Elastic scattering of positrons off rare-gas atoms

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A simple potential model proposed for the elastic scattering of positrons off rare-gas atoms is used to compute low-energy phase shifts and differential scattering cross sections $\sigma(\theta)$ for positrons incident on $_{10}$Ne, $_{18}$Ar, and $_{36}$Kr at energies 20, 3.4, and 6.67 eV, respectively. The calculated results for $\sigma(\theta)$ are in good agreement with currently available experimental values and are as reliable as the numbers obtained from much more elaborate calculations. It is pointed out that an important virtue of the present model is its simplicity.

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I. INTRODUCTION

It is widely believed that positrons (e^+) are very sensitive probes for neutral atomic targets, and studies in e^+-atom scattering constitute an exciting field of investigation. With the exception of positronium formation [1], all available computational methods for electronic systems can easily be adapted for positronic systems by regarding the positron as a distinguishable electron (e^-) of positive charge. As in the case of e^--atom scattering, studies in e^+-atom scattering become increasingly difficult as one moves along the periodic table and, practically, detailed variational and nonvariational calculations [2] assume the status of a formidable task even for currently available computer facilities. In contrast to this, the approach based on model potentials is simple enough to admit straightforward applications to large-Z atoms. In the potential model approach, the scattering interaction is assumed to consist of two parts having different dynamical origins. The first part corresponds to the so-called static potential and is taken care of by employing results from some *ab initio* calculation. The second part gets a contribution from polarization of the atomic target by the incident particle. The polarization effects are incorporated by the use of simple functions with adjustable parameters. The use of model potentials in the study of e^+-atom scattering has an old root in the atomic literature. However a very significant contribution with respect to this has been made by Nakanishi and Schrader (NS) [3], who clearly demonstrate that choosing the adjustable parameter in the polarization potential based on physically founded assumptions leads to potential models for simple and accurate calculations of e^+-atom elastic scattering.

In the model by NS, the leading term of the dipole polarization was bootstrapped with a short-range cutoff function characterized by a disposable parameter, called the effective radius, so as to account for other residual interactions that may be associated with the atomic polarizability. Asymptotically, the cutoff function goes to unity giving the long-range behavior of the dipole term. The effective radius for each atom was adjusted to reproduce the well-known reference values, via solutions of the radial Schrödinger equation. More recently, Jain [4] has constructed an approximate parameter-free polarization potential, which he calls the correlation polarization potential (CPP). The CPP was determined from the correlation energy of one positron in a homogeneous electron gas. The present paper is an effort along the line of thought initiated by NS and studied in more detail by Jain [4] and by Baluja *et al.* [5]. We shall discuss the e^+-atom scattering problem within the framework of a potential model, which from a physical and mathematical point of view is intermediate in complexity between that of NS and that of Jain.

We devote Sec. II to our choice of the model potential. In particular, for the static part of the e^+-atom interaction we use an electrostatic potential constructed by Salvat *et al.* [6] by means of an analytical fitting procedure to Dirac-Hartree-Fock-Slater self-consistent data. The reliability of this potential has been demonstrated by Salvat [7] himself in the context of scattering of fast positrons by atoms.

The Buckingham potential [8] appears to be the first semiempirical polarization potential to be used in e^--atom scattering calculations. Since then there have been myriad attempts to search for more realistic models, and the works of NS [3] and of Jain [4] constitute two such independent attempts. Here we shall work with a form of the polarization potential $V_p(r)$ [9], which accurately represents the effect of both static and dynamic polarizabilities of the atomic target induced by the projectile. Additional remarks on the form of $V_p(r)$ will be presented in due course. In particular, the free parameter characterizing it will be determined by making use of an argument given in Condon and Shortley [10] and by taking recourse to the so-called quantum defect theory (QDT) [11]. For the present study we shall not differentiate between the e^+-atom and e^--atom polarization potentials. This is not expected to affect the low-

energy scattering data since the second-order perturbation energy is independent of the sign of the projectile charge.

In Sec. III we summarize our method for calculating the scattering phase shift. Rather than solving the Schrödinger equation, we work with the variable-phase approach [12] to potential scattering because it is a direct method for computing scattering phase shifts and has certain distinct advantages over the traditional wave-function method. Here one works with a first-order equation, albeit a nonlinear one. This fact, on the one hand, decreases the number of computations and, on the other hand, makes it possible to use a number of known results from the theory of differential equations. In Sec. IV we present results for the differential cross sections for scattering of positrons from $_{10}$Ne, $_{18}$Ar, and $_{36}$Kr for some selected values of projectile energy.

