experiment for the cross section for the electron ionization of atomic hydrogen. To get this agreement it is necessary to use an electron velocity distribution of the form  $(v_0/v_1)^3 e^{-v_0/v_1}$ ; since this distribution is very different from the exact velocity distribution its use cannot be justified theoretically. However, this semiempirical procedure could partially be justified if it gave good results for other atomic systems. Unfortunately, this is not the case. For example, if we compare the cross sections obtained from Gryzinski's semiempirical formula with the Bethe formulas<sup>14</sup> for electron ionization of the states of hydrogen with principal quantum numbers n=2, 3, and 4 we find that at high energies the semiempirical classical formula is in error by factors of 2, 3, and 4, respectively.

It is interesting to note in Table I that the two classical cross sections obtained by replacing V by  $(v_1^2+v_2^2)^{1/2}$  tend to agree quite closely with the experimental cross section at low energies. Since the result of this approximation is to eliminate collisions with long interaction times it has been suggested<sup>2</sup> that since it has the same effect as the inclusion of the atomic nucleus it

<sup>14</sup> H. Bethe, Ann. Physik 5, 325 (1930).

is a better approximation than the original classical approximation. By comparing columns one, two, and five of Table I we see that this suggestion is true.

### CONCLUSION

At large impact energies we cannot expect the classical inelastic electron-atom scattering cross sections to agree with experiment, for the classical theory cannot describe an electron-atom collision correctly. However, at incident electron energies of a few atomic units the classical description of a collision is valid and the classical cross sections should be as accurate as the Born-approximation cross sections. If the incident electron energy is close to the ionization or excitation threshold the electron-electron interaction is not the dominant interaction and we cannot expect either the classical or the Born approximations to give accurate cross sections.

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## Polarization Effects in the Elastic Scattering of Electrons from Helium\*†

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The cross section for elastic scattering of electrons from helium atoms has been computed for an energy range from 0 to 50 eV. The formalism used here was obtained from an extension of Hartree-Fock theory wherein the distortion induced in the atom by the scattering electron is approximated by a polarization potential. The method is similar to the "adiabatic-exchange" treatment of electron-hydrogen scattering by Temkin and Lamkin. The computed scattering phase shifts and cross sections are compared with various other calculations and experimental data. A scattering length of  $1.13 a_0$  is extrapolated from the phase shifts after correcting them for the effects of truncating the polarization interaction as required in the iteration process. The computed total cross sections compare favorably at low energies with the data of Ramsauer and Kollath and at very low energies with the modified effective-range theory of O'Malley, Spruch, and Rosenberg. The differential scattering cross sections follow the effective-range theory at higher energies. The momentum-transfer cross sections agree well with recent microwave drift-velocity measurements, especially those of Pack, Phelps, and Frost.

### I. INTRODUCTION

THIS paper is concerned with the elastic scattering of electrons from atomic helium in the energy region from 0 to 50 eV. For this problem, as in all lowenergy electron-atom scattering problems, two major effects must be included in the formalism to give adequate description of the scattering. These are the exchange interactions between the scattering electron and the atomic electrons arising from the exclusion principle and the distortion induced in the atomic system by the presence of the scattering electron.

Exchange effects in scattering have been studied by

<sup>\*</sup> A preliminary account of this work was given at the Pasadena meeting of the American Physical Society [Bull. Am. Phys. Soc. 8, 608 (1963)].

 $<sup>\</sup>dagger$  This work was supported in part by the U. S. Bureau of Naval Weapons,

many authors, including Morse and Allis who treated the cases of hydrogen and helium.<sup>1</sup> From these investigations it is clear that exchange effects must be contained in any theory which treats electron-atom scattering at low energies. This may be done either by explicit antisymmetrization of the total wave function for the system or implicitly in an eigenfunction expansion over a complete set of states for the system. In the present study, a completely antisymmetrized wave function is used to include exchange.

As yet no simple procedure exists for adequately treating the more subtle distortion effects. There is in fact a sequence of interrelated effects as the electron moves in through the atom. These effects may be characterized by the magnitude of the separation distance between the electron and atom. For very large separations, the system consists of a point charge and neutral atom between which there will exist a  $-\alpha/r^4$  polarization potential due to the dipole moment induced in the atom (polarizability  $\alpha$ ) by the electric field of the point charge.<sup>2,3</sup> As the separation decreases, the electron is accelerated by the attractive polarization potential and although it may have started at infinity with a velocity far below that of the atomic electrons, it soon attains a velocity of similar magnitude. This leads to velocitydependent interactions. When the scattering electron penetrates the atom, correlation effects between it and the atomic electrons become important since the atomic configuration must adjust for the close proximity of this additional electron.

To date, only the first of these effects has been given much consideration. In this case the usual procedure is to assume that the velocity of the incident electron remains substantially smaller than that of the atomic electrons so that the entire electronic configuration of the atom instantaneously readjusts for each position of the incident electron. From the resulting distortion, usually only the dipole polarization part is retained. This method is commonly called the "adiabatic" approximation and has been applied with some success to hydrogen by Temkin and Lamkin.<sup>4</sup> Their treatment included the Pauli principle explicitly in determining the polarization and the resulting formalism then incorporates some dynamic effects.

