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The Elastic Scattering of Electrons by Neutral Hydrogen Atoms by the Variational Method

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Two variational methods are proposed for computing the phase shifts for an electron scattered by a neutral atom. These methods are shown to be different formulations of the same physical principle, i.e., the stationary property of the phase shift. By applying one of these methods to the S scattering of an electron by a hydrogen atom, the phase shifts are computed for various kinetic energies. A comparison is finally made with the results which Morse and Allis have derived from the solution of the Fock equation.

I. INTRODUCTION

THE problem of the elastic scattering of electrons by hydrogen atoms has been considered by Chandrasekhar and Breen,¹ Massey and Mohr,² McDougall,³ and Morse and Allis.⁴ While the latter authors solved the appropriate Fock equations⁵ and determined the phase shifts, the others used the Hartree field. As both the Fock equation and the Hartree field are derived from a variational principle on the assumption that the coordinates of the free and the bound electron are separable, it would be of interest to see if one can formulate a similar principle without such an assumption. For the case of S states, the author has shown that⁶ such a formulation is feasible. And the use of this later variation method has the further advantage that the numerical work involved is much less than is required for the solution of the Fock equation.

The method we shall adopt is an extension of the work done by Hulthén⁷ and by Tamm.⁸ Both of these authors have treated nuclear scattering and consequently limited the problem to the encounter of two

particles. In the problem which we propose to consider, three particles are involved in each encounter; a more general formulation of the variational principles of Hulthén and Tamm is necessary. We shall formulate the necessary generalization. It may also be stated here that of the two formulations, that of Hulthén appears to be the more general while Tamm's has the merit of being more simple and direct.

We shall first present these two formulations in their generalized forms and then show their equivalence. Finally, we shall illustrate the principles by considering the S -scattering of free electrons by a neutral hydrogen atom in the ground state.

II. THE VARIATIONAL PRINCIPLE

If we adopt the Bohr radius and $R\hbar$ as the unit of length and of energy, respectively, the wave equation corresponding to a free electron in the field of a neutral hydrogen atom is

$$(L-E)\psi=0, \quad (1)$$

where

$$L = -\nabla_1^2 - \nabla_2^2 - 2/r_1 - 2/r_2 + 2/r_{12}. \quad (2)$$

The effect of the term in r_{12} has been mostly neglected; and we are particularly interested in it. However, this term does not affect the formulation of the variational principle. Insofar as the potential field in which the free electron is moving tends to zero faster than $1/r^p$ (where $p > 1$) for $r \rightarrow \infty$ (this is evidently the case for motion of an electron in the field of a neutral atom), we can write

¹ S. Chandrasekhar and F. H. Breen, *Astrophys. J.* **103**, 41 (1946).

² H. S. W. Massey and C. B. O. Mohr, *Proc. Roy. Soc.* **A136**, 289 (1932).

³ J. McDougall, *Proc. Roy. Soc.* **A136**, 549 (1932).

⁴ P. M. Morse and W. P. Allis, *Phys. Rev.* **44**, 269 (1933).

⁵ V. Fock, *Zeits. f. Physik* **61**, 126 (1930).

⁶ S. S. Huang, *Phys. Rev.* **75**, 980 (1949).

⁷ L. Hulthén, *K. Fysiogr. Sällsk. Lund Förhandl.* **14**, No. 21 (1944).

⁸ E. E. Tamm, *J. Exper. Theor. Phys. (Russian)* **18**, No. 4 (1948).

the asymptotic form for the wave function:

$$\begin{aligned} \psi_i(\infty) = & [(2l+1)/(4\pi)]^{1/2} [(e^{-r_1}/r_2) \\ & \times P_l(\cos\theta_2) \sin(kr_2 - l\pi/2 + \eta_l) \\ & \pm (e^{-r_2}/r_1) P_l(\cos\theta_1) \sin(kr_1 - l\pi/2 + \eta_l)], \quad (3) \end{aligned}$$

the sign being plus or minus according as the state is symmetrical or antisymmetrical, respectively. This asymptotic form represents a final state in which the bound electron is in its ground state and the free electron is at infinity with a kinetic energy k^2 . In addition, the wave function should, of course, not have any singularity at $r_1=0$, or $r_2=0$.

