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Energy Eigenvalues for the Coulomb Potential with Cut-Off. Part I.

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In this paper, the Schrödinger equation is solved analytically for the Coulomb potential with horizontal cut-off. For this purpose, a detailed mathematical study of the confluent hypergeometric functions is carried out and their similarity to Bessel and Neumann functions is put on a quantitative basis. The resulting formulas for the energy levels are valid for all cases except when the energy is lying very little above the cut-off.

THE Coulomb potential with a cut-off (see Fig. 1) has been proposed as an approximate potential energy for certain quantum mechanical problems in the theory of solids.[1] It has actually been used for such a purpose by Tibbs, who solved the problem in one particular case by numerical integration methods.[2] But, in fact, the problem is capable of an analytic, though not rigorous, solution which is to be derived in the following.

The problem is to solve the equation

$$\frac{d^2F}{dr^2}+\left(-\frac{\alpha^2}{k^2}+\frac{2\alpha}{r_0}-\frac{l(l+1)}{r^2}\right)F=0 \qquad (1)$$

for $r<r_0$ and

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

for $r>r_0$, and to join them with continuous derivative at $r=r_0$. The usual conditions are to be added at the origin and infinity. The energy parameter is written here in the form $-\alpha^2/k^2$, where α is a given constant and k is our unknown to be determined.

1. BESSEL-LIKE AND NEUMANN-LIKE FUNCTIONS

The solutions of Eq. (2) are called confluent hypergeometric functions and are discussed in Whittaker and Watson.[3] The two solutions may be either distinguished by their behavior at the origin or their behavior at infinity. In the notation of WW, we have one solution, $M_{k,l+\frac{1}{2}}(2\alpha r/k)$, which is finite at the origin while the other, $M_{k,-l-\frac{1}{2}}(2\alpha r/k)$, has a pole of order l. At plus infinity, one solution, $W_{k,l+\frac{1}{2}}(2\alpha r/k)$, is finite while the other tends to infinity. It is well known that whenever the expression $k-l$ is a positive integer, the solution which is finite at the origin also happens to be finite at $+\infty$. Hence $k=l+1, l+2, l+3, \cdots$ are the eigenvalues of k in the case of the Coulomb potential without cut-off. If there is a cut-off at r_0, then $W_{k,l+\frac{1}{2}}(z)$ is the correct wave function beyond r_0, but the values of k will no longer be integer.

The similarity between the functions M and the Bessel functions is well known.[4] In order to bring it out we introduce a new variable x which is defined thus:

$$x=2(2\alpha r)^{\frac{1}{2}}=2(kz)^{\frac{1}{2}} \qquad (3)$$

and instead of M we introduce $J_p{}^k(x)$,

$$J_p{}^k(x)=\frac{z^{-\frac{1}{2}}k^{\frac{1}{2}p}}{p!}M_{k,\frac{1}{2}p}(z). \qquad (4)$$

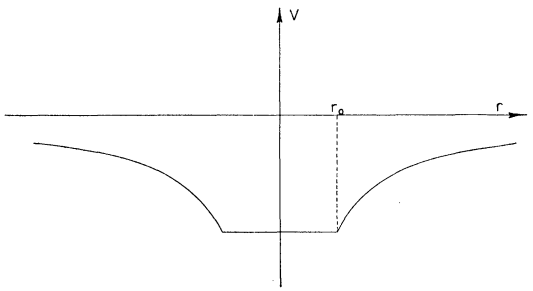

FIG. 1. Coulomb potential with cut-off. Solving the Schrödinger equation for such a potential is the problem of this paper.

[1] G. H. Wannier, Phys. Rev. **52**, 191 (1937).
[2] S. R. Tibbs, Trans. Faraday Soc. **35**, 1471 (1939).
[3] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press), Chapter XVI. In the following quoted as WW.
[4] H. A. Bethe, *Handbuch der Physik*, second edition, Vol. XXIV, 1, p. 287.

It can be verified by substitution into Eq. (2) that

$$\lim_{k\to\infty} J_p^k(x) = J_p(x),$$

i.e., the zero energy Schroedinger eigenfunction is a Bessel function. In addition, by comparing power series, one finds that the first two terms of the series agree for all values of k. A better standard of comparison is gained by a study of their integral representations. The well-known Bessel integral may take the following form

$$J_p(x) = \frac{1}{2\pi i}\int \exp\left[\tfrac{1}{2}x\left(u-\frac{1}{u}\right)\right]u^{-p-1}du. \quad (5)$$

