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Potential-Scattering Model for Electrons on Helium and Other Atoms*

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An independent-particle potential-scattering model is proposed for electron scattering by atoms, which is similar in approach to the recent study by Green *et al.* for bound states of atoms. The general model is discussed, including specific scattering considerations, and specialized to the case of helium. Results of calculations for e-He elastic scattering are given and compared with experimental results and with the calculations by LaBahn and Callaway. By allowing the polarization part of the potential to be slowly energy dependent, the agreement becomes quite satisfactory. The relevance of this study to future efforts to develop an optical model for elastic electron scattering by atoms and molecules is discussed.

I. INTRODUCTION

The nuclear independent-particle model (IPM),[1] based upon analytic shell and optical-model potentials, has contributed greatly to the development of techniques for calculating elastic and inelastic scattering cross sections, transition probabilities, and other important nuclear properties. A simple analytic IPM for bound states of electrons in atoms, which maintains a close relationship to the Hartree-Fock model, has been found in a recent study.[2] The intent of the present effort is to explore simple optical models to deal with elastic scattering of electrons by atoms. These two studies would lay the foundation for a later attack on inelastic electron scattering using a variant of the distorted-wave Born approximation (DWBA).

The study of electron scattering by atoms has had a lengthy history. An early review article is that of Brode,[3] who summarizes both theoretical and experimental results available at that date (1933). More recent references are given by Goldberger and Watson.[4]

For electron energies greater than or of the order of a kilovolt, one can use analytical approximations to Hartree-Fock potentials in atoms to predict scattering properties in terms of a single, static potential.[5] At these high energies, the effects of polarization of the atom and of electron exchange are usually ignored.

These latter effects are known to be quite important for the low energy region around one rydberg (13.6 eV) or less.[6] Various analytical forms for the polarization potential have been used, one of the most popular, introduced by Buckingham and by Bates and Massey,[7] is given in Eq. (4) below. Resonance effects are also known to be rather large in this energy region.[8]

It is in the intermediate region (around 100 eV), where our primary interests lie at present. There are several reasons for focusing on this region. Here excitation and ionization processes are quite important[9] and may have some effect on the elastic cross sections. Also, at these energies, isolated resonances should have little effect on the elastic cross sections.

The present effort is devoted to elastic scattering of electrons by helium. This system is studied from a somewhat different viewpoint in a companion paper.[10] Recent experiments[11] now give reliable angular distributions for e-He scattering, whose absolute normalization is, hopefully, accurately determined. Furthermore, a detailed microscopic theory of elastic electron scattering has recently been given by LaBahn and and Callaway[12]; thus providing a point of contact between experiment, microscopic theory, and the more phenomenological approaches. The LaBahn-Callaway and other[13] calculations indicate that polarization effects are important in this energy region also.

A summary of the types of potentials which are used in the particular case of helium as well as one which may be of use in the more general case is given in Sec. II. The calculational procedure is discussed in some detail in Sec. III, and the results of applying the method to electron scattering by He in the energy range 100–500 eV are given in Sec. IV. The implications of the results of these calculations are discussed in Sec. V.

II. ELECTRON-ATOM INTERACTION POTENTIALS

It should perhaps be stressed that what is being sought in the general study of which this is a part, is a representation of the interaction between an atom and a colliding electron in terms of relatively simple analytic potentials.

A major part of the interaction is the electrostatic potential due to the nucleus and the electron cloud. For helium, an estimation of this potential can be obtained from the simple Hylleraas varia-

tional wave function[14]

$$U(r) = (\mu^3/8\pi)^{1/2} e^{-(\mu/2)r}, \quad (1)$$

where $\mu = 3.375\ a_0^{-1}$, where a_0 is the Bohr radius. The charge density of the He two-electron cloud is

$$\rho(r) = -ZeU^2(r) = (-Ze\mu^3/8\pi)\, e^{-\mu r}. \quad (2)$$

The potential energy of an external electron in the field of the nucleus $(-2Z/r)$ together with the repulsive potential energy of the electron due to the exponential cloud is given by

$$V_S(r) = (-2Z/r)(1 + \tfrac{1}{2}\mu r)\, e^{-\mu r}, \quad (3)$$

where $V_S(r)$ (and all other potentials) are given in units of rydbergs (1 Ry $\approx$ 13.6 eV) and lengths are in units of the Bohr radius a_0.

