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NEW PARAMETER-FREE POLARIZATION POTENTIALS IN LOW-ENERGY POSITRON COLLISIONS

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ABSTRACT

The polarization potential plays a decisive role in shaping up the cross sections in low–energy positron collisions with atoms and molecules. However, its inclusion without involving any adjustable parameter, is still a challange. Here we summarise various other techniques employed so far for positron collisions and discuss a new, nonadjustable and very simple form of the polarization potential for positron–atom (molecule) collisions below the threshold of positronium formation. This new potential, recently proposed by us, is based on the correlation energy (ϵ_{corr}) of a single positron in a homogeneous electron gas. The ϵ_{corr} has been calculated by solving the Schrödinger equation of the positron–electron system and fitted to an analytical form in various ranges of the density parameter. In the outside region, the ϵ_{corr} is joined smoothly with the correct asymptotic form ($-\frac{\alpha_0}{2r^4}$, where α_0 is the polarisibility of the target). We tested this new positron correlation polarization (PCOP) potential on several atomic and molecular targets such as the Ar, CO, and CH_4. The results on the total and differential cross sections on these targets are shown here alongwith the experimental data where ever they are available.

I. Introduction

In the positron(e^+) scattering with multi–electron atom (or molecule), a true e^+ polarization potential is very difficult to incorporate without involving any adjustable parameter. Two simple stratagems have been quite popular: one, to use the electron polarization potential as such for the corresponding positron collisions and two, to employ a phenomenological form under the tuning procedure. However, both approaches are unsatisfactory and usually fail at the differential cross section (DCS) and annihilation parameter (Z_{eff}) level; although one may be succesful in getting good agreement for the integral quantities.

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(1–8); however, these rigorous calculations are not totally parameter–free and suffer from including near–the–target nonadiabatic effects and also the correct values in the asymptotic region. Although, the question of nonadiabaticity may not as crucial for the positron projectile as it is for the electron case (see later). The polarization effects dominate the scattering process at very low energies (below about 5 eV). At somewhat higher energies (roughly above 5 eV), the DCS's are still quite sensitive to such charge distortion effects. Here we are concerned only at low energies, particularly below the positronium formation and/or any electronic excitation thresholds. For the one–electron positron–hydrogen case, the issue of polarization potential has recently been discussed by Abdel –Raouf[9]. A very recent and comprehensive review[10] on the e^+–molecule scattering gives details on various approaches used so far to include polarization effects in positron scattering.

It is, therefore, always desirable to find some kind of simple form of the polarization force without involving any fitting parameter. At low impact energies, where the impinging positron is moving very slowly relative to the target electron, the distortion of the electronic charge cloud is quite different than the corresponding electron impact case. Asymptotically, the polarization potential can be assumed to be the same for both the projectiles (which is true up to the second-order perturbative theory only); however, at near–the–target encounters, both the charged projectiles interact differently with the charge cloud of the target. In this talk, we discuss a new parameter–free form of an approximate e^+ polarization potential which is simply a function of the target charge density and in addition is energy–independent.

A summary of earlier usage of various models for polarization potential in positron–molecule collisions is given by Morrison and coworkers(1−2). Recently, Elza et al[8] have investigated various aspects of polarization/correlation effects in low–energy positron–N_2 collisions via a two–parameter model. Tennyson[3] and Tennyson and Morgan[4] have applied the R–matrix technique to positron–molecule (H_2, N_2 and CO) collisions. However, the inclusion of polarization force in all these the so called *ab initio* methods is not either satisfactory nor complete. From numerical point of view, these procedures are not easy to apply for a general positron–molecule system. The collision of positrons with polyatomic targets is even more complicated. We(11−12) have reviewed the situation on the polyatomic molecules with respective to the polarization effects and the comparison with the experimental data.

In the next section, we describe the new positron polarization potential and in section III, the numerical techniques are summarised. In order to demonstrate the success of the new positron correlation polarization (PCOP) potential, in section IV, we present some calculations on the differential and integral elastic cross sections for the atomic (Ar) and molecular (CO and CH_4) targets below the positronium (Ps) formation threshold (i.e. $E \leq 10$ eV). Concluding remarks are given in the last section.

II. The New Positron–Correlation–Polarization (PCOP) Potential

Asymptotically, for a general e^+–molecule collision system, the polarization potential behaves as

$$V_{pol}(r,\theta,\phi) = \frac{-1}{2r^4}[\alpha_0(4\pi)^{\frac{1}{2}}S_0^{01} + \alpha_2(\frac{4}{5}\pi)^{\frac{1}{2}}S_2^{01} + \alpha_2^1(\frac{4}{15}\pi)^{\frac{1}{2}}S_2^{21}], \qquad (1)$$

where the S_ℓ^{mq} is a real spherical harmonic (see Ref. 13 for its definition and various properties), (r,θ,ϕ) are the coordinates of the projectile referring to the center of the target and the spherical (α_0) and nonspherical (α_2 and α_2^1) polarisibilities are expressed in terms of the polarisibility tensor α_{ii} of the target, namely,

$$\alpha_0 = \frac{1}{3}(\alpha_{11}+\alpha_{22}+\alpha_{33}); \ \alpha_2 = \frac{2}{3}(\alpha_{33} - \frac{1}{2}\alpha_{11} - \frac{1}{2}\alpha_{22}); \ \alpha_2^1 = \alpha_{11} - \alpha_{22}.$$

The above form (Eq. 1) of the polarization potential is accurate at large r values up to the second–order perturbation theory. The problem arises when the projectile is near the target. A simple way to remedy this difficulty has been to multiply Eq. (1) by a cut–off function depending upon some adjustable parameter; however, this approach is unsatisfactory , although the results may be forced to agree with observations (see for example, Darewych[14], Horbatsch and Darewych[15]). For positron collisions, most of the calculations prior to 1984 used an electron polarization potential (EPP) assuming that such polarization effects are not sensitive to the sign of the charge of the projectile. Morrison and his group (Morrison et al[1]; Morrison[2]; Elza et al[8]) strongly advocated for a need to generate a true positron polarization potential (PPP) rather than employing the EPP; they strengthened their point by presenting detailed calculations on the positron–H_2 and N_2 systems and comparing them with experimental data. Although earlier calculations on the positron collisions using the EPP gave good results as compared to experimental σ_t values, however, these theoretical results are generally poor at low energies and not qualitatively good at all for differential cross sections at any energy$^{(16-17)}$. Unfortunately, the more rigorous calculations based on the variational polarised–orbital theories are not satisfactory either; Elza et al[8] have to introduce a cut–off function in both the short and long ranges and adjust two parameters to make theory and measurement in close agreement. Even in a more sophisticated R–matrix approach, an accurate inclusion of polarization effects has not been achieved yet$^{(3-5)}$.

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 virtually free from any adjustable parameter. The basic philosophy of the present approach is similar to the method of O'Connel and Lane[18] 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 potential is also based on the correlation energy of a localized positron in an electron gas and its hybridization with the correct asymptotic form. Here, we think 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 e^+ correlation energy ϵ_{corr} in an electron gas has been evaluated phenomenologically$^{(19-20)}$ as well as using the Bethe–Goldstone type approach[21]. Recently, Arponen and Pajanne[22] have applied a completely new approach to the problem of a light impurity in an electron gas. In their method[22] the electron gas is described by a set of interacting bosons representing the collective excitations of the random–phase–approximation (RPA). Very recently, Boronski and Nieminen[23] have described the density functional theory of the electron–positron system and presented the results on the positron–electron correlation energy as a function of the density parameter $\mathbf{r}_s$ (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.

