approximately 0.25. On the other hand, for 660-kev photons, the total Compton cross section appears to be independent of the electron binding energy. It is interesting to note that at 660 kev, the small- and large-angle behavior of $d\sigma_K$ has a compensating effect in which the total cross-section ratio, σ_K/σ_F, is approximately equal to unity for both tin and gold.

ACKNOWLEDGMENTS

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Electron Scattering from Hydrogen*

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Kohn's variational principle has been used to calculate S-wave elastic scattering of electrons from atomic hydrogen, using up to 50 trial functions of the type introduced by Hylleraas to describe the bound states of two-electron atoms. The phase shifts calculated at several energies up to 10 ev appear to have converged well, leaving residual uncertainties mostly less than one thousandth of a radian. Taking extra pains to include the effect of the long-range force at zero energy, we have also determined very accurate values for the scattering lengths.

INTRODUCTION

THE scattering of electrons from hydrogen atoms has been the subject of a great many calculations since it presents what is probably the simplest nontrivial real problem in scattering theory. We undertook a program of computing definitive values of the S-wave elastic phase shifts for this system, making no approximations other than those imposed by the finite speed and capacity of modern computing machines. Our use of the variational method[1] for this scattering problem completes, in a sense, the famous work on the bound states of two-electron atoms begun more than thirty years ago by Hylleraas.

Probably the most interesting, and quite unexpected, result of this program has been the realization of the extraordinary nature of the convergence of the "stationary" phase shift. It has been recognized for some time[2] that, in contrast with bound-state problems, the addition of more variational parameters in a scattering calculation does not necessarily lead to a better answer. This behavior is blamed on the nonexistence of any minimum (or maximum) principle. The error in a variational calculation may be represented by

$$\int \Delta(E-H)\Delta d\tau \qquad (1)$$

where Δ is the unknown error in the trial wave function. Only for systems where one knows the (finite) number of eigenvalues of H below the value E can one possibly state that the expression (1) must be negative.[3] For scattering at any finite energy it is clearly impossible to make any such statement. We have discussed elsewhere[4] how, by taking a great deal of numerical data, one can draw smooth curves and see an effectively regular convergence for the general scattering problem at any energy. This paper will present the results of this treatment for the e-H problem.

We use Kohn's variational principle,

$$[\tan\delta/k]=\tan\delta/k+(2m/\hbar^2)\int\psi(E-H)\psi d\tau_1 d\tau_2, \qquad (2)$$

where

$$(2m/\hbar^2)(E-H)=k^2-1+\nabla_1^2+\nabla_2^2+(2/r_1)+(2/r_2)-(2/r_{12}),$$

with lengths in units of $\hbar^2/me^2$; and our trial wave function is (for singlet or triplet states) $\psi=\varphi+\chi$,

$$\varphi=(1\pm P_{12})2e^{-r_2}[\sin kr_1/kr_1+\tan\delta\cos kr_1/kr_1(1-e^{-(\kappa/2)r_1})]/4\pi\sqrt{2}, \qquad (3a)$$

$$\chi=\sum_{l,m,n\geq 0} C_{lmn}e^{-(\kappa/2)(r_1+r_2)}r_{12}{}^l\times(r_1{}^m r_2{}^n\pm r_1{}^n r_2{}^m)/4\pi\sqrt{2}, \qquad (3b)$$

* Supported in part by the Advanced Research Projects Administration through the U. S. Office of Naval Research.

[1] A calculation identical to ours but limited to zero energy and using only a small number of parameters has recently been reported by Y. Hara, T. Ohmura, and T. Yamanouchi, Progr. Theoret. Phys. (Kyoto) **25**, 467 (1961).

[2] See, for example, H. S. W. Massey in *Handbuch der Physik* edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 36.

[3] L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. **119**, 164 (1960), have in this manner established minimum principles for scattering at zero energy. These authors have recently extended their method to positive energies, but only by mutilating the potentials.

[4] C. Schwartz, Ann. Phys. (to be published).

where P_{12} exchanges coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, and κ is the variable scale parameter which is so important in studying the convergence. The actual variation of parameters yields the standard linear problem

$$\sum_j M_{ij}C_j=-R_i, \quad (i, j=1, 2, \cdots, N),$$

$$M_{ij}=(2m/\hbar^2)\int \chi_i(E-H)\chi_j d\tau_1 d\tau_2, \tag{4}$$

$$R_i=(2m/\hbar^2)\int \chi_i(E-H)\varphi d\tau_1 d\tau_2,$$

and the final variation of $\tan\delta$ is also a trivial linear problem. We have specifically avoided the temptation of being selective in the choice of parameters in (3b) in order to get some "best" result for a given total number N of parameters. The numbers $N=3$, 7, 13, 22, 34, and 50 in the following results identify the order of the matrix including *all* terms in (3b) through total powers, $(l+m+n)$, from 2 to 7 for the triplet state and 1 to 6 for the singlet state, respectively.