In more complex atoms, where a simple result of the above sort is unattainable, one would expect to use potentials obtained perhaps from Hartree-Fock (HF) self-consistent potentials. A recent study by Green *et al.* showed that a simple one- or two-parameter potential gave excellent fits to Hartree-Fock-Slater (HFS) screening functions and to experimental as well as to HF and HFS single-particle energies. The single-particle potential for a neutral atom of atomic number Z, as used by these authors, is

$$V(r) = -2r^{-1}[(Z-1)\,\Omega(r) + 1], \quad (4)$$

where $\Omega(r) = [H(e^{r/D} - 1) + 1]^{-1}$, $H = D\alpha(Z-1)^{0.4}$, and, for all practical purposes, α could be fixed at the valve $\alpha = 1$. The parameter D has been tabulated[12] for all $2 \le Z \le 103$. It should be noted that $\Omega(0) = 1$, $\Omega(\infty) = 0$. One modification of Eq. (4) which may be useful for electron scattering by a neutral atom is simply

$$V_S(r) = -2r^{-1} Z\Omega(r), \quad (5)$$

with $\Omega(r)$ determined as given above. The potentials V_S given by Eqs. (2) and (4) will be referred to as the static potential.

It must also be recognized that the target atom is polarized by the Coulomb field of the incident electron. This gives rise to a polarization potential, which at large radial distances behaves as r^{-4}. In the present paper we consider a polarization potential of the form

$$V_P(r) = -\alpha/(r^2 + d^2)^2, \quad (6)$$

where α and d characterize the strength and range of the potential. The quantity α is the electrostatic dipole polarizability of the atom and has the value 1.39 a_0^3 for He. The range or "screening length" d will be treated phenomenologically as an adjustable energy-dependent parameter. For comparison, however, Mittleman and Watson[15] estimate d to be

$$d^4 = (\tfrac{1}{2}\alpha)\, Z^{-1/3}. \quad (7)$$

This gives, for He, $d \simeq 0.86$ or $d^2 \simeq 0.74$, which is a similar value to that found empirically in the present paper (see Sec. IV).

In addition to a static and a polarization potential, it is reasonable to expect that an imaginary term in the total potential will be necessary. Although the general form of such a potential is unknown, it is possible to make reasonable guesses about its form and attempt empirically to determine the constants involved. One such form that we are using is

$$V_I = -iAr^n e^{-qr}, \quad (8)$$

where q is chosen as the Hylleraas value 3.375 a_0^{-1} in the e-He case. A and n are adjustable constants.

In the present work, the electron-atom interaction is taken to be a sum of V_S and V_P given in Eqs. (3) and (6). Some preliminary results obtained using more general forms for the potential are referred to in Sec. IV. For this reason, as well as for completeness, the above discussion has been expanded to include these potentials.

III. CALCULATIONAL PROCEDURE

The calculational procedure employed here is a standard one for the most part. The approach will be described in some detail in order to point out those special considerations which are used.

The Schrödinger equation for the lth partial-wave radial function for electron energy $E = k^2$ is

$$d^2u_l/dr^2 + [k^2 - l(l+1)/r^2 - V(r)]\,u_l = 0, \quad (9)$$

where units are as given after Eq. (3). Equation (9) is solved subject to the boundary conditions $u_l(0) = 0$ and

$$u_l \to rj_l(kr) + kA_l(-rn_l + irj_l) \quad \text{as } r \to \infty,$$

where j_l and n_l are the spherical Bessel and Neumann functions. The coefficients A_l are related to the phase shifts δ_l by

$$A_l = [e^{2i\delta_l} - 1]/2ik. \quad (10)$$

The phase shifts are complex quantities when $V(r)$ is complex; otherwise, they are real.

