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Transformation coefficients between oscillator harmonics and hyperspherical harmonics in two space dimensions

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Abstract. The transformation coefficients between oscillator harmonics and hyperspherical harmonics are derived analytically for an arbitrary number of particles with arbitrary masses, which allows us to express the transformation coefficients among the hyperspherical harmonics with different sets of variables in terms of those for oscillator harmonics and facilitates the variational calculations with hyperspherical harmonics. The diagonalization of the Hamiltonian for D^- system in a quantum well is given as an example to demonstrate the applications.

1. Introduction

It is well known that hyper-spherical harmonics and oscillator harmonics are the two most important basis functions in numerical diagonalizations of Hamiltonians for finite systems (atoms and nuclei). In recent years, there has been increasing interest in the study of finite systems in two dimensions such as few anyons in a harmonic potential [1–3], few electrons in parabolic quantum dots [4–9], electron–hole complex and the like [10]. In the study of low-dimensional few-body problems, hyperspherical harmonics and oscillator harmonics continue to be the most powerful and extensively used basis functions. Those who are used to the variational calculations with these functions are aware of the difficulties in calculating the particle–particle interaction matrix elements and symmetrizing the basis functions when dealing with identical-particle systems. The difficulties can be overcome if the transformation coefficient of harmonics with different sets of internal coordinates as arguments are known. In a previous paper [11], we presented the transformation coefficients for oscillator harmonics, which can be most easily derived in the formalism of second quantization operators, while a direct derivation of the transformation coefficients for hyper-spherical harmonics turns out to be complicated and lengthy. Instead of deriving the transformation coefficients for hyper-spherical harmonics, if the transformation coefficients between hyper-spherical harmonics and oscillator harmonics are known, the transformation coefficients for hyper-spherical harmonics are also known. In section 2, we use this strategy to derive the transformation coefficients for hyper-spherical harmonics. In section 3, an example is given to illustrate their applications.

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2. The formalism

2.1. Oscillator harmonics and hyper-spherical harmonics

Let us consider an N-body quantum mechanical system with arbitrary masses. Let $\{\vec{\eta}_\nu;\, \nu = 1, \ldots, N-1\}$ be a set of Jacobi coordinates such that each $\vec{\eta}_\nu$ is the displacement of the centre-of-mass (c.m.) of a particle cluster from the c.m. of another particle cluster and such that no two such vectors connect the same c.m. The reduced mass associated with $\vec{\eta}_\nu$ is denoted by μ_ν. We define

$$\vec{\xi}_\nu = \sqrt{\frac{\mu_\nu \omega}{\hbar}}\vec{\eta}_\nu \tag{1}$$

where ω is the oscillator frequency. Then the Hamiltonian for the relative motion in a harmonic potential is

$$H_{rel} = \sum_{\nu=1}^{N-1} \tfrac{1}{2}(p_{\xi_\nu}^2 + \xi_\nu^2)\hbar\omega. \tag{2}$$

Its eigenvalues and eigenfunctions are well known,

$$\Psi_{\{k\}} = \prod_{\nu=1}^{N-1}\left\{R_{n_\nu l_\nu}(\xi_\nu)\frac{\mathrm{e}^{(\mathrm{i}l_\nu\varphi_\nu)}}{\sqrt{2\pi}}\right\} \tag{3}$$

$$E_{rel} = \sum_{\nu=1}^{N-1}(2n_\nu + |l_\nu| + 1)\hbar\omega \tag{4}$$

$$L = \sum_{\nu=1}^{N-1} l_\nu \tag{5}$$

where $\{k\}$ denotes the full set of $2(N-1)$ quantum numbers $n_1, \ldots, n_{N-1}; l_1, \ldots, l_{N-1}$ in brevity, φ_ν is the polar angle of $\vec{\xi}_\nu$ and

$$R_{nl}(\xi) = N_{nl}\xi^l L_n^{|l|}(\xi^2)\mathrm{e}^{(-\xi^2/2)} \tag{6}$$

where $N_{nl} = \sqrt{2n!/\Gamma(n+|l|+1)}$, $L_n^{|l|}$ is a Laguerre polynomial. For the following purpose, we rewrite equation (3) into

$$\Psi_{\{k\}} = \sum_{m_1=0}^{n_1}\cdots\sum_{m_{N-1}=0}^{n_{N-1}}\left\{D(\{k\}; m_1, \ldots, m_{N-1})\prod_{\nu=1}^{N-1}\xi_\nu^{2m_\nu+|l_\nu|}\frac{\mathrm{e}^{(\mathrm{i}l_\nu\varphi_\nu)}}{\sqrt{2\pi}}\right\}\mathrm{e}^{-\xi^2/2} \tag{7}$$

$$D(\{k\}; m_1, \ldots, m_{N-1}) = \prod_{\nu=1}^{N-1}\frac{(-)^{m_\nu}\sqrt{2n_\nu!(n_\nu+|l_\nu|)!}}{m_\nu!(n_\nu-m_\nu)!(m_\nu+|l_\nu|)!}. \tag{8}$$

