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The Solution of the Schrödinger Equation for an Approximate Atomic Field*

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An approximate atomic potential having an "effective nuclear charge for potential," that is, bilinear in the radial distance from the nucleus, is discussed and shown to approximate reasonably well to Hartree or Fermi-Thomas potentials. The Schrödinger equation with the approximate potential is solved as a series of hydrogenic wave functions and as a power series in $Ar/(1+Ar)$ (A being a parameter of the potential). Some illustrative numerical results pertaining to the mercury atom are presented.

1. THE APPROXIMATE POTENTIAL

THE atomic potentials[1] $-Z_p(r)/r$ of Hartree and Fermi-Thomas may be represented adequately for many purposes through the simple formula for Z_p,

$$Z_{pA}=Z/(1+Ar).$$

Figure 1 gives a comparison of the different potentials for the mercury atom.[2]

Figure 2 tests the formula by showing $A(r)=(Z/Z_p-1)/r$ as a function of r for different atoms, Z_p being that given by Hartree.[3] It is seen that Z_{pA} is quite satisfactory out to radii for which Z_p is from 10 to 20 percent of Z, and is certainly too big beyond these radii. An analysis of the curves in the regions where they are flat shows that a good average value for A is $1.525Z^{1/3}$. The approximate potential may of course be improved substantially by adding terms with higher powers of r in the denominator of Z_{pA}; usually a quadratic and a cubic term suffice to give high accuracy over essentially the whole range of r. However, the cost of this in extra mathematical complexity is too great for any but the simplest of atomic calculations.

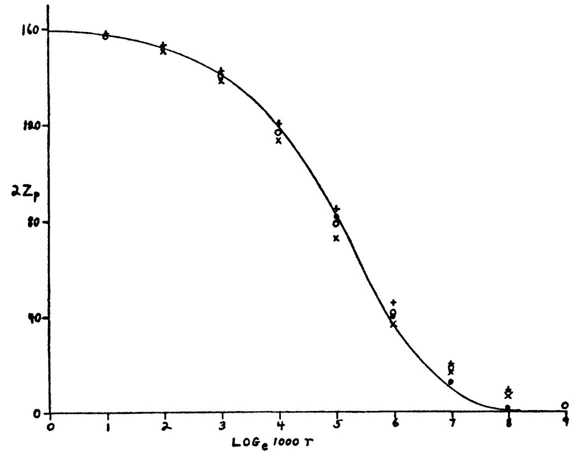

FIG. 1. Comparison of Z_p's for mercury. Smooth curve: Hartree $2Z_p$; ● = Fermi-Thomas $2Z_p$; $\times=2Z_{pA}$ for $A=8$; ○ $=2Z_{pA}$ for $A=7$; $+=2Z_{pA}$ for $A=6$.

The Fermi-Thomas φ function, satisfying $x^{1/2}\varphi''=\varphi^{3/2}$ with $r=0.88534x/Z^{1/3}=bx$, is given by $\varphi_A=(1+Abx)^{-1}$ in our approximation. Figure 2 gives $Ab=(\varphi^{-1}-1)/x$ (φ being that for a neutral atom) as a function of x. A comparison of the expansions of φ and φ_A near the origin shows that $A(Z)\simeq 1.79Z^{1/3}$, while direct substitution of φ_A in the Fermi-Thomas equation shows that $A\simeq 1.34Z^{1/3}$ for x near $2^{1/3}/3=0.42$. The solutions φ_0 of the Fermi equation corresponding to positive ions, i.e., those which are zero at a finite x, say, x_0, may be simply and precisely approximated for all x by $\varphi_q=(1-x/x_0)/(1+qx)$, where q depends (although insensitively) on x_0. This is tested in Fig. 2, where $q=(1-x/x_0-\varphi_0)/(\varphi_0 x)$ is plotted against x for a few x_0's. The parameter q could be calculated from the Fermi-Thomas boundary condition $x_0\varphi'(x_0)=(N-Z)/Z$, N being the number of electrons in the ion, but this gives a spurious q value because φ_q does not have the right slope at x_0. The φ_q has an accuracy comparable to that of the relatively complicated Sommerfeld[4] approximate solution of the Fermi equation. Also, the error in φ_q as a representation of φ_0 is mainly in the