The physical picture of the positron correlation in an electron gas is 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 positrons in such an electron–positron plasma, can be written as[23]

$$-\frac{1}{2}\nabla^2\psi_i^+(\mathbf{r}) + [\mu_{xc}(n_+(\mathbf{r})) - \phi(\mathbf{r}) + \frac{\delta E_c^{e-p}(n_+,n_-)}{\delta n_+(\mathbf{r})}]\psi_i^+(\mathbf{r}) = \epsilon_i^+\psi_i^+(\mathbf{r}), \tag{2}$$

here μ_{xc} is the exchange–correlation potential (which is zero in the present one–positron case), $\phi(\mathbf{r})$ is the Hartree-Coulomb potential and E_c^{e-p} is the positron–electron correlation energy functional. The Eq. (2) has been solved numerically in a self-consistent manner[23]. Based on the paper of Arponen and Pajanne[22], Boronski and Nieminen[23] have given explicit expressions for the positron–electron correlation energy, $\epsilon_{corr}(\mathbf{r}_s)$ 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 $\mathbf{r}_s$ (Kallio et al[24]). In their work, Arponen and Pajanne[22] have developed a new approach to solve the problem of a charged impurity in an electron gas. The correlation energy, ϵ_{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 ϵ_{corr}, the positron–electron interaction has also been considered (see Eq. 2). The analytic interpolated expressions for the ϵ_{corr} in the whole range of the density parameter $\mathbf{r}_s$ ($\frac{4}{3}\pi\mathbf{r}_s^3\rho(\mathbf{r}) = 1$, where $\rho(\mathbf{r})$ is the undistorted electronic density of the target) are given as follows:

$$2\epsilon_{corr}(\mathbf{r}_s) = -\frac{1.56}{\sqrt{\mathbf{r}_s}} + (0.051 \ln \mathbf{r}_s - 0.081) \ln \mathbf{r}_s + 1.14; \qquad r_s \leq 0.302, \qquad (3a)$$

$$2\epsilon_{corr}(\mathbf{r}_s) = -0.92305 - \frac{0.05459}{\mathbf{r}_s^2}; \qquad 0.302 \leq r_s \leq 0.56, \qquad (3b)$$

$$2\epsilon_{corr}(\mathbf{r}_s) = \frac{13.15111}{(\mathbf{r}_s + 2.5)^2} + \frac{2.8655}{(\mathbf{r}_s + 2.5)} - 0.6298; \qquad 0.56 \leq r_s \leq 8.0, \qquad (3c)$$

and finally,

$$2\epsilon_{corr}(n(\mathbf{r}_s)) = -179856.2768 n^2 + 186.4207 n - 0.524; \qquad 8.0 \leq r_s \leq \infty, \qquad (3d)$$

where $n(\mathbf{r}_s)$ is the electronic density corresponding to the density parameter $\mathbf{r}_s$.

The PCOP potential, defined as a functional derivative of the correlation energy with respect to $\rho(\mathbf{r})$, can be derived conveniently from the following equation in terms of functional derivative of the density parameter[24],

$$V_{corr}(\mathbf{r}) = \left(1 - \frac{1}{3}\mathbf{r}_s \frac{d}{d\mathbf{r}_s}\right) \epsilon_{corr}(\mathbf{r}_s). \qquad (4)$$

Finally, we obtain the following form of the $V_{corr}(\mathbf{r})$ (in atomic units) from Eqs. (3)–(4): for $r_s \leq 0.302$,

$$2V_{corr}(\mathbf{r}) = \frac{-1.30}{\sqrt{\mathbf{r}_s}} + (0.051 \ln(\mathbf{r}_s) - 0.115) \ln(\mathbf{r}_s) + 1.167; \qquad (5a)$$

for $0.302 \leq r_s \leq 0.56$,

$$2V_{corr}(\mathbf{r}) = -0.92305 - \frac{0.09098}{\mathbf{r}_s^2}; \qquad (5b)$$

and for $0.56 \leq r_s \leq 8.0$,

$$2V_{corr}(\mathbf{r}) = -\frac{8.7674\mathbf{r}_s}{(\mathbf{r}_s + 2.5)^3} + \frac{-13.151 + 0.9552\mathbf{r}_s}{(\mathbf{r}_s + 2.5)^2} + \frac{2.8655}{(\mathbf{r}_s + 2.5)} - 0.6298. \qquad (5c)$$

Note that for molecular systems the short–range $\epsilon_{corr}(\mathbf{r}_s)$ is to be divided by a factor of $(2\ell + 1)/\sqrt{4\pi}$ to account for molecular orientation not considered by Arponen and Pajanne[22]. Here we do not worry about the $8.0 \leq r_s \leq \infty$ region, as this range is beyond the crossing point where the polarization potential is accurately described by the asymptotic term (Eq. 1). It is to be noted that the interpolation formulae for the correlation energy (Eqs. (3)) 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 scattering case, we realize that in the $r_s \to \infty$ limit, the correlation energy approaches the correct asymptotic form of the polarization potential (the same prescription as suggested by O'Connel and Lane[18]).

Thus, the PCOP interaction potential, $V_{pol}^{PCOP}(\mathbf{r})$, for the e$^+$–molecule/atom system is given by,

$$V_{pol}^{PCOP}(\mathbf{r}) = V_{corr}(\mathbf{r}), \qquad r \leq r_c, \qquad (6a)$$

and by Eq. (1) for the $r \geq r_c$ range. Here r_c is the radius where the V_{corr} and $-\alpha_0/2r^4$ (or $\alpha_2/2r^4$) terms cross each other for the first time. In addition, we will also report the similar cross sections under the ECOP potential, which has recently been employed for positron–molecule scattering (Jain$^{(26-27)}$, Gianturco et al[28]). Even though the EPP results are encouraging for some molecular targets (Jain and Thompson[29]), we feel that it is more appropriate to find a true positron polarization interaction.

The new PCOP potential (Eq. 6) has several favourable points worth mentioning here: first, it involves a true correlation of the incoming positron with the target electrons at short distance encounters and exihibits correct behavior in the asymptotic region; second, it is very easy to calculate and convenient to incorporate into any model potential approach; third, it is quite different from the corresponding EPP and finally, (see later), it gives qualitative good results for the total cross sections for several atomic and molecular targets as compared with experimental data.

III. Scattering Parameters

In fact, the numerical techniques to solve the scattering equation for the e^+ wave function are standard as employed for the electron scattering case. For the atomic target (Ar), we use the variable–phase–approach (VPA)[30] in order to determine phase–shifts at each energy; more details of the VPA approach are given in Ref. 31. The optical potential of the e^+–Ar system is determined very accurately from the numerical Hartree–Fock wave functions of the target[32]. In order to preserve numerical accuracy, convergence tests were carried out with respect to radial integration and number of partial waves retained in the evaluation of various cross sections[16].

For the diatomic molecule (CO) case, the scattering equations are set up in the single center formalism under the body–fixed (BF) adiabatic–nuclei–approximation (ANA). The final coupled scheme is formulated in the integral equation method[33]. More details for the positron-CO calculations can be found in our earlier$^{(26-27)}$ and recent[17] papers.

