# Representation of cusps in a hyperspherical basis set

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The wave functions of Coulomb systems have cusps at points corresponding to two-particle coelescences. In this paper, we derive series representing the cusps in terms of hyperspherical harmonics multiplied by functions of the hyperradius. When the hyperspherical method is applied to Coulomb systems, the harmonics which appear in these series should be included in the hyperangular basis set.

## 1. Introduction

The Schrödinger equation of a system of $N$ particles can be written in the form

$$\left[-\tfrac{1}{2}\Delta + V(\mathbf{x}) - E\right]\psi(\mathbf{x}) = 0\,, \tag{1}$$

where $\Delta$ is the generalized Laplacian operator [1,2]:

$$\Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} = \frac{1}{r^{d-1}}\frac{\partial}{\partial r} r^{d-1}\frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2}\,, \qquad d = 3N\,. \tag{2}$$

In eq. (2), $r$ is the hyperradius, defined by

$$r^2 \equiv \sum_{j=1}^{d} x_j^2\,, \tag{3}$$

while $\Lambda^2$ is the grand angular momentum operator:

$$\Lambda^2 \equiv -\sum_{i>j}^{d}\left(x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i}\right)^2. \tag{4}$$

In eqs. (1)–(4), $x_1, x_2, \ldots x_d$, $d = 3N$, are the mass-weighted Cartesian coordinates of the system's $N$ particles.

One can try to build up solutions to the Schrödinger equation from basis functions of the form

$$\Phi_{n\lambda\mu} = R_{n\lambda}(r)\, Y_{\lambda\mu}(\mathbf{u}), \tag{5}$$

where $Y_{\lambda\mu}(\mathbf{u})$ is a hyperspherical harmonic [1,2] satisfying

$$\left[\Lambda^2 - \lambda(\lambda + d - 2)\right] Y_{\lambda\mu}(\mathbf{u}) = 0, \qquad \lambda = 0, 1, 2, \ldots, \tag{6}$$

and where

$$\mathbf{u} \equiv \frac{\mathbf{x}}{r} = \frac{1}{r}(x_1, x_2, \ldots, x_d) \tag{7}$$

is a $d$-dimensional unit vector. This approach offers many advantages in the treatment of correlation, since independent-particle approximations are avoided. However, a problem arises when hyperspherical harmonics are used as a basis for treating systems interacting through Coulomb forces: The wave functions of Coulomb systems have cusps at points corresponding to two-particle coalescences [3,4]. To represent such cusps accurately, large values of $\lambda$ are required; but for each value of $\lambda$, there are

$$\omega = \frac{(d + 2\lambda - 2)(d + \lambda - 3)!}{\lambda!(d-2)!} \tag{8}$$

linearly independent hyperspherical harmonics, a degeneracy which becomes extremely large when $\lambda$ is large. It is therefore interesting to ask exactly which hyperspherical harmonics are needed to represent the cusps of a Coulomb system, since this knowledge will allow us to achieve good accuracy with a hyperangular basis set of moderate size.

## 2. Electron-nuclear cusps

Let us consider the case of an $N$-electron atom with a fixed nucleus. Then

$$V(\mathbf{x}) = \sum_{a=1}^{N} \left( -\frac{Z}{r_a} + \sum_{b>a}^{N} \frac{1}{|\mathbf{r}_a - \mathbf{r}_b|} \right), \tag{9}$$

where

$$\begin{aligned} r_1 &\equiv \sqrt{x_1^2 + x_2^2 + x_3^2}, \\ r_2 &\equiv \sqrt{x_4^2 + x_5^2 + x_6^2}, \\ &\vdots \quad \vdots \quad \vdots \end{aligned} \tag{10}$$

In the neighborhood of a point where $\mathbf{r}_a = 0$, the $N$-electron wave-function has a cusp of the form

$$\Psi \sim e^{-Zr_a} . \tag{11}$$

In order to see how this cusp may be represented in terms of hyperspherical harmonics, we will try to construct a series of the form

$$e^{-Zr_a} = \sum_{\lambda=0,2,..}^{\infty} f_\lambda(r)\, Y_{\lambda a}(\mathbf{u}) . \tag{12}$$

To do this, we will need to make use of some of the properties of hyperspherical harmonics.

