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# Positronium formation in positron–alkali-metal-atom collisions: An optical potential approach

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Integral and differential cross sections for the Ps-formation channel for $e^+$–alkali-metal-atom collisions are calculated, with considerable success, by means of a model optical potential. The atomic targets discussed here are Li, Na, and K. The potential is obtained without empirical parameters via a global modeling of the dynamical polarization potential and of the short-range correlation forces, with the use of generalized damping functions. The absorption part of the potential is obtained by means of a dispersion relation. We present here a full account of this simple and promising technique. [S1050-2947(96)02707-2]

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## I. INTRODUCTION

The interest in positron-atom collisions is rapidly increasing owing to the recent progress in positron-beam technology, which gives experimental research a new tool for investigating the properties of atomic, molecular, and solid-state matter. It is now possible to make comparisons between $e^+$ and $e^-$ collision data and learn about the relative importance of the interaction terms by comparing similar dynamical attributes in the two processes. Together with the change of sign for the static interaction, the main difference between these two kinds of probe is that the positron is distinguishable from the target electrons. As there are no symmetry requirements for the total wave function, the nonlocal exchange part of the potential can be dropped, with a consequent simplification of the whole quantum-mechanical problem.

Among the various inelastic atomic collisions, the formation of a bound $e^+e^-$ state plays indeed a special role, and, additionally, the relative cross section is often found to be dominant in the low-energy region with respect to the other channels, including the elastic one.

Positronium-formation cross sections for alkali-metal vapors (Na,K) have been recently measured by Zhou *et al.* [1] and have been found to be two orders of magnitude larger than the analogous cross-section measurements for room-temperature gases [2–4] and atomic hydrogen [5]. This specific feature, together with the fact that it is only for $e^+$–alkali-metal-atom collisions that the reaction

$$e^+ + A \rightarrow A^+ + \mathrm{Ps} \tag{1}$$

is exothermic (the ionization potentials are in fact lower than the Ps ground-state binding energy), renders the positron interaction with this class of atoms a very interesting subject for investigation.

There are several theoretical results for Ps formation in $e^+$-Li scattering [6–10], while the literature is still rather poor as regards sodium and potassium targets. We give below an extensive list of the most recent $e^+$-Na,K theoretical studies and further report the corresponding approximations: Abdel-Raouf [11,12] carried out a two-state close-coupling (CC) computation, Mandal and Guha [13] used the first Born approximation, Nahar and Wadehera [15] and Guha and Mandal [14] employed the distorted-wave approach, while Hewitt, Noble, and Bransden [16] carried out full coupled-channels computations, further extended by McAlinden, Kernoghan, and Walters [10,17]. These calculations gave only the integral Ps($1s$)-formation cross sections, except for the CC calculations of Refs. [10,16,17] where are reported the cross sections for Ps formation in the lower excited states. It is also worth noting here that there is a marked lack of systematic studies of differential cross sections for any of the processes involved in Ps formation.

In this work we aim to extend to this class of atoms a technique which has been successfully used [18] when investigating the hydrogen and helium positron scattering parameters. This method is based on the projection operator formalism, by which—defining an effective Hamiltonian—we project the solutions of the Schrödinger equation onto an arbitrarily chosen basis set (in this case, the asymptotic incoming and outgoing channels). This feature radically simplifies the solution of the scattering equations as one can concentrate on finding a good model for the optical potential rather than on making approximations to both the interaction potential and the total wave function. With this purpose, we develop below a model for the nonadiabatic, energy-dependent polarization potential. We also describe the short-range correlation forces by means of a set parameter-free damping functions which correct the short-range diverging terms in the Rayleigh-Schrödinger expansion series. Finally, we obtain the imaginary part of the optical potential by using an integral relation which connects it to the real part of $V^{\mathrm{opt}}$.

The search for simpler methods is certainly an attractive challenge for a theoretical study, as models always give some additional physical insight within their formulation. We will show below how the present method turns out to be more efficient than the lengthy procedures involved in the CC calculations, while, however, still giving comparably good results, a feature which renders it suitable for applications to a wide range of collision problems.

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## II. OPTICAL POTENTIAL AND DISPERSION RELATIONS

The projection operator formalism has been successfully used in nuclear and atomic physics research during the last three decades, since the time that it was introduced in its mature form in Feshbach's seminal paper [19]. We will briefly review in the following the fundamental aspects of this theory, showing how it naturally leads to the definition of a complex optical potential and to a dispersion relation between its real and imaginary parts. This mathematical feature undoubtedly plays a central role in the present study and will be exploited when constructing our final equations.