Another case in which the adiabatic approximation has been applied with greater success, although restricted to very low energies, is the modified effectiverange theory of O'Malley, Spruch, and Rosenberg.<sup>5</sup> For

this, the long-range  $-\alpha/r^4$  polarization potential was shown to be the major interaction determining the scattering in the limit of zero energy. The usual effectiverange theory developed for nuclear problems was then modified to account for this long-range potential and an expansion in energy was derived for the cross section. Application of this theory to low-energy scattering from helium and other rare gases has been given by O'Malley with good results for energies up to a few  $eV.^6$ 

The demonstration by modified effective-range theory of the importance of the adiabatic polarization interaction at low energies prompted us to examine this approximation in more detail, and over a larger energy region. In particular we have included polarization effects in a Hartree-Fock calculation of electron scattering from helium where we have found substantial improvement in the cross sections for the energy region from 0 to 50 eV as compared to those of previous calculations. The derivation of the extended Hartree-Fock equation follows the procedure of Temkin and Lamkin,<sup>4</sup> and is discussed in Secs. II and III.

A further comment should be made concerning the close-range correlation effects mentioned above. These effects are necessarily neglected in the present formalism. To include them, one must use a more powerful method such as "close-coupling" which has been applied to hydrogen.7 However, this approach requires knowledge of all the eigenfunctions of the atom being treated in order to get just the adiabatic polarization effect and as such holds little promise in its present form for any atoms other than hydrogen as far as elastic scattering is concerned.<sup>8</sup> An extension of this method wherein only a few of the low-lying states are kept in the eigenfunction expansion and the remaining states approximated by an "optical" potential has, however, been considered by Pu.9

The reduction of the scattering equation to a form suitable for computer solution and the methods used to solve it are given in Sec. IV. The results obtained from this formalism are presented and compared with other calculations and with experiment in Sec. V.

# II. DERIVATION OF THE SCATTERING EQUATION

The procedure used to obtain the equation for the scattering wave function follows the standard Hartree-Fock (H-F) method. One requires that the variation of the integral

$$I = \int \Psi^* (H - E) \Psi d\tau \tag{1}$$

<sup>&</sup>lt;sup>1</sup> P. M. Morse and W. P. Allis, Phys. Rev. 44, 269 (1933). <sup>2</sup> We have assumed here, as is the case for helium, that the isolated atom possesses no intrinsic quadrupole moment. If such should exist as in the case of oxygen, a potential proportional to  $1/r^3$  would be present which would have more important long-range effects than the induced dipole moment.

Atomic units are used throughout this paper in which  $\hbar = 1$ ,  $e^2 = 2$ , and  $m = \frac{1}{2}$ . The unit of length is the Bohr radius and that of

 <sup>&</sup>lt;sup>4</sup> A. Temkin and J. C. Lamkin, Phys. Rev. 121, 788 (1961).
 <sup>5</sup> T. F. O'Malley, L. Spruch, and L. Rosenberg, Phys. Rev. Letters 5, 375 (1960); J. Math. Phys. 2, 491 (1961); Phys. Rev. 125, 1300 (1962).

<sup>&</sup>lt;sup>6</sup> T. F. O'Malley, Phys. Rev. **130**, 1020 (1963). <sup>7</sup> See for example the comprehensive review of electron-hydrogen scattering by P. G. Burke and K. Smith, Rev. Mod. Phys. 34, 458 (1962).

<sup>&</sup>lt;sup>8</sup> The "close-coupling" approach has been found to be a powerful method for treating inelastic collisions since any particular channel of interest can be examined almost independently of the others.

<sup>&</sup>lt;sup>9</sup> R. Pu, University of California Radiation Laboratory Rept. UCRL-10878, 1963 (unpublished).

be zero, where, for helium the total Hamiltonian is given by

$$H = -\nabla_{1}^{2} - \nabla_{2}^{2} - \nabla_{3}^{2} - \frac{4}{r_{1}} - \frac{4}{r_{2}} - \frac{4}{r_{3}} + \frac{2}{r_{12}} + \frac{2}{r_{13}} + \frac{2}{r_{23}}, \quad (2)$$
  

$$r_{ij} = |\mathbf{r}_{i} - \mathbf{r}_{j}|,$$
  
and the energy is  

$$E = E_{4} + k^{2} \quad (3)$$

and the

$$E = E_A + k^2 \tag{3}$$

with  $E_A$  the ground-state energy of the atom and  $k^2$  the energy of the scattering electron.