The scattering amplitude $f(\theta)$ and the differential cross section $d\sigma/d\Omega$ are obtained in principle from the A_l's and the Legendre Polynomials P_l by the relations

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1)\, A_l P_l(\cos\theta) \quad (11)$$

and

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2. \quad (12)$$

The usual procedure is then followed. Equation (9) is integrated numerically for partials waves $0 \le l \le L$. (The manner in which L is chosen is discussed below.) A power-series expansion for u_l is used near $r = 0$ after which Numerov's method[16] is used to integrate outward to a "matching radius" r_m. The mesh size is doubled periodically in the vicinity of $r = 0$ to allow a small grid where the potential is changing rapidly and a larger grid farther out. At the matching radius, the derivative of u_l is computed numerically and the equation

$$\frac{u_l'}{u_l}\,(\text{numerical}) = \frac{(rj_l)' + A_l k(-rn_l + irj_l)'}{(rj_l) + A_l k(-rn_l + rj_l)} \qquad (13)$$

is used to obtain A_l and therefore δ_l from Eq. (10) and $d\sigma/d\Omega$ from Eqs. (11) and (12).

For potentials which fall away sufficiently rapidly as r becomes large, the above procedure permits the scattering cross section to be determined. However, since the potentials under consideration here include the polarization potential Eq. (6), which has the asymptotic form r^{-4} for large r, the above procedure must be modified in two ways. First, one must allow for contribution to δ_l due to the remaining potential outside of $r = r_m$. Second, one must include an infinite number of partial waves in Eq. (11). These two points can be treated as follows.

From phase-amplitude considerations,[17] one can derive a power-series expansion in r_m^{-1} for the contribution to the total phase difference between r_m and infinity due to potentials such as that given in Eq. (6). The difference between the series with and without the potential gives the correction to the phase shift due to the remaining potential outside of r_m. This correction term is given (to order r_m^{-6}) by

$$\Delta_l = \frac{\alpha}{2kr_m^3}\left[\frac{1}{3} + \frac{1}{r_m^2}\left(\frac{l(l+1)-2}{10k^2} - \frac{8d^2}{15}\right)\right], \qquad (14)$$

where α and d are from Eq. (6) and provided that $l(kr_m)^{-1} \ll 1$. The δ_l's and the A_l's can be corrected by adding Δ_l to the value of δ_l found from Eq. (13).

For sufficiently large l, the only contribution to the scattering amplitude comes from the polarization potential. The Born approximation can be used to take this potential into account for all l's, at least approximately. In this approximation, Eq. (6) gives the scattering amplitude

$$f_p^B(\theta) = -K^{-1}\int_0^\infty r \sin Kr V_p(r)\, dr$$

$$= (\alpha\pi/4d)\, e^{-Kd}\,, \qquad (15)$$

where $K = k[2(1-\cos\theta)]^{1/2} = 2k\sin\tfrac{1}{2}\theta \qquad (16)$

is the momentum transfer.

The total scattering amplitude is now rewritten by adding and subtracting $f_p^B(\theta)$ and its partial wave decomposition in Eq. (11), which gives[18]

$$f(\theta) = f_p^B(\theta) + \sum_{l=0}^{\infty}(2l+1)(A_l - B_l)\,P_l(\cos\theta)\,, \qquad (17)$$

where $B_l = \tfrac{1}{2}\int_{-1}^{1} f_p^B(\cos\theta)\,P_l(\cos\theta)\,d(\cos\theta)\,. \qquad (18)$

The assumption is now made (and calculations confirm this assumption) that the series in Eq. (17) effectively terminates at a finite value L. This is equivalent to the assumption that the phase shift δ_l can be approximated by the Born approximation of δ_l using the polarization potential alone. More details are given below for specific cases.

In addition to $d\sigma/d\Omega$ given by Eq. (12) using Eq. (17) for $f(\theta)$, the integrated elastic and reaction cross sections σ_e and σ_r are needed in Sec. IV. They are given by

$$\sigma_e = 4\pi\sum_{l=0}(2l+1)(|A_l|^2)$$

$$= \sigma_e^B + 4\pi\sum_l (2l+1)(|A_l|^2 - B_l^2)\,, \qquad (19)$$

where $\sigma_e^B = (\pi^3\alpha^2/8k^2d^4)[1-(1+2kd)\,e^{-2kd}] \qquad (20)$

and $\sigma_r = \sum_l (2l+1)(1-|e^{2i\delta_l}|^2)\,. \qquad (21)$

The reaction cross section becomes nonzero only when δ_l is complex, i.e., when $V(r)$ is complex.

