Concerning the Choice of Physically Acceptable Solutions of the Schrödinger Equation for the Hydrogen Atom

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IN a calculation of the stationary states of hydrogen atoms a representation of the wave function in the form

$$\Psi(r,\ \vartheta,\ \varphi) = R(r)\, P_l^m(\cos\vartheta)\, e^{\pm im\varphi} \tag{1}$$

leads to the following differential equation for R and $E < 0$ (in atomic units):

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(2E + \frac{2Z}{r} - \frac{l(l+1)}{r^2}\right)R = 0, \tag{2}$$

The characteristic equation corresponding to the differential equation (2) has two roots l and $-(l+1)$ at the point $r = 0$. Consequently, the expansions of the particular solutions R_1 and R_2 begin with the term r^l or $r^{-(l+1)}$, respectively. The eigenfunction R_2, which behaves in the expansion as $r^{-(l+1)}$, is discarded for $l \geq 1$ since the condition of quadratic integrability cannot be satisfied. For $l = 0$ Sommerfeld and Kramers[1] and Rellich[2] proposed that there is no basis for discarding the second eigensolution, since all eigensolutions are normalizable. Subsequently, Falk and Marschall[3] showed that the second particular solution R_2 still should be discarded because of the normalization condition, and the problem appeared to be clarified.

The proposals of Sommerfeld, Kramers and Rellich are indeed incorrect. However, the proof of Falk and Marschall is applicable only for the case $1 - 2z/\varkappa = -n$, $n = 0, 1, 2\ldots$ and therefore, it tacitly assumes the continuity of the solution at $r = 0$. The purpose of the present letter is to show that for the case $l = 0$ there is only one solution which can be normalized. It will also be shown below that it is necessary to impose some local condition at the point $r = 0$ in order to obtain the correct spectrum of eigenvalues.

For $l = 0$ we have the following independent eigensolutions:

$$R_1 = e^{-\rho/2}\,{}_1F_1\left(1 - \frac{2Z}{\varkappa}, 2, \rho\right), \tag{3}$$

$$R_2 = e^{-\rho/2}\,\Phi\left(1 - \frac{2Z}{\varkappa}, 2, \rho\right).$$

The following abbreviations were introduced in Eq. (3):

$$2E = -\varkappa^2/4;\ \ \varkappa r = \rho > 0. \tag{4}$$

${}_1F_1$ denotes the confluent hypergeometric series, and Φ is the second independent solution of the confluent hypergeometric differential equation.

As is well known[4], Φ may be written

$$\Phi(a,\ b,\ x) = \frac{\Gamma(1-a)}{2\pi i}\, e^{-a\pi i} \times \int_{\infty\cdot e^{i\varphi}}^{(0+)} e^{-xt}\, t^{a-1}(1+t)^{b-a-1}\, dt, \tag{5}$$

$$-\pi/2 \leqslant \varphi < \pi/2.$$

The asymptotic form of this function for $x \to +\infty$ is

$$\Phi(a,\ b,\ x) = x^{-a}\,[1 + 0(1/x)]. \tag{6}$$

Therefore, our second solution R_2 has the following form for $\rho \to +\infty$:

$$R_2 = e^{-\rho/2}\rho^{-[1-(2Z/\varkappa)]}\,[1 + 0(1/\rho)]. \tag{7}$$

This formula shows that the second eigenfunction R_2 can be normalized for large r. For small r the relation

$$\lim_{x \to +0} x^{b-1}\,\Phi(a,\ b,\ x) = \Gamma(b-1)/\Gamma(a);\ \ b > 1 \tag{8}$$

shows that R_2 approaches in the limit of $\rho \to +0$ the expression

$$\lim_{\rho \to +0} R_2 = \frac{e^{-\rho/2}}{\Gamma[1-(2Z/\varkappa)]}\,\frac{1}{\rho}. \tag{9}$$

