

Independent eigenstates of angular momentum in a quantum N -body system

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The global rotational degrees of freedom in the Schrödinger equation for an N -body system are completely separated from the internal ones. After removing the motion of the center of mass, we find a complete set of $(2\ell+1)$ independent base functions with angular momentum ℓ . These are homogeneous polynomials in the components of the coordinate vectors and the solutions of the Laplace equation, where the Euler angles do not appear explicitly. Any function with given angular momentum and given parity in the system can be expanded with respect to the base functions, where the coefficients are the functions of the internal variables. With the right choice of the base functions and the internal variables, we explicitly establish the equations for those functions. Only $(3N-6)$ internal variables are involved both in the functions and in the equations. The permutation symmetry of the wave functions for identical particles is discussed.

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I. INTRODUCTION

For a quantum N -body system with a pair potential, the Schrödinger equation is invariant under spatial translation, rotation, and inversion. It is well known that, due to the translation symmetry of the system, the wave function can be separated into a product of two parts. One describes the motion of the center of mass as a free particle, and the other describes the motion of the system in the center-of-mass frame. It is no loss of generality to suppose the center of mass of the system to be at rest, so that the configuration is completely specified by $(N-1)$ vectors \mathbf{r}_{cj} , $1 \leq j \leq N-1$, which are usually chosen as the Jacobi coordinate vectors \mathbf{R}_j for simplicity [1–3] (see Sec. II). On the other hand, due to the symmetries of the global rotation and space inversion of the system, the three rotational degrees of freedom should be separated completely from the internal ones so that only $(3N-6)$ internal variables, called the shape coordinates in some papers, are involved both in the functions and in the equations. This is the aim of this paper.

The hydrogen atom is a typical quantum two-body system, where there is only one Jacobi coordinate vector, which is proportional to the relative position vector $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. The Schrödinger equation for the hydrogen atom becomes a partial differential equation with respect to the three components of \mathbf{r} . Because of the spherical symmetry, the angular momentum is conserved, and the wave function can be expressed as a product of a radial function $\phi(r)$ and a spherical harmonic function $Y_m^\ell(\theta, \varphi)$,

$$\Psi_m^\ell(\mathbf{r}) = \phi(r) Y_m^\ell(\theta, \varphi), \quad (1)$$

where the radial function $\phi(r)$ satisfies the radial equation containing only one radial variable. The generalization of this method to a quantum N -body system is an important and fundamental problem that has been attacked by many groups.

Wigner studied this problem using group theory [4]. The global rotation of a system can be described by a space rotation $R = R(\alpha, \beta, \gamma)$, rotating the center-of-mass frame into the body-fixed frame, where α , β , and γ are the Euler angles. Briefly denoting all the internal variables for simplicity by ξ , which is invariant in the global rotation, one may express the wave function with a given angular momentum as $\Psi_m^\ell(R, \xi) = \Psi_m^\ell(\alpha, \beta, \gamma, \xi)$. Let P_S be the transformation operator for a scalar function $\psi(x)$ in the transformation S , $P_S \psi(x) = \psi(S^{-1}x)$ (see p. 105 in Ref. [4]). In a rotation $S \in \text{SO}(3)$, the function $\Psi_m^\ell(R, \xi)$ transforms as

$$P_S \Psi_m^\ell(R, \xi) = \Psi_m^\ell(S^{-1}R, \xi) = \sum_{m'=-\ell}^{\ell} \Psi_{m'}^\ell(R, \xi) D_{m'm}^\ell(S).$$

$\Psi_m^\ell(R, \xi)$ was called by Wigner [4] the function belonging to the m th row of the representation $D^\ell(\text{SO}(3))$. Letting $R = R(0, 0, 0)$ be the identity element, one obtains

$$\Psi_m^\ell(S^{-1}, \xi) = P_S \Psi_m^\ell(0, 0, 0, \xi) = \sum_{m'=-\ell}^{\ell} \phi_{m'}^\ell(\xi) D_{m'm}^\ell(S),$$

where $\phi_{m'}^\ell(\xi) = \Psi_{m'}^\ell(0, 0, 0, \xi)$ depends only on the internal variables, called the generalized radial functions in this paper. Due to the spherical symmetry, one only needs to study the eigenfunctions of angular momentum with the largest eigenvalue of L_z ($m = \ell$), which in this paper are simply called the wave functions with angular momentum ℓ for simplicity. Their partners with the smaller eigenvalues of L_z can be calculated from them by the lowering operator L_- . Letting $S^{-1} = R(\alpha, \beta, \gamma)$, one obtains [see Eq. (19.6) in [4]]

$$\Psi_m^\ell(\alpha, \beta, \gamma, \xi) = \Psi_m^\ell(R, \xi) = \sum_{m'=-\ell}^{\ell} D_{m'm}^\ell(\alpha, \beta, \gamma) \phi_{m'}^\ell(\xi), \quad (2)$$

where the commonly used form of the D function [5] is adopted. In Eq. (2) $D_{m'm}^\ell(\alpha, \beta, \gamma)$ plays the role of the base function. What Wigner proved is that $(2\ell+1)$ functions

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$D_{\ell m}^{\ell}(\alpha, \beta, \gamma)^*$ constitute a complete set of independent base functions with the angular momentum ℓ , and any wave function with the angular momentum ℓ can be expanded with respect to those base functions. Due to the singularity of the Euler angles, the generalized radial equations satisfied by the generalized radial functions are quite difficult to derive based on Eq. (2). Hirschfelder and Wigner [6] studied the problem of the generalized radial equations. Later, the generalized radial equations were improved by several authors [7–9]. The equations seem quite cumbersome [7]. In the present paper we are going to rechoose the base functions as the homogeneous polynomials in the components of the coordinate vectors so that the derivation of the generalized radial equations becomes very simple.

The generalized radial equations for a quantum three-body system have been discussed in more detail [10–12]. Recently, by making use of the body-fixed frame, the expression for the kinetic energy operator was built in terms of the partial angular momentum operators and radial derivatives containing $(3N-6)$ internal variables [13,14]. A coupled angular momentum basis was used to prediagonalize the kinetic energy operator, where some off-diagonal elements remain nonvanishing. Those results have been generalized to nonorthogonal vectors [15,16]. In those calculations, a function with a given angular momentum was obtained from the partial angular momentum states using Clebsch-Gordan coefficients. Since the partial angular momenta are generally not conserved, one has to deal with, in principle, an infinite number of partial angular momentum states. This problem also occurs in the hyperspherical harmonic function method and its improved versions [17–22]. It causes unnecessary degeneracy of the hyperspherical harmonic states because, as Wigner proved, only $(2\ell+1)$ base functions with angular momentum ℓ are involved in the calculation.

Eckart [1] presented another method, called the principal axis transformation, to distinguish the global rotation and the internal motion in a classical N -body system. From the $(N-1)$ Jacobi coordinate vector \mathbf{R}_j , he defined an $(N-1) \times (N-1)$ real symmetric matrix $\mathcal{R}_{jk} = \mathbf{R}_j \cdot \mathbf{R}_k$, which is semipositive definite. \mathcal{R} can be diagonalized by a real orthogonal similarity transformation X , $X\mathcal{R}X^{-1} = \Gamma$:

$$\left(\sum_{s=1}^{N-1} X_{js} \mathbf{R}_s \right) \cdot \left(\sum_{t=1}^{N-1} X_{kt} \mathbf{R}_t \right) = \delta_{jk} \Gamma_{jj}. \quad (3)$$

Since there are at most three orthogonal vectors in a three-dimensional space, the vectors can be expressed as

$$\sum_{k=1}^{N-1} X_{jk} \mathbf{R}_k = \begin{cases} \mathbf{e}_a r_a & \text{when } j = a \leq 3 \\ \mathbf{0} & \text{when } 4 \leq j \leq N-1, \end{cases} \quad (4)$$

where \mathbf{e}_a are three orthonormal vectors in the usual three-dimensional space and $r_a^2 = \Gamma_{aa}$. Three orthonormal vectors \mathbf{e}_a contain three Euler angles describing the global rotation of the system [1]. Thus, from Eqs. (3) and (4), Eckart obtained

$$\mathbf{R}_j = \sum_{a=1}^3 \mathbf{e}_a r_a X_{aj}, \quad 1 \leq j \leq N-1. \quad (5)$$

X_{aj} are the first three rows of the matrix X and contain $(3N-9)$ independent parameters. Therefore, $r_a X_{aj}$ contain $(3N-6)$ internal variables, and the rotational variables (Euler angles) can be completely separated in the kinetic energy expression from the internal variables [1]. This approach has been further studied and quantized in recent years [2,23–25]. The internal coordinates and their conjugate momenta were quantized to derive the kinetic energy expression through generalized angular momentum operators. However, the formal formula (5) does not give the explicit functional relation of the internal coordinates with the components of the Jacobi coordinate vectors, so that the kinetic energy expression cannot be transformed directly from the usual kinetic energy term in the Schrödinger equation by replacement of variables. It is very difficult to obtain the wave function on the position vectors \mathbf{r}_k (or on the Jacobi coordinate vectors \mathbf{R}_j) from a solution on these internal coordinates. The intermediate calculations for the kinetic energy expression are so complicated that, as said in Ref. [25], the expression for a quantum six-body system has not been obtained probably due to a few mistakes in calculations.

Let us return to the hydrogen atom problem. After removing the motion of the center of mass, the configuration space is parametrized in terms of the rectangular coordinates $\mathbf{r} = (x, y, z)$ or the spherical coordinates (r, θ, φ) , where r specifies the internal (radial) motion and (θ, φ) specify the overall rotation. There is another way to separate the rotational degrees of freedom and obtain the same radial function and the radial equation as those derived from Eq. (1). One may avoid explicitly introducing the rotational angles θ and φ using the harmonic polynomial $\mathcal{Y}_m^{\ell}(\mathbf{r}) = r^{\ell} Y_m^{\ell}(\theta, \varphi)$, which is a homogeneous polynomial of degree ℓ in the rectangular coordinates (x, y, z) and satisfies the Laplace equation as well as the eigenequation of the angular momentum. Using $\mathcal{Y}_m^{\ell}(\mathbf{r})$, Eq. (1) becomes

$$\Psi_m^{\ell}(\mathbf{r}) = \{r^{-\ell} \phi(r)\} \mathcal{Y}_m^{\ell}(\mathbf{r}).$$

Under the action of the Laplace operator, we have

$$\begin{aligned} \Delta \Psi_m^{\ell}(\mathbf{r}) &= \mathcal{Y}_m^{\ell}(\mathbf{r}) [\Delta r^{-\ell} \phi(r)] + 2 \nabla [r^{-\ell} \phi(r)] \cdot \nabla \{\mathcal{Y}_m^{\ell}(\mathbf{r})\} \\ &= \mathcal{Y}_m^{\ell}(\mathbf{r}) r^{-1} \partial_r^2 r [r^{-\ell} \phi(r)] \\ &\quad + 2 \partial_r [r^{-\ell} \phi(r)] r^{-1} \mathbf{r} \cdot \nabla \{\mathcal{Y}_m^{\ell}(\mathbf{r})\} \\ &= \mathcal{Y}_m^{\ell}(\mathbf{r}) r^{-\ell} \{r^{-1} \partial_r^2 r \phi(r) + \ell(\ell+1) r^{-2} \phi(r) \\ &\quad + 2(-\ell r^{-1}) [\partial_r \phi(r) + r^{-1} \phi(r)]\} \\ &\quad + 2\{-\ell r^{-\ell-1} \phi(r) + r^{-\ell} \partial_r \phi(r)\} \{\ell r^{-1} \mathcal{Y}_m^{\ell}(\mathbf{r})\} \\ &= Y_m^{\ell}(\theta, \varphi) \{r^{-1} \partial_r^2 r \phi(r) - \ell(\ell+1) r^{-2} \phi(r)\}, \end{aligned}$$

where and hereafter $\partial_r \psi$ denotes $\partial \psi / \partial r$, and so on. The results are the same. In the traditional approach, the property that $Y_m^{\ell}(\theta, \varphi)$ is the eigenfunction of L^2 is used, and, in this approach, the property that $\mathcal{Y}_m^{\ell}(\mathbf{r})$ is a homogeneous polynomial in the rectangular coordinates and is a solution to the Laplace equation is used. It is worth emphasizing that the rotational angles θ and φ do not appear explicitly in this

approach. Since the differential calculus with respect to θ and φ is not complicated, this approach is similar to the traditional one in a two-body system. However, it may be easier in an N -body system due to the complicated calculus with respect to the Euler angles. In the present paper we will separate the global rotational variables in the Schrödinger equation for an N -body system from the internal ones by a generalized method following the approach described above. In our approach, the number of base functions with the given angular momentum is finite, but that number in the hyper-spherical harmonic function method and its improved versions [13,17–22] is infinite due to the unconserved partial angular momenta. We also avoid the heavy differential calculus with respect to the Euler angles which is sometimes necessary for expressing kinetic energy operators.