Assuming the CO molecule in its ground electronic ($1\sigma^2 2\sigma^2 3\sigma^2 4\sigma^2 1\pi^4$; ${}^1\Sigma$) and vibrational states, the equation of the continuum positron wave function, $P(\mathbf{r})$ in the single center formalism under the BF ANA can be written as,

$$[\nabla^2 + k^2 - 2V(\mathbf{r})]P(\mathbf{r}) = 0, \tag{7}$$

where k^2 is the positron energy in Rydbergs and the interaction potential $V(\mathbf{r})$ includes the repulsive static and attractive polarization forces. Expanding the $V(\mathbf{r})$ in terms of Legendre projections, v_λ,

$$V(\mathbf{r}) = V_{st}(\mathbf{r}) + V_{pol}(\mathbf{r}) = \sum_{\lambda=0}^{\lambda_{max}} [v_\lambda^{ST}(r) + v_\lambda^{POL}(r)]P_\lambda(\cos\theta), \tag{8}$$

we obtain the following set of coupled differential equations for the continuum function $P(\mathbf{r})$ for a given symmetry Λ,

$$[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2]P^\Lambda_{\ell\ell_0}(r) = \sum_{\ell'} V_{\ell\ell'}(r)P^\Lambda_{\ell'\ell_0}(r), \tag{9}$$

where the potential matrix $V_{\ell\ell'}$ is determined as usual[34]. Here Λ corresponds to $\Sigma(\Lambda = 0)$, $\Pi(\Lambda = 1)$, $\Delta(\Lambda = 2)$, $\Phi(\Lambda = 3)$ etc. symmetries. There are several methods to solve equation (9), but we adopt an integral–equation technique by converting the differential equation (9) into an integral equation[33],

$$P^{\Lambda}_{\ell\ell_0}(r) = j_\ell(kr)\delta_{\ell\ell_0} + \sum_{\ell'} \int_0^r G_\ell(r,r')V_{\ell\ell'}(r')P^{\Lambda}_{\ell'\ell_0}(r')dr', \tag{10}$$

where the Green's function is defined by

$$G_\ell(r,r') = k^{-1}[\eta_\ell(kr)j_\ell(kr') - j_\ell(kr)\eta_\ell(kr')], \tag{11}$$

in which $j_\ell(kr)$ and $\eta_\ell(kr)$ are Riccati–Bessel functions. Note that in the expansion (Eq. 8) of polarization term, we have only $\lambda = 0$ and 2 terms.

The CO molecule is a polar molecule which needs special attention in a BF adiabatic–nuclei theory where the forward DCS and σ_t are undefined[35]. In this respect, we employ the multipole–extracted–adiabatic–nuclei (MEAN) scheme of Norcross and Padial[36], in which the DCS for the $J \rightarrow J'$ rotational transition are given as

$$\frac{d\sigma}{d\Omega}(JJ') = \frac{d\sigma^{FBA}}{d\Omega}(JJ') + \frac{k_{J'}}{4k_J}\sum_{l_t}[C(Jl_tJ';00)]^2\frac{1}{k^2}\sum_{\lambda=0}^{\lambda_{max}}(B_{\lambda,l_t} - B^{FBA}_{\lambda,l_t})P_\lambda(\cos\theta), \tag{12}$$

where the first term is the usual closed form for the (JJ') rotational excitation DCS in the space–fixed first–Born–approximation (FBA); k_J and $k_{J'}$ are respectively the wavevectors in the initial and the final channels; C (...) is a Clebsch–Gordan coefficient; l_t is the angular momentum transferred during the collision; B_{λ,l_t} are the DCS expansion coefficients and B^{FBA}_{λ,l_t} are the corresponding quantities in the FBA evaluated in the BF frame of reference. The channel vectors are related by the relation,

$$k_J^2 - k_{J'}^2 = B[J'(J'+1) - J(J+1)], \tag{13}$$

where B is the rotational constant of the CO molecule. Finally, the expressions for total ($\sigma_t^{JJ'}$) and the momentum transfer ($\sigma_m^{JJ'}$) cross sections are evaluated from equation (11) for any (JJ') transition. Total (summed over all final rotational states J') integrated (σ_t) and momentum transfer (σ_m) cross sections can easily be obtained from

$$\sigma_{t\ or\ m} = \sum_{J'} \sigma^{JJ'}_{t\ or\ m}\ , \tag{14}$$

However, for a proper comparison with experiment, we average the σ_t and σ_m over the Boltzmann distribution of rotational states at 300 K (represented as $\langle\sigma_t\rangle$ and $\langle\sigma_m\rangle$). This is quite easy since in the present energy region the sum over J' in equaton (14) is insensitive to J.

Finally, for a polyatomic molecule, we employ totally a different set of computer codes to obtain scattering parameters. The details are given elsewhere(13,37). For a polyatomic target, it is again convenient to make use of the ANA and set up the scattering equations in the single–center–expansion scheme under the close–coupling formalism. The equation for the scattered positron function $P(\mathbf{r})$ is the same as given in Eq. (7), however, now the single–center–expansion scheme is quite different. The angular basis functions belong to the irreducible representation (IR) of the molecular point group. The $P(\mathbf{r})$, V_{st} and V_{pol} are expanded around the center–of–mass (COM) of the molecule in question. For example, the $P(\mathbf{r})$ is expanded as[13],

$$P(\mathbf{r}) = \sum_{\ell h p\mu} r^{-1}G^{(p\mu)}_{\ell h}(r)X^{(p\mu)}_{\ell h}(\hat{\mathbf{r}}), \tag{15}$$

where the $X_{\ell h}^{p\mu}$ are symmetry–adapted angular functions belonging to a particular irreducible representation $p\mu$ of the molecular point group. The static potential V_{st} is given by

$$V_{st}(\mathbf{r}) = \int |\psi_0|^2 \sum_{j=1}^{N} |\mathbf{r} - \mathbf{r_j}|^{-1} d\mathbf{r_1} d\mathbf{r_2} \cdots d\mathbf{r_N} - \sum_{i=1}^{M} Z_i |\mathbf{r} - \mathbf{R_i}|^{-1}, \tag{16}$$

where ψ_0 is the target ground state wavefunction given as a single Slater determinant of one–electron spin orbitals $\phi_\alpha(\mathbf{r})$, N is the total number of electrons and M the number of nuclei in the molecule.

Finally, the scattering amplitude for e^+ with initial direction $\hat{\mathbf{k}}$ and the final direction $\hat{\mathbf{r}}$ is

$$f(\hat{\mathbf{k}}.\hat{\mathbf{r}}) = \frac{2\pi}{ik} \sum X_{\ell h}^{p\mu}(\hat{\mathbf{k}}) X_{\ell' h'}^{p\mu}(\hat{\mathbf{r}}) i^{\ell - \ell'} (\mathbf{S}_{\ell h, \ell' h'}^{p\mu} - \delta_{\ell\ell'}\delta_{hh'}), \tag{17}$$

where the sum being over ℓ, h, ℓ', h', p and μ. The **S** matrix is related with the **K** matrix in the usual fashion. The amplitude (Eq. 17) is defined in the BF frame of reference. In order to transform it into the space–fixed (SF) or the laboratory frame coordinate system, we employ the standard technique in terms of rotation matrices[13], $\Re(\alpha, \beta, \gamma)$ (the $(\alpha\beta\gamma)$ are the three Euler's angles). If $\mathbf{r}'$ represents the coordinates of the positron with respect to SF coordinate system, the transformed amplitude, $f(\hat{\mathbf{k}}.\hat{\mathbf{r}}')$, is employed to determine the rotationally inelastic transition amplitude under the ANA theory, i.e.,

$$f(\mathbf{i} \rightarrow \mathbf{f}) = \langle \mathbf{i} | f(\hat{\mathbf{k}}.\hat{\mathbf{r}}'; \alpha\beta\gamma) | \mathbf{f} \rangle,$$

where $\langle \mathbf{i}|$ and $\langle \mathbf{f}|$ are respectively the initial and final rotational eigenfunctions. The total elastic cross sections are obtained by summing over all final rotational states and averaging over all initial states. The expressions for the differential, integral and momentum transfer cross sections are given for general non–linear polyatomic molecules in Ref. 13.

