$\kappa=1.7926$: anomalous magnetic moment of proton in nuclear magneton unit

$\alpha=e^2/4\pi\hbar c=1/137.0$: fine structure constant

$a_0=4\pi\hbar^2/me^2=0.529\times10^{-8}$ cm: first Bohr radius of hydrogen atom

$r_0=e^2/4\pi mc^2=2.818\times10^{-13}$ cm: classical electronic radius

$u(p)$, $\bar{u}(p')$: Dirac spinors (positive energy) of free electron

$U(P)$, $\bar{U}(P')$: Dirac spinors (positive energy) of free proton

$A\cdot B=\mathbf{A}\cdot\mathbf{B}-A_0B_0$: scalar product of two 4-vectors A and B

$q=p+k-p'=P'-P$

$q'=-r=p-p'=P'-P-k$

$Q=P+P'$

$R=p+p'$

$\sigma_{\mu\nu}=(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu)/2i$

$\lambda=p\cdot k$

$\lambda'=p'\cdot k$

$\Lambda=P\cdot k$

$\Lambda'=P'\cdot k$

$$a=\frac{P\cdot e}{\Lambda}-\frac{P'\cdot e}{\Lambda'}$$

$$a'=\frac{P\cdot e}{\Lambda}+\frac{P'\cdot e}{\Lambda'}$$

$$b=\frac{p\cdot e}{\lambda}-\frac{p'\cdot e}{\lambda'}$$

$$b'=\frac{p\cdot e}{\lambda}+\frac{p'\cdot e}{\lambda'}$$

$F_1(q^2)$, $F_2(q^2)$: covariant form factors of charge and current distributions of proton. For the exponential distributions one has $F_{1,2}(q^2)=[1+(a_{1,2}q)^2]^{-2}$, where $a_1=a_2=(\langle r^2\rangle/12)^{\frac{1}{2}}$ and $(\langle r^2\rangle)^{\frac{1}{2}}=0.8\times10^{-13}$ cm.

$d\Omega_e$: differential solid angle along the direction of outgoing electron

$d\Omega_k$: differential solid angle along the direction of outgoing photon.

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Effect of Virtual Excitations on the Elastic Scattering of Electrons and Positrons by Atomic Hydrogen*

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Total elastic cross sections for the scattering of electrons and positrons (neglecting positronium formation) from the $1s$ state of atomic hydrogen have been calculated allowing for virtual excitation to the $2s$ and $3s$ states. The S-, P-, and D-wave contributions to $Q_{1s\text{-}1s}$ have been computed for incident energies below 10 ev. The results for positron scattering show that virtual excitation to the $2s$ and $3s$ states only slightly affects the phase shifts calculated in the static approximation. The influence of the $2s$ state appears to be much more important for electrons. The scattering lengths of these exploratory calculations are compared with the results of other calculations.

INTRODUCTION

IN low-energy positron or electron scattering from atomic hydrogen, it is to be expected that the charge distribution of the hydrogen atom will be appreciably distorted due to the impinging particle spending a great deal of time in its vicinity. It is possible to allow for this distortion, theoretically, in a variety of ways.

We shall be interested in incident energies too low for excitation of the target hydrogen atom and too low for positronium formation. However, virtual excitation to higher atomic states and also virtual positronium formation could be used to allow for the distortive effects. The latter process has been considered by Moussa[1] and Spruch and Rosenberg.[2] These authors

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[1] A. H. A. Moussa, Proc. Phys. Soc. (London) **74**, 101 (1959).

[2] L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960).

have used variational methods to show that virtual positronium formation changes the results of the "static approximation" considerably. It is the purpose of this paper to examine the former effect, about which nothing is known yet, in the positron problem. In the electron problem, Geltman[3] has used a variational method to examine the effect of virtual excitation of the 2*s* and 3*s* states.