II. MODEL POTENTIAL

We write the scattering potential $V(r)$ for e^+-atom scattering in the form

$$V(r)=V_s(r)+V_{\rm pol}(r) \ . \tag{1}$$

The static potential $V_s(r)$ used by us is taken from Salvat *et al.* [6] and is written as

$$V_s(r)=z\frac{Z}{r}\sum_{i=1}^{n} A_i e^{-\alpha_i r} \ , \tag{2}$$

where Z stands for the atomic number of the target and z is the projectile charge. Obviously, for the positron, $z=+1$. As noted earlier, the values of strength and screening parameters A_i and α_i were obtained through a suitable fit to the numerical potentials obtained from self-consistent calculations. The number of Yukawa terms in Eq. (2) varies from atom to atom. The analytical screening functions presented here improve on other alternatives used previously for the static field. On a very general ground one knows that the mean static interaction for atoms other than hydrogen has a long-range Coulomb tail. This poses typical difficulties in the computation of scattering phase shifts. Since $V_s(r)$ in Eq. (2) involves only Yukawaian terms, the Coulomb difficulties will no longer complicate the computational procedure.

As for the polarization potential $V_{\rm pol}(r)$ we shall work with [9]

$$V_{\rm pol}(r)=-\frac{\alpha_d}{r^4}[1-e^{-(r/r_c)^6}]-\frac{\alpha_q-6\beta}{r^6}[1-e^{-(r/r_c)^{10}}] \ , \tag{3}$$

where α_d and α_q are static dipole and quadrupole polarizabilities of the core, and β is the nonadiabatic electric-dipole core polarizability. The term *core* used here refers to the following.

In an alkali-metal atom, the core is composed of the inner groups of electrons and has an inert structure. The core is polarized by the field of the outer electron so that the valence electron's motion is perturbed by the polarization potential [10]. For low-energy e^+–rare-gas-atom scattering, we postulate that a *slow incident positron polarizes the atomic target in the same way as a valence electron does for the alkali-metal atom core.* This is not a drastic approximation as long as we agree to remain within the accuracy of the second-order perturbation theory, which fortunately is good enough for low-energy scattering. An important virtue of $V_{\rm pol}(r)$ in Eq. (3) is that it is regular at the origin and has only one open parameter r_c, the outer cutoff radius. For alkali-metal atoms, r_c is a function of the orbital angular momentum l of the outer electron. The leading terms of $V_{\rm pol}(r)$ are obtained for values of $r \gg r_c$. The choice of r_c in the case of e^+-atom scattering is an involved problem. However, we shall follow the above viewpoint to compute numerical results for r_c. We defer details with respect to this (particularly, the rationale of QDT) until we come to the discussion of our results. Throughout this paper we shall work in Hartree atomic units ($\hbar=m=e=1$).

III. DIFFERENTIAL CROSS SECTION

If a positron of incident energy $E=k^2/2$ is elastically scattered by an atomic target through an angle θ, the differential cross section $\sigma(\theta)$ is given by

$$\sigma(\theta)=\frac{1}{k^2}\left|\sum_{l=0}^{l_{\max}}(2l+1)e^{i\delta_l(k)}\sin\delta_l(k)P_l(\cos\theta)\right|^2 \ , \tag{4}$$

where $P_l(\cos\theta)$ is a Legendre polynomial of order l. The scattering phase shift $\delta_l(k)$ in Eq. (4) is generally obtained by integrating the radial Schrödinger equation for the potential in Eq. (1) from the origin to the asymptotic region and then comparing the phase of the wave function with that of an appropriate circular function. But we have already remarked in the Introduction that we shall work with a direct method for computating $\delta_l(k)$. In the literature, this is referred to as the variable-phase approach [12] or phase-function method (PFM) [13]. The determination of $\delta_l(k)$ by the PFM consists in solving a first-order, nonlinear differential equation written as

$$\delta_l'(k,r)=-\frac{V(r)}{k}[\hat{j}_l(kr)\cos\delta_l(k,r)-\hat{\eta}_l(kr)\sin\delta_l(k,r)]^2 \ , \tag{5}$$

where the prime denotes differentiation with respect to r and $\hat{j}_l(kr)$ and $\hat{\eta}_l(kr)$ stand for the Riccati-Bessel and Neumann functions, respectively. The function $\delta_l(k,r)$ is called the phase function and Eq. (5) is subject to the initial condition, $\delta_l(k,0)=0$. The scattering phase shift is defined by

$$\delta_l(k)=\lim_{r\to\infty}\delta_l(k,r) \ . \tag{6}$$

It appears that Eqs. (5) and (6) have also been used by Baluja *et al.* [5] to compute the scattering phase shift. In this context we note the following.