RESULTS

Figure 1 shows the stationary values of $[(\tan\delta)/k]$ as computed for the triplet S wave at $k=0.4$ (about 2 ev). This is our most thoroughly studied case, the curves shown representing some 150 points in this region. Even so, a great deal of structure is not shown here. At $\kappa=1.55$, the 7×7 curve shows the singularity characteristic of the scattering problem (see reference 4). Similar singularities certainly do exist for all the larger matrices, but they are so narrow (as a function of κ) that we have not resolved them. At $\kappa<0.4$, all the curves pass through $+\infty$ and then come up again from $-\infty$ to a value of $[(\tan\delta)/k]$ of about -2.73 as $\kappa\to 0$. Convergence is inferred from the apparent behavior that for the larger number of parameters the curves become flatter and closer together. Our collection of final results (see Table I) is derived from such curves as this, where we have by inspection extrapolated to an answer and assigned our uncertainty (which should be interpreted as a very likely error).

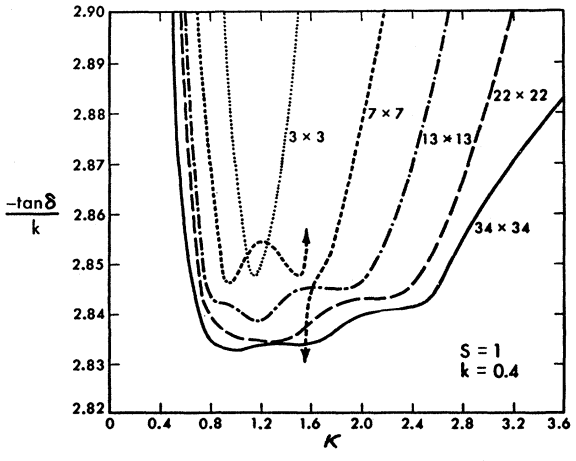

FIG. 1. Triplet phase shift at $k=0.4$: the most thoroughly studies case, over 150 points represented.

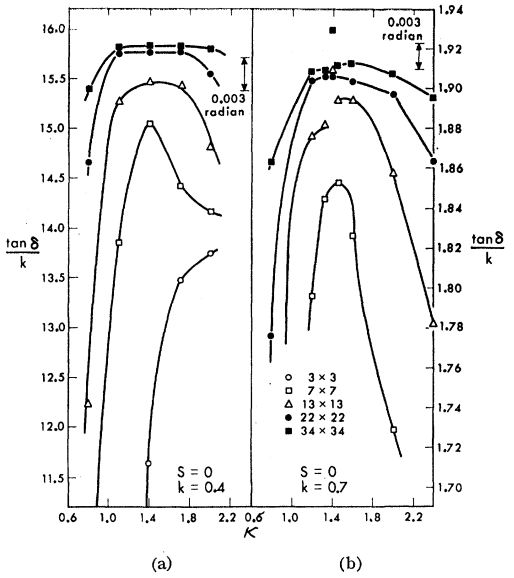

FIG. 2. (a) Singlet phase shift at $k=0.4$; typical well-behaved results using only five κ values. (b) Singlet phase shift at $k=0.7$; typical result with wild values at $\kappa=1.4$.

It may be thought that a reasonable measure of the goodness of calculations of this type is given by the fractional difference between the stationary value of $[\tan\delta]$ and the minimizing value of $\tan\delta$. A brief investigation has shown us that this measure is smallest (say as a function of κ) where the curves are flat, but it can easily lead to a gross overestimate of the accuracy; it actually passes through zero, and its mean square value in this good region is much less than the proper error in the calculation as deduced from the apparent rate of convergence.

Most of our results were obtained from only a few ($\geqq 5$) κ values; Fig. 2(a) shows a typical case. Figure 2(b) shows a case where one of the first 5 points ($\kappa=1.4$) gave results noticeably "out of line" with its neighbors, for the 13 and 34 size matrices. The extra

TABLE I. Results of variational calculations of S-wave e-H scattering. The numbers in parentheses give the uncertainty in the last digit quoted.