The Pauli principle requires that the total wave function for the system be antisymmetric in the interchange of any two electrons. To include this and adiabatic distortion effects, the Ansatz for the total wave function is taken as an antisymmetric combination of the perturbed wave functions for the atomic orbitals and the scattering electron. Since the atomic configuration forms a singlet spin state, only one orientation of the scattering electron spin need be considered. Furthermore, since exchange is explicitly included, the perturbed atomic orbitals must be properly paired with the wave function for the scattering electron. From these considerations, the Ansatz is taken to be

$$\Psi(1,2,3) = (3)^{-1/2} [\psi^{(3)}(1,2)\varphi(3)\mathbf{S}(1,2)\alpha(3) + \psi^{(2)}(3,1)\varphi(2)\mathbf{S}(3,1)\alpha(2) + \psi^{(1)}(2,3)\varphi(1)\mathbf{S}(2,3)\alpha(1)], \quad (4)$$

where  $\mathbf{S}$  is the singlet spin function,

$$\mathbf{S}(i,j) = (2!)^{-1/2} [\boldsymbol{\alpha}(i)\boldsymbol{\beta}(j) - \boldsymbol{\alpha}(j)\boldsymbol{\beta}(i)], \qquad (5)$$

 $\alpha$  and  $\beta$  are single electron spinors with projections  $m_s = +\frac{1}{2}$  and  $-\frac{1}{2}$ , respectively;  $\varphi$  is the wave function of the scattering electron, and  $\psi^{(n)}(i,j)$  denotes the space part of the H-F wave function for the atomic orbitals, electrons i and j, perturbed by the field of a separated electron *n*. The functions  $\psi^{(n)}(i,j)$  are assumed to be known, and are not varied. The Ansatz is also seen to be an eigenfunction of the total spin of the system.

The atomic wave functions are determined to first order in the interaction with the "scattering electron." According to Temkin these will be of the form <sup>10</sup>

$$\psi^{(n)}(i,j) = \psi_{100}(i)\psi_{100}(j) + \psi_{100}(i)\chi(j;n) + \psi_{100}(j)\chi(i;n), \quad (6)$$

where  $\psi_{100}$  denotes the unperturbed H-F wave function for the helium ground state and X(j; n) is the first-order perturbed wave function for the state of atomic electron j acted on by the field of separated electron n.

For future reference, the unperturbed wave functions satisfy the ordinary H-F equation

$$[-\nabla_1^2 - 4/r_1 + V_{\epsilon}(r_1) - \epsilon] \psi_{100}(\mathbf{r}_1) = 0, \qquad (7)$$

where  $\epsilon$  is the H-F single electron energy eigenvalue and  $V_c$  is the self consistent electron interaction given by

$$V_{c}(\mathbf{r}_{1}) = \int |\psi_{100}(\mathbf{r}_{2})|^{2} \frac{2}{r_{12}} d\tau_{2}.$$
 (8)

<sup>10</sup> A. Temkin, Phys. Rev. 107, 1004 (1957).

We do not use the rather complicated H-F perturbation theory, but instead assume that the perturbed function satisfy the equation<sup>11</sup>

$$\begin{bmatrix} -\nabla_{i}^{2} - \frac{4}{r_{i}} + V_{c}(r_{i}) - \epsilon \end{bmatrix} \chi(\mathbf{r}_{i}; \mathbf{r}_{n}) = [\mu(r_{n}) - \upsilon(\mathbf{r}_{i}, \mathbf{r}_{n})] \psi_{100}(\mathbf{r}_{i}), \quad (9)$$

where

μ

$$(\mathbf{r}_n) = \int |\psi_{100}(\mathbf{r}_i)|^2 \mathfrak{V}(\mathbf{r}_i, \mathbf{r}_n) d\tau_i \qquad (10)$$

is the first-order perturbation energy and  $\mathcal{U}(\mathbf{r}_i,\mathbf{r}_n)$  is the perturbation potential acting on electron i due to electron n. The terms deleted from the H-F perturbation theory are Coulomb and exchange integrals between the perturbed and unperturbed wave functions and neglect of them should be justified since they are smaller than the terms retained.

The perturbation potentials v are the corresponding two-body parts of the total interaction between the scattering electron and the atom,

$$V_{in}(1,2,3) = -\frac{4}{r_3} + \frac{2}{r_{13}} + \frac{2}{r_{23}}.$$

These may be expanded in the Legendre polynomial series

$$\upsilon(\mathbf{r}_{i},\mathbf{r}_{n}) = \frac{2}{r_{in}} = 2 \sum_{l=0}^{\infty} \frac{r_{<^{l}}}{r_{>^{l+1}}} P_{l}(\cos\theta_{in}), \qquad (11)$$

where  $r_{\leq}$  is the smaller and  $r_{>}$  the larger of  $r_i$  and  $r_n$ . A common assumption is to consider the atomic orbitals perturbed only where the scattering electron is "outside" of the atomic electrons  $(r_n > r_i)$ , the perturbation vanishing otherwise.<sup>12</sup> For the case being treated here, we have used a slightly different approach wherein some contribution from the region where the scattering electron is inside of the atomic electrons is retained as explained in the following.