The path comes from $-\infty$, circles around the origin in a positive direction and returns to $-\infty$ (Fig. 2). A similar integral exists for $J_p^k(x)$. Whittaker and Watson introduce an integral representation for $W_{k,m}$ only.[5] The same integral will also be valid for $M_{k,m}$ if the path is suitably altered. Transforming their integral with (3) and (4) and introducing a new variable of integration u through

$$t = -\tfrac{1}{2}(xu - z) = -\tfrac{1}{2}x[u + (x/4k)],$$

we get

$$J_p^k(x) = \frac{1}{2\pi i}\int e^{\frac{1}{2}xu}\left(u+\frac{x}{4k}\right)^{-k-\frac{1}{2}(p+1)} \times\left(u-\frac{x}{4k}\right)^{k-\frac{1}{2}(p+1)} du. \quad (6a)$$

The path in WW must be altered to encircle both singular points of the integrand in a counterclockwise direction and then to return to $-\infty$ (Fig. 3). This statement is verified as

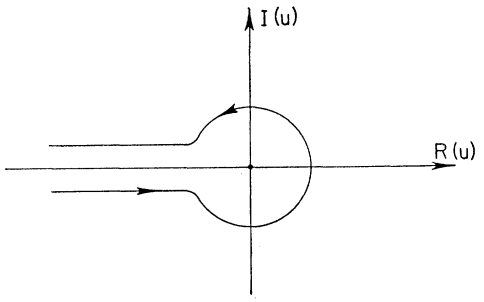

FIG. 2. Path of integration to be followed in the definition of the Bessel function by the Bessel integral [Eq. (5)].

[5] WW, section 16·12.

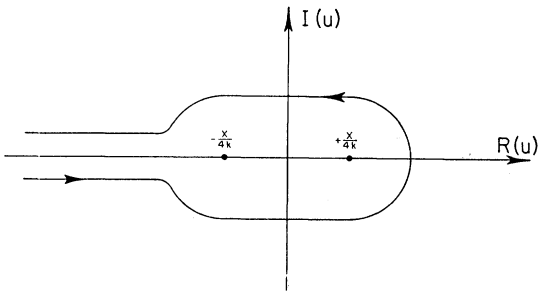

FIG. 3. Path of integration to be followed in defining the Bessel-like function by a contour integral [Eq. (6)].

follows: If we substitute t back again into (6) we get

$$J_p^k(x) = -\exp\left(-\frac{x^2}{8k}\right)(\tfrac{1}{2}x)^p(1/2\pi i) \times\int e^{-t}(-t)^{-p-1}[1+(x^2/4kt)]^{k-\frac{1}{2}(p+1)}dt.$$

Since the path encircles both singularities it can be deformed to make $|t| > x^2/4k$. Hence the binomial can be developed into a power series, and the series can be integrated term by term. The resulting series, by (3) and (4), agrees with the series given for M in WW.

To bring out the similarity between (5) and (6) we write the latter in the form

$$J_p^k(x) = (1/2\pi i) \times\int \exp\left[\tfrac{1}{2}x\left(u-\frac{1}{u}\right)\right]u^{-p-1}\phi(x/4ku)du, \quad (6b)$$

with

$$\phi(s) = (1-s^2)^{-\frac{1}{2}(p+1)}\left[e^{2s}\frac{1-s}{1+s}\right]^k = 1+\tfrac{1}{2}(p+1)s^2-\tfrac{2}{3}ks^3+\cdots. \quad (7)$$

Since $|u|$ may be made larger than 1 in the integrand, we can conclude that

$$J_p^k(x) = J_p(x)\left[1+0\left(\frac{x^2}{16k^2}\right)\right]. \quad (8)$$

It is possible, incidentally, to derive a development of the Bessel-like function $J_p^k(x)$ in a series of Bessel functions, following up the reasoning just indicated. It can be stated as follows: If we write for the series (7)

$$\phi(s) = \sum_{\nu=0}^{\infty} b_\nu s^\nu, \quad (9a)$$

then

$$J_p^k(x)=\sum_{\nu=0}^{\infty} b_\nu(x/4k)^\nu J_{p+\nu}(x). \tag{9b}$$

The convergence is quite rapid, but there are other, more physical ways of constructing improved expressions for $J_p^k(x)$ which are outlined in Sections 3 and 4 below.