In the present CH_4 case, we do not face any convergence problem in the summation over various angular momentum quantum numbers. In fact, even the DCS's can be obtained easily with proper convergence within a reasonable size of the scattering matrix. For more details about the actual numerical parameters we recommend our previous paper[29]. In the present results on the positron–CH_4 collisions, we have kept the same single–center expansion and K-matrix parameters as described in Ref. 29.

Jain and Thompson[29] used three different approximations for the polarization interaction; all the three models were exactly the same as employed for electron scattering(38–40). However, the most successful was the one based on the second–order perturbation theory under the Pople Shofield method[41] in which the distortion in each molecular orbital is the same. The non–adiabatic effects were included via the non–penetration criterion of Temkin[42]. This electron polarization potential[40] (to be denoted by JT) has so far been quite successful in positron–CH_4 collisions. Unfortunately, the JT potential has never been employed for any atomic system; however, it has been employed for the e^+–N_2 case[43] with fair success. The other two EPP used by Jain and Thompson[29] were based on the asymptotic form multiplied by the cut–off function. Although the use of non–penetrating scheme for the positron case may be questionable, however, we argue here that the non–adiabatic effects in e^+ case are not much effective due to relatively smaller local kinetic energy of the impinging positron in the vicinity of the target. Therefore, we emphasize here that in any polarised–orbital variational approach, the non–adiabatic correction may not be taken very seriously. In the findings of Elza et al[8], these non–adiabatic effects seem to change the results; however, it is hard to draw any conclusion since they introduce fitting parameters which makes physics less clear.

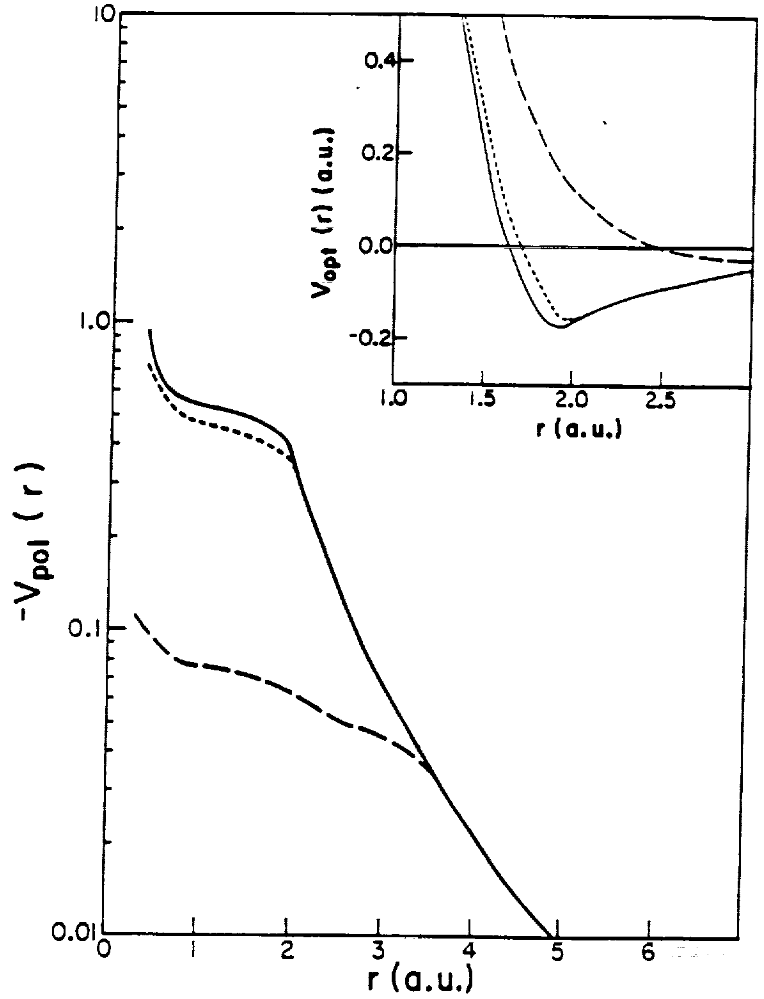

Fig. 1. Various polarization potentials for the e^+–Ar system. The potentials PCOP1, PCOP2 and ECOP are shown, respectively, by solid, dashed and long–dashed lines. The various notations are explained in the text. In the inset are shown the total optical potentials (sum of repulsive static and attractive polarization potentials) with various models: solid line, $V_{st} + V_{pol}^{PCOP2}$; dashed line, $V_{st} + V_{pol}^{PCOP1}$; long–dashed line, $V_{st} + V_{pol}^{ECOP}$.

IV. Results and Discussion

First, we display the new PCOP terms in Fig. 1 for the e$^+$–Ar system. We have considered two forms of the PCOP model; one, the correlation potential defined by Eq. (6) (to be denoted by PCOP2) and two, the correlation energy itself (Eq. 3, to be denoted by PCOP1). Both the PCOP1 and PCOP2 terms are plotted in Fig. 1. Also shown in this figure is the corresponding ECOP potential. We see a significant difference between the ECOP and PCOP curves. In general, the PCOP is stronger then the ECOP approximation. This simply means that the $e^+ - e^-$ correlation energy is stronger, thus giving rise to a more attractive polarization potential. It seems realistic since the e^+ is expected to distort the target charge cloud deeper due to strong correlation of electron and positron particles. A similar situation exists for molecular targets (CO and CH_4) (not shown).

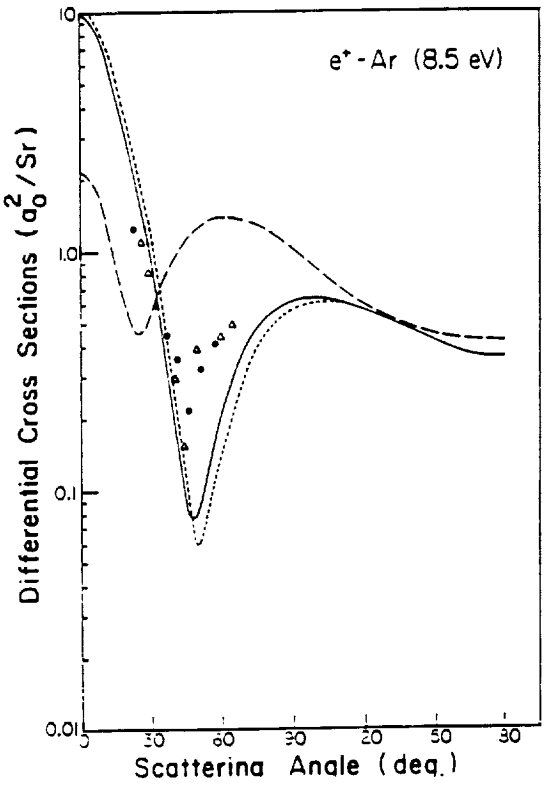

Fig. 2 Differential cross sections for the e$^+$-Ar elastic collision at 8.5 eV. Present theory: solid curve, PCOP2 model; dashed curve, PCOP1 model; long-dashed curve, ECOP model. The experimental points are taken from Refs. 44 and 45.