For helium, we have not solved for the H-F perturbed wave functions since we are considering only the direct polarization potential effects at present. Instead, we have used the polarization potential given by Bethe<sup>13</sup> which he derived using the simple  $\exp(-zr)$  variational wave functions for the atomic orbitals. Bethe's considerations were actually directed toward finding the second order correction to the energy of the atom for one electron in a highly excited state. In this, then, he also included the region where the outer electron was inside of the 1s electron since the probability of such was not negligible. By doing this, he obtained different

<sup>&</sup>lt;sup>11</sup> The complete form of the perturbed wave function equation given by Temkin in Ref. 10 is slightly in error. The proper form is given in its entirety by J. Callaway, Phys. Rev. 106, 868 (1957).

<sup>&</sup>lt;sup>12</sup> A. Temkin, Phys. Rev. 116, 358 (1959).
<sup>13</sup> H. A. Bethe, *Handbuch der Physik* (Edwards Brothers, Inc., Ann Arbor, Michigan, 1943), Vol. 24, Pt. 1, pp. 339 ff.

.

perturbed wave functions for the "inner" and "outer" regions which then had to be matched at the boundary.

Since Bethe assumed that the 1s wave function is simply an exponential instead of the actual H-F wave function, a matching problem arises. This is overcome by noting that it is mainly the asymptotic form of the polarization potential which is important,<sup>12</sup> so that as long as we match this to the proper  $-\alpha/r^4$  form, reasonable results should be obtained in the adiabatic approximation. This matching is discussed further in Sec. III. The choice of Bethe's polarization potential over that given by Callaway<sup>11</sup> (or Temkin<sup>12</sup> which is the same) was motivated by the fact that Bethe's varies like  $r^2$ at the origin while Callaway's goes like r and semiclassical considerations indicate that a  $r^2$  dependency is appropriate.

The scattering equation is then obtained by substituting (2), (3), and (4) into (1), integrating over spin and carrying out the variation on  $\varphi^*$ . This results in the equation

$$\int \psi^{*(3)}(1,2) \{H-E\} \\ \times [\psi^{(3)}(1,2)\varphi(3) - \psi^{(2)}(3,1)\varphi(2)] d\tau_1 d\tau_2 = 0 \quad (12)$$

for the scattering electron wave function  $\varphi$ , where, in obtaining this, we have used the fact that the perturbed atomic wave functions in the exchange part are identical as far as the integral in (12) is concerned.

Equation (12) sometimes appears in a form in which the unperturbed atomic function appears on the left in the integrand. This is suggested, but is by no means required by the definition of the full scattering wave function as the projection of total wave function on the unperturbed target atom wave function.<sup>14</sup> That procedure may have some justification if one can choose an approximate wave function for the system which is extremely close to the exact wave function, so that the Schrödinger equation alone,

$$(H-E)\Psi = 0 \tag{13}$$

is approximately satisfied. One may then multiply by anything on the left and integrate out the undesired coordinates without appreciably changing the validity of the results. This is just the philosophy behind the "close-coupling" approach to scattering problems.

#### **III. REDUCTION OF THE SCATTERING EQUATION**

The adiabatic-exchange approximation for the scattering equation is obtained by keeping the perturbed atomic wave functions only in the direct terms while neglecting them completely in the exchange terms in (12). Thus, all terms in (6) are retained for the first integral in (12) while only the first term of (6) is retained in the second integral. In addition, any *dynamic* terms of the form  $\nabla_n^2 \chi(\mathbf{r}_i; \mathbf{r}_n)$  are neglected as are all thirdand higher order terms. Making these substitutions and using (7) and (9) to reduce the resulting terms gives the adiabatic-exchange equation for  $\varphi$  as

$$\begin{bmatrix} -\nabla_{3}^{2} - \frac{4}{r_{3}} + 2V_{c}(r_{3}) + 2V_{p}(r_{3}) - k^{2} \end{bmatrix} \varphi(\mathbf{r}_{3})$$

$$= \begin{bmatrix} (\epsilon - k^{2}) \int \psi_{100}^{*}(\mathbf{r}_{2}) \varphi(\mathbf{r}_{2}) d\tau_{2} \\ + \int \psi_{100}^{*}(\mathbf{r}_{2}) \frac{2}{r_{23}} \varphi(\mathbf{r}_{2}) d\tau_{2} \end{bmatrix} \psi_{100}(\mathbf{r}_{3}), \quad (14)$$

where  $V_p$  is the polarization potential and given by

$$V_{p}(r_{3}) = \int \psi_{100}^{*}(\mathbf{r}_{1}) \mathcal{U}(\mathbf{r}_{1},\mathbf{r}_{3}) \chi(\mathbf{r}_{1};\,\mathbf{r}_{3}) d\tau_{1}, \quad (15)$$

in general. For our case, only the dipole part of  $\mathcal{U}$  was retained [the l=1 term of (11)] and the corresponding polarization potential was given by Bethe<sup>13</sup> as

$$2V_{p}(r) = -\frac{9}{(zr)^{4}} \left\{ 1 - \frac{1}{3} e^{-2zr} \left[ 1 + 2zr + 6(zr)^{2} + \frac{20}{3} (zr)^{3} + \frac{4}{3} (zr)^{4} \right] - \frac{2}{3} e^{-4zr} (1 + zr)^{4} \right\}, \quad (16)$$

where z is chosen so that the asymptotic form of (16) approaches

$$2V_p(r) \rightarrow -\alpha/r^4$$
, for  $r \rightarrow \infty$ , (16a)

which gives

$$z = (9/\alpha)^{1/4} \tag{17}$$

with  $\alpha$  the experimental polarizability.