We further define the hyper-radius ρ and hyper-angles $\phi_1, \ldots, \phi_{N-2}$ which are related to the norm of $\vec{\xi}_\nu$ by

$$\xi_\nu = \rho\left(\prod_{j=0}^{\nu-1}\sin\phi_j\right)\cos\phi_\nu. \tag{9}$$

In this expression, $\phi_0 \equiv \pi/2$ and $\phi_{N-1} \equiv 0$ are understood.

With hyper-spherical coordinates, H_{rel} is then given by

$$H_{rel} = \frac{\hbar\omega}{2}\left[-\frac{1}{\rho^{2N-3}}\frac{\partial}{\partial\rho}\rho^{2N-3}\frac{\partial}{\partial\rho} + \frac{\Lambda^2(\Omega)}{\rho^2} + \rho^2\right] \tag{10}$$

where $\Lambda^2(\Omega)$ is the grand orbital operator, defined by

$$\Lambda^2(\Omega) = \sum_{\nu=0}^{N-3} K^{(\nu)}(\phi_{N-2-\nu}) - \sum_{\nu=1}^{N-1} \frac{\hat{\ell}^2(\varphi_\nu)}{(\prod_{j=0}^{\nu-1}\sin^2\phi_j)\cos^2\phi_\nu} \tag{11}$$

$$K^{(\nu)}(\phi_{N-2-\nu}) = \frac{1}{\prod_{j=0}^{N-3-\nu}\sin^2\phi_j}\left\{\frac{\partial^2}{\partial\phi_{N-2-\nu}^2} + \left[(1+2\nu)\frac{\cos\phi_{N-2-\nu}}{\sin\phi_{N-2-\nu}} - \frac{\sin\phi_{N-2-\nu}}{\cos\phi_{N-2-\nu}}\right]\frac{\partial}{\partial\phi_{N-2-\nu}}\right\} \tag{12}$$

where $\hat{\ell}(\varphi) = -\mathrm{i}\partial/\partial\varphi$, Ω denotes a set of $2N-3$ angular variables $\phi_1,\ldots,\phi_{N-2}$, $\varphi_1,\ldots,\varphi_{N-1}$. By setting $\Phi = \mathrm{Re}\,(\rho)Y(\Omega)$, then the eigenequation $H_{rel}\Phi = E_{rel}\Phi$ splits into

$$\frac{\hbar\omega}{2}\left[\left(-\frac{1}{\rho^{2N-3}}\frac{\mathrm{d}}{\mathrm{d}\rho}\rho^{2N-3}\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{\lambda(\lambda+2N-4)}{\rho^2}\right) + \rho^2\right]\mathrm{Re}\,(\rho) = E_{rel}\mathrm{Re}\,(\rho) \tag{13}$$

$$\Lambda^2(\Omega)Y(\Omega) = \lambda(\lambda+2N-4)Y(\Omega). \tag{14}$$

The eigenvalues of equation (13) are $E_{rel} = \hbar\omega(2n_\rho+\lambda+N-1)$, the associated eigenfunctions are

$$\Re_{n_\rho\lambda}(\rho) = N_{n_\rho\lambda}\rho^\lambda L_{n_\rho}^{\lambda+N-2}(\rho^2)\mathrm{e}^{-\rho^2/2}. \tag{15}$$