The total optical potential shown in the inset of Fig. 1 is a sum of repulsive static and attractive polarization terms; thus there is a zero–potential point and an attractive well. The position of the zero–point potential and the shape of the attractive well decide the penetration and sign of various partial waves. Here the role of polarization interaction is important and the low–energy scattering is strongly influenced by these cancellation effects not present in the electron scattering case. Thus the form of the polarization potential in the zero–potential and the attractive well region is very crucial to determine the scattering process.

Fig. 2 illustrates the DCS for the e$^+$-Ar system at 8.5 eV alongwith the ECOP results and the measurements of Refs. 44–45. We see a significant qualitative improvement represented by these PCOP curves. The dip in the experimental DCS around 50^0 is neatly reproduced by the new model, while the ECOP dip occurs at smaller angle (30^0). We have not shown other calculations[46–49] due to their semi-empirical nature. We have seen similar agreement between theory and experiment at other energies (lower and higher than 8.5 eV) also[16]. In order to further see the success of the PCOP model at lower energies, we have calculated the scattering length in the zero energy limit. The value of the PCOP scattering length is -4.89 (au), which compares very well with the experimental value[50] of -4.4 ± 0.5 (au); the ECOP model gives this value only 1.7 (au). It is thus quite clear that in this low energy limit a true positron polarization interaction makes big difference in the scattering parameters.

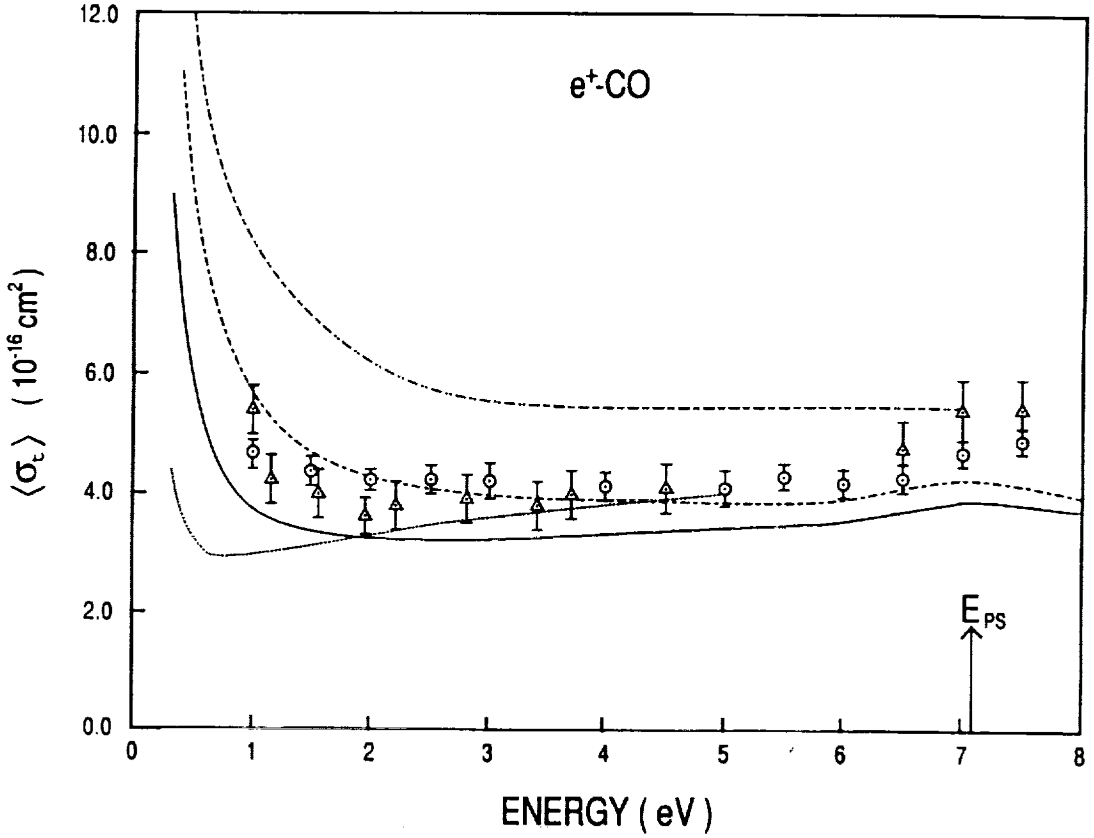

Fig. 3. Positron–CO $\langle\sigma_t\rangle$ cross sections in various theoretical models (including the R–matrix results[3]*, shown as dash-dot-dot curve) and experimental observations (circles, Kwan et al*[51]*; triangle, Sueoka and Mori*[52]*). Our PCOP results are shown using experimental value of the dipole moment (solid curve) and also the theoretical value of the dipole moment (dashed curve). The ECOP data*[16] *are plotted as the dotted curve.*

We now discuss our e^+–CO calculations on the $\langle\sigma_t\rangle$ parameter. Fig. 3 shows the present PCOP $\langle\sigma_t\rangle$ alongwith the ECOP[28], R–matrix[4] and the experimental(51–52) results. We have shown two versions of the present PCOP (Eq. 6) model: one, with the present theoretical value of the dipole moment (D=0.099 a.u.), shown as dashed curve in Fig. 3 and two, by using the experimental value (D=0.044 au), shown as a solid line. Below 4 eV, the use of theoretical value of the dipole moment makes large changes in the $\langle\sigma_t\rangle$. The R–matrix results do not compare well with the measurements; one reason being that they employ their theoretical dipole moment value in the MEAN approximation and the second reason is related with their polarization force which still needs to be improved[53]. The inclusion of the polarization force makes large changes (about a factor of two or more) in the pure static results. It seems that the ECOP approximation is better at higher ($E \geq 2$ eV) energies; however, this conclusion may not be true as the two sets of DCS's differ significantly and we expect that the PCOP DCS's are better than the cooresponding ECOP cross sections [17].