This paper is organized as follows. In Sec. II we will briefly review the method of separating the motion of the center of mass by the Jacobi coordinate vectors. In Sec. III we will define $(3N-6)$ internal variables from the Jacobi coordinate vectors \mathbf{R}_j and find the $(2\ell+1)$ base functions with total orbital angular momentum ℓ , which are the homogeneous polynomials in the components of \mathbf{R}_j and the solutions of the Laplace equation. Then we will prove that the base functions constitute a complete set, namely, any function with the angular momentum ℓ and the given parity in the system can be expanded with respect to the base functions, where the coefficients depend only on the internal variables. Since the base functions are polynomials, we are able to derive easily the generalized radial equations satisfied by the coefficients explicitly in Sec. IV. The permutation symmetry for the total wave function when some or all of the particles in the system are identical particles is discussed in Sec. V. In Sec. VI we will derive the radial equations in a general case where the Jacobi coordinate vectors \mathbf{R}_j (orthogonal vectors) are replaced by arbitrary coordinate vectors \mathbf{r}_{c_j} in the center-of-mass frame (nonorthogonal vectors). In Sec. VII we will discuss a physical application of our approach. Some conclusions are given in Sec. VIII.

II. SEPARATION OF MOTION OF CENTER OF MASS

For a quantum N -body system, we denote the position vectors and the masses of N particles by \mathbf{r}_k and by m_k , $k=1,2,\dots,N$, respectively. $M=\sum_k m_k$ is the total mass. The Schrödinger equation for the N -body system is

$$-\frac{\hbar^2}{2} \sum_{k=1}^N m_k^{-1} \Delta_{\mathbf{r}_k} \Psi + V\Psi = E\Psi, \quad (6)$$

where $\Delta_{\mathbf{r}_k}$ is the Laplace operator with respect to the position vector \mathbf{r}_k , and V is a pair potential, depending upon the distance of each pair of particles, $|\mathbf{r}_j - \mathbf{r}_k|$.

Now, we replace the position vectors \mathbf{r}_k by the Jacobi coordinate vectors \mathbf{R}_j :

$$\mathbf{R}_0 = M^{-1/2} \sum_{k=1}^N m_k \mathbf{r}_k,$$

$$\mathbf{R}_j = \left(\frac{m_j M_{j+1}}{M_j} \right)^{1/2} \left(\mathbf{r}_j - \sum_{k=j+1}^N \frac{m_k \mathbf{r}_k}{M_{j+1}} \right),$$

$$1 \leq j \leq (N-1), \quad M_j = \sum_{k=j}^N m_k, \quad M_1 = M, \quad (7)$$

where \mathbf{R}_0 describes the position of the center of mass, \mathbf{R}_1 describes the mass-weighted separation from the first particle to the center of mass of the remaining particles, \mathbf{R}_2 describes the mass-weighted separation from the second particle to the center of mass of the remaining $N-2$ particles, and so on. The mass-weighted factors in front of the formulas for \mathbf{R}_j are determined by the condition

$$\sum_{k=1}^N m_k \mathbf{r}_k^2 = \sum_{j=0}^{N-1} \mathbf{R}_j^2,$$

where an additional factor \sqrt{M} is included in \mathbf{R}_j for convenience. One may determine the factors one by one from the following schemes. In the center-of-mass frame, if the first $j-1$ particles are located at the origin and the last $N-j$ particles coincide with each other, the factor in front of \mathbf{R}_j is determined by

$$\mathbf{r}_{j+1} = \mathbf{r}_{j+2} = \dots = \mathbf{r}_N = -m_j \mathbf{r}_j / M_{j+1}, \quad \sum_{k=j}^N m_k \mathbf{r}_k^2 = \mathbf{R}_j^2. \quad (8)$$

A straightforward calculation by replacement of variables shows that the Laplace operator in Eq. (6) and the orbital angular momentum operator \mathbf{L} are directly expressed in \mathbf{R}_j :

$$\Delta = \sum_{k=1}^N m_k^{-1} \Delta_{\mathbf{r}_k} = \sum_{j=0}^{N-1} \Delta_{\mathbf{R}_j},$$

$$\mathbf{L} = -i\hbar \sum_{k=1}^N \mathbf{r}_k \times \nabla_{\mathbf{r}_k} = -i\hbar \sum_{j=0}^{N-1} \mathbf{R}_j \times \nabla_{\mathbf{R}_j}. \quad (9)$$

In the center-of-mass frame, $\mathbf{R}_0=0$. Since the Laplace operator does not contain mixed derivative terms, the Jacobi coordinate vectors are also called orthogonal vectors [14]. The Laplace operator obviously has the symmetry of the $O(3N-3)$ group with respect to $(3N-3)$ components of $(N-1)$ Jacobi coordinate vectors. The $O(3N-3)$ group contains a subgroup $SO(3) \times O(N-1)$, where $SO(3)$ is the usual rotation group. The space inversion and the different definitions for the Jacobi coordinate vectors in the so-called Jacobi tree [19] can be obtained by $O(N-1)$ transformations. For a system of identical particles, the permutation group among particles is also a subgroup of the $O(N-1)$ group. As a matter of fact, after the transposition $(k, k+1)$ between the k th and the $(k+1)$ th particles, the new Jacobi coordinate vectors, denoted by \mathbf{R}'_j , satisfy

$$\mathbf{R}'_j = \mathbf{R}_j \quad \text{when } j \neq k \quad \text{or } k+1,$$

$$\begin{aligned}
\mathbf{R}'_k &= \left[\frac{m_{k+1}}{M_k(m_k + M_{k+2})} \right]^{1/2} \left[(m_k + M_{k+2})\mathbf{r}_{k+1} - m_k\mathbf{r}_k \right. \\
&\quad \left. - \sum_{j=k+2}^N m_j\mathbf{r}_j \right] \\
&= -\mathbf{R}_k \cos \theta_k + \mathbf{R}_{k+1} \sin \theta_k, \\
\mathbf{R}'_{k+1} &= \left[\frac{m_k}{(m_k + M_{k+2})M_{k+2}} \right]^{1/2} \left[M_{k+2}\mathbf{r}_k - \sum_{j=k+2}^N m_j\mathbf{r}_j \right] \\
&= \mathbf{R}_k \sin \theta_k + \mathbf{R}_{k+1} \cos \theta_k, \\
\cos \theta_k &= \left[\frac{m_k m_{k+1}}{M_{k+1}(m_k + M_{k+2})} \right]^{1/2}, \\
\sin \theta_k &= \left[\frac{M_k M_{k+2}}{M_{k+1}(m_k + M_{k+2})} \right]^{1/2}. \tag{10}
\end{aligned}$$

This is obviously an $O(N-1)$ transformation. For a system of identical particles, $\cos \theta_k = (N-k)^{-1}$.

It is easy to obtain the inverse transformation of Eq. (7):

$$\mathbf{r}_j = \left[\frac{M_{j+1}}{m_j M_j} \right]^{1/2} \mathbf{R}_j - \sum_{k=1}^{j-1} \left[\frac{m_k}{M_k M_{k+1}} \right]^{1/2} \mathbf{R}_k + M^{-1/2} \mathbf{R}_0, \tag{11}$$

$$\begin{aligned}
\mathbf{r}_j - \mathbf{r}_k &= \left[\frac{M_{j+1}}{m_j M_j} \right]^{1/2} \mathbf{R}_j - \sum_{i=k+1}^{j-1} \left[\frac{m_i}{M_i M_{i+1}} \right]^{1/2} \mathbf{R}_i \\
&\quad - \left[\frac{M_k}{m_k M_{k+1}} \right]^{1/2} \mathbf{R}_k. \tag{12}
\end{aligned}$$

Thus, the potential V is a function of $\mathbf{R}_j \cdot \mathbf{R}_k$.

The Jacobi coordinate vectors \mathbf{R}_j are invariant in translation and constitute a complete set of coordinate vectors in the center-of-mass frame. If a complete set of arbitrary coordinate vectors \mathbf{r}_{c_j} is chosen to replace the Jacobi coordinate vectors,

$$\mathbf{r}_{c_j} = \sum_{k=1}^{N-1} \mathbf{R}_k D_{kj}, \quad \det D \neq 0, \tag{13}$$

where D_{kj} are functions of the masses m_j , the Laplace operator and the angular momentum operator become

$$\begin{aligned}
\Delta &= \sum_{j,k=1}^{N-1} S_{jk} \nabla_{\mathbf{r}_{c_j}} \cdot \nabla_{\mathbf{r}_{c_k}}, \quad S_{jk} = \sum_{i=1}^{N-1} D_{ij} D_{ik}, \\
\mathbf{L} &= -i\hbar \sum_{j=1}^{N-1} \mathbf{r}_{c_j} \times \nabla_{\mathbf{r}_{c_j}}. \tag{14}
\end{aligned}$$

A typical example is $\mathbf{r}_{c_j} = \mathbf{r}_j - M^{-1/2} \mathbf{R}_0$ [see Eq. (11)]. When the matrix S is not diagonal, \mathbf{r}_{c_j} are called the nonorthogonal vectors [15,16]. We will not discuss the nonorthogonal vectors until Sec. VI.

III. BASE FUNCTIONS WITH THE GIVEN ANGULAR MOMENTUM

Because of the spherical symmetry, the angular momentum is conserved. We are going to discuss the wave functions with the given angular momentum and parity. From the given form (9), the eigenfunctions of the angular momentum \mathbf{L}^2 are homogeneous polynomials in the components R_{jb} of the Jacobi coordinate vectors \mathbf{R}_j .

For a quantum two-body system, there is only one Jacobi coordinate vector $\mathbf{R} = \mathbf{r}$, and the eigenfunction of the angular momentum is the spherical harmonic function $Y_m^\ell(\theta, \varphi)$. What is the generalization of the spherical harmonic function for a quantum N -body system? A naive idea for generalization is to introduce the Euler angles, as was done by Wigner [4,7-9]. Is it necessary to introduce angular variables in the eigenfunction of the angular momentum?

As is well known, the harmonic polynomial $\mathcal{Y}_m^\ell(\mathbf{r}) = r^\ell Y_m^\ell(\theta, \varphi)$ is a homogeneous polynomial of degree ℓ in the components of \mathbf{r} , which satisfies the Laplace equation as well as the eigenequation of the angular momentum. It does not contain angular variables explicitly. The number of linearly independent homogeneous polynomials of degree ℓ in the components of \mathbf{r} is

$$N(\ell) = \sum_{s=0}^{\ell} (\ell - s + 1) = (\ell + 1)(\ell + 2)/2. \tag{15}$$

The number of homogeneous polynomials that can be expressed as a product of $\mathbf{r} \cdot \mathbf{r}$ and a homogeneous polynomial of degree $(\ell - 2)$ is $N(\ell - 2)$. Because $N(\ell) - N(\ell - 2) = 2\ell + 1$, the remaining homogeneous polynomials of degree ℓ are nothing but the harmonic polynomials $\mathcal{Y}_m^\ell(\mathbf{r})$.