	S=0		S=1	
k	$[\tan\delta/k]$	δ (radians)	$[\tan\delta/k]$	δ (radians)
0.1	−6.68(2)	2.553(1)	−2.056(4)	2.9388(4)
0.2	−9.23(2)	2.0673(9)	−2.260(3)	2.7171(5)
0.3	−26.4(1)	1.6964(5)	−2.492(4)	2.4996(8)
0.4	+15.87(4)	1.4146(4)	−2.833(2)	2.2938(4)
0.5	5.17(2)	1.202(1)	−3.384(3)	2.1046(4)
0.6	2.845(8)	1.041(1)	−4.40(1)	1.9329(8)
0.7	1.917(5)	0.930(1)	−6.74(2)	1.7797(6)
0.8	1.530(5)	0.886(1)	−17.2(6)	1.643(3)
0.866	···	···	+150(20)	1.563(1)

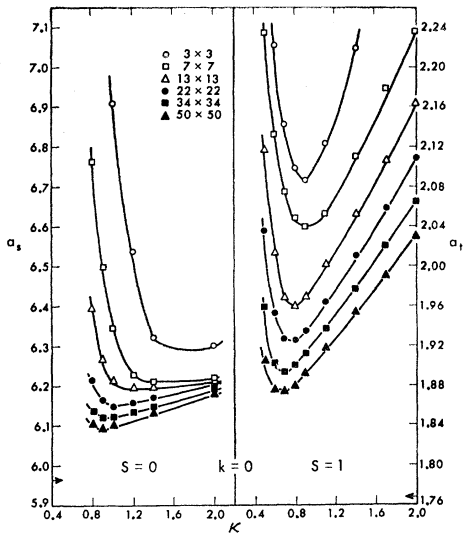

FIG. 3(a) and (b). First zero-energy results.

data taken nearby, at $\kappa=1.33$ and 1.45 support our general rule that in these proceedings one should disregard the singular points and use only the smoothest results. Returning to Fig. 1, it seems possible that there may be a smooth region between $\kappa=1.8$ and 2.4, but it is in the $\kappa=1.0$ to 1.6 region that the "best" (smooth and convergent from one curve to the next) behavior is seen.

Having satisfied the requirements given in reference 3, we are guaranteed at $k=0$ a strict minimum principle for the scattering length, $a=-\tan\delta/k$ $(k\to 0)$. Figure 3(a) and (b) show our results which do appear as smooth parabolas; but it is also clear that the convergence here is very poor. A crude analysis of the differences of successive minima of these curves suggests a convergence like $\sum 1/N^2$, and an extrapolation on this basis gives $a_s=5.95$, $a_t=1.77$, which values are in fact quite close to the much better results described in the next section.

Another convergence problem arises at the other end of the elastic energy region. Above excitation of the $n=2$ levels the asymptotic part of the wave function will have a term $e^{ik'r}$, where $k'=(k^2-\frac{3}{4})^{\frac{1}{2}}$. Thus just below threshold k' is a small imaginary number and the correct wave function will have a long tail, which our localized trial functions will find it difficult to reproduce. In fact we were unable to make any sensible deductions from our data for the singlet state at $k=0.866$; the triplet state at this energy was more approachable, probably because the phase shift is very close to $\pi/2$ (the resonance dominates).

PROBLEM OF THE LONG-RANGE FORCE

It is well known that, in the adiabatic approximation, the potential seen at large distances from a hydrogen atom is $-(\hbar^2/2m)(\alpha/r^4)$, and it has been pointed out[5] that in such a circumstance the asymptotic form of the wave function at zero energy is

$$1-(a/r)-(\alpha/2r^2).$$

The slow convergence noted above for our first work at $k=0$ can be blamed on the difficulty of expanding a function[6] which dies off as slowly as $1/r^2$ in terms of $r^n e^{-r}$. At finite energies it may be inferred that the long-range potential has been effectively "washed out."

It is not hard to show that for the scattering of a particle of unit charge from a neutral spin-zero atomic system with ground-state wave function $\Phi^{(0)}$, the total wave function has the following expansion for large values of the coordinate r_0 of the scattering particle.

$$\Psi=\Phi^{(0)}\left[1-\frac{a}{r_0}-\frac{\alpha}{2r_0^2}\right]+\frac{\mathbf{r}_0\cdot\boldsymbol{\Phi}^{(1)}}{r_0^3}+O(r_0^{-3}), \tag{5}$$

where $\boldsymbol{\Phi}^{(1)}$ is the polarized target wave function,

$$(E_0-H_0)\boldsymbol{\Phi}^{(1)}=\mathbf{D}\Phi^{(0)}. \tag{6}$$

$\mathbf{D}$ is the dipole moment operator for the atomic system and α is its static polarizability,

$$\alpha=-\tfrac{2}{3}(\Phi^{(0)},\mathbf{D}\cdot\boldsymbol{\Phi}^{(1)}). \tag{7}$$

Thus an improved choice for the asymptotic wave function (3a) is[7]

$$\varphi=(1\pm P_{12})2e^{-r_2}\left[1-\frac{a}{r_1}f_1-\frac{2.25}{r_1^2}f_2-\cos\theta_{12}\frac{(r_2+r_2^2/2)}{r_1^2}f_3\right]\Big/4\pi\sqrt{2}, \tag{8}$$

where the f's are functions used to shield the singularities at $r\to 0$:

$$f_n=r_1^n\int_0^d\frac{p^{n-1}dp}{(n-1)!}e^{-pr_1}. \tag{9}$$

The manual labor of setting up all the integrals with this improved φ was very great; the value of d was fixed at 1.0, and the scale parameter κ in χ was varied independently.

