Low-energy positron-argon collisions by using parameter-free positron correlation polarization potentials

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We report differential, integral, and momentum-transfer cross sections and the scattering length (A_0) for positron (e^+)-argon scattering at low energies below the positronium formation threshold. An optical-potential approach is employed in which the repulsive Coulombic interaction is calculated exactly at the Hartree-Fock level and the attractive polarization and correlation effects are included approximately via a parameter-free positron correlation polarization (PCP) potential recently proposed by us. The PCP model is based on the correlation energy ε_{corr} of one positron in a homogeneous electron gas; in the outside region, the ε_{corr} is joined smoothly with the correct asymptotic form of the polarization interaction ($-\alpha_0/2r^4$, where α_0 is the target polarizability) where they cross each other for the first time. The total optical potential of the e^+-argon system is treated exactly in a partial-wave analysis to extract the scattering parameters. It is found that the PCP potential gives much better qualitative results, particularly for the differential cross sections and the scattering length, than the corresponding results obtained from an electron polarization potential used as such for the positron case. We also discuss the "critical" points (representing the minima in the differential scattering) in the low-energy e^+-Ar scattering. The present results involve no fitting procedure.

I. INTRODUCTION

Recently, we[1] discussed the issue of polarization potentials in low-energy positron collisions with atoms and molecules. It is a well-known fact that in the positron (e^+)-atom (or molecule) collisions, a true e^+ polarization potential is very difficult to incorporate without involving any adjustable parameter. It is only recently that several theoretical attempts have been made to consider the polarization of the target atom (or molecule) by the e^+ at the *ab initio* level;[2-7] however, these rigorous calculations are not totally parameter-free. In some collision systems, an electron polarization potential (EPP) works reasonably well for the positron case also,[5-6] although there is no justification for doing that. In order to obtain a truer positron polarization potential (PPP) than the corresponding electron one (i.e., EPP), we need to go beyond the second-order perturbation theory, which is a formidable task. The second-order perturbation energy is independent of the sign of the projectile charge, i.e., the same for electron and positron particles. For many-electron systems, the calculation of a true nonadjustable PPP from more elaborate theories such as the polarized-orbital or the multistate optical-potential approaches (see Ref. 7 and references therein), becomes an arduous task computationally. In most of the previous work on the e^+-atom collisions, either an EPP has been employed for the e^+ case or some semiempirical form of the polarization interaction has been derived (e.g., see Nakanishi and Schrader[8]).

Recently, we proposed a new parameter-free model polarization potential for the low-energy collisions of positrons with atoms and molecules.[1] Our results on the total cross section (σ_t) for the positron-CO system[9] were found to be in very good agreement with the available experimental data. In this paper, we present our calculations on the argon atom at 1–10 eV. Our main emphasis is on the differential cross section (DCS), which is very sensitive (as compared to σ_t) to the polarization of the target. Our calculated DCS at 2.2, 3.4, 6.5, and 8.5 eV are compared with the available experimental data[10-13] at these energies. Further, we discuss the critical points which represent minima in the DCS as a function of incident energy and the scattering angle. In addition, we also report our value for the scattering length (A_0) for the e^+-Ar system.

In the next section, we describe the new positron polarization potential and in Sec. II A we summarize our method of calculation. Section II B presents the discussion on the differential and integral elastic cross sections below the positronium (Ps) formation threshold (i.e., $E \leq 10$ eV), while in Sec. II C the present calculation of the critical points is described. The results on the scattering length are given in Sec. II D. The final concluding remarks are made in Sec. III. We employ atomic units throughout this paper.

II. NEW POSITRON CORRELATION POLARIZATION (PCP) POTENTIAL

Asymptotically, the polarization potential has the simple form $-\alpha_0/2r^4$ for both the electron and positron projectiles. The difficulty arises when the projectile is in the vicinity of the target charge cloud. A simple way to remedy this difficulty has been to multiply the $-\alpha_0/2r^4$ form by a cutoff function depending upon some adjustable parameter; however, this approach is unsatisfactory, although the results may be, fortuitously, very good.

Here, our goal is to look for a computationally simple form of the positron polarization potential, which is different from the corresponding electron potential and free from any adjustable parameter. The basic philosophy of the present approach is akin to the method of O'Connel and Lane[14] for the case of electron scattering based on the correlation energy of the target in the presence of an incoming electron. The present positron polarization potentials are also based on the correlation energy of a localized positron in an electron gas and its hybridization with the correct asymptotic form $(-\alpha_0/2r^4)$. Here, we consider the incoming e^+ as a charged impurity at a fixed distance in an homogeneous electron gas. In positron annihilation experiments, a fundamental question to be asked is how the electron-positron interaction distorts the electronic structure of the system under investigation.