The usual starting point is to define, given a complete basis set $|\phi_i\rangle$, the projection operators $P$ and $Q$ by the familiar expressions

$$P=\sum_{i\in P}|\phi_i\rangle\langle\phi_i|, \quad Q=I-P. \tag{2}$$

The choice of the basis set can be adjusted to the physical nature of the studied phenomena. When the interactions are supposed to be short range, e.g., nuclear interactions, the most natural choice is to project the solutions of the scattering problem outside a sphere of a given radius, as in the outside region the nuclear forces can be neglected. In dealing with atomic collisions, a convenient choice is to use the incoming and outgoing scattering channels, in either the coordinate or the momentum representation [20], as a suitable basis set. Applying those operators to the Schrödinger equation, one can then write a completely equivalent projected equation where the potential in the Hamiltonian is substituted by an optical potential:

$$(E-T-V^{\mathrm{opt}})P|\psi\rangle=0. \tag{3}$$

The term $T+V^{\mathrm{opt}}$ is called the *effective Hamiltonian*. In the same notation, $V^{\mathrm{opt}}$, is shown to be equivalent to

$$V^{\mathrm{opt}}(E)=PVP+PVQ\,\frac{1}{E-QHQ}\,QVP. \tag{4}$$

If the $P$ space is spanned by the asymptotic states only, the scattering problem reduces to a two-state one. It follows that the whole dynamics of the colliding system is embodied in the effective Hamiltonian, which is strictly connected to the resolvent of the QHQ operator, as shown in Eq. (4). To get a full understanding of the effects that some of the following approximations have on the scattering parameters, some preliminary considerations on the operators spectrum are required. An important assumption in Feshbach's theory, which has been rigorously demonstrated by Bertero [21] in the three-body case, is that the eigenvalue distribution of the QHQ operator is similar to the spectrum of the full Hamiltonian $H$. In other words, we have a point spectrum in the open interval $[0,\epsilon)$—with isolated eigenvalues of finite multiplicity—and a continuous spectrum for higher energies. Since the energy-dependent optical potential can have an imaginary part only in the interval $[\epsilon,\infty)$, all the energies at which the $Q$-projected channels become open will be larger than $\epsilon$. The probability flux is in general not conserved within the $P$ space as it goes into the other channels as they become energetically accessible. For this reason the optical potential defined in Eq. (4) is complex and hence non-Hermitian.

In our present model the $Q$ space gathers all the excited states of both the target and the outgoing compound, so that $\epsilon$ equals the energy of the lowest inelastic channel. In the kind of collisions studied in the present work, $\epsilon$ is the transition energy to the first excited level of the atom, $\mathscr{E}_1$.

We may regard the optical potential as a function of the complex variable $E$, of which in general it will not be an analytic function. However, by requiring the $V^{\mathrm{opt}}$ to be analytic in the $E$ plane, with a branch cut in $[\epsilon,\infty)$, a useful dispersion relation can be obtained. As a first step, we split $V^{\mathrm{opt}}(E)$ into three terms:

$$V^{\mathrm{opt}}(E)=V^S+V^P(E)+iV^A(E), \tag{5}$$

where $V^S$ represents the interaction of the impinging positron with the unperturbed atom, while $V^P(E)$ and $V^A(E)$ are, respectively, the polarization and absorption model potentials. It can be further shown [22] that the following integral relation holds:

$$V^P(E)=\frac{1}{\pi}\,\mathrm{P}\int_{\mathscr{E}_1}^{\infty}\frac{V^A(E')}{E'-E}\,dE'. \tag{6}$$

This equation resembles the well known Konig-Kramers relations for a linear response function, although we wish to point out some specific differences from the latter: the integration is not extended onto the real axis, but starts from $\mathscr{E}_1$, and Eq. (6) does not have a symmetric counterpart. Further, the interaction potential is in general nonlocal. However, the present colliding particle is distinguishable from the atomic electrons, so that the difficulties arising from nonlocality are automatically removed. In the present approach the polarization potential is considered to be a known function, and hence Eq. (6) becomes a Fredholm equation of the first kind. This feature brings about some difficulties as this kind of integral equation is ill conditioned, and therefore the mathematical problem has to be handled carefully. Further, $V^A(E)$ has an arbitrary number of unphysical solutions outside the integration domain, so that the optical potential obtained with the help of Eq. (6) cannot be used for projectile energies lower than $\mathscr{E}_1$.

