The hydrogen atom via the four-dimensional spherical harmonics

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Using the fact that the Schrödinger equation for the stationary states of the hydrogen atom is equivalent to an integral equation on the unit sphere in a four-dimensional space, the eigenvalues, the eigenfunctions, and a dynamical symmetry group for this problem are obtained from the four-dimensional spherical harmonics and the group of rotations on the sphere. It is shown that the four-dimensional spherical harmonics separable in Euler angles correspond to solutions of the time-independent Schrödinger equation that are separable in parabolic coordinates.

Keywords: Hydrogen atom; hidden symmetries; four-dimensional spherical harmonics.

Usando el hecho de que la ecuación de Schrödinger para los estados estacionarios del átomo de hidrógeno es equivalente a una ecuación integral sobre la esfera de radio 1 en un espacio de dimensión cuatro, los eigenvalores, las eigenfunciones y un grupo de simetría dinámica para este problema se obtienen a partir de los armónicos esféricos en dimensión cuatro y el grupo de rotaciones sobre la esfera. Se muestra que los armónicos esféricos en dimensión cuatro separables en ángulos de Euler corresponden a soluciones de la ecuación de Schrödinger que son separables en coordenadas parabólicas.

Descriptores: Átomo de hidrógeno; simetrías ocultas; armónicos esféricos en dimensión cuatro.

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1. Introduction

The problem of a charged spinless particle in a Coulomb field, in the framework of nonrelativistic quantum mechanics, which in what follows will be referred to as the problem of the hydrogen atom, is perhaps the favorite example of a system with hidden symmetries. The "obvious" rotational invariance of the Hamiltonian implies that the energy eigenvalues cannot depend on the magnetic quantum number, m, but actually the energy eigenvalues do not depend on m nor on the azimuthal quantum number, l.

This "accidental" degeneracy is related to the existence of operators (the quantum analogs of the components of the Runge–Lenz vector) that, just like the components of the angular momentum, commute with the Hamiltonian. In fact, the components of the angular momentum and those of the analog of the Runge–Lenz vector, restricted to the subspace $H = E$, with $E < 0$, are the basis of a Lie algebra isomorphic to that of the group of rotations in four dimensions, SO(4) [1–4]. One remarkable feature of the hydrogen atom is that, by a suitable change of variables, the time-independent Schrödinger equation can be expressed in such a form that the invariance under rotations in a four-dimensional space becomes obvious [5–7].

In this paper we use the fact that the time-independent Schrödinger equation for the hydrogen atom can be transformed into an equation on the unit sphere in the four-dimensional Euclidean space to find the energy levels and the stationary states explicitly, obtaining a relationship between the generating function of the generalized associated Legendre functions and that of the associated Laguerre polynomials. We also show that the Runge–Lenz vector can be derived from the expressions for the generators of rotations in a four-dimensional space. A similar treatment for the two-dimensional hydrogen atom has been given in Refs. 8 and 9.

In Sec. 2 the Schrödinger equation for the stationary states of the hydrogen atom is expressed as an integral equation over the unit sphere in the four-dimensional Euclidean space, which makes obvious a hidden SO(4) symmetry of the original equation (see also Refs. 5 and 7). In Sec. 3, some elementary facts about the four-dimensional spherical harmonics are given, showing that these functions are the solutions of the integral equation given in Sec. 2 (see also Ref. 7). In Sec. 4, following a procedure similar to that employed in Ref. 8, we find the explicit expression for the wavefunctions for the stationary states of the hydrogen atom in spherical coordinates, starting from the four-dimensional spherical harmonics in the spherical coordinates of $\mathbb{R}^4$. In Sec. 5 it is explicitly shown that the infinitesimal generators of the rotations in $\mathbb{R}^4$ correspond to the components of the angular momentum and the quantum analog of the Runge–Lenz vector (*cf.* Ref. 7). In Sec. 6 it is shown that the four-dimensional spherical harmonics expressed in terms of Euler angles correspond to the wavefunctions in parabolic coordinates (*cf.* Ref. 7), which leads to a relation between the Wigner D functions (or the Jacobi polynomials) and products of associated Laguerre polynomials.

2. Symmetry of the Schrödinger equation

By expressing the solution of the time-independent Schrödinger equation for the hydrogen atom

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

where k is a positive constant, as a Fourier transform,

$$\psi(\mathbf{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int \Phi(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}d^3\mathbf{p}, \tag{2}$$

using the fact that $\int (1/r)e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar}d^3\mathbf{r} = 4\pi\hbar^2/|\mathbf{p}-\mathbf{p}'|^2$, one obtains the integral equation

$$(p^2 - 2ME)\Phi(\mathbf{p}) = \frac{Mk}{\pi^2\hbar}\int \frac{\Phi(\mathbf{p}')}{|\mathbf{p}-\mathbf{p}'|^2}d^3\mathbf{p}', \tag{3}$$

where $p \equiv |\mathbf{p}|$. In what follows we shall consider bound states only, for which $E < 0$. Then, by means of the stereographic projection, the vector $\mathbf{p}$ can be replaced by a *unit* vector $\mathbf{n} = (n_1, n_2, n_3, n_4)$ according to [5,7]

$$\mathbf{p} = (p_x, p_y, p_z) = p_0\frac{(n_1, n_2, n_3)}{1 - n_4}, \tag{4}$$

where

$$p_0 \equiv \sqrt{-2ME}. \tag{5}$$

Under the correspondence between $\mathbf{p}$ and $\mathbf{n}$ given by Eq. (4), the three-dimensional space is mapped into the unit sphere in $\mathbb{R}^4$.