This equation is equivalent to the adiabatic-exchange equation solved by Temkin and Lamkin<sup>4</sup> and hence the conflicting viewpoints discussed at the end of the previous section only give differences in the form of the polarization exchange terms which are neglected here.

The neglect of the polarization exchange terms in (14) corresponds to actually neglecting some first-order terms while the second-order polarization potential is retained. The justification for this approximation lies in the fact that all of the exchange terms neglected will contain factors which fall off exponentially with increasing  $r_3$  since they are always mlutiplied by a bound-state wave function. The polarization potential, on the other hand, falls off only as  $r_3^{-4}$  and thus, although of higher order in a formal sense than neglected terms, is of sufficiently greater range to be of more importance than the exponentially decaying terms. This is readily seen to be true for hydrogen when one observes the changes in the phase shifts as the various orders of approximation were included in the work of Temkin and Lamkin. A similar situation is believed to hold for helium. A more elaborate analysis including most of the deleted terms will be considered in subsequent work.

<sup>14</sup> A. Temkin, J. Math. Phys. 2, 336 (1961).

The solution of (14) is achieved by first expanding  $\varphi$  in the spherical harmonic series

$$\varphi(\mathbf{r}) = r^{-1} \sum_{l} u_{l}(r) Y_{l}^{0}(\Omega) \qquad (18)$$

substituting this into (14), multiplying by  $r_3 Y_l^{0*}(\Omega_2)$ and integrating over  $d\Omega_3$  to get an integrodifferential equation for the  $u_l(r)$ . This equation is then solved for the  $u_l$  subject to the boundary conditions

$$u_l(r) \to r^{l+1}, \qquad \text{for} \quad r \to 0,$$

$$u_l(r) \rightarrow \text{const} \times \sin(kr - l\pi/2 + \eta_l), \text{ for } r \rightarrow \infty,$$
 (19)

where  $\eta_l$  is the resulting phase shift. The scattering cross sections are then obtained from the phase shifts by the standard partial-wave expansions.

## IV. SOLUTION OF THE SCATTERING EQUATION

The radial equation obtained after intergrating out the angular dependence in (14) is adapted for computer solution by writing it in the form

$$\frac{d^{2}}{dr_{3}^{2}}u_{l}(r_{3}) = \left[\frac{l(l+1)}{r_{3}^{2}} - \frac{4}{r_{3}} + 2V_{c}(r_{3}) + 2V_{p}(r_{3}) - k^{2}\right]u_{l}(r_{3})$$
$$-\frac{2}{2l+1}R_{1s}(r_{3})\left[\left\{B_{l} + \frac{1}{2}A_{l}(\epsilon - k^{2})\delta_{l,0}\right\}r_{3}^{l+1} + r_{3}^{-l}\int_{0}^{r_{3}}R_{1s}(r_{2})u_{l}(r_{2})r_{2}^{l+1}dr_{2} - r_{3}^{l+1}\int_{0}^{r_{3}}R_{1s}(r_{2})u_{l}(r_{2})r_{2}^{-l}dr_{2}\right], \quad (20)$$

where  $A_l$  and  $B_l$  are two constants given by

$$A_{l} = \int_{0}^{\infty} R_{1s}(r_{2})u_{l}(r_{2})r_{2}^{l+1}dr_{2},$$

$$B_{l} = \int_{0}^{\infty} R_{1s}(r_{2})u_{l}(r_{2})r_{2}^{-l}dr_{2},$$
(21)

and  $R_{1s}$  is the normalized (and real) radial part of the unperturbed H-F 1s wave function for the helium atom, related to the  $\psi_{100}$  by  $\psi_{100}(\mathbf{r}) = R_{1s}(\mathbf{r}) Y_0^0(\Omega)$ .

The H-F wave functions used here were those given in analytical form by Roothan, Sachs, and Weiss for which the corresponding energy eigenvalue is  $\epsilon = -1.835912$ Rv.<sup>15</sup> The value used for the polarizability of helium,  $\alpha$ , was that given by Wikner and Das<sup>16</sup> as 1.376  $a_0^3$ .