The positron correlation energy in an homogeneous electron gas has been calculated phenomenologically[15,16] as well as using the Bethe-Goldstone-type approach.[17] Recently, Arponen and Pajanne[18] have applied a completely different approach to the problem of a light impurity in an electron gas. In their method,[18] the target electrons are described by a set of interacting bosons representing the collective excitations of the random-phase approximation (RPA). Very recently, Boronski and Nieminen[19] have described the density functional theory of the electron-positron system and presented the results on the correlation energy as a function of the density parameter r_s (see later) for different $n_+(\mathbf{r})/n_-(\mathbf{r})$ ratios including the case of one positron in a homogeneous electron gas. Here n_+ and n_- denote the densities of positrons and electrons, respectively.

We can give the physical picture of the positron correlation in an electron gas as follows. When the incoming positron enters the target electronic charge cloud, we can assume the positron as localized instantaneously and correlating with the surrounding electrons of a given density $n_-(\mathbf{r})$. The wave function of the positron in such an electron-positron plasma can be written as[19]

$$-\tfrac{1}{2}\nabla^2\psi_i^+(\mathbf{r})+\left[\mu_{\rm xc}(n_+(\mathbf{r}))-\phi(\mathbf{r})+\frac{\delta E_c^{e\text{-}p}(n_+,n_-)}{\delta n_+(\mathbf{r})}\right]\psi_i^+(\mathbf{r})=\varepsilon_i^+\psi_i^+(\mathbf{r})\ , \quad (1)$$

where $\mu_{\rm xc}$ is the exchange-correlation potential (which vanishes in the present one-positron case), $\phi(\mathbf{r})$ is the Hartree-Coulomb potential, and $E_c^{e\text{-}p}$ is the e^+-e^- correlation energy functional. Equation (1) has been solved self-consistently.[19] Following the paper of Arponen and Pajanne,[18] Boronski and Nieminen[19] have provided explicit expressions for the e^+-e^- correlation energy ($\varepsilon_{\rm corr}$), interpolating it for the whole radial region. These expressions are obtained without giving any divergence problems in the calculations of annihilation rates over the entire range of the density parameter r_s.[19,20] Arponen and Pajanne[18] have developed a new approach to solve the problem of a charged impurity in an electron gas. The e^+-e^- correlation energy $\varepsilon_{\rm corr}$ is calculated from the ground-state expectation value of the Hamiltonian which describes the electron gas plus the incoming positron fixed at a distance. In the evaluation of $\varepsilon_{\rm corr}$, the e^--e^+ interaction has also been considered[18] [see Eq. (1)]. The analytic interpolated expressions for the $\varepsilon_{\rm corr}$ in the whole range of the density parameter r_s [$\frac{4}{3}\pi r_s^3\rho(r)=1$, where $\rho(r)$ is the target undistorted electronic density], measured in atomic units (a_0), are given as follows:

$$2\varepsilon_{\rm corr}(r_s)=-\frac{1.56}{(r_s)^{1/2}}+(0.051\ln r_s-0.081)\ln r_s+1.14, \quad r_s\le 0.302 \quad (2a)$$

$$2\varepsilon_{\rm corr}(r_s)=-0.923\,05-\frac{0.054\,59}{r_s^2}\ , \quad 0.302\le r_s\le 0.56 \quad (2b)$$

$$2\varepsilon_{\rm corr}(r_s)=\frac{-13.151\,11}{(r_s+2.5)^2}+\frac{2.8655}{(r_s+2.5)}-0.6298\ , \quad 0.56\le r_s\le 8.0 \quad (2c)$$

and finally,

$$2\varepsilon_{\rm corr}[n(r_s)]=-179\,856.2768n^2+186.4207n-0.524, \quad 8.0\le r_s\le\infty \quad (2d)$$

where $n(r_s)$ is the electronic density corresponding to the density parameter r_s.

The positron correlation polarization (PCP) potential defined as a functional derivative of the correlation energy with respect to $\rho(r)$, can be derived conveniently from the following equation in terms of functional derivative of the density parameter:[21]

$$V_{\rm corr}(r)=\left[1-\frac{1}{3}r_s\frac{d}{dr_s}\right]\varepsilon_{\rm corr}(r_s)\ . \quad (3)$$

Finally, we obtain the following form of the $V_{\rm corr}(r)$ (in atomic units) from Eqs. (2) and (3) for $r_s\le 0.302$

$$2V_{\rm corr}(r)=\frac{-1.82}{(r_s)^{1/2}}+[0.051\ln(r_s)-0.115]\ln(r_s)+1.167\ , \quad (4a)$$

for $0.302\le r_s\le 0.56$

$$2V_{\rm corr}(r)=-0.923\,05-\frac{0.090\,98}{r_s^2}\ , \quad (4b)$$

and for $0.56\le r_s\le 8.0$

$$2V_{\rm corr}(r)=-\frac{8.7674r_s}{(r_s+2.5)^3}+\frac{-13.151+0.9552r_s}{(r_s+2.5)^2}+\frac{2.8655}{(r_s+2.5)}-0.6298\ . \quad (4c)$$

