Equivalent Linear Two-Body Equations for Many-Body Systems
Alexander L. Zubarev and Yeong E. Kim
Department of Physics, Purdue University
West Lafayette, Indiana 47907

Abstract

A method has been developed for obtaining equivalent linear two-body equations (ELTBE) for the system of many \( N \) bosons using the variational principle. The method has been applied to the one-dimensional \( N \)-body problem with pair-wise contact interactions (McGurie-Yang \( N \)-body problem) and to the dilute Bose-Einstein condensation (BEC) of atoms in anisotropic harmonic traps at zero temperature. For both cases, it is shown that the method gives excellent results for large \( N \).

PACS numbers: 03.75.Fi, 03.65.Db, 05.30.Jp, 67.90.+z
In this paper we present an approximate method of obtaining the eigenvalue solutions of the system of interacting $N$ bosons using an equivalent two-body method similar to that used by Feshbach and Rubinov [1] for the triton ($^3H$) three-body ($N=3$) bound state. They [1] used both (i) the variational principle and (ii) a reduced coordinate variable (not the hyperradius) to obtain an equivalent two-body equation for the three-body bound state ($^3H$). For many-body problems, use of one reduced coordinate variable (the hyperradius [2]) was made to obtain equivalent two-body equations by keeping only a finite sum of terms of the hyperspherical expansion with $K = K_{\text{min}}$ ($K$ is the global angular momentum). This method has been applied to the ground state of the $N$-body system composed of distinguishable particles or of bosons and also to nuclear bound states [3,4]. It was shown that the method leads to the correctly behaved nuclear bound states in the limit of large $A$ ($A$ is the nucleon number) [4]. Recently, it has been used to describe the Bose-Einstein condensation (BEC) of atoms in isotropic harmonic traps [5].

In this paper we apply our method to the one-dimensional $N$-body problem with pairwise contact interactions (the McGuire-Yang $N$-body problem [6, 7]) and to the dilute BEC of atoms in anisotropic harmonic traps at zero temperature. We show that the method gives excellent results for large $N$ for both cases.

For the $N$-body system, our method for obtaining the equivalent linear two-body equation (ELTBE) consists of two steps. The first step is to give the $N$-body wave function $\Psi(r_1, r_2, \ldots)$ a particular functional form

$$\Psi(r_1, r_2, \ldots) \approx \tilde{\Psi}(\zeta_1, \zeta_2, \zeta_3),$$

where $\zeta_1, \zeta_2,$ and $\zeta_3$ are known functions. We limit $\zeta$’s to three variables in order to obtain the ELTBE. The second step is to derive an equation for $\tilde{\Psi}(\zeta_1, \zeta_2, \zeta_3)$ by requiring that $\tilde{\Psi}$ must satisfy a variational principle

$$\delta \int \tilde{\Psi}^* \tilde{\Psi} d\tau = 0$$

(2)

with a subsidiary condition $\int \tilde{\Psi}^* \tilde{\Psi} d\tau = 1$. This leads to a linear two-body equation, from which both eigenvalues and eigenfunctions can be obtained. The lowest eigenvalue is an upper bound of the lowest eigenvalue of the original $N$-body problem. To test our ELTBE method, we apply the method to the one-dimensional $N$-body problem and to the BEC of atoms in anisotropic traps at zero temperature in the following.
There are only several known cases of exactly solvable three-body and four-body problems. For $N = 3$ case it was shown [8] that the Faddeev equations [9] for one-dimensional three-body problem with pair-wise contact interactions are exactly solvable. For the one-dimensional $N = 4$ case, analytical solutions of the four-body Faddeev-Yakubovsky were obtained in [10]. We note that for nuclear three body systems with short-range interactions, the Schrödinger equation in three-dimension is reformulated into the Faddeev equations [9] which can be solved numerically after making partial wave expansion [11] or without partial wave expansion [12]. In the following, we consider an exactly solvable one-dimensional $N$-body system as a test case for our method.