In working with Bessel-like functions of integer index p we are faced with a difficulty which is well known from the theory of Bessel functions. Usually, J_p^k and J_{-p}^k form a complete solution of our differential Eq. (2), but whenever p becomes integer the two solutions become identical, apart from a constant factor. We must therefore define an auxiliary function to use beside J_p^k, and it is natural to look for a function which may be compared with the Neumann function $N_p(x)$ (called $Y_p(x)$ in some books). In the latter case, the definition runs

$$N_p(x)\sin p\pi=J_p(x)\cos p\pi-J_{-p}(x). \tag{10}$$

The right-hand side of this equation is constructed so as to vanish identically for integer p. The same principle must be applied in constructing a Neumann-like function N_p^k from the two Bessel-like functions J_p^k and J_{-p}^k. The relationship between the latter two may be obtained from their power series. If we add to this relationship two requirements which we wish to impose, namely,

$$\lim_{x=0}\frac{N_p^k(x)}{N_p(x)}=1 \quad \text{for all } k$$

and

$$\lim_{k\to\infty}\frac{N_p^k(x)}{N_p(x)}=1 \quad \text{for all } x,$$

then the new function is completely determined:

$$N_p^k(x)\sin p\pi$$
$$=\frac{(k+\frac{1}{2}p-\frac{1}{2})!}{(k-\frac{1}{2}p-\frac{1}{2})!k^p}J_p^k(x)\cos p\pi-J_{-p}^k(x). \tag{11}$$

We can expect the new function to equal $N_p(x)$ under the same condition (8) as in the previous case.[6]

The Bessel-like and the Neumann-like function form a complete system of solutions for (2), and therefore, our wave function $W_{k,m}(z)$ is expressible in terms of them. These relationships are well known.[7] We may write the relation relevant to our case

$$z^{-\frac{1}{2}}W_{k,m}(z)\sin 2m\pi$$
$$=(k+m-\tfrac{1}{2})!k^{-m}J_{2m}^k(x)\sin(k+m-\tfrac{1}{2})\pi$$
$$-(k-m-\tfrac{1}{2})!k^mJ_{-2m}^k(x)\sin(k-m-\tfrac{1}{2})\pi. \tag{12}$$

This relation reduces to $0=0$ for integer or half integer m. But if we eliminate J_{-2m}^k with the help of (11) we get a non-trivial relation for all m

$$z^{-\frac{1}{2}}W_{k,m}(z)$$
$$=(k+m-\tfrac{1}{2})!k^{-m}J_{2m}^k(x)\cos(k-m-\tfrac{1}{2})\pi$$
$$-(k-m-\tfrac{1}{2})!k^mN_{2m}^k(x)\sin(k-m-\tfrac{1}{2})\pi. \tag{13}$$

Through its trigonometric factors, the formula shows up clearly the oscillating character of W as a function of k. Every time $k-m+\frac{1}{2}$ is a positive integer the term in N will drop out. The oscillatory character does not continue, however, into the region where $k<m$ because the vanishing of the sine is cancelled by the pole in the factorial.

2. A SIMPLE APPROXIMATE SOLUTION OF THE PROBLEM

Our problem consists in fitting the solution of (1), namely,

$$F_1=xJ_{l+\frac{1}{2}}\left(\frac{x^2}{2x_0}\left(1-\frac{x_0^2}{16k^2}\right)^{\frac{1}{2}}\right), \tag{14}$$

where we have defined consistently with (3)

$$x_0=2(2\alpha r_0)^{\frac{1}{2}} \tag{15}$$

and the solution of (2), which may be written according to (13),

$$F_2=xJ_{2l+1}^k(x)\cos k\pi$$
$$+\frac{(k-l-1)!k^{2l+1}}{(k+l)!}xN_{2l+1}^k(x)\sin k\pi. \tag{16}$$

[6] It appears at first sight that the factor in front of J_p^k alters the situation because it is possible to satisfy the requirement (8)

$$x\ll 4k$$

and yet to have that factor markedly different from 1 by having

$$p\sim 2k.$$

But these two conditions imply also

$$x<p$$

and under these conditions, the lowest negative power in J_{-p}^k outweighs all other contributions to the function N.

[7] WW, section 16·41.

It is possible to get a quick and simple answer by observing the following. We have a condition under which the Bessel-like and Neumann-like function can be replaced by their namesakes, namely,

$$x \ll 4k. \tag{17}$$

Now it is very fortunate that for physical reasons a somewhat weaker condition is always satisfied at the cut-off $x=x_0$:

$$x < 4k. \tag{18}$$

We obtain the condition by demanding that the total energy be higher than the potential energy at the cut-off. Condition (17) will, in fact, apply to all but some of the lowest levels although the latter are no doubt the most important ones. Keeping this restriction in mind we shall construct an approximate solution valid for most states by setting equal at $x=x_0$ the logarithmic derivatives of the following functions

$$F_1 = xJ_{l+\frac{1}{2}}(x^2/2x_0) \tag{19}$$

and

$$F_2 = xJ_{2l+1}(x)\cos k\pi + \frac{(k-l-1)!k^{2l+1}}{(k+l)!} xN_{2l+1}(x)\sin k\pi. \tag{20}$$