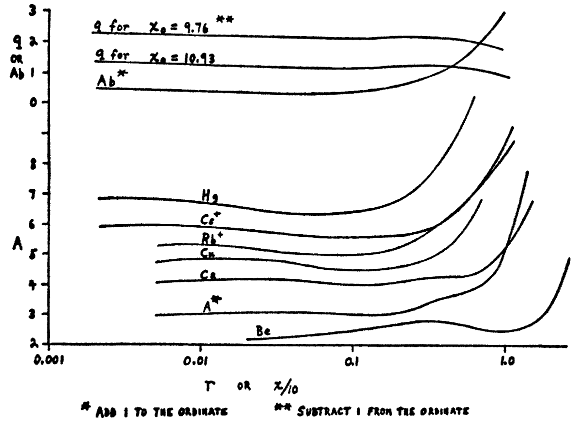

FIG. 2. The upper two curves show q as a function of $x/10$; x is the Fermi-Thomas variable and x_0 is the ionic radius. The next curve shows Ab as a function of $x/10$ using the Fermi-Thomas function φ for neutral atoms. The lower seven curves show A as a function of r for different atoms, using values of Z_p given by Hartree.

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* Some of this work was a part of the author's doctoral thesis at Cornell University.

[1] Atomic units will be used throughout the discussion.

[2] D. R. Hartree, Phys. Rev. **46**, 743 (1934); Proc. Roy. Soc. (London) **149**, 210 (1935).

[3] D. R. Hartree, Proc. Cambridge Phil. Soc. **24**, 89 (1928); Proc. Roy. Soc. (London) **143**, 506 (1934) and **166**, 450 (1938).

[4] A. Sommerfeld, Z. Physik, **78**, 283 (1932).

direction of making it more "Hartree-like" if q is given a value which makes φ_0 and φ_q agree at smaller r, since then φ_q is somewhat smaller than φ_0 for large r while φ_0 is somewhat larger than the Hartree function for such r.

Our final potential for an ion is now

$$-V_a=\frac{Z(1-r/r_0)}{r(1+ar)}+\frac{Z-N}{r_0}\qquad r<r_0$$
$$=(Z-N)/r\qquad r>r_0,$$

where r_0 is the ionic radius and $a=q/b\sim Z^{\frac{1}{3}}$. In the special case where r_0 is large we get the potential $-V_A(r)=Z/r(1+Ar)$. For the present, we shall principally discuss V_A as a generator of Schrödinger wave functions, postponing a consideration of Dirac functions as well as a more extensive treatment of V_a and of various atomic calculations for a later report. Since V_A is close to the Hartree potential over a range of r where most wave functions have their largest amplitudes, we may expect V_A to yield a set of useful functions for electrons in the atomic core but not in the outermost shells. Without too serious consequences we will not distinguish between separate potentials for separate electron groups and the approximate potential itself. Our wave functions therefore will be orthogonal. Some evaluation of the accuracy of wave functions calculated with V_A is provided by a work of Slater,[5] who has shown that empirical approximations (correct to within about one percent) to Hartree functions are generated by potentials which, compared with the Hartree potentials, are very poor at large r and for r in the vicinity of the roots of his functions, sometimes being off by a factor of two or more and having the wrong sign as well. It is to be presumed that the wave functions arising from V_A are in many cases sufficiently close to Hartree functions.

2. THE SOLUTION OF THE WAVE EQUATION

For the potential V_A we may write the radial wave function in the usual way as $R=r^le^{-\epsilon r}g(r)$ with $\epsilon=+(-2E)^{\frac{1}{2}}$. Then, introducing the independent variable $x=Ar$ and the abbreviations $\alpha=\epsilon/A$ and $\beta=Z/A$, the differential equation for g is

$$\frac{d^2g}{dx^2}+\frac{dg}{dx}\left\{\frac{2(l+1)}{x}-2\alpha\right\}+g\left\{\frac{2\beta}{x(1+x)}-\frac{2\alpha(l+1)}{x}\right\}=0,$$
$$0\leq x\leq\infty\qquad(1)$$