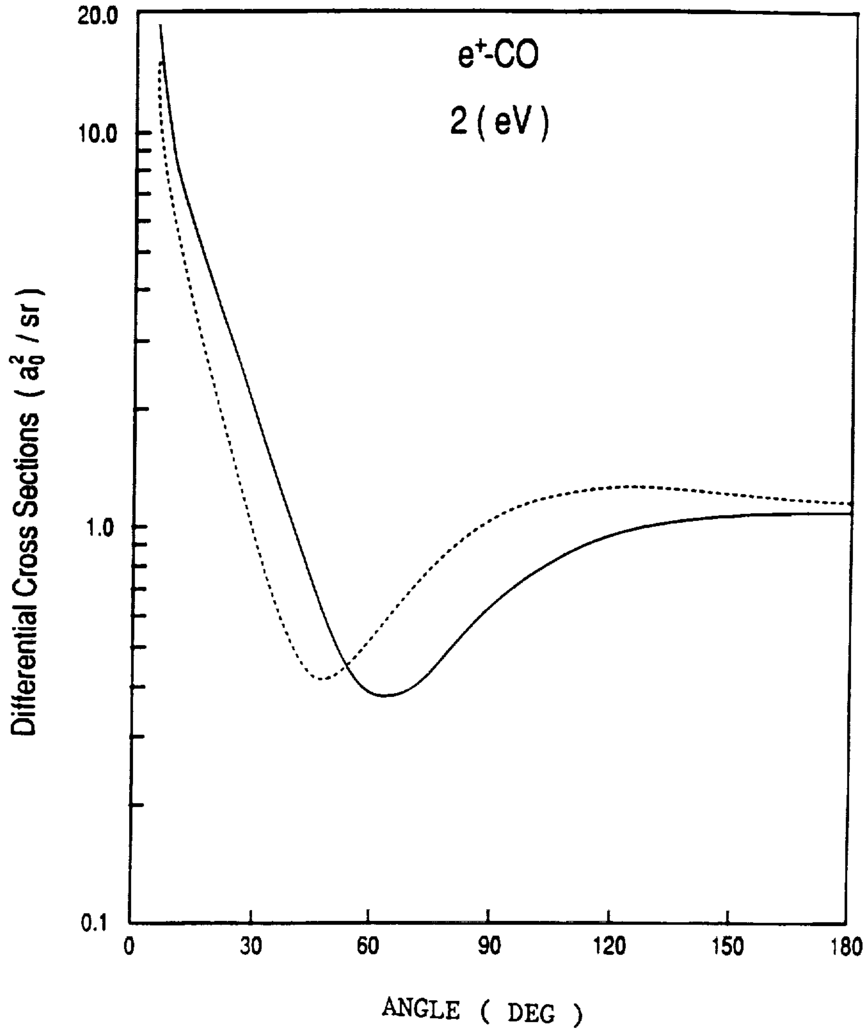

Fig. 4. Positron–CO DCS at 2 eV in the PCOP (solid curve) and ECOP (dashed curve)[26] *polarization models.*

In order to see the qualitative differences between the ECOP and PCOP models for the positron collisions with CO molecules, we have shown in Fig. 4, the differential cross sections at 2 eV. We see a qualitative difference between the two curves of Fig. 4 . The dip in the ECOP approximation occurs at lower angles while the PCOP dip in the DCS's curve occurs at somewhat larger angles; the difference between the positions of the two dips is about 20^0. The disagreement between these two polarization model is seen at all angles (Fig. 4). It is interesting to note that the total cross sections at this energy is almost same in both the PCOP and ECOP approximations. Thus, the integral cross sections are sometimes confusing and therefore a theoretical model should be judged from the angular functions which are more sensitive to model potential results. It would be very interesting to see the position of the dip in an experimental investigation. So far, we believe that the PCOP dip is more realistic.

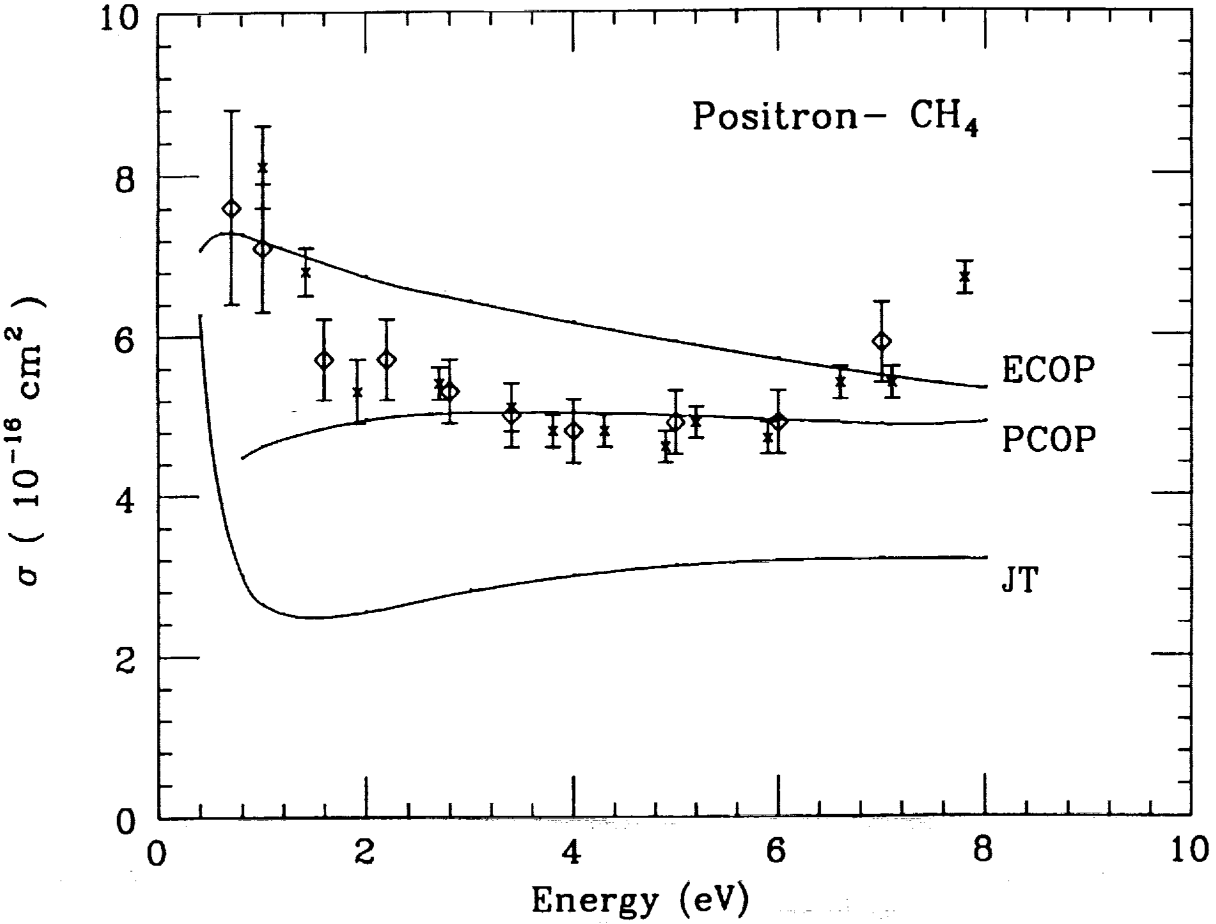

Fig. 5. The positron–CH$_4$ σ_t cross sections using the PCOP , ECOP[28] and JT[29] theoretical models. All the curves are labelled with respect to all these approximations. The experimental data are taken from Refs. 54 and 55.

From Fig. 3, we thus see that the PCOP model is quite successful in reproducing the experimental data, particularly at low energies where the ECOP calculations totally fail. At higher energies (above 3 eV) where the ECOP approximation seems to work well, the difference between the two sets of DCS is significant (see Fig. 4); for example, at 2 eV, the positions of the dips in the ECOP and PCOP curves occur at 40^0 and 50^0 angles respectively.