Interestingly, for each of the familiar theorems satisfied by spherical harmonics, there is a $d$-dimensional generalization [1]. Thus, for example, hyperspherical harmonics obey an orthonormality relation

$$\int d\Omega\; Y^*_{\lambda'\mu'} Y_{\lambda\mu} = \delta_{\lambda'\lambda}\delta_{\mu'\mu} , \tag{13}$$

where $d\Omega$ is the generalized solid angle element defined by

$$dx = dx_1 dx_2 ... dx_d = r^{d-1} dr d\Omega . \tag{14}$$

Here $\mu$ stands for a set of indices labeling the hyperspherical harmonics belonging to a particular value of $\lambda$. Like the familiar spherical harmonics in a 3-dimensional space, the hyperspherical harmonics also obey a sum rule:

$$\sum_\mu Y^*_{\lambda\mu}(\mathbf{u}')\, Y_{\lambda\mu}(\mathbf{u}) = \frac{\lambda+\alpha}{\alpha I(0)} C^\alpha_\lambda(\mathbf{u}\cdot\mathbf{u}') . \tag{15}$$

Here

$$\alpha \equiv \frac{d-2}{2} \tag{16}$$

while $C^\alpha_\lambda(\mathbf{u}\cdot\mathbf{u}')$ is a Gegenbauer polynomial:

$$C^\alpha_\lambda(\mathbf{u}\cdot\mathbf{u}') = \frac{1}{\Gamma(\alpha)} \sum_{t=0}^{[\lambda/2]} \frac{(-1)^t \Gamma(\alpha+\lambda-t)(2\mathbf{u}\cdot\mathbf{u}')^{\lambda-2t}}{t!(\lambda-2t)!} . \tag{17}$$

In eq. (15), $I(0)$ represents the total solid angle:

$$I(0) \equiv \int d\Omega = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})} . \tag{18}$$

When $d = 3$ and $\alpha = 1/2$, eq. (15) reduces to the familiar sum rule for spherical harmonics; and in fact, the Legendre polynomials which appear in the familiar sum rule are a special case of Gegenbauer polynomials. In 3-dimensional space, a plane wave can be expanded in terms of Legendre polynomials and spherical Bessel functions; and this expansion has a $d$-dimensional generalization:

$$e^{i(k_1x_1+...+k_dx_d)} = e^{ikr\mathbf{u}_k\cdot\mathbf{u}} = (d-4)!!\sum_{\lambda=0}^{\infty} i^\lambda(d+2\lambda-2)j_\lambda^d(kr)C_\lambda^\alpha(\mathbf{u}_k\cdot\mathbf{u}),$$
$$\mathbf{u}_k \equiv \frac{\mathbf{k}}{k} = \frac{1}{k}(k_1,k_2,...,k_d), \tag{19}$$

where

$$j_\lambda^d(kr) \equiv \frac{\Gamma(\alpha)2^{\alpha-1}J_{\alpha+\lambda}(kr)}{(d-4)!!(kr)^\alpha} = \sum_{t=0}^{\infty}\frac{(-1)^t(kr)^{2t+\lambda}}{(2t)!!(d+2t+2\lambda-2)!!} \tag{20}$$

might be called a "hyperspherical Bessel function".