Here we do not worry about the asymptotic $8.0\le r_s\le\infty$ region, as this range is beyond the crossing point where the polarization potential is accurately given by the $-\alpha_0/2r^4$ term. We mention here that the interpo-

lation formulas for the correlation energy [Eqs. (2)] were formulated in such a way that for the limit $r_s \to \infty$, the ε_{corr} reaches the value of Ps^- ion energy, i.e., -0.262 a.u. In the present positron case, we realize that in the $r_s \to \infty$ limit, the correlation energy should approach the correct asymptotic form of the polarization potential, i.e., $-\alpha_0/2r^4$. We use the same *ad hoc* prescription as O'Connel and Lane[14] by switching from correlation energy to the asymptotic polarization potential at their crossing point.

Thus the PCP potential $V_{pol}^{PCP}(r)$ for the e^+-atom system is taken to be

$$V_{pol}^{PCP}(r)=V_{corr}(r), \quad r \le r_c \tag{5a}$$

and

$$V_{pol}^{PCP}(r)=-\frac{\alpha_0}{2r^4}, \quad r \ge r_c \tag{5b}$$

where r_c is the crossing radius. We have used here two versions of the PCP potential: one, by employing just the correlation energy ε_{corr} in Eq. (5a) (to be designated by PCP1); and two, by taking Eq. (5a) as such with V_{corr} from Eqs. (4a)–(4c) (to be represented as the PCP2 model). In addition, we will also present the similar cross sections under the electron correlation polarization (ECP) potential,[14] which has recently been used for positron-molecule scattering[22] also.

The present PCP prescription is an approximate model approach in order to continue our search for a true positron polarization potential that is different from the corresponding electron potential and involves no adjustable parameter. However, the PCP potential [Eq. (5)] has several favorable points worth mentioning here: First, it involves a true short-range correlation of the incoming positron with the target electrons at short distances and exhibits correct behavior in the asymptotic region; second, it is quite simple to evaluate and convenient to incorporate into any optical potential partial-wave analysis or close-coupling techniques; third, it is quite different from the corresponding ECP; and finally, it gives qualitatively good results, particularly for the DCS parameter. Furthermore, the scattering length calculated with the new potential compares very well with the measured values (see later).

A. Scattering calculations

Here, we summarize the method of obtaining the scattering parameters. In the usual potential scattering problem, we solve the following differential equation for the scattered electron function R_l for the lth partial wave at an energy of k^2, i.e.,

$$\frac{d^2R_l(r)}{dr^2}+\left[k^2-\frac{l(l+1)}{r^2}-2V_{opt}(r)\right]R_l(r)=0 , \tag{6}$$

where $V_{opt}(r)$ is a local real optical potential for the e^+-Ar system written as a sum of repulsive static $[V_{st}(r)]$ and the attractive polarization $[V_{pol}(r)$; PCP1, PCP2, and ECP models] potentials. The evaluation of the V_{st} and the V_{pol} requires the charge density $\rho(r)$ of the target. In order to generate the $\rho(r)$ at all r values, the one-electron radial orbitals of the argon atom were computed by the self-consistent Hartree-Fock method[23] (for details see Ref. 24). The value of the polarizability of argon atom is taken to be 11.08 a.u.

In order to solve the partial-wave equation (6) for the scattering phase shifts, we use the variable-phase-approach[25–26] (VPA) technique. In the VPA method,[25] the differential equation (6) is converted in terms of first derivative of the phase function $\chi_l(kr)$. We rewrite the first-order phase function equation as follows:

$$\chi_l'(kr)=-\frac{2}{k}[2V_{opt}(r)X^2] , \tag{7}$$

where

$$X=\cos\chi_l(kr)j_l(kr)-\sin\chi_l(kr)\eta_l(kr) , \tag{8}$$

and $j_l(kr)$ and $\eta_l(kr)$ are the usual Ricatti-Bessel functions.[25] Equation (7) is integrated up to a sufficiently large r value different for different l and k values. The corresponding phase shift χ_l is extracted in the $r \to \infty$ limit. In terms of the scattering S matrix $S_l(k)=\exp(i2\chi_l)$, the σ_t and DCS are calculated from