Let

$$\mathcal{L} = \int \int_{\infty} \psi_i(L-E)\psi_i d\tau_1 d\tau_2, \quad (4)$$

and consider the variation. By Green's theorem,

$$\begin{aligned} \int \psi_i \nabla_1^2 \delta\psi_i d\tau_1 = & \int \delta\psi_i \nabla_1^2 \psi_i d\tau_1 \\ & + \oint [\psi_i(\partial\delta\psi_i/\partial r_1) - \delta\psi_i(\partial\psi_i/\partial r_1)] dS_1. \quad (5) \end{aligned}$$

The surface integral in Eq. (5) can be evaluated at $r_1 \rightarrow \infty$ by using the asymptotic expansion (3) of the wave function. It can, in fact, be shown that

$$\int \int_{\infty} \psi_i \nabla_1^2 \delta\psi_i d\tau_1 d\tau_2 = \int \int_{\infty} \delta\psi_i \nabla_1^2 \psi_i d\tau_1 d\tau_2 - \pi k \delta\eta_1. \quad (6)$$

The corresponding integral with subscript 2 can be similarly transformed. Thus,

$$\delta\mathcal{L} = 2 \int \int_{\infty} \delta\psi_i(L-E)\psi_i d\tau_1 d\tau_2 + 2\pi k \delta\eta_1. \quad (7)$$

If ψ_i satisfies the wave equation, we have

$$\delta\mathcal{L} = 2\pi k \delta\eta_1, \quad (8)$$

which will reduce to

$$\delta\mathcal{L} = 0 \quad (9)$$

if the phase shift η_l is stationary. Or, in other words, under the stationary condition of η_l , the wave equation assumes a variational form which is given by Eq. (9). Regarding now

$$\mathcal{L} = 0 \quad (10)$$

as an equation which determines η_l , we can conversely impose the stationary condition by making use of Eq. (9). A practical procedure which this principle suggests is the following. Form an approximate wave function ψ_i which satisfies the required boundary conditions and at the same time contains n parameters. Then Eqs. (9)

and (10) will give $n+1$ equations which will determine completely η_l and the n parameters. It is thus seen that the phase shift plays in the continuous spectrum the same role as the energy in the discrete spectrum. It is due to this reason that Hulthén⁷ introduced the name "eigenphase" for η_l .

As the wave function should approach the asymptotic expansion (3) when the free electron is at infinity and be finite when it is at the origin, it is natural to write it in the approximate form:

$$\begin{aligned} \psi_i = & [(2l+1)/(4\pi)]^{1/2} [F(r_1, \theta_1, r_2, r_{12}) P_l(\cos\theta_2)/r_2 \\ & \pm F(r_2, \theta_2, r_1, r_{12}) P_l(\cos\theta_1)/r_1], \quad (11) \end{aligned}$$

where

$$\begin{aligned} F(r_1, \theta_1, r_2, r_{12}) = & (\pi k r_2 / 2)^{1/2} J_{l+1/2}(k r_2) f(r_1, \theta_1, r_2, r_{12}) \\ & + (\pi k r_2 / 2)^{1/2} J_{-l-1/2}(k r_2) g(r_1, \theta_1, r_2, r_{12}), \quad (12) \end{aligned}$$

such that

$$f \rightarrow e^{-r_1} \cos\eta_l \quad \text{and} \quad g \rightarrow e^{-r_1} \sin\eta_l \quad (13)$$

as $r_2 \rightarrow \infty$. In Eq. (12), $J_{\pm(l+1/2)}(kr)$ represent Bessel functions of order $\pm(l+1/2)$, respectively.

III. A RESTRICTED FORM OF VARIATIONAL PRINCIPLE

In spite of the general nature of the method derived in Section II, the mathematical formulas for actually working out the variational integral are very complicated. It would, therefore, seem that a somewhat less general but a mathematically simpler formulation of the principle is more suitable. For states with spherical symmetry and zero angular momentum this can be accomplished in the following way: In this case⁹ the wave function can be completely expressed in terms of three coordinates r_1 , r_2 , and r_{12} .