The eigenfunctions of equation (14) are hyper-spherical harmonic functions in two space dimensions, given by

$$Y_{[\lambda]}(\Omega) = \left[\prod_{\nu=1}^{N-2} P_{\nu,\tilde{n}_\nu}^{\lambda_{\nu+1},l_\nu}(\phi_\nu)\right]\left[\prod_{j=1}^{N-1}\frac{\mathrm{e}^{(\mathrm{i}l_j\varphi_j)}}{\sqrt{2\pi}}\right] \tag{16}$$

where $[\lambda]$ denotes a set of $2N-3$ quantum numbers $\tilde{n}_1,\ldots,\tilde{n}_{N-2},l_1,\ldots,l_{N-1}$; $\lambda_{N-1} = |l_{N-1}|$, $\lambda_i = 2\tilde{n}_i + \lambda_{\nu+1} + |l_i|$, $\lambda_1 = 2\tilde{n}_1 + \lambda_2 + |l_1|$; $\lambda = \sum_{\nu=1}^{N-1}\lambda_\nu$,

$$P_{\nu,n_\nu}^{\lambda_{\nu+1},l_\nu}(\phi) = \Theta_\nu^{\lambda_{\nu+1}+(N-2-\nu),l_\nu}\sum_{m=0}^{\nu}(-)^{\nu-m}\binom{\nu+\lambda_{\nu+1}+(N-2-\nu)}{m}\binom{\nu+|l_\nu|}{\nu-m} \times(\cos\phi)^{2m+|l_\nu|}(\sin\phi)^{2(\nu-m)+\lambda_{\nu+1}} \tag{17}$$

where $\Theta_n^{l,l'} = \sqrt{2(2n+l+|l'|+1)n!(n+l+|l'|)!/[(n+l)!(n+|l'|)!]}$ are the normalization constants, such that

$$\int \mathrm{d}\Omega\, Y_{[\lambda]}^*(\Omega)Y_{[\lambda']}(\Omega) = \delta_{[\lambda],[\lambda']} \tag{18}$$

where $\mathrm{d}\Omega = \prod_{i=1}^{N-2}[(\sin\phi_i)^{2(N-i)-3}\cos\phi_i\,\mathrm{d}\phi_i]\prod_{j=1}^{N-1}\mathrm{d}\varphi_j$.

2.2. Some auxiliary formula

(a) Since the $P_{i,n}^{ll'}(\phi)$ defined in equation (17) form a complete set in the domain $(0 \leqslant \phi \leqslant \pi/2)$, we have

$$\sin^k\phi\cos^{k'}\phi = \sum_n F_{ill'n}^{k,k'}P_{i,n}^{ll'}(\phi) \tag{19}$$

where the expansion coefficient is

$$F_{ill'n}^{kk'} = \int_0^{\pi/2}\mathrm{d}\phi\,(\sin\phi)^{2(N-i)+k-3}(\cos\phi)^{k'+1}P_{i,n}^{ll'}(\phi)$$
$$= \theta_n^{l+(N-i-2),l'}\sum_{m=0}^{n}(-)^{n-m}\binom{n+l+(N-i-2)}{m}\binom{n+|l'|}{n-m}$$

$$\times I_{2(N+n-m-i)+l+k-3,2m+|l'|+k'+1} \tag{20}$$

$$I_{i,i'} = \epsilon_{ii'} \frac{(i-1)!!(i'-1)!!}{(i+i')!!} \qquad \epsilon_{ii'} = \begin{cases} \dfrac{\pi}{2} & \text{for even } l_1 \text{ and } l_1' \\ 1 & \text{others.} \end{cases} \tag{21}$$

(b) With $k - \lambda =$ even, we have

$$\rho^k \mathrm{e}^{-\rho^2/2} = \sum_{n_\rho} G^k_{n_\rho\lambda} \mathrm{Re}_{\,n_\rho\lambda}(\rho) \tag{22}$$

where the expansion coefficients are

$$\begin{aligned} G^k_{n_\rho\lambda} &= \int_0^\infty \rho^{(k+2N-3)} \mathrm{e}^{-\rho^2/2} \mathrm{Re}_{\,n_\rho\lambda}(\rho)\, \mathrm{d}\rho \\ &= \frac{1}{2} N_{n_\rho\lambda} \sum_{m=0}^{n_\rho} \frac{(-)^m}{m!} \binom{n_\rho + \lambda + N - 2}{n_\rho - m} \left(\frac{k + 2m + \lambda + 2N - 4}{2}\right)!. \end{aligned} \tag{23}$$

2.3. *The transformation coefficients*

Using equations (20) and (22), we have

$$\xi_1^{s_1} \ldots \xi_{N-1}^{s_{N-1}} = \sum_{n''_\rho} \sum_{\tilde{n}''_1} \ldots \sum_{\tilde{n}''_{N-2}} G^K_{n''_\rho\lambda} \mathrm{Re}_{\,n''_\rho\lambda''}(\rho) \prod_{j=1}^{N-2} \left\{ F^{s_j t_j}_{j\lambda''_{j+1} l_j} P^{\lambda''_{j+1}, l_j}_{j,\tilde{n}''_j}(\phi_j) \right\} \tag{24}$$

where $K = \sum_{i=1}^{N-1} s_i$, $t_j = \sum_{i=j+1}^{N-1} s_i$.

