

Distortion Effects in the Elastic Scattering of 100- to 400-eV Electrons from Helium

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The elastic scattering of 100- to 400-eV electrons from helium is analyzed by explicit calculations of the scattering phase shifts including the effects of both adiabatic and non-adiabatic distortion of the target atom. The calculations involve numerical solution of the appropriate single-channel scattering equation for low angular momentum states and analytical estimation of the phase shifts for high angular momentum states of the scattering electron. The adiabatic and nonadiabatic distortion effects are represented by the appropriate central potentials derived in earlier works. Results of these calculations are compared with recent experimental data and other calculations. Atomic distortion causes the differential cross section to have a relatively high peak in the forward direction at all energies considered. The nonadiabatic corrections to the adiabatic polarization are required to sharpen and reduce this forward-scattering peak somewhat. As a whole, the inclusion of adiabatic and nonadiabatic distortion gives a rather good description of the differential scattering cross sections throughout the 100- to 400-eV range.

I. INTRODUCTION

In recent years, electron-atom collision processes have been of considerable theoretical and experimental interest.¹ A substantial effort has been directed toward examining the details of electron-atom scattering at very low energies and at or near excitation thresholds. However, there have been relatively few investigations of elastic electron-atom scattering at energies significantly above the ionization thresholds.

There has been a long standing disagreement between Born-approximation calculations and some early experiments, such as those of Hughes, McMillen, and Webb² on electron-helium scattering. The disagreement is pronounced at small scattering angles where experiment shows much greater forward scattering than is predicted by first Born-approximation calculations. The discrepancies were believed to be due to neglect of polarization of the atom by the scattering electron, which is not accounted for in the first Born approximation. Subsequent calculations by Massey and Mohr³ attempted to include polarization through use of the second Born approximation, and yielded a logarithmically infinite forward-scattering amplitude. However, it was pointed out by Kingston and Skinner⁴ that Massey and Mohr's use of the second Born approximation was inconsistent in some respects, thus leaving the question of the importance of polarization still unresolved.

In 1963-1965, Khare and Moiseiwitsch⁵ re-examined the problem by incorporating an adiabatic polarization potential to represent the distortion interaction. They considered electron-helium scattering over a range of energies between 25 and

700 eV. Although the adiabatic polarization potential is obtained under the assumption that the velocity of the scattering electron is significantly less than that of the bound electron (which is not the case for energies greater than 50 eV), their results were in qualitative agreement with available experimental data. The experimental results of Hughes, McMillen, and Webb² do not give absolute cross sections so that Khare and Moiseiwitsch normalized this data to fit their calculations at each energy. For all energies less than 500 eV, their calculations, including the polarization potential, gave relatively large forward scattering similar to that exhibited by the experimental data. For energies 500 eV and above, they found adequate agreement between experiment and Born-approximation calculations.

Recently, absolute differential cross sections for electron-helium elastic scattering have been measured by Vriens, Kuyatt, and Mielczarek,⁶ for scattering angles between 5° and 30°. The normalization of these measurements has subsequently been reanalyzed by Cooper and Chamberlain,⁷ and found to be incorrect, especially at the lower energies. The properly renormalized data of Vriens, Kuyatt, and Mielczarek still exhibit much greater forward scattering than predicted by the Born approximation. On the other hand, comparison of the corrected experimental data at 100 and 200 eV with the calculations of Khare and Moiseiwitsch⁵ shows relatively good agreement except that the calculations predict greater forward scattering than is found experimentally.