We can use these general properties of hyperspherical harmonics to construct the series shown in eq. (12). We begin by remembering that the 3-dimensional Fourier transform of $e^{-Zr_a}$ is given by

$$e^{-Zr_a} = \frac{1}{(2\pi)^{3/2}}\int d^3k\, e^{i\mathbf{k}\cdot\mathbf{r}_a}\sqrt{\frac{2}{\pi}}\,\frac{2Z}{(k^2+Z^2)^2}, \tag{21}$$

where

$$\int d^3k \equiv \int_0^\infty dk\, k^2\int d\Omega_k,$$
$$\int d\Omega_k \equiv \int_0^{2\pi} d\phi_k\int_0^\pi \sin\theta_k\, d\theta_k. \tag{22}$$

We now define a set of $d$-dimensional unit vectors $\mathbf{w}_a$ by

$$\mathbf{w}_1 \equiv \frac{1}{k}(k_1,k_2,k_3,0,0,0,0,...,0),$$
$$\mathbf{w}_1 \equiv \frac{1}{k}(0,0,0,k_1,k_2,k_3,0,...,0),$$
$$\vdots\quad\vdots\quad\vdots$$
$$\mathbf{w}_N \equiv \frac{1}{k}(0,0,0,0,...,0,k_1,k_2,k_3), \tag{23}$$

so that

$$e^{i\mathbf{k}\cdot\mathbf{r}_a} = e^{ikr\mathbf{u}\cdot\mathbf{w}_a}, \tag{24}$$

where $\mathbf{u}$ is defined by eq. (7). Then from (19) we have

$$e^{i\mathbf{k}\cdot\mathbf{r}_a} = (d-4)!!\sum_{\lambda=0}^{\infty} i^{\lambda}(d+2\lambda-2)j_{\lambda}^{d}(kr)C_{\lambda}^{\alpha}(\mathbf{u}\cdot\mathbf{w}_a)\,. \tag{25}$$

Substituting (25) into (21), we obtain

$$e^{-Zr_a} = \frac{(d-4)!!Z}{\pi^2}\sum_{\lambda=0}^{\infty} i^{\lambda}(d+2\lambda-2)\int_0^{\infty}\frac{dk\,k^2 j_{\lambda}^{d}(kr)}{(k^2+Z^2)^2}\int d\Omega_k\; C_{\lambda}^{\alpha}(\mathbf{u}\cdot\mathbf{w}_a)\,. \tag{26}$$

The function

$$U_{\lambda}^{a}(\mathbf{u}) \equiv \frac{1}{4\pi}\int d\Omega_k\; C_{\lambda}^{\alpha}(\mathbf{u}\cdot\mathbf{w}_a) \tag{27}$$

is an eigenfunction of the generalized angular momentum operator $\Lambda^2$, since, from eqs. (6) and (15), we have

$$\left[\Lambda^2 - \lambda(\lambda+d-2)\right]C_{\lambda}^{\alpha}(\mathbf{u}\cdot\mathbf{w}_a) = 0\,, \tag{28}$$

so that

$$\Lambda^2 U_{\lambda}^{a}(\mathbf{u}) \equiv \frac{1}{4\pi}\int d\Omega_k\; \Lambda^2 C_{\lambda}^{\alpha}(\mathbf{u}\cdot\mathbf{w}_a) = \lambda(\lambda+d-2)U_{\lambda}^{a}(\mathbf{u})\,. \tag{29}$$

The integration over $d\Omega_k$ in (27) can be carried out explicitly, using the fact that (for example)

$$\mathbf{u}\cdot\mathbf{w}_1 = \frac{1}{r}(x_1\cos\theta_k\cos\phi_k + x_2\cos\theta_k\sin\phi_k + x_3\sin\theta_k)\,. \tag{30}$$

From (22) and (30) we obtain

$$\begin{aligned}\frac{1}{4\pi}\int d\Omega_k(2\mathbf{u}\cdot\mathbf{w}_a)^{\lambda-2t} &= \frac{1}{2}\left(\frac{2r_a}{r}\right)^{\lambda-2t}\int_0^{\pi} d\theta_k\sin\theta_k(\cos\theta_k)^{\lambda-2t}\\ &= \begin{cases}\frac{1}{\lambda-2t+1}\left(\frac{2r_a}{r}\right)^{\lambda-2t}, & \lambda = \text{even},\\ 0, & \lambda = \text{odd}.\end{cases}\end{aligned} \tag{31}$$