This is a confluent form of the Heun differential equation,[6] having regular singularities at $x=0$ and $x=-1$, and an irregular singularity at infinity. In the case that $\alpha=0$, (1) is a hypergeometric equation. If $l=0$, (1) may be reduced by the transformations $g=e^{\alpha x}(1+x)f(x)$, $z=1+2x$ to a case of the spheroidal wave equation studies in detail by Chu and Stratton.[7] A confluent Heun equation arises also in the hydrogen molecule ion problem,[8] which is mathematically closely related to the present one. It will be observed that for either of the potentials V_A or V_a the integrals of the WKB approximation may be evaluated in terms of the standard elliptic integrals, since the integrand is a rational function of r and the square root of a quartic polynomial in r.[9]

The eigensolutions to (1) may be conveniently expanded in hydrogenic functions, as in perturbation theory. This has the advantage that the largest terms can often be picked out. Instead of the Laguerre polynomials proper, we will use the equivalent confluent fluent hypergeometric polynomials. Setting

$$g=\sum_{\nu=0}^{\infty}c_\nu F(-\nu,\,2l+2,\,2\alpha x),$$

and using the recurrence formulas for the F functions, it is found that the c_ν are given by the recurrence relation

$$c_{\nu+1}(\nu+1)(\nu+l+2)/2+c_\nu\{\beta-\alpha(l+\nu+1)-(l+\nu+1)^2\}$$
$$+c_{\nu-1}(\nu+l)(\nu+2l+1)/2\quad \nu=0,1,2,\cdots;c_{-1}=0.\qquad(2)$$

A more general potential, involving higher powers of r in Z_{pA} as mentioned before, may be treated similarly through repeated application of the recurrence formulas for the F functions; each successive additional power of r beyond the first, in either the numerator or denominator of Z_{pA}, gives two extra terms in the recurrence formulas for the c_ν. The convergence of expansions of the present kind, when α is an eigenvalue, has been proven by McCrea and Newing.[10]

Another useful expansion is suggested by Jaffe's[11] discussion of the hydrogen molecule ion problem. In (1), let $g=(1+x)^{-l-1}h(x)$ and then let $\xi=x/(x+1)$. Then

$$\xi(1-\xi)^2h''+\{2(l+2)\xi^2-2(\alpha+2l+3)\xi+2(l+1)\}h'$$
$$+\{2\beta-2\alpha(l+1)-2(l+1)^2+(l+1)(l+2)\xi\}h=0,$$
$$0\leq\xi\leq1.$$

Developing h in a power series about the origin, $h=\sum_{\nu=0}^{\infty}a_\nu\xi^\nu$, it is found, upon substitution in the differential equation and after some reduction, that the a_ν are given by

$$\tfrac{1}{2}(\nu+1)(\nu+2l+2)a_{\nu+1}+\{\beta-\alpha(\nu+l+1)$$
$$-(\nu+l+1)^2\}a_\nu+\tfrac{1}{2}(\nu+l)(\nu+l+1)a_{\nu-1}=0,$$
$$\nu=0,1,2,\cdots;\quad a_{-1}=0.$$

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[5] J. C. Slater, Phys. Rev. 42, 33 (1932).

[6] E. L. Ince, *Ordinary Differential Equations* (Longmans, Green and Company, London, 1927), p. 394.

[7] L. J. Chu and J. A. Stratton, J. Math. Phys. **20**, 259 (1941).

[8] W. G. Baber and H. R. Hasse, Proc. Cambridge Phil. Soc. **31**, 564 (1935).

[9] E. T. Whittaker and G. N. Watson, *Modern Analysis* (The Macmillan Company, New York, 1943), article 22.7.

[10] McCrea and Newing, Proc. London Math. Soc. **37**, 520 (1934).

[11] G. Jaffe, Z. Physik **87**, 535 (1935).

If now one sets $a_\nu = b_\nu f(\nu)$ and determines $f(\nu)$ so that $f(\nu+1)/f(\nu) = (\nu+l+2)/(\nu+2l+2)$, i.e., so that

$$f(\nu) = \binom{l+\nu+1}{\nu} \Big/ \binom{2l+\nu+1}{\nu},$$

then b_ν satisfies just the same difference equation as the c_ν of Eq. (2). As in the hydrogen molecule ion problem, the series is convergent for all ξ in $0 \leq \xi \leq 1$. Thus, the evaluation of *one* set of expansion coefficients provides *two* representations of the wave function.

