

Interbasis expansion and SO(3) symmetry in the two-dimensional hydrogen atom

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Making use of the SO(3) symmetry of the two-dimensional hydrogen atom, each of the bases for the bound states formed by the separable solutions of the Schrödinger equation in polar and parabolic coordinates are expressed in terms of the other.

Keywords: Hydrogen atom; dynamical symmetry; rotation group

Usando la simetría SO(3) del átomo de hidrógeno en dos dimensiones, cada una de las bases para los estados ligados formadas por las soluciones separables de la ecuación de Schrödinger en coordenadas polares y parabólicas se expresa en términos de la otra.

Descriptores: Átomo de hidrógeno; simetría dinámica; grupo de rotaciones

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1. Introduction

The hydrogen atom in n dimensions, with $n \geq 2$, has a “hidden” SO($n + 1$) symmetry group [1–3] which is related to the conservation of the Runge–Lenz vector. This symmetry is also related to the separability of the Schrödinger equation in two or more coordinate systems. In the case of the two-dimensional hydrogen atom, the corresponding Schrödinger equation is separable in polar coordinates, as a consequence of the “obvious” rotational symmetry of the Hamiltonian, and is also separable in parabolic coordinates, in spite of the fact that both coordinates are non-ignorable. The separability in parabolic coordinates leads to the existence of a conserved quantity that turns out to be the Runge–Lenz vector.

Each energy level of the two-dimensional hydrogen atom has a degeneracy of the form $2l + 1$ with $l = 0, 1, \dots$ and for a given energy eigenvalue, the separable solutions in polar or parabolic coordinates form a basis for the states with that energy. Therefore, it must be possible to express each of these bases in terms of the other. This relationship has been previously studied in Ref. 4, making use of the explicit expressions of the eigenfunctions and some relations between the special functions involved. Here we follow a simpler procedure taking advantage of the relationship of the hydrogen atom in two dimensions with a free particle on a sphere [1, 3, 5]. In Sect. 2 we summarize the relevant results concerning the separable solutions of the Schrödinger equation for the two-dimensional hydrogen atom with negative energy in polar and parabolic coordinates and the relationship of these solutions with the usual spherical harmonics. In Sect. 3 the separable solutions of the two-dimensional hydrogen atom in polar and parabolic coordinates are expressed in terms of each other. A

similar relation is derived for the separable solutions of the two-dimensional isotropic harmonic oscillator in polar and Cartesian coordinates.

2. Separable solutions of the hydrogen atom and spherical harmonics

The Schrödinger equation for the bound states of the two-dimensional hydrogen atom

$$-\frac{\hbar^2}{2M}\nabla^2\psi - \frac{k}{r}\psi = E\psi, \quad (1)$$

is separable in polar and parabolic coordinates. The normalized separable solutions of Eq. (1) in polar coordinates (r, φ) are given, up to a phase factor, by

$$\psi_{lm}(r, \varphi) = \frac{p_0}{\hbar} (-i)^m \left[\frac{2l+1}{2\pi} \frac{(l-|m|)!}{(l+|m|)!} \right]^{1/2} \frac{2^{|m|+1}}{2l+1} \\ \times e^{-p_0 r/\hbar} \left(\frac{p_0 r}{\hbar} \right)^{|m|} L_{l-|m|}^{2|m|} \left(\frac{2p_0 r}{\hbar} \right) e^{im\varphi}, \quad (2)$$

where

$$p_0 \equiv \sqrt{-2ME} = \frac{2Mk}{\hbar(2l+1)}, \quad (3)$$

L_n^k denote the associated Laguerre polynomials [6, 7], $l = 0, 1, 2, \dots$, and $m = 0, \pm 1, \dots, \pm l$. The separation constant m is the eigenvalue of $(1/\hbar)L_z$, where L_z is the angular momentum operator

$$L_z = -i\hbar \frac{\partial}{\partial \varphi}. \quad (4)$$

The normalized separable solutions of Eq. (1) in the parabolic coordinates (u, v) , defined by