We find the following result

$$\frac{(k-l-1)!k^{2l+1}}{(k+l)!}\tan k\pi = -\frac{J_{2l}(x)J_{l+\frac{1}{2}}(\frac{1}{2}x) - J_{2l+1}(x)J_{l-\frac{1}{2}}(\frac{1}{2}x)}{N_{2l}(x)J_{l+\frac{1}{2}}(\frac{1}{2}x) - N_{2l+1}(x)J_{l-\frac{1}{2}}(\frac{1}{2}x)}, \tag{21}$$

where we have replaced for brevity the cut-off coordinate x_0 by x. Equation (21) is explicit in that it contains on the right a function of the cut-off coordinate only and on the left a function of the unknown k, the "effective" principal quantum number. For s states the formula is particularly attractive:

$$\tan k\pi = -\frac{J_0(x)\sin\frac{1}{2}x - J_1(x)\cos\frac{1}{2}x}{N_0(x)\sin\frac{1}{2}x - N_1(x)\cos\frac{1}{2}x}. \tag{22}$$

To realize the power of this simple formula we shall recompute with its help the results of Tibbs.[2] Tibbs calculated in a particular case the energy values for the $1s$, $2s$, and $2p$ states. His cut-off is located at

$$x = 2.62$$

and he found for k:

$$k = 1.154 \pm .002 \quad \text{in the } 1s \text{ state,}$$
$$k = 2.143 \pm .019 \quad \text{in the } 2s \text{ state.}$$

Formula (22) gives

$$k = n + 0.158 \quad \text{for all } s \text{ states.}$$

The agreement may be partly accidental because it is upset if a refined approximation is used for one of the wave functions only. However, it is not impossible that formula (22) is actually better than it appears from this paper and that the deduction of the author is not doing it full justice. In any case, formulas (21) and (22) are very useful for a rough location of the energy levels.

What follows first from (21) and (22) is that while the energy correction is of course smaller for high energy levels, the correction to the principal quantum number is of the same order for all levels having the same angular momentum quantum number. It is actually the same (within the restrictions of this section) for all s states and tends to be the same for sufficiently high energy in the other cases. If we turn to comparing states of different l, then s states are more disturbed than p states, and so forth. One can appreciate that difference particularly well if one assumes x sufficiently small to permit power series development of the Bessel and Neumann functions. We get in that case from (21)

$$k = n + \left(1-\frac{1}{n^2}\right)\left(1-\frac{4}{n^2}\right)\cdots\left(1-\frac{l^2}{n^2}\right) \times \frac{(\frac{1}{2}x)^{4l+4}}{(2l+1)!(2l+3)!},$$

where n is the next lower integer, i.e., the principal quantum number in the correct sense of the word. The limiting formula for large x is also very simple if the Bessel and Neumann functions can be replaced by their trigonometric equivalents and if the ratio of factorials can be set equal to 1. We get

$$k = n + (x/2\pi) - \tfrac{1}{2}l - \tfrac{1}{4}.$$

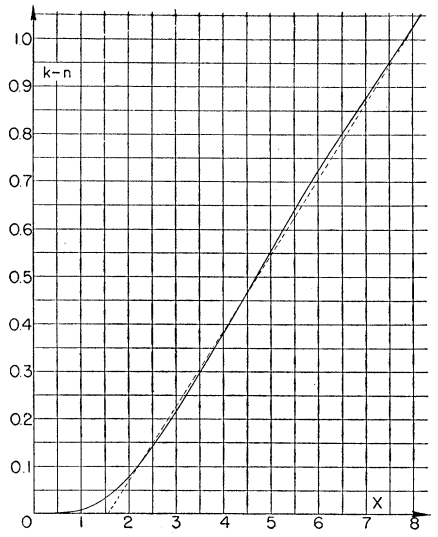

FIG. 4. Plotting energy against cut-off radius according to Eq. (22). The abscissa x goes as the square root of the radius [Eq. (3)] and the ordinate contains the difference of the principal quantum number n and a number k which must be substituted into the Balmer formula to give the energy levels. The graph applies only to s states under the restriction (17).

The validity of this formula is somewhat restricted because x must be large compared to l, yet condition (17) must not be broken. A graphical evaluation of formula (22), plotting $k-n$ against x for s states is given in Fig. 4. One sees that the curve oscillates about the asymptote which we discussed just above.

3. A MORE PRECISE SOLUTION FOR s STATES

It has been pointed out that the solution of Section 2 is correct if condition (17) holds while only condition (18) is fulfilled in many actual cases. In this section, we shall improve Eq. (22) by applying various corrections to the approximation (20), so as to make it quantitatively correct everywhere except in the immediate neighborhood of $x=4k$.

When one studies the approximate wave functions (20) numerically and compares them with the Schrödinger eigenfunctions in the case of integer k, one finds of course complete disagreement beyond $x=4k$. Below that point the two functions show the same general structure, but vary somewhat in detail. It is possible to cancel out most of this discrepancy by the following two steps.