In a recent series of papers, the present authors have analyzed the effects of adiabatic distortion on the elastic scattering of low-energy electrons from

helium.^{8,9} In the latest paper of this series,⁹ we have discussed an extended polarization potential approximation which includes some of the non-adiabatic corrections necessary to the adiabatic theory to account for finite velocities of the scattering electron. Similar analyses of the nonadiabatic corrections were independently made by Kleinman, Hahn and Spruch,¹⁰ and Eissa and Öpik.¹¹ In our earlier papers, only the low-energy (0–30 eV) region was considered. In the work reported here we have applied the extended polarization-potential approximation to elastic scattering of electrons from helium in the 100- to 400-eV region to test the validity of this theory in a high-energy region. The plan of this paper is as follows. In Sec. II we briefly discuss the theory involved in these calculations. Section III presents the results of our calculations, and the comparison with the corrected⁷ experimental data of Vriens, Kuyatt, and Mielczarek.⁶

II. THEORY

The extended polarization-potential approximation is thoroughly discussed in Ref. 9. The procedure may be summarized as follows. The distortion induced in the target atom by the scattering electron is treated by Hartree-Fock perturbation theory. The adiabatic hypothesis is used in which the distorted wave function for the atom is calculated for any position of a stationary external point charge. The resulting perturbed atomic wave function is then used to derive a single-channel scattering equation for the wave function of the scattered particle. Additional simplifications are made in this analysis by neglecting distortion effects in the exchange interaction. The resulting scattering equation is similar to the static-exchange approximation considered years ago by Morse and Allis,¹² differing only by the inclusion of extra potential terms in the direct interaction.

The additional potential terms which arise are the adiabatic polarization potential and the nonadiabatic correction to this, which we call the distortion potential. The adiabatic polarization potential is simply the second-order interaction energy between the atom and a stationary external point charge as given by perturbation theory. The distortion potential arises from operation of the kinetic-energy operator for the scattering electron upon the perturbed atomic wave function. This term has no analog in ordinary perturbation theory for a stationary perturbing charge and represents a correction to the adiabatic polarization potential for finite speed of the perturbing charge. The combination of the adiabatic polarization plus the nonadiabatic distortion potential is termed the "extended polarization potential" (EP). The intent of this work is to test, by comparison with experiment, the utility of this approximation pro-

cedure in a high-energy region.

Asymptotic forms for the multipole components of the polarization and distortion potentials are discussed in Ref. 9. These are shown to be of the form (in atomic units with energy in rydbergs),

$$V_p(R) \sim - \sum_{n=1}^{\infty} \frac{\alpha_n}{R^{2n+2}}, \quad \text{as } R \rightarrow \infty, \quad (1)$$

for the polarization potential, and

$$V_d(R) \sim \sum_{n=1}^{\infty} \frac{\beta_n}{R^{2n+4}}, \quad \text{as } R \rightarrow \infty, \quad (2)$$

for the distortion potential. The $n=0$ components of both V_p and V_d vanish exponentially in the asymptotic region. Explicit expressions for α_n and β_n are given in Ref. 9 for atoms or ions possessing only 1s electrons whose unperturbed states may be represented by hydrogenic wave functions. The coefficient α_1 is equal to the electrostatic dipole polarizability of the atom while α_2 is the corresponding quadrupole polarizability. For small R , both V_p and V_d have rather complicated forms which cut off the interactions in a well-behaved manner at $R=0$.

The calculations reported in this paper were performed as follows. The scattering equation including the $n=0, 1$, and 2 components of V_p and $n=0$ and 1 components of V_d was solved numerically to determine the partial-wave phase shifts for $l=0$ through 10 at energies of 100, 150, 200, 300, and 400 eV. However, for these energies, phase shifts of higher l are required to determine adequately the differential cross section. We found that including all phases through $l=50$ gave differential cross sections accurate to at least 1.5% for non-zero scattering angles. At zero scattering angle, the contributions from the successive partial waves add constructively in the differential cross section and convergence of the summation over l is very slow. To be certain of convergence in this case, we included all phases through $l=10051$ to obtain the differential cross sections at zero scattering angle. Since exchange effects are entirely negligible for $l \geq 10$, we obtained the phase shifts for $l \geq 11$ by analytical approximations.

The analytical approximations for higher l phase shifts were based on two considerations. When exchange is neglected, we are considering simple potential scattering. The scattering potential contains two parts; the short-range static potential of the unperturbed atom and the long-range extended polarization potential. The contributions to the phase shifts from both of these potential terms are small, and so we can find the phase shifts due to each separately and add the results.