Making use of equations (7) and (24), we finally obtain the explicit expression for the transformation coefficient

$$\begin{aligned} E(\{k\}, \{n_\rho, [\lambda]\}) &\equiv \langle \Psi_{\{k\}}(\xi_1, \ldots, \xi_{N-1}) | \Phi_{\{n_\rho,[\lambda]\}}(\rho, \Omega) \rangle \\ &= \sum_{m_1=0}^{n_1} \ldots \sum_{m_{N-1}=0}^{n_{N-1}} D(\{k\}; m_1 \ldots m_{N-1}) G^K_{\tilde{n}_\rho\lambda} \prod_{j=1}^{N-2} F^{(2m_j+|l_j|), t_j}_{\tilde{n}_j \lambda_{j+1} l_j}. \end{aligned} \tag{25}$$

2.4. *The transformation coefficients for hyper-spherical harmonics in terms of the transformation coefficient for oscillator harmonics*

Let us define the transformation coefficients for oscillator harmonics by

$$B(\{k\}\alpha; \{k'\}\beta) = \langle \Psi_{\{k\}}(\xi_1^\alpha, \ldots, \xi_{N-1}^\alpha) | \Psi_{\{k'\}}(\xi_1^\beta, \ldots, \xi_{N-1}^\beta) \rangle \tag{26}$$

where $\{\xi_i^\alpha\}$ and $\{\xi_i^\beta\}$ are two different sets of Jacobi coordinates assigned to the system. Explicit expression for $B(\{k\}\alpha; \{k'\}\beta)$ has been given in [11] .

Let us define the transformation coefficients for hyper-spherical harmonics by

$$Z([\lambda]\alpha; [\lambda']\beta) = \langle Y_{[\lambda]}(\Omega^\alpha) | Y_{[\lambda']}(\Omega^\beta) \rangle \tag{27}$$

which we are going to derive. Then we have

$$\begin{aligned} Z([\lambda]\alpha; [\lambda']\beta) &= \langle \Phi_{\{0,[\lambda]\}}(\rho, \Omega^\alpha) | \Phi_{\{0,[\lambda']\}}(\rho, \Omega^\beta) \rangle \\ &= \sum_{\{k\}} \sum_{\{k'\}} \langle \Phi_{\{0,[\lambda]\}}(\rho, \Omega^\alpha) | \Psi_{\{k\}}(\xi_1^\alpha, \ldots, \xi_{N-1}^\alpha) \rangle \\ &\quad \times \langle \Psi_{\{k\}}(\xi_1^\alpha, \ldots, \xi_{N-1}^\alpha) | \Psi_{\{k'\}}(\xi_1^\beta, \ldots, \xi_{N-1}^\beta) \rangle \\ &\quad \times \langle \Psi_{\{k'\}}(\xi_1^\beta, \ldots, \xi_{N-1}^\beta) | \Phi_{\{0,[\lambda']\}}(\rho, \Omega^\beta) \rangle \\ &= \sum_{\{k\}} \sum_{\{k'\}} E(\{k\}, \{0, [\lambda]\}) \cdot B(\{k\}\alpha; \{k'\}\beta) \cdot E(\{k\}, \{0, [\lambda']\}) \end{aligned} \tag{28}$$

where the sums are subject to the conservation of energy and angular momentum.

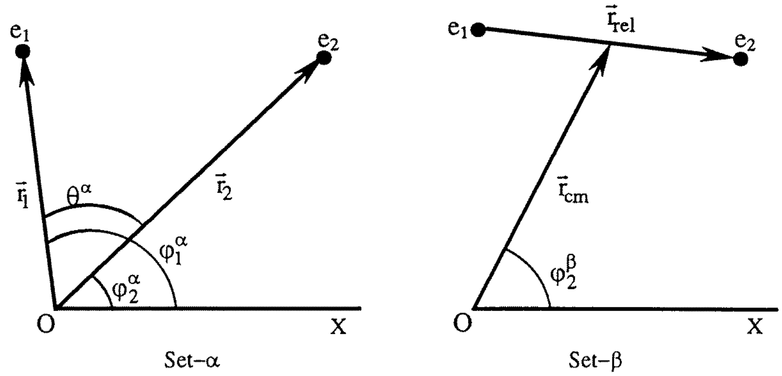

Figure 1. Schematic definition of coordinates set-α and set-β.