For the one-dimensional N-body problem with the Hamiltonian

$$H = -\sum_{i=1}^{N} \frac{d^2}{dx_i^2} + 2c \sum_{i<j} \delta(x_i - x_j) \quad (\text{with } \hbar = m = 1),$$

the Schrödinger equation is exactly solvable. The bound and scattering states for this system have been found by McGuire [6] and by Yang [7]. For the case $c < 0$, there are bound states [6] for the system of $N$ bosons with the wave function $\Psi = \exp[(c/2) \sum_{i<j} |x_i - x_j|]$. The energy of this bound state is

$$E_{\text{exact}} = -\frac{c^2 N(N^2 - 1)}{12}. \quad (3)$$

The McGuire-Yang N-body problem gives a unique possibility to check the validity of various approximations made for the Schrödinger equation describing $N$ particles interacting via short range potential.

For this case, we seek for eigenfunction $\Psi$ of $H$ in the form of

$$\Psi \approx \tilde{\Psi}(\rho) = \frac{F(\rho)}{\rho^{(N-2)/2}},$$

where $\rho = \frac{1}{N} \sum_{i<j} (x_i - x_j)^2$. We shall derive an equation for $F(\rho)$ by requiring that $\tilde{\Psi}$ must satisfy a variational principle (2). This requirement leads to the equation

$$[-\frac{d^2}{d\rho^2} + \frac{(N - 2)(N - 4)}{4\rho^2} + V(\rho)]F(\rho) = EF(\rho), \quad (4)$$

where

$$V(\rho) = cN(N - 1) \frac{\Gamma(N/2 - 1/2)}{\sqrt{2\pi} \Gamma(N/2 - 1)} \frac{1}{\rho}. \quad (5)$$

We note that Eq. (4) is exactly the form of the Schrödinger two-body equation in which $\Psi = (F(\rho)/\rho)Y_{lm}$, and a centrifugal potential energy is given by $(N - 2)(N - 4)/(4\rho^2r)$ with identification of angular momentum quantum number $l = N/2 - 1$. Eq. (4) with the
Coulomb like potential $V(\rho)$, Eq. (5), can be solved analytically, and we obtain for $E$ the following expression [13]

$$E = -\frac{c^2}{2\pi^2} \left[ \frac{N(N - 1)\Gamma(N/2 - 1/2)}{(N - 2)\Gamma(N/2 - 1)} \right]^2.$$  \hspace{1cm} (6)

In the case of large $N$, using the asymptotic formulas for $\Gamma$ function, $\lim_{|z| \to \infty} \frac{\Gamma(z + \alpha)}{\Gamma(z + \beta)} = z^{\alpha - \beta}(1 + O(\frac{1}{z}))$, we obtain $E = -\frac{c^2}{12}N^3$ for the leading term of Eq. (6). On the other hand we have for large $N$ case from Eq. (1), $E_{\text{exact}} = -\frac{c^2}{12}N^3(1 + O(\frac{1}{N^2}))$. Therefore, for the McGuire-Yang N-body problem we have demonstrated that the ELT BE method, Eqs. (4) and (5), is a very good approximation for the case of large $N$ (the relative error for binding energy is about 4.5%). Furthermore, our approximation, Eq. (6), agrees remarkably well with exact value, Eq. (3), for any $N$ (the maximum value of binding energy relative error occurs for $N = 3$ and is about 10%).

Now, let us consider $N$ identical bosonic atoms confined in a harmonic anisotropic trap with the following Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \Delta_i + \frac{1}{2} \sum_{i=1}^{N} m(\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2) + \sum_{i<j} V_{\text{int}}(\mathbf{r}_i - \mathbf{r}_j),$$  \hspace{1cm} (7)

where we assume $V_{\text{int}}$ in the dilute condensate case to be the following form [14]

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

with $s$-wave scattering length, $a$.

For eigenfunction $\Psi$ of $H$, we assume the solution for $\Psi$ has the following form

$$\Psi(\mathbf{r}_1, ... \mathbf{r}_N) \approx \frac{\tilde{\Psi}(x, y, z)}{(xyz)^{(N-1)/2}}$$  \hspace{1cm} (8)

where $x^2 = \sum_{i=1}^{N} x_i^2$, $y^2 = \sum_{i=1}^{N} y_i^2$, $z^2 = \sum_{i=1}^{N} z_i^2$.