The larger of the two contributions comes from the extended polarization potential ($V_p + V_d$). In this case we used the first Born approximation for the phase shifts for potential scattering. This gives (in atomic units)

$$\eta_l(k) = -k \int_0^\infty [V_p(r) + V_d(r)] j_l^2(kr) r^2 dr. \quad (3)$$

To avoid messy numerical integrations in using this formula, we have approximated the extended polarization potential by the simple form

$$V_p(r) + V_d(r) = \sum_{n=1}^N \frac{a_n}{(d_n^2 + r^2)^{2n}}, \quad (4)$$

where a_n and d_n were chosen to match the actual form of $V_p + V_d$ over as large a range of r as possible. We found that upon taking $N=3$ and $d_1^2 = d_2^2 = d_3^2 = 0.4$, a good fit to $V_p + V_d$ could be obtained for $a_1 = -1.395$, $a_2 = 0.4935$, and $a_3 = 6.395$ for all $r \geq 2a_0$. The resulting integral in Eq. (3) was then found analytically from which the phase shift for any desired l and k was obtained.

The same procedure was applied to the case where the distortion interaction includes only the dipole polarization potential. The resulting interaction then has the asymptotic form $-\alpha_1/R^4$. This is commonly referred to as the "adiabatic-exchange dipole" (AED) approximation.⁸ This is fundamentally the same approximation as used by Khare and Moiseiwitsch,⁵ although as shown in the next section our results in this case predict still greater forward scattering than they obtained.

The phase shifts for large l for the case of the static potential can be found from an equation similar to (3). However, when the static potential is

obtained from analytic Hartree-Fock wave functions, the Born-approximation calculation yielded functions somewhat inconvenient to evaluate numerically. In this case, we employed instead the simpler semiclassical formula¹³ (in atomic units)

$$\eta_l(k) = - \int_{r_0}^\infty V_S(r) [k^2 - (l + \frac{1}{2})^2/r^2]^{-1/2} dr, \quad (5)$$

where r_0 is the classical turning point, $r_0 = (l + \frac{1}{2})/k$, and k is the magnitude of the wave vector for the scattering electron. We have used Eq. (5) to determine the phase shifts for $11 \leq l \leq 25$ due to the short-range static potential (V_S) for the energies involved (for $l > 25$, the contribution to the phase shifts from V_S is negligible compared to that from the distortion terms).

All approximations were checked by comparison with results from the numerical solution of the scattering equation for $7 \leq l \leq 10$. Satisfactory agreement was obtained in all cases, giving confidence in the validity of the analytic procedure.

III. RESULTS AND DISCUSSION

The phase shifts from the extended polarization-potential calculations of this work are given in Table I. The first 11 phase shifts for each energy were obtained by numerical solution of the scattering equation, and these results are considered accurate to the significant figures shown. Only a sampling of the phase shifts for higher l are shown since these were obtained by analytic approximation and believed to be accurate only to about 2%.

Differential scattering cross sections were computed from these phase shifts, and the results are shown by the solid curves (EP) in Figs. 1 through 5. Also shown in these figures are the correspond-

TABLE I. Partial-wave phase shifts in radians for electron-helium scattering in the extended polarization-potential approximation.

l	η_l (100 eV)	η_l (150 eV)	η_l (200 eV)	η_l (300 eV)	η_l (400 eV)
0	1.1118	0.9628	0.8678	0.7540	0.6872
1	0.3469	0.3397	0.3342	0.3258	0.3187
2	0.1410	0.1527	0.1592	0.1672	0.1720
3	0.0686	0.0811	0.0888	0.0982	0.1042
4	0.0371	0.0473	0.0543	0.0631	0.0688
5	0.0216	0.0292	0.0350	0.0429	0.0481
6	0.0135	0.0189	0.0234	0.0301	0.0348
7	0.008 90	0.0128	0.0162	0.0217	0.0257
8	0.006 17	0.008 98	0.0115	0.0159	0.0194
9	0.004 45	0.006 52	0.008 46	0.0119	0.0148
10	0.003 31	0.004 88	0.006 37	0.009 11	0.0115
15	0.0011	0.0016	0.0020	0.0030	0.0039
25	0.000 24	0.00036	0.00048	0.000 71	0.000 93
50	0.000 03	0.000 05	0.000 06	0.000 09	0.000 12