3. Example of applications

Let us consider a system of two electrons bound to a donor ion in an x–y plane (denoted by D^-) [12–24]. The Schrodinger equation is,

$$\left\{\sum_{j=1}^{2}\left[\frac{p_j^2}{2m_e^*}-\frac{e^2}{4\pi\epsilon r_j}\right]+\frac{e^2}{4\pi\epsilon r_{12}}\right\}\Psi(\vec{r}_1,\vec{r}_2)=E\Psi(\vec{r}_1,\vec{r}_2) \tag{29}$$

where m_e^* is the effective mass of an electron, ϵ is the dielectric constant, $\vec{r}_j$ is the displacement of the jth electron from the donor ion (see figure 1).

With the effective atomic units (i.e., energy unit is $m_e^* e^4/(4\pi\epsilon\hbar)^2$, length unit is $4\pi\epsilon\hbar^2/m_e^* e^2$), equation (29) can be more succinctly written as,

$$\left\{\sum_{j=1}^{2}\left[-\frac{1}{2}\nabla_{\vec{r}_j}-\frac{1}{r_j}\right]+\frac{1}{r_{12}}\right\}\Psi(\vec{r}_1,\vec{r}_2)=E\Psi(\vec{r}_1,\vec{r}_2). \tag{30}$$

Let (x_j, y_j) be the position of the jth electron. We introduce two different sets of hyper-spherical coordinates to describe the system as follows,

$$\begin{aligned}(x_1,y_1)&=(R\cos\phi^\alpha\cos\varphi_1^\alpha,\,R\cos\phi^\alpha\sin\varphi_1^\alpha)\\(x_2,y_2)&=(R\sin\phi^\alpha\cos\varphi_2^\alpha,\,R\sin\phi^\alpha\sin\varphi_2^\alpha)\end{aligned} \tag{31}$$

and

$$\begin{aligned}(x_{rel},y_{rel})&\equiv(x_2-x_1,y_2-y_1)=(\sqrt{2}R\cos\phi^\beta\cos\varphi_1^\beta,\,\sqrt{2}R\cos\phi^\beta\sin\varphi_1^\beta)\\(x_{cm},y_{cm})&\equiv\left(\frac{x_1+x_2}{2},\frac{y_1+y_2}{2}\right)=\left(\sqrt{\frac{1}{2}}R\sin\phi^\beta\cos\varphi_2^\beta,\,\sqrt{\frac{1}{2}}R\sin\phi^\beta\sin\varphi_2^\beta\right)\end{aligned} \tag{32}$$

where (x_{rel}, y_{rel}) denote the relative coordinates, and (x_{cm}, y_{cm}) denote the c.m. coordinates of the two electrons. With hyper-spherical coordinates, equation (30) can be rewritten as,

$$\left\{-\frac{1}{2}\left[\frac{\partial^2}{\partial R^2}+\frac{3}{R}\frac{\partial}{\partial R}-\frac{\Lambda^2(\Omega)}{R^2}\right]+\frac{U(\Omega)}{R}\right\}\Psi(R,\Omega)=E\Psi(R,\Omega) \tag{33}$$

where

$$\begin{aligned}\Lambda^2(\Omega)&=\frac{\partial^2}{\partial\phi^2}+\left(\frac{\cos\phi}{\sin\phi}-\frac{\sin\phi}{\cos\phi}\right)\frac{\partial}{\partial\phi}+\frac{\hat{\ell}^2(\varphi_1)}{\cos^2\phi}+\frac{\hat{\ell}^2(\varphi_2)}{\sin^2\phi}\\U(\Omega)&=\frac{1}{\sqrt{2}\cos\phi^\beta}-\frac{1}{\cos\phi^\alpha}-\frac{1}{\sin\phi^\alpha}\end{aligned} \tag{34}$$

where $\Omega \equiv \{\phi, \varphi_1, \varphi_2\}$ refers either to $\{\phi^\alpha, \varphi_1^\alpha, \varphi_2^\alpha\}$ or to $\{\phi^\beta, \varphi_1^\beta, \varphi_2^\beta\}$.

