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SOLVING THE SCHROEDINGER EQUATION FOR A COULOMB POTENTIAL WITH CUT-OFF.

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The problem of solving the Schroedinger equation for a cut off Coulomb potential,
viz.

$$\frac{d^2\Psi}{d\,r^2} + \left(- \frac{\alpha^2}{k^2} - V(r) - \frac{l(l+1)}{r^2} \right) \Psi = 0 \qquad (1)$$

with

$$\begin{aligned} V(r) &= - \frac{2\alpha}{r_o} \qquad \text{for} \qquad r \leqq r_o \\ V(r) &= - \frac{2\alpha}{r} \qquad \text{for} \qquad r \geqq r_o \end{aligned} \qquad (2)$$

has some importance in certain calculations concerning the excited states of solids[1]. The problem has actually been solved numerically for a particular case by Tibbs[2]. Numerical methods are always very specialized and have to be repeated in every new case. It is the purpose of this note to call attention to the fact that such problems are often capable of analytic solution comprising most of the possible cases

Formulating the problem as we did in eqs. (1) and (2), we accept for the energy the usual Balmer formula, but replace the integer n by some undetermined number k which we may continue to call the principal quantum number; we wish to determine the eigenvalues of this number which will solve equation (1) for $l = 0, 1, 2, 3, 4, 5 \;\ldots$ in such a way that the solution is simultaneously finite at the origin and infinity. In our case, when there is a break in the potential curve, the required type of solution can be written down immediately on either side, and k is to be determined by the requirement of continuity for the function and its first derivative at the joining point.

The solution below $r = r_o$ is given by

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1 Mott and Gurney, Electronic processes in ionic crystals. Oxford University Press. pp. 88 and 113.
Gregory H. Wannier, Phys. Rev. *52,* 191, 1937.

2 S. R. Tibbs, Trans. Faraday Soc. *35,* 1471, 1939.

$$\Psi = \sqrt{r}\, J_{l+\frac{1}{2}} \left(\sqrt{\frac{2\alpha}{r_o} - \frac{\alpha^2}{k^2}}\; r \right) \tag{3}$$

and above $r = r_o$

$$\Psi = W_{k,l+\frac{1}{2}} \left(\frac{2\alpha}{k}\, r \right) \tag{4}$$

where $W_{k,l+\frac{1}{2}}$ is the confluent hypergeometric function which is finite at infinity as defined by Whittaker and Watson[3]. If k happens to be a positive integer obeying the inequality

$$k > l$$

this function happens to be also finite at the origin, and hence if the cut-off radius shrinks to zero we get the well known eigenvalues

$$k = n = l + 1,\ l + 2,\ l + 3, \quad . \ . \ . \ . \ .$$

For finite cut-off we make use of the fact first pointed out by Bethe[4] that there is a great similarity between the confluent hypergeometric functions and certain Bessel functions, at least below the limit of the classical orbit (which is by necessity the region in which the joining point must lie.).

we bring this out by defining a new variable x :

$$x = 2\ (2\ \alpha\ r)^{\frac{1}{2}} \tag{5}$$

and a Bessel-like Function

$$J^{k}_{2m}(x) = \frac{(2\ \alpha\ r)^{-\frac{1}{2}}\ k^{m+\frac{1}{2}}}{2m\,!}\ M_{k,m}\left(\frac{2\ \alpha\ r}{k}\right) \tag{6}$$

where $M_{k,m}$ is the confluent hypergeometric function of given behavior at the origin, as defined in Whittaker and Watson[3]. The similiarity between this Bessel-like function $J^{k}_{p}(x)$ and the Bessel function $J_p(x)$ can be brought out by comparing their representations by contour integrals:

$$J^{k}_{2m}(x) = \frac{1}{2\pi i}\int e^{\frac{1}{2}xu}\left(u + \frac{x}{4k}\right)^{-k-m-\frac{1}{2}}\left(u - \frac{x}{4k}\right)^{-k-m-\frac{1}{2}} du$$

$$J_{2m}(x) = \frac{1}{2\pi i}\int e^{\frac{1}{2}x\left(u - \frac{1}{u}\right)}\ u^{-2m-1} du$$

The path of integration is the same in the two cases, going from $-\infty$ in a positive sense round the singularities present and

[3] Whittaker and Watson, Modern Analysis, Cambridge University press, chapter XVI, particularly 16.1, 16.12, 16.41.

