ON THE HYDROGEN SYMMETRY

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We construct O(4)-invariant hydrogen wave function in coordinate representation.
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The symmetry mentioned above is the famous O(4)-symmetry of the nonrelativistic hydrogen atom, which was transformed by V.A. Fock from the hidden form to the explicit one [1]. Fock considered the problem at the wave-function level: he pointed out that Schroedinger equation in omentum representation is nothing else as the defining property of the 4-dimensional spherical harmonics.

At the operator level this symmetry was well known long ago: 10 years before Fock the hydrogen energy was quantized by W. Pauli [2] just using two conserved operators - orbital momentum L and Laplace vector K. As was shown by V. Bargmann [3] both are generators of the O(4)-symmetry.

For more than 60 years still remains without answer the question - how to see this symmetry immediately in coordinate representation? Aside of a simple curiosity this question is also of practical meaning because it is more easy to work with symmetric quantities.

Indeed, what is the symmetry? In a simplest case it is an independence of the function on the corresponding variable. For example, an axial symmetry means that function has not angle φ among its arguments. Another example, isotropy, means that the mentioned axis may be rotated in an arbitrary mode -- now the angle θ drops out of consideration. The isotropic function depends not on three variables x,y,z but only on the one combination of them $r = \sqrt{x^2 + y^2 + z^2}$. Just this contraction is the main cause of most simplifications when working with symmetric entities.

Let us turn to the hydrogen problem. Its Hamiltonian

$$H = \vec{p}^2 / 2m - Ze^2 / r \qquad (1)$$

is explicitly isotropic. This property is usually used to separate the angles from radius, factorizing the spherical function $Y_{lm}(\theta,\varphi)$ from the radial $R_{nl}(r)$ one.

But then the Fock symmetry becomes completely elusive: indeed, O(4)--symmetry mixes the states with different values of the quantum number while during separation of the angles this number is kept fixed. Therefore our goal may be achieved only in the one way: to find the wave function of the given energy state without expanding in the partial waves -- it must be some linear combination of the "standard" radial-angular solutions.

First we separate the asymptotic factor exp(-λr) bearing in mind that state is bound, E<0, and λ=(2mE/ $\hbar^2$)$^{1/2}$. Schroedinger equation takes on the form

$$\left\{\nabla^2 - 2\frac{R}{R}\nabla - \frac{2}{R}(1 - i\xi)\right\}\Phi(R) = 0, \qquad (2)$$

where we have introduced the dimensionless radius $R = \lambda r$ and insert the notation $\xi = Ze^2/\hbar v$ for the dimensionless *Coulomb* parameter.

Axially symmetric wave function $\Phi(R)$ must not depend on the angle φ. Thus, two possible arguments R-z and R+z remain. The wave function, which depends only on one of them u=R+z[1],

$$\Phi(R) = f(u), \qquad (3)$$

has a property being constant on the paraboloid u=R+z -- displacements along its surface do not change it.

One of these displacements is motion along the "parallel" and is simply a rotation around the z-axis; it generates the axial symmetry mentioned above. But the other one -- displacement along the "meridian" -- is something new. Parametrizing the paraboloid as

$$R=u\cos^2\tau, \quad z=u\sin^2\tau \qquad (4)$$

we can change the angle τ by arbitrary additive: τ→τ+δ. The τ is that same third angle needed for the 4-dim symmetry!

To "liberate" the z -axis it is sufficient to write the argument as $u = R + \mu R$ using unit vector μ. No property will be lost, only the axis of the paraboloid will change its direction, now pointing along that vector.

It is not difficult to treat the positive energies: the asymptotic factor will be exp(ikr) with k=(+2mE/ $\hbar^2$)$^{1/2}$ dimensionless radius becomes to be $R = kr$ and u=ik(r+μr).

[1] The choice v=R-z is also possible but gives nothing new because of parity conservation.

Unlike to momentum representation, where Fock symmetry is realized differently: on the sphere when E<0 and on the hyperboloid when E>0 (see [3,4]), in our case all the wave functions are living on the same paraboloid
independently on the sign of the energy.

It must be mentioned that in classical limit this paraboloid obtains a simple visual sense: it represents the surface, whose interior is unattainable for positively charged particles falling on the nucleus.

Another interesting and important property is that homogeneous flux of particles falling inside of paraboloid, after being gathered in its focus is diverging in space according to Rutherford law:

$$dN/d\Omega \sim [\sin(\theta/2)]^{-4} . \qquad (5)$$

This property explains a mysterious coincidence of the quantum and classical cross-sections for Coulomb scattering (for more details see [5]).

APPENDIX: SOLUTIONS IN EXPLICIT FORM

Here some technical questions are sampled together. Equation (2) under assumption (3) takes on the form

$$u\Phi''(u) + (1-u)\Phi'(u) - \eta\Phi(u) = 0 , \qquad \eta = 1 - i\xi . \qquad (a.1)$$

Its solution for the bound states ($i\xi = n = 1,2,\ldots$) is simply a Laguerre polynomial

$$\Phi_n(u) = L_{n-1}(u) = F_{11}(1-n;1|u) \qquad (a.2)$$

where $F_{11}(a;b|u)$ is degenerate hyper-geometric function.

Despite of its simplicity, this expression contains much information. Its expansion in Legendre polynomials

$$\Phi_n(u) = \sum_{l=0}^{n-1} C_{nl} P_l(\cos\theta) R_{nl}(R) ,$$
$$C_{nl} = \frac{(n-1)!}{(n-l-1)!(2l)!} \qquad (a.3)$$

generates all the radial functions $R_{nl}(R) = (2R)^l F_{11}(l+1-n;2l+2|2R)$ belonging to the n-th energy level. For example, the n=3 wave function

$$\Phi_3(u) = L_2(u) = 1 - 2u + u^2/2 \qquad (a.4)$$

contain all the three angular states S,P,D: $\Phi_3 = \tilde{R}_0(R) + \tilde{R}_1(R)P_1(\cos\theta) + \tilde{R}_2(R)P_2(\cos\theta)$ with well-known radial functions:

$$\tilde{R}_0(R) = 1 - 2R + 2R^2/3 ;$$
$$\tilde{R}_1(R) = R(2-R) ;$$
$$\tilde{R}_2(R) = R^2/3 . \qquad (a.5)$$

Fourier-transformation of the considered solutions

$$f_n(\vec{p}) = \int e^{i\vec{p}\vec{r}} e^{-\lambda r} \Phi_n[\lambda(r+z)] d^3r \qquad (a.6)$$

after evaluation

$$f_n(p) = \frac{8\pi n}{\lambda^3(1+p^2)^2}\left(\frac{1+ip}{1-ip}\right)^{n-1} \qquad (a.7)$$

coincides with appropriately transformed expression of V. Fock.

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