For scattering on a relatively long-range interaction like that in Eq. (1), a large number of partial waves contribute to the differential cross section. In higher partial-wave phase-shift calculations, generation of the

numerical values for $\hat{j}_l(kr)$ and $\hat{\eta}_l(kr)$ for $kr \ll l$ poses several problems originating from underflow and overflow, respectively. Klozenberg [14] has tried to deal with the situation by implementing the algorithms of Carbató and Uretsky [15] as well as generating the function $\hat{\eta}_l(kr)$. This is, however, quite a job. Thus we have tried to circumvent them by working with a generalized phase equation [12]

$$\gamma_l'(k,r) = -\frac{1}{k}\left[\frac{l(l+1)}{r^2} + V(r)\right]\sin^2(kr+\gamma_l(k,r)) , \tag{7}$$

with the initial condition $\gamma(k,0)=0$ supplemented by $\gamma_l'(k,0) = -kl/(l+1)$. Here the scattering phase shift $\delta_l(k)$ is given by

$$\delta_l(k) = \gamma_l(k,\infty) + \frac{l\pi}{2} . \tag{8}$$

While the significance of Eqs. (7) and (8) was thoroughly discussed by Calogero [12], it appears that the differential equation (7) was never used to compute scattering phase shifts, presumably because it is rather tricky to incorporate the tangent condition $\gamma_l'(k,0) = -kl/(l+1)$, which plays a crucial role in the uniqueness of the desired solution [16]. To take care of this, we introduce the value of the phase function $\gamma_l(k,r)$ at the next adjacent point of zero by [17]

$$\gamma_l'(k,0) = \lim_{h\to 0}\frac{\gamma_l(k,h)-\gamma_l(k,0)}{h} = -\frac{kl}{l+1} . \tag{9}$$

Given the result in Eqs. (7)–(9), the higher partial-wave scattering phase shifts can be computed without generating the values for Riccati-Bessel functions at every integration step. But the price we pay for this is that it is now necessary to integrate Eq. (7) from the origin to a large distance even for short-range potentials because of the slow asymptotic vanishing of the centrifugal term.

IV. RESULTS AND DISCUSSION

The values of the parameters for the potential in Eq. (2) for $_{10}$Ne, $_{18}$Ar, and $_{36}$Kr have been given in Salvat *et al.* [6]. The results used by us for the polarizabilities α_d, α_q, and β occurring in Eq. (3) are given in Table I. All numbers in this table except the result for α_q of $_{36}$Kr are given in Bransden [18]. This result was generated by making judicious use of Eq. (5-63b) in Ref. [18]. In addition to the polarizabilities, the polarization potential involves a free parameter r_c. As advocated in Sec. II, for the values of r_c we shall work with the core radii of alkali-metal atoms. The spectra of alkali-metal atoms can often be described quite accurately in terms of simple physical models and the QDT [11] serves a useful purpose in this respect. Here the energy eigenspectrum is still described by a hydrogenic formula, with the principal quantum number n being replaced by an effective quantum number n^*, and the quantum defect Δ is written as

$$\Delta = n - n^* . \tag{10}$$

TABLE I. Parameters in the long-range part $[V_{\text{pol}}(r)]$ of the effective potential in Eq. (1).

	Polarizabilities (a.u.)		
Atom	α_d	α_q	β
$_{10}$Ne	2.67	9.0	1.27
$_{18}$Ar	11.1	72.9	8.33
$_{36}$Kr	16.8	113.9	14.5

The quantity Δ is almost constant in a particular series (constant l and varying n) of terms and is obtained traditionally by fitting the experimental binding energy. Recently, we have derived a method for computation of the values for Δ without resorting to the use of experimental data [19]. As an added advantage, we have found that this theory simultaneously yields values for r_c. This was achieved by making use of the Thomas-Fermi model [20] of the atom and demanding that Δ be stationary with respect to variation in the values of inert atomic core radii. In the atomic unit of length ($a_0=1$), the numbers computed by us for r_c to be associated with $_{10}$Ne, $_{18}$Ar, and $_{36}$Kr are found to be 1.8310, 2.1469, and 2.5237, respectively.