The method of solving the problem employed here is that of the eigenfunction expansion approach of Mott and Massey,[4] together with the Hartree-Fock variational principle.[5] Namely, the over-all wave function of the incident projectile plus hydrogen atom system is expanded in terms of the complete set of functions which are eigenfunctions of the target Hamiltonian. The contribution from the continuum in this expansion is neglected. Furthermore, only the first three *S*-state eigenfunctions are retained from the denumerably infinite discrete set of eigenfunctions. That is, if virtual excitation can be considered as giving rise to distortive effects, only spherical distortions will be considered here. Thus, the present calculation is primarily exploratory.

In order to examine nonspherical distortive effects, the $L>0$ states would have to be included. Such a program is being developed by the authors in collaboration with V. M. Burke and H. Schey for the electron problem. The formation for including real or virtual positronium formation, as well as excitation effects, using the eigenfunction approach and Kohn's[5] variational principle has been developed by Cody and Smith[6] and it is hoped that numerical results based on this formalism will form the basis of future reports.

In Sec. I the mathematical problem is discussed. The positron results are presented in Sec. II and the electron results are presented in Sec. III. All cross sections are given in units of πa_0^2, where a_0 is the Bohr radius of the hydrogen atom. Scattering lengths and wave numbers, k, are given in units of a_0 and $1/a_0$, respectively.

I. MATHEMATICAL METHOD

The mathematical problem (neglecting electron exchange, or positronium formation) reduces to solving a system of N coupled second-order differential equations, where N is the number of *S*-state terms taken in the eigenfunction expansion. The solutions to these equations, $F_n(x)$, are interpreted as describing the motion of the incident or emerging projectiles relative to the target. Since we shall be interested in incident energies below excitation thresholds, we require solutions with exponential decaying asymptotic forms in all channels except the incident channel. In the incident channel, we require the solution to be oscillatory; from this solution we calculate the phase shift and consequently the corresponding partial wave elastic cross section.

Exploiting the exponential asymptotic boundary conditions is the novel feature of this paper. Two methods have been used here.

In the first method, which is an analogous procedure to that used by Smith[7] for the electron problem above excitation thresholds, the differential equations are numerically integrated out from the origin into the asymptotic region, N times. For N second-order equations, $2N$ constants must be specified in some way before the numerical solution can begin. The condition that the solutions vanish at the origin determines N constants, the remaining N are arbitrary. For $l=0$, the N arbitrary constants are identified with the first derivatives at the origin. The second derivatives are related to these arbitrary constants. With this information, it is possible to use the Runge-Kutta method (see Gill[8]) to solve the system of equations. For $l=1$, the P waves, the first derivatives also vanish and the arbitrary constants are identified with the second derivatives at the origin. It is possible, once more, to solve the equations using the Runge-Kutta method. For $l>1$, and for the interactions used in this class of problems, the second derivatives also vanish and the Runge-Kutta method cannot be used starting from the origin. However, it is possible to perform an expansion in an ascending power series of the independent variable x. This series can then be used to evaluate the functions and their derivatives at some small x and the numerical integration started from that point. In this method, the solutions in the inelastic channels contain some positive exponential which dominates the decaying exponential at large x. In order to avoid this, a second method was devised which imposed the asymptotic conditions at the outset.

In the second method, the forward solution of the systems of equations was stopped at some point, x_0 say, which is not in the asymptotic region. The solution is restarted in the asymptotic region, imposing the asymptotic boundary condition (which amounts to specifying the $N-1$ logarithmic derivatives) and performing a backward numerical integration to x_0. Since only $N-1$ constants can be specified unambiguously, it is necessary to obtain $N+1$ linearly independent solutions in the outer region. The N forward solutions and the $N+1$ backward solutions, and their first derivatives, are matched at x_0. Explicitly, the matching condition at x_0 is

$$\sum_{\alpha=1}^{N} u_\alpha \begin{pmatrix} F_i(x_0) \\ F_i'(x_0) \end{pmatrix}_\alpha = \sum_{\beta=1}^{N+1} w_\beta \begin{pmatrix} F_i(x_0) \\ F_i'(x_0) \end{pmatrix}_\beta, \quad i=1,2,\cdots N,$$

where u_α and w_β are arbitrary coefficients to be determined from these equations. The N inner solutions,

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[3] S. Geltman, Phys. Rev. **119**, 1283 (1960).

