A z^{(N-1)/2} \exp[-m\tilde{\omega}(z/\gamma)^2/(2\hbar)], \]

where

\[ A = \sqrt{2/\Gamma(N/2)(m\tilde{\omega}/(\alpha^2\hbar))^{N/4}}, \]
\[ \alpha = \tilde{n}^{1/5}\tilde{\omega}/\omega_x, \beta = \tilde{n}^{1/5}\tilde{\omega}/\omega_y, \gamma = \tilde{n}^{1/5}\tilde{\omega}/\omega_z, \tilde{\omega} = (\omega_x\omega_y\omega_z)^{1/3}, \tilde{n} = n\tilde{c}, n = 2\sqrt{\tilde{\omega}m/(2\pi\hbar)}Na \]
\[ \tilde{c} = \left(\frac{4}{\pi}\right)^{5/2}\frac{15}{8}\sqrt{\pi} \approx 0.82. \]

Eqs. (25-28) give the exact ground-state solution of Eq. (24) for large $N$. Thus we have found an analytical solution for the ground-state wave function describing collective dynamics in variables $(x,y,z)$ in the large $N$ limit.

We note that the slope of the Thomas-Fermi wave function becomes infinity at the surface, leading to logarithmic singularity in the kinetic energy. Hence it is necessary to modify the Thomas-Fermi wave function near the surface [12-14]. In contrast, we do not have such problems for our solution, Eq. (25-28).

It is also interesting to compare our results with the ELTB method [4,5]. For this situation (contact force, Eq. (23) and large $N$ limit), the ELTB method corresponds to $\tilde{c}^{2/5} = 1$. It shows that the ELTB method is a very good approximation with relative error of about 8% for parameter $\tilde{c}^{2/5}$.

In summary, we have investigated the general structure of the ground-state solution of the Schrödinger equation for $N$ identical interacting particles (bosons or fermions) confined in a harmonic anisotropic trap in the large $N$ limit. The main results and conclusions are as follows

(i) It has been shown that in the case of large $N$ the ground-state wave function can be written in separable form, Eq. (1).
(ii) Using this form, we have found an analytical solution for the ground-state wave function, Eqs. (25-29), describing collective dynamics in collective variables \((x,y,z)\) for \(N\) trapped bosons interacting via contact repulsive forces.

(iii) Our results can be used for checking various approximations (both existing and future) made for the Schrödinger equation describing \(N\) identical interacting particles (bosons or fermions) confined in a harmonic anisotropic trap.
Appendix

To prove Eq. (19) we consider the contact potential case

$$ V_{int}(r_i - r_j, \sigma) = \delta(r_i - r_j)\eta(\sigma), \quad (A.1) $$

where $\eta$ depends on spin variables. Using Eq. (A.1) we can rewrite Eq. (9) as

$$ V_{[K][\kappa]}(x, y, z) = \gamma_{[K][\kappa]} \frac{N(N - 1)}{xyz}, \quad (A.2) $$

where $\gamma_{[K][\kappa]}$ does not depend on $x, y, z$.

Substitution of Eq. (A.2) into Eq. (13) gives

$$ H_{[K][\kappa]}(\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x'^i \alpha_y'^j \alpha_z'^k) \bigg/ (\hbar \tilde{\omega} N) = (1/2) S(\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x'^i \alpha_y'^j \alpha_z'^k) $$

$$ \times \left[ \delta_{[K][\kappa]} \frac{1 + (\alpha_x^i)^2 (\alpha_y'^j)^2 \beta_z^2}{(\alpha_x^i)^2 + (\alpha_y'^j)^2} + \frac{1 + (\alpha_y^j)^2 (\alpha_y'^j)^2 \beta_y^2}{(\alpha_y^j)^2 + (\alpha_y'^j)^2} + \frac{1 + (\alpha_z^k)^2 (\alpha_z'^k)^2 \beta_z^2}{(\alpha_z^k)^2 + (\alpha_z'^k)^2} \right] $$

$$ + \sqrt{((\alpha_x^i)^2)((\alpha_y^j)^2)((\alpha_y'^j)^2)((\alpha_z^k)^2)((\alpha_z'^k)^2)} \frac{\Gamma((N - 1)/2)}{\Gamma(N/2)} \frac{\Gamma(N - 1/2)}{3!} $$

$$ \times (\frac{m \tilde{\omega}}{\hbar})^{3/2} N - 1 \sqrt{8} \gamma_{[K][\kappa]} \bigg], \quad (A.3) $$

where $\beta_t = \omega_t / \tilde{\omega}$ for $t = x, y, \text{ or } z$.

For large $N$, $S(\alpha_x^i \alpha_y^j \alpha_z^k, \alpha_x'^i \alpha_y'^j \alpha_z'^k)$, Eq. (14), reduces to the Kronecker deltas $\delta_{ii'} \delta_{jj'} \delta_{kk'}$, and hence from Eq. (A.3) we obtain Eq. (19).
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