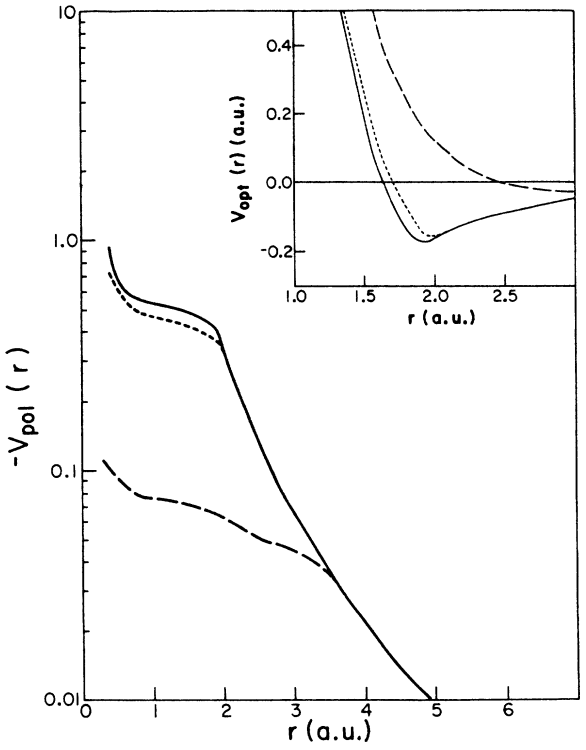

FIG. 1. Various polarization potentials (in atomic units) for the e^+-Ar system. The potentials PCP2, PCP1, and ECP are shown respectively by solid, dashed, and long-dashed lines. The various notations are explained in the text. In the inset are shown the total optical potentials (repulsive static plus the attractive polarization terms) with various approximations: solid line, $V_{st}+V_{pol}^{PCP2}$; dashed line, $V_{st}+V_{pol}^{PCP1}$; long-dashed line, $V_{st}+V_{pol}^{ECP}$.

$$\sigma_l^l=\frac{\pi}{k^2}(2l+1)|1-S_l(k)|^2,\quad \sigma_t=\sum_{l=0}^{l_{\max}}\sigma_t^l\ , \tag{9}$$

and

$$\frac{d\sigma}{d\Omega}=\frac{1}{4k^2}\left|\sum_{l=0}^{l_{\max}}(2l+1)[S_l(k)-1]P_l(\cos\theta)\right|^2, \tag{10}$$

where $P_l(\cos\theta)$ is a Legendre polynomial of order l. The momentum-transfer cross sections (σ_m) are evaluated from the integration of Eq. (10) with a weighting factor of $1-\cos\theta$.

We made convergence tests preserving numerical accuracy up to 0.0001 with respect to radial distance and the step size. In addition, the convergence criterion in the number of partial waves were chosen to be the 0.000 01. In this low-energy region, we do not need a large number of partial waves, i.e., $l_{\max}$; a value of $l_{\max}=20$ is sufficient for well-converged DCS at the highest energy considered here.

In Fig. 1, we show the present PCP potentials (PCP1 and PCP2 both) along with the corresponding ECP curve. There is a significant difference between the ECP and PCP curves. The PCP1 approximation [using $\varepsilon_{\rm corr}$, Eqs. (2)] is about 10% less attractive than the corresponding PCP2 [using the $V_{\rm corr}$, Eq. (3)] term. The crossing points (with the asymptotic polarization potential) for the PCP and the ECP potentials are, respectively, 2.0 (PCP1 and PCP2 values are very close to each other) and 3.6 a.u. This simply means that the e^+-e^- correlation energy is stronger, thus giving rise to a more attractive positron polarization potential than the corresponding electron potential. It seems realistic since the positron is expected to distort the target charge cloud deeper due to strong positron-electron correlation. This difference in the ECP and PCP models gives totally different DCS and a_0 parameters in the present low-energy region (see later).

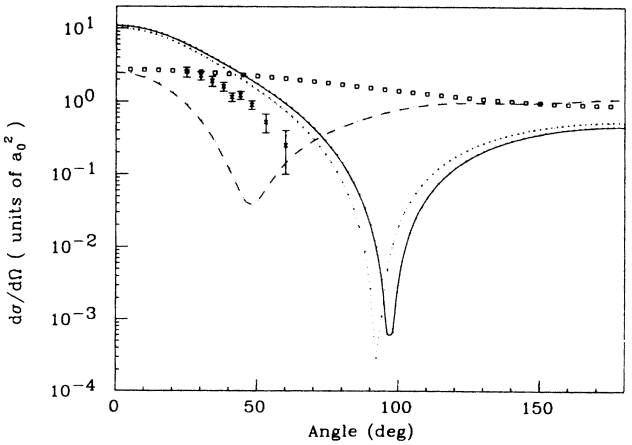

FIG. 2. Differential cross sections (in units of a_0^2/sr) for the e^+-Ar elastic scattering at 2.2 eV. Present theory: solid curve, PCP2 model; dotted curve, PCP1 model; dashed curve, ECP model. The squares are the theoretical results without including any polarization effects. The experimental points (crosses) are due to Coleman and McNutt (Ref. 10).

