Generalized Radial Equations in a Quantum N-Body Problem

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We demonstrate how to separate the rotational degrees of freedom in a quantum N-body problem completely from the internal ones. It is shown that any common eigenfunction of the total orbital angular momentum ($\ell$) and the parity in the system can be expanded with respect to $(2\ell + 1)$ base-functions, where the coefficients are the functions of the internal variables. We establish explicitly the equations for those functions, called the generalized radial equations, which are $(2\ell + 1)$ coupled partial differential equations containing only $(3N - 6)$ internal variables.

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Symmetry is an important property of a physical system. The symmetry of a quantum system can simplify its Schrödinger equation and remove some variables in the equation. The simplest example is the hydrogen atom problem, where, due to the spherical symmetry, the wavefunction is expressed as a product of a radial function and a spherical harmonic function,

$$\Psi^\ell_m(r) = \phi(r)Y^\ell_m(\theta, \varphi), \quad (1)$$

and the Schrödinger equation reduces to a radial equation with only one radial variable.

For a quantum N-body problem with a pair potential, the Schrödinger equation is invariant under the spatial translation, rotation, and inversion. From those symmetries, one should be able to separate the motion of center-of-mass and the global rotation of the system from the internal motions so as to reduce the Schrödinger equation to the generalized "radial" equation that contains only internal variables. However, this problem has not been solved. In this letter we will solve this problem completely. Using the appropriately chosen $(3N - 6)$ internal variables and the $(2\ell + 1)$ base-functions for the total orbital angular momentum $\ell$, we establish explicitly the generalized radial equations.

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without any approximation. Only \((3N - 6)\) internal variables are involved in both the generalized radial functions and the equations.

Denote by \(r_j\) the position vectors of \(N\)-particles with masses \(m_j\) in the laboratory frame (LF), respectively. The Schrödinger equation for the \(N\)-body problem is

\[
-\left(\frac{\hbar^2}{2}\right) \sum_{j=1}^{N} m_j^{-1} \Delta r_j \Psi + V \Psi = E \Psi, \tag{2}
\]

where \(V\) is assumed to be a pair potential, depending on the distances of each pair of particles. Therefore, the potential \(V\) is a function of only the internal variables. It is well known that, due to the translation symmetry of the system, the motion of center-of-mass can be separated completely from others by making use of the Jacobi coordinate vectors in the center-of-mass frame (CF) [1-3],

\[
R_k = \left(\frac{m_k W_{k+1}}{W_k}\right)^{1/2} \left(r_k - \sum_{j=k+1}^{N} \frac{m_j r_j}{W_{k+1}}\right), \quad 1 \leq k \leq (N - 1). \tag{3}
\]

where \(W_j = \sum_{t=j}^{N} m_t\). In CF, the Laplace operator and the total orbital angular momentum operator \(L\) can be directly expressed with respect to \(R_k\):

\[
\Delta = \sum_{j=1}^{N} m_j^{-1} \Delta r_j = \sum_{k=1}^{N-1} \Delta R_k,
\]

\[
L = -i\hbar \sum_{j=1}^{N} r_j \times \nabla r_j = -i\hbar \sum_{k=1}^{N-1} R_k \times \nabla R_k, \tag{4}
\]

The Laplace operator obviously has the symmetry of \(O(3N - 3)\) group with respect to \((3N - 3)\) variables. The \(O(3N - 3)\) group contains a subgroup \(SO(3) \times O(N - 1)\), where \(SO(3)\) is the usual rotational group. The space inversion and the different definitions for the Jacobi vectors in the so-called ”Jacobi tree” [4] can be obtained by \(O(N - 1)\) transformations. For the system of identical particles, the permutation group among particles is also a subgroup of \(O(N - 1)\) group.