Defining the spherical coordinates in $\mathbb{R}^4$, (r, χ, θ, ϕ), by means of

$$\begin{aligned}
x_1 &= r\sin\chi\sin\theta\cos\phi, \\
x_2 &= r\sin\chi\sin\theta\sin\phi, \\
x_3 &= r\sin\chi\cos\theta, \\
x_4 &= r\cos\chi, \tag{6}
\end{aligned}$$

according to Eq. (4), the vector $\mathbf{p}$ can be expressed in terms of the spherical coordinates of the unit vector $\mathbf{n}$ as

$$\begin{aligned}
\mathbf{p} &= \frac{p_0}{1 - \cos\chi}(\sin\chi\sin\theta\cos\phi, \sin\chi\sin\theta\sin\phi, \sin\chi\cos\theta) \\
&= p_0\cot(\chi/2)(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta); \tag{7}
\end{aligned}$$

therefore,

$$p = p_0\cot(\chi/2),$$

$$d^3\mathbf{p} = \frac{p_0^3\, d^3\Omega}{(1 - n_4)^3} = \tfrac{1}{8}p_0^3\csc^6(\chi/2)\, d^3\Omega, \tag{8}$$

where $d^3\Omega = \sin^2\chi\sin\theta\, d\chi d\theta d\phi$ is the solid angle element (or volume element) of S^3, the unit sphere in $\mathbb{R}^4$, and

$$\begin{aligned}
|\mathbf{p} - \mathbf{p}'| &= \frac{p_0|\mathbf{n} - \mathbf{n}'|}{(1 - n_4)^{1/2}(1 - n_4')^{1/2}} \\
&= \tfrac{1}{2}p_0\csc(\chi/2)\csc(\chi'/2)|\mathbf{n} - \mathbf{n}'|, \tag{9}
\end{aligned}$$

where $\mathbf{n}'$ is the unit vector corresponding to $\mathbf{p}'$ according to Eq. (4). Substituting Eqs. (5), (8) and (9) into Eq. (3) one gets

$$\csc^4(\chi/2)\Phi(\mathbf{n}) = \frac{Mk}{2\pi^2\hbar p_0}\int \frac{\csc^4(\chi'/2)\Phi(\mathbf{n}')}{|\mathbf{n} - \mathbf{n}'|^2}d^3\Omega';$$

hence, by introducing

$$\begin{aligned}
\hat{\Phi}(\mathbf{n}) &\equiv 2^{-2}p_0^{3/2}\csc^4(\chi/2)\Phi(\mathbf{n}) \\
&= p_0^{3/2}\left[\frac{p^2 + p_0^2}{2p_0^2}\right]^2\Phi(\mathbf{p}), \tag{10}
\end{aligned}$$

one obtains the integral equation

$$\hat{\Phi}(\mathbf{n}) = \frac{Mk}{2\pi^2\hbar p_0}\int \frac{\hat{\Phi}(\mathbf{n}')}{|\mathbf{n} - \mathbf{n}'|^2}d^3\Omega'. \tag{11}$$

The constant factors included in definition (10) are chosen in such a way that $\hat{\Phi}$ is dimensionless and $\hat{\Phi}$ is normalized over the sphere if and only if ψ is normalized over the space [7].

Since the distance between points on the sphere and the solid angle element $d^3\Omega$ are invariant under rotations of the sphere, Eq. (11) is explicitly invariant under these transformations, thus showing that the rotation group SO(4) is a symmetry group of the original equation (1) for $E < 0$. As we shall show in the following section, the solutions of the integral equation (11) are the four-dimensional spherical harmonics [7]. Substituting Eqs. (7), (8) and (10) into Eq. (2), one obtains the wave function $\psi(\mathbf{r})$ in terms of the solution of the integral equation (11)

$$\psi(x, y, z) = \frac{1}{2}\left(\frac{p_0}{2\pi\hbar}\right)^{3/2}\int \hat{\Phi}(\chi, \theta, \phi)\csc^2(\chi/2)$$

$$\times e^{ip_0\cot(\chi/2)(x\sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta)/\hbar}d^3\Omega. \tag{12}$$

3. Energy eigenvalues

The integral equation (11) contains the inverse of the *squared* distance between two points of $\mathbb{R}^4$, which can be expanded with the aid of the generating function of the (generalized) Legendre polynomials in four dimensions [10]:

$$\frac{1}{1 - 2xt + t^2} = \sum_{n=0}^{\infty}(n + 1)P_{n,4}(x)t^n, \tag{13}$$

where $P_{n,4}$ denotes the Legendre polynomial of order n in four dimensions. These polynomials are related to the Tchebichef polynomials of the second kind, U_n, the ultraspherical, $P_n^{(1)}$, or Gegenbauer polynomials, C_n^1, by

$$(n + 1)P_{n,4}(x) = U_n(x) = P_n^{(1)}(x) = C_n^1(x) \tag{14}$$

(see, for example, Refs. 11 and 12).