[4] H. Bethe, Handbuch der Physik, second edition, XXIV/1, p. 287.

returning to $-\infty$; and the powers which appear are to be chosen so that they are positive when x is positive and when u cuts the positive real axis. Both integrals can be verified directly by checking the power series in x which results from them. From those two integrals we can deduce

$$\lim_{k\to\infty} J^{k}_{p}(x) = J_p(x)$$

or more precisely

$$J^{k}_{p}(x) = J_p(x) + O\left(\frac{x^2}{16k^2}\right) \tag{7}$$

We must now define also a Neumann-like function because the two solutions $J^{k}_{p}(x)$ and $J^{k}_{-p}(x)$ cease to be linearly independent for integer p. Our formula apes of course the corresponding definition of the Neumann function:

$$N^{k}_{2m}(x) \sin 2m\pi = - J^{k}_{-2m}(x) + \frac{(k+m-\frac{1}{2})!}{(k-m-\frac{1}{2})!\,k^{2m}} J^{k}_{2m}(x)\cos 2m\pi \tag{8}$$

The formula differs from its analogue only by the factor in front of J^{k}_{2m} which tends to 1 for large k. The factor is necessary, however, if the right side is to vanish simultaneously with the left for $m = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, - - - -$

Now we are ready for the basic step. We know that beyond the cut-off our solution is actually W as defined by (4). This W is expressible in terms of the M's as pointed out in Whittaker and Watson[3]. Substituting into their formula our equations (6) and (8) we get

$$\left(\frac{x^2}{4k}\right)^{-\frac{1}{2}} W_{k,m}\left(\frac{x^2}{4k}\right) = (k+m-\tfrac{1}{2})!\,k^{-m}J^{k}_{2m}(x) \cos(k-m-\tfrac{1}{2})\pi + (k-m-\tfrac{1}{2})!\,k^{m}N^{k}_{2m}(x)\sin(k-m-\tfrac{1}{2})\pi \tag{9}$$

Now k is determined by the condition of smooth joining at the cut-off radius $x = x_o$

$$x_oJ_{1+\frac{1}{2}}\left(\frac{x_o}{2}\sqrt{1-\frac{x_o^2}{16k^2}}\right) \times \frac{d}{dx}\left[W_{k,1+\frac{1}{2}}\left(\frac{x^2}{4k}\right)\right]_{x=x_o} - \frac{d}{dx}\left[xJ_{1+\frac{1}{2}}\left(\frac{x^2}{2x_o}\sqrt{1-\frac{x_o^2}{16k^2}}\right)\right]_{x=x_o} \times W_{k,1+\frac{1}{2}}\left(\frac{x_o^2}{4k}\right) = 0$$

Into this equation we substitute for W its expression (9). The result simplifies drastically whenever $x_o << 4k$ because (7) can be used for simplification. In this latter case we find the result

$$\frac{(k-l-1)!\,k^{2l+1}}{(k+l)!}\tan k\pi = \tag{10}$$

$$= -\frac{J_{2l}(x_o)J_{l+\frac{1}{2}}(\frac{1}{2}x_o) - J_{2l+1}(x_o)J_{l-\frac{1}{2}}(\frac{1}{2}x_o)}{N_{2l}(x_o)J_{l+\frac{1}{2}}(\frac{1}{2}x_o) - N_{2l+1}(x_o)J_{l-\frac{1}{2}}(\frac{1}{2}x_o)}$$

The right hand side depends only on the joining point, the left only on the unknown k. Hence solution with respect to k is a simple matter. A particularly easy formula results for $l = o$

$$\tan k\pi = -\frac{J_o(x_o)\sin\frac{1}{2}x_o - J_1(x_o)\cos\frac{1}{2}x_o}{N_o(x_o \sin\frac{1}{2}x_o - N_1(x_o)\cos\frac{1}{2}x_o} \tag{11}$$

Formula (11) can be applied directly to reproduce the numerical results of Tibbs. He calculates the two lowest s-levels for $x_o = 2.62$ and gets

$$k_1 = 1.154$$
$$k_2 = 2.15$$

while our formula gives

$$k_1 = 1.158$$
$$k_2 = 2.158$$
$$k_3 = 3.158 \qquad \text{etc}$$

The close agreement is partly accidental, but it leaves no doubt about the power of the method.

Formula (10) holds only good for $x_o \ll 4k$ and must break down when a level gets relatively close to the bottom of the trough. However, $x_o < 4k$ is always satisfied for energy reasons, and an extension to all cases appears thus possible. This extension is being carried out by the author and will be published elsewhere.

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