Because of the spherical symmetry, the angular momentum is conserved. The hydrogen atom problem is a typical quantum two-body problem, where there is only one Jacobi coordinate vector, usually called the relative position vector \(r\). For a quantum \(N\)-body problem, equation (1) should be generalized in three aspects. The first is how to define the internal variables, which describe the internal motions completely. The second is
how to find the complete set of the independent base-functions with the given angular momentum. The total wavefunction is expanded with respect to the base-functions, where the coefficients are the generalized radial functions which only depend on the internal variables. The last is how to derive the generalized radial equations that only contain $(3N - 6)$ internal variables. As a matter of fact, these three aspects are connected. The parity should also be considered in the generalization. Due to the spherical symmetry, one only needs to study the eigenfunctions of angular momentum with the largest eigenvalue of $L_3 (m = \ell)$, which are simply called the wavefunctions with the angular momentum $\ell$ in this letter for simplicity. Their partners with the smaller eigenvalues of $L_3$ can be calculated from them by the lowering operator $L_-$. 

Denote by $R = R(\alpha, \beta, \gamma)$ a spatial rotation, transforming CF to the body-fixed frame (BF), and by $\xi$ all the internal variables in a quantum $N$-body problem for simplicity. Although Wigner did not separate the motion of center-of-mass by the Jacobi vectors, he proved from the group theory that any wavefunction with the angular momentum $\ell$ in the system can be expressed as follows (see Eq. (19.6) in [5]):

$$\Psi_\ell(\alpha, \beta, \gamma, \xi) = \sum_{q=\ell}^{\ell} D_{\ell q}(\alpha, \beta, \gamma)^* \psi_q(\xi),$$

where we adopt the commonly used form of the $D$-function [6]. In Eq. (5) $D_{\ell q}(\alpha, \beta, \gamma)^*$ plays the role of the base-function with the angular momentum $\ell$, and $\psi_q(\xi)$ is the generalized radial function. What Wigner proved is that there are only $(2\ell + 1)$ independent base-functions with the angular momentum $\ell$. Unfortunately, due to the singularity of the Euler angles, the generalized radial equations are very difficult to derive based on Eq. (5). Wigner did not discuss the generalized radial equations, and to our knowledge, those equations have not yet been established in the literature. It is obvious that the generalized radial equations are very easy to obtain for the $S$ wave [7]. However, it seems quite difficult to obtain even for $P$ wave in a three-body problem [8,9].

Recently, a coupled angular momentum basis was used to prediagonalize the kinetic energy operator [10], where some off-diagonal elements remain non-vanishing. In their calculation, the function with a given angular momentum was combined from the partial angular momentum states by the Clebsch-Gordan coefficients. Since the partial angular momenta are not conserved, one has to deal with, in principle, an infinite number of
the partial angular momentum states. This problem also occurs in the hyperspherical harmonic function method and its improved ones [2,4,11,12]. However, as Wigner proved, only \((2\ell + 1)\) partial angular momentum states are involved in constructing the base-functions with the angular momentum \(\ell\).

Arbitrarily choose two Jacobi coordinate vectors, say \(\mathbf{R}_1\) and \(\mathbf{R}_2\). Let \(\mathbf{R}_1\) be parallel with the \(Z\)-axis of BF, and \(\mathbf{R}_2\) be located in the \(XZ\) plane with a non-negative \(X\)-component in BF. The rotational degrees of freedom of the system are described by a rotation \(R(\alpha, \beta, \gamma)\), transforming CF to BF. Define \((3N - 6)\) internal variables, which should be invariant in the global rotation \(R(\alpha, \beta, \gamma)\):

\[
\xi_j = \mathbf{R}_j \cdot \mathbf{R}_1, \quad \eta_j = \mathbf{R}_j \cdot \mathbf{R}_2, \quad \zeta_j = \mathbf{R}_j \cdot (\mathbf{R}_1 \wedge \mathbf{R}_2), \quad 1 \leq j \leq (N - 1),
\]

where \(\eta_1 = \xi_2\) and \(\zeta_1 = \zeta_2 = 0\). It is worth mentioning that \(\xi_j\) and \(\eta_j\) have even parity, but \(\zeta_j\) has odd parity. From them we have

\[
\Omega_j = (\mathbf{R}_1 \wedge \mathbf{R}_j) \cdot (\mathbf{R}_1 \wedge \mathbf{R}_2) = \xi_j \eta_j - \zeta_j \zeta_j,
\]