The solutions to (1) may also be expanded in series of bessel functions, in powers of $(1+Ar)^{-1}$, and in other ways. For the potential V_a, an expansion of the wave function R in powers of $(1-r/r_0)/(1+ar)$ (for $r < r_0$) is convenient, since the boundary conditions of a smooth junction of R at r_0 with the hydrogenic solution beyond r_0 is easily met by specifying the first two expansion coefficients.

In a three-term recurrence formula such as (2), the eigenvalues of α must be found before the formula can be used to compute the c_ν. Formulas of this type are ordinarily handled by a method of continued fractions first used by Ince[12] in connection with Mathieu's equation. The method was improved by Bouwkamp[13] for use with the spheroidal wave equation. Although applicable in principle to most second-order difference equations, this method turns out to be uncommonly awkward in practice for Eq. (2). Alternatively, (2) may be looked upon as an infinite set of linear equations in the c_ν. For the self-consistency of the equations, the determinant Δ of the coefficients of the c_ν must be zero. Then $\Delta(\alpha) = 0$ is a transcendental equation in α whose roots are the eigenvalues. Since c_{n-l-1} may be expected to be among the largest c_ν, n meaning the principal quantum number, the determinant can be conveniently written around the "main term" $\beta - \alpha n - n^2$.

As a zeroth approximation to $\Delta = 0$, one may take $\beta - \alpha n - n^2 = 0$, so that $\epsilon_0 = Z/n - nA$. In the limit $A = 0$ we have then the hydrogenic value for ϵ. A much better approximation would be

$$\begin{vmatrix} \beta - \alpha(n-1) - (n-1)^2, & n(n-1-l)/2, & 0 \\ (n-1)(n+l)/2 \quad, & \beta - \alpha n - n^2 \;, & (n-l)(n+1)/2 \\ 0 \quad, & n(n+l+1)/2, & \beta - \alpha(n+1) \\ & & -(n+1)^2 \end{vmatrix} = 0. \tag{3}$$

This mode of expanding the determinant is like that used for the infinite determinant for characteristic values arising from Hill's differential equation.[14] An approximate root of (3) is found explicitly by introducing $\alpha_0 = \epsilon_0/A$ into the corner terms of the determinant. The result is

$$\epsilon_1 = \frac{Z}{n} - nA + \frac{A^2}{4} \frac{(n+l+1)(n-l)(n+1)}{(Z/n) + (n+1)A} - \frac{A^2}{4} \frac{(n-l-1)(n+l)(n-1)}{(Z/n) + (n-1)A}. \tag{4}$$

Equations (3) and (4) are useful for quickly obtaining approximate eigen-ϵ.

The roots of the infinite determinant may be calculated with arbitrary accuracy with the following technique. First, rewrite (2) for simplicity as

$$c_{\nu-1} d_{\nu,\,\nu-1} + c_\nu d_{\nu\nu} + c_{\nu+1} = 0,$$

$$d_{\nu,\,\nu-1} = \frac{(\nu+l)(\nu+2l+1)}{(\nu+1)(\nu+l+2)},$$

$$d_{\nu\nu} = \frac{2[\beta - \alpha(\nu+l+1) - (\nu+l+1)^2]}{(\nu+1)(\nu+l+2)},$$

so that the characteristic equation for α is

$$\Delta = \begin{vmatrix} d_{00} & 1 & 0 & \cdots & & & & \\ d_{10} & d_{11} & 1 & 0 & \cdots & & & \\ 0 & d_{21} & d_{22} & 1 & \cdots & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \\ & \cdots & 0 & d_{m,\,m-1} & d_{m,\,m} & 1 & 0 & \cdots \\ & & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix} = 0.$$