We now derive an equation for $\tilde{\Psi}(x, y, z)$ by requiring that $\tilde{\Psi}(x, y, z)$ must satisfy the variational principle (2). This requirement leads to the equation

$$H \tilde{\Psi} = E \tilde{\Psi},$$  \hspace{1cm} (9)

where

$$H = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) + \frac{\hbar^2}{2m} \left( \frac{(N - 1)(N - 3)}{4} \left( \frac{1}{x^2} + \frac{1}{y^2} + \frac{1}{z^2} \right) + \frac{g}{xyz} \right).$$  \hspace{1cm} (10)
with \( g = g_0(2\pi)^{-3/2}(\Gamma(N/2)/\Gamma(N/2 - 1/2))^3 N(N - 1)/2 \) and \( g_0 = 4\pi \hbar^2 a/m \). To the best of our knowledge, Eqs. (9) and (10) have not been discussed in the literature.

For the positive scattering length case, \( a > 0 \), we look for the solution of Eq. (9) of the form

\[
\tilde{\Psi}(x, y, z) = \sum_{i,j,k} c_{ijk} \Phi^{(1)}_i(x) \Phi^{(2)}_j(y) \Phi^{(3)}_k(z),
\]

where \( \Phi^{(1)}_i(x) = x^{N-1/2} \exp[-(x/\alpha_i)^2/2] \), \( \Phi^{(2)}_j(y) = y^{(N-1)/2} \exp[-(y/\beta_j)^2/2] \), \( \Phi^{(3)}_k(z) = z^{(N-1)/2} \exp[-(z/\gamma_k)^2/2] \), and \( c_{ijk} \) are solutions of the following equations

\[
\sum_{l,m,n} H_{ijk,lmn} c_{lmn} = E \sum_{l,m,n} \lambda_{ijk,lmn} c_{lmn}
\]

where

\[
H_{ijk,lmn} = \frac{\hbar \bar{\omega} N \lambda_{ijk,lmn}}{2} [1 + \alpha_i^2 \alpha_j \alpha_k^2 + 1 + \beta_j^2 \beta_m \alpha_k^2 + 1 + \gamma_k^2 \gamma_m \alpha_l^2 + \gamma_n^2 \gamma_k \alpha_l^2] + \bar{g},
\]

with \( \bar{g} = \frac{(N-1)}{2\sqrt{2N}} \tilde{n}, \tilde{n} = 2\sqrt{\bar{\omega}m/(2\pi \hbar)} N, \tilde{\omega} = (\omega_x \omega_y \omega_z)^{1/3}, \alpha_x = \omega_x/\tilde{\omega}, \alpha_y = \omega_y/\tilde{\omega}, \) and \( \alpha_z = \omega_z/\tilde{\omega} \).

For the case of large \( N \), we have \( \lambda_{ijk,lmn} \approx \delta_{il}\delta_{jm}\delta_{kn}, \ H_{ijk,lmn} \approx E \delta_{il}\delta_{jm}\delta_{kn} \). For the ground state energy, using \( \frac{\partial E}{\partial \alpha_i} = \frac{\partial E}{\partial \alpha_j} = \frac{\partial E}{\partial \alpha_k} = 0 \), we obtain

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

We note that Eq. (13) is the exact ground state solution of Eq. (9) for large \( N \). For the case of large \( N \) we can obtain an essentially exact expression for the ground state energy by neglecting the kinetic energy term in the Ginzburg-Pitaevskii-Gross (GPG) equation [16] (the Thomas-Fermi approximation [15]) as

\[
\frac{E_{TF}}{N\hbar \bar{\omega}} = \frac{5}{7} \left( \frac{15}{8} \sqrt{\pi} \right)^2 \tilde{n}^{5/2}
\]

Comparing Eq. (13) with Eq. (14), we can see that for the case of large \( N \) the ELTBE method (Eqs. (9) and Eq. (10)) is a very good approximation, with a relative error of about 8% for the binding energy.

When the scattering length is negative, the effective interaction between atoms is attractive. It has been claimed that the BEC in free space is impossible [17] because the
attraction makes the system tend to an ever dense phase. For $^7\text{Li}$, the s-wave scattering length is $a = (-14.5 \pm 0.4)\text{Å}$ [18]. For bosons trapped in an external potential there may exist a metastable BEC state with a number of atoms below the critical value $N_{cr}$ [19-27].