\[
\omega_j = (\mathbf{R}_2 \wedge \mathbf{R}_j) \cdot (\mathbf{R}_1 \wedge \mathbf{R}_2) = \xi_j \eta_j - \eta_j \zeta_j,
\]

\[
\mathbf{R}_j \cdot \mathbf{R}_k = \Omega_2^{-1} (\Omega_j \eta_k - \omega_j \xi_k + \zeta_j \zeta_k),
\]

where \(\Omega_1 = \omega_2 = 0\), and \(\Omega_2 = -\omega_1 = (\mathbf{R}_1 \wedge \mathbf{R}_2)^2\).

Recall that two Jacobi vectors \(\mathbf{R}_1\) and \(\mathbf{R}_2\) completely determine BF and three Euler angles. The base-functions with the angular momentum \(\ell\) should be combined from the products of two spherical harmonic functions \(Y^q_m(\mathbf{R}_1)\) and \(Y^p_{m'}(\mathbf{R}_2)\) by the Clebsch-Gordan coefficients \(\langle q, m, p, m'|\ell, (m + m')\rangle\). Define [3,11]

\[
Q^\ell_{q}(\mathbf{R}_1, \mathbf{R}_2) = \frac{(R_{11} + iR_{12})^{q-\tau}(R_{21} + iR_{22})^{\ell-q}}{(q-\tau)!(\ell-q)!} \{(R_{11} + iR_{12})R_{23} - R_{13}(R_{21} + iR_{22})\}^{\tau},
\]

\[
\tau \leq q \leq \ell, \quad \tau = 0, 1.
\]

where \(R_{ja}\) is the \(a\)th component of the Jacobi vector \(\mathbf{R}_j\). \(Q^\ell_{q}(\mathbf{R}_1, \mathbf{R}_2)\) is the common eigenfunction of \(L^2, L_3, \Delta_{\mathbf{R}_k}\), and the parity with the eigenvalues \(\ell(\ell + 1), \ell, 0,\) and \((-1)^{\ell+\tau}\), respectively. As a matter of fact, the following combination of products of two spherical harmonic functions is proportional to \(Q^\ell_{q}(\mathbf{R}_1, \mathbf{R}_2)\)

\[
\sum_{m} \zeta_{\eta_1}^{q/2} Y^q_m(\mathbf{R}_1) |\eta_{2}^{\ell-q+\tau}/2 Y_{\ell-m}^{\ell-q+\tau}(\mathbf{R}_2) \langle q, m, (\ell - q + \tau), (\ell - m)|\ell, \ell\rangle = C Q^\ell_{q}(\mathbf{R}_1, \mathbf{R}_2),
\]

\(\zeta_{\eta_1}\)
where \( C \) is a normalization factor. Now, we come to the theorem.

**Theorem.** Any function \( \Psi^\ell_\ell\alpha(R_1, \ldots, R_{N-1}) \) with the angular momentum \( \ell \) and the parity \((-1)^{\ell+\lambda}\) in a quantum \( N \)-body problem can be expanded with respect to \( Q^\ell_\ell\alpha(R_1, R_2) \) with the coefficients \( \psi^\ell_\ell\alpha(\xi, \eta, \zeta) \), which depend on \((3N - 6)\) internal variables:

\[
\Psi^\ell_\ell(R_1, \ldots, R_{N-1}) = \sum_{\tau=0}^{1} \sum_{q=\tau}^{\ell} \psi^\ell_\ell\alpha(\xi, \eta, \zeta) Q^\ell_\ell(R_1, R_2),
\]

where the parity of \( \psi^\ell_\ell\alpha(\xi, \eta, \zeta) \) is \((-1)^{\lambda - \tau} \).