$$x = \frac{1}{2}(u^2 - v^2), \quad y = uv \quad (5)$$

or, equivalently, by

$$x + iy = \frac{1}{2}(u + iv)^2, \quad (6)$$

are given, up to a phase factor, by

$$\tilde{\psi}_{lm_y} = \frac{p_0}{\hbar} \frac{i^{l-m_y} e^{-p_0(u^2+v^2)/2\hbar} H_{l+m_y}(\sqrt{p_0/\hbar}u) H_{l-m_y}(\sqrt{p_0/\hbar}v)}{\sqrt{2^{2l-1}(2l+1)\pi(l+m_y)!(l-m_y)!}}, \quad (7)$$

where the H_n are Hermite polynomials and $m_y = 0, \pm 1, \dots, \pm l$ [5, 8–10]. The separation constant m_y is the eigenvalue of $-A_x/(p_0\hbar)$, where A_x is the x -component of

$$\mathbf{A} \equiv \frac{1}{2}(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{Mk\mathbf{r}}{r}, \quad (8)$$

$\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and $\mathbf{p} = -i\hbar\nabla$ [5].

For each value of l , there must exist complex scalars, $c_{m_y m}^l$, such that

$$\tilde{\psi}_{lm_y}(u, v) = \sum_{m=-l}^l c_{m_y m}^l \psi_{lm}(r, \varphi). \quad (9)$$

As we shall show, the coefficients $c_{m_y m}^l$ can be readily obtained using the fact that the solutions of the Schrödinger equation for the bound states of the two-dimensional hydrogen atom can be expressed in the form

$$\psi(x, y) = \frac{p_0}{2\sqrt{2}\pi\hbar} \int \hat{\Phi}(\theta, \phi) \csc \frac{\theta}{2} \times e^{ip_0 \cot(\theta/2)(x \cos \phi + y \sin \phi)/\hbar} d\Omega \quad (10)$$

[Ref. 5, Eq. (12)], where $\hat{\Phi}$ is a spherical harmonic, of degree l given by Eq. (3), $d\Omega$ is the solid angle element and the integral is over the unit sphere. The wave function $\psi(x, y)$ is normalized over the plane if and only if $\hat{\Phi}$ is normalized over the sphere.

The inverse of the integral transform (10) is given by

$$\hat{\Phi}(\theta, \phi) = \frac{p_0}{4\sqrt{2}\pi\hbar} \frac{1}{\sin^3 \frac{\theta}{2}} \int \psi(x, y) \times e^{-ip_0 \cot(\theta/2)(x \cos \phi + y \sin \phi)/\hbar} dx dy. \quad (11)$$

Making use of the relationship between spherical harmonics and solutions of Eq. (1), for a fixed value of E , given by Eqs. (10) and (11), one finds that the angular momentum operators on the sphere, \hat{L}_x , \hat{L}_y , \hat{L}_z , which have the explicit expressions

$$\begin{aligned} \hat{L}_x &= i\hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right), \\ \hat{L}_y &= i\hbar \left(-\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right), \\ \hat{L}_z &= -i\hbar \frac{\partial}{\partial \phi}, \end{aligned}$$

correspond to A_y/p_0 , $-A_x/p_0$, and L_z , respectively [5]. That is, if the integral transform (10) is denoted by $\psi = \mathcal{T}[\hat{\Phi}]$, then $\mathcal{T}[\hat{L}_x \hat{\Phi}] = (1/p_0)A_y \mathcal{T}[\hat{\Phi}]$, $\mathcal{T}[\hat{L}_y \hat{\Phi}] = (-1/p_0)A_x \mathcal{T}[\hat{\Phi}]$, and $\mathcal{T}[\hat{L}_z \hat{\Phi}] = L_z \mathcal{T}[\hat{\Phi}]$. Therefore, the wave functions $\psi_{lm}(r, \varphi)$, which are eigenfunctions of L_z , correspond to the spherical harmonics $\hat{\Phi}(\theta, \phi)$ that are eigenfunctions of \hat{L}_z , i.e., the usual spherical harmonics $Y_{lm}(\theta, \phi)$. In fact, in Ref. 5 it was explicitly shown that if one substitutes $\hat{\Phi}(\theta, \phi) = Y_{lm}(\theta, \phi)$ into Eq. (10) and the Cartesian coordinates are replaced by polar coordinates, then one obtains the wave function $\psi_{lm}(r, \varphi)$ given by Eq. (2) (including the phase factor $(-i)^m$).