For a quantum three-body system there are two Jacobi coordinate vectors \mathbf{R}_1 and \mathbf{R}_2 and three internal variables in the center-of-mass frame:

$$\xi_1 = \mathbf{R}_1 \cdot \mathbf{R}_1, \quad \xi_2 = \mathbf{R}_1 \cdot \mathbf{R}_2, \quad \eta_2 = \mathbf{R}_2 \cdot \mathbf{R}_2. \tag{15}$$

The internal variables are invariant in the global rotation and the space inversion of the system. We are going to construct base functions for angular momentum that do not contain a function of the internal variables as a multiplying factor, because the factor should be incorporated into the generalized radial functions. The number of linearly independent homogeneous polynomials of degree ℓ in the components of the Jacobi coordinate vectors is $M(\ell)$:

$$M(\ell) = \frac{1}{5!} (\ell + 1)(\ell + 2)(\ell + 3)(\ell + 4)(\ell + 5).$$

The number of homogeneous polynomials of degree ℓ that do not contain a function of the internal variables as a factor is

$$\begin{aligned}
K(\ell) &= M(\ell) - 3M(\ell - 2) + 3M(\ell - 4) - M(\ell - 6) \\
&= 4\ell^2 + 2, \quad \ell \geq 1.
\end{aligned}$$

On the other hand, the wave function with angular momentum ℓ can be obtained from $\mathcal{Y}_m^q(\mathbf{R}_1)\mathcal{Y}_{m'}^{\ell-q}(\mathbf{R}_2)$ by use of the Clebsch-Gordan coefficients $\langle q, m, \ell - q, \mu - m | L, \mu \rangle$ [5]:

$$\mathcal{Y}_{L\mu}^q(\mathbf{R}_1, \mathbf{R}_2) = \sum_m \mathcal{Y}_m^q(\mathbf{R}_1)\mathcal{Y}_{\mu-m}^{\ell-q}(\mathbf{R}_2) \times \langle q, m, \ell - q, \mu - m | L, \mu \rangle. \quad (16)$$

$\mathcal{Y}_{L\mu}^q(\mathbf{R}_1, \mathbf{R}_2)$ is a homogeneous polynomial of degree ℓ in the components of the Jacobi coordinate vectors \mathbf{R}_j . Simultaneously, it is the common eigenfunction of \mathbf{L}^2 , L_z , and the space inversion with eigenvalues $L(L+1)$, μ , and $(-1)^\ell$, respectively. When $\mu = L = \ell$ ($0 \leq q \leq \ell$) and $(\ell - 1)$ ($1 \leq q \leq \ell - 1$), we have

$$\begin{aligned} \mathcal{Y}_{L\mu}^q(\mathbf{R}_1, \mathbf{R}_2) &= (-1)^\ell \left\{ \frac{[(2q+1)!(2\ell-2q+1)!]^{1/2}}{q!(\ell-q)!2^{\ell+2}\pi} \right\} \\ &\quad \times (R_{1x} + iR_{1y})^q (R_{2x} + iR_{2y})^{\ell-q}, \\ \mathcal{Y}_{(\ell-1)(\ell-1)}^q(\mathbf{R}_1, \mathbf{R}_2) &= (-1)^{\ell-1} \left\{ \frac{(2q+1)!(2\ell-2q+1)!}{2q\ell(\ell-q)} \right\}^{1/2} \\ &\quad \times \{(q-1)!(\ell-q-1)!2^{\ell+1}\pi\}^{-1} \\ &\quad \times (R_{1x} + iR_{1y})^{q-1} (R_{2x} + iR_{2y})^{\ell-q-1} \\ &\quad \times \{(R_{1x} + iR_{1y})R_{2z} - R_{1z}(R_{2x} + iR_{2y})\}. \end{aligned} \quad (17)$$

It is evident that these expressions do not contain a function of the internal variables as a factor; neither do their partners with smaller μ due to the spherical symmetry. The number of these eigenfunctions is

$$(2\ell+1)(\ell+1) + (2\ell-1)(\ell-1) = 4\ell^2 + 2 = K(\ell), \quad \ell \geq 1.$$

That is, any of the remaining eigenfunctions $\mathcal{Y}_{L\mu}^q(\mathbf{R}_1, \mathbf{R}_2)$ with $L < \ell - 1$ can be expressed as a combination, where each term is a product of a function of the internal variables and a homogeneous polynomial of degree less than ℓ [26]. For example,

$$\begin{aligned} \mathcal{Y}_{00}^{21}(\mathbf{R}_1, \mathbf{R}_2) &= -\frac{\sqrt{3}}{4\pi}\xi_2, \\ \mathcal{Y}_{00}^{42}(\mathbf{R}_1, \mathbf{R}_2) &= \frac{\sqrt{5}}{8\pi}\{3\xi_2^2 - \xi_1\eta_2\}, \\ \mathcal{Y}_{22}^{42}(\mathbf{R}_1, \mathbf{R}_2) &= 5\frac{\sqrt{21}}{56\pi}\{\eta_2(R_{1x} + iR_{1y})^2 + \xi_1(R_{2x} + iR_{2y})^2 \\ &\quad - 3\xi_2(R_{1x} + iR_{1y})(R_{2x} + iR_{2y})\}. \end{aligned}$$

In other words, any eigenfunction with angular momentum ℓ is a combination of those homogeneous polynomials $\mathcal{Y}_{\ell\ell}^q(\mathbf{R}_1, \mathbf{R}_2)$ and $\mathcal{Y}_{\ell\ell}^{(\ell+1)q}(\mathbf{R}_1, \mathbf{R}_2)$, where the combinative coefficients are functions of the internal variables. Since the normalization factor can be ignored, we rewrite $\mathcal{Y}_{\ell\ell}^{(\ell+\lambda)q}(\mathbf{R}_1, \mathbf{R}_2)$ in a simplified form as $Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$ by removing a constant factor:

$$Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2) = \frac{X^{q-\lambda}Y^{\ell-q}Z^\lambda}{(q-\lambda)!(\ell-q)!}, \quad \lambda \leq q \leq \ell, \quad \lambda = 0, 1, \\ X \equiv R_{1x} + iR_{1y}, \quad Y \equiv R_{2x} + iR_{2y}, \quad Z \equiv XR_{2z} - R_{1z}Y. \quad (18)$$

Note that

$$Q_q^{\ell-1}(\mathbf{R}_1, \mathbf{R}_2) = Q_{q-1}^{(\ell-1)0}(\mathbf{R}_1, \mathbf{R}_2)Z. \quad (19)$$

$Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$, called the generalized harmonic polynomial, is a homogeneous polynomial of degree $(\ell + \lambda)$ in the components of the Jacobi coordinate vectors. It is the common eigenfunction of \mathbf{L}^2 , L_z , $\mathbf{L}_{\mathbf{R}_1}^2$, $\mathbf{L}_{\mathbf{R}_2}^2$, $\Delta_{\mathbf{R}_1}$, $\Delta_{\mathbf{R}_2}$, $\nabla_{\mathbf{R}_1} \cdot \nabla_{\mathbf{R}_2}$, and the space inversion with the eigenvalues $\ell(\ell+1)$, ℓ , $q(q+1)$, $(\ell-q+\lambda)(\ell-q+\lambda+1)$, 0 , 0 , 0 , and $(-1)^{\ell+\lambda}$, respectively, where $\mathbf{L}_{\mathbf{R}_1}^2$ ($\mathbf{L}_{\mathbf{R}_2}^2$) is the square of the partial angular momentum, and $\Delta_{\mathbf{R}_1}$ ($\Delta_{\mathbf{R}_2}$) is the Laplace operator with respect to the Jacobi coordinate vector \mathbf{R}_1 (\mathbf{R}_2) [see Eq. (9)]. Any wave function with the given angular momentum ℓ and the parity $(-1)^{\ell+\lambda}$ can be expressed as follows:

$$\Psi_{\ell}^\wedge(\mathbf{R}_1, \mathbf{R}_2) = \sum_{q=\lambda}^{\ell} \psi_q^\wedge(\xi_1, \xi_2, \eta_2) Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2), \quad \lambda = 0, 1. \quad (20)$$

That is, for a three-body system the generalized harmonic polynomials $Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$ constitute a complete set of base functions with angular momentum ℓ and parity $(-1)^{\ell+\lambda}$. Only $\ell + 1 - \lambda$ partial angular momentum states are involved in constructing a function with angular momentum ℓ and parity $(-1)^{\ell+\lambda}$, and the contributions from the infinite number of remaining partial angular momentum states are incorporated into those of the radial functions. Substituting Eq. (20) into the Schrödinger equations (6) and (9), one is able to easily derive the generalized radial equations for the generalized radial functions $\psi_q^\wedge(\xi_1, \xi_2, \eta_2)$ [3,27]:

$$\begin{aligned} \Delta \psi_q^\wedge + 4q\partial_{\xi_1}\psi_q^\wedge + 4(\ell-q+\lambda)\partial_{\eta_2}\psi_q^\wedge + 2(q-\lambda)\partial_{\xi_2}\psi_{q-1}^\wedge \\ + 2(\ell-q)\partial_{\xi_2}\psi_{q+1}^\wedge = -\frac{2}{\hbar^2}(E-V)\psi_q^\wedge, \\ \Delta \psi_q^\wedge(\xi_1, \xi_2, \eta_2) = \{4\xi_1\partial_{\xi_1}^2 + 4\eta_2\partial_{\eta_2}^2 + 6(\partial_{\xi_1} + \partial_{\eta_2}) \\ + (\xi_1 + \eta_2)\partial_{\xi_2}^2 + 4\xi_2(\partial_{\xi_1} + \partial_{\eta_2})\partial_{\xi_2}\} \\ \times \psi_q^\wedge(\xi_1, \xi_2, \eta_2), \quad \lambda \leq q \leq \ell, \quad \lambda = 0, 1. \end{aligned} \quad (21)$$

For a quantum N -body system, there are $(N-1)$ Jacobi coordinate vectors. We arbitrarily choose two Jacobi coordi-

nate vectors, say, \mathbf{R}_1 and \mathbf{R}_2 . We fix the body-fixed frame such that \mathbf{R}_1 is parallel with its Z axis, and \mathbf{R}_2 is located in its XZ plane with a non-negative X component. Define $(3N-6)$ internal variables, which are invariant in the global rotation of the system:

$$\begin{aligned} \xi_j &= \mathbf{R}_j \cdot \mathbf{R}_1, & \eta_j &= \mathbf{R}_j \cdot \mathbf{R}_2, & \zeta_j &= \mathbf{R}_j \cdot (\mathbf{R}_1 \times \mathbf{R}_2), \\ 1 \leq j \leq (N-1), & & \eta_1 &= \xi_2, & \zeta_1 &= \zeta_2 = 0. \end{aligned} \quad (22)$$

It is worth mentioning that ξ_j and η_j have even parity, but ζ_j has odd parity. From them we have

$$\begin{aligned} \Omega_j &= (\mathbf{R}_1 \times \mathbf{R}_j) \cdot (\mathbf{R}_1 \times \mathbf{R}_2) = \xi_1 \eta_j - \xi_2 \xi_j, \\ \omega_j &= (\mathbf{R}_2 \times \mathbf{R}_j) \cdot (\mathbf{R}_1 \times \mathbf{R}_2) = \xi_2 \eta_j - \eta_2 \xi_j, \\ \Omega_1 &= \omega_2 = 0, & \Omega_2 &= -\omega_1 = (\mathbf{R}_1 \times \mathbf{R}_2)^2. \end{aligned} \quad (23)$$

Due to our choice of the body-fixed frame, the components of \mathbf{R}_1 and \mathbf{R}_2 are in the frame $(0, 0, \xi_1^{1/2})$ and $[(\Omega_2/\xi_1)^{1/2}, 0, \xi_2 \xi_1^{-1/2}]$, respectively. From Eq. (22) we are able to express all the components \mathbf{R}'_{jb} of the Jacobi coordinate vectors \mathbf{R}_j in the body-fixed frame by the internal variables:

$$R'_{jx} = \Omega_j (\xi_1 \Omega_2)^{-1/2}, \quad R'_{jy} = \zeta_j \Omega_2^{-1/2}, \quad R'_{jz} = \xi_j \xi_1^{-1/2}. \quad (24)$$

The formulas (24) also hold for $j=1$ and 2 . The volume element of the configuration space can be calculated from the Jacobi determinant by replacement of variables:

$$\begin{aligned} \prod_{j=1}^{N-1} dR_{jx} dR_{jy} dR_{jz} &= \frac{1}{4} \Omega_2^{3-N} \sin \beta d\alpha d\beta d\gamma d\xi_1 d\xi_2 d\eta_2 \\ &\times \prod_{j=3}^{N-1} d\xi_j d\eta_j d\zeta_j. \end{aligned} \quad (25)$$

The range of definition of the Euler angle is well known; the ranges of definition of ξ_1 and η_2 are $(0, \infty)$ and the ranges of definition of the remaining variables are $(-\infty, \infty)$.