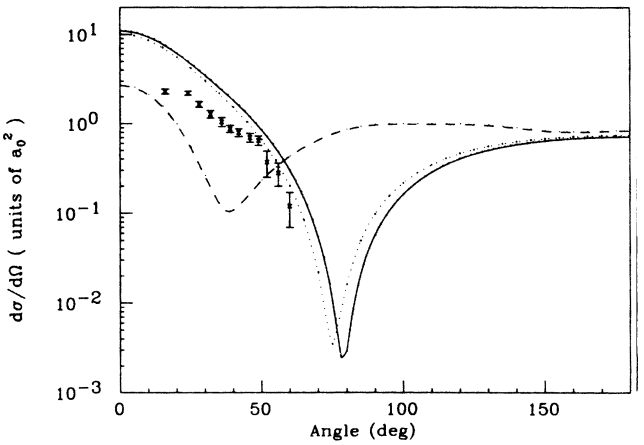

FIG. 3. Same as in Fig. 2, but at 3.4 eV.

The total optical potential $V_{\rm opt}(r)$, displayed in the inset of Fig. 1, is a sum of repulsive static and attractive polarization terms; thus there exists a zero-potential [$V_{\rm opt}(r)=0$] point which is quite different for the PCP and ECP cases. Certainly, the role of the position of the zero-point potential is important in shaping up the scattering cross sections since this point decides the penetration and sign of various partial waves. The two versions of the PCP potential also have a small difference with respect to the zero point. Thus the e^+ scattering is more sensitive to the inclusion of the polarization potential than the corresponding e^- case, where exchange interaction also contributes significantly in reproducing the features of the cross sections. In the zero-energy limit, the role of the position of the zero-point potential is even more critical (see Sec. II C).

B. Differential, integral and momentum transfer cross sections

We now present our DCS and integral (σ_t and σ_m) cross sections by using the PCP (both versions, i.e., PCP1 and PCP2) model for the e^+-Ar elastic scattering at low energies below the Ps formation threshold, where a wealth of experimental data for total[27–39] and differential[10–13] cross sections are available for comparison. We would, however, compare our σ_t values with a few selected measurements only to avoid crowded points in the figure. It is only recently that the DCS for the positron scattering can be measured in the laboratory. Such a pioneering experiment was first performed by Coleman and McNutt[10] at low energies below the first excitation threshold. Later, Hyder *et al.*[11] measured the e^+-Ar DCS for 100, 200, and 300 eV energies at 30°–135° angles, while more recently this group reported their relative DCS measurements at lower energies and other angles also.[12] More recently, Floeder *et al.*[13] reported their relative DCS for the e^+-Ar system at 8.5 and 30 eV between 26° and 65° angles. Since these recently measured values (except the work of Ref. 10) are not absolute, their comparison with various theoretical DCS data[7,40] involves a normalization procedure.

Figures 2–5 display our DCS at 2.2, 3.4, 6.7, and 8.5

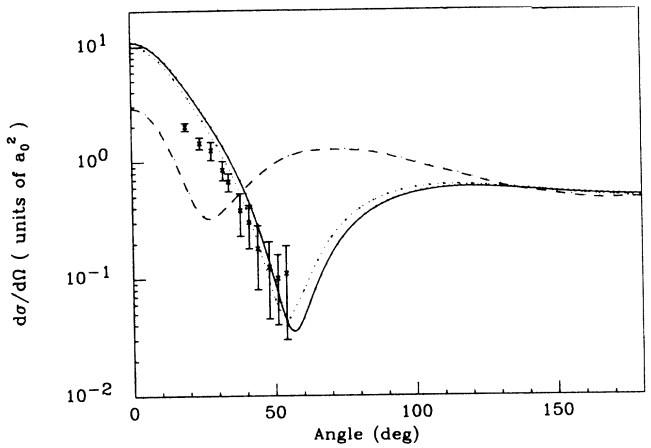

FIG. 4. Same as in Fig. 2, but at 6.7 eV.

eV energies, respectively. We have plotted all the three models (PCP1, PCP2, and ECP) along with the experimental points from Refs. 10–13. From these figures we clearly see that the PCP model is more realistic than the corresponding ECP one. We must remember that the present results involve no fitting parameter as compared to previous calculations.[8,40–42] However, the agreement between experiment and these previous semiempirical calculations[8,40–42] is only satisfactory. From Fig. 10 of Ref. 8, where the positron-Ar DCS below Ps threshold is compared with measurements, the situation is not quite clear since the theoretical results are plotted only up to a 70° angle and the experimental points are shown only up to 60°. Here, we have reported our calculations at all angles. The experimental data of Bielefeld and Detroit groups for the 8.5- and 6.7-eV DCS clearly exhibit a dip in the DCS at middle angles; this structure is approximately reproduced by the present PCP models, while the ECP potential is unable to give the right shape of these angular distributions. We also notice a significant discrepancy between the relative measurements of Refs. 12 and 13. The present PCP DCS seems to agree with the measurements of Floeder *et al.* rather than the data of Smith *et al.* at 8.7 eV.