[4] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, New York, 1949), 2nd ed., Chap. VIII.

[5] W. Kohn, Phys. Rev. **74**, 1763 (1948).

[6] W. J. Cody and K. Smith, Argonne National Laboratory Report, ANL-6121, 1960 (unpublished).

[7] K. Smith, Phys. Rev. **120**, 845 (1960).

[8] S. Gill, Proc. Cambridge Phil. Soc. **47**, 96 (1951).

TABLE I. Phase shifts (rad) for the scattering of positrons by hydrogen atoms. Row (a): static approximation; row (b): strong-coupling approximation (1*s*-2*s*); row (c): 1*s*-2*s*-3*s* coupling.

k_0a_0 \ l		0	1	2
0.8	(a)	−0.3713	−0.0584	−0.0082
	(b)	−0.3569	−0.0549	−0.0077
	(c)	−0.3537		
0.6	(a)	−0.3043	−0.0322	−0.0028
	(b)	−0.2936	−0.0305	−0.0027
	(c)	−0.2914		
0.5	(a)	−0.2636	−0.0214	
	(b)	−0.2547	−0.02	
	(c)	−0.2529		
0.4	(a)	−0.2181	−0.0121	−0.0005
	(b)	−0.2110	−0.0114	−0.0006
	(c)	−0.2095		
0.2	(a)	−0.1145	−0.0018	
	(b)	−0.1109	−0.0017	
	(c)	−0.1102		
0.1	(a)	−0.0580	−0.0002	
	(b)	−0.0562		
	(c)			

multiplied by their corresponding coefficients u_α, are then added together; similarly for the $N+1$ outer solutions. The phase shift is calculated from the matched solution in the incident channel.

When electron exchange (or positronium formation) is included, the mathematical problem involves the solution of systems of coupled integro-differential equations. We adopted a straightforward iteration procedure. In the first iteration, the integral terms are neglected and the matched solution to the resulting truncated system of homogeneous equations is calculated by the method discussed above. This matched solution is then substituted into the integral terms and the resulting system of inhomogeneous equations is solved once in the inner region, $x \leqslant x_0$, and once in the outer region, $x \geqslant x_0$. The matching condition is now

$$\begin{pmatrix} \mathcal{F}_i(x_0) \\ \mathcal{F}_i'(x_0) \end{pmatrix}_{\text{in}} + \sum u_\alpha \begin{pmatrix} F_i(x_0) \\ F_i'(x_0) \end{pmatrix} = \begin{pmatrix} \mathcal{F}_i(x_0) \\ \mathcal{F}_i'(x_0) \end{pmatrix}_{\text{out}} + \sum w_\beta \begin{pmatrix} F_i(x_0) \\ F_i'(x_0) \end{pmatrix},$$

where $\mathcal{F}$ are the solutions to the inhomogeneous equations. There are $2N$ equations, but $2N+1$ fitting parameters u_α and w_β. An additional equation can be constructed due to the over-all normalization of the problem being arbitrary. The new matched solution is then substituted back into the integral terms and the cycle repeated. The iteration procedure was assumed to have converged when the resulting phase shift did not change by more than a specified epsilon from one iteration to the next.

II. POSITRON RESULTS

The static approximation is the name given to those calculations which assume only one term, e.g., the 1*s* state, in the eigenfunction expansion of the total wave function of the incident projectile plus hydrogen atom system. When two terms are assumed, e.g., 1*s* and 2*s* states, the approximation is called the strong-coupling approximation.

Phase shifts calculated in the static (1*s* state only) and strong coupling (1*s*-2*s*) approximations are presented in Table I. In Fig. 1, we plot $-k \cot\eta_0$ versus k^2 in order to obtain an estimate of the scattering length. In Fig. 2, we plot the elastic scattering cross section versus the energy.