Furthermore,

$$\mathbf{R}_j \cdot \mathbf{R}_k = \Omega_2^{-1} (\Omega_j \eta_k - \omega_j \xi_k + \zeta_j \zeta_k). \quad (26)$$

It is easy to see from Eqs. (12) and (26) that the potential V is a function of only the internal variables. Since \mathbf{R}_1 and \mathbf{R}_2 determine the body-fixed frame completely, it also can be seen from Eq. (24) that each of the components of the Jacobi coordinate vectors \mathbf{R}_j can be expressed as a linear combination of \mathbf{R}_{1b} and \mathbf{R}_{2b} with the coefficients depending on the internal variables. In fact, denote the rotation transforming the center-of-mass frame to the body-fixed frame by $R(\alpha, \beta, \gamma)$ with three Euler angles [5]

$$R(\alpha, \beta, \gamma) = \begin{pmatrix} c_\alpha c_\beta c_\gamma - s_\alpha s_\gamma & -c_\alpha c_\beta s_\gamma - s_\alpha c_\gamma & c_\alpha s_\beta \\ s_\alpha c_\beta c_\gamma + c_\alpha s_\gamma & -s_\alpha c_\beta s_\gamma + c_\alpha c_\gamma & s_\alpha s_\beta \\ -s_\beta c_\gamma & s_\beta s_\gamma & c_\beta \end{pmatrix}, \quad (27)$$

where $c_\alpha = \cos \alpha$, $s_\alpha = \sin \alpha$, and so on. It is straightforward to obtain from Eqs. (18), (24), and (27) that

$$\begin{aligned} X &= R_{1x} + iR_{1y} = \xi_1^{1/2} e^{i\alpha} s_\beta, \\ Y &= R_{2x} + iR_{2y} = (\Omega_2/\xi_1)^{1/2} e^{i\alpha} (c_\beta c_\gamma + i s_\gamma) + \xi_2 \xi_1^{-1/2} e^{i\alpha} s_\beta, \\ R_{1z} &= \xi_1^{1/2} c_\beta, & R_{2z} &= -(\Omega_2/\xi_1)^{1/2} s_\beta c_\gamma + \xi_2 \xi_1^{-1/2} c_\beta, \\ Z &= (R_{1x} + iR_{1y})R_{2z} - R_{1z}(R_{2x} + iR_{2y}) \\ &= -\Omega_2^{1/2} e^{i\alpha} (c_\gamma + i c_\beta s_\gamma), \\ R_{jx} + iR_{jy} &= \Omega_2^{-1} \{ -\omega_j X + \Omega_j Y - i\zeta_j Z \}, \\ (R_{jx} + iR_{jy})R_{kz} - R_{jz}(R_{kx} + iR_{ky}) \\ &= \Omega_2^{-1} \{ i(\eta_j \zeta_k - \eta_k \zeta_j) X - i(\xi_j \zeta_k - \xi_k \zeta_j) Y \\ &\quad + (\xi_j \eta_k - \xi_k \eta_j) Z \}. \end{aligned} \quad (28)$$

Therefore, each harmonic polynomial $\mathcal{Y}^\ell(\mathbf{R}_j)$ can be expressed as a combination of $Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$ with the coefficients depending on the internal variables. This means that the generalized harmonic polynomials $Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$ given in Eq. (18) do constitute a complete set of independent base functions with the given angular momentum ℓ for a quantum N -body system, just as they do for a quantum three-body system.

Because this conclusion plays a key role in separating the global rotational degrees of freedom from the internal ones in the quantum N -body system, we are going to prove it by another method. From Eq. (28) we have

$$\begin{aligned} e^{i\alpha} s_\beta &= \xi_1^{-1/2} X, & e^{i\alpha} (c_\gamma + i c_\beta s_\gamma) &= -\Omega_2^{-1/2} Z, \\ e^{i\alpha} (c_\beta c_\gamma + i s_\gamma) &= -\xi_2 (\xi_1 \Omega_2)^{-1/2} X + (\xi_1 / \Omega_2)^{1/2} Y, \end{aligned} \quad (30)$$

$$Z^2 = \eta_2 X^2 - 2\xi_2 XY + \xi_1 Y^2. \quad (31)$$

That is, a homogeneous polynomial of degree ℓ in three variables $e^{i\alpha} s_\beta$, $e^{i\alpha} (c_\beta c_\gamma + i s_\gamma)$, and $e^{i\alpha} (c_\gamma + i c_\beta s_\gamma)$ can be expanded with respect to $Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$ where the coefficients only depend on the internal variables ξ_j , η_j , and ζ_j . On the other hand, the Wigner D function is [5]

$$\begin{aligned} D_{\ell(\pm m)}^\ell(\alpha, \beta, \gamma)^* &= (-1)^{\ell-m} 2^{-\ell} \left[\frac{(2\ell)!}{(\ell+m)!(\ell-m)!} \right]^{1/2} \\ &\quad \times e^{i(\ell \pm m \gamma)} s_\beta^{\ell-m} (1 \pm c_\beta)^m \\ &= (-1)^{\ell-m} 2^{-\ell} \left[\frac{(2\ell)!}{(\ell+m)!(\ell-m)!} \right]^{1/2} \\ &\quad \times (e^{i\alpha} s_\beta)^{\ell-m} [e^{i\alpha} (c_\gamma + i c_\beta s_\gamma) \\ &\quad \pm e^{i\alpha} (c_\beta c_\gamma + i s_\gamma)]^m, \end{aligned} \quad (32)$$

where $m \geq 0$. Therefore, $D_{\ell m}^\ell(\alpha, \beta, \gamma)^*$ can be expanded with respect to $Q_q^\ell(\mathbf{R}_1, \mathbf{R}_2)$, where the coefficients depend only on the internal variables. $D_{\ell m}^\ell(\alpha, \beta, \gamma)^*$ constitute a

complete set of independent base functions with the angular momentum ℓ , and so do $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$. Now, we come to the theorem.

Theorem. Any function $\Psi^{\ell\lambda}(\mathbf{R}_1, \dots, \mathbf{R}_{N-1})$ with the angular momentum ℓ and the parity $(-1)^{\ell+\lambda}$ in a quantum N -body system can be expanded with respect to the generalized harmonic polynomials $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$ with the coefficients $\psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta)$ depending on $(3N-6)$ internal variables:

$$\begin{aligned} \Psi^{\ell\lambda}(\mathbf{R}_1, \dots, \mathbf{R}_{N-1}) &= \sum_{\tau=0}^1 \sum_{q=\tau}^{\ell} \psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta) Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2), \\ \psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta) & \\ &= \psi_{q\tau}^{\ell\lambda}(\xi_1, \dots, \xi_{N-1}, \eta_2, \dots, \eta_{N-1}, \zeta_3, \dots, \zeta_{N-1}), \\ \psi_{q\tau}^{\ell\lambda}(\xi, \eta, -\zeta) &= (-1)^{\lambda-\tau} \psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta), \end{aligned} \quad (33)$$

where the last equality means that the parity of $\psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta)$ is $(-1)^{\lambda-\tau}$.

IV. THE GENERALIZED RADIAL EQUATIONS

From the theorem above, the set of $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$, just like the set of $D_{\ell m}^{\ell}(\alpha, \beta, \gamma)^*$, is a complete set of base functions

with angular momentum ℓ in the quantum N -body system. Each function with angular momentum ℓ in the system can be expanded like Eq. (33) or Eq. (2). However, Eq. (33) has two important characteristics, which make it easier to derive the generalized radial equations. One is that the generalized harmonic polynomial $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$ is a homogeneous polynomial in the components of two Jacobi coordinate vectors \mathbf{R}_1 and \mathbf{R}_2 , where the Euler angles do not appear explicitly. The other is the well-chosen internal variables (22), where the internal variables ζ_j have odd parity. It is due to the existence of ζ_j that $Q_q^{\ell 0}(\mathbf{R}_1, \mathbf{R}_2)$ and $Q_q^{\ell 1}(\mathbf{R}_1, \mathbf{R}_2)$ appear together in the expansion of the wave function. By comparison, all internal variables in a quantum three-body system have even parity ($\zeta_j=0$) so that in the expansion (20) of a wave function with a given parity only the base functions with the same parity appear [3,4,27,28].

Because of these two characteristics, it is easy to derive the generalized radial equations by substituting Eq. (33) into the Schrödinger equation (6) with the Laplace operator (9). The main calculation in the derivation is to apply the Laplace operator (9) to the function $\Psi^{\ell\lambda}(\mathbf{R}_1, \dots, \mathbf{R}_{N-1})$ in Eq. (33). The calculation consists of three parts. The first is to apply the Laplace operator to the generalized radial functions $\psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta)$:

$$\begin{aligned} \Delta \psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta) &= \left\{ 4\xi_1 \partial_{\xi_1}^2 + 4\eta_2 \partial_{\eta_2}^2 + (\xi_1 + \eta_2) \partial_{\xi_2}^2 + 4\xi_2 (\partial_{\xi_1} + \partial_{\eta_2}) \partial_{\xi_2} + 6(\partial_{\xi_1} + \partial_{\eta_2}) \right. \\ &+ \sum_{j=3}^{N-1} [\xi_1 \partial_{\xi_j}^2 + \eta_2 \partial_{\eta_j}^2 + \Omega_2 \partial_{\zeta_j}^2 + 2\xi_2 \partial_{\xi_j} \partial_{\eta_j} + 4(\xi_j \partial_{\xi_j} + \zeta_j \partial_{\zeta_j}) \partial_{\xi_1} + 4(\eta_j \partial_{\eta_j} + \zeta_j \partial_{\zeta_j}) \partial_{\eta_2} + 2(\eta_j \partial_{\xi_j} + \xi_j \partial_{\eta_j}) \partial_{\xi_2}] \\ &+ \Omega_2^{-1} \sum_{j,k=3}^{N-1} [(\Omega_j \eta_k - \omega_j \xi_k + \zeta_j \zeta_k) (\partial_{\xi_j} \partial_{\xi_k} + \partial_{\eta_j} \partial_{\eta_k}) - 2(\omega_j \zeta_k - \omega_k \zeta_j) \partial_{\xi_j} \partial_{\zeta_k} + 2(\Omega_j \zeta_k - \Omega_k \zeta_j) \partial_{\eta_j} \partial_{\zeta_k} \\ &\left. + (\Omega_j \Omega_k + \omega_j \omega_k + \xi_1 \zeta_j \zeta_k + \eta_2 \zeta_j \zeta_k) \partial_{\zeta_j} \partial_{\zeta_k} \right\} \psi_{q\tau}^{\ell\lambda}(\xi, \eta, \zeta). \end{aligned} \quad (34)$$