Transforming Eq. (1) into new coordinates, we get

$$\begin{aligned} & (\partial^2\psi/\partial r_1^2) + (2/r_1)(\partial\psi/\partial r_1) + (\partial^2\psi/\partial r_2^2) \\ & + (2/r_2)(\partial\psi/\partial r_2) + 2(\partial^2\psi/\partial r_{12}^2) + (4/r_{12})(\partial\psi/\partial r_{12}) \\ & + [(r_1^2 - r_2^2 + r_{12}^2)/r_1 r_{12}](\partial^2\psi/\partial r_1 \partial r_{12}) \\ & + [(r_2^2 - r_1^2 + r_{12}^2)/r_2 r_{12}](\partial^2\psi/\partial r_2 \partial r_{12}) \\ & + [E + 2(1/r_1 + 1/r_2 - 1/r_{12})]\psi = 0. \quad (14) \end{aligned}$$

Similar to Tamm's treatment⁸ we make the substitution,

$$\begin{aligned} \psi(r_1, r_2, r_{12}) \\ = & (e^{-r_1}/r_2) [\sin k r_2 + u(r_1, r_2, r_{12}) \cos k r_2]. \quad (15) \end{aligned}$$

Equation (14) now becomes

$$\begin{aligned} & [(\partial^2 u/\partial r_1^2) + (2/r_1)(\partial u/\partial r_1) - 2(\partial u/\partial r_1) + (\partial^2 u/\partial r_2^2) \\ & + 2(\partial^2 u/\partial r_{12}^2) + (4/r_{12})(\partial u/\partial r_{12})] \cos k r_2 \\ & - 2k(\partial u/\partial r_2) \sin k r_2 + [(r_1^2 - r_2^2 + r_{12}^2)/r_1 r_{12}] \\ & \times [(\partial^2 u/\partial r_1 \partial r_{12}) - (\partial u/\partial r_{12})] \cos k r_2 \\ & + [(r_2^2 - r_1^2 + r_{12}^2)/r_2 r_{12}] [(\partial^2 u/\partial r_2 \partial r_{12}) \cos k r_2 \\ & - (\partial u/\partial r_{12})(\cos k r_2/r_2) - k(\partial u/\partial r_{12}) \sin k r_2] \\ & + 2[(1/r_2) - (1/r_{12})] (\sin k r_2 + u \cos k r_2) = 0. \quad (16) \end{aligned}$$

⁹ E. A. Hylleraas, *Zeits. f. Physik* **54**, 347 (1929); H. Bethe, *Handbuch der Physik* (1933), Vol. 24, p. 354.

In making the substitution we have used the energy relation

$$E = -1 + k^2, \quad (17)$$

which is true in $R\hbar$ unit.

From Eq. (15) it is apparent that $u(r_1, r_2, r_{12})$ becomes the tangent of phase shift as $r_2 \rightarrow \infty$. Accordingly, we may call Eq. (16) as the equation for the eigenphase. The boundary conditions on $u(r_1, r_2, r_{12})$ are therefore

$$\left. \begin{aligned} u &= 0 & \text{as } r_2 &= 0 \\ u &= u(k) & \text{as } r_2 &\rightarrow \infty \end{aligned} \right\} \quad (18)$$

As Eq. (14) is symmetrical in r_1 and r_2 , the wave function appropriate to the physical problem can be written in the form

$$\psi_0 = \psi(r_1, r_2, r_{12}) \pm \psi(r_2, r_1, r_{12}), \quad (19)$$

where $\psi(r_1, r_2, r_{12})$ is defined in Eq. (15). In Eq. (19)

we have the plus or minus sign according as we are dealing with the singlet or triplet state.

It can now be shown that Eq. (16) is the Euler equation of the variational integral:

$$\delta\mathfrak{F} = 0;$$

$$\mathfrak{F} = \int_0^\infty dr_2 \int_0^\infty dr_1 \int_{|r_1-r_2|}^{r_1+r_2} dr_{12} \times F(u_1, u_2, u_{12}, u; r_1, r_2, r_{12}), \quad (20)$$

where

$$\begin{aligned} F = & e^{-2r_1} \cos^2 kr_2 [r_1 r_{12} (u_1^2 + u_2^2 + 2u_{12}^2) / r_2 \\ & + (r_1^2 - r_2^2 + r_{12}^2) u_1 u_{12} / r_2 \\ & + r_1 (r_2^2 - r_1^2 + r_{12}^2) u_2 u_{12} / r_2^2 \\ & - (2r_1 r_{12} / r_2) (1/r_2 - 1/r_{12}) (2u \tan kr_2 + u^2)] \end{aligned} \quad (21)$$

and

$$u_1 = \partial u / \partial r_1, \quad u_2 = \partial u / \partial r_2, \quad u_{12} = \partial u / \partial r_{12}. \quad (22)$$