As in the case of the (usual) Legendre polynomials in three dimensions, the generalized Legendre polynomials

$P_{n,4}$ are the regular angular parts of the axially symmetric solutions of the Laplace equation [10]. In terms of the spherical coordinates of $\mathbb{R}^4$, defined by Eq. (6), the solutions of the Laplace equation in four dimensions that depend on r and χ only are of the form

$$\sum_{n=0}^{\infty}(A_n r^n + B_n r^{-n-2})P_{n,4}(\cos\chi),$$

where the A_n, B_n are constants. The Laplace operator of $\mathbb{R}^4$ is given by

$$\nabla^2 = \frac{1}{r^3}\frac{\partial}{\partial r}\left(r^3\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left\{\frac{1}{\sin^2\chi}\frac{\partial}{\partial\chi}\left(\sin^2\chi\frac{\partial}{\partial\chi}\right)\right.$$
$$\left. + \frac{1}{\sin^2\chi}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right\},$$

and one finds that the solutions of the Laplace equation are of the form

$$\sum_{n=0}^{\infty}\sum_{l=0}^{n}\sum_{m=-l}^{l}(A_{nlm}r^n + B_{nlm}r^{-n-2})P_{n,4}^l(\cos\chi)Y_{lm}(\theta,\phi),$$

where the A_{nlm}, B_{nlm} are constants, the $P_{n,4}^l$ are the generalized associated Legendre functions

$$P_{n,4}^l(x) \equiv (1-x^2)^{l/2}\frac{\mathrm{d}^l}{\mathrm{d}x^l}P_{n,4}(x) \qquad (15)$$

$(l = 0, 1, \ldots, n)$ and the Y_{lm} are the usual spherical harmonics.

The functions

$$\mathcal{Y}_{nlm}(\chi,\theta,\phi) = N_{nl}P_{n,4}^l(\cos\chi)Y_{lm}(\theta,\phi)$$

are four-dimensional spherical harmonics. N_{nl} is a normalization constant such that

$$1 = \int |\mathcal{Y}_{nlm}(\chi,\theta,\phi)|^2 \mathrm{d}^3\Omega$$

$$= \int_0^{\pi} |N_{nl}P_{n,4}^l(\cos\chi)|^2 \sin^2\chi\,\mathrm{d}\chi.$$

The spherical harmonics $\mathcal{Y}_{nlm}$ satisfy the addition theorem

$$P_{n,4}(\cos\gamma) = \frac{2\pi^2}{(n+1)^2}$$
$$\times \sum_{l=0}^{n}\sum_{m=-l}^{l}\mathcal{Y}_{nlm}^*(\chi',\theta',\phi')\mathcal{Y}_{nlm}(\chi,\theta,\phi),$$

where γ is the angle between the directions defined by (χ',θ',ϕ') and (χ,θ,ϕ) (the factor $2\pi^2$ is the solid angle of the sphere S^3, while $(n+1)^2$ is the number of terms on the right hand side); therefore,

$$\frac{1}{|\mathbf{n}-\mathbf{n}'|^2} = 2\pi^2$$
$$\times \sum_{n=0}^{\infty}\sum_{l=0}^{n}\sum_{m=-l}^{l}\frac{1}{n+1}\mathcal{Y}_{nlm}^*(\chi',\theta',\phi')\mathcal{Y}_{nlm}(\chi,\theta,\phi), \quad (16)$$

where (χ,θ,ϕ) and (χ',θ',ϕ') are the spherical coordinates of $\mathbf{n}$ and $\mathbf{n}'$, respectively.

The integral equation (11) can be easily solved using the fact that the spherical harmonics form a complete set for the functions defined on the sphere; therefore the function $\hat{\Phi}$ can be expanded in the form

$$\hat{\Phi}(\chi,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{l=0}^{n}\sum_{m=-l}^{l} a_{nlm}\mathcal{Y}_{nlm}(\chi,\theta,\phi), \qquad (17)$$

where the a_{nlm} are some constants. Substituting Eq. (17) into Eq. (11), and making use of the expansion (16) and of the orthonormality of the spherical harmonics, one obtains

$$\sum_{n=0}^{\infty}\sum_{l=0}^{n}\sum_{m=-l}^{l}\left[1 - \frac{Mk}{\hbar p_0(n+1)}\right] a_{nlm}\mathcal{Y}_{nlm}(\chi,\theta,\phi) = 0,$$

which implies that, in order to have a nontrivial solution, $Mk/(\hbar p_0)$ must be a natural number; hence, according to Eq. (5),

$$E = -\frac{Mk^2}{2\hbar^2(n+1)^2} \qquad (18)$$

$(n = 0, 1, 2, \ldots)$, which coincides with the expression obtained in the standard manner, identifying $n+1$ with the *principal quantum number* (usually denoted by n). Furthermore, for the value of n appearing in Eq. (18), the $(n+1)^2$ coefficients a_{nlm} $(l = 0, 1, \ldots, n; m = -l, -l+1, \ldots, l)$ are arbitrary and $a_{n'lm} = 0$ for all $n' \neq n$. Thus, the degeneracy of the energy level (18) is $(n+1)^2$; all the spherical harmonics of order n are solutions of Eq. (11), corresponding to the energy (18).