For the D^- system, $N = 3$. The eigenfunctions for $\Lambda^2(\Omega)$ are (see equation (16)),

$$Y_{[\lambda]} = P_{1,\tilde{n}}^{l_2,l_1}(\phi) \prod_{j=1}^{2} \frac{\mathrm{e}^{\mathrm{i}l_j\varphi_j}}{\sqrt{2\pi}} \tag{35}$$

with eigenvalues $\lambda = 2\tilde{n} + |l_1| + |l_2|$.

We expand the wavefunction in equation (33) in terms of hyper-spherical harmonics $Y_{[\lambda]}(\Omega)$,

$$\Psi(R, \Omega) = \sum_{[\lambda]} F_{[\lambda]}(R) Y_{[\lambda]}(\Omega). \tag{36}$$

Then we obtain a set of coupled second-order differential equations for $\{F_{[\lambda]}(R)\}$,

$$-\frac{1}{2}\left[\frac{\mathrm{d}^2}{\mathrm{d}R^2} + \frac{3}{R}\frac{\mathrm{d}}{\mathrm{d}R} - \frac{\lambda(\lambda+2)}{R^2}\right] F_{[\lambda]}(R) + \frac{1}{R}\sum_{[\lambda']} U_{[\lambda],[\lambda']} F_{[\lambda']}(R) = E F_{[\lambda]}(R) \tag{37}$$

where $U_{[\lambda],[\lambda']}$ are the coupling constants,

$$U_{[\lambda],[\lambda']} = \int Y^*_{[\lambda]}(\Omega) U(\Omega) Y_{[\lambda']}(\Omega)\, \mathrm{d}\Omega. \tag{38}$$

Until now we have not specified the angular variables for the basis functions. In practice, we use $\{R, \phi^\beta, \varphi_1^\beta, \varphi_2^\beta\}$ as the independent variables for the basis functions. This has the advantage that imposing exchange symmetry will be straightforward: since the exchange of electrons $1 \rightleftharpoons 2$ is equivalent to $\varphi_1^\beta \to \varphi_1^\beta + \pi$, we take $l_1 = odd$ for spin-singlet states and $l_1 = even$ for spin-triplet states. The coupling constants $U_{[\lambda],[\lambda']}$ turn out to be

$$\begin{aligned}
U_{[\lambda],[\lambda']} &= \frac{1}{\sqrt{2}} \int Y^*_{[\lambda]}(\Omega^\beta) \frac{1}{\cos\phi^\beta} Y_{[\lambda]}(\Omega^\beta)\, \mathrm{d}\Omega^\beta - \int Y^*_{[\lambda]}(\Omega^\beta) \frac{1}{\cos\phi^\alpha} Y_{[\lambda']}(\Omega^\beta)\, \mathrm{d}\Omega^\beta \\
&\quad - \int Y^*_{[\lambda]}(\Omega^\beta) \frac{1}{\sin\phi^\alpha} Y_{[\lambda']}(\Omega^\beta)\, \mathrm{d}\Omega^\beta \\
&= \frac{1}{\sqrt{2}} \int Y^*_{[\lambda]}(\Omega^\beta) \frac{1}{\cos\phi^\beta} Y_{[\lambda]}(\Omega^\beta)\, \mathrm{d}\Omega^\beta \\
&\quad - \sum_{[\lambda'']} \sum_{[\lambda''']} Z([\lambda]\beta, [\lambda'']\alpha) Z([\lambda']\beta, [\lambda''']\alpha) \int Y^*_{[\lambda'']}(\Omega^\alpha) \frac{1}{\cos\phi^\alpha} Y_{[\lambda''']}(\Omega^\alpha)\, \mathrm{d}\Omega^\alpha \\
&\quad - \sum_{[\lambda'']} \sum_{[\lambda''']} Z([\lambda]\beta, [\lambda'']\alpha) Z([\lambda']\beta, [\lambda''']\alpha) \int Y^*_{[\lambda'']}(\Omega^\alpha) \frac{1}{\sin\phi^\alpha} Y_{[\lambda''']}(\Omega^\alpha)\, \mathrm{d}\Omega^\alpha \\
&= \frac{1}{\sqrt{2}} H_{[\lambda],[\lambda']} - 2 \sum_{[\lambda'']} \sum_{[\lambda''']} Z([\lambda]\beta, [\lambda'']\alpha) Z([\lambda']\beta, [\lambda''']\alpha) H_{[\lambda''],[\lambda''']}
\end{aligned} \tag{39}$$