It is of interest to note that the integral \mathfrak{F} reduces to that given by Tamm in the special case where $u = u(r_2)$ only, and where $-2(1/r_2 - 1/r_{12})$ can be approximated by an expression which involves r_2 only (as for example, by a potential $V(r_2)$ of the Hartree field of the hydrogen atom). For in this special case the integration with respect to r_{12} and r_1 can be effected directly, and the final integral

$$\mathfrak{F} = \int_0^\infty dr_2 [u_2^2 \cos^2 kr_2 + V u^2 \cos^2 kr_2 + V u \sin 2kr_2] \quad (23)$$

is identical with what Tamm has given.

To derive the variational principle expressed by Eq. (20) from Eq. (9) is a straightforward matter, although it is quite long and tedious. We may therefore indicate

the various steps briefly. Substituting Eq. (15) into Eq. (9) we carry out the variation; one part would be equal to zero on account of Eq. (16); the remaining terms are then reduced by integration by parts; the integrated terms do not contribute anything as the variation vanishes on the boundary surface; most of other terms cancel one another, and we are finally left with

$$\delta\mathcal{L} = \frac{1}{2} \delta\mathfrak{F}. \quad (24)$$

IV. S-SCATTERING OF ELECTRONS BY THE HYDROGEN ATOM

Here we shall apply Eq. (20) to derive the phase shift of the S waves for the case of a free electron scattered by a hydrogen atom. As our trial function, we shall suppose that

$$u = (1 - e^{-r_2}) [a + (b + cr_{12}) e^{-r_2}], \quad (25)$$

where a , b , and c are three parameters which are to be determined. Substituting the foregoing form for u in Eq. (20) we carry out the integration. In order to express our result simply, it is convenient to define the functions:

$$F_n(\alpha, m; k) = \int_0^\infty (1 - e^{-r})^n e^{-\alpha r} r^m \cos^2 kr dr \quad (n \geq 0, m \geq -n), \quad (26)$$

$$G_n(\alpha, m; k) = \int_0^\infty (1 - e^{-r})^n e^{-\alpha r} r^m \sin 2kr dr \quad (n \geq 0, m \geq -n - 1), \quad (27)$$

$$I_n(\alpha; k) = \int_0^\infty (1 - e^{-r})^n (1 - e^{-2r}) (e^{-\alpha r} / r^2) \cos^2 kr dr \quad (n \geq 1), \quad (28)$$

$$J_n(\alpha; k) = \int_0^\infty (1 - e^{-r})^n (1 - e^{-2r}) (e^{-\alpha r} / r^2) \sin 2kr dr \quad (n \geq 0), \quad (29)$$

and

$$M(\alpha; k) = \int_0^\infty (1 - e^{-2r}) (e^{-\alpha r} / r) \cos^2 kr dr, \quad (30)$$

where m and n are integers. In terms of these functions \mathfrak{F} is a quadratic function in the parameters a , b , and c .

The variational principle would then give three equations for the three parameters. It is found that these three equations have the following forms.

$$\partial\mathfrak{F} / \partial a = A_1 a + B_1 b + C_1 c - D_1 = 0, \quad (31)$$

$$\partial\mathfrak{F} / \partial b = A_2 a + B_2 b + C_2 c - D_2 = 0, \quad (32)$$

$$\partial\mathfrak{F} / \partial c = A_3 a + B_3 b + C_3 c - D_3 = 0, \quad (33)$$

TABLE I. Coefficients of u .