4. Explicit form of the wavefunctions

According to the preceding results, the solutions of the Schrödinger equation (1), for $E < 0$, are given by Eq. (12),

$$\psi(x,y,z) = 2\left(\frac{p_0}{2\pi\hbar}\right)^{3/2}\int \hat{\Phi}(\chi,\theta,\phi)\cos^2(\chi/2)$$
$$\times e^{ip_0\cot(\chi/2)(x\sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta)/\hbar}\mathrm{d}\chi$$
$$\times \sin\theta\mathrm{d}\theta\mathrm{d}\phi, \qquad (19)$$

where $\hat{\Phi}(\chi,\theta,\phi)$ is a four-dimensional spherical harmonic. Hence, with $\hat{\Phi} = \mathcal{Y}_{nlm}$, making use of the expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l j_l(kr)Y_{lm}^*(\hat{k})Y_{lm}(\hat{r}),$$

where $\hat{k}$ and $\hat{r}$ are unit vectors in the direction of **k** and **r**, respectively (see, *e.g.*, Ref. 13), and the orthonormality of the usual spherical harmonics, we have

$$\psi_{nlm}(\mathbf{r}) = 8\pi \left(\frac{p_0}{2\pi\hbar}\right)^{3/2} N_{nl} \mathrm{i}^l$$
$$\times \left[\int\limits_0^\pi P_{n,4}^l(\cos\chi) j_l\Big((p_0 r/\hbar)\cot(\chi/2)\Big)\right.$$
$$\left.\times \cos^2(\chi/2)\mathrm{d}\chi\right] Y_{lm}(\hat{r}), \tag{20}$$

which shows that the separable spherical harmonics in the spherical coordinates of $\mathbb{R}^4$ correspond to separable eigen-

functions of the Hamiltonian of the hydrogen atom in the spherical coordinates of $\mathbb{R}^3$.

The recurrence relation for the ultraspherical polynomials [11]

$$\frac{\mathrm{d}}{\mathrm{d}x} P_{n+1}^{(1)}(x) - \frac{\mathrm{d}}{\mathrm{d}x} P_{n-1}^{(1)}(x) = 2(n+1) P_n^{(1)}(x)$$

leads to

$$2(n+1)^2 \sin\chi P_{n,4}^l(\cos\chi) = (n+2) P_{n+1,4}^{l+1}(\cos\chi)$$
$$-n P_{n-1,4}^{l+1}(\cos\chi)$$

[see Eqs. (14) and (15)]; hence, introducing an auxiliary parameter t, we find that, for fixed l,

$$\sum_{n=l}^\infty 2(n+1)^2 P_{n,4}^l(\cos\chi) t^{n+1} = \frac{1}{\sin\chi}\left[\sum_{n=l}^\infty (n+2) P_{n+1,4}^{l+1}(\cos\chi) t^{n+1} - \sum_{n=l+2}^\infty n P_{n-1,4}^{l+1}(\cos\chi) t^{n+1}\right]$$
$$= \frac{1}{\sin\chi}\left[\sum_{n=l+1}^\infty (n+1) P_{n,4}^{l+1}(\cos\chi) t^n - \sum_{n=l+1}^\infty (n+1) P_{n,4}^{l+1}(\cos\chi) t^{n+2}\right]$$
$$= \frac{1-t^2}{\sin\chi} \sum_{n=l+1}^\infty (n+1) P_{n,4}^{l+1}(\cos\chi) t^n$$
$$= \frac{(1-t^2)}{\sin\chi} \frac{(l+1)!(2t)^{l+1}\sin^{l+1}\chi}{(1-2t\cos\chi+t^2)};$$

the last equality is obtained by differentiating $l+1$ times the generating function (13) and making use of the definition (15).

Then, denoting by $R_{nl}(r)$ the integral between brackets in Eq. (20), we have

$$\sum_{n=l}^\infty 2(n+1)^2 R_{nl} t^{n+1} = \int\limits_0^\pi \frac{(1-t^2)}{\sin\chi} \frac{(l+1)!(2t)^{l+1}\sin^{l+1}\chi}{(1-2t\cos\chi+t^2)} j_l\Big((p_0 r/\hbar)\cot(\chi/2)\Big) \cos^2(\chi/2)\mathrm{d}\chi$$

and, by replacing the variable χ by $\mu \equiv \cot(\chi/2)$ and using the relation $j_l(x) = \sqrt{\dfrac{\pi}{2x}} J_{l+1/2}(x)$, one finds that

$$\sum_{n=l}^\infty 2(n+1)^2 R_{nl} t^{n+1} = (4t)^{l+1} \frac{(1-t^2)(l+1)!}{(1-t)^{2l+4}} \sqrt{\frac{\pi\hbar}{2p_0 r}} \int\limits_0^\infty \frac{\mu^{l+3/2} J_{l+1/2}\Big((p_0 r/\hbar)\mu\Big)}{\left[\mu^2 + \left(\frac{1+t}{1-t}\right)^2\right]^{l+2}} \mathrm{d}\mu.$$