Thus, from the definition of the Gegenbauer polynomials, we have for even $\lambda$

$$U_{\lambda}^{a}(\mathbf{u}) = \sum_{t=0}^{\lambda/2} b_{\lambda,t}\left(\frac{2r_a}{r}\right)^{\lambda-2t}, \tag{32}$$

where

$$b_{\lambda,t} \equiv \frac{(-1)^t\Gamma(\lambda+\alpha-t)}{\Gamma(\alpha)t!(\lambda-2t+1)!}\,. \tag{33}$$

The odd values of $\lambda$ do not enter the series shown in eq. (26) because the integral in eq. (31) vanishes when $\lambda$ is odd.

Apart from a normalization constant, $U_\lambda^a(\mathbf{u})$ is the special hyperspherical harmonic which we need for the series of eq. (12). The normalizing constant can be found by making use of the sum rule for hyperspherical harmonics and the definition of the Gegenbauer polynomials, from which it follows that

$$\begin{aligned}\frac{(4\pi)^2}{I(0)}\int d\Omega |U_\lambda^a(\mathbf{u})|^2 &= \int d\Omega_k \int d\Omega_{k'}\left[\frac{1}{I(0)}\int d\Omega C_\lambda^\alpha(\mathbf{u}\cdot\mathbf{w}_a)C_{\lambda'}^\alpha(\mathbf{u}\cdot\mathbf{w}'_a)\right]\\ &= \frac{\alpha}{\lambda+\alpha}\int d\Omega_k\int d\Omega_{k'} C_\lambda^\alpha(\mathbf{w}_a\cdot\mathbf{w}'_a)\\ &= \frac{\alpha}{(\lambda+\alpha)\Gamma(\alpha)}\sum_{t=0}^{[\lambda/2]}\frac{(-1)^t\Gamma(\lambda+\alpha-t)}{t!(\lambda-2t)!}\\ &\quad\times\int d\Omega_k\int d\Omega_{k'}(2\mathbf{w}_a\cdot\mathbf{w}'_a)^{\lambda-2t}\,. \end{aligned} \tag{34}$$

But

$$\mathbf{w}_a\cdot\mathbf{w}'_a = \frac{1}{k'k}\mathbf{k}\cdot\mathbf{k}' = \cos\theta_k \tag{35}$$

so that

$$\int d\Omega_k\int d\Omega_{k'}(\mathbf{w}_a\cdot\mathbf{w}'_a)^{\lambda-2t} = \frac{(4\pi)^2}{\lambda-2t+1}\,. \tag{36}$$

Therefore

$$\frac{1}{I(0)}\int d\Omega|U_\lambda^a(\mathbf{u})|^2 = \frac{\alpha}{\lambda+\alpha}\sum_{t=0}^{[\lambda/2]} b_{\lambda,t}(2)^{\lambda-2t}\,, \tag{37}$$

where $b_{\lambda,t}$ is defined by eq. (33). Eq. (37) can be simplified by noticing that

$$C_{\lambda+1}^{\alpha-1}(\xi) = \frac{1}{\Gamma(\alpha-1)}\sum_{t=0}^{[(\lambda+1)/2]}\frac{(-1)^t\Gamma(\lambda+\alpha-t)(2\xi)^{\lambda+1-2t}}{t!(\lambda-2t+1)!}\,. \tag{38}$$

Comparing eqs. (37) and (38), and making use of the fact that [1]

$$C_{\lambda+1}^{\alpha-1}(1) = \frac{(\lambda+d-4)!}{(\lambda+1)!(d-5)!}\,, \tag{39}$$

we can rewrite (37) in the form

$$\frac{1}{I(0)}\int d\Omega |U_\lambda^a(\mathbf{u})|^2 = \frac{\alpha(\lambda+d-4)!}{(\lambda+\alpha)(\lambda+1)!(d-4)!}\,. \tag{40}$$