In a similar manner, the wave function $\tilde{\psi}_{lm_y}(u, v)$, which is an eigenfunction of A_x , corresponds to a spherical harmonic of degree l that is an eigenfunction of \hat{L}_y with eigenvalue m_y (which is not separable in the coordinates (θ, ϕ)).

Let $\hat{\mathcal{R}}_0$ be the rotation about the origin in three-dimensional Euclidean space that maps the ordered basis $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ into $\{\mathbf{k}, \mathbf{i}, \mathbf{j}\}$; then, the rotated functions $\hat{\mathcal{R}}_0 Y_{lm}$ are eigenfunctions of $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ and \hat{L}_y , with eigenvalues $l(l+1)\hbar^2$ and $m_y\hbar$, respectively [3, 11–13]. (The action of $\hat{\mathcal{R}}_0$ on an arbitrary function, f , is defined by $(\hat{\mathcal{R}}_0 f)(\mathbf{r}) \equiv f(\hat{\mathcal{R}}_0^{-1}(\mathbf{r}))$.) The Euler angles (ϕ, θ, ψ) corresponding to $\hat{\mathcal{R}}_0$ in the “ y convention” [14] can be taken as $(\pi/2, \pi/2, \pi)$ and, therefore,

$$\hat{\mathcal{R}}_0 Y_{lm_y} = \sum_{m=-l}^l D_{mm_y}^l \left(\frac{\pi}{2}, \frac{\pi}{2}, \pi \right) Y_{lm}, \quad (12)$$

where $D_{m'm}^l(\phi, \theta, \psi)$ are the Wigner functions [3, 11–13]. The Wigner D functions are given by

$$D_{m'm}^l(\phi, \theta, \psi) = e^{-im'\phi} d_{m'm}^l(\theta) e^{-im\psi}, \quad (13)$$

with

$$\begin{aligned} d_{m'm}^l(\theta) &= \sqrt{(l+m)!(l-m)!(l+m')!(l-m')!} \\ &\times \sum_k \frac{(-1)^k \left(\sin \frac{\theta}{2} \right)^{m-m'+2k} \left(\cos \frac{\theta}{2} \right)^{2l-m+m'-2k}}{k!(l+m'-k)!(l-m-k)!(m-m'+k)!}, \quad (14) \end{aligned}$$

hence

$$\hat{\mathcal{R}}_0 Y_{lm_y} = (-1)^{m_y} \sum_{m=-l}^l (-i)^m d_{mm_y}^l \left(\frac{\pi}{2} \right) Y_{lm}. \quad (15)$$

We claim that the wave function $\tilde{\psi}_{lm_y}(u, v)$, given by Eq. (7), corresponds to $\hat{\mathcal{R}}_0 Y_{lm_y}$ by means of (10), i.e.,

$$\begin{aligned} \tilde{\psi}_{lm_y}(u, v) &= \frac{p_0}{2\sqrt{2}\pi\hbar} \int (\hat{\mathcal{R}}_0 Y_{lm_y}) \csc \frac{\theta}{2} \\ &\times e^{ip_0 \cot(\theta/2)(\cos\phi(u^2-v^2)/2 + \sin\phi uv)/\hbar} d\Omega. \quad (16) \end{aligned}$$

According to the preceding discussion, we only need to check that $\tilde{\psi}_{lm_y}(u, v)$ has the appropriate phase. From Eq. (7) we see that under complex conjugation, $(\tilde{\psi}_{lm_y})^* = (-1)^{m_y-l} \tilde{\psi}_{lm_y}$ and that $\tilde{\psi}_{lm_y}(u, v) = (-1)^l \tilde{\psi}_{lm_y}(-v, u)$. On the other hand, using the fact that $(\hat{\mathcal{R}}_0 Y_{lm_y})^* = (-1)^{m_y} \hat{\mathcal{R}}_0 Y_{l, -m_y}$, one verifies that under complex conjugation the right-hand side of Eq. (16) obeys the same relationship as $\tilde{\psi}_{lm_y}$. This implies that the two sides of Eq. (16) can differ at most by a real factor with absolute value equal to 1; the relations derived from Eq. (16) show that the two sides of this equation indeed coincide (see, e.g., Eq. (20) below).