For the $a < 0$ case, we can see that potential energy in Eq. (10),

$$V(x, y, z) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2) + \frac{\hbar^2}{2m} \frac{(N - 1)(N - 3)}{4} \left( \frac{1}{x^2} + \frac{1}{y^2} + \frac{1}{z^2} \right) - \left| \frac{g}{xyz} \right|,$$

for $N < N_{cr}$ has a single metastable minimum which leads to the metastable BEC state. We note that for the case of large $N_{cr}$, the ELTBE method leads to the same $N_{cr}$ as the variational GPG stationary theory [26]. To show this, let us consider an anisotropic trap, $\omega_x = \omega_y = \omega_\perp$, $\omega_z = \lambda\omega_\perp$. Local minimum conditions $\hat{\lambda} > 0$, where $\hat{\lambda}$ is a matrix with matrix elements $A_{ij} = \partial^2 V/\partial x_i \partial x_j$, can be written for this case as

$$n^2/2\delta_\perp^2 \delta_z^4 - n - \lambda^2 \delta_\perp \delta_z^2/32 + O(1/N) < 0,$$

where $\delta_z = (2m\omega_\perp/\hbar N_{cr})^2$, $\delta_\perp = (2m\omega_\perp/\hbar N_{cr})^2 x^2$, and $n = 2(\omega_\perp / 2\pi \hbar)^1/2 N_{cr} \ | \ a \ |$. Setting the left-hand side of Eq. (16) to zero and neglecting $O(1/N)$ terms, we obtain the following equations for $N_{cr}$

$$1 - 2\delta_\perp^2 = \delta_\perp^2(1 + 8\lambda^2)^{1/2},\ 1 - \lambda^2 \delta_z^2 = \delta_z \delta_\perp [1 + (1 + 8\lambda^2)^{1/2}],\ n = \delta_\perp \delta_z^2 [1 + (1 + 8\lambda^2)^{1/2}]$$

Eqs. (17) are exactly the same as equations for determining $N_{cr}$ obtained from the variational GPG approach [26]. Taking the experimental values of $^7\text{Li}$ trap parameters [28], $\omega_\perp / 2\pi = 152$ Hz, and $\omega_z / 2\pi = 132$ Hz, we obtain $N_{cr} = 1456$. This value of $N_{cr}$ is consistent with theoretical predictions [23-27] and is in agreement with those observed in a recent experiment [28].

We note that the ELTBE method for a general anisotropic trap can be improved using a generalization of hyperspherical expansion

$$\Psi(r_1, ... r_N) = \sum_{K_x, K_y, K_z} \sum_{\nu_x, \nu_y, \nu_z} \Psi_{K_x, K_y, K_z}(x, y, z) Y_{K_x}^{\nu_x}(\Omega_x) Y_{K_y}^{\nu_y}(\Omega_y) Y_{K_z}^{\nu_z}(\Omega_z),$$

where the hyperspherical harmonics $Y_{K_x}^{\nu_x}(\Omega_x)$, $Y_{K_y}^{\nu_y}(\Omega_y)$, and $Y_{K_z}^{\nu_z}(\Omega_z)$ are eigenfunctions of the angular parts of the Laplace operators $\sum_{i=1}^N \frac{\partial^2}{\partial x_i^2}$, $\sum_{i=1}^N \frac{\partial^2}{\partial y_i^2}$, and $\sum_{i=1}^N \frac{\partial^2}{\partial z_i^2}$, respectively. However, we do not expect a fast convergence of the expansion, Eq. (18), because of nonuniformity of the convergence of the expansion of $\sum_{i<j} V_{int}(r_i - r_j)$ in $x$, $y$, and $z$. 
In summary, we have presented a method for obtaining an equivalent linear two-body equation for the system of $N$ bosons. We have applied the method to the McGuire-Yang $N$-body problem and also to the dilute Bose-Einstein condensation in anisotropic harmonic traps at zero temperature. For both cases we have shown that the method gives excellent results for large $N$. 
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