Equation (5) coincides with Eq. (10), because either of the set of \( D^\ell_\ell\alpha(\alpha, \beta, \gamma)^* \) and the set of \( Q^\ell_\ell(R_1, R_2) \) is a complete set of base-functions of the angular momentum. However, equation (10) has three important characteristics, which make it possible to derive the generalized radial equations. The first is that the Euler angles do not appear explicitly in the base-functions \( Q^\ell_\ell(R_1, R_2) \). The second is that the well chosen internal variables (6). The third is that the internal variables \( \zeta_j \) have odd parity. It is due to the existence of \( \zeta_j \) that the base-functions \( Q^\ell_\ell\alpha_0(R_1, R_2) \) and \( Q^\ell_\ell(R_1, R_2) \) appear together in one total wavefunction. By comparison, all the internal variables in a quantum three-body problem have even parity \((\zeta_j = 0)\) so that in a total wavefunction with a given parity, only the base-functions with the same parity appear [5,12].

Now, substituting Eq. (10) into the Schrödinger equation (2) with the Laplace operator (4), we obtain the generalized radial equations by a straightforward calculation:

\[
\triangle \psi^\ell_0 + 4 \{ q \partial_{\xi_1} + (\ell - q) \partial_{\eta_\tau} \} \psi^\ell_0 + 2q \partial_{\xi_\tau} \psi^\ell_{(q-1)0} + 2(\ell - q) \partial_{\xi_\zeta} \psi^\ell_{(q+1)0} \\
+ \sum_{j=3}^{N-1} 2\Omega_2^{-1} \left\{ -\omega_j q \partial_{\xi_j} + \Omega_j (\ell - q) \partial_{\eta_j} + \eta_2 \zeta_j q \partial_{\xi_j} + \xi_1 \zeta_j (\ell - q) \partial_{\xi_j} \right\} \psi^\ell_0 \\
- q \left[ \omega_j \partial_{\eta_j} + \xi_2 \zeta_j \partial_{\xi_j} \right] \psi^\ell_{(q-1)0} + (\ell - q) \left[ \Omega_j \partial_{\xi_j} - \xi_2 \zeta_j \partial_{\xi_j} \right] \psi^\ell_{(q+1)0} \\
- i \eta_2 q (\ell - 1) \left[ \zeta_j \partial_{\eta_j} - \Omega_j \partial_{\xi_j} \right] \psi^\ell_{(q-1)1} \\
- i q \left[ \eta_2 \zeta_j q \partial_{\xi_j} - \xi_2 \zeta_j (2\ell - 2q + 1) \partial_{\eta_j} + \eta_2 \omega_j q \partial_{\zeta_j} + \xi_2 \Omega_j (2\ell - 2q + 1) \partial_{\xi_j} \right] \psi^\ell_q \\
+ i(\ell - q) \left[ \xi_2 \zeta_j (2q + 1) \partial_{\xi_j} - \xi_1 \zeta_j (\ell - q) \partial_{\eta_j} + \xi_2 \omega_j (2q + 1) \partial_{\zeta_j} + \xi_1 \Omega_j (\ell - q) \partial_{\xi_j} \right] \psi^\ell_{(q+1)1} \\
- i \xi_1 (\ell - q) (\ell - q - 1) \left[ \zeta_j \partial_{\xi_j} + \omega_j \partial_{\zeta_j} \right] \psi^\ell_{(q+2)1} = - \left( \frac{2}{\hbar^2} \right) [E - V] \psi^\ell_0,
\]

\((11a)\)
\[ \Delta \psi_{q1}^{\ell\lambda} + 4 \{ q \partial_{\xi_1} + (\ell - q + 1) \partial_{\eta_2} \} \psi_{q1}^{\ell\lambda} + 2(q - 1) \partial_{\xi_2} \psi_{(q-1)1}^{\ell\lambda} + 2(\ell - q) \partial_{\xi_2} \psi_{(q+1)1}^{\ell\lambda} + \sum_{j=3}^{N-1} 2\Omega_2^{-1} \{ \left[ -\omega_j q \partial_{\xi_j} + \Omega_j (\ell - q + 1) \partial_{\eta_j} + \eta_2 \zeta_j q \partial_{\xi_j} + \xi_1 \zeta_j (\ell - q + 1) \partial_{\xi_j} \right] \psi_{(q-1)1}^{\ell\lambda} 
\]
\[ \quad - (q - 1) \left[ \omega_j \partial_{\eta_j} + \xi_2 \zeta_j \partial_{\xi_j} \right] \psi_{(q-1)0}^{\ell\lambda} - (\ell - q) \left[ \Omega_j \partial_{\xi_j} - \xi_2 \zeta_j \partial_{\xi_j} \right] \psi_{(q+1)1}^{\ell\lambda} 
\]
\[ - i \left[ \zeta_j \partial_{\eta_j} - \Omega_j \partial_{\xi_j} \right] \psi_{(q-1)0}^{\ell\lambda} - i \left[ \zeta_j \partial_{\xi_j} + \omega_j \partial_{\eta_j} \right] \psi_{(q-1)0}^{\ell\lambda} = - \left( 2/\hbar^2 \right) [ E - V ] \psi_{q1}^{\ell\lambda}, \quad (11b) \]