In the static approximation, we note that the $l=0$ phase shifts at $k_0a_0=0.5$ and 0.2 agree with those calculated by Massey and Moussa.[9] In Fig. 1, for the static approximation, as $k \rightarrow 0$, $k \cot\eta_0 \rightarrow -1.718$. This

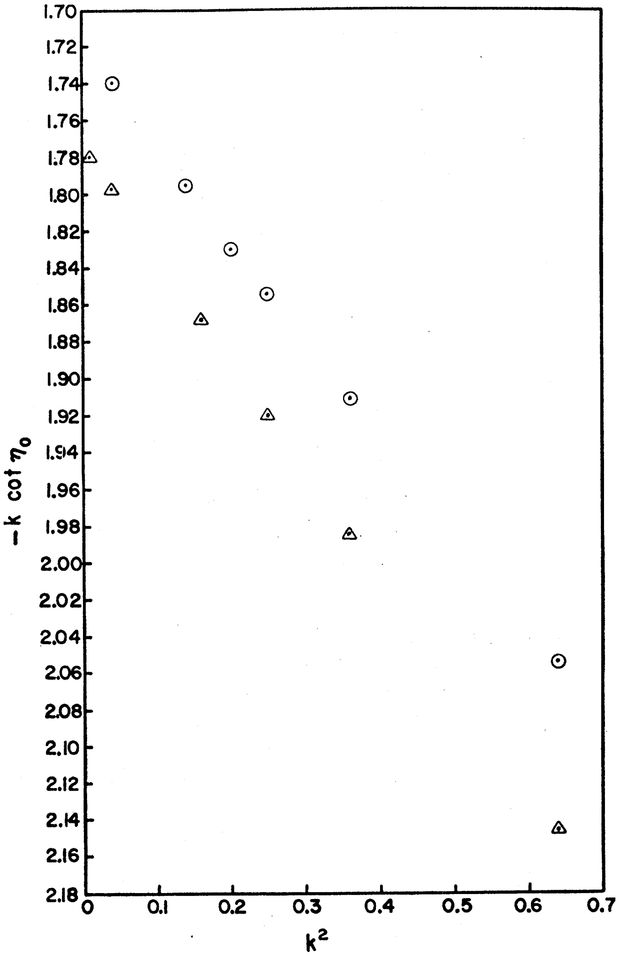

FIG. 1. Plot of $-k \cot\eta_0$ vs k^2 for positrons incident on atomic hydrogen. ⊙: static approximation; △: strong-coupling approximation.

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[9] H. S. W. Massey and A. H. A. Moussa, Proc. Phys. Soc. (London) 71, 38 (1958).

TABLE II. Phase shifts for the elastic scattering of electrons (neglecting exchange) by hydrogen atoms. Rows (a), (b), and (c) have the same significance as in Table I.

k_0a_0 \ l		0	1	2
0.8	(a)	0.9633	0.0752	0.0087
	(b)	0.8962	0.0927	0.0095
	(c)	0.8575	0.0938	0.0096
0.6	(a)	1.0210	0.0406	0.0030
	(b)	0.5887	0.0464	0.0032
	(c)	0.2516	0.0471	0.0032
0.5	(a)	1.0446	0.0263	
	(b)	0.0238	0.0294	
	(c)	2.5769		
0.4	(a)	1.0575	0.0147	0.0005
	(b)	2.4960	0.0163	0.0006
	(c)	2.1596	0.0165	0.0006
0.2	(a)	0.9725	0.0021	
	(b)	2.3172	0.0023	
	(c)	2.1216	0.0023	
0.1	(a)	0.7212	0.0003	
	(b)	2.6015		

corresponds to a scattering length $A_0=+0.582$, where A_0 is defined by $\lim_{k\to 0} k \cot\eta_0 \to -1/A_0$.