The two versions of PCP (i.e., PCP1 and PCP2) differ only slightly. At 8.7 eV, the position of the minimum is strikingly in fair agreement with the measurements; however, there is some discrepancy between our PCP curves and the experimental points with respect to magnitude. We have not used any further normalization procedure than the one already taken care of by these experimentalists. At further lower energies (2.2 and 3.4 eV, Figs. 2 and 3), our PCP curves compare qualitatively very well with the absolute data of Coleman and McNutt.[10] The trend of the PCP DCS follows the absolute experimental values of Ref. 10. Here also, the ECP model does not give the right shape of the cross sections. There is large difference in the position and magnitude of the dip structure given by the PCP and ECP models; the ECP dip occurs at about 40° less than the position of the PCP minimum. No other parameter-free theoretical calculations (except the empirical ones) are available at such low energies. Since the PCP approximation is parameter-free, its success over the ECP one cannot be ignored, and therefore the former model deserves further attention. Nevertheless, we do expect some discrepancy between theory and experiment due to the fact that the process of virtual Ps formation is neglected here and also the model nature of the PCP potential. In addition, the accuracy of the relative measurements[11–13] is also not very clear.

We now discuss our integral cross sections. Figure 6 shows the σ_t and σ_m scattering parameters for the e^+-Ar system in the 1–10 eV range. Also shown in this figure are the two sets of experimental data (σ_t) from Refs. 29 and 39 only and the theoretical semiempirical results of Nakanishi and Schrader[8] (for both the σ_t and σ_m cross sections). Again, we see from Fig. 6 that the PCP models compare reasonably well with the measured data, particularly in reproducing the general shape of the cross sections in the whole energy region considered here. It is to be noted that the ECP approximation works well for the electron scattering.[14] The PCP curves (Fig. 6) are in qualitative agreement with the semiempirical calculations of Nakanishi and Schrader.[8] At somewhat higher energies ($E \geq 3$ eV), the ECP σ_t curve is in better agreement with the recent measurements of Charlton *et al.*[39] However, we must emphasize here that the success of any model potential calculation should be judged from the differential cross section point of view. The PCP σ_t cross sections along with the calculations of Nakanishi and Schrader[8] agree with the experimental values of Kauppila, Stein, and Gesion[29] rather than the recent observations of Charlton *et al.*[39] The two sets of experimental data shown in Fig. 6 differ significantly with each other in the 4–10 eV energy region.

The σ_m values in all the three approximations (PCP1, PCP2, and ECP) are displayed in the lower part of Fig. 6. Also shown in this part of Fig. 6 are the theoretical semiempirical results of Nakanishi and Schrader.[8] Here, the ECP curve is quite different from the other three curves shown in Fig. 6 for the σ_m. At very low energies

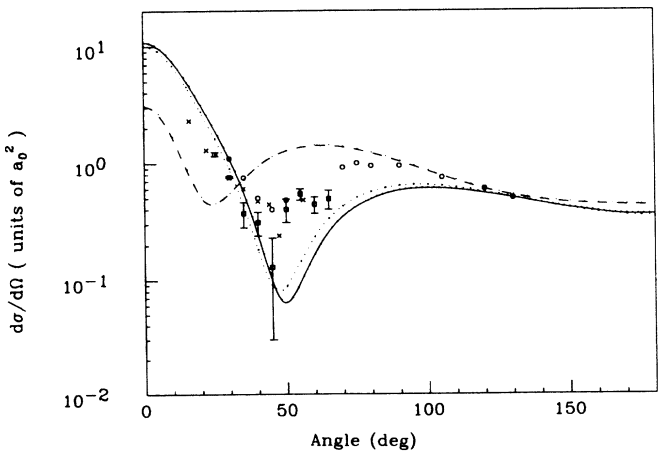

FIG. 5. Same as in Fig. 2, but at 8.7 eV. The circles are the measured values of Smith *et al.* (Ref. 12), while the experimental data (at 8.5 eV) of Floeder *et al.* (Ref. 13) are plotted as squares.