\[ \Delta \psi_{q7}^{\ell\lambda}(\xi, \eta, \zeta) = \{ 4\xi_1 \partial_{\xi_1}^2 + 4\eta_2 \partial_{\eta_2}^2 + (\xi_1 + \eta_2) \partial_{\xi_2}^2 + 4\xi_2 (\partial_{\xi_1} + \partial_{\eta_2}) \partial_{\xi_2} + 6 (\partial_{\xi_1} + \partial_{\eta_2}) \}
\]
\[ + \sum_{j=3}^{N-1} \left[ \xi_1 \partial_{\xi_j}^2 + \eta_2 \partial_{\eta_j}^2 + \Omega_2^{-1} \left( \eta_j \Omega_j - \xi_j \omega_j + \zeta_j^2 \right) \left( \partial_{\xi_j}^2 + \partial_{\eta_j}^2 \right) \right]
\]
\[ + \Omega_2^{-1} \left( \Omega_2^2 + \Omega_j^2 + \omega_j^2 + \xi_1 \zeta_j^2 + \eta_2 \zeta_j^2 \right) \partial_{\xi_j}^2 + 4 \left( \xi_j \partial_{\eta_j} + \zeta_j \partial_{\xi_j} \right) \partial_{\xi_j}
\]
\[ + 4 \left( \eta_j \partial_{\eta_j} + \zeta_j \partial_{\xi_j} \right) \partial_{\eta_j} + 2 \left( \eta_j \partial_{\xi_j} + \xi_j \partial_{\eta_j} \right) \partial_{\xi_j} + 2 \xi_j \partial_{\xi_j} \partial_{\eta_j} \} \psi_{q7}^{\ell\lambda}(\xi, \eta, \zeta). \quad (11c) \]

Due to the limited size of a letter, we have to leave the proof of the theorem and the detailed calculation elsewhere. When establishing BF we arbitrarily choose two Jacobi coordinate vectors \( \mathbf{R}_1 \) and \( \mathbf{R}_2 \). Those two vectors may be replaced with any other two Jacobi vectors. One may change the choice according to the characteristics of the physical problem under study, such as some or all particles in the quantum \( N \)-body problem are the identical particles.

In deriving the generalized radial equations, the key is to discover the base-functions \( Q_q^{\ell\lambda}(\mathbf{R}_1, \mathbf{R}_2) \) of the angular momentum and to choose the right internal variables, some of which have odd parity. From Eq. (9) we see that only finite number of partial angular momentum states are involved in constructing the base-functions \( Q_q^{\ell\lambda}(\mathbf{R}_1, \mathbf{R}_2) \). Namely, the contributions from the remaining partial angular momentum states have been incorporated into those from the generalized radial functions.

The two features in this method, that the numbers of both functions \( \psi_{q7}^{\ell\lambda}(\xi, \eta, \zeta) \) and equations are finite, and they depend only on \((3N-6)\) internal variables, are important for calculating the energy levels and wavefunctions in a quantum \( N \)-body problem. In fact, in the numerical experiment for the quantum three-body problem by the series expansion, much fewer terms have to be taken to achieve the same precision of energy than with other methods. The calculation error will be less in comparison with the method to truncate the series on the partial angular momentum states. As the number of the particles in the
system increases, we believe, to remove three independent variables will greatly decrease the calculation capacity requirement.

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