In the strong-coupling approximation, the effect of virtual excitation to the $2s$ atomic state of hydrogen is to give a slightly lower value for the scattering length, $A_0=+0.564$, and to decrease the elastic scattering cross sections by a few percent. This decrease in the cross section is consistent with the conjecture of Massey and Moussa,[9] which was based on the measurements of Marder *et al.*[10] on the low energy scattering of positrons by helium, neon, and argon atoms, and with the calculations of Moiseiwitsch.[11]

Recently, Moussa[1] and Spruch and Rosenberg[2] have taken into account the possibility of virtual positronium formation. If the positron is not bound to the hydrogen atom, then the result of the latter authors is the better of the two, since their calculations are based on a rigorous minimum principle. However, both authors obtained a much larger effect than that observed here. In fact, Spruch and Rosenberg[2] obtained a negative scattering length. The qualitative consequence of this result is that the positron is attracted toward the hydrogen atom at very low energies. In view of this serious disagreement with the model assumed here, calculations based on the formalism given in Cody and Smith[6] must be carried out to determine the very low energy behavior of the cross section. Furthermore, the effect of positronium formation might cause an appreciable change in the excitation cross sections as calculated by Smith *et al.*[12] in the strong-coupling approximation.

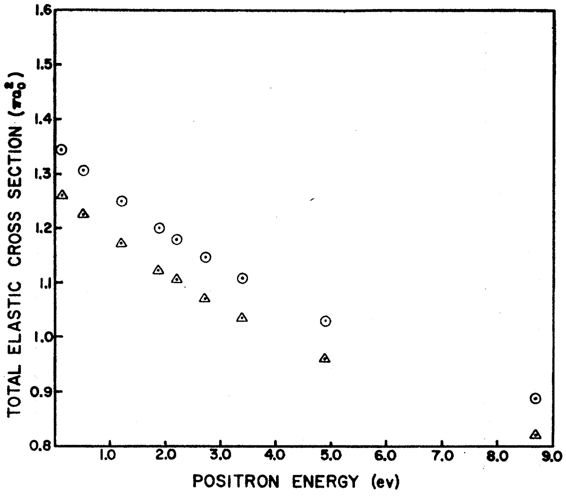

FIG. 2. Total elastic scattering cross section for positrons incident on atomic hydrogen. ⊙: static approximation; △: strong-coupling approximation.

III. ELECTRON RESULTS

Phase shifts for the elastic scattering of electrons by hydrogen atoms, neglecting exchange and including exchange are presented in Tables II and III, respectively. The total elastic cross sections, no-exchange strong-coupling approximation, are presented in Fig. 3.

The phase shifts calculated in the static approximation agree with those of Chandrasekhar and Breen[13] at $k=0.5$, 0.2, and 0.1. These phase shifts extrapolate to give a scattering length of $-9.35a_0$. The elastic scattering cross section increases smoothly, with decreasing energy, over the entire range of interest.

A very interesting feature of the strong-coupling, no-exchange approximation is the vanishing of the zero-order partial wave cross section at an energy just below 3.4 ev. To verify that this effect was not spurious, the calculations were carried out at $k=0.4$ under many conditions. Firstly, both methods described in Sec. II were used; secondly, the power series expansion was used and the phase shift was seen to be independent of the starting x. The result was also independent of the step size used in the integration scheme, as well as being independent of the location of x_0. The introduc-

TABLE III. Zero-order partial wave phase shifts (rad) for the elastic scattering of electrons by hydrogen atoms, including the effect of virtual excitation to the $2s$-state. Row (a): no-exchange; row (b): triplet; row (c): singlet. The scattering lengths are given in the last column.

	ka_0				
	0.1	0.075	0.05	0.01	0.0
(a)	2.602	2.715	2.845	3.080	6.135
(b)	2.901	2.916	3.022	3.108	2.33
(c)	2.404	2.591	2.767	3.065	7.5

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[10] S. Marder, V. W. Hughes, C. S. Wu, and W. Bennett, Phys. Rev. **103**, 1258 (1956).

[11] B. L. Moiseiwitsch, Proc. Phys. Soc. (London) **72**, 139 (1958).