The last integral has been calculated in Ref. 8:

$$\int\limits_0^\infty \frac{(2m+1)!}{2^m m!} \frac{s x^{m+1} J_m(xy)}{(x^2+s^2)^{m+3/2}} \mathrm{d}x = y^m \mathrm{e}^{-ys},$$

hence, making use of the duplication formula of the Gamma function,

$$\sum_{n=l}^\infty 2(n+1)^2 R_{nl} t^{n+1} = 2^l \pi t^{l+1} (p_0 r/\hbar)^l \mathrm{e}^{-p_0 r/\hbar} \frac{\mathrm{e}^{-(2p_0 r/\hbar)t/(1-t)}}{(1-t)^{2l+2}}.$$

Recalling that

$$\frac{e^{-xz/(1-z)}}{(1-z)^{k+1}} = \sum_{n=0}^{\infty} L_n^k(x) z^n,$$

where L_n^k denote the associated Laguerre polynomials (see, *e.g.*, Ref. 10), we obtain

$$\sum_{n=l}^{\infty} 2(n+1)^2 R_{nl} t^{n+1} = \pi (2p_0 r/\hbar)^l e^{-p_0 r/\hbar}$$

$$\times \sum_{n=l}^{\infty} L_{n-l}^{2l+1}(2p_0 r/\hbar) t^{n+1};$$

therefore,

$$R_{nl}(r) = \frac{\pi}{2(n+1)^2}(2p_0 r/\hbar)^l e^{-p_0 r/\hbar} L_{n-l}^{2l+1}(2p_0 r/\hbar),$$

and substituting this result into Eq. (20) one finds that the wavefunction corresponding to the spherical harmonic $\mathcal{Y}_{nlm}$ is given by

$$\psi_{nlm}(r,\theta,\phi) = \left(\frac{p_0}{2\pi\hbar}\right)^{3/2} \frac{4\pi^2 N_{nl} i^l}{(n+1)^2}(2p_0 r/\hbar)^l$$

$$\times e^{-p_0 r/\hbar} L_{n-l}^{2l+1}(2p_0 r/\hbar) Y_{lm}(\theta,\phi). \quad (21)$$

(Recall that n differs by one unit from the usual principal quantum number.)

5. The generators of the symmetry

As we have shown, Eq. (12) gives a correspondence between the solutions of the integral equation (11) and those of the

Schrödinger equation (1). As remarked above, Eq. (11) is explicitly invariant under the rotations of the sphere and a set of generators of these rotations are the six operators

$$\hat{L}_j \equiv -i\hbar \varepsilon_{jkm} x_k \partial_m, \quad \hat{K}_j \equiv -i\hbar(x_j \partial_4 - x_4 \partial_j) \quad (22)$$

$(i,j,k,\ldots = 1,2,3)$, expressed in terms of Cartesian coordinates (x_1, x_2, x_3, x_4), which satisfy the commutation relations

$$[\hat{L}_i, \hat{L}_j] = i\hbar \varepsilon_{ijk} \hat{L}_k,$$

$$[\hat{L}_i, \hat{K}_j] = i\hbar \varepsilon_{ijk} \hat{K}_k,$$

$$[\hat{K}_i, \hat{K}_j] = i\hbar \varepsilon_{ijk} \hat{L}_k. \quad (23)$$

The ˆ indicates that these operators act on functions defined on the sphere.

In terms of the spherical coordinates of $\mathbb{R}^4$, the operators $\hat{L}_i$ and $\hat{K}_i$ are given explicitly by

$$\hat{L}_1 = i\hbar \left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right),$$

$$\hat{L}_2 = i\hbar \left(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right),$$

$$\hat{L}_3 = -i\hbar \frac{\partial}{\partial\phi}, \quad (24)$$

and

$$\hat{K}_1 = i\hbar \left(\sin\theta \cos\phi \frac{\partial}{\partial\chi} + \cot\chi \cos\theta \cos\phi \frac{\partial}{\partial\theta} - \cot\chi \csc\theta \sin\phi \frac{\partial}{\partial\phi} \right),$$

$$\hat{K}_2 = i\hbar \left(\sin\theta \sin\phi \frac{\partial}{\partial\chi} + \cot\chi \cos\theta \sin\phi \frac{\partial}{\partial\theta} + \cot\chi \csc\theta \cos\phi \frac{\partial}{\partial\phi} \right), \quad (25)$$

$$\hat{K}_3 = i\hbar \left(\cos\theta \frac{\partial}{\partial\chi} - \cot\chi \sin\theta \frac{\partial}{\partial\theta} \right).$$

By means of correspondence (12) we can find the operators on the wave functions that correspond to the generators of rotations (24) and (25). From Eqs. (2), (7) and (10) it follows that the function $\hat{\Phi}$ on the sphere corresponding to a wave function $\psi(\mathbf{r})$ is

$$\hat{\Phi}(\mathbf{n}) = \frac{p_0^{3/2} \sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \psi(\mathbf{r}) e^{-ip_0 \cot(\chi/2)(x\sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta)/\hbar} d^3\mathbf{r}. \quad (26)$$