ing cross sections for the AED calculations and the corrected⁷ experimental data of Vriens, Kuyatt, and Mielczarek.⁶ Differential cross sections were also calculated from the phase shifts computed with complete neglect of the distortion interactions. This method is commonly called the static-exchange approximation, and the resulting cross sections are shown by the dashed curves (SE) in the figures for reference purposes.

Finally, the differential cross sections calculated by Khare and Moiseiwitsch⁵ as quoted in Ref. 6 are shown by the crosses in Figs. 1 and 3. Their calculations were made within the adiabatic-exchange dipole approximation and thus should compare closely with our AED results. However, these do not agree at small angles for reasons as yet unclear to us. The number of partial waves included by Khare and Moiseiwitsch is not given in their paper.

Observation of Figs. 1 through 5 shows several interesting features. Inclusion of polarization effects is definitely required to account for the high

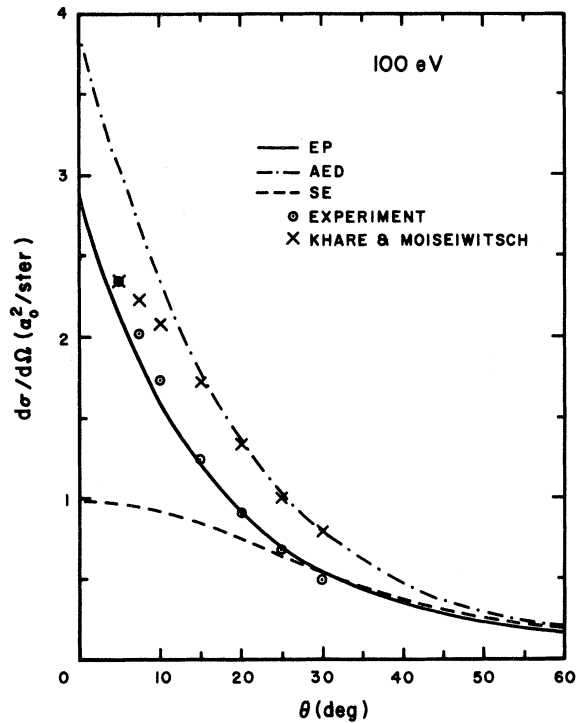


FIG. 1. Differential cross sections for the elastic scattering of 100-eV electrons by helium. Curve EP represents the extended polarization-potential calculations, curve AED the adiabatic-exchange dipole calculations, and curve SE the static-exchange calculations of this work. The experimental data is from Vriens, Kuyatt, and Mielczarek (Ref. 6) as corrected by Cooper and Chamberlain (Ref. 7). The crosses are from the calculations of Khare and Moiseiwitsch (Ref. 5) as quoted in Ref. 6.

forward scattering found experimentally. The use of just the adiabatic dipole polarization potential (AED) yields forward scattering greatly in excess of experiment. This implies that nonadiabatic effects are significant at these energies. The inclusion of nonadiabatic effects through the extended