## III. THEORETICAL DEVELOPMENT OF THE MODEL

It is apparent from Eq. (6) that an energy dependency for the polarization potential is also required and therefore the atomic polarization potential cannot be derived adiabatically. In fact, in the adiabatic approximation one describes the atomic orbitals as instantaneously relaxing in a perturbed configuration, and of course this is not true if the perturbating field varies with time, i.e., when a charged particle moves in the atomic neighborhood. In this case the dynamical polarization potential will be shallower than the adiabatic potential.

The polarization potential $V^P(r,E)$ is usually expanded as

$$V^P(r,E)=-\frac{\alpha_1}{2r^4}-\frac{\alpha_2}{2r^6}+\frac{1}{2r^6}\,(6\beta+48\gamma E)+O(r^{-7}) \tag{7}$$

where the dipole and quadrupole polarizabilities and the first two nonadiabatic corrections have been included. Considering the actual values of those coefficients for alkali-metal atoms, it is straightforward to show that, if the energies involved are larger than a few eV, the energy-independent nonadiabatic term is negligible with respect to the energy-dependent term. So, by dropping the $\beta$ term, the polarizability expansion can be written as

$$V^P(r,E) = -\frac{\alpha_1}{2r^4} - \frac{\alpha_2}{2r^6} + \frac{1}{2r^6}\,48\gamma E \tag{8}$$

and neglecting the $r^{-8}$ terms we have

$$V^P(r,E) = V^P_{\mathrm{ad}}(r)\left(1 - \frac{48\gamma}{\alpha_1}\,\frac{E}{r^2}\right), \tag{9}$$

where $V^P_{\mathrm{ad}}(r)$ is the full adiabatic polarizability. The last expression for $V^P(r,E)$ gives a proper account of the charge-atom interaction only for large values of $r$. We now define the adiabatic correlation-polarization potential as $V^{\mathrm{CP}}_{\mathrm{ad}}(r)$, which is aimed at improving the asymptotic expansion and, at this point of the discussion, is supposed to reproduce the correct atomic adiabatic polarizability both in the internal region of the atom and at large distances. We will describe below the procedure adopted to model the short-range correlation forces.

We can now factorize $V^P$:

$$V^P(r,E) = V^{\mathrm{CP}}_{\mathrm{ad}}(r)\,\Gamma(r,E), \tag{10}$$

where $\Gamma(r,E)$ is an energy-dependent function which still has to be defined. There are some intuitively obvious constraints that can be used when making a model to describe this function.

(i) When the perturbing charge is fixed, the energy-dependent polarization potential equals the adiabatic potential, so $\Gamma(r,E) \to 1$ as $E \to 0$.

(ii) For high projectile velocities, the atom has not the time to polarize under the influence of that high-frequency perturbing field, so we have $\Gamma(r,E) \to 0$ as $E \to \infty$.

(iii) When the energy is fixed, the field varies more rapidly in time as the positron gets closer to the atom, thus $\Gamma(r,E) \to 0$ for $r \to 0$.

(iv) On the contrary, if, the energy being fixed, the charged particle is far enough from the target, the perturbation has only very low frequencies and so the adiabatic approximation is correct: $\Gamma(r,E) = 1$ for $r \to \infty$.

(v) As a last condition, we require that the product $V^{\mathrm{CP}}_{\mathrm{ad}}(r)\Gamma(r,E)$ reproduces for large values of $r$ the asymptotic polarization potential in its simplified version given by Eq. (9).

In this study a functional form (which is, of course, not unique) has been chosen for $\Gamma(r,E)$ following the one already used by Thirumalai, Staszewaska, and Truhlar [22] for electron-atom scattering problems:

$$\Gamma(r,E) = \frac{1}{1 + \eta(E/r^2)}. \tag{11}$$

It is straightforward to verify that the previous conditions (i)–(iv) are satisfied by the above expression. Further, by making a series expansion (for $r \gg \eta E$) we get

$$\Gamma(r,E) = 1 - \frac{\eta E}{r^2} + \cdots , \tag{12}$$

so, with $\eta = 48\gamma/\alpha_1$, the last condition is also satisfied. The present derivation is somewhat different from the one given in Ref. [22], as the latter was developed in the framework of the average energy approximation, and therefore the two derivations lead to different values of the coefficient $\eta$.