Equations (7) and (9) show that R_2 can be normalized for all eigenvalues $E < 0$. Thus there always exists a solution that can be normalized. Further-

more, we note that the normalization conditions are not sufficient to obtain the correct spectrum of eigenvalues. This deficiency can be overcome by imposing an additional regional condition, namely, the condition that the function be regular at the origin. If we demand that $1-(2Z/\varkappa) = -n$, $n = 0, 1, 2\ldots$, then Φ goes into the Laguerre polynomial, and consequently, the function R_2 is regular at $r = 0$. For $1-(2Z/\varkappa) = -n$ the functions R_1 and R_2 are lineraly dependent and for $1-(2Z/\varkappa) \neq -n$ they are linearly independent. In conclusion, we note that for $l = 0$ the theory of Weyl also demands some regional condition. In the present case the demand that the solution be regular corresponds to the choice of some fully determined boundary condition of Weyl for $r = 0$. In this way the demand of regularity guarantees the physical correctness of the spectrum of eigenvalues. It is also possible to substantiate the regional condition at $r = 0$ by making a use of the Hermiticity conditions[5].

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Nuclear Capture of Neutrons with an Energy of Several MEV

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THE object of the present note is to calculate the cross section for neutron capture by excitation of the nuclear volume vibrations.

The incident neutron, interacting with the vibrational motion, gives up its energy and goes into a bound state in the nucleus. We consider the excitation of the first radial vibration, the frequency of which ω_0 corresponds to an energy of the order 10 mev.[1] The corresponding level has an appreciable width γ as a result of dissipation. However, such a mechanism of capture makes sense if the width of the level is not too large compared with the vibrational energy.

The Schrödinger equation of the system, nucleus + neutron, is

$$[-(\hbar^2/2M)\nabla^2 + U_0(r) + U(\mathbf{r}, Q) + T + W]\Psi = E\Psi, \quad (1)$$

where $\mathbf{r}$ is the radius vector of the neutron, U_0 is a spherically symmetrical potential well of depth V_0 and radius R; $U(\mathbf{r}, Q)$ is the potential arising from the nuclear density vibrations described by coordinates Q; T and W are the kinetic and potential energies of vibration. According to Ref. 1, for a two-fluid compressible model of the nucleus

$$W = \frac{1}{2}\int (a\delta\rho_p^2 + 2b\delta\rho_p\delta\rho_n + a\delta\rho_n^2)\, d\tau, \quad (2)$$

where $\delta\rho_p$ and $\delta\rho_n$ are the deviations of neutron and proton densities from their static values and $\delta\rho_{n,p} = f_{n,p}(\mathbf{r})\, Q$;

$$f_p(r) = D_{1p}j_0(q_1 r) + D_{2p}j_0(q_2 r); \quad (3)$$

$$f_n(r) = D_{1n}j_0(q_1 r) + D_{2n}j_0(q_2 r).$$

Here the constants D and q depend only on the number of neutrons and protons in the nucleus; j_l is the spherical Bessel function of order l.

In zero order

$$\Psi = \psi(\mathbf{r})\varphi(Q);$$

$$-\frac{\hbar^2}{2M}\nabla^2\psi + U_0\psi = E^{(0)}\Psi; \quad (T+W)\varphi = \varepsilon\varphi.$$

Bearing in mind the short range of nuclear force, we consider that the interaction energy of the neutron with the vibrations is proportional to the density deviation $\delta\rho = \delta\rho_n + \delta\rho_p$ at that point where the neutron is located. We define the coefficient of proportionality such that the interaction with a single-fluid static distribution of charge could be described by a potential U_0.

After summation over all final states of the captured neutron, the cross section is, to first approximation in perturbation theory;

$$\sigma = \sum_{nl}\sigma_{nl} = (2\pi/\hbar)\sum_{nl}|U_{nl}|^2, \quad (4)$$

where l is the angular momentum of the captured neutron, n is the quantum number of the bound state with momentum l;