IV. RESULTS OF THE CALCULATIONS

We show the results of our calculations in Fig. 1. In the figure, the circles represent the data[11] for 100–400 eV, from Vriens *et al.* as renormalized[12] and for 500 eV, from Bromberg. The dashed curve is the calculation of LaBahn and Callaway[12] and the solid curve is ours. The results of our calculations which are shown in Fig. 1 were obtained using a real total potential given by

$$V(r) = V_S(r) + V_P(r)\,, \qquad (22)$$

where $V_S(r)$ is given in Eq. (3) and $V_P(r)$ is given in Eq. (6).

The integrated elastic cross section [Eq. (19)] is tabulated on Table I along with the results of Ref. 12.

As indicated in Sec. II, the quantity d^2 has been treated as an adjustable parameter for each energy. The values which were used in obtaining the illustrated results are given in Table II. One should notice that numerically they are roughly the same as that obtained in Sec. II from a result of Mittleman and Watson. There is, however, a rather smooth energy dependence to the values of d^2 which are given in the table. Roughly speaking, d^2 is given by

$$d^2 = \tfrac{1}{200}\,E + 0.4\,. \qquad (23)$$

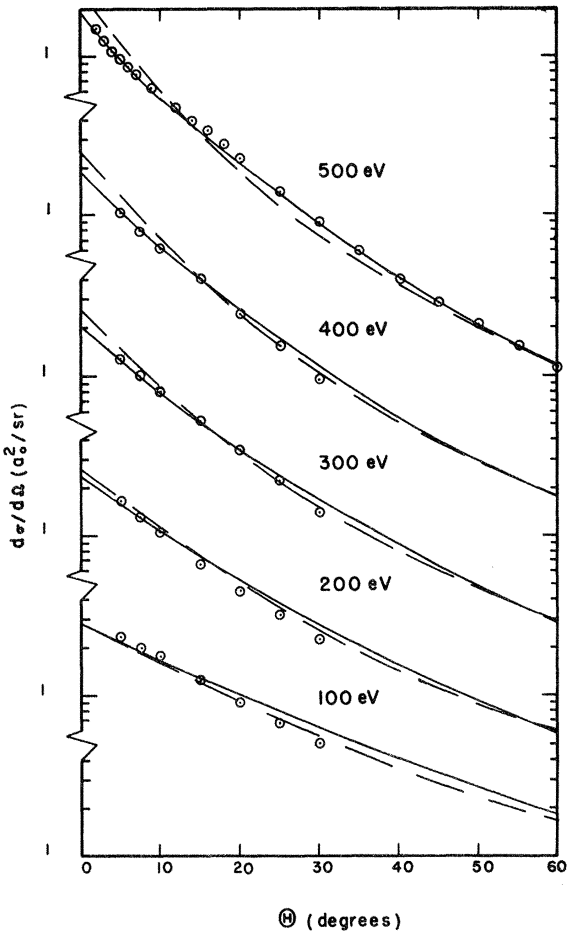

FIG. 1. Comparison of differential cross sections for electron scattering by He. The circles are data (see text), the dashed curves are theoretical results of La-Bahn and Callaway, and the solid curves are the present author's results.

It should be noted that Ganas *et al.*[10] have obtained quite similar results to those given here using a different calculational approach. Since the 400- and 500-eV data give essentially the same d^2, the above relationship clearly is not completely accurate over the entire set of results. We return to this point in Sec. V.

In the calculation, the method given in Sec. III was followed. The upper limit on the sum in Eq. (17) was kept fixed at $L = 15$ and the matching radius was fixed at $r_m = 20\ a_0$. Differential cross sections computed in this manner are stable to at least 1% by making rather large variations in L and r_m as well as in the number of integration mesh points.