Hence, by applying, for example, the operator $\hat{L}_3$ to both sides of the last equation we obtain

$$\hat{L}_3 \hat{\Phi} = \frac{p_0^{3/2} \sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \psi(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} p_0 \cot(\chi/2)(x\sin\theta\sin\phi - y\sin\theta\cos\phi) d^3\mathbf{r}$$

$$= \frac{p_0^{3/2} \sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \psi(\mathbf{r}) i\hbar(x\partial_y - y\partial_x) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} d^3\mathbf{r}$$

$$= \frac{p_0^{3/2} \sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int [-i\hbar(x\partial_y - y\partial_x)\psi(\mathbf{r})] e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} d^3\mathbf{r},$$

after integrating by parts. Thus, under the correspondence between the functions $\hat{\Phi}$, defined on the sphere, and the wavefunctions $\psi(\mathbf{r})$, given by Eq. (26), $\hat{L}_3$ corresponds to the operator $-\mathrm{i}\hbar(x\partial_y - y\partial_x)$, which is just the z-component of the angular momentum. In a similar way, one finds that the operators $\hat{L}_1$ and $\hat{L}_2$ correspond to the x- and y-component of the angular momentum.

On the other hand, by applying the operator $\hat{K}_3$ to both sides of Eq. (26) we obtain

$$\hat{K}_3\hat{\Phi} = -\frac{p_0^{3/2}\sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \psi(\mathbf{r})\mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar}\{2\mathrm{i}\hbar\cot(\chi/2)\cos\theta + p_0\cot^2(\chi/2)[x\sin\theta\cos\theta\cos\phi$$

$$+ y\sin\theta\cos\theta\sin\phi + z(\cos^2\theta - \sin^2\theta)/2] + p_0 z/2\}\mathrm{d}^3\mathbf{r}$$

$$= \frac{p_0^{1/2}\sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \psi(\mathbf{r})\hbar^2[2\partial_z + x\partial_x\partial_z + y\partial_y\partial_z - (z/2)(\partial_x^2 + \partial_y^2 - \partial_z^2) - p_0^2 z/(2\hbar^2)]\mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar}\mathrm{d}^3\mathbf{r}$$

$$= \frac{p_0^{1/2}\sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \{\hbar^2[\partial_z + x\partial_x\partial_z + y\partial_y\partial_z - (z/2)(\partial_x^2 + \partial_y^2 - \partial_z^2) - p_0^2 z/(2\hbar^2)]\psi(\mathbf{r})\} \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar}\mathrm{d}^3\mathbf{r},$$

where we have integrated by parts. Assuming that ψ satisfies Eq. (1), the last term of the expression between brackets can be replaced according to $p_0^2\psi = \hbar^2\nabla^2\psi + (2Mk/r)\psi$, and one finds that

$$\hat{K}_3\hat{\Phi} = \frac{p_0^{3/2}\sin^{-4}(\chi/2)}{4(2\pi\hbar)^{3/2}} \int \left\{\frac{1}{p_0}\left[\frac{1}{2}(p_x L_y + L_y p_x - p_y L_x - L_x p_y) - \frac{Mkz}{r}\right]\psi(\mathbf{r})\right\} \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar}\,\mathrm{d}^3\mathbf{r},$$

which is of the form (26), with ψ replaced by $(1/p_0)A_z\psi$, where A_z is the z-component of the quantum analog of the Runge–Lenz vector

$$\mathbf{A} = \frac{1}{2}(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}) - \frac{Mk\mathbf{r}}{r}, \tag{27}$$

and $\mathbf{p}$ and $\mathbf{L}$ are the usual linear and angular momentum operators. Thus, under the correspondence given by Eq. (26), $\hat{K}_3$ corresponds to $(1/p_0)A_z$.

In a similar manner, one finds that the operators $\hat{K}_1$ and $\hat{K}_2$ correspond to $(1/p_0)A_x$ and $(1/p_0)A_y$, respectively, restricted to the subspace formed by the states with a fixed energy $E = -p_0^2/(2M)$. Thus, the Runge–Lenz vector (27) is associated with the manifest SO(4) symmetry of Eq. (11), and the operators L_i, $(1/p_0)A_i$, obey the same commutation relations as $\hat{L}_i$, $\hat{K}_i$, namely [see Eq. (23)]

$$[L_i, L_j] = \mathrm{i}\hbar\varepsilon_{ijk}L_k,$$

$$[L_i, A_j] = \mathrm{i}\hbar\varepsilon_{ijk}A_k,$$

$$[A_i, A_j] = -\mathrm{i}\hbar\varepsilon_{ijk}2ME L_k. \tag{28}$$

Note that a similar procedure can be followed to find the action on the wavefunctions of a finite transformation belonging to SO(4).