3. Interbasis expansions

Owing to the linearity of the integral transform (10), from Eq. (15) it follows that

$$\tilde{\psi}_{lm_y}(u, v) = (-1)^{m_y} \sum_{m=-l}^m (-i)^m d_{mm_y}^l \left(\frac{\pi}{2} \right) \psi_{lm}(r, \varphi), \quad (17)$$

which is the desired relation (9). Since the inverse of a rotation with Euler angles (ϕ, θ, ψ) is the rotation with Euler angles $(-\psi, -\theta, -\phi)$, from Eqs. (12) and (13) and the fact that the matrices $D_{m'm}^l$ form a linear representation of the rotation group we obtain

$$\begin{aligned} Y_{lm} &= \sum_{m_y=-l}^l D_{m_y m}^l \left(-\pi, -\frac{\pi}{2}, -\frac{\pi}{2} \right) \hat{\mathcal{R}}_0 Y_{lm_y} \\ &= i^m \sum_{m_y=-l}^l (-1)^{m_y} d_{m_y m}^l \left(-\frac{\pi}{2} \right) \hat{\mathcal{R}}_0 Y_{lm_y}, \quad (18) \end{aligned}$$

which implies that

$$\psi_{lm}(r, \varphi) = i^m \sum_{m_y=-l}^l (-1)^{m_y} d_{m_y m}^l \left(-\frac{\pi}{2} \right) \tilde{\psi}_{lm_y}(u, v). \quad (19)$$

Making use of Eqs. (2) and (7) it follows that, for $m \geq 0$, Eq. (19) is equivalent to

$$(u+iv)^{2m} L_{l-m}^{2m}(u^2+v^2) = \frac{1}{2^l} \sqrt{\frac{(l+m)!}{(l-m)!}} \sum_{m'=-l}^l (-1)^{m'-m} d_{m' m}^l \left(\frac{\pi}{2} \right) \frac{H_{l+m'}(u) H_{l-m'}(v)}{\sqrt{(l+m')!(l-m')!}}. \quad (20)$$

Owing to the procedure employed here, Eq. (20) holds for $l = 0, 1, \dots$, and $m = 0, 1, \dots, l$; however, it can be verified that Eq. (20) also holds when l and m are half-integers. Taking $m = 0$ in the last equation one obtains

$$L_l(u^2+v^2) = \frac{(-1)^l}{2^{2l}} \sum_{k=0}^l \frac{H_{2k}(u) H_{2l-2k}(v)}{k!(l-k)!} \quad (21)$$

(cf. Ref. 7, Chap. 4).

Since \hat{L}_z is the infinitesimal generator of rotations about the z -axis on the sphere and L_z is the infinitesimal generator of rotations about the origin on the plane, the fact that \hat{L}_z corresponds to L_z under the integral transform (10) implies that if $\mathcal{R}_z(\alpha)$ denotes the rotation on the plane about the origin through the angle α and $\hat{\mathcal{R}}_z(\alpha)$ denotes the rotation on the sphere about the z -axis through the angle α , then

$$\mathcal{R}_z(\alpha) \mathcal{T}[\hat{\Phi}] = \mathcal{T}[\hat{\mathcal{R}}_z(\alpha) \hat{\Phi}].$$

Thus, taking $\hat{\Phi} = \hat{\mathcal{R}}_0 Y_{lm_y}$ in the last identity we obtain

$$\mathcal{R}_z(\alpha) \mathcal{T}[\hat{\mathcal{R}}_0 Y_{lm_y}] = \mathcal{T}[\hat{\mathcal{R}}_z(\alpha) \hat{\mathcal{R}}_0 Y_{lm_y}]. \quad (22)$$