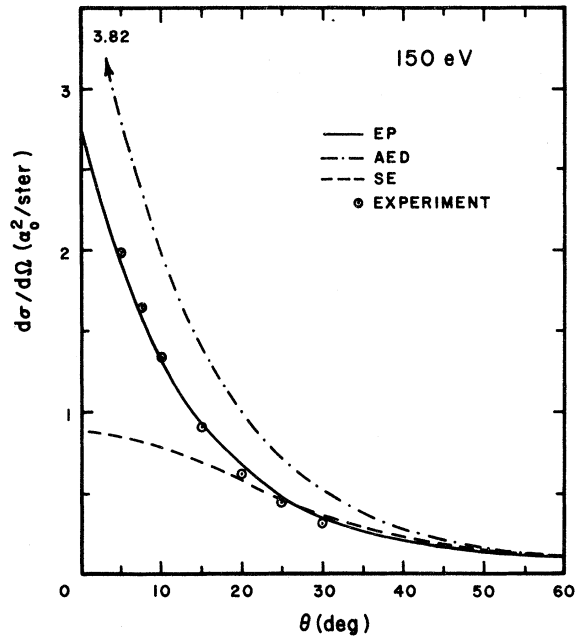


FIG. 2. Differential cross sections for the elastic scattering of 150-eV electrons by helium. (See caption of Fig. 1 for identification of curves.)

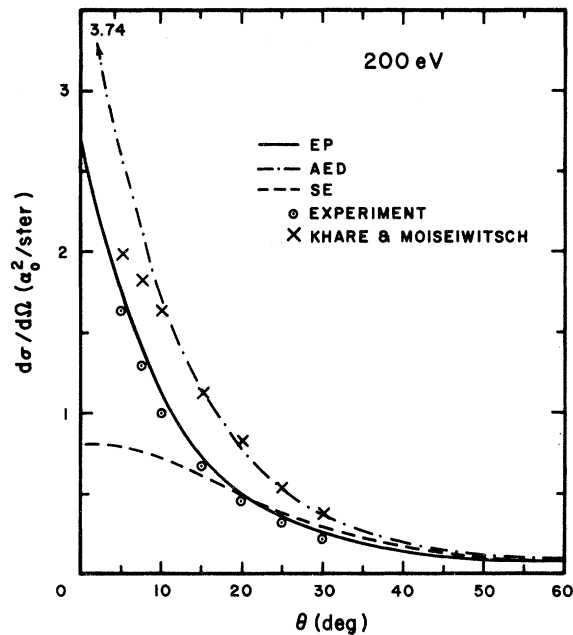


FIG. 3. Differential cross sections for the elastic scattering of 200-eV electrons from helium. (See caption of Fig. 1 for identification of curves.)

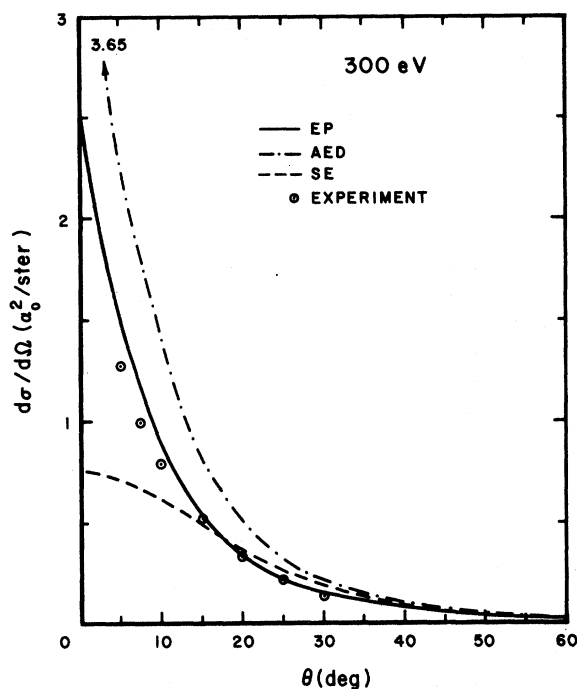


FIG. 4. Differential cross sections for the elastic scattering of 300-eV electrons from helium. (See caption of Fig. 1 for identification of curves.)