The second is to apply it to the generalized harmonic polynomials $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$. This part is vanishing because $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$ satisfies the Laplace equation. The last is the mixed application

$$\begin{aligned} &2 \left\{ (\partial_{\xi_1} \psi_{q\tau}^{\ell\lambda}) 2\mathbf{R}_1 + (\partial_{\xi_2} \psi_{q\tau}^{\ell\lambda}) \mathbf{R}_2 \right. \\ &+ \sum_{j=3}^{N-1} [(\partial_{\xi_j} \psi_{q\tau}^{\ell\lambda}) \mathbf{R}_j + (\partial_{\zeta_j} \psi_{q\tau}^{\ell\lambda}) (\mathbf{R}_2 \times \mathbf{R}_j)] \left. \right\} \cdot \nabla_{\mathbf{R}_1} Q_q^{\ell\tau} \\ &+ 2 \left\{ (\partial_{\xi_2} \psi_{q\tau}^{\ell\lambda}) \mathbf{R}_1 + (\partial_{\eta_2} \psi_{q\tau}^{\ell\lambda}) 2\mathbf{R}_2 \right. \\ &+ \sum_{j=3}^{N-1} [(\partial_{\eta_j} \psi_{q\tau}^{\ell\lambda}) \mathbf{R}_j + (\partial_{\zeta_j} \psi_{q\tau}^{\ell\lambda}) (\mathbf{R}_j \times \mathbf{R}_1)] \left. \right\} \cdot \nabla_{\mathbf{R}_2} Q_q^{\ell\tau}. \end{aligned}$$

In terms of Eqs. (18) and (29) we obtain

$$\begin{aligned} \mathbf{R}_1 \cdot \nabla_{\mathbf{R}_1} Q_q^{\ell\tau} &= q Q_q^{\ell\tau}, \quad \mathbf{R}_2 \cdot \nabla_{\mathbf{R}_2} Q_q^{\ell\tau} = (\ell - q + \tau) Q_q^{\ell\tau}, \\ \mathbf{R}_2 \cdot \nabla_{\mathbf{R}_1} Q_q^{\ell\tau} &= (\ell - q + 1) Q_q^{\ell\tau-1}, \\ \mathbf{R}_1 \cdot \nabla_{\mathbf{R}_2} Q_q^{\ell\tau} &= (q - \tau + 1) Q_q^{\ell\tau+1}, \\ \mathbf{R}_j \cdot \nabla_{\mathbf{R}_1} Q_q^{\ell 0} &= \Omega_2^{-1} \{-\omega_j q Q_q^{\ell 0} + \Omega_j (\ell - q + 1) Q_q^{\ell 0} - i \zeta_j Q_q^{\ell 1}\}, \\ \mathbf{R}_j \cdot \nabla_{\mathbf{R}_2} Q_q^{\ell 0} &= \Omega_2^{-1} \{-\omega_j (q + 1) Q_q^{\ell 0} + \Omega_j (\ell - q) Q_q^{\ell 0} - i \zeta_j Q_q^{\ell 1}\}, \end{aligned}$$

$$\begin{aligned} \mathbf{R}_j \cdot \nabla_{\mathbf{R}_1} Q_q^{\prime 1} &= \Omega_2^{-1} \{ -i \eta_2 \zeta_j q^2 Q_q^{\prime 0} + i \xi_2 \zeta_j (2q-1) \\ &\quad \times (\ell - q + 1) Q_{q-1}^{\prime 0} - i \xi_1 \zeta_j (\ell - q + 2) \\ &\quad \times (\ell - q + 1) Q_{q-2}^{\prime 0} - \omega_j q Q_q^{\prime 1} \\ &\quad + \Omega_j (\ell - q + 1) Q_{q-1}^{\prime 1} \}, \end{aligned}$$

$$\begin{aligned} \mathbf{R}_j \cdot \nabla_{\mathbf{R}_2} Q_q^{\prime 1} &= \Omega_2^{-1} \{ -i \eta_2 \zeta_j (q+1) q Q_{q+1}^{\prime 0} + i \xi_2 \zeta_j q \\ &\quad \times (2\ell - 2q + 1) Q_q^{\prime 0} - i \xi_1 \zeta_j (\ell - q + 1)^2 Q_{q-1}^{\prime 0} \\ &\quad - \omega_j q Q_{q+1}^{\prime 1} + \Omega_j (\ell - q + 1) Q_q^{\prime 1} \}, \end{aligned}$$

$$\begin{aligned} (\mathbf{R}_2 \times \mathbf{R}_j) \cdot \nabla_{\mathbf{R}_1} Q_q^{\prime 0} &= \Omega_2^{-1} \{ \eta_2 \zeta_j q Q_q^{\prime 0} - \xi_2 \zeta_j (\ell - q + 1) \\ &\quad \times Q_{q-1}^{\prime 0} - i \omega_j Q_q^{\prime 1} \}, \end{aligned}$$

$$\begin{aligned} (\mathbf{R}_j \times \mathbf{R}_1) \cdot \nabla_{\mathbf{R}_2} Q_q^{\prime 0} &= \Omega_2^{-1} \{ -\xi_2 \zeta_j (q+1) Q_{q+1}^{\prime 0} \\ &\quad + \xi_1 \zeta_j (\ell - q) Q_q^{\prime 0} + i \Omega_j Q_{q+1}^{\prime 1} \}, \end{aligned}$$

$$\begin{aligned} (\mathbf{R}_2 \times \mathbf{R}_j) \cdot \nabla_{\mathbf{R}_1} Q_q^{\prime 1} &= \Omega_2^{-1} \{ -i \eta_2 \omega_j q^2 Q_q^{\prime 0} + i \xi_2 \omega_j (2q-1) \\ &\quad \times (\ell - q + 1) Q_{q-1}^{\prime 0} - i \xi_1 \omega_j (\ell - q + 2) \\ &\quad \times (\ell - q + 1) Q_{q-2}^{\prime 0} + \eta_2 \zeta_j q Q_q^{\prime 1} \\ &\quad - \xi_2 \zeta_j (\ell - q + 1) Q_{q-1}^{\prime 1} \}, \end{aligned}$$

$$\begin{aligned} (\mathbf{R}_j \times \mathbf{R}_1) \cdot \nabla_{\mathbf{R}_2} Q_q^{\prime 1} &= \Omega_2^{-1} \{ i \eta_2 \Omega_j (q+1) q Q_{q+1}^{\prime 0} \\ &\quad - i \xi_2 \Omega_j q (2\ell - 2q + 1) Q_q^{\prime 0} \\ &\quad + i \xi_1 \Omega_j (\ell - q + 1)^2 Q_{q-1}^{\prime 0} \\ &\quad - \xi_2 \zeta_j q Q_{q+1}^{\prime 1} + \xi_1 \zeta_j (\ell - q + 1) Q_q^{\prime 1} \}. \end{aligned} \quad (35)$$

Now the generalized radial equations are

$$\begin{aligned} \Delta \psi_{q_0}^{\wedge} &+ 4 \{ q \partial_{\xi_1} + (\ell - q) \partial_{\eta_2} \} \psi_{q_0}^{\wedge} + 2q \partial_{\xi_2} \psi_{(q-1)0}^{\wedge} + 2(\ell - q) \partial_{\xi_2} \psi_{(q+1)0}^{\wedge} + \sum_{j=3}^{N-1} 2\Omega_2^{-1} \{ [-\omega_j q \partial_{\xi_j} + \Omega_j (\ell - q) \partial_{\eta_j} + \eta_2 \zeta_j q \partial_{\xi_j} \\ &\quad + \xi_1 \zeta_j (\ell - q) \partial_{\xi_j}] \psi_{q_0}^{\wedge} - q [\omega_j \partial_{\eta_j} + \xi_2 \zeta_j \partial_{\xi_j}] \psi_{(q-1)0}^{\wedge} + (\ell - q) [\Omega_j \partial_{\xi_j} - \xi_2 \zeta_j \partial_{\xi_j}] \psi_{(q+1)0}^{\wedge} - i \eta_2 q (q-1) [\zeta_j \partial_{\eta_j} - \Omega_j \partial_{\xi_j}] \\ &\quad \times \psi_{(q-1)1}^{\wedge} - i q [\eta_2 \zeta_j q \partial_{\xi_j} - \xi_2 \zeta_j (2\ell - 2q + 1) \partial_{\eta_j} + \eta_2 \omega_j q \partial_{\xi_j} + \xi_2 \Omega_j (2\ell - 2q + 1) \partial_{\xi_j}] \psi_{q_1}^{\wedge} + i (\ell - q) [\xi_2 \zeta_j (2q + 1) \\ &\quad \times \partial_{\xi_j} - \xi_1 \zeta_j (\ell - q) \partial_{\eta_j} + \xi_2 \omega_j (2q + 1) \partial_{\xi_j} + \xi_1 \Omega_j (\ell - q) \partial_{\xi_j}] \psi_{(q+1)1}^{\wedge} - i \xi_1 (\ell - q) (\ell - q - 1) [\zeta_j \partial_{\xi_j} + \omega_j \partial_{\xi_j}] \psi_{(q+2)1}^{\wedge} \} \\ &= - (2/\hbar^2) [E - V] \psi_{q_0}^{\wedge}, \end{aligned} \quad (36a)$$

$$\begin{aligned} \Delta \psi_{q_1}^{\wedge} &+ 4 \{ q \partial_{\xi_1} + (\ell - q + 1) \partial_{\eta_2} \} \psi_{q_1}^{\wedge} + 2(q-1) \partial_{\xi_2} \psi_{(q-1)1}^{\wedge} + 2(\ell - q) \partial_{\xi_2} \psi_{(q+1)1}^{\wedge} + \sum_{j=3}^{N-1} 2\Omega_2^{-1} \{ [-\omega_j q \partial_{\xi_j} + \Omega_j (\ell - q + 1) \partial_{\eta_j} \\ &\quad + \eta_2 \zeta_j q \partial_{\xi_j} + \xi_1 \zeta_j (\ell - q + 1) \partial_{\xi_j}] \psi_{q_1}^{\wedge} - (q-1) [\omega_j \partial_{\eta_j} + \xi_2 \zeta_j \partial_{\xi_j}] \psi_{(q-1)1}^{\wedge} + (\ell - q) [\Omega_j \partial_{\xi_j} - \xi_2 \zeta_j \partial_{\xi_j}] \psi_{(q+1)1}^{\wedge} \\ &\quad - i [\zeta_j \partial_{\eta_j} - \Omega_j \partial_{\xi_j}] \psi_{(q-1)0}^{\wedge} - i [\zeta_j \partial_{\xi_j} + \omega_j \partial_{\xi_j}] \psi_{q_0}^{\wedge} \} = - (2/\hbar^2) [E - V] \psi_{q_1}^{\wedge}, \end{aligned} \quad (36b)$$

where $\Delta \psi_{q\tau}^{\wedge}$ was given in Eq. (34). When $N=3$, Eq. (36) reduces to Eq. (21), where, because all internal variables have even parity, the generalized radial functions $\psi_{q\tau}^{\wedge}(\xi, \eta, \zeta)$ with $\lambda \neq \tau$ have to be vanishing.

V. PERMUTATION PROPERTY OF WAVE FUNCTIONS

When some or all particles in a quantum N -body system are identical particles, one has to consider the permutation property of the spatial wave function, which depends on the total spin of identical particles. Since the spatial wave function $\Psi^{\wedge}(\mathbf{R}_1, \dots, \mathbf{R}_{N-1})$ is expanded with respect to the base functions $Q_q^{\prime \tau}(\mathbf{R}_1, \mathbf{R}_2)$, we need to study only the prop-

erty of $Q_q^{\prime \tau}(\mathbf{R}_1, \mathbf{R}_2)$ in the transposition $(k, k+1)$ between two neighboring particles. The transformation property of the Jacobi coordinate vectors \mathbf{R}_j in the transposition $(k, k+1)$ was given in Eq. (10). Therefore, the base function $Q_q^{\prime \tau}(\mathbf{R}_1, \mathbf{R}_2)$ remains invariant in the transposition $(k, k+1)$ with $k \geq 3$. In the following we are going to study the transformation property of $Q_q^{\prime \tau}(\mathbf{R}_1, \mathbf{R}_2)$ in the transpositions $(1, 2)$ and $(2, 3)$. Denote by P_1 and P_2 the transformation operators for the base function in the transpositions $(1, 2)$ and $(2, 3)$, respectively. In the following formulas we neglect the argument $\mathbf{R}_1, \mathbf{R}_2$ in $Q_q^{\prime \tau}(\mathbf{R}_1, \mathbf{R}_2)$ and briefly denote $\sin \theta_1$, $\sin \theta_2$, $\cos \theta_1$, and $\cos \theta_2$ by s_1 , s_2 , c_1 , and c_2 for simplicity.