The integral equation (6) has an analytical solution for the functional form of $V^P(r,E)$ as given in Eq. (11); thus we have for the absorption potential

$$V^A(r,E) = V^{\mathrm{CP}}_{\mathrm{ad}}(r)\left(\frac{E - \mathscr{E}_1}{E + (\alpha_1 r^2/12\gamma)}\right)^{1/2}. \tag{13}$$

It should be noted that, as discussed before, the above potential is not defined for $E < \mathscr{E}_1$, so this theory cannot make predictions for $e^+$-atom impact energies lower than about 2 eV (for alkali-metal atoms).

The following step is helpful to estimate the correct behavior of the adiabatic polarization potential for short positron-atom distances. The asymptotic expansion of the polarizability, which has the form

$$V^P_{\mathrm{ad}}(r) = -\sum_{l=1}^{\infty} \frac{\alpha_l}{2r^{2l+2}}, \tag{14}$$

is divergent at the origin, as each term has a pole at $r = 0$. A natural way to deal with this difficulty is to introduce some damping function aimed at rendering the behavior of $V^P_{\mathrm{ad}}(r)$ correct at all distances. In this work we adopt a damping technique developed in our group [23,24] which has given remarkably good results in electron- and positron-atom scattering problems. It starts by noting that the necessary correlation-polarization potential can be expressed as a series of products of functions over the whole range of distances:

$$V^{\mathrm{CP}}(r) = -\sum_{2l+2}^{\infty} f_{2l+2}(r)\,\frac{\alpha_l}{2r^{2l+2}}, \tag{15}$$

where $f_{2l+2}(r)$ are still unknown functions. It can be shown that the polarization series approximated to the second order is given by

$$V^{P(2)}_{\mathrm{ad}} = -\frac{1}{\epsilon}\left\langle \phi_0 \left| \left[\frac{1}{r_p}\sum_{l=1}^{\infty}\left(\frac{r_e}{r_p}\right)^l P_l(\cos\theta)\right]^2 \right| \phi_0 \right\rangle, \tag{16}$$

where $|\phi_0\rangle$ is the atomic ground state, $r_e$ and $r_p$ are, respectively, the electron-nucleus and positron-nucleus distances, $\theta$ is the angle between the $e^+$ and $e^-$ position vectors, and $\epsilon$ is the average atomic excitation energy. Using the orthogonality of the Legendre polynomials we have

$$V^{P(2)}_{\mathrm{ad}} = -\sum_{l=1}^{\infty} \frac{K_l}{2r_p^{2l+2}} \int_0^{\infty} \rho_0(r_e)\, r_e^{2l+2}\, dr_e , \tag{17}$$

where $K_l$ contains all the coefficients and the normalization constant of the corresponding Legendre polynomial, while $\rho_0(r_e)$ is the electronic density of the atomic ground state. A direct comparison with Eq. (14) gives the following expression for the polarizability coefficients:

$$a_l = K_l \int_0^\infty \rho_0(r_e) r_e^{2l+2} dr_e . \tag{18}$$

The fundamental assumption of this model is now that only the electronic density inside the sphere of radius $r_p$ contributes to the target polarizability. The coefficients $\alpha_l$ are now dependent on the positron coordinate $r_p$, so we have

$$\alpha_l(r_p) = K_l \int_0^{r_p} \rho_0(r_e) r_e^{2l+2} dr_e , \tag{19}$$

which can be written as

$$\alpha_l(r_p) = f_{2l+2}(r_p)\alpha_l , \tag{20}$$

and finally we obtain the expression for the damping functions:

$$f_{2l+2}(r_p) = \frac{\int_0^{r_p} \rho_0(r_e) r_e^{2l+2} dr_e}{\int_0^\infty \rho_0(r_e) r_e^{2l+2} dr_e} , \tag{21}$$

where $\rho_0(r_e)$ is the electronic density of the atomic ground state. Observe that these functions correctly go to zero faster than $r_c^{2l+2}$ and approach unity as the positron distance becomes large.

The present approach does not preclude a multielectron treatment [18]. We adopt, however, a single-electron model (frozen-core approximation), which is a natural and widely accepted simplification when dealing with alkali-metal atoms. Additionally, the positron trajectory usually runs over barely penetrating orbits at these energies. Further, from Eqs. (10) and (15) it is apparent that the parameters which determine the size of the $T$ matrix element are the polarizability coefficients $\alpha_l$ and those coefficients are much larger—for alkali metals—when referred to the valence electron than the corresponding values for the core electrons.

An important approximation within this model is the following: the nuclear charge is considered as perfectly screened by the electronic cloud, so our ''atom'' is treated as a pure multipole source. In ignoring the effects of the partial screening, we have tried to be consistent with our physical picture of this reaction. The target electron is considered to go through successive excitations of the polarized orbitals, which for this class of atoms are considerably spread in space, and not simply ejected via the interaction with the impinging positron. We may conclude that the static short-range part of the potential should not affect strongly the collision dynamics in the energy range considered here and therefore we do not need to calculate it explicitly.