Before computing results for scattering phases on the basis of Eqs. (1)–(3) and (7)–(9), one would like to examine the effectiveness of our semiempirical potential in Eq. (3) to produce experimentally determined positron-atom scattering lengths that exhibit a marked sensitivity to the target polarization. To deal with this we have made use of the interpolating equation

$$a'(r) = v(r)[r - a(r)]^2 , \tag{11}$$

with $a(0)=0$ to compute the s-wave scattering length defined as

$$a = \lim_{r\to\infty} a(r) . \tag{12}$$

The computed values of a for different targets is also expressed in atomic units. For $_{10}$Ne we obtained $a=-0.5213$. This value is in excellent agreement with the experimental result $[-(0.53+0.15)]$ of Tsai, Lebow, and Paul [21] and is somewhat improved over the corresponding theoretical result -0.7283 obtained by NS [3]. Our result $a=-6.0812$ for $_{18}$Ar may appear a little disappointing since it is lower than the experimental value $[-(4.4+0.5)]$ of Lee and Jones [22]. In this context we note that McEachran, Ryman, and Stauffer [23] obtained $a=-5.30$ from a polarized orbital method calculation. However, we shall see that the results for differential scattering cross section computed by the use of the above quoted r_c value for $_{18}$Ar are in good agreement with the recently calculated values of Jain [24]. The scattering length for $_{36}$Kr was found to be -2.6801 and could not be compared with earlier results for want of data.

In Table II we present our results for the phase shift. The projectile energy (E) for each of the atomic targets was chosen in such a way as to permit comparison with

TABLE II. Partial-wave phase shifts for positrons elastically scattered from Ne, Ar, and Kr at energies 20 eV, 3.4 eV, and 6.67 eV, respectively. The numbers in parentheses are from Ref. [3] (for Ne and Ar) and Ref. [25] (for Kr).

		Phase shifts $\delta_l(k)$ (rad) for values of l						
Target atom	E (eV)	0	1	2	3	4	5	6
$_{10}$Ne	20.0	−0.6621	−0.0452	0.0552	0.0353	0.0186	0.0110	0.0070
		(−0.5526)	(−0.0148)	(0.0644)	(0.0342)	(0.0172)		
$_{18}$Ar	3.4	−0.0043	0.2696	0.0887	0.0305	0.0130	0.0089	0.0069
		(−0.0730)	(0.2121)	(0.0778)	(0.0278)	(0.0126)		
$_{36}$Kr	6.67	−0.4417	0.2208	0.2054	0.0949	0.0420	0.0250	0.0130
		(−0.4427)	(0.2200)	(0.2170)	(0.0970)	(0.0429)	(0.0219)	(0.0127)

relevant theoretical and experimental data. The numbers in parentheses for $_{10}$Ne and $_{18}$Ar are from NS [3] and those for $_{36}$Kr are from McEachran, Stauffer, and Campbell [25]. As for $_{10}$Ne we note that our phase-shift results are slightly lower than the corresponding numbers of NS for $l \leq 2$. For $l > 2$, this trend becomes the opposite. However, we have clearly demonstrated the convergence of $\delta_l(k)$ at higher partial waves. In the case of $_{18}$Ar, the values of our phase shifts are always augmented compared to those of NS. The maximum discrepancy is 9% and occurs in the s-wave case. The discrepancy consistently diminishes as we go to higher partial waves. It is of interest to note that the two sets of phase shifts for $_{36}$Kr are in good agreement. This indicates that the result for the associated scattering length computed by us may also be in good agreement with the data to be obtained from forthcoming experiments.

In Figs. 1–3 we plot the values of the differential cross section $\sigma(\theta)$ as a function of the scattering angle θ for e^+-Ne at $E = 20$ eV, e^+-Ar at $E = 3.4$ eV, and e^+-Kr at $E = 6.67$ eV. We represent the variation of our results by solid curves. The appropriate experimental results are shown by hollow triangles. We use dashed curves to exhibit θ dependence of earlier theoretical results. As for $_{10}$Ne, the earlier theoretical results are due to NS [3]. Looking into Fig. 1, we see that at all scattering angles our values of $\sigma(\theta)$ are slightly augmented compared to those of NS and therefore in better agreement with the experiment of Kauppila *et al.* [26]. Although in Table II we have quoted the phase-shift values of NS [3] for $_{18}$Ar, we have compared in Fig. 2 our results for $\sigma(\theta)$ with those of Jain [24], presumably because Jain's results are more recent and appeared to be somewhat improved over the corresponding results by NS. The two sets of results do not differ appreciably and each of the sets are only in reasonable agreement with the experimental points of Coleman and McNutt [27]. In Fig. 3, our results for $_{36}$Kr are not discernible from those of McEachran, Stauffer, and Campbell [25], at least for the logarithmic scale used by us. Thus our potential model in this case exactly reproduces the polarized orbital data. But, unfortunately, the recent experimental results of Dou *et al.* [28] are only in qualitative agreement with the theoretical values.