6. Separation of variables in parabolic coordinates

As is well known, the Schrödinger equation (1) admits separable solutions in the parabolic coordinates

$$x = 2\xi\eta\cos\phi, \quad y = 2\xi\eta\sin\phi, \quad z = \xi^2 - \eta^2 \tag{29}$$

(see also Ref. 2). In fact, in these coordinates, the Schrödinger equation (1) reads

$$-\frac{\hbar^2}{2M}\frac{1}{4\xi\eta(\xi^2+\eta^2)}\left[\eta\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) + \xi\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)\right.$$

$$\left. + \frac{\xi^2+\eta^2}{\xi\eta}\frac{\partial^2}{\partial\phi^2}\right]\psi - \frac{k}{\xi^2+\eta^2}\psi = E\psi$$

and looking for solutions of the form $\psi(\xi,\eta,\phi) = f(\xi)g(\eta)h(\phi)$, one obtains the separate equations

$$\frac{1}{\xi}\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\xi\frac{\mathrm{d}f}{\mathrm{d}\xi}\right) + \left(\frac{4Mk}{\hbar^2} + \frac{8ME\xi^2}{\hbar^2} - \frac{m^2}{\xi^2}\right)f = \lambda f,$$

$$\frac{1}{\eta}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\eta\frac{\mathrm{d}g}{\mathrm{d}\eta}\right) + \left(\frac{4Mk}{\hbar^2} + \frac{8ME\eta^2}{\hbar^2} - \frac{m^2}{\eta^2}\right)g = -\lambda g,$$

$$\frac{\mathrm{d}^2 h}{\mathrm{d}\phi^2} = -m^2 h, \tag{30}$$

where m is an integer and λ is another separation constant. By combining Eqs. (30), so as to eliminate E, one finds that

$$\frac{1}{\xi^2+\eta^2}\left[\frac{\eta^2}{\xi}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) - \frac{\xi^2}{\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)\right.$$

$$\left. - \frac{\xi^4-\eta^4}{\xi^2\eta^2}\frac{\partial^2}{\partial\phi^2} - \frac{4Mk}{\hbar^2}(\xi^2-\eta^2)\right]\psi = \lambda\psi$$

and a straightforward computation shows that the operator on the left-hand side of this equation is $4A_z/\hbar^2$. Hence,

the separable solutions of the Schrödinger equation (1) in parabolic coordinates are eigenfunctions of L_z and A_z and correspond, via the relation (26), to eigenfunctions of $\hat{L}_3$ and $\hat{K}_3$. As we shall show below, such eigenfunctions are the four-dimensional spherical harmonics separable in Euler angles (see also Ref. 7).

Since by means of an appropriate rotation about the origin in $\mathbb{R}^4$, one can map the $x_1 x_2$-plane onto any other two-plane, all the operators $\hat{L}_i$ and $\hat{K}_i$ are unitarily related to each other and, therefore, have the same spectrum. Hence, for a given value of n (the order of the four-dimensional spherical harmonics), the eigenvalues of $\hat{K}_3$ are of the form $m\hbar$, where $m = -n, -n + 1, \ldots, n$, with degeneracies $n + 1 - |m|$, as in the case of $\hat{L}_3$.

We conclude that, for a given value of n, the separation constant λ, appearing in Eqs. (30), can take on the values $\lambda = 4p_0 q/\hbar$, with $q = -n, -n + 1, \ldots, n$, and, by making use of the expression (18) for E, one obtains, for example,

$$\frac{1}{u}\frac{\mathrm{d}}{\mathrm{d}u}\left(u\frac{\mathrm{d}f}{\mathrm{d}u}\right) + \left[4(n+1) - 4u^2 - \frac{m^2}{u^2} - 4q\right]f = 0,$$

where $u \equiv \sqrt{p_0/\hbar}\,\xi$. The solution of this last equation is given in terms of associated Laguerre polynomials by

$$f = u^{|m|}\mathrm{e}^{-u^2}L^{|m|}_{(n-|m|-q)/2}(2u^2)$$

or, equivalently,

$$f(\xi) = (\sqrt{p_0/\hbar}\,\xi)^{|m|}\mathrm{e}^{-p_0\xi^2/\hbar}L^{|m|}_{(n-|m|-q)/2}(2p_0\xi^2/\hbar) \quad (31)$$

and, therefore,

$$g(\eta) = (\sqrt{p_0/\hbar}\,\eta)^{|m|}\mathrm{e}^{-p_0\eta^2/\hbar}L^{|m|}_{(n-|m|+q)/2}(2p_0\eta^2/\hbar). \quad (32)$$

In place of the spherical coordinates of $\mathbb{R}^4$ defined in (6), we can also parameterize the sphere by means of the Euler angles α, β, γ, defined by

$$x_1 = \cos(\beta/2)\cos\alpha,$$
$$x_2 = \cos(\beta/2)\sin\alpha,$$
$$x_3 = \sin(\beta/2)\cos\gamma,$$
$$x_4 = \sin(\beta/2)\sin\gamma, \quad (33)$$

with $0 \leqslant \alpha \leqslant 2\pi$, $0 \leqslant \beta \leqslant \pi$, $0 \leqslant \gamma \leqslant 2\pi$. Then one readily finds that the standard metric of $\mathbb{R}^4$, restricted to the sphere, is

$$(\mathrm{d}x_1)^2 + (\mathrm{d}x_2)^2 + (\mathrm{d}x_3)^2 + (\mathrm{d}x_4)^2 = \cos^2(\beta/2)(\mathrm{d}\alpha)^2$$
$$+ \tfrac{1}{4}(\mathrm{d}\beta)^2 + \sin^2(\beta/2)(\mathrm{d}\gamma)^2;$$

therefore, the Laplace–Beltrami operator of the sphere, Δ_{S^3}, is given by

$$\Delta_{\mathrm{S}^3}f = \frac{1}{\cos^2(\beta/2)}\frac{\partial^2 f}{\partial\alpha^2} + \frac{4}{\sin\beta}\frac{\partial}{\partial\beta}\left(\sin\beta\frac{\partial f}{\partial\beta}\right)$$
$$+ \frac{1}{\sin^2(\beta/2)}\frac{\partial^2 f}{\partial\gamma^2}$$

and the solid angle element

$$\mathrm{d}^3\Omega = \frac{1}{4}\sin\beta\,\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}\gamma.$$