Right now there are no other DCS's (theoretical or experimental) available for comparison for the positron–CO elastic collisions. It would have been interesting to have a comparison between the PCOP and the R-matrix angular functions. It is possible that the DCS's for the positron–CO system be measured in the laboratory in future. Only then one can conclude finally about the usefulness of the PCOP model in the e$^+$–CO case. In passing, we would like to mention that at further lower energies (below 1 eV) the difference between various DCS calculations may be dramatic due to a stronger dependence of the collision dynamics on the polarization/correlation effects.

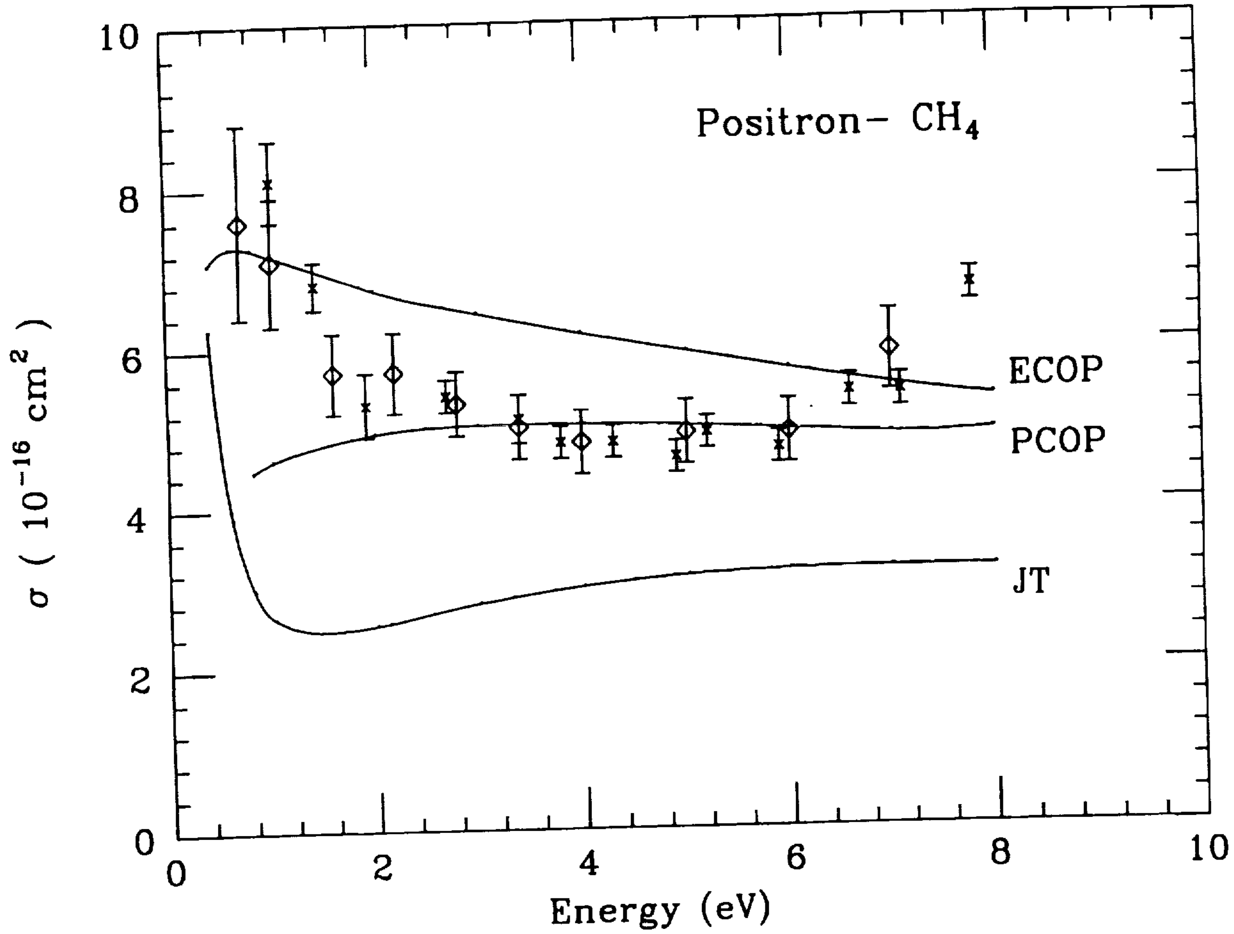

Fig. 5. The positron-CH_4 σ_t cross sections using the PCOP , ECOP[28] and JT[29] theoretical models. All the curves are labelled with respect to all these approximations. The experimental data are taken from Refs. 54 and 55.

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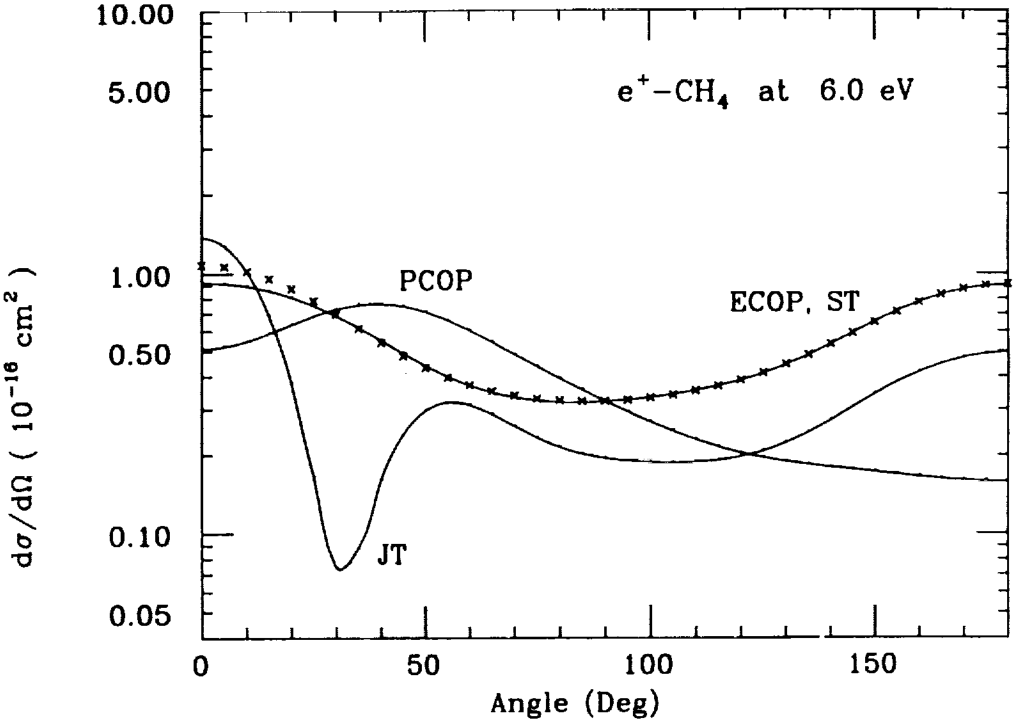

Fig. 6. DCS's for the e^+–CH_4 collisions at 6 eV using the PCOP, ECOP and JT[29] models for the polarization potential. The points (+) are the static only results.

Finally, in Fig. 5, we demonstrate our e^+–CH_4 σ_t values along with experimental points. Also shown in this Fig. 4 are the calculations using EPP models of Jain and Thompson[29] and Gianturco et al[28]. The measured data are taken from Dababneh et al[54] and Sueoka and Mori[55]. Again we see that the new PCOP gives very encouraging results as compared to other theoretical models based on the EPP. However, if we look into the corresponding DCS (Fig. 6) at 6 eV, the three models give totally different type of results. We need experimental data on the DCS in order to see which polarization approximation describes the collision properly. It is clear from Fig. 6 that even if there is some agreement in the total cross sections, the DCS's may be quite different both in quality and quantity.