From Eqs. (12) and (18) we have

$$\begin{aligned} \hat{\mathcal{R}}_z(\alpha) \hat{\mathcal{R}}_0 Y_{lm_y} &= \sum_{m'=-l}^l D_{m' m_y}^l \left(\frac{\pi}{2}, \frac{\pi}{2}, \pi \right) \hat{\mathcal{R}}_z(\alpha) Y_{lm} \\ &= \sum_{m, k=-l}^l D_{m m_y}^l \left(\frac{\pi}{2}, \frac{\pi}{2}, \pi \right) D_{km}^l(\alpha, 0, 0) Y_{lk} \\ &= \sum_{m, k, m'_y=-l}^l D_{m m_y}^l \left(\frac{\pi}{2}, \frac{\pi}{2}, \pi \right) D_{km}^l(\alpha, 0, 0) \\ &\quad \times D_{m'_y k}^l \left(-\pi, -\frac{\pi}{2}, -\frac{\pi}{2} \right) \hat{\mathcal{R}}_0 Y_{lm'_y}. \end{aligned}$$

The composition of a rotation with Euler angles $(-\pi, -\pi/2, -\pi/2)$ followed by a rotation with Euler angles $(\alpha, 0, 0)$, followed then by a rotation with Euler angles $(\pi/2, \pi/2, \pi)$ is the rotation with Euler angles $(-\pi/2, \alpha, \pi/2)$, as can be verified, for example, using the fact that the rotation with Euler angles (ϕ, θ, ψ) is repre-

sented by the SU(2) matrix

$$\begin{pmatrix} e^{-i(\phi+\psi)/2} \cos \frac{\theta}{2} & -e^{-i(\phi-\psi)/2} \sin \frac{\theta}{2} \\ e^{i(\phi-\psi)/2} \sin \frac{\theta}{2} & e^{i(\phi+\psi)/2} \cos \frac{\theta}{2} \end{pmatrix}.$$

Therefore, using again that the D functions form a linear representation of the rotation group, it follows that

$$\begin{aligned} \hat{\mathcal{R}}_z(\alpha) \hat{\mathcal{R}}_0 Y_{lm_y} &= \sum_{m'_y=-l}^l D_{m'_y m_y}^l \left(-\frac{1}{2}\pi, \alpha, \frac{1}{2}\pi \right) \hat{\mathcal{R}}_0 Y_{lm'_y} \\ &= (-i)^{m_y} \sum_{m'_y=-l}^l i^{m'_y} d_{m'_y m_y}^l(\alpha) \hat{\mathcal{R}}_0 Y_{lm'_y} \end{aligned}$$

and by means of the integral transform (10), this last relation amounts to

$$\mathcal{R}_z(\alpha) \tilde{\psi}_{lm_y} = (-i)^{m_y} \sum_{m'_y=-l}^l i^{m'_y} d_{m'_y m_y}^l(\alpha) \tilde{\psi}_{lm'_y}. \quad (23)$$

More explicitly, since a rotation about the origin through an angle α in the xy -plane corresponds to a rotation about the origin through an angle $\alpha/2$ in the uv -plane [as can be seen from Eq. (6)], we have

$$\begin{aligned} \tilde{\psi}_{lm_y} \left(u \cos \frac{\alpha}{2} + v \sin \frac{\alpha}{2}, v \cos \frac{\alpha}{2} - u \sin \frac{\alpha}{2} \right) &= \\ &= (-i)^{m_y} \sum_{m'_y=-l}^l i^{m'_y} d_{m'_y m_y}^l(\alpha) \tilde{\psi}_{lm'_y}(u, v) \end{aligned}$$

(cf. Ref. 4). Using Eq. (7), one finds that the last equation is equivalent to

$$\frac{H_{l+m} \left(u \cos \frac{1}{2}\alpha + v \sin \frac{1}{2}\alpha \right) H_{l-m} \left(v \cos \frac{1}{2}\alpha - u \sin \frac{1}{2}\alpha \right)}{\sqrt{(l+m)!(l-m)!}} = \sum_{m'=-l}^l d_{m' m}^l(\alpha) \frac{H_{l+m'}(u) H_{l-m'}(v)}{\sqrt{(l+m')!(l-m')!}}. \quad (24)$$

(An alternative derivation of this relation can be found in Ref. 15.)