A. Transposition (1,2)

$$P_1 Q_q^{\ell 0} = \frac{1}{q!(\ell-q)!} [-Xc_1 + Ys_1]^q [Xs_1 + Yc_1]^{\ell-q} \\ = \sum_{p=0}^{\ell} Q_p^{\ell 0} D_{pq}^{\ell(1)}(\theta_1), \quad (37)$$

where

$$D_{pq}^{\ell(1)}(\theta_1) = \sum_n \frac{(-1)^{q-n} p!(\ell-p)! c_1^{\ell-p+q-2n} s_1^{2n+p-q}}{(q-n)!(\ell-p-n)! n!(n+p-q)!}. \quad (38)$$

Because of Eq. (19) and $P_1 Z = -Z$, we obtain

where

$$P_1 Q_q^{\ell 1} = - \sum_{p=1}^{\ell} Q_p^{\ell 1} D_{(p-1)(q-1)}^{\ell(1)}(\theta_1). \quad (39)$$

B. Transposition (2,3)

$$P_2 Q_q^{\ell 0} = \frac{X^q [-s_2 \omega_3 X + (s_2 \Omega_3 - c_2 \Omega_2) Y - i s_2 \zeta_3 Z]^{\ell-q}}{q!(\ell-q)! \Omega_2^{\ell-q}} \\ = \sum_{p=q}^{\ell} Q_p^{\ell 0} D_{pq}^{\ell(2)}(\theta_2) + i \sum_{p=q+1}^{\ell} Q_p^{\ell 1} D_{pq}^{\ell(3)}(\theta_2), \quad (40)$$

$$D_{(q+n)q}^{\ell(2)} = \frac{(q+n)!(\ell-q-n)! s_2^{\ell-q}}{q!(\ell-q)! \Omega_2^{\ell-q}} \sum_m \binom{\ell-q}{2m} (-1)^{n+m} \zeta_3^{2m} \sum_{rt} \binom{\ell-q-2m}{n-r} \binom{m}{t} \binom{m-t}{r-2t} \xi_1^{m-r+t} \eta_2^t (2\xi_2)^{r-2t} \omega_3^{n-r} \\ \times (\Omega_3 - \Omega_2 c_2 / s_2)^{\ell-q-n-2m+r}, \\ D_{(q+n)q}^{\ell(3)} = \frac{(q+n-1)!(\ell-q-n)! s_2^{\ell-q}}{q!(\ell-q)! \Omega_2^{\ell-q}} \sum_m \binom{\ell-q}{2m+1} (-1)^{n+m} \zeta_3^{2m+1} \sum_{rt} \binom{\ell-q-2m-1}{n-r-1} \binom{m}{t} \binom{m-t}{r-2t} \\ \times \xi_1^{m-r+t} \eta_2^t (2\xi_2)^{r-2t} \omega_3^{n-r-1} (\Omega_3 - \Omega_2 c_2 / s_2)^{\ell-q-n-2m+r}, \quad (41)$$

where the combinatorics $\binom{a}{b} = a! / b!(a-b)!$, and the ranges of the summation indices m , r , and t are determined by the conditions that those combinatorics are not vanishing:

$$P_2 Q_q^{\ell 1} = \Omega_2^{-1} \{i s_2 \xi_2 \zeta_3 X - i s_2 \xi_1 \zeta_3 Y + (s_2 \Omega_3 - c_2 \Omega_2) Z\} [P_2 Q_{q-1}^{\ell(1)0}] \\ = i s_2 \zeta_3 \Omega_2^{-1} \sum_{p=q}^{\ell} \{Q_p^{\ell 0} p \xi_2 - Q_{p-1}^{\ell 0} (\ell-p+1) \xi_1\} D_{(p-1)(q-1)}^{\ell(1)(2)}(\theta_2) + i (s_2 \Omega_3 - c_2 \Omega_2) \Omega_2^{-1} \\ \times \sum_{p=q+1}^{\ell} \{Q_p^{\ell 0} p (p-1) \eta_2 - 2 Q_{p-1}^{\ell 0} (p-1) (\ell-p+1) \xi_2 + Q_{p-2}^{\ell 0} (\ell-p+2) (\ell-p+1) \xi_1\} D_{(p-1)(q-1)}^{\ell(1)(3)}(\theta_2) \\ + \Omega_2^{-1} (s_2 \Omega_3 - c_2 \Omega_2) \sum_{p=q}^{\ell} Q_p^{\ell 1} D_{(p-1)(q-1)}^{\ell(2)}(\theta_2) - s_2 \zeta_3 \Omega_2^{-1} \\ \times \sum_{p=q+1}^{\ell} \{Q_p^{\ell 1} (p-1) \xi_2 - Q_{p-1}^{\ell 1} (\ell-p+1) \xi_1\} D_{(p-1)(q-1)}^{\ell(3)}(\theta_2). \quad (42)$$

In real calculations the cases with small angular momentum may be more interesting. In the following we explicitly list the above formulas for $\ell = 1$ and 2 (the formulas for the case with $\ell = 0$ are trivial):

$$P_1 Q_1^{10} = -c_1 Q_1^{10} + s_1 Q_0^{10}, \quad P_1 Q_0^{10} = s_1 Q_1^{10} + c_1 Q_0^{10},$$

$$P_1 Q_1^{11} = -Q_1^{11},$$

$$P_1 Q_2^{20} = c_1^2 Q_2^{20} - c_1 s_1 Q_1^{20} + s_1^2 Q_0^{20},$$

$$P_1 Q_1^{20} = -2c_1 s_1 Q_2^{20} - (c_1^2 - s_1^2) Q_1^{20} + 2c_1 s_1 Q_0^{20},$$

$$P_1 Q_0^{20} = s_1^2 Q_2^{20} + c_1 s_1 Q_1^{20} + c_1^2 Q_0^{20},$$

$$P_1 Q_2^{21} = c_1 Q_2^{21} - s_1 Q_1^{21}, \quad P_1 Q_1^{21} = -s_1 Q_2^{21} - c_1 Q_1^{21}.$$

$$P_2 Q_1^{10} = Q_1^{10},$$

$$P_2 Q_0^{10} = s_2 \Omega_2^{-1} [-\omega_3 Q_1^{10} + (\Omega_3 - \Omega_2 c_2 / s_2) Q_0^{10} - i \zeta_3 Q_1^{11}],$$

$$P_2 Q_1^{11} = s_2 \Omega_2^{-1} [i \xi_2 \zeta_3 Q_1^{10} - i \xi_1 \zeta_3 Q_0^{10} \\ + (\Omega_3 - \Omega_2 c_2 / s_2) Q_1^{11}],$$

$$P_2 Q_2^{20} = Q_2^{20},$$

$$P_2 Q_1^{20} = s_2 \Omega_2^{-1} [-2 \omega_3 Q_2^{20} + (\Omega_3 - \Omega_2 c_2 / s_2) Q_1^{20} - i \zeta_3 Q_2^{21}],$$

$$P_2 Q_0^{20} = s_2^2 \Omega_2^{-2} \{ (\omega_3^2 - \eta_2 \zeta_3^2) Q_2^{20} + [-\omega_3 (\Omega_3 - \Omega_2 c_2 / s_2) \\ + \xi_2 \zeta_3^2] Q_1^{20} + [(\Omega_3 - \Omega_2 c_2 / s_2)^2 - \xi_1 \zeta_3^2] Q_0^{20} \\ + i \omega_3 \zeta_3 Q_2^{21} - i \zeta_3 (\Omega_3 - \Omega_2 c_2 / s_2) Q_1^{21} \},$$

$$P_2 Q_2^{21} = s_2 \Omega_2^{-1} \{ i 2 \xi_2 \zeta_3 Q_2^{20} - i \xi_1 \zeta_3 Q_1^{20} \\ + (\Omega_3 - \Omega_2 c_2 / s_2) Q_2^{21} \},$$

$$P_2 Q_1^{21} = s_2^2 \Omega_2^{-2} \{ -2 i \zeta_3 [\xi_2 \omega_3 + \eta_2 (\Omega_3 - \Omega_2 c_2 / s_2)] Q_2^{20} \\ + i \zeta_3 [\xi_1 \omega_3 + 3 \xi_2 (\Omega_3 - \Omega_2 c_2 / s_2)] Q_1^{20} - 4 i \xi_1 \zeta_3 \\ \times (\Omega_3 - \Omega_2 c_2 / s_2) Q_0^{20} \\ + [\xi_2 \zeta_3^2 - \omega_3 (\Omega_3 - \Omega_2 c_2 / s_2)] Q_2^{21} \\ + [(\Omega_3 - \Omega_2 c_2 / s_2)^2 - \xi_1 \zeta_3^2] Q_1^{21} \}.$$

VI. NONORTHOGONAL VECTORS

Now, we turn to the general case where arbitrary coordinate vectors \mathbf{r}_{c_j} in the center-of-mass frame [see Eq. (13)] are used to replace the Jacobi coordinate vectors \mathbf{R}_j . In this

case the Laplace operator contains mixed derivative terms [see Eq. (14)]. All the conclusions in Sec. III hold for the present case except that the Jacobi coordinate vectors should be replaced with the coordinate vectors \mathbf{r}_{c_j} and the volume element of the configuration space (25) changes due to the linear transformation (13). In particular, the generalized harmonic polynomial $Q_q^\lambda(\mathbf{R}_1, \mathbf{R}_2)$ now becomes $Q_q^\lambda(\mathbf{r}_{c_1}, \mathbf{r}_{c_2})$, where \mathbf{r}_{c_1} and \mathbf{r}_{c_2} are two arbitrarily chosen coordinate vectors.

Any function $\Psi_q^\lambda(\mathbf{r}_{c_1}, \dots, \mathbf{r}_{c_{(N-1)}})$ with angular momentum q and parity $(-1)^{q+\lambda}$ in a quantum N -body system can be expanded with respect to $Q_q^\lambda(\mathbf{r}_{c_1}, \mathbf{r}_{c_2})$ with the coefficients $\psi_{q\tau}^\lambda(\xi, \eta, \zeta)$ depending on $(3N-6)$ invariant variables,

$$\Psi_q^\lambda(\mathbf{r}_{c_1}, \dots, \mathbf{r}_{c_{(N-1)}}) = \sum_{\tau=0}^1 \sum_{q=\tau}^q \psi_{q\tau}^\lambda(\xi, \eta, \zeta) Q_q^\lambda(\mathbf{r}_{c_1}, \mathbf{r}_{c_2}), \quad (43)$$

where, instead of Eq. (22), the internal variables ξ_j , η_j , and ζ_j are redefined as

$$\xi_j = \mathbf{r}_{c_j} \cdot \mathbf{r}_{c_1}, \quad \eta_j = \mathbf{r}_{c_j} \cdot \mathbf{r}_{c_2}, \quad \zeta_j = \mathbf{r}_{c_j} \cdot (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}), \\ 1 \leq j \leq (N-1), \quad \eta_1 = \xi_2, \quad \zeta_1 = \zeta_2 = 0. \quad (44)$$