k	3-parameter approximation			2-parameter approximation		1-parameter approximation
	a	b	c	a	c	a
0	0	0	0	0	0	0
0.05	-0.4038	+0.16954	-0.4199	-0.4067	-0.3944	+0.3102
0.10	-0.8499	+0.3572	-0.8938	-0.8576	-0.8425	+0.6066
0.15	-1.3978	+0.5883	-1.4970	-1.4160	-1.4208	+0.8777
0.20	-2.158	+0.9099	-2.368	-2.202	-2.274	+1.1155
0.25	-3.394	+1.4348	-3.840	-3.520	-3.765	+1.3162
0.50	+5.254	-2.246	+7.147	+4.616	+6.146	+1.8280
0.75	+2.037	-0.9067	+2.947	+1.8132	+2.649	+1.8969
1.00	+1.6636	-0.8899	+2.071	+1.4068	+1.7846	+1.8572
1.50	+1.8372	-1.3059	+1.6403	+1.3687	+1.1761	+1.7809
2.00	+2.059	-1.4506	+1.6050	+1.4722	+1.0362	+1.7484
2.50	+2.280	-1.5294	+1.7069	+1.6127	+1.0567	+1.7253
3.00	+2.580	-1.7028	+1.9399	+1.7897	+1.1607	+1.6924
4.00	+3.656	-2.523	+2.909	+2.309	+1.5629	+1.5891
6.00	+25.635	-20.46	+22.87	+5.389	+4.045	+1.3282
8.00	-5.763	+5.076	-5.501	-24.69	-19.758	+1.1004
10.00	-2.743	+2.564	-2.722	-4.098	-3.403	-0.9262
20.00	-0.8622	+0.9841	-0.9083	-0.9303	-0.8192	-0.4983
50.00	-0.3102	+0.3276	-0.3330	-0.3181	-0.2853	-0.2037
100.00	-0.1535	+0.1616	-0.1649	-0.1562	-0.1404	-0.1022

where

$$A_1 = F_0(2, 0; k) - 2F_2(2, 0; k) - 2F_2(2, -1; k), \quad (34)$$

$$A_2 = B_1 = F_0(3, 0; k) - F_1(2, 0; k) - 2F_2(3, 0; k) - 2F_2(3, -1; k), \quad (35)$$

$$A_3 = C_1 = F_0(3, 1; k) - F_1(2, 1; k) + F_1(2, 0; k) + \frac{3}{2}F_1(4, 0; k) - \frac{1}{2}F_0(5, 0; k) - F_1(2, -1; k) + 2F_1(3, -1; k) + 3F_1(4, -1; k) - 2I_2(1; k) - I_1(2; k), \quad (36)$$

$$B_2 = F_2(2, 0; k) - 2F_2(4, 0; k) - 2F_1(3, 0; k) + F_0(4, 0; k) - 2F_2(4, -1; k), \quad (37)$$

$$B_3 = C_2 = F_2(2, -1; k) - 2F_1(3, -1; k) - F_1(4, -1; k) + 7F_1(5, -1; k) - \frac{3}{2}F_2(4, 0; k) - F_2(2, 0; k) + 2F_1(5, 0; k) + F_1(3, 0; k) - \frac{1}{2}F_0(6, 0; k) + F_2(2, 1; k) - 2F_1(3, 1; k) + F_0(4, 1; k) - I_1(2; k), \quad (38)$$

$$C_3 = F_2(2, 2; k) - 2F_1(3, 2; k) + F_0(4, 2; k) - 2F_2(2, 1; k) + 2F_1(3, 1; k) + 5F_2(2, 0; k) - F_2(4, 0; k) - 6F_1(3, 0; k) + 3F_0(4, 0; k) - 4F_2(2, -1; k) - 2F_2(4, -1; k), \quad (39)$$

$$D_1 = G_1(2, 0; k) + G_1(2, -1; k), \quad (40)$$

$$D_2 = G_1(3, 0; k) + G_1(3, -1; k), \quad (41)$$

$$D_3 = J_1(1; k) - \frac{1}{2}G_1(3, -1; k). \quad (42)$$

The formal solution of Eqs. (31)–(33) will be given in terms of determinants as follows:

$$a = (DBC)/(ABC), \quad b = (ADC)/(ABC), \quad c = (ABD)/(ABC). \quad (43)$$

Before we give the result of the calculations, we shall indicate some steps in the evaluation of the functions defined by Eqs. (26)–(30). First we may observe that the following recurrence formula holds,

$$F_n(\alpha, m; k) = F_{n-1}(\alpha, m; k) - F_{n-1}(\alpha+1, m; k), \quad (44)$$

provided every function in the formula is convergent. Similar formulas can be written down for $G_n(\alpha, m; k)$,

$I_n(\alpha; k)$, and $J_n(\alpha; k)$. Also there exists the relation between F_n and G_n ,

$$\partial F_n(\alpha, m; k)/\partial k = -G_n(\alpha, m+1; k). \quad (45)$$

Another relation which is useful in the numerical work is

$$\partial F_n(\alpha, m; k)/\partial \alpha = -F_n(\alpha, m+1; k). \quad (46)$$

Similar formula exists for $G_n(\alpha, m; k)$.