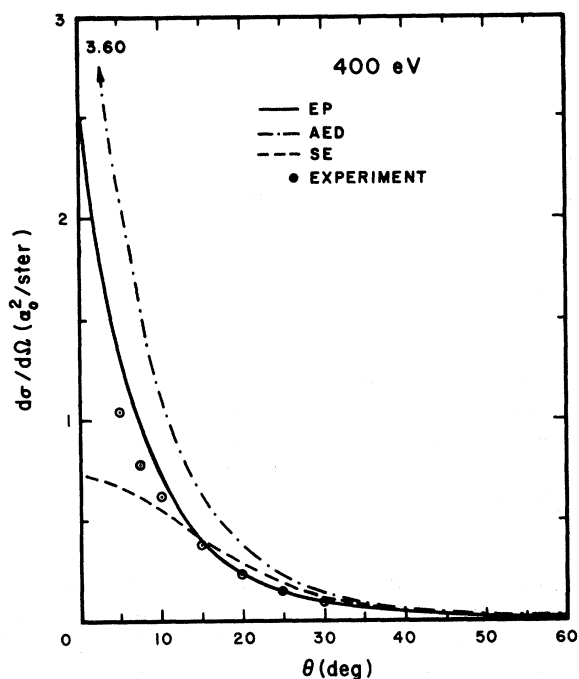


FIG. 5. Differential cross sections for the elastic scattering of 400-eV electrons from helium. (See caption of Fig. 1 for identification of curves.)

polarization (EP) approximation results in predictions for the differential cross sections which are in good agreement with experiment at all energies considered. This result is consistent with earlier calculations at much lower energies,⁹ although in these the differences between AED and EP calculations were not so pronounced. Even so, it was found that nonadiabatic effects were important to give an accurate prediction of the scattering down to zero energy.^{8,9}

Total scattering cross sections were computed from the phase shifts calculated in the AED and EP approximations and these are presented in Table II. Because of the normalization errors⁷ in the Vriens, Kuyatt, and Mielczarek⁶ data, their total cross section estimates are also in error by an unknown amount. We thus show in Table II the results of only their Born-approximation calculations for comparison purposes.

TABLE II. Total cross sections for the elastic scattering of electrons from helium.

Energy (eV)	Total cross section σ/a_0^2		
	AED	EP	Born ⁶
100	2.754	2.230	1.24
150	1.767	1.377	0.889
200	1.288	0.977	0.6905
300	0.828	0.609	0.4756
400	0.608	0.441	0.3622

The substantial degree of success of these calculations in predicting differential cross sections at high energy supports the contention that methods based on the general polarized orbital procedure¹⁴ are of considerable utility in electron-atom scattering. This conclusion is at variance with recent comments of Mittleman and Peacher.¹⁵ The success is unexpected, to some extent, in view of expectations that the effective optical potential might show significant energy dependence.¹⁶ Our results may, however, be interpreted in a fashion consistent with this view. If we accept the stated accuracy of the experimental results, and consider the scattering phase shifts to be obtained by solutions of an effective Schrödinger equation with an energy-dependent optical potential, we see that the optical potential must remain attractive at large distances to account for the high forward scattering, but that it shows some tendency to weaken, that is to become less attractive as the energy increases. It appears that the EP procedure furnishes a reasonably good approximation to the effective optical potential, and that the residual explicit energy dependence which we do not include is not very large.

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Formation of Molecular Helium During the Early Afterglow*

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It is shown that in the early afterglow, of a somewhat typical helium plasma, molecular excited-state densities develop pronounced spatial gradients. This study emphasizes the physics of the formation and maintenance of the observed molecular nonuniformities. Two models are proposed in an attempt to explain the phenomenon. One is a collisional-equilibrium model and the other is a nonuniform-formation model.

I. INTRODUCTION

Experimental studies, of the formation and behavior of molecular helium during the early afterglow of helium plasmas, date back to the early 1960's.¹⁻⁶ Conclusions drawn from these studies are not consistent and in some cases, contradictory. It appears that some of the reported phe-

nomena are traits of the particular discharge tube used in the investigation. A possible explanation for this is the failure to account for spatial nonuniformities of plasma parameters. The existence of nonuniformities of plasma parameters during the early afterglow of helium plasmas is well documented.^{7,8} Many of the plasmas in which the molecular helium studies were performed are