These new zero-energy results, shown in Fig. 4(a) and (b), do exhibit a much improved convergence, at a rate approximately equal to $\sum 1/N^4$, which was anticipated. Our final results are $a_s=5.965\pm0.003$, $a_t=1.7686\pm0.0002$.

In our earlier discussion[4] of these computations it was

[5] L. Spruch, T. F. O'Malley, and L. Rosenberg, Phys. Rev. Letters, **5**, 375 (1960).

[6] We have made a simplified analysis of this expansion problem, supporting the previously noted $1/N^2$ rate of convergence.

[7] At an earlier stage of these investigations we used only the first new term in this expression, being then ignorant of the $\cos\theta/r^2$ term. The results were essentially no better than in the original attempt.

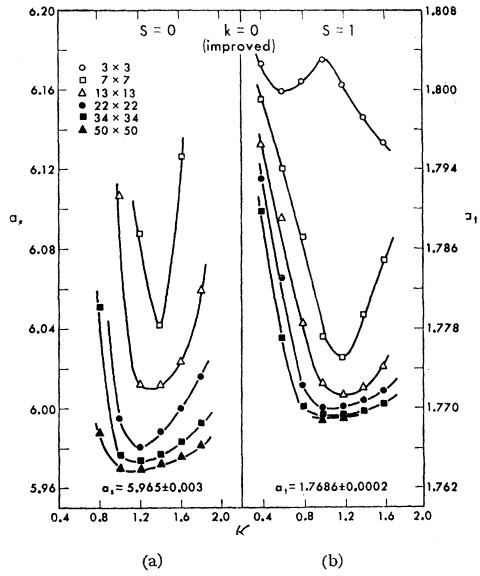

FIG. 4 (a) and (b). Improved zero-energy results.

mentioned that numerical inaccuracies [round-off errors accumulated in solving Eq. (4)] could be a serious problem. In particular, we could not determine the stationary value from our 50×50 matrix at zero energy (the old way) to any better than about 1%. However, with this improved calculation the numerical uncertainties were much reduced. There thus seems to be a correlation between good convergence and good numerical accuracy at each step.[8] This is a very interesting phenomenon for which we do not have any general theoretical understanding, but it appears to be a rather general property of variational calculations.

The computations reported here were carried out on the IBM 704 facility of the University of California Computation Center.

TABLE II. e^+-H phase shifts.

ka_0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
δ (radians)	0.151	0.188	0.168	0.120	0.062	0.007	−0.054

POSITRON SCATTERING

A few simple modifications of the programs allowed us to calculate elastic S-wave phase shifts for the scattering of positrons by atomic hydrogen. Since without the space symmetry we now need more terms in (3b) for each total power, $(l+m+n)$; the results do not converge as rapidly as for e^-. The results, shown in Table II, have probable errors of about ±0.001 radian. For the scattering length we find the upper bound $a_+ \leqq -2.10$; and from the apparent rate of convergence we believe that a_+ will not be as little[9] as −2.11.

[8] This behavior was also noted at the end of Appendix 2 of reference 4.

[9] Compare with previous results of L. Spruch and L. Rosenberg, Phys. Rev. **117**, 143 (1960).

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Continuous Photoelectric Absorption Cross Section of Helium*

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The continuous photoelectric absorption cross section of helium has been measured in the spectral region extending from 180 to 600 A with greater accuracy and the observations are found to agree with the calculations of Huang and Stewart and Wilkinson. A grazing incidence spectrometer with a photomultiplier was used for a single measurement at 180 A while the remaining measurements were carried out in a normal incidence spectrometer utilizing photographic techniques. Whereas in previous experiments the absorbing gas sample was allowed to fill the entire spectrometer chamber, in the current measurements the gas was confined to a small cell provided with sufficiently transparent windows. The use of an absoprtion cell reduces contamination and facilitates the measurement of gas pressures. The results indicate that the cross section varies from a value of 0.98±0.04 Mb at 180 A to a value of 7.7±0.3 Mb at the absorption edge located at 504 A.

I. INTRODUCTION

FOLLOWING recent success in the development of windows which are transparent to extreme ultraviolet radiation, we have carried out measurements of the continuous photoelectric absorption cross section of helium. The use of such windows in the construction of a gas cell permits confinement of the gas sample to a restricted volume. This technique has certain advantages over earlier methods[1,2] which used the entire

* Supported in part by the Office of Naval Research.

[1] P. Lee and G. L. Weissler, Phys. Rev. **99**, 540 (1955).

[2] N. Axelrod and M. P. Givens, Phys. Rev. **115**, 97 (1959).