Equation (20) is thus in a form suitable for iteration from the origin out once starting values for  $A_0$  and  $B_l$ are determined. For this, the differential equation was iterated by Milne's method<sup>17</sup> with the integrals done

by Simpson's rule. To begin the iteration, Milne's method necessitated knowledge of the first four points and these were obtained by expanding  $u_l$  in a power series, substituting this into (20) and solving for the first few coefficients. In addition, the required starting values for  $A_0$  and  $B_l$  were found by solving (20) with the last part set equal to zero (the no-exchange approximation). The resulting wave functions were then used in (21) to estimate the constants  $A_0$  and  $B_l$ .

Having a set of starting values, the entire integrodifferential equation was iterated through a selfconsistent field procedure. For this, the iteration was carried out to the point where new values of the constants  $A_l$  and  $B_l$  could be obtained with sufficient accuracy (the exponential decay of the atomic orbitals causes the integrands to vanish to a good approximation for  $r \ge 15$ ). The new value of  $A_l$  was then compared with the starting value and if they disagreed to some present accuracy, the new values of  $A_l$  and  $B_l$  were used for starters and the iteration repeated. This procedure was repeated until an essentially self-consistent solution was obtained wherein the constant  $A_l$  changed by less than 0.1% from iteration to iteration. At this point, the solution was assumed self-consistant and the iteration carried out to r = 25. The constant  $B_l$  was not explicitly checked in this since experience showed it to converge more rapidly, changing by less than 0.01% when the change in  $A_l$  had decreased to 0.1%.

The mesh size used in this iteration was varied from 0.01 to 0.1 in the following pattern;  $\Delta r = 0.01$  for  $0 \le r \le 0.15$ ,  $\Delta r = 0.05$  for  $0.15 \le r \le 2.0$  and  $\Delta r = 0.1$  for  $2.0 \le r \le 25$ . This was done to allow accurate starting values for the iteration to be obtained with only the first few terms in the power-series expansion of  $u_l$  and at the same time get good accuracy from Milne's method over the region where the nuclear Coulomb potential has a very large derivative. However, varying the mesh in this way led to difficulties in using Simpson's rule for the integrals when passing the points where the mesh was changed. These difficulties were surmounted by using the trapezoidal rule for the integrals for the first increment in the region of a changed mesh size.

Approximate phase shifts were extracted from the iterated  $u_l$  around r=R=25 by matching these to the spherical Bessel functions in the form

$$u_l(r) = Cj_l(kr) - Dn_l(kr)$$
(22)

from which the phase shifts were then found from

$$\eta_l(R) = \tan^{-1}(D/C) \tag{23}$$

mod  $\pi$ , where  $\eta_l(R)$  indicates the phase shift induced by the interaction between the origin and the point r=R. To determine the actual phase shift  $\eta_l$ , both the proper multiple of  $\pi$  to be added to (23) and the effect of terminating the iteration at some finite R were examined as follows.

The proper multiple of  $\pi$  was determined from

<sup>&</sup>lt;sup>15</sup> C. C. J. Roothan, L. M. Sachs, and A. W. Weiss, Rev. Mod. Phys. 32, 186 (1960).
<sup>16</sup> E. G. Wikner and T. P. Das, Phys. Rev. 107, 497 (1957).
<sup>17</sup> W. E. Milne, *Numerical Calculus* (Princeton University Press, Princeton, New Jersey, 1949), p. 140.

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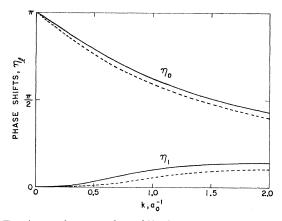


FIG. 1. s- and p-wave phase shifts for electrons scattered from helium. Dashed curves are the results of Morse and Allis where distortion effects were neglected.

Swan's<sup>18</sup> conjecture on Levinson's theorem as discussed by Temkin.<sup>14</sup> For this since there are no bound states for the He<sup>-</sup> ion with two electrons in the  $1s^2$  ground state, only the effects of the Pauli principle act to make the s-wave phase shift equal to  $\pi$  at k=0 and all higher partial-wave phase shifts approach zero.

The effects of terminating the iteration at R=25was to truncate the polarization interaction. This has most serious effects upon the very low-energy phase shifts and corrections to these were thus a necessity.

The corrections were obtained from the formalism developed by Levy and Keller<sup>19</sup> for pure potential scattering. (This is applicable here since only the polarization potential exists in the region of interest,  $25 \le r < \infty$ .) From their work, integration of the expres-

TABLE I. Partial-wave phase shifts in radians.

k	Energy eV	s wave		d wave
ĸ	C V	3 wave	p wave	u wave
0ª	0	1.132		
0.01	0.00136	3.13016	0.000029	0.000004
0.05	0.034	3.0822	0.00080	0.00010
0.10	0.136	3.0186	0.0033	0.00044
0.1917	0.50	2.8972	0.0129	0.0016
0.25	0.85	2.8189	0.0228	0.0027
0.2712	1.00	2.7904	0.0272	0.0031
0.3835	2.00	2.6417	0.0576	0.0063
0.4287	2.50	2.5832	0.0730	0.0080
0.50	3.40	2.4934	0.1006	0.0111
0.6063	5.00	2.3652	0.1472	0.0168
0.75	7.65	2.2050	0.2142	0.0267
0.8575	10.00	2.0953	0.2623	0.0356
1.00	13.60	1.9632	0.3176	0.0491
1.25	21.25	1.7651	0.3862	0.0753
1.50	30.60	1.6034	0.4235	0.1017
1.75	41.65	1.4704	0.4405	0.1256
2.00	54.40	1.3601	0.4460	0.1460

• The k = 0 entry is the scattering length computed from the k = 0.01 and 0.05 s-wave phase shifts. The numerical accuracy of the quoted results are to about 2 in the last decimal place.

