RELATIONSHIP BETWEEN WAVE FUNCTIONS OF TWO-DIMENSIONAL HYDROGEN ATOM IN PARABOLIC AND POLAR COORDINATES

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Abstract

We show, for the two-dimensional hydrogen atom, the relationship between its wave functions in polar and parabolic coordinates.

Keywords

Two-dimensional hydrogen atom; polar and parabolic coordinates

Introduction.

The Schrödinger equation for bounded states of the hydrogen atom in two dimensions:

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

has the following normalized wave functions in polar coordinates (r,φ) [1,2]:

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

where $p_0 = \sqrt{-2ME} = \frac{2M\tilde{K}}{\hbar(2l+1)}$ $, l = 0,1,\ldots; m = 0,\pm 1,\ldots,\pm l$ *and* L_b^a are the associated Laguerre polynomials [3-5].

In parabolic coordinates (*u,v*) defined by:

$$x = \frac{1}{2}\left(u^2 - v^2\right) \quad , \quad y = uv \quad , \qquad (3)$$

The normalized solutions of (1) are given by [1,2]:

$$\tilde{\psi}_{lq}(u,v) = \frac{p_0\, i^{l-q} e^{-\frac{p_0}{2\hbar}(u^2+v^2)} H_{l+q}\left(\sqrt{\frac{p_0}{\hbar}}\,u\right) H_{l-q}\left(\sqrt{\frac{p_0}{\hbar}}\,v\right)}{\hbar\left[2^{2l-1}\pi\,(2l+1)(l+q)!(l-q)!\right]^{1/2}} \qquad (4)$$

where $q = 0,\pm 1,\ldots,\pm l$ and the H_n are the Hermite polynomials [3-5].

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The problem is to express (2) in terms of (4), which it is resolved in [6] employing non-trivial relations from group theory, with the following answer:

$$\psi_{lm}(r,\varphi) = i^m \sum_{q=-l}^{l} (-1)^q \, d^l_{qm}(-\frac{\pi}{2}) \, \tilde{\psi}_{lq}(u,v) \tag{5}$$

such that [6,7]

$$d^l_{qm}(\theta) = \left[(l+m)!(l-m)!(l+q)!(l-q)!\right]^{1/2} \cdot \sum_{k=0}^{l} \frac{(-1)^k (Sen\frac{\theta}{2})^{m-q+2k} (Cos\frac{\theta}{2})^{2l-m+q-2k}}{k!(l+q-k)!(l-m-k)!(m-q+k)!} \tag{6}$$

In the next Sec. we shall show –for special values of *m*- expressions between ψ and $\tilde{\psi}$ (alternative ones to (5)) which can be obtained without using group theory. In fact, it is sufficient to use known relations for the Laguerre and Hermite polynomials; our procedure accepts easy generalization to arbitrary values of parameter *m*.

Relationship between polar and parabolic wave functions..

When we search for writing ψ_{lm} in terms of $\tilde{\psi}_{lq}$ it results that the identity [5]:

$$L_a\left(\xi^2+\eta^2\right) = \frac{(-1)^a}{2^{2a}} \sum_{k=0}^{a} \frac{H_{2k}(\xi) H_{2a-2k}(\eta)}{k!(a-k)!} \tag{7}$$

is basic in our process, which we illustrate in two cases:

a).- $\underline{m=0}$.

From (2) we have the following solutions for arbitrary l:

$$\psi_{l0} = \frac{p_0}{\hbar}\left[\frac{2}{\pi(2l+1)}\right]^{1/2} e^{-\frac{p_0 r}{\hbar}} L_l\left(\frac{2p_0 r}{\hbar}\right), \tag{8}$$

there we put $r = \frac{1}{2}\left(u^2+v^2\right)$, then we employ (7) with $a=l$, $\xi = \sqrt{\frac{p_0}{\hbar}}\, u$, $\eta = \sqrt{\frac{p_0}{\hbar}}\, v$ and we remember (4) to deduce the following expression ($\Gamma(z)$ denotes the gamma function) :

$$\psi_{l0} = \frac{(-1)^l}{2^{2l}} \sum_{q=-l}^{l} \frac{\sqrt{(l+q)!(l-q)!}}{\Gamma\left(\frac{l+q}{2}+1\right)\Gamma\left(\frac{l-q}{2}+1\right)} Cos\left[\frac{(q-l)\pi}{2}\right] \tilde{\psi}_{lq} , \tag{9}$$

much more simple in computations than the corresponding relation obtained from (5) for $m=0$; in (9) it is clear that $\Gamma\left(\frac{l\pm q}{2}+1\right) = \left(\frac{l\pm q}{2}\right)!$ when $\left(\frac{l\pm q}{2}\right)$ is an integer.