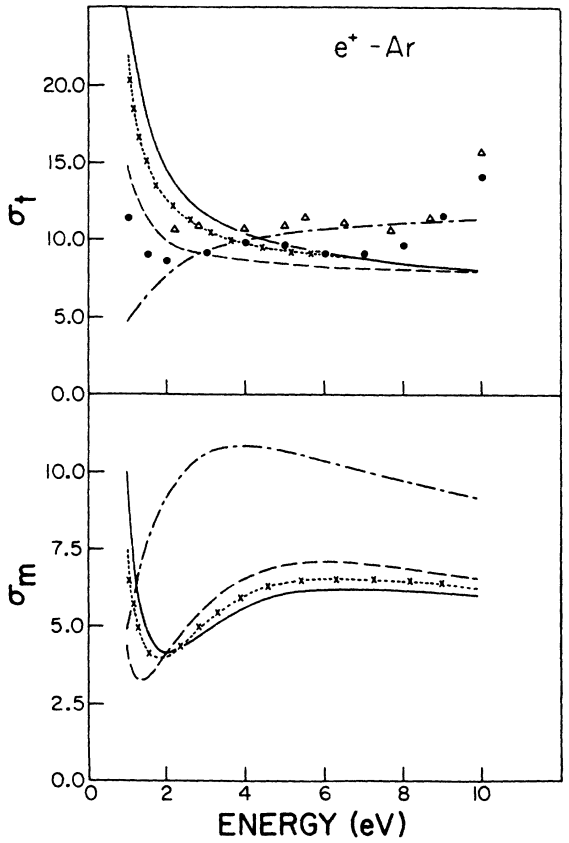

FIG. 6. Integral (σ_t) are momentum transfer (σ_m) cross sections (in units of 10^{-16} cm^2) for the e^+-Ar elastic collisions at 1–10 eV. The various models are shown by solid (PCP2), cross-dashed (PCP1), and dot-dashed (ECP) curves. The theoretical semiempirical results of Nakanishi and Schrader (Ref. 8) are plotted as a dashed curve. The experimental data are taken from Kauppila, Stein, and Gesion (Ref. 29) (closed circles) and Charlton, *et al.* (Ref. 39) (triangles). For various notations see the text.

(below 3 eV) the ECP model seems to give totally different results than the expected shape of the integral (σ_t or σ_m) cross sections. From Fig. 6, it is quite clear that the PCP model describes the low-energy e^+-Ar elastic scattering more realistically than the corresponding ECP approximation; this fact is further supported by the calculation of scattering length (see below).

C. Critical points

The critical points are related with the minima in the DCS. In the present low-energy region, the position and the magnitude of the minimum in the DCS are highly sensitive to the polarization potential (see Figs. 2–5). However, the higher partial waves (mostly $l \geq 2$) are not affected by the details of the polarization potential in the target region. For the present e^+-Ar case, for example, at 2.2 eV, only the s and p waves change with various polarization models (also the contribution of these higher-order partial waves is not crucial in the present discussion). Thus, assuming only the two-wave scattering [s ($l=0$) and p ($l=1$) waves], the minima in the DCS occur at angle $\theta_{\min}$ defined by[43]

$$\cos\theta_{\min} = -\tfrac{1}{3}\cos(\chi_0-\chi_1)[\sin(\chi_0)/\sin(\chi_1)] \ . \tag{11}$$

In Table I, we have listed χ_0, χ_1, χ_2, χ_3, and $\theta_{\min}$ at 2.2 eV in several models PCP1, PCP2, and ECP) including the semiempirical calculations of Nakanishi and Schrader.[8] From Table I, we see that the higher-order phase shifts ($l \geq 2$) are the same in all models, while the $l=0$ and 1 phase shifts are very sensitive to the treatment of polarization. This means that the phase shifts with $l \geq 2$ do not penetrate the target region and scatter mainly with the asymptotic polarization potential, which is known correctly. The value of $\theta_{\min}$ increases with the strength of the polarization in the target region. The values of the critical parameters (angle, θ_{cr}; energy, E_{cr}; DCS_{cr}) in all the present models are given in Table I along wigh the estimates of Wadehra, Stein, and Kauppila[43] (they used the phase shifts calculated by McEachran, Ryman, and Stauffer[40]). Again we see that the PCP approximation is close to other theoretical estimates. It could not be possible to find these critical points in the ECP model; this further supports our findings that the ECP is not a right choice for the positron case.

D. Scattering length (A_0)

The calculation of the A_0 involves the collision problem in the zero-energy limit. The role of polarization interaction becomes very critical for the calculation of A_0 or Z_{eff} (not considered here). In the positron case, the zero-energy scattering is even more difficult due to strong polarization and correlation effects and the cancellation between attractive polarization and repulsive static potentials. In this energy region, only the s wave ($l=0$) is significant, and therefore higher-order partial waves can be neglected in this part of the calculation. We now test our PCP parameter-free prescription by calculating the scattering length A_0, which is defined in the zero-energy limit as follows (neglecting higher-order terms in k^2):