As in the case with the orthogonal vectors, the main calculation in deriving the generalized radial equations in the present case is to apply the Laplace operator (14) to the function $\Psi_q^\lambda(\mathbf{r}_{c_1}, \dots, \mathbf{r}_{c_{(N-1)}})$ in Eq. (43). Similarly, the calculation consists of three parts, and the second part is vanishing. But the first part [see Eq. (34)] becomes

$$\Delta \psi_{q\tau}^\lambda(\xi, \eta, \zeta) = \{ (4S_{11} \xi_1 \partial_{\xi_1}^2 + 4S_{22} \eta_2 \partial_{\eta_2}^2) + (S_{11} \eta_2 + S_{22} \xi_1 + 2S_{12} \xi_2) \partial_{\xi_2}^2 + 4(S_{11} \xi_2 + S_{12} \xi_1) \partial_{\xi_1} \partial_{\xi_2} + 4(S_{22} \xi_2 + S_{12} \eta_2) \partial_{\xi_2} \partial_{\eta_2} \\ + 8S_{12} \xi_2 \partial_{\xi_1} \partial_{\eta_2} + 6(S_{11} \partial_{\xi_1} + S_{22} \partial_{\eta_2} + S_{12} \partial_{\xi_2}) \} \psi_{q\tau}^\lambda(\xi, \eta, \zeta) + \sum_{j=3}^{N-1} \{ 4(S_{11} \xi_j + S_{1j} \xi_1) \partial_{\xi_1} \partial_{\xi_j} \\ + 4(S_{22} \eta_j + S_{2j} \eta_2) \partial_{\eta_2} \partial_{\eta_j} + 4(S_{12} \xi_j + S_{1j} \xi_2) \partial_{\xi_1} \partial_{\eta_j} + 4(S_{12} \eta_j + S_{2j} \xi_2) \partial_{\eta_2} \partial_{\xi_j} \\ + 2(S_{11} \eta_j + S_{12} \xi_j + S_{1j} \xi_2 + S_{2j} \xi_1) \partial_{\xi_2} \partial_{\xi_j} + 2(S_{22} \xi_j + S_{12} \eta_j + S_{1j} \eta_2 + S_{2j} \xi_2) \partial_{\xi_2} \partial_{\eta_j} \\ + 4\zeta_j (S_{11} \partial_{\xi_1} + S_{22} \partial_{\eta_2} + S_{12} \partial_{\xi_2}) \partial_{\xi_j} + 6(S_{1j} \partial_{\xi_j} + S_{2j} \partial_{\eta_j}) \} \psi_{q\tau}^\lambda(\xi, \eta, \zeta) \\ + \sum_{j,k=3}^{N-1} \{ (2S_{1j} \xi_k + S_{jk} \xi_1) \partial_{\xi_j} \partial_{\xi_k} + (2S_{2j} \eta_k + S_{jk} \eta_2) \partial_{\eta_j} \partial_{\eta_k} + 2(S_{1k} \eta_j + S_{2j} \xi_k + S_{jk} \xi_2) \partial_{\xi_j} \partial_{\eta_k} \\ + 2(S_{1j} \zeta_k + S_{1k} \zeta_j) \partial_{\xi_j} \partial_{\xi_k} + 2(S_{2j} \zeta_k + S_{2k} \zeta_j) \partial_{\eta_j} \partial_{\xi_k} + (2S_{1j} \omega_k - 2S_{2j} \Omega_k + S_{jk} \Omega_2) \partial_{\xi_j} \partial_{\xi_k} \} \psi_{q\tau}^\lambda(\xi, \eta, \zeta) \\ + \sum_{j,k=3}^{N-1} \Omega_2^{-1} \{ (\Omega_j \eta_k - \omega_j \xi_k + \zeta_j \zeta_k) (S_{11} \partial_{\xi_j} \partial_{\xi_k} + S_{22} \partial_{\eta_j} \partial_{\eta_k} + 2S_{12} \partial_{\xi_j} \partial_{\eta_k}) \\ + 2[-S_{11} (\omega_j \zeta_k - \omega_k \zeta_j) + S_{12} (\Omega_j \zeta_k - \Omega_k \zeta_j)] \partial_{\xi_j} \partial_{\xi_k} + 2[S_{22} (\Omega_j \zeta_k - \Omega_k \zeta_j) - S_{12} (\omega_j \zeta_k - \omega_k \zeta_j)] \partial_{\eta_j} \partial_{\xi_k} \\ + [S_{11} (\omega_j \omega_k + \eta_2 \zeta_j \zeta_k) + S_{22} (\Omega_j \Omega_k + \xi_1 \zeta_j \zeta_k) - 2S_{12} (\omega_j \Omega_k + \xi_2 \zeta_j \zeta_k)] \partial_{\xi_j} \partial_{\xi_k} \} \psi_{q\tau}^\lambda(\xi, \eta, \zeta). \quad (45)$$

The last part contains the mixed application

$$\begin{aligned}
& 2 \sum_{j=1}^{N-1} \sum_{k=1}^{N-1} S_{jk} \nabla_{\mathbf{r}_{c_j}} \psi_{q\tau}^{\wedge} \cdot \nabla_{\mathbf{r}_{c_k}} \mathcal{Q}_q^{\prime\tau} \\
&= 2 \left\{ \mathbf{r}_{c_1} \left[2S_{11} \partial_{\xi_1} + S_{12} \partial_{\xi_2} + \sum_{j=3}^{N-1} S_{1j} \partial_{\xi_j} \right] + \mathbf{r}_{c_2} \left[S_{11} \partial_{\xi_2} + 2S_{12} \partial_{\eta_2} + \sum_{j=3}^{N-1} S_{1j} \partial_{\eta_j} \right] + \sum_{j=3}^{N-1} [\mathbf{r}_{c_j} (S_{11} \partial_{\xi_j} + S_{12} \partial_{\eta_j}) \right. \\
&\quad \left. + (\mathbf{r}_{c_2} \times \mathbf{r}_{c_j}) S_{11} \partial_{\xi_j} + (\mathbf{r}_{c_j} \times \mathbf{r}_{c_1}) S_{12} \partial_{\xi_j} + (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}) S_{1j} \partial_{\xi_j} \right] \psi_{q\tau}^{\wedge} \cdot \nabla_{\mathbf{r}_{c_1}} \mathcal{Q}_q^{\prime\tau} + 2 \left\{ \mathbf{r}_{c_1} \left[2S_{12} \partial_{\xi_1} + S_{22} \partial_{\xi_2} + \sum_{j=3}^{N-1} S_{2j} \partial_{\xi_j} \right] \right. \\
&\quad \left. + \mathbf{r}_{c_2} \left[S_{12} \partial_{\xi_2} + 2S_{22} \partial_{\eta_2} + \sum_{j=3}^{N-1} S_{2j} \partial_{\eta_j} \right] + \sum_{j=3}^{N-1} [\mathbf{r}_{c_j} (S_{12} \partial_{\xi_j} + S_{22} \partial_{\eta_j}) + (\mathbf{r}_{c_2} \times \mathbf{r}_{c_j}) S_{12} \partial_{\xi_j} \right. \right. \\
&\quad \left. \left. + (\mathbf{r}_{c_j} \times \mathbf{r}_{c_1}) S_{22} \partial_{\xi_j} + (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}) S_{2j} \partial_{\xi_j} \right] \right\} \psi_{q\tau}^{\wedge} \cdot \nabla_{\mathbf{r}_{c_2}} \mathcal{Q}_q^{\prime\tau}. \tag{46}
\end{aligned}$$

In addition to the formulas (35), where \mathbf{R}_j should be replaced with \mathbf{r}_{c_j} , we also need the following formulas:

$$\begin{aligned}
& (\mathbf{r}_{c_2} \times \mathbf{r}_{c_j}) \cdot \nabla_{\mathbf{r}_{c_2}} \mathcal{Q}_q^{\prime 0} = \Omega_2^{-1} \{ \eta_2 \zeta_j (q+1) \mathcal{Q}_{q+1}^{\prime 0} - \xi_2 \zeta_j (\ell - q) \mathcal{Q}_q^{\prime 0} - i \omega_j \mathcal{Q}_{q+1}^{\prime 1} \}, \\
& (\mathbf{r}_{c_j} \times \mathbf{r}_{c_1}) \cdot \nabla_{\mathbf{r}_{c_1}} \mathcal{Q}_q^{\prime 0} = \Omega_2^{-1} \{ -\xi_2 \zeta_j q \mathcal{Q}_q^{\prime 0} + \xi_1 \zeta_j (\ell - q + 1) \mathcal{Q}_{q-1}^{\prime 0} + i \Omega_j \mathcal{Q}_q^{\prime 1} \}, \\
& (\mathbf{r}_{c_2} \times \mathbf{r}_{c_j}) \cdot \nabla_{\mathbf{r}_{c_2}} \mathcal{Q}_q^{\prime 1} = \Omega_2^{-1} \{ -i \xi_1 \omega_j (\ell - q + 1)^2 \mathcal{Q}_{q-1}^{\prime 0} + i \xi_2 \omega_j q (2\ell - 2q + 1) \mathcal{Q}_q^{\prime 0} - i \eta_2 \omega_j (q+1) q \mathcal{Q}_{q+1}^{\prime 0} \\
&\quad - \xi_2 \zeta_j (\ell - q + 1) \mathcal{Q}_q^{\prime 1} + \eta_2 \zeta_j q \mathcal{Q}_{q+1}^{\prime 1} \}, \\
& (\mathbf{r}_{c_j} \times \mathbf{r}_{c_1}) \cdot \nabla_{\mathbf{r}_{c_1}} \mathcal{Q}_q^{\prime 1} = \Omega_2^{-1} \{ i \xi_1 \Omega_j (\ell - q + 1) (\ell - q + 2) \mathcal{Q}_{q-2}^{\prime 0} - i \xi_2 \Omega_j (\ell - q + 1) (2q - 1) \mathcal{Q}_{q-1}^{\prime 0} + i \eta_2 \Omega_j q^2 \mathcal{Q}_q^{\prime 0} \\
&\quad + \xi_1 \zeta_j (\ell - q + 1) \mathcal{Q}_{q-1}^{\prime 1} - \xi_2 \zeta_j q \mathcal{Q}_q^{\prime 1} \}, \\
& (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}) \cdot \nabla_{\mathbf{r}_{c_1}} \mathcal{Q}_q^{\prime 0} = -i \mathcal{Q}_q^{\prime 1}, \\
& (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}) \cdot \nabla_{\mathbf{r}_{c_2}} \mathcal{Q}_q^{\prime 0} = -i \mathcal{Q}_{q+1}^{\prime 1}, \\
& (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}) \cdot \nabla_{\mathbf{r}_{c_1}} \mathcal{Q}_q^{\prime 1} = -i \eta_2 q^2 \mathcal{Q}_q^{\prime 0} + i \xi_2 (\ell - q + 1) (2q - 1) \mathcal{Q}_{q-1}^{\prime 0} - i \xi_1 (\ell - q + 2) (\ell - q + 1) \mathcal{Q}_{q-2}^{\prime 0}, \\
& (\mathbf{r}_{c_1} \times \mathbf{r}_{c_2}) \cdot \nabla_{\mathbf{r}_{c_2}} \mathcal{Q}_q^{\prime 1} = i \xi_2 q (2\ell - 2q + 1) \mathcal{Q}_q^{\prime 0} - i \xi_1 (\ell - q + 1)^2 \mathcal{Q}_{q-1}^{\prime 0} - i \eta_2 q (q+1) \mathcal{Q}_{q+1}^{\prime 0}. \tag{47}
\end{aligned}$$