In order to express $I_n(\alpha; k)$ in terms of other more easily calculable functions, we intergrate by parts, and find

$$I_n(\alpha; k) = \int_0^\infty \{d[(1-e^{-r})^\alpha(1-e^{-2r}) \times e^{-\alpha r} \cos^2 kr]/dr\} (dr/r) \\ = kG_n(\alpha+2, -1; k) - kG_n(\alpha, -1; k) - \alpha F_n(\alpha, -1; k) + nF_n(\alpha+1, -1; k) + (\alpha+n+2)F_n(\alpha+2, -1; k). \quad (47)$$

In a similar manner it can be shown that

$$J_n(\alpha; k) = 2kF_n(\alpha+2, -1; 0) - 2kF_n(\alpha, -1; 0) + 4kF_n(\alpha, -1; k) - 4kF_n(\alpha+2, -1; k) - \alpha G_n(\alpha, -1; k) + nG_n(\alpha+1, -1; k) + (\alpha+n+2)G_n(\alpha+2, -1; k). \quad (48)$$

Also in deriving Eqs. (34)–(42) we have made use of the obvious identity:

$$M(\alpha; k) = F_1(\alpha, -1; k) + F_1(\alpha+1, -1; k). \quad (49)$$

It is therefore sufficient to evaluate only a few fundamental functions occurring in Eqs. (34)–(42). The rest

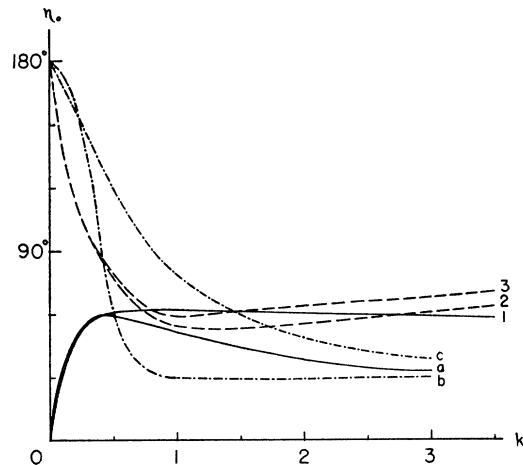


FIG. 1. Phase shifts η_0 of the S wave in degrees against electron velocities k in atomic units. The curves labeled 1, 2, and 3 are computed from the 1-, 2-, and 3-parameter trial functions, respectively, in the present paper. The curves labeled a , b , and c are Morse and Allis' results. Curve a is obtained for an electron moving in the Hartree field. Curves b and c give the phase shifts of symmetrical and antisymmetrical waves, respectively, when the effect of exchange is taken into consideration.

can be obtained by making use of the relations Eqs. (44)–(49). And the basic functions are:

$$F_0(\alpha, 0; k) = 1/(2\alpha) + \alpha/[2(\alpha^2 + 4k^2)], \quad (50)$$

$$\begin{aligned} F_1(\alpha, -1; k) &= \int_{\infty}^{\alpha} [\partial F_1(\alpha', -1; k)/\partial \alpha'] d\alpha' \\ &= - \int_{\infty}^{\alpha} F_1(\alpha', 0; k) d\alpha' \\ &= \frac{1}{2} \log[(\alpha+1)/\alpha] \\ &\quad + \frac{1}{4} \log\{[(\alpha+1)^2 + 4k^2]/(\alpha^2 + 4k^2)\}, \quad (51) \end{aligned}$$

$$G_1(\alpha, 0; k) = 2k/(\alpha^2 + 4k^2) - 2k/[(\alpha+1)^2 + 4k^2], \quad (52)$$

$$\begin{aligned} G_1(\alpha, -1; k) &= \int_{\infty}^{\alpha} [\partial G_1(\alpha', -1; k)/\partial \alpha'] d\alpha' \\ &= \tan^{-1}[(\alpha+1)/(2k)] - \tan^{-1}[\alpha/(2k)]. \quad (53) \end{aligned}$$

That this integral vanishes at the lower limit is as obvious as that of the integral (51), if we combine the two terms into one term according to the trigonometrical identity.