The determinant of the $(m+1)$th order, Δ_{m+1}, equal to Δ with all rows and columns beyond the mth omitted, may be expanded in minors starting at the lower right-hand corner where d_{mm} is situated:

$$\Delta_{m+1} = d_{mm}\Delta_m - d_{m,\,m-1}\Delta_{m-1}. \tag{5}$$

With the conventions $\Delta_0 = 1$, $\Delta_1 = d_{00}$, (5) permits the computation in succession of the determinants Δ_m up to any order desired. Let α_0 be an approximate root of Δ. Performing a variation of (5) with respect to α, one has

$$\delta\Delta_{m+1} = \Delta_m \delta d_{mm} + d_{mm}\delta\Delta_m - d_{m,\,m-1}\delta\Delta_{m-1}$$

$$\delta d_{mm} = \frac{-2(l+m+1)}{(m+1)(m+l+2)}\delta\alpha. \tag{6}$$

With the approximate α_0, the Δ_m and $\delta\Delta_m$ may be found in succession, and for sufficiently large m it can be required that

$$\Delta_{m+1}(\alpha_0 + \delta\alpha) = \Delta_{m+1}(\alpha_0) + \frac{\delta\Delta_{m+1}}{\delta\alpha}\delta\alpha = 0,$$

which determines a correction $\delta\alpha$ to α_0. The $\delta\alpha$ deduced in this way turn out to be remarkably independent of m beginning at relatively low m (see Table I), so that a good value for α can be found with little

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[12] E. L. Ince, Phil. Mag. **6**, 547 (1928).

[13] C. J. Bouwkamp, J. Math. Phys. **26**, 79 (1947).

[14] Reference 9, §19.42.

TABLE I. Example of calculation of eigenvalues and expansion coefficients; $Z=80$, $1S$ state, $A=1/.145$, $\beta=11.6$.

m	d_{mm}	Δ_{m+1}	$\delta\Delta_{m+1}/\delta\alpha$	$\delta\alpha$	$d_{m+1,m}$	$2/m+2$
Initial $\alpha=10.673$						
0	-0.0730	$-0.0730\ \_$	$-1.0\ \_$		$0.3\bar{3}$	$1.0\_$
1	$-4.5820\_$	$0.001152\bar{6}$	$4.630\bar{6}$		0.5	$0.6\bar{6}$
2	$-4.9031\bar{6}$	0.03084828	-22.205506	$+1.3892\times10^{-3}$	$0.6\_$	0.50
3	-4.70920	-0.14596234	101.77943	$+1.4341\times10^{-3}$	$0.6\bar{6}$	$0.4\underline{0}$
4	$-4.451\underline{0}$	0.62911285	-438.16792	$+1.4358\times10^{-3}$	0.71428571	$0.3\bar{3}$
5	$-4.211\bar{3}$	-2.5451451	1772.3918	$+1.4360\times10^{-3}$	$0.7\underline{5}0$	0.28571428
6	$-4.003\underline{9}643$	9.7188354	-6767.3314	$+1.4361\times10^{-3}$	$0.7\bar{7}$	$0.2\underline{5}0$
7	$-3.827\bar{3}$	-35.217665			0.8	$0.2\bar{2}$
			$\delta\alpha=+1.44\times10^{-3}$			
New $\alpha=10.67444$					$\delta\Delta_{m+1}$	$\Delta_{m+1}\vert$corr.
0	-0.07444	-0.07444	-1.0		$+5.02432\times10^{-6}$	-7.443498×10^{-2}
1	$-4.58296\underline{0}$	0.007822209	4.6325867		-2.32756×10^{-5}	$+7.798933\times10^{-3}$
2	$-4.90388\bar{6}$	-0.001139227	-22.221591		$+1.11648\times10^{-4}$	-1.027578×10^{-3}
3	-4.7097760	0.0006721776	101.87962	-6.5978×10^{-6}	-5.11876×10^{-4}	$+1.60301\times10^{-4}$
4	-4.4514800	-0.002232700	-438.70092	-5.0893×10^{-6}	$+2.20426\times10^{-3}$	-2.8434×10^{-5}
5	-4.2117448	0.008923438	1774.9258	-5.0275×10^{-6}	-8.91780×10^{-3}	$+5.634\times10^{-6}$
6	-4.0043243	-0.034057814	-6778.3550	-5.0245×10^{-6}	$+0.0340566$	-1.15×10^{-6}
7	-3.8276533	0.12342105	24564.703	-5.0243×10^{-6}	-0.12342	$+0\times10^{-5}$
			$\delta\alpha=-5.0243\times10^{-6}$			
Final $\alpha=10.674434976$						

labor. With obvious modifications this method could be applied to any three-term recurrence relation like (2). The similarity to Bouwkamp's method will be evident. It follows from Eqs. (2) and (5) that $c_\nu=(-1)^\nu\Delta_\nu$; hence the calculations may be performed directly with the c_ν.