In the first step, we carry out a change in the abscissa scale so as to bring the nodes of the true wave function and its approximation to coincidence; i.e., we write the wave function in the form

$$F=x_kZ_1(x_k),$$

where $Z_1(x)$ stands for the linear combination (20) of Bessel and Neumann functions. x_k is an unknown function of x differing from it very little as long as condition (17) holds. If we introduce a corresponding r_k through (3) we get for F the equation

$$\left(\frac{d^2F}{dr_k^2}\right)+\left(\frac{2\alpha}{r_k}\right)F=0,$$

while as a function of r, it obeys Eq. (2),

$$\frac{d^2F}{dr^2}+\left(-\frac{\alpha^2}{k^2}+\frac{2\alpha}{r}\right)F=0.$$

These two equations give for r_k as a function of r

$$-\frac{\alpha^2}{k^2}+\frac{2\alpha}{r}=\frac{2\alpha}{r_k}\left(\frac{dr_k}{dr}\right)^2-\frac{1}{F}\frac{dF}{dr_k}\frac{d^2r_k}{dr^2}.$$

It is approximately correct to leave off the second term on the right-hand side because $(1/F)(dF/dr_k)$ is an expression of alternating sign which will make little long range contribution to $(dr_k/dr)^2$. The remainder of the equation reads then

$$\frac{dr_k}{dr}=r_k^{\frac{1}{2}}\left(\frac{1}{r}-\frac{\alpha}{2k^2}\right)^{\frac{1}{2}}$$

or passing over to x coordinates with the help of (3)

$$\frac{dx_k}{dx}=\left(1-\frac{x^2}{16k^2}\right)^{\frac{1}{2}}$$

which integrates to

$$x_k=\tfrac{1}{2}x\left(1-\frac{x^2}{16k^2}\right)^{\frac{1}{2}}+2k\arcsin\frac{x}{4k}. \qquad (23)$$

TABLE I. Approximations of the $2s$ eigenfunction.

$2\alpha r$	x	$F_{(20)}$	$F_{(23)}$	F
0	0.000	0.000	0.000	0.000
1	2.000	1.154	1.168	1.168
4	4.000	−0.264	0.010	0.000
6	4.899	−1.540	−1.308	−1.337
8	5.657	−1.861	−2.181	−2.164
9	6.000	−1.660	−2.414	−2.370
12	6.928	−0.180	−2.642	−2.392
16	8.000	1.876	$-\infty$	−1.758

The behavior of x_k/k as a function of x/k is shown in Fig. 5. At first, they are very similar, but as the latter approaches 4, the former falls back and approaches π with zero slope.

This correction brings the nodes quite well to coincidence. One finds now the main discrepancy in the size of the loops, the true loops increasing somewhat more sharply with r than the approximate ones. To correct this, we introduce as our second step an unknown factor f into the wave function, writing

$$F=f\cdot\Phi,$$

where

$$\Phi=x_kZ_1(x_k).$$

It is clear from the purpose of the correction that f may be assumed to vary slowly compared to Φ. Substituting into (2) and using the equation for Φ, *viz.*,

$$\frac{d^2\Phi}{dr^2}-\frac{d^2r_k/dr^2}{dr_k/dr}\frac{d\Phi}{dr}+\left(-\frac{\alpha^2}{k^2}+\frac{2\alpha}{r}\right)\Phi=0,$$

we find

$$\frac{d^2f}{dr^2}\Phi+\left\{2\frac{df}{dr}+f\frac{d^2r_k/dr^2}{dr_k/dr}\right\}\frac{d\Phi}{dr}=0.$$

According to our assumption, the first term can be neglected compared to the others and we get

$$f=\left(\frac{dr_k}{dr}\right)^{-\frac{1}{2}}=\frac{x}{x_k^{\frac{1}{2}}x_k^{*\frac{1}{2}}}, \tag{24}$$

where we have introduced the abbreviation

$$x_k^*=\frac{dx_k}{dx}x=x\left(1-\frac{x^2}{16k^2}\right)^{\frac{1}{2}}. \tag{25}$$

Thus we get finally for F

$$F=xx_k^{\frac{1}{2}}x_k^{*-\frac{1}{2}}\{J_1(x_k)\cos k\pi+N_1(x_k)\sin k\pi\}. \tag{26}$$

It is perhaps worth while to explain the corrections of this section by physical reasoning. The function

$$xZ_1(x)$$

is the correct solution of (2) for zero energy. According to the Wentzel-Kramers-Brillouin approximation, the true wave function for a negative energy state must differ from it on two counts:

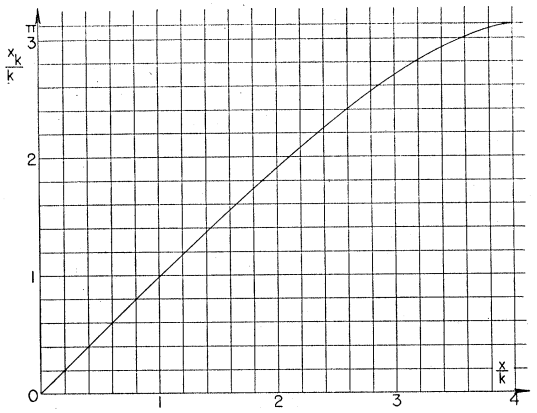

FIG. 5. Plotting the scale-corrected argument x_k against the true x [Eq. (23)]. x_k must be used instead of x as the argument in the Bessel or Neumann function to make our approximation quantitatively correct. It is an essential feature of the method that it does not extend beyond $x=4k$.

(a) The wave-length, obeying De Broglie's relation, must be longer. This reasoning leads to a change in the abscissa scale which agrees exactly with (23).

(b) The amplitude of the wave function is inversely proportional to the square root of the classical velocity. Hence we should multiply our wave function with a factor f which equals

$$f=\left(\frac{\text{false velocity at false position}}{\text{right velocity at right position}}\right)^{\frac{1}{2}}.$$

This formula reproduces exactly (24).

It is an inevitable consequence of such reasoning that the corrected wave function breaks down at $x=4k$ because this is the limit of the classical orbit. But until the neighborhood of that point is reached, the approximation is greatly improved numerically. To illustrate this fact, the Schrödinger wave function for the $2s$ state is given in Table I, and the approximations (20) and (26) are compared with it.

Fitting the wave function (26) to the wave function (15) at the point $x=x_0$ is now a straightforward matter. One finds

$$\tan k\pi=-\frac{J_0(x_k)\sin\frac{1}{2}x_k^*-J_1(x_k)\cos\frac{1}{2}x_k^*+\frac{1}{2}\{(x^2/x_k^{*3})-(1/x_k)\}J_1(x_k)\sin\frac{1}{2}x_k^*}{N_0(x_k)\sin\frac{1}{2}x_k^*-N_1(x_k)\cos\frac{1}{2}x_k^*+\frac{1}{2}\{(x^2/x_k^{*3})-(1/x_k)\}N_1(x_k)\sin\frac{1}{2}x_k^*}. \tag{27}$$

x_k and x_k^* are derived from the cut-off coordinate $x=x_0$ by the formulas (23) and (25). x_0 itself is derived from r_0 through (15).

Formula (27) is of course less convenient to use than (22) because the unknown k is contained implicitly in the right-hand expression. That expression varies, however, much more slowly with k than the left (except in the excluded case when x is very close to $4k$) and hence the formula is suitable for successive approximations, starting with an approximate k on the right. One or two steps are amply sufficient to get the answer.

Applying the formula to the case of Tibbs[2] we get

$$k=1.153 \quad \text{for the } 1s \text{ state}$$
$$k=2.159 \quad \text{for the } 2s \text{ state}$$

in complete agreement with his results.

4. SOLUTION FOR OTHER STATES

The method of Section 3 is applicable in the same form to states of non-vanishing angular momentum. We shall restrict ourselves therefore to the discussion of new features and the quotation of results.

Following the same reasoning as previously we are led to an equation for the scale-corrected radius r_{kl}

$$\left(\frac{dr_{kl}}{dr}\right)^2=\frac{\dfrac{2\alpha}{r_{kl}}-\dfrac{l(l+1)}{r_{kl}^2}}{\dfrac{2\alpha}{r}-\dfrac{l(l+1)}{r^2}-\dfrac{\alpha^2}{k^2}}.$$

We notice that this expression is considerably more involved than in the previous case. This is explained with the help of Fig. 6, which shows the potential for radial motion. In the actual negative energy state the classical orbit has now an inner limit b as well as an outer limit c which are the two roots of the denominator above; and the zero-energy orbit has an inner limit a, which is the root of the numerator. It follows from this that r_{kl} will be a complex function of r unless the constant of integration is picked in such a way that when

$$r=b$$

then

$$r_{kl}=a.$$

Such a choice has the additional advantage that it brings the first inflexion points of the approximate and the true F automatically to coincidence. We find thus

$$(r_{kl}-a)^{\frac{1}{2}}-a^{\frac{1}{2}}\arctan\left(\frac{r_{kl}-a}{a}\right)^{\frac{1}{2}}=\tfrac{1}{2}\left(\frac{(r-b)(c-r)}{b+c}\right)^{\frac{1}{2}}+\tfrac{1}{2}(b+c)^{\frac{1}{2}}\arctan\left(\frac{r-b}{c-r}\right)^{\frac{1}{2}}-a^{\frac{1}{2}}\arctan\left[\frac{\dfrac{1}{b}-\dfrac{1}{r}}{\dfrac{1}{r}-\dfrac{1}{c}}\right]^{\frac{1}{2}}. \quad (28)$$