Finally, we obtain the generalized radial equations as follows:

$$\begin{aligned}
& \Delta \psi_{q_0}^{\wedge} + 2[2S_{11} q \partial_{\xi_1} + \ell S_{12} \partial_{\xi_2} + 2(\ell - q) S_{22} \partial_{\eta_2}] \psi_{q_0}^{\wedge} + 2q(2S_{12} \partial_{\xi_1} + S_{22} \partial_{\xi_2}) \psi_{(q-1)0}^{\wedge} + 2(\ell - q)(S_{11} \partial_{\xi_2} + 2S_{12} \partial_{\eta_2}) \psi_{(q+1)0}^{\wedge} \\
& + \sum_{j=3}^{N-1} 2\Omega_2^{-1} \{ [(\ell - q)(\Omega_j S_{12} \partial_{\xi_j} + \Omega_j S_{22} \partial_{\eta_j} + \Omega_2 S_{j2} \partial_{\eta_j} + \xi_1 \zeta_j S_{22} \partial_{\xi_j}) + q(\Omega_2 S_{j1} - \omega_j S_{11}) \partial_{\xi_j} - \omega_j q S_{12} \partial_{\eta_j} \\
& + \zeta_j (\eta_2 q S_{11} - \xi_2 \ell S_{12}) \partial_{\xi_j}] \psi_{q_0}^{\wedge} + q[(\Omega_2 S_{j2} - \omega_j S_{12}) \partial_{\xi_j} - \omega_j S_{22} \partial_{\eta_j} + \zeta_j (\eta_2 S_{12} - \xi_2 S_{22}) \partial_{\xi_j}] \psi_{(q-1)0}^{\wedge} + (\ell - q) \\
& \times [S_{11} \Omega_j \partial_{\xi_j} + (S_{j1} \Omega_2 + S_{12} \Omega_j) \partial_{\eta_j} + \zeta_j (\xi_1 S_{12} - \xi_2 S_{11}) \partial_{\xi_j}] \psi_{(q+1)0}^{\wedge} - i \eta_2 q (q-1) \\
& \times [\zeta_j (S_{12} \partial_{\xi_j} + S_{22} \partial_{\eta_j}) + (\omega_j S_{12} - \Omega_j S_{22} + \Omega_2 S_{j2}) \partial_{\xi_j}] \psi_{(q-1)1}^{\wedge} - i q [\eta_2 q (\zeta_j S_{11} \partial_{\xi_j} + \zeta_j S_{12} \partial_{\eta_j} + \omega_j S_{11} \partial_{\xi_j} - \Omega_j S_{12} \partial_{\xi_j} \\
& + \Omega_2 S_{j1} \partial_{\xi_j}) - \xi_2 (2\ell - 2q + 1) (\zeta_j S_{12} \partial_{\xi_j} + \zeta_j S_{22} \partial_{\eta_j} + \Omega_2 S_{j2} \partial_{\xi_j} - \Omega_j S_{22} \partial_{\xi_j} + \omega_j S_{12} \partial_{\xi_j})] \psi_{q_1}^{\wedge} \\
& + i(\ell - q) [(2q + 1) \xi_2 (\zeta_j S_{11} \partial_{\xi_j} + \zeta_j S_{12} \partial_{\eta_j} + \Omega_2 S_{j1} \partial_{\xi_j} + \omega_j S_{11} \partial_{\xi_j} - \Omega_j S_{12} \partial_{\xi_j}) - \xi_1 (\ell - q) (\zeta_j S_{12} \partial_{\xi_j} + \zeta_j S_{22} \partial_{\eta_j} + \omega_j S_{12} \partial_{\xi_j} \\
& - \Omega_j S_{22} \partial_{\xi_j} + \Omega_2 S_{j2} \partial_{\xi_j})] \psi_{(q+1)1}^{\wedge} - i \xi_1 (\ell - q) (\ell - q - 1) [\zeta_j (S_{11} \partial_{\xi_j} + S_{12} \partial_{\eta_j}) + (\omega_j S_{11} - \Omega_j S_{12} + \Omega_2 S_{j1}) \partial_{\xi_j}] \psi_{(q+2)1}^{\wedge} \} \\
& = -(2/\hbar^2) [E - V] \psi_{q_0}^{\wedge}, \tag{48a}
\end{aligned}$$

$$\begin{aligned}
& \Delta \psi_{q1}^\wedge + 2\{2qS_{11}\partial_{\xi_1} + (\ell+1)S_{12}\partial_{\xi_2} + 2(\ell-q+1)S_{22}\partial_{\eta_2}\}\psi_{q1}^\wedge + 2(q-1)(2S_{12}\partial_{\xi_1} + S_{22}\partial_{\xi_2})\psi_{(q-1)1}^\wedge + 2(\ell-q) \\
& \times (S_{11}\partial_{\xi_2} + 2S_{12}\partial_{\eta_2})\psi_{(q+1)1}^\wedge + \sum_{j=3}^{N-1} 2\Omega_2^{-1}\{-i[\zeta_j(S_{12}\partial_{\xi_j} + S_{22}\partial_{\eta_j}) + (\Omega_2 S_{j2} - \Omega_j S_{22} + \omega_j S_{12})\partial_{\xi_j}]\psi_{(q-1)0}^\wedge \\
& - i[\zeta_j(S_{11}\partial_{\xi_j} + S_{12}\partial_{\eta_j}) + (\omega_j S_{11} - \Omega_j S_{12} + \Omega_2 S_{j1})\partial_{\xi_j}]\psi_{q0}^\wedge + [q(\Omega_2 S_{j1} - \omega_j S_{11})\partial_{\xi_j} - \omega_j q S_{12}\partial_{\eta_j} \\
& + \zeta_j(\eta_2 q S_{11} - \xi_2(\ell+1)S_{12})\partial_{\xi_j} + (\ell-q+1)(\Omega_j S_{12}\partial_{\xi_j} + \Omega_2 S_{j2}\partial_{\eta_j} + \Omega_j S_{22}\partial_{\eta_j} + \xi_1 \zeta_j S_{22}\partial_{\xi_j})]\psi_{q1}^\wedge \\
& + (q-1)[(\Omega_2 S_{j2} - \omega_j S_{12})\partial_{\xi_j} - \omega_j S_{22}\partial_{\eta_j} + \zeta_j(\eta_2 S_{12} - \xi_2 S_{22})\partial_{\xi_j}]\psi_{(q-1)1}^\wedge + (\ell-q)[\Omega_j S_{11}\partial_{\xi_j} + (\Omega_2 S_{j1} + \Omega_j S_{12})\partial_{\eta_j} \\
& + \zeta_j(-\xi_2 S_{11} + \xi_1 S_{12})\partial_{\xi_j}]\psi_{(q+1)1}^\wedge\} = -(2/\hbar^2)[E-V]\psi_{q1}^\wedge. \tag{48b}
\end{aligned}$$

VII. PHYSICAL APPLICATION

In a quantum N -body system, any function with angular momentum ℓ and parity $(-1)^{\ell+\lambda}$ can be expanded with respect to the generalized harmonic polynomials $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$, where the coefficients, called the generalized radial functions, depend only on $(3N-6)$ internal variables. Since $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$ is a homogeneous polynomial in the components of the Jacobi coordinate vectors and a solution of the Laplace equation, we have derived the generalized radial equations easily. That the rotational variables (the Euler angles) are not involved in either the generalized radial functions or the equations will greatly decrease the amount of calculation in solving the Schrödinger equation numerically for the N -body system. As a first step, we applied this approach to the calculation of the energy levels of a helium atom and a positronium ion [29–31]. In the following we sketch the method and give some more calculation results.

Once the generalized radial equations have been derived, one may choose any other complete set of internal variables to simplify the calculation. The generalized radial equations for the new variables can easily be obtained by replacement of variables. In a Coulombic three-body system, such as a helium atom, we choose the hyperradius ρ and two dimensionless quantities η and ζ as the internal variables, so as to make the potential a meromorphic function:

$$\rho = (\mathbf{R}_1^2 + \mathbf{R}_2^2)^{1/2}, \quad \eta = \frac{|\mathbf{r}_2 - \mathbf{r}_3|}{\rho}, \quad \zeta = \frac{|\mathbf{r}_1 - \mathbf{r}_2|}{\rho} + \frac{|\mathbf{r}_1 - \mathbf{r}_3|}{\rho}, \tag{49}$$

where \mathbf{r}_1 denotes the position vector of the helium nucleus and \mathbf{r}_2 and \mathbf{r}_3 the position vectors of two electrons. After expanding the wave function as a Taylor series with respect to η and ζ up to the order n , we obtain an ordinary differential matrix equation for the coefficients $R(\rho)$. In the real calculation, we calculate the propagating matrix $F(\rho)$ and its inverse matrix $G(\rho)$ by the Taylor series method instead of the function $R(\rho)$ in order to avoid the logarithmic singularities at $\rho=0$ in the forms of $\rho^a(\ln \rho)^b$ [32–34]:

$$\rho \frac{dR(\rho)}{d\rho} = F(\rho)R(\rho). \tag{50}$$

We are able to obtain the energy levels of a helium atom in the different spectra $^{2S+1}L^{e(o)}$ with high accuracy by choosing $n=10$ (for the S and P states) or $n=9$ (for the D states) due to the fast convergence of the series, where S is the total spin of two electrons, $e(o)$ describes the parity, and $L=S, P, D$ for the angular momentum states. In order to compare our calculation results with those obtained by the variational methods where the nucleus mass is usually assumed to be infinite, we also calculate the energy level with a large mass ratio M of the nucleus to the electron ($M=10^{20}$). Both calculated results are listed in Table I for comparison. Fewer terms in the truncated series are taken in our calculation than those in the hyperspherical harmonic function method [22] and in the variational methods [36].

VIII. CONCLUSIONS

For a quantum N -body system we have found a complete set of independent base functions $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$ for the given angular momentum and parity. Any function with angular momentum ℓ and parity $(-1)^{\ell+\lambda}$ in the system can be expanded with respect to the $(2\ell+1)$ generalized harmonic polynomials $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$, where the combinative coefficients are functions of the $(3N-6)$ internal variables. We have established the generalized radial equations explicitly; they are simultaneous partial differential equations in the internal variables. The number of both the functions and the equations is $(2\ell+1)$ when $N \geq 4$, and it becomes $(\ell+1)$ or ℓ when $N=3$, depending on the parity. Only a finite number of partial angular momentum states are involved in constructing the generalized harmonic polynomials $Q_q^{\ell\tau}(\mathbf{R}_1, \mathbf{R}_2)$. That is, the contributions from the remaining partial angular momentum states have been incorporated into those from the generalized radial functions. We have generalized the formulas to the case with nonorthogonal vectors.

When establishing the body-fixed frame we fix it with two arbitrarily chosen Jacobi coordinate vectors \mathbf{R}_1 and \mathbf{R}_2 . Those two vectors may be replaced by any other two coordinate vectors according to the characteristics of the physical problem under study.

The choice of the complete set of base functions is not unique. However, the right choices of both the base functions and the internal variables play a key role in establishing the

TABLE I. Numerical calculation for the energy levels of a helium atom in atomic units.

Spectral term $2S+1L^{e(o)}$	Our results		Variational calculation [35]
	$M = 7296.28$	$M = 10^{20}$	$M \sim \infty$
$1S^e$	2.9033046	2.903724377034116	2.9037243770341195
$3S^e$	2.1749303	2.1752293777	2.1752293782
$1P^e$	0.5801748	0.5802464725	0.5802465 ^a
$3P^e$	0.7105002	0.7103965	0.710499 ^a
$1P^o$	2.1235456	2.1238430778	2.1238430865
$3P^o$	2.1328807	2.133164187	2.133164191
$1D^o$	0.5637256	0.5638004	
$3D^o$	0.5592482	0.5593283	
$3D^e$	2.0553230	2.055871	2.0556363
$1D^e$	2.0553055	2.0555693	2.0556207

^aThe calculation in Ref. [36].

generalized radial equations. Those two choices are the main progress of the present paper in comparison with the previous work of Wigner [4] and Eckart [1]. Once the generalized radial equations have been derived, one may choose any other complete set of internal variables to simplify the calculation. The generalized radial equations for the new variables can easily be obtained by replacement of variables, just as we did in Sec. VII for the three-body system.

The two features in this method, that the numbers of both functions $\psi_{q\tau}^{\wedge}(\xi, \eta, \zeta)$ and equations are finite, and they depend on only $(3N-6)$ internal variables, are important for calculating the energy levels and wave functions in a quantum N -body system. In fact, in numerical experiments for a quantum three-body system we calculated the lowest energy levels of a helium atom in P states [29] and in D states [30] with total spin 1 and zero, and some energy levels of a pos-

itronium negative ion [31] by a series expansion. Because three rotational variables are removed, fewer terms have to be taken to achieve the same precision of energy as in other methods to truncate the series of partial angular momentum states. As the number of particles in the system increases, we believe that removing three independent variables related to the global rotation will greatly decrease the amount of calculation.

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