From the discussion presented above, it is clear that

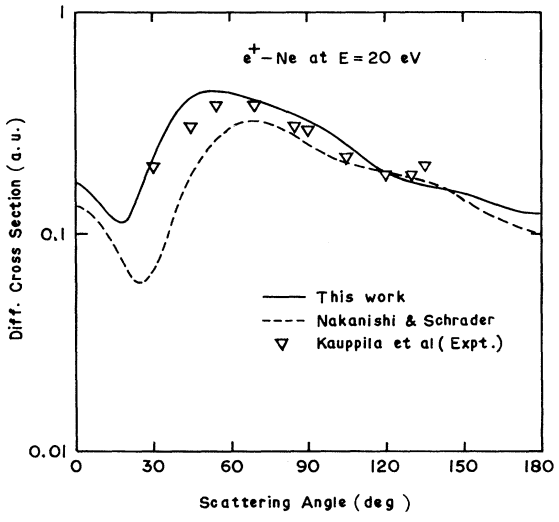

FIG. 1. Differential cross section (DCS) for positrons elastically scattered from $_{10}$Ne as a function of scattering angle at an incident energy 20 eV.

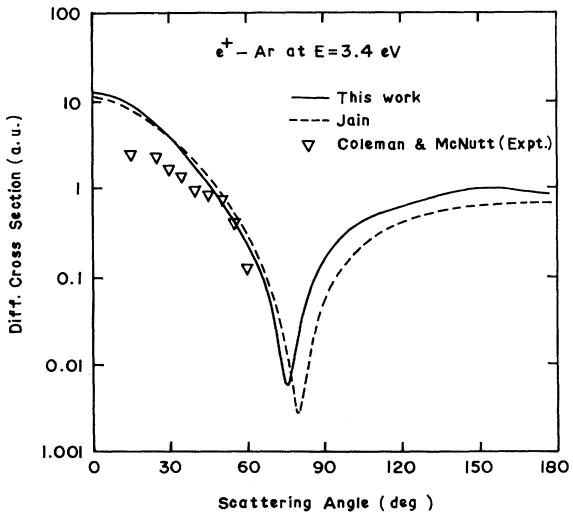

FIG. 2. DCS for e^+-Ar elastic scattering at 3.4 eV.

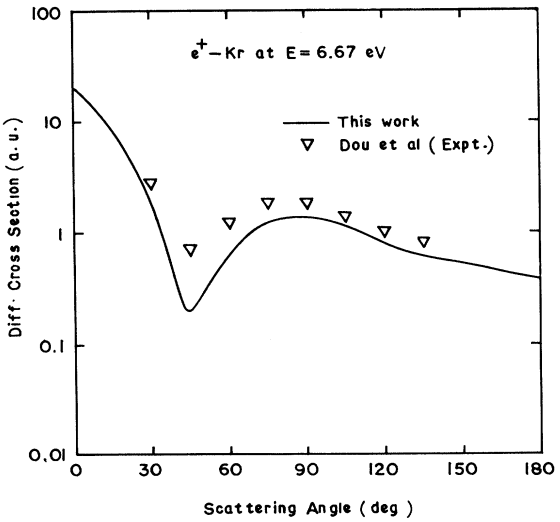

FIG. 3. DCS for e^+-Kr elastic scattering at 6.67 eV.

the potential model used by us for the study of e^+–rare-gas-atom scattering is quite realistic and reproduces numbers for $\sigma(\theta)$ that are comparable in accuracy with those obtained from more detailed calculations. But one can still improve on the results by working with the polarization potential of Valone, Truhlar, and Thirumalai [29]. In this work the expression for $V_p(r)$ was constructed by using a low-energy approximation to the second-order optical potential and subsequently modeling it in terms of imaginary-frequency susceptibilities of the target due to a point charge. In contrast to the expression in Eq. (3), the model potential of Ref. [29] is free from any cutoff parameter and is physically more appealing because of its association with a position-dependent frequency. The usefulness of the potential has already been tested for e^-–rare-gas-atom scattering [30] to get encouraging results and, admittedly, the next logical step will be to envisage a similar study for the e^+-atom scattering.

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