The approximate c_ν (or Δ_ν) computed with the approximate α can be easily corrected after $\delta\alpha$ has itself been determined. An illustrative example is given in Table I for the $1S$ state of mercury assuming $A=1/0.145=6.896$ and $\beta=Z/A=11.6$. As in the example, one characteristically finds that the Δ_m diverge in opposite senses for α which are slightly above or below the correct value. This provides a good check on the calculations. Another check comes from the fact that $\delta\alpha$ may be found at every step, and for a good initial α is observed to converge rapidly to a limit. If the initial α is poor, this convergence is poor, and it is best to correct α before going too far and to start over. Not more than one or two such iterations, depending on the accuracy sought, provides both an eigenvalue and a set of expansion coefficients having many significant digits in most cases. An hour with a desk calculator suffices to determine an α correct to within one part in a million, frequently better than this.

TABLE II. Comparison of eigenvalues of ϵ for $Z=80$.

		From Eq. (4)		From infinite determinant	
n, l	Hartree	$A=6.986$	$A=6$	$A=6.896$	$A=6$
$1S$	74.48	73.61	74.39	73.62	74.40
$2S$	30.41	29.23	30.40	29.44	30.46
$2P$	29.87	28.56	29.86	28.72	29.98
$3S$	14.76	12.97	14.40	14.23	15.29
$3P$	14.19	12.39	13.91	13.35	14.73
$3D$	13.08	11.24	12.93	12.16	13.57
$4S$	6.87	4.72	5.47	7.22	8.08
$4P$	6.34	3.29	5.09	6.69	7.61
$4D$	5.27	2.43	4.34	5.61	6.69
$4F$	3.09	1.15	3.20	3.91	5.18

In practice, it is usually not necessary to go beyond $m=10$ or 20, except for states with the largest quantum numbers corresponding to optical states. For example, some fifty or sixty terms must be computed for the $n=5$ states of mercury before the divergence of the c_ν is evident (although only about fifteen are needed for the $n=4$ states). Neither the approximate potential nor the expansions that have been used for the wave functions are suitable for such states.

The evaluation of the c_ν is completed by an examination of their behavior for large ν. In (2), let $c_\nu=k_\nu/(l+\nu+1)$. Then

$$\tfrac{1}{2}(\nu+1)k_{\nu+1}+k_\nu\{[\beta/(l+\nu+1)]-(\alpha+l+\nu+1)\}+\tfrac{1}{2}k_{\nu-1}(\nu+2l+1)=0. \quad (7)$$

In the limit of large ν, $\beta/(l+\nu+1)$ is negligible in comparison with $\alpha+l+\nu+1$, and (7) becomes a difference equation of hypergeometric type[15] with the asymptotic solutions

$$k(\nu)=\exp[\pm2(2\alpha)^{\frac{1}{2}}(\nu+2l+1)^{\frac{1}{2}}]\times(\nu+2l+1)^{l+\frac{1}{4}}\{1\pm O(1/\nu^{\frac{1}{2}})\}.$$

The ± signs correspond to the independent solutions of the difference equation, the minus sign giving convergent expansions of the wave functions.

A few results obtained with the aforementioned procedures are given in Table II and Fig. 3. Table II shows eigen-ϵ computed from (4) and from the infinite determinant in comparison with Hartree's values, for $Z=80$. Figure 3 shows how the $2S$ and $2P$ levels split as the non-coulomb potential $-Z_{pA}/r$ is turned on

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[15] P. M. Batchelder, *Linear Difference Equations* (Harvard University Press, Cambridge, 1927), p. 175. The difference equation is of the "irregular" type, having a characteristic equation with equal roots.