[12] K. Smith, W. F. Miller, and A. J. P. Mumford, Proc. Phys. Soc. (London) **76**, 559 (1960).

[13] S. Chandrasekhar and F. Breen, Astrophys. J. **103**, 41 (1946).

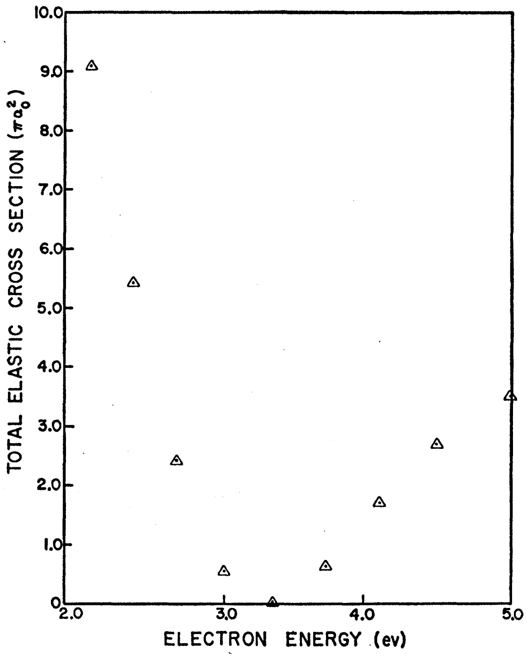

FIG. 3. Total elastic scattering cross sections for electrons incident on atomic hydrogen: strong-coupling approximation (no-exchange).

tion of an extra loop in the wave function was seen to take place by observing the decrease in the slope of the function with decrease in energy, until the slope actually changed sign and started to increase.

This dip in the total cross section, see Fig. 3, is not predicted in the static approximation whether exchange is included or not,[14] nor is it observed in the strong-coupling approximation using variational methods.[3] However, Lippmann and Schey,[15] using an optical-model analysis of the low-energy electron-hydrogen atom scattering, have found that the triplet cross section does have a sharp minimum in the energy region close to that drawn in Fig. 3.

Another interesting feature of this approximation is the low energy behavior of the $l=0$ phase shift. In Tables II and III it is seen that $\eta(0)$ tends to π, which differs appreciably from the static approximation, where $\eta(0)$ tends to zero. Extrapolation of the plot of $k\cot\eta_0$ vs k^2 back to $k^2=0$ predicts a scattering length equal to $+6.135a_0$, which is comparable to the best singlet scattering lengths calculated by variational methods.[16]

In Table III, we present a few preliminary results calculated in the strong-coupling approximation with exchange. In order to test the code, the method was applied to P waves at $k=0.4$ (singlet), 0.2 (triplet), and 0.1 (singlet); the results agreed to four decimal places with those of McEachran and Fraser[17] who solved the strong-coupling approximation in the form of integral equations. It should be remarked that the phase shift at $k=0.1$, was -0.0003, which has the opposite sign to the value calculated by Geltman.[3]

We note that both the triplet and singlet zero-order partial wave phase shifts tend to π as k tends to zero. Furthermore, the triplet phase shifts are almost the same as those calculated in the static exchange approximation[14] and by variational methods.[18] However, the singlet phase shifts are somewhat smaller and therefore give a larger scattering length.

A generalized version of the program used to calculate the numbers reported here has been written and is being tested. With this program, which includes all atomic states with $n\leqslant 3$, we hope to calculate the total elastic cross section in the strong-coupling exchange approximation over the entire energy region and so be able to compare the results with the experimental results of Bederson *et al.*[19] and Brackman *et al.*[20]

ACKNOWLEDGMENTS

The authors would like to thank J. W. Butler for discussions on the numerical analysis and B. S. Garbow and L. T. Michel for advice on the codes for Argonne's IBM-704.

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[19] B. Bederson, H. Malamud, and J. Hammer, Bull. Am. Phys. Soc. **2**, 172 (1957).

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