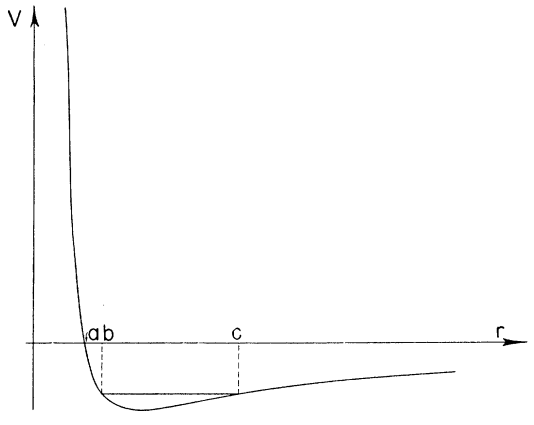

FIG. 6. Radial potential for a particle having non-vanishing angular momentum which moves under the influence of a Coulomb force.

The new formula is seen to go over into (23) in the special case when $a=b=0$.

No special difficulty arises in the determination of the factor f. If we define as in (3)

$$x_{kl}=2(2\alpha r_{kl})^{\frac{1}{2}} \quad (29)$$

and as in (25)

$$x_{kl}^*=\frac{dx_{kl}}{dx}x=x\left[\frac{1-\dfrac{4l(l+1)}{x^2}-\dfrac{x^2}{16k^2}}{1-\dfrac{4l(l+1)}{x_k^2}}\right]^{\frac{1}{2}}, \quad (30)$$

then we get for the wave function F:

$$F=xx_{kl}^{\frac{1}{2}}x_{kl}^{*-\frac{1}{2}}Z_{2l+1}(x_{kl}),$$

where $Z_{2l+1}(x)$ is a combination of Bessel and Neumann functions of order $2l+1$. It seems logical to follow the procedure that led to (26), that is, to substitute for Z the linear combination (20). However, such a procedure is incorrect because the substitution of x_{kl} for x has brought in some constant factors. x_{kl}, through (28), (29), and (3), is a regular function of x right through the inner limit point of the orbit $x_{kl}=2[l(l+1)]^{\frac{1}{2}}$; the same applies to x_{kl}^* as defined by (30). They both are also equal to zero simultaneously with x, and their ratio x_{kl}^*/x_{kl}, tends to 1 in that limit; but the ratio x_{kl}/x does not do so. We find

$$\lim_{x=0}\frac{x_{kl}}{x}=\left[\frac{\left(1+\dfrac{[l(l+1)]^{\frac{1}{2}}}{k}\right)^{\{k/[l(l+1)]^{\frac{1}{2}}\}+1}}{\left(1-\dfrac{[l(l+1)]^{\frac{1}{2}}}{k}\right)^{\{k/[l(l+1)]^{\frac{1}{2}}\}-1}\cdot e^2}\right]^{\frac{1}{2}}$$

which is a quantity lying between 1 and 0.8578. Now the Bessel-like and Neumann-like functions are characterized by their behavior at the origin where they are to behave as

$$\frac{(\frac{1}{2}x)^{2l+1}}{(2l+1)!}\quad\text{and}\quad-\frac{(2l)!(\frac{1}{2}x)^{-2l-1}}{\pi},$$

respectively. Hence, if we define

$$C_{kl}=\left[\frac{\left(1-\dfrac{[l(l+1)]^{\frac{1}{2}}}{k}\right)^{\{k/[l(l+1)]^{\frac{1}{2}}\}-1}\cdot e^2}{\left(1+\dfrac{[l(l+1)]^{\frac{1}{2}}}{k}\right)^{\{k/[l(l+1)]^{\frac{1}{2}}\}+1}}\right]^{l+\frac{1}{2}},\qquad(31)$$

we get F equal to

$$F=xx_{kl}^{\frac{1}{2}}x_{kl}^{*-\frac{1}{2}}\left\{C_{kl}^{\frac{1}{2}}J_{2l+1}(x_{kl})\cos k\pi+C_{kl}^{-\frac{1}{2}}\frac{(k-l-1)!k^{2l+1}}{(k+l)!}N_{2l+1}(x_{kl})\sin k\pi\right\}.\qquad(32a)$$

A comparison of the Schrödinger wave function with its approximation (32a) is carried out in Table II. The factor C_{kl} equals 1.424 in this case and could certainly not be neglected.