where

$$\begin{aligned}
H_{[\lambda],[\lambda']} &\equiv \int Y^*_{[\lambda]}(\Omega) \frac{1}{\cos\phi} Y_{[\lambda']}(\Omega)\, \mathrm{d}\Omega \\
&= \delta_{l_1,l_1'} \delta_{l_2,l_2'} \sum_{k=0}^{\nu} \sum_{k'=0}^{\nu'} (-)^{\nu+\nu'-k-k'} \binom{\nu+|l_2|}{k} \binom{\nu+|l_1|}{\nu-k} \binom{\nu'+|l_2|}{k'} \binom{\nu'+|l_1|}{\nu'-k'} \\
&\quad \times I_{2(\nu+nu'-k-k'+|l_2|)+1,2(k+k'+|l_1|)}.
\end{aligned} \tag{40}$$

In equation (37), as $R \to \infty$, $F_{[\lambda]}(R) \to \exp(-R/\zeta)$, where $\zeta = 1/\sqrt{-2E}$. Therefore we make the substitution $\rho = 2R/\zeta$, and rewrite $F_{[\lambda]}(R)$ into

$$F_{[\lambda]}(R) = u_{[\lambda]}(\rho) \mathrm{e}^{-\rho/2}. \tag{41}$$

Table 1. Groundstate energies of the D^- system in two space dimensions. N_{LP} is the number of Laguerre polynomials and N_{HH} is the number of hyper-spherical harmonics used in the calcalations.

	N_{LP}				
N_{HH}	3	4	5	6	7
36	−2.192 0710	−2.193 0423	−2.193 0885	−2.193 0851	−2.193 0831
49	−2.202 1833	−2.203 6324	−2.203 7466	−2.203 7486	−2.203 7469
64	−2.209 3718	−2.211 2460	−2.211 4402	−2.211 4512	−2.211 4501
100	−2.217 9319	−2.220 4753	−2.220 8324	−2.220 8698	−2.220 8717
196	−2.225 7341	−2.229 0709	−2.229 6825	−2.229 7803	−2.229 7930
256	−2.227 6958	−2.231 2664	−2.231 9663	−2.232 0902	−2.232 1091

Substituting equation (41) into (37), we obtain the eigenequations for $u_{[\lambda]}(\rho)$,

$$\frac{\mathrm{d}^2u_{[\lambda]}(\rho)}{\mathrm{d}\rho^2} + \left(\frac{3}{\rho} - 1\right)\frac{\mathrm{d}u_{[\lambda]}}{\mathrm{d}\rho} - \frac{3}{2\rho}u_{[\lambda]}(\rho) - \frac{\lambda(\lambda+2)}{\rho^2}u_{[\lambda]}(\rho) = \frac{\zeta}{\rho}\sum_{[\lambda']} U_{[\lambda],[\lambda']}u_{[\lambda']}(\rho). \tag{42}$$

We expand $u_{[\lambda]}(\rho)$ in terms of Laguerre polynomials $L_n^\gamma(\rho)$ with $\gamma = 2$,

$$u_{[\lambda]}(\rho) = \sum_n C_{n,[\lambda]}L_n^\gamma(\rho). \tag{43}$$

Substituting equation (43) into (42), multiplying $\sqrt{n!/(\gamma+n)!}\rho^4\mathrm{e}^{-\rho}L_n^\gamma(\rho)$ to equation (42) and integrating over ρ, we obtain the recurrence formula for the expansion coefficients, $C_{n,[\lambda]}$,

$$\begin{aligned}(n + \tfrac{5}{2})(n+3)C_{n+1,[\lambda]} &- [\lambda(\lambda+2) + (n + \tfrac{3}{2})(2n+3)]C_{n,[\lambda]} + (n + \tfrac{1}{2})nC_{n-1,[\lambda]} \\ &+\zeta\sum_{[\lambda']} U_{[\lambda],[\lambda']}[(n+3)C_{n+1,[\lambda']} - (2n+3)C_{n,[\lambda']} + nC_{n-1,[\lambda']}] = 0.\end{aligned} \tag{44}$$

The secular equation of the linear and homogeneous equation (44) is solved to obtain the eigenenergies and eigenfunctions.

In table 1, we present the groundstate energies of the D^- system, which is a state with singlet spin and $L = 0$. N_{LP}, the numbers of Laguerre polynomials used in our calculations, are 3, 4, 5, 6, 7; while, N_{HH}, the numbers of hyper-spherical harmonics, are 36, 49, 64, 81, 196, 256. From table 1, we see that the convergence of the groundstate energy is very fast with N_{LG}, i.e., a small value of N_{LG} is sufficient to obtain accurate groundstate energies. In contrast, a large value of N_{HH} is required.