From (40) and (32) it follows that the special hyperspherical harmonics needed for representation of the cusp $e^{-Zr_a}$ are given by

$$Y_{\lambda a}(\mathbf{u}) = \mathcal{N}\sum_{t=0}^{\lambda/2} b_{\lambda,t}\left(\frac{2r_a}{r}\right)^{\lambda-2t}, \tag{41}$$

where

$$\mathcal{N} = \sqrt{\frac{(\lambda+\alpha)(\lambda+1)!(d-4)!}{\alpha I(0)(\lambda+d-4)!}}\,. \tag{42}$$

Using the fact that

$$\int d\Omega\ Y_{\lambda' a}(\mathbf{u})\,Y_{\lambda a}(\mathbf{u}) = \delta_{\lambda'\lambda} \tag{43}$$

we can obtain from (12) the relationship

$$f_\lambda(r) = \int d\Omega\ Y_{\lambda a}(\mathbf{u})e^{-Zr_a}\,. \tag{44}$$

Then, since

$$e^{-Zr_a} = \sum_{n=0}^{\infty}\frac{(-Zr)^n}{n!}\left(\frac{r_a}{r}\right)^n, \tag{45}$$

eqs. (41)–(44) give us a Taylor series representation of $f_\lambda(r)$:

$$f_\lambda(r) = \sum_{n=0}^{\infty} c_n r^n\,, \tag{46}$$

where

$$c_n = \frac{(-Z)^n}{n!}\mathcal{N}\sum_{t=0}^{\lambda/2} b_{\lambda,t}2^{\lambda-2t}\int d\Omega\left(\frac{r_a}{r}\right)^{\lambda+n-2t}. \tag{47}$$

The hyperangular integral in (47) can be evaluated explicitly, since [17]

$$\frac{1}{I(0)}\int d\Omega\left(\frac{r_a}{r}\right)^{\nu} = \frac{\Gamma(\frac{\nu+3}{2})\Gamma(\frac{d}{2})}{\Gamma(\frac{3}{2})\Gamma(\frac{\nu+d}{2})}\,. \tag{48}$$

For all values of $\lambda$ except $\lambda = 0$, the coefficient $c_0$ vanishes in the Taylor series of eq. (46). This can be seen from eqs. (43)–(45), since from (43) we have

$$\int d\Omega\ Y_{\lambda a}(\mathbf{u}) = 0, \qquad \lambda \neq 0, \tag{49}$$

while from (44) and (45) we have

$$f_\lambda(r) = \int d\Omega\ Y_{\lambda a}(\mathbf{u})\left[1 - Zr\left(\frac{r_a}{r}\right) + \ldots\right]. \tag{50}$$

From (49) it follows that the leading term in (50) vanishes when $\lambda \neq 0$. When $\lambda = 0$, eqs. (41) and (42) yield

$$Y_{0a}(\mathbf{u}) = \mathcal{N} = \frac{1}{\sqrt{I(0)}} \tag{51}$$

and (50) becomes

$$f_0(r) = \frac{1}{\mathcal{N}I(0)}\int d\Omega\ \left[1 - Zr\left(\frac{r_a}{r}\right) + \ldots\right]. \tag{52}$$

Then, with the help of (48), we obtain the leading terms:

$$f_0(r) = \mathcal{N}^{-1}\left[1 - \frac{\Gamma(2)\Gamma(\frac{d}{2})}{\Gamma(\frac{3}{2})\Gamma(\frac{d+1}{2})}Zr + \ldots\right]. \tag{53}$$