TABLE II. Energy dependence of the parameter d^2.

E(eV)	100	150[a]	200	300	400	500
$d^2(a_0^2)$	0.9	1.2	1.5	1.9	2.4	2.4

[a]The value for $E = 150$ eV has been included in the table, but, for convenience, the curves are not given in Fig. 1.

It was of interest to see the effect of including an imaginary part such as that given in Eq. (8) to the potential. Preliminary results indicate that it is possible to find fixed values for A and n in Eq. (8) which give roughly the right reaction cross section[9] over a range of energies using Eq. (20). The angular distributions, particularly the forward angles, are not seriously affected; but a slight readjustment of the value of d^2 in the polarization potential seems necessary.

Further preliminary results indicate that the static potential given in Eq. (5) will be quite satisfactory for higher-Z atoms.

These last two points – the imaginary part and the general static potential – are subjects for further study.

V. DISCUSSION OF RESULTS

One conclusion to be drawn from this work is that a real potential – with a static part resulting from the nucleus and electron cloud and a simple polarization term – is sufficient to allow a description of elastic scattering of electrons by helium atoms. This conclusion is not a new one by any means. However, the fact that the polarization potential should be somewhat energy dependent is qualitatively in agreement with LaBahn and Callaway. However, treating this effect in the above manner is much simpler and should present many practical advantages over a detailed microscopic theory.

One rather troublesome point is that the data from 100 to 400 eV seem to be qualitatively different from those at 500 eV. It may perhaps be dangerous to draw this conclusion from the rather simple model calculation done here, but the sharp

TABLE I. Comparisons of total elastic cross section.

	E(eV) = 100	150	200	300	400	500
LaBahn-Callaway	$\sigma_e(a_0^2) = 2.230$	1.377	0.977	0.609	0.441	(0.346)[a]
Present calculation	$\sigma_e(a_0^2) = 2.512$	1.469	1.003	0.6145	0.4306	0.3449

[a]The 500-eV result is not given in Ref. 12. It was obtained by using their published phase shifts and computing the higher partial waves by Born approximation essentially as described in Sec. II.

break in d^2 versus E in going 400–500 eV (see Table II) is suggestive that the data from the two different laboratories are not totally consistent. If so, the problem of obtaining accurate absolute normalizations for differential cross sections may still be present.

With the above test case rather satisfactorily accounted for by the simple model described in Sec. II, we expect now to consider the more general problem of looking for an "optical model" for electron scattering by atoms. The problem is more complex for larger-Z atoms both because the static potential is generally less well known and because existent data are perhaps less satisfactory than for He. Preliminary results indicate that the considerations given in Sec. II should be adequate to carry us quite far into the general problem.

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Modified Born Approximation and the Elastic Scattering of Electrons from Helium†

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We discuss the elastic scattering of electrons from helium atoms in terms of an energy-dependent central-potential model having the form

$$V(r) = 2Z \lim_{\Lambda \to \mu} \left(\frac{-\Lambda^2}{\Lambda^2 - \mu^2} \frac{e^{-\mu r}}{r} + \frac{\mu^2}{\Lambda^2 - \mu^2} \frac{e^{-\Lambda r}}{r} \right) - \frac{\alpha}{(r^2 + d^2)^2},$$

where μ, α are fixed constants (for He, $\mu = 3.375$ and $\alpha = 1.39$), and d is an energy-dependent phenomenological parameter. The method of partial waves is adapted for a generalized Yukawa potential and a polarization potential. Phase shifts and scattering cross sections are calculated from our potential model using the first Born approximation and a modified form of it. We develop an effective-range theory for a generalized Yukawa and a polarization potential, and apply it to generate a set of energy-dependent electron-helium phase shifts in the region 0–500 eV. Recent experimental angular distribution data in the region 100–500 eV are rather satisfactorily accounted for by our potential model. Our results compare favorably with those of LaBahn and Callaway.

I. INTRODUCTION

The general aspects of the elastic scattering of electrons from helium atoms have been discussed in Paper I.[1] Here we examine the same problem within the framework of the first Born approxima-