The two-dimensional hydrogen atom is also known to be related to the two-dimensional isotropic harmonic oscillator (TIHO) [8–10, 16, 17]. The normalized separable solutions of the Schrödinger equation for the TIHO in Cartesian coordinates are, up to a phase factor,

$$\psi_{n_1 n_2}(x, y) = \sqrt{\frac{M\omega}{\hbar\pi 2^{n_1+n_2} n_1! n_2!}} e^{-M\omega(x^2+y^2)/2\hbar} H_{n_1} \left(\sqrt{\frac{M\omega}{\hbar}} x \right) H_{n_2} \left(\sqrt{\frac{M\omega}{\hbar}} y \right)$$

($n_1, n_2 = 0, 1, \dots$) and the corresponding energy eigenvalue is $(n_1 + n_2 + 1)\hbar\omega$. Hence, from Eq. (20) we find that

$$\sqrt{\frac{(l-m)! M\omega}{(l+m)! \hbar\pi}} e^{-M\omega r^2/2\hbar} r^{2m} e^{2im\varphi} L_{l-m}^{2m} \left(\frac{M\omega r^2}{\hbar} \right) = \sum_{m'=-l}^l (-1)^{m'-m} i^{l-m'} d_{m m'}^l \left(\frac{\pi}{2} \right) \psi_{l+m', l-m'}(x, y), \quad (25)$$

is a normalized separable solution of the Schrödinger equation of the TIHO in polar coordinates with energy $(l+1)\hbar\omega$ (with $l = 0, 1/2, 1, \dots$) and Eq. (25) gives the relationship between the separable solutions of the Schrödinger equation of the TIHO in polar and Cartesian coordinates.

4. Concluding remarks

We have shown that the mapping given by Eqs. (10) and (11) allows us to make use of some well-known results about the rotation of the spherical harmonics in order to find the expression of the separable solutions (2) in terms of the separable solutions (7) and viceversa. Following this procedure, identities like Eqs. (16), (20), (21), and (24) are readily obtained. It may be noticed, for instance, that it is not even evident that the result of the integration in the right-hand side of Eq. (16) is the product of two separate functions of u and v and it seems that a direct proof of the validity of Eq. (16) would be very difficult.

The solutions of the Schrödinger equation for the two-dimensional hydrogen atom with zero energy can be related

to the solutions of the Helmholtz equation in the Euclidean plane, $\nabla^2 \Phi = -\Phi$, by means of expressions analogous to Eqs. (10) and (11) [5]. In this case, the separable solutions of $\nabla^2 \Phi = -\Phi$ that are eigenfunctions of the linear momentum operators P_x and P_y are of the form $e^{i\mathbf{s}\cdot(x,y)}$ with $|\mathbf{s}| = 1$ and correspond to the separable solutions of the Schrödinger equation (1) with zero energy in parabolic coordinates, while the functions of the form $J_m(\rho)e^{im\theta}$ are separable solutions of $\nabla^2 \Phi = -\Phi$ in polar coordinates (ρ, θ) that correspond to the separable solutions of Eq. (1) with $E = 0$ in polar coordinates. The analog of Eq. (15) is given by $e^{i\mathbf{s}\cdot(x,y)} = \sum_{m=-\infty}^{\infty} i^m e^{-im\alpha} J_m(\rho) e^{im\theta}$, where $\mathbf{s} = (\cos \alpha, \sin \alpha)$.

It is an interesting fact that even though Eq. (24) corresponds to rotations in the plane and, hence, to an action of

the group SO(2), the coefficients appearing in Eq. (24) come from the representation of SO(3) given by the D functions. Even if one is not considering the hydrogen atom with nega-

tive energy or the TIHO (which have SO(3) and SU(2) symmetry, respectively), the Hermite polynomials turn out to be related to the rotation group SO(3).

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