$$\lim_{k\to 0} k\cot\delta_0(k) = -\frac{1}{A_0} \ , \tag{12}$$

where δ_0 is the s-wave phase shift at energy k^2. Here we report our A_0 values in the PCP1, PCP2, and ECP approximations at very low energy ($E=0.0001$ eV) along with the experimental and other theoretical values available in the literature. (We checked the convergence or the zero-energy limit at several lower energies 0.0001, 0.0005, and 0.001 eV with A_0 to be -4.89, -4.88, and -4.81, respectively, in the PCP1 case; there is virtually no change in the A_0 value below 0.0001 eV.) The PCP values for A_0 (-4.89 a.u. in PCP1 and -5.42 a.u. in PCP2 approximations) can be compared with several measurements, e.g., $-(4.4\pm0.5)$ a.u. by Lee and Jones,[44] $-(2.8\pm0.7)$ a.u. by Tsai, Lebow, and Paul,[45] and $-(3.5\pm0.5)$ a.u. by Hara and Fraser.[46] The corresponding theoretical A_0 value of Nakanisi and Schrader[8] is -4.5 a.u. while McEachran, Ryman, and Stauffer[40] report their number to be -5.30 a.u.

TABLE I. Phase-shifts and the value of the θ_{min} for positron-Ar scattering at 2.2 eV in various theoretical models. The θ_{cr}, E_{cr}, and DCS_{cr} are, respectively, the values of critical angle, critical energy, and the DCS at θ_{cr} and E_{cr} for the positron-Ar system in various models (see the text for notations).

Quantity	PCP1	PCP2	ECP	Semiempirical calculation (Ref. 8 or 43)
χ_0	0.1324	0.169	−0.22	0.0543[a]
χ_1	0.202	0.208	0.120	0.1857[a]
χ_2	0.053	0.052	0.052	0.052[a]
χ_3	0.018	0.018	0.018	0.018[a]
θ_{min} (deg)	102.6	105.7	35.0	99.6[a]
θ_{cr} (deg)	93.5	93.8		95.1[b]
E_{cr} (eV)	2.15	2.35		1.67[b]
$DCS_{cr}(a_0^2)$	0.0002	0.000 273		0.000 14[b]

[a]Reference 8.
[b]Reference 43.

On the other hand, the present ECP value of −1.68 for A_0 seems to be way off from the correct value. This can also be seen from Fig. 6, where the ECP σ_t and σ_m cross sections have wrong behavior at low energies (below 1 eV). It is a well-known fact that the relation [Eq. (10)] is true for those long-range potentials which asymptotically fall off as r^{-s}, where $s \geq 3$ (see Ref. 47), i.e., the polarization interaction in the present case. A lower value of A_0 in the ECP model than the corresponding PCP or experimental values simply means that the ECP potential is too weak to actually represent the polarization of the target due to positron impact. Thus even in the zero-energy scattering case, the behavior of polarization potential at short distances has substantial effect on the scattering parameters.

III. CONCLUSIONS

In this paper, we have employed an approximate parameter-free positron correlation polarization potential to investigate the low-energy collisions of positrons with argon atoms. The new PCP potential is determined from the correlation energy ε_{corr} of one positron in a homogeneous electron gas. For the ε_{corr}, we have employed the recent accurate results of Boronski and Nieminen[19] based on the theroy of Arponen and Pajanne[18] for ε_{corr} in the whole radial region. The ε_{corr} is simply a function of the target electronic density and very easy to calculate computationally. At large distances, the correlation term is replaced by the correct asymptotic form of the polarization potential ($-\alpha_0/2r^4$) by following the crossing point procedure suggested first by O'Connel and Lane.[14] We tested two versions of this PCP prescription: one, just the ε_{corr} energy as such (PCP1) and two, the correlation potential V_{corr} [PCP2, Eq. (4)], which should be an appropriate way to obtain correlation potential from the ε_{corr} energy (see Refs. 48 and 49).

For the present positron-argon case, we found that the PCP (both PCP1 and PCP2) model gives qualitative as well as quantitative agreement with experimental results, while the corresponding electron polarization potential used as such for the positron case fails to reproduce observed features in the cross sections. This fact is further proved by calculating the scattering length (A_0) in all the three PCP1, PCP2, and ECP models; we find that the PCP values for A_0 are much closer to the experimental data than the corresponding ECP result. We also noticed that the difference between the PCP1 and PCP2 parameters is not significant; however, at very low energies (below 3 eV), the small difference between the PCP1 and PCP2 models is enough to change the position of the dip in the DCS by about 5°. In the zero-energy limit, the value of A_0 changes by 8% by switching from PCP1 to PCP2 approximation. We also reported our results on the critical points in the DCS and found that there the PCP model is in reasonable agreement with previous estimates.[43]

It is thus quite obvious that for the positron-scattering we need a different polarization potential than the one used for electron case. This conclusion is quite similar to the one discussed properly by Morrision, Gibson, and Austin for the positron-molecule case.[2,3] In particular, the use of an electron polarization potential for the positron case should not be carried out for the DCS and the zero-energy parameters such as the A_0.

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