A second approach to the radial functions, $f_\lambda(r)$, is through evaluation of the $k$-integral in eq. (26). From (12), (26) and (27) we have

$$f_\lambda(r) = 2Z\mathcal{N}^{-1}i^\lambda(d-4)!!(d+2\lambda-2)\frac{2}{\pi}\int_0^\infty dk\frac{k^2 j_\lambda^d(kr)}{(k^2+Z^2)^2}. \tag{54}$$

Using eq. (20), we can express $j_\lambda^d(kr)$ in terms of ordinary Bessel functions:

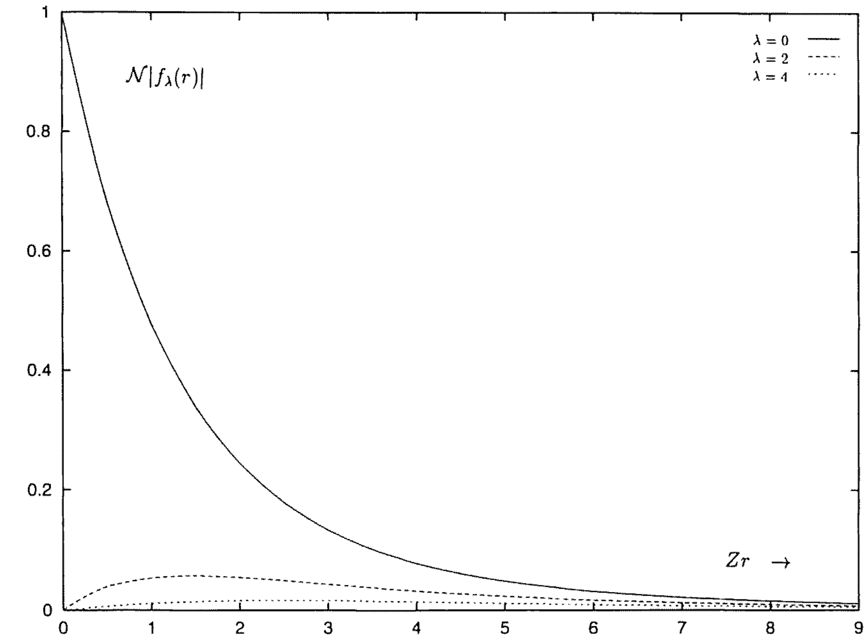
$$j_\lambda^d(kr) = \frac{\Gamma(\alpha)2^{\alpha-1}J_{\alpha+\lambda}(kr)}{(d-4)!!(kr)^\alpha}, \tag{55}$$

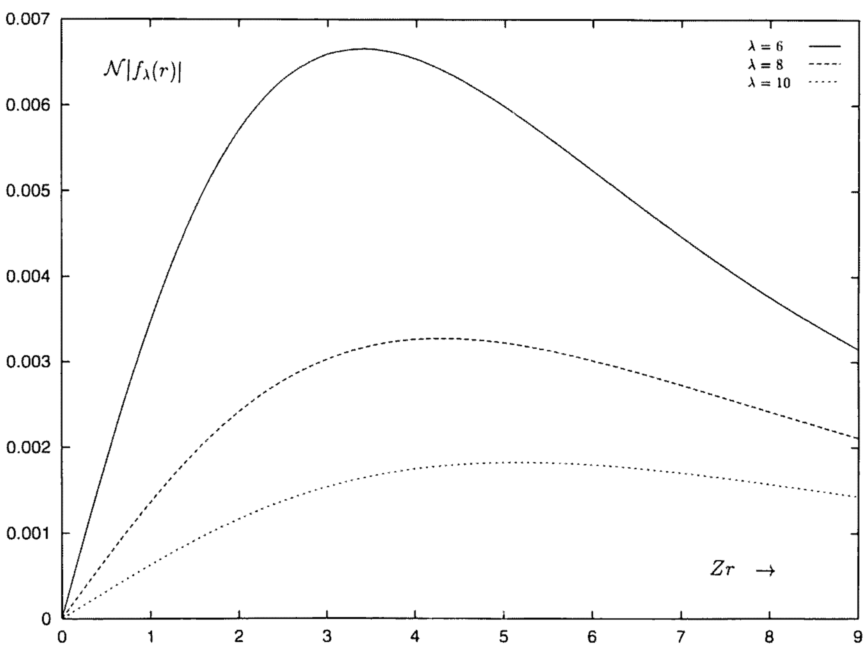
where $\alpha$ is defined by eq. (16). Thus