Instead of computing the values of a , b , and c from Eqs. (43) for various values of k , it is simpler to get the numerical solution directly from Eqs. (31)–(33) once their coefficients have been evaluated. The results of the calculation are given in Table I. For comparison, the results for a 2-parameter (a , c) and a 1-parameter (a), trial functions are also included; they are labeled as 2-parameter and 1-parameter approximation, respectively.

As the phase shift η_0 is given by

$$\tan \eta_0 = \lim_{r_2 \rightarrow \infty} u = a, \quad (54)$$

and the cross section of S wave by

$$q_0 = 4\pi(\sin \eta_0/k)^2,$$

they can be computed directly from Table I; they are given in Table II. The phase shifts are further plotted in Fig. 1 where Morse and Allis's results are also shown.

TABLE II. Phase shifts and cross sections of the S wave.

k	3-parameter approximation		2-parameter approximation		1-parameter approximation	
	η_0	q_0	η_0	q_0	η_0	q_0
0	180°	—	180°	—	0°	—
0.05	158° 0'.7	704.7	157° 52'.3	713.2	17° 13'.9	441.1
0.10	139° 38'.2	527.1	139° 23'.0	532.6	31° 14'.5	338.0
0.15	125° 34'.8	369.4	125° 13'.8	372.7	41° 16'.4	243.0
0.20	114° 52'.0	258.6	114° 25'.2	260.5	48° 7'.5	174.18
0.25	106° 25'.0	185.00	105° 51'.6	186.04	52° 46'.4	127.48
0.50	79° 13'.5	48.51	77° 46'.5	48.01	61° 19'.2	38.69
0.75	63° 51'.2	18.001	61° 7'.4	17.131	62° 12'.2	17.482
1.00	58° 59'.4	9.231	54° 35'.6	8.348	61° 42'.0	9.741
1.50	61° 26'.4	4.309	53° 50'.9	3.642	60° 41'.1	4.246
2.00	64° 5'.7	2.542	55° 48'.8	2.150	60° 13'.9	2.368
2.50	66° 19'.1	1.686	58° 11'.9	1.453	59° 54'.2	1.505
3.00	68° 48'.6	1.214	60° 48'.3	1.064	59° 25'.3	1.035
4.00	74° 42'.2	0.730	66° 34'.9	0.661	57° 49'.1	0.563
6.00	87° 46'.0	0.348	79° 29'.2	0.338	53° 1'.4	0.222
8.00	99° 50'.6	0.191	92° 19'.2	0.196	47° 44'.2	0.108
10.00	110° 1'.8	0.111	103° 42'.9	0.118	42° 48'.3	0.058
20.00	139° 14'.0	0.014	137° 4'.1	0.015	26° 29'.3	0.006
50.00	162° 45'.9	0.0004	162° 21'.2	0.0005	11° 30'.8	0.0003
100.00	171° 16'.4	0.00003	171° 7'.4	0.00003	5° 50'.0	0.00001

Our results are not in agreement with theirs and unfortunately no experimental data are available for comparison. But one common feature between the results of Morse and Allis's and ours is worth noticing. While the 1-parameter trial function which does not contain a term in r_{12} gives a variation of the phase shift, similar to that computed from the Hartree field, approaching 0° as $k \rightarrow 0$, the introduction of the r_{12} term (the 3-parameter and the 2-parameter approximations) makes $\eta_0 \rightarrow 180^\circ$ as $k \rightarrow 0$; in this respect it is similar to the introduction of the exchange effect in the manner of Morse and Allis. There is, however, an important difference between these two results. So far as the phase shift is concerned, there is no difference in our formulation for symmetrical and antisymmetrical states, but Morse and Allis give different values of η_0 for these two states.

In a later paper we propose to use the wave functions derived here to the evaluation of the radiative cross sections for the free-free transition of an electron in the field of a neutral hydrogen atom.¹⁰

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¹⁰ S. Chandrasekhar and F. H. Breen, *Astrophys. J.* **104**, 430 (1946).