TABLE II. Comparison of the $4d$ wave function with approximation (32a).

x^2	x^2_{kl}	$F_{(32a)}$	F
0.0	0.0	0.000	0.000
26.8	24.0	0.782	0.782
50.0	43.2	1.639	1.632
80.0	65.6	0.940	0.913
120.0	91.5	−1.295	−1.323
160.0	112.5	−2.53	−2.39
229.2	132.6	∞	

To get our equation for k we must fit (32) to (14) at the cut-off. The result is

$$\tan k\pi=-C_{kl}\frac{(k+l)!}{(k-l-1)!k^{2l+1}}\cdot\frac{J_{2l}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)-J_{2l+1}(x_{kl})J_{l-\frac{1}{2}}(\frac{1}{2}x_k^*)\dfrac{x_k^*}{x_{kl}^*}+\psi J_{2l+1}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)}{N_{2l}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)-N_{2l+1}(x_k)J_{l-\frac{1}{2}}(\frac{1}{2}x_k^*)\dfrac{x_k^*}{x_{kl}^*}+\psi N_{2l+1}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)}.\qquad(33a)$$

The factor ψ equals

$$\psi=\frac{2l+1}{x_{kl}^*}-\frac{2l+1}{x_{kl}}+\frac{1}{2\left(1-\dfrac{4l(l+1)}{x_{kl}^2}\right)}\times\left(\frac{1}{x_{kl}}+\frac{x^2}{x_{kl}^{*3}}-2\frac{x_k^{*2}}{x_{kl}^{*3}}\right).\qquad(34)$$

In spite of appearances to the contrary, the factor ψ tends to zero for small x and remains finite for $x_k=2[l(l+1)]^{\frac{1}{2}}$. The variables entering into (33a) and (34) are defined in (3), (25), (28), (29), (30), and (31).

It is an interesting accident that the factor entering (33a), namely,

$$C_{kl}\frac{(k+l)!}{(k-l-1)!k^{2l+1}},$$

is almost 1 for all possible values of k and l.

For instance, for $k=2$, $l=1$, we find 1.011, for $k=3$, $l=1$, we find 1.002 and so on. It reaches its largest value for $k=\infty$, $l=k-1$, namely, 1.074, while for $l\leqq k-2$, it is smaller than 1.026. Thus we may often neglect it entirely, and write for F, apart from a constant factor

$$F=xx_{kl}^{\frac{1}{2}}x_{kl}^{*-\frac{1}{2}}\{J_{2l+1}(x_{kl})\cos k\pi + N_{2l+1}(x_{kl})\sin k\pi\} \quad (32b)$$

and instead of (33a)

$$\tan k\pi=-\frac{J_{2l}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)-J_{2l+1}(x_{kl})J_{l-\frac{1}{2}}(\frac{1}{2}x_k^*)\dfrac{x_k^*}{x_{kl}^*}+\psi J_{2l+1}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)}{N_{2l}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)-N_{2l+1}(x_{kl})J_{l-\frac{1}{2}}(\frac{1}{2}x_k^*)\dfrac{x_k^*}{x_{kl}^*}+\psi N_{2l+1}(x_{kl})J_{l+\frac{1}{2}}(\frac{1}{2}x_k^*)}. \quad (33b)$$

If we apply Formula (33) to the $2p$ state studied by Tibbs[2] we find

$$k=2.004.$$

The approximate formula (21) gives

$$k=2.005.$$

Unfortunately a check with his result does not mean very much here because his value may lie anywhere between 2.00 and 2.041.

It seems to the author that the elimination of purely numerical work in quantum mechanics is very desirable because of the greater generality gained. The present paper makes the cut-off Coulomb field an analytically soluble case except for energy levels which are so close to the cut-off in the potential energy that only an exponential tail is situated beyond the cut-off radius. More precise criteria, together with formulas to replace (21), (27), and (33) will be given in another paper.

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Theory of Static Fields

I. A Phenomenological Attempt to Determine the Proper Field of an Electron

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According to the phenomenological theory of quantum fields, fluctuation phenomena correspond even to the lowest energy state of a system. The average value of field quantities is zero in the case of a vacuum. This value changes, however, if we introduce a particle into the field. The determination of the average value of the field fluctuation leads immediately to the expressions of the proper field of an electron. The calculation becomes considerably simplified by an appropriate use of Dirac's theory.

A. INTRODUCTION

1. Purpose of the Paper

IT is well known that classical theory does not represent, so far, a consistent scheme of physical phenomena, even if we apply it to a simple problem as the problem of the motion of an electron. Even the value of kinetic energy of an electron cannot be obtained from classical physics in a satisfactory way since the value given by the mechanical picture does not agree at all with the value one would expect from the transformation properties of static electromagnetic fields.