For example, (9) implies that $\psi_{00} = \tilde{\psi}_{00}$ and :

$$\psi_{10}=\frac{1}{\sqrt{2}}\left(\tilde{\psi}_{1-1}-\tilde{\psi}_{11}\right) \quad , \quad \psi_{20}=\frac{1}{2}\left[\sqrt{\frac{3}{2}}\left(\tilde{\psi}_{22}+\tilde{\psi}_{2-2}\right)-\tilde{\psi}_{20}\right] \quad ,$$

$$\psi_{30}=\frac{1}{4}\left[\sqrt{5}\left(\tilde{\psi}_{3-3}-\tilde{\psi}_{33}\right)+\sqrt{3}\left(\tilde{\psi}_{31}-\tilde{\psi}_{3-1}\right)\right] \quad , \text{ etc.} \tag{10}$$

in accordance with (5).

b).- $m=1$.

The equation (2) gives us the wave functions :

$$\psi_{l1}=-2i\left(\frac{p_0}{\hbar}\right)^2\left[\frac{2}{\pi(2l+1)(l+1)l}\right]^{1/2} r\, e^{-\frac{p_0 r}{\hbar}} L_{l-1}^{2}\left(\frac{2p_0 r}{\hbar}\right) e^{i\varphi} \tag{11}$$

where we employ $e^{i\varphi}=\frac{1}{2r}(u+iv)^2$ and the same expressions for $r\,,\xi\,,\eta$ as used in ψ_{l0}, resulting thus that:

$$\psi_{l1}=-i\frac{p_0}{\hbar}\left[\frac{2}{\pi(2l+1)(l+1)l}\right]^{1/2} e^{-\frac{p_0 r}{\hbar}}(\xi+i\eta)^2 L_{l-1}^{2}\left(\xi^2+\eta^2\right) \tag{12}$$

On the other hand, by repeated partial differentiation of (7) with respect to ξ and/or η for $a = l+1$, and the use of the known properties [5]:

$$\frac{d}{dz}H_n(z)=2n\cdot H_{n-1}(z)\,,\quad \frac{d}{dz}L_n^{a}(z)=-L_{n-1}^{a+1}(z) \tag{13}$$

It is easy to show the interesting identity:

$$(\xi+i\eta)^2 L_{l-1}^{2}\left(\xi^2+\eta^2\right)=\frac{(-1)^l}{2^{2l}}\sum_{q=0}^{l}\frac{1}{q!(l-q)!}\left[(l-2q)\cdot H_{2q}(\xi)H_{2l-2q}(\eta)-2i(l-q)H_{2q+1}(\xi)H_{2l-2q-1}(\eta)\right] \tag{14}$$

which jointly with (4) and (12) lead to the expansion:

$$\psi_{l1}=\frac{i(-1)^l}{2^l\sqrt{l(l+1)}}\sum_{q=-l}^{l}\sqrt{(l+q)!(l-q)!}\cdot\left[\frac{q\,Cos\left(\frac{q-l}{2}\pi\right)}{\Gamma\left(\frac{l+q}{2}+1\right)\Gamma\left(\frac{l-q}{2}+1\right)}+\frac{2(-1)^{q-l}\,Sen\left(\frac{q-l}{2}\pi\right)}{\Gamma\left(\frac{l+q-1}{2}+1\right)\Gamma\left(\frac{l-q-1}{2}+1\right)}\right]\tilde{\psi}_{lq} \tag{15}$$

which is more economical – in calculations - than (5) for *m=1.* Then (15) implies:

$$\psi_{11}=-i\left[\tfrac{1}{2}\left(\tilde{\psi}_{1-1}+\tilde{\psi}_{11}\right)+\tfrac{1}{\sqrt{2}}\tilde{\psi}_{10}\right],\quad \psi_{21}=+\tfrac{i}{2}\left(\tilde{\psi}_{22}-\tilde{\psi}_{2-2}+\tilde{\psi}_{21}-\tilde{\psi}_{2-1}\right),\ \text{etc.} \tag{16}$$

Similarly, with (7) for $a = l+2$ we can obtain an expression for $(\xi+i\eta)^4\ L_{l-2}^{4}(\xi^2+\eta^2)$ and then to deduce ψ_{l2} in terms of the $\tilde{\psi}_{lq}$, and so on; therefore, our method admits application for any value of *m*. From (2) we have that $\psi_{l-m} = \overline{\psi}_{lm}$, implying that it is only necessary to develop expressions for $m \geq 0$

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