From the normalization condition with variables of set-α,

$$1 = \int |\Psi(R,\phi^\alpha,\varphi_1^\alpha,\varphi_2^\alpha)|^2R^3\cos\phi^\alpha\sin\phi^\alpha\,\mathrm{d}R\,\mathrm{d}\phi^\alpha\,\mathrm{d}\varphi_1^\alpha\,\varphi_2^\alpha \tag{45}$$

we define a shape-density function in the manner,

$$\rho_s(R,\phi^\alpha,\theta^\alpha) = |\Psi(R,\phi^\alpha,\varphi_1^\alpha,\varphi_2^\alpha)|^2R^3\cos\phi^\alpha\sin\phi^\alpha \tag{46}$$

which gives the probability density for the system to stay at a certain size and shape of geometric configuration [25]. Due to the rotational symmetry, ρ_s depends on the polar angles φ_1^α and φ_2^α through $\theta^\alpha \equiv \varphi_2^\alpha - \varphi_1^\alpha$.

In figure 2, the shape density for the groundstate is presented as a function of $[\phi^\alpha, \theta^\alpha]$ for different values of R. In the $[\phi^\alpha, \theta^\alpha]$ plane, point $[45^\circ, 180^\circ]$ corresponds to a collinear structure with the donor ion at the midpoint of the two electrons (hereafter referred to as a dumbbell), which provides the optimal binding; point $[45^\circ, 0]$ corresponds to the overlap of the two electrons. In figure 2, when R is small, the electron–electron interaction does not play a role, the distribution of ρ_s is rather smooth. As R increases, a minimum appears at $[45^\circ, 0]$,

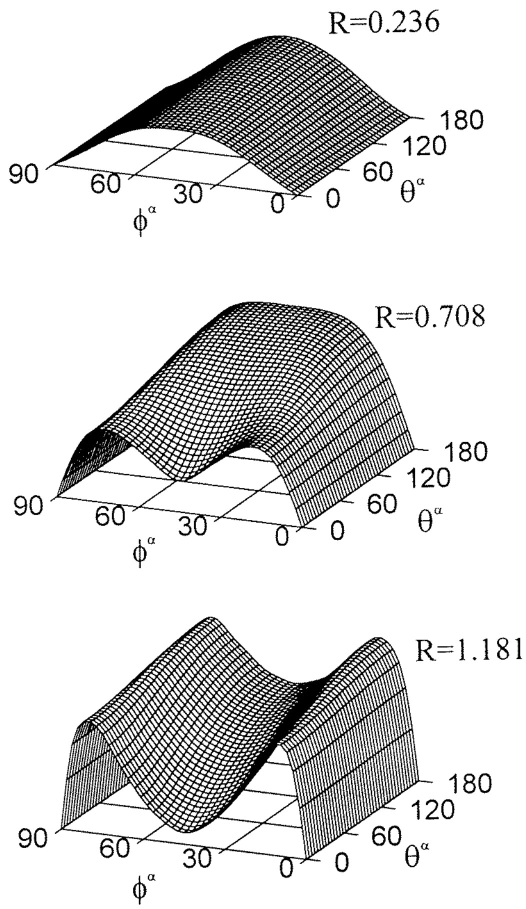

Figure 2. Distribution of the shape-density function $\rho_s(R, \phi^\alpha, \theta^\alpha)$ in the $[\phi^\alpha, \theta^\alpha]$ plane with different values of R for the groundstate . The unit for R is $m_e^* e^2/(4\pi\epsilon\hbar^2)$.

indicating an attempt to avoid the overlap of the two electrons. As R increases further, the minimum evolves continuously into a valley along the $\theta^\alpha = 45^\circ$ axis, indicating a preference to the configuration with one electron being very close to the donor ion and another electron being far away from it when R is large. In any case, however, since the two electrons have to rotate in the opposite directions to keep their total orbital angular momentum to be zero, the distribution of ρ_s does not suggest the existence of an very optimal value of θ^α.

To summarize, we have presented a formula for calculating the transformation coefficients for hyper-spherical harmonics. The D^- system has been given as an example to demonstrate how the formula can be used to solve the few-body problems in two space dimensions. When a system including more electrons is considered, imposing the exchange symmetry on the basis functions will be much more complicated. The transformation coefficients also provide a tool to construct symmetrized basis functions [26].

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