<sup>18</sup> P. Swan, Proc. Roy. Soc. (London) A228, 10 (1955).
 <sup>19</sup> B. R. Levy and J. B. Keller, J. Math. Phys. 4, 54 (1963).

sion for the phase shift under a pure central potential V(r) yields the correction formula

( -

$$k = \tan \eta_l(R)$$
  
-  $k \int_R^\infty V(r) [j_l(kr) - n_l(kr) \tan \eta_l(r)]^2 r^2 dr, \quad (24)$ 

where the appropriate potential here is the asymptotic form of the polarization potential given in (16a). In addition, the first-order approximation was made in replacing  $\eta_l(r)$  inside the integral by the constant  $\eta_l(R)$ . This approximation is quite good here since only small corrections are obtained for R as large as 25.

## V. RESULTS AND DISCUSSION

The scattering phase shifts for the s, p, and d waves have been computed and corrected as outlined above and the results are given in Table I. The s- and p-wave phase shifts are also plotted in Fig. 1 for comparison with those computed by Morse and Allis with the distortion effects neglected. The effects of applying the correction formula (24) to the approximate phase shifts found in (23) were most important for energies below 2 eV and for the *p*- and *d*-wave phase shifts. Only a very small effect was noted in the s-wave phase shifts and primarily in the value of the scattering length obtained from them. We shall first discuss this scattering length.

The scattering length given under the k=0 entry (a) in Table I was obtained from the k=0.01 and 0.05 s-wave phase shifts using the first two terms of the modified effective range theory expansion<sup>5</sup>

$$\tan \eta_0 = -Ak - (\pi \alpha/3)k^2 - (4\alpha A/3)k^3 \ln k - \cdots, \quad (25)$$

where A is the scattering length. (The magnitude of the remaining terms are assumed negligible compared to those retained.) This value of 1.132  $a_0$  for the scattering length lies within the range of values from 1.19 to 1.06  $a_0$  as found by various experimenters and reviewed by O'Malley.<sup>6</sup> Our uncorrected phase shifts gave a scattering length of 1.178  $a_0$ .

The lower value of the corrected scattering length is more in accord with the recent experimental data. However, as evidenced the wide range of experimental values, there is considerable discrepancy in the experimental scattering length for helium. This is in part due to the fact that the experimental values are obtained from measurements of the cross sections for a teneous gas of atoms rather than for an isolated atom. Because of this, there is also a correction necessary in the experimental values to account for the finite separation between atoms of the gas which leads to an effective screening of the polarization interaction at some finite distance. Further comparisons with experimental scattering lengths will thus be deferred to a later date when better experimental methods are devised to overcome the proximity problem.

Comparison of the phase shifts in Fig. 1 shows that

inclusion of some distortion has two major effects upon the phases. These are: a change in slope near k=0for both the s and p waves; and, a larger over-all change in magnitude for the p wave as compared to the s-wave phase shift. These effects are important, first, in giving the opposite slope to the total cross section at very low energies (Fig. 3) and, secondly, producing a high backward asymmetry in the differential cross sections at low energies (Fig. 2). These changes then result in better correspondence with other data at low energies as discussed in the following.

The differential scattering cross sections computed from the phase shifts in Table I for a selection of the energies considered are shown in Fig. 2. These show a large backward asymmetry for low energies which reverses to a forward asymmetry as the energy increases. The shape at low energies is not in accordance with the experimental data of Ramsauer and Kollath<sup>20</sup> or Bullard and Massey.<sup>21</sup> For higher energies the shape matches these quite closely. However, at low energies, the modified effective-range theory predicts a shape given by<sup>6</sup>

 $d\sigma/d\Omega = A^2 + 4\alpha A k \sin(\theta/2) + (8\alpha A^2/3)k^2 \ln k + \cdots, (26)$ 

which reaches a maximum for  $\theta = \pi$ . It thus appears that a high backward asymmetry should be observed

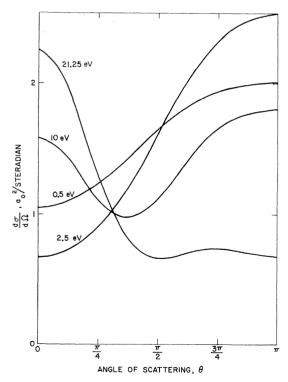


FIG 2. Differential scattering cross sections for electrons on helium by the adiabatic-exchange approximation.

