THE FUNDAMENTAL SOLUTIONS OF THE SCHRÖDINGER EQUATION FOR THE HYDROGEN ATOM

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The problem for the hydrogen atom, as one of the few that allows an exact analytical solution, is considered for methodological reasons in most textbooks on quantum mechanics. One of the two independent solutions of the Schrödinger equation is square integrable and satisfies the boundary conditions at the coordinate origin ($r = 0$) and at infinity ($r \to \infty$). For states with orbital angular momentum $l \geq 1$, the second singular solution gives the divergence of the normalization integral at the point $r = 0$.

However, for the angular momentum $l = 0$, the singularity of the second solution is expressed weakly and does not lead to the divergence of the integral at the origin, but it is rejected by guiding various arguments in various textbooks. These arguments can be classified into three groups. The first argument of textbooks indicates the unsatisfactory boundary conditions of the second solution at the origin. Another argument indicated that this solution does not satisfy the Schrödinger equation at the origin of coordinates $r = 0$ due to the appearance of the Dirac function $\delta(r)$ [1]. In the practical textbook [2], there is argued that in the singular state of $l=0$ the mean value of the kinetic energy takes the infinite, therefore this solution is unacceptable.

We tried to deal with this variety of arguments also because if the singular solution for the orbital moment $l = 0$ is possible to normalize, then it represents a state with limited energy of the system but an infinite average kinetic energy ($+ \infty$) and infinite potential energy ($-\infty$), that is, the sum of two infinite quantities is finite

$$E = \langle \Psi | \hat{H} | \Psi \rangle = \langle E_k \rangle + \langle E_\Pi \rangle = (+\infty) + (-\infty). \tag{1}$$

To demonstrate our investigation about the singular solution we briefly repeat one of the methods for obtaining the analytical solution of the Schrödinger equation with the Coulomb potential. In the Schrödinger equation

$$\hat{H}\Psi(\vec{r}) = E\Psi(\vec{r}) \tag{2}$$

with the Coulomb potential for the hydrogen atom

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} + \frac{\alpha}{r} , \tag{3}$$

where μ is a reduced mass of the atom, one separates the variables in the spherical coordinate system

$$\Psi(\vec{r}) = \Psi(r, \theta, \varphi) = R_l(r)Y_{lm}(\theta, \varphi) = \frac{u_l(r)}{r}Y_{lm}(\theta, \varphi), \tag{4}$$

where $Y_{lm}(\theta, \varphi)$ is the spherical harmonics. For radial function $u_l(r)$, we obtain the equation

$$u_l'' + \left(-k^2 - \frac{l(l+1)}{r^2} + \frac{2A}{r}\right) \cdot u_l(r) = 0, \tag{5}$$

where l is the orbital angular momentum, and parameters k and A have the same dimension and are given by expressions

$$k^2 = \frac{2\mu|E|}{\hbar^2}, \quad A = \frac{e^2\mu}{\hbar^2} \tag{6}$$

The normalization of the radial function $u(r)$ looks as

$$\int_0^\infty u_l^2(r) \cdot dr = 1. \tag{7}$$

At large distance $(r \to \infty)$ equation (5) takes the form

$$u'' - k^2 \cdot u(r) = 0, \tag{8}$$

and has two independent solutions e^{-kr} and e^{+kr}. Since the normalization condition is fulfilled for the asymptotic $(r \to \infty)$ solution e^{-kr}, the radial function of equation (5) is sought in the form

$$u(r) = f(r) \cdot e^{-kr}, \tag{9}$$

which leads to an equation for the unknown function $f(r)$

$$f'' - 2kf' - \frac{l(l+1)}{r^2}f + \frac{2A}{r}f = 0. \tag{10}$$

We shall now look for solution of equation (10) by the power series method

$$f(r) = r^s \cdot \sum_{j=0}^\infty a_j r^j, \quad a_0 \neq 0, \tag{11}$$

where s and a_j are unknown parameters that are determined from the substitution of function (11) into equation (10) with subsequent zeroing of coefficients for each power of variable r. The coefficient at the lowest power gives the equation for determining the parameter s

$$a_0(s^2 - s - l^2 - l) = 0. \tag{12}$$

This equation has two solutions $s_1 = l + 1$ and $s_2 = -l$. Since the roots of the indicial equation (12) differ by an integer, according to [3] two independent solutions of the differential equation are defined in the way

$$f_1(r) = r^{l+1} \cdot \sum_{j=0}^\infty a_j r^j, \tag{13}$$

$$f_2(r) = r^{-l} \cdot \sum_{q=0}^\infty b_q r^q + g \cdot f_1(r) \cdot \ln(r), \tag{14}$$

where unknown coefficients a_j, b_q and g are successively determined by substituting the formulas (13) and (14) into equation (10) and equating to zero the coefficients for powers of the variable r.

We want to emphasize that for the hydrogen atom with Coulomb potential and for deuteron wave function [4], the logarithmic term in (14) ensures the correct behavior of the solution at the origin. However, for other potentials, it can appear that the coefficient g in equation (14) is zero [5, 6].

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МІЖНАРОДНА КОНФЕРЕНЦІЯ МОЛОДИХ ВЧЕНИХ ТА АСПІРАНТІВ

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PROGRAMME AND ABSTRACTS

Збірник містить матеріали конференції. Доповіді присвячені дослідженню явищ, що відбуваються у різноманітних атомних системах у газоподібному та конденсованому станах. Представлено також роботи з технологічних та фізичних особливостей отримання деяких речовин із заданими властивостями.

This book presents proceedings of the conference. The contributions are dedicated to the studies of the phenomena occurring in different atomic systems in free and condensed states. The papers on the studies of technological and physical peculiarities of the production of certain substances with preset properties are also included.

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