V. Conclusions

We conclude that a true positron polarization approximation is essential to investigate the low–energy positron collisions with atoms and molecules. Even if the EPP and PCOP total cross sections are identical, the DCS differ significantly. We are in the process to test the sensitivity of the Z_{eff} parameter with respect to EPP and PCOP polarization models. We mention here that in the positron scattering, the question of nonadiabaticity may not be as serious as in the case of electron collisions: the reason being that the positron being repelled by the nucleus of the target is not speeded up in the vicinity of the target; thus reducing the non-adiabatic effects.

In this article, we have discussed a new parameter–free positron polarization potential which is obtained by short range $e^+ - e^-$ correlation energy and the correct long range behaviour of the polarization potential. It should be realized that the inclusion of correlation/polarization effects in positron collisions is a very hard problem. In model approaches, such as the one discussed here, one has to compromise with the local and energy–dependent form of the polarization against its non–local and non–adiabatic nature. The use of model polarization potentials will still continue due to their simplicity and significant success even at the DCS level. We emphasize that all the positron polarization models should be tested with respect to differential cross sections and the very low energy parameters such as the scattering length and the annihilation paremeter.

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Some useful discussion with Jonathan Tennyson about his R–matrix calculation is thankfully acknowledged. We thank the Florida State University Computing Center for providing supercomputer time. We acknowledge the support by the Florida State University Supercomputer Computations Research Institute which is partially funded by the U.S. Department of Energy through Contract No. DE-FC05-85ER250000.

REFERENCES

1. Morrison M A, Gibson T L and Austin D, J. Phys.B; At. Mol. Phys. **17**, 2725 (1984)
2. Morrison M A, *Proc 3rd Int. Conf. on Positron(Electron) Gas scattering* eds. Kauppila et al (World Scientific, Singapore, 1986) p. 100
3. Tennyson J, J. Phys. B: AT. Mol. Phys., **19**, 4255 (1986)
4. Tennyson J and Morgan L, J. Phys. B: At. Mol. Phys. **20**, L641 (1987)
5. Tennyson J and Danby G , *Atomic Physics with Positrons* eds. J. W. Humberston (Plenum, New York 1987) p. 111
6. Armour E A G , Phys. Rep. **169**, 1–98 (1988)
7. Barschat K, McEachran R P and Stauffer A D, J. Phys. **B21**, 2789 (1988)
8. Elza B K, Gibson T L, Morrison M A and Saha B C , J. Phys. **B22**; At. Mol. Phys., 113 (1988)
9. Abdel - Raouf M A, Acta Phys. Hungarica, **63**, 21 (1988)
10. Armour E A G, Phys. Rep., **169** , 1 (1988)
11. Jain A, Proc. 3rd. Int. Conf. on " Positron (Electron)–Gas Scattering ", Eds. Kauppila et al (World Scientific, Singapore 1986)
12. Jain A, Proc. 4th Int. Conf. on " Atomic Physics with Positrons ", Eds Humberston and Armour (Plenum, NY 1987)
13. Gianturco F A and Jain A, Phys. Rep., **143**, 347 (1986)
14. Darewych J W, J. Phys. B: At. Mol. Phys. **15**, L415 (1982)
15. Horbatsch M and Darewych J W, J. Phys. B: At. Mol. Phys. **16**, 4059 (1983)
16. Jain A, Phys. Rev. **A39** (in press, August 1989)
17. Jain A, J. Phys. B: At. Mol. Phys., (in press, 1989)
18. O'Connel J O and Lane N F, Phys. Rev. **A27**, 1893 (1983)

19. Sjolander S and Scott M J,Solid State Comm. **8**, 1881 (1970)
20. Sjolander S and Scott M J, Phys. Rev **B5**, 2109 (1972)
21. Hodges C H and Scott M J, Phys. Rev. **B7**, 73 (1973)
22. Arponen J and Pajanne E, Ann. Phys. **121**, 343 (1979)
23. Boronski E and Nieminen R M, Phys. Rev. **B34**, 3820 (1986)
24. Kallio A, Pietilanen P and Lantto L J, Phys. Scr. **25**, 943 (1982)
25. Kohn W and Sham L J, Phys. Rev. **140**, A1133 (1965)
26. Jain A, J. Phys. B: At. Mol. Phys. **B19**, L105–L110 (1986)
27. Jain A, J. Phys. B: At. Mol. Phys. **B19**, L379–L384 (1986)
28. Gianturco F A, Jain A and Pantano L C, Phys. Rev. **A36**, 4637 (1987)
29. Jain A and Thompson D G, J. Phys. B: At. Mol. Phys. **16** 1113 (1983)
30. Calogero F, " Variable Phase Approach to Potential Scattering", (New York, 1973)
31. Jain A, Phys. Rev. **A34**, 3707 (1986)
32. Karim K R and Jain A, Phys. Scripta, **39**, 238 (1989)
33. Morrison M A, Lane N F and Collins L A, Phys. Rev. **A15**, 2186 (1977)
34. Burke P G, Chandra N and Gianturco F A, J. Phys. **B3** 641 (1974)
35. Collins L A and Norcross D W, Phys. Rev. **A18**, 478 (1978)
36. Norcross D W and Padial N T, Phys. Rev. **A25**, 226 (1982)
37. Jain A, Ph.D thesis, The Queen's University, Belfast (1983)
38. Gianturco F A and Thompson D G, J. Phys. **B9**, L383 (1976)
39. Gianturco F A and Thompson D G, J. Phys. **B13**, 613 (1980)
40. Jain A and Thompson D G, J. Phys. **B15**, L631 (1982)
41. Pople J A and Shofield P, Phil. Mag., **2**, 591, (1957)
42. Temkin A, Phys. Rev. **107**, 1004 (1957)
43. Gillespie E S and Thompson D G, J. Phys. **B8**, 2858 (1975)
44. Coleman P G, McNutt J D, Phys. Rev. Lett. **42**, 1130 (1979)
45. Floeder K, Honer P, Raith W, Schwab A, Sinapius G and Spicher G, Phys. Rev. Lett. **23**, 2363 (1987)
46. Nakanishi H and Schrader D M, Phys. Rev. **A34**, 1823 (1986)
47. McEachran R P, Ryman A G and Stauffer A D, J. Phys. **B12**, 1031(1979)
48. Schrader D M, Phys. Rev. **A20**, 918 (1979)
49. Datta S K, Mandal S K, Khan P and Ghosh A S, Phys. Rev. **A32**, 633 (1985)
50. Lee G F and Jones G, Cand. J. Phys. **52**, 17 (1974)
51. Kwan Ch K, Hsieh Y F, Kauppila W E, Smith S J, Stein T S , Uddin M N and Dababneh M S 1983, Phys. Rev. **A27**, 1328
52. Sueoka O and Mori S, J. Phys. Soc. Japan **53**, 2491 (1984)
53. Tennyson J, private communication
54. Dababneh M S, Hseih Y -F, Kauppila W E, Kwan C K, Smith S J Stein T S and Uddin M N, Phys. Rev. **A38**, 1207 (1988)
55. Sueoka O and Mori J, J. Phys. **B19**, 4035 (1986)