$$f_\lambda(r) = Zr\Gamma(\alpha)\mathcal{N}^{-1}i^\lambda(d+2\lambda-2)\frac{2^{\alpha+1}}{\pi}\int_0^\infty dt\frac{t^{2-\alpha}J_{\lambda+\alpha}(t)}{(t^2+Z^2r^2)^2}. \tag{56}$$

The integral in (56) can be evaluated in terms of hypergeometric functions using Gradshteyn and Ryzhik's eq. 6.565(8) [5], or by numerical integration.

The radial functions $f_\lambda(r)$ for $\lambda = 0, 2, 4, 6, 8, 10$ are illustrated in Figs. 1–3. The functions shown in the figures correspond to $d = 3N = 9$. The functions were evaluated by numerical integration of (56) for large values of $r$, and using the series defined by eqs. (46)–(48) for small values of $r$. As we would expect from eq. (50), $f_0(0) = \mathcal{N}^{-1}$, while for $\lambda \neq 0, f_\lambda(0) = 0$.




Figs. 1 and 2. These figures show the hyperradial functions $\mathcal{N}|f_\lambda(r)|$ of eq. (56) for the first few values of $\lambda$. Because of the factor $i^\lambda$, the functions alternate in sign, $f_0(r)$ being positive for $0 < r < \infty$, while $f_2(r)$ is negative, and so on; but in the figures we show the absolute values of the functions.

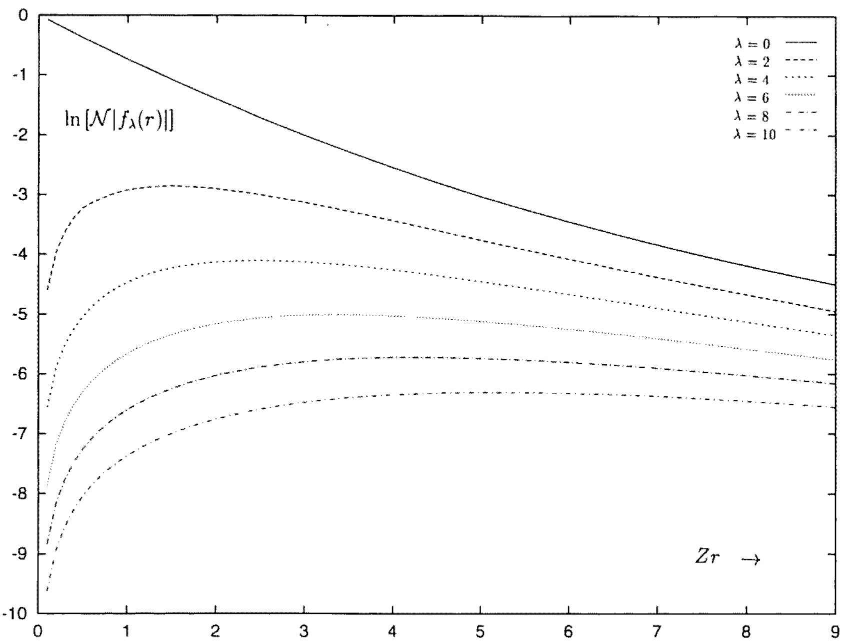



Fig. 3. This figure shows $\ln[\mathcal{N}|f_\lambda(r)|]$. It can be seen from the figure that for large values of the hyperradius, $r$, the functions $|f_\lambda(r)|$ have an almost exponential behaviour. One can also see from this figure that the functions fall off rapidly in magnitude with increasing values of $\lambda$.