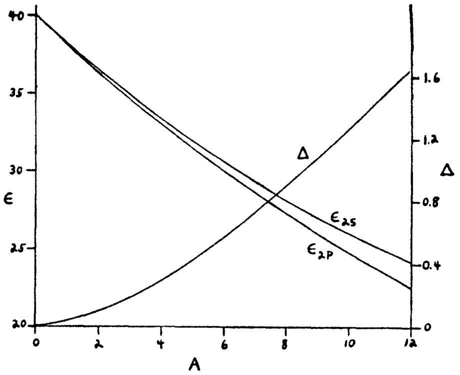

FIG. 3. ϵ as a function of A for Z fixed at 80 and for the $2S$ and $2P$ states. $\Delta = \epsilon_{2S} - \epsilon_{2P}$ shows the splitting of the states as the non-coulomb character of the potential is amplified through increasing A.

through increasing A. Normalization factors for the wave functions may be easily found in terms of the c_ν by making use of the orthogonality of the F functions and the recurrence formulas for them. Such quantities as transition probabilities are also computed in a straightforward way from tables of c_ν and one may see the separate hydrogenlike contributions to the final value.

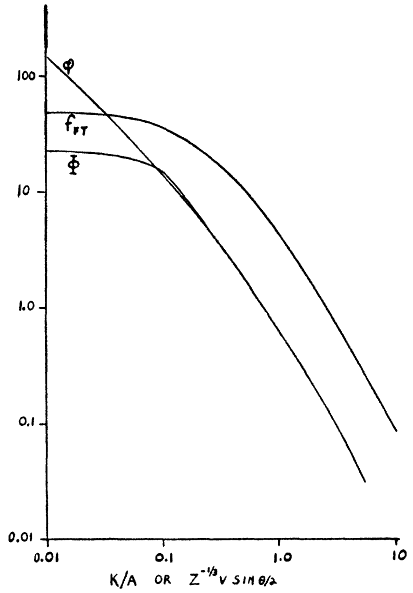

FIG. 4. Comparison of scattering amplitudes in Born approximation. φ is calculated directly with the approximate potential $-Z_{PA}/r$. Φ is calculated with the potential cut-off at R for the case that $AR=26$. f_{FT} is the Fermi-Thomas scattering amplitude.

An example of the use of the approximate potential directly is the calculation of the scattering amplitude $f(\theta)$ for a fast electron in the potential. In the Born approximation,

$$
\begin{aligned}
f(\theta) &= \frac{8\pi^2 m}{h^2}\int_0^\infty \frac{\sin Kr}{Kr}\,\frac{Z}{r(1+Ar)}r^2dr \\
&= \frac{8\pi^2 mZ}{h^2A^2}\left\{\frac{\sin(K/A)\mathrm{Ci}(K/A)+\cos(K/A)[\pi/2-\mathrm{Si}(K/A)]}{K/A}\right\} \\
&= \frac{8\pi^2 mZ}{h^2A^2}\varphi\left(\frac{K}{A}\right),
\end{aligned}
\tag{8}
$$

where $K=(4\pi mv/h)\sin(\theta/2)$, mv being the incident electron momentum and θ the scattering angle. In the limit of small K/A, $\varphi(x)$ diverges as $[x\log(1.781x)+\frac{1}{2}\pi-x]/x$, reflecting the fact the approximate potential is too large at large r so that the incident electron is affected too much in a distant collision. If one cuts off the potential at $r=R$, then (8) is replaced by

$$
\begin{aligned}
f(\theta) &= \frac{8\pi^2 mZ}{h^2A^2}\left\{\frac{\sin(K/A)[\mathrm{Ci}(K/A)-\mathrm{Ci}((1+AR)K/A)]+\cos(K/A)[\mathrm{Si}((1+AR)K/A)-\mathrm{Si}(K/A)]}{K/A}\right\} \\
&= \frac{8\pi^2 mZ}{h^2A^2}\Phi\left(\frac{K}{A}\right).
\end{aligned}
$$

For small K/A, $\Phi(K/A)=AR-\log(1+AR)$. The functions φ, Φ, and that $f(\theta)$, f_{FT}, arising from the Fermi-Thomas potential[16] may be conveniently compared on a log-log graph. This is done in Fig. 4, where f_{FT} is plotted against $Z^{-\frac{1}{3}}v\sin(\theta/2)$ and φ and Φ (for $AR=26$) are plotted against K/A. It is seen that φ and Φ are indistinguishable except at small K/A, and that Φ and f_{FT} agree satisfactorily.

In conclusion, the writer wishes to thank Professors Richard P. Feynman and Hans A. Bethe for friendly discussion and criticism.

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[16] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1949).