The spherical harmonics of order n are the eigenfunctions of Δ_{S^3} with eigenvalue $-n(n+2)$ (see, for example, Ref. 10); hence, the separable spherical harmonics of order n in the Euler angles (α, β, γ) are of the form

$$\mathrm{e}^{\mathrm{i}m\alpha}\mathrm{e}^{\mathrm{i}q\gamma}B_{nqm}(\cos\beta), \quad (34)$$

where m and q are integers and $B_{nqm}(x)$ is a solution of the ordinary differential equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}B_{nqm}}{\mathrm{d}x}\right] + \left[\frac{n}{2}\left(\frac{n}{2}+1\right) - \frac{1}{2}\frac{m^2+q^2}{1-x^2}\right.$$
$$\left. + \frac{1}{2}\frac{(m^2-q^2)x}{1-x^2}\right]B_{nqm} = 0. \quad (35)$$

The solutions to this equation can be expressed in terms of Jacobi polynomials or of Wigner D functions. The spherical harmonics (34) are simultaneous eigenfunctions of ∂_α and ∂_γ and, by means of a straightforward computation, making use of Eqs. (33), one finds that these two operators amount to $x_1\partial_2 - x_2\partial_1$ and $x_3\partial_4 - x_4\partial_3$, respectively, that is, to the operators $\hat{L}_3/(-\mathrm{i}\hbar)$ and $\hat{K}_3/(-\mathrm{i}\hbar)$ [see Eq. (22)].

Thus, the wavefunctions corresponding to the spherical harmonics (34) are eigenfunctions of L_z and A_z and must be, therefore, the separable solutions of the Schrödinger equation (1) in the parabolic coordinates. Substituting Eqs. (4), (8), (10), (29), (33), and (34) into Eq. (2) one obtains

$$\psi(\xi,\eta,\phi) = \frac{p_0^{3/2}}{4(2\pi\hbar)^{3/2}}\int \mathrm{e}^{\mathrm{i}m\alpha}\mathrm{e}^{\mathrm{i}q\gamma}B_{nqm}(\cos\beta)$$
$$\times \exp\left[\frac{\mathrm{i}p_0(\xi^2-\eta^2)\sin(\beta/2)\cos\gamma}{\hbar(1-\sin(\beta/2)\sin\gamma)}\right]$$
$$\times \exp\left[\frac{2\mathrm{i}p_0\xi\eta\cos(\beta/2)}{\hbar(1-\sin(\beta/2)\sin\gamma)}\cos(\phi-\alpha)\right]$$
$$\times \frac{\sin\beta\mathrm{d}\alpha\mathrm{d}\beta\mathrm{d}\gamma}{1-\sin(\beta/2)\sin\gamma}.$$

Making use of the Jacobi–Anger expansion,

$$\mathrm{e}^{\mathrm{i}x\sin\theta} = \sum_{m'=-\infty}^{\infty}\mathrm{e}^{\mathrm{i}m'\theta}J_{m'}(x)$$

and integrating on α one finds

$$\psi(\xi,\eta,\phi) = \frac{\pi p_0^{3/2}}{2(2\pi\hbar)^{3/2}}\mathrm{e}^{\mathrm{i}m\phi}\int \mathrm{e}^{\mathrm{i}q\gamma}B_{nqm}(\cos\beta)$$
$$\times \exp\left[\frac{\mathrm{i}p_0(\xi^2-\eta^2)\sin(\beta/2)\cos\gamma}{\hbar(1-\sin(\beta/2)\sin\gamma)}\right]$$
$$\times \mathrm{i}^m J_m\left(\frac{2p_0\xi\eta\cos(\beta/2)}{\hbar(1-\sin(\beta/2)\sin\gamma)}\right)$$
$$\times \frac{\sin\beta\mathrm{d}\beta\mathrm{d}\gamma}{1-\sin(\beta/2)\sin\gamma},$$

which is clearly an eigenfunction of L_z; according to the previous results, the double integral appearing in the last expression must be the product of the functions (31) and (32), up to a constant factor.

7. Concluding remarks

As pointed out in Ref. 7, the hydrogen atom in two or more dimensions shows several regularities. The results of this paper and those of Ref. 8 suggest the existence of a relation between the generalized associated Legendre functions in any dimension and the associated Laguerre polynomials [see Eqs. (20) and (21)].

Among the advantages of the approach followed in this paper in the solution of the hydrogen atom, we have found that the relationship of the components of the quantum analog of the Runge–Lenz, A_i, with the generators of rotations in four dimensions allows us to conclude that all the operators A_i/p_0 have the same spectrum as L_z, in spite of the differences in the commutation relations satisfied by these operators [Eqs. (28)].

Acknowledgment

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