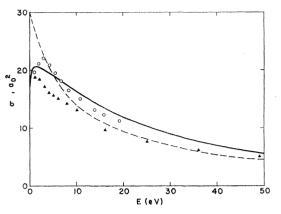


FIG. 3. Total scattering cross sections for electrons on helium. The adiabatic-exchange approximation is compared with the computations of Morse and Allis (dashed curve) and experimental data by Ramsauer and Kollath (circles) and Normand (triangles).

and further considerations will be deferred to a later date when the data of Golden and Bandel<sup>22</sup> becomes available.

The total scattering cross sections have been computed for all of the energies considered and are plotted in Fig. 3. These are compared with the cross sections computed by Morse and Allis<sup>1</sup> and those measured by Ramsauer and Kollath<sup>20</sup> and by Normand.<sup>23</sup> The comparison with experimental data is seen to be good in both cases and especially with the Ramsauer-Kollath data at low energies. For the medium energy region (10 to 30 eV), the adiabatic-exchange cross sections exceed both experimental data and we believe that this is due in part to the dynamic effects neglected here.

The very low-energy cross sections computed by the adiabatic-exchange approximation are compared with the values predicted by the modified effective-range theory (ERT) in Table II. The effective range theory values were computed from the expansion<sup>5,6</sup>

$$\sigma = 4\pi [A^{2} + (2\pi\alpha A/3)k + (8\alpha A^{2}/3)k^{2} \ln k + [(8\alpha A^{2}/6) \ln(\alpha/16) + A^{3}r_{p0} + (2\pi A/3)(A^{2} - \alpha)\alpha^{1/2} - 22\pi^{2}\alpha^{2}/225]k^{2} + \cdots ].$$
(27)

where only the largest terms in the coefficient of the

TABLE II. Comparison of electron-helium total scattering cross sections by the adiabatic-exchange approximation and modified effective-range theory.

E (eV)	Adiabatic-exchange	Modified ERT	
0.00136	16.425	16.483	
0.034	17.749	17.632	
0.136	18.958	18.529	
0.50	20.201	19.220	
0.85	20.541	19.276	
1.00	20.602	19.253	
2.00	20.499	18.891	

22 D. E. Golden and H. W. Bandel, Bull. Am. Phys. Soc. 9, 90 (1964). <sup>28</sup> C. E. Normand, Phys. Rev. 35, 1217 (1930).

<sup>&</sup>lt;sup>20</sup> C. Ramsauer and R. Kollath, Ann. Physik 3, 536 (1929); 12.

<sup>529 (1932).</sup> <sup>21</sup> F. C. Bullard and H. S. W. Massey, Proc. Roy. Soc. (London)

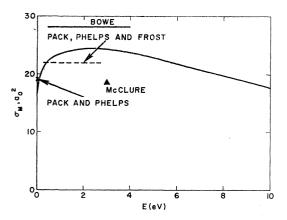


FIG. 4. Momentum transfer cross sections for electrons on helium. The adiabatic-exchange approximation is compared with recent microwave drift velocity measurements.

 $k^2$  term have been retained and  $r_{p0}$  is the modified "effective range." The value used for  $r_{p0}$  in (27) was obtained here by extrapolation from the  $k^2$  coefficient used by O'Malley<sup>6</sup> in matching the Ramsauer-Kollath data. This value is  $r_{p0} = 3.7 a_0$  and closely corresponds to the point where the short-range potential interaction in (14) vanishes. Our value of 1.132  $a_0$  was used for the scattering length.

The comparison with modified effective-range theory is seen to be good in general with the main exception being a steeper slope for our data. It is possible this discrepancy would be reduced if the polarization-exchange terms neglected on the right side of (14) were retained.

We finally show in Fig. 4 the cross sections for momentum transfer computed from the phases of Table I and compared with various other data. For these, more recent measurements are available through microwave drift velocity experiments but the results differ widely in absolute magnitude. These results are the values labeled Bowe,24 Pack and Phelps,25 Pack, Phelps, and Frost,<sup>26</sup> and McClure<sup>27</sup> with the latter being the most recent. The comparison is seen to be quite good with earlier experimental data but exceeds the most recent data.

The comparison of the adiabatic-exchange approximation with experimental data is seen to be superior at low energies to the previous calculations which neglected distortion effects. However, the present calculations are not an optimum fit to the experimental data over the entire 0- to 50-eV energy range. An attempt will be made at a later date to ascertain whether inclusion of exchange-polarization effects improves the agreement with experiment.

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   <sup>25</sup> J. L. Pack and A. V. Phelps, Phys. Rev. 121, 798 (1961).
   <sup>26</sup> J. L. Pack, A. V. Phelps, and L. S. Frost, Phys. Rev. 117, 470
- (1960).
  - <sup>27</sup> B. T. McClure, Bull. Am. Phys. Soc. 9, 90 (1964).