## 3. Electron-electron cusps

For high accuracy, it is necessary to include in our basis set the harmonics $Y_{\lambda a}(\mathbf{u})$, which are needed for a good representation of the electron-nuclear cusps; but this is not enough: We must also include the functions which are needed for a good representation of the cusps which occur at electron-electron coalescences, as has been emphasized by Morgan [4]. The representation of electron-electron cusps can be considered as a special case of a more general question: Can we represent an arbitrary function of the interparticle distance $r_{ab}$,

$$g(r_{ab}) \equiv g(|\mathbf{r}_a - \mathbf{r}_b|) , \tag{57}$$

as a series of hyperspherical harmonics multiplied by functions of the hyperradius? We can, in fact, do this, using a method almost identical to eqs. (21)–(56). In this way we obtain the series

$$g(r_{ab}) = \sum_{\lambda=0,2,\ldots}^{\infty} g_\lambda(r)\, Y_{\lambda(ab)}(\mathbf{u}) , \tag{58}$$

where

$$Y_{\lambda(ab)}(\mathbf{u}) = \mathcal{N} \sum_{t=0}^{\lambda/2} b_{\lambda,t} \left( \frac{\sqrt{2} r_{ab}}{r} \right)^{\lambda - 2t} \tag{59}$$

and

$$g_\lambda(r) = \mathcal{N}^{-1} i^\lambda (d-4)!!(d+2\lambda-2) \sqrt{\frac{2}{\pi}} \int_0^\infty dk\, k^2 j_\lambda^d(\sqrt{2}kr) g^t(k) . \tag{60}$$

In eqs. (58)–(60), $b_{\lambda,t}$ and $\mathcal{N}$ are defined by eqs. (33) and (42), while $g^t(k)$ is the Fourier transform of the function $g(r_{ab})$:

$$g^t(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty dr_{ab}\, r_{ab}^2 j_0(kr_{ab}) g(r_{ab}) , \tag{61}$$

$j_0$ being a spherical Bessel function. The harmonics in eq. (59) are normalized in such a way that

$$\int d\Omega\; Y_{\lambda'(ab)}(\mathbf{u}) Y_{\lambda(ab)}(\mathbf{u}) = \delta_{\lambda'\lambda} . \tag{62}$$

However, two harmonics corresponding to the same value of $\lambda$ but to different values of the particle indices are not orthogonal:

$$\int d\Omega\; Y_{\lambda(ab)}(\mathbf{u}) Y_{\lambda(cd)}(\mathbf{u}) \neq 0 . \tag{63}$$

It is interesting to notice that in the series of eqs. (58)–(61), the harmonics $Y_{\lambda(ab)}(\mathbf{u})$ are independent of the form of $g(r_{ab})$. Thus, for example, any potential of the form

$$V(\mathbf{x}) = \sum_{b>a}^{N} \sum_{a}^{N} g(r_{ab}) \tag{64}$$

can be represented by a series of the form

$$V(\mathbf{x}) = \sum_{\lambda=0,2,\ldots}^{\infty} g_\lambda(r) \sum_{b>a}^{N} \sum_{a}^{N} Y_{\lambda(ab)}(\mathbf{u}) . \tag{65}$$

Since the $\lambda$-projection of the potential is a "potential harmonic" of the type introduced into nuclear physics by Fabre de la Ripelle [6,7], eq. (67) shows us that the harmonics needed for accurate representation of electron–electron cusps are closely related to potential harmonics.

We conclude from the present study that harmonics of the type $Y_{\lambda a}(\mathbf{u})$ (eq. (41)) and $Y_{\lambda(ab)}(\mathbf{u})$ (eq. (59)) should be included in the basis set when the hyperspherical method is applied to Coulomb systems.

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