Figure 1 displays the real and imaginary parts of the optical potential for the Li target at different energies, obtained with the present modeling. The complicated structure of the potential at small distances is due to the nodes in the electronic density, which in turn define the damping functions.

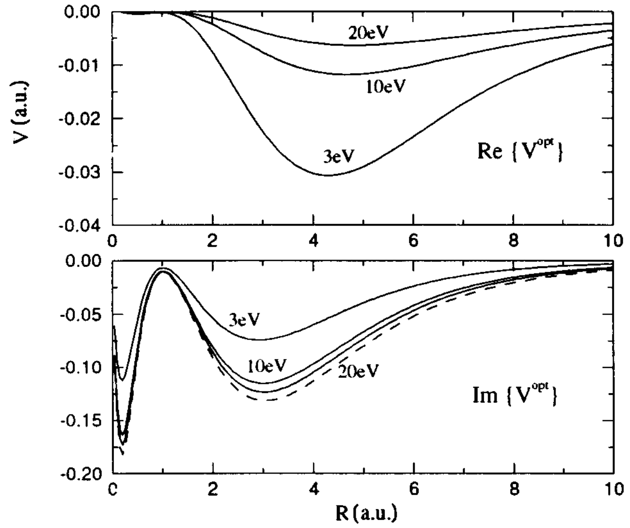

FIG. 1. Computed real and imaginary parts of the present optical potential for positron scattering from lithium atoms. Top: real component. Bottom: imaginary component. The various curves refer to different collision energies while the dashed curve represents the asymptotic behavior of Im$V^{\text{opt}}$.

## IV. THE SCATTERING EQUATIONS

The transition matrix for a two-state system—in this case the asymptotic states onto which the Schrödinger equation has been projected—has a very simple expression:

$$T_{fi} = \langle f | V^{\text{opt}} | i \rangle . \tag{22}$$

This equation is exact if we know the exact potential, that is, if we use a complete basis set. In actual *ab initio* calculations, the spectral series of the $QHQ$ eigenstates is always truncated, so researchers use the Lippman-Schwinger equation—of which Eq. (22) can be seen as a zero-order implementation—in order to obtain a double-basis representation for the $T$ matrix. The use of this procedure is indeed more problematic (if not impossible) when dealing with model potentials, as in this case there is not, in our opinion, a transparent way to distinguish the ''residual'' states in the $P$ space. However, we argue, leaving it as a task for further investigations, that a suitable basis in the $P$ space could be the set of the (outgoing) positronium excited-state channels.

Writing Eq. (22) in a more explicit form, we have therefore that

$$T_{fi}(\mathbf{k}_f,\mathbf{k}_i) = \int e^{-i\mathbf{k}_f\cdot\mathbf{R}} \chi_0(\rho) V^{\text{opt}}(r_p,k_i) e^{i\mathbf{k}_i\cdot\mathbf{r}_p} \phi_0(r_e) d\mathbf{r}_p d\mathbf{r}_e , \tag{23}$$

where $\mathbf{r}_e$ and $\mathbf{r}_p$ are the electron and positron coordinates, $\chi_0(\rho)$ and $\phi_0(r_e)$ are the positronium and atomic ground states, respectively, and $\mathbf{R} = \frac{1}{2}(\mathbf{r}_p + \mathbf{r}_e)$, $\rho = |\mathbf{r}_p - \mathbf{r}_e|$.

Imposing the conservation of the total energy of the system, and remembering that the scattering problem from a central potential has a cylindrical symmetry, it is possible to reduce the number of variables in the $T$ matrix element. We have thus

$$T_{fi}(\mathbf{k}_f,\mathbf{k}_i)\rightarrow T_{fi}(\theta,E),$$

where $E$ and $\theta$ are the initial projectile energy and the scattering angle. Finally, we can write the differential cross section (with the reduced masses put as $\mu_P=1$ and $\mu_{\text{Ps}}=2$, in atomic units)

$$\frac{d\sigma}{d\Omega}(\theta,E)=\frac{1}{\sqrt{2}\pi^2}\left(\frac{E+E_{\text{Ps}}-E_I}{E}\right)^{1/2}|T(\theta,E)|^2, \quad (24)$$

where $E_{Ps}$ is the binding energy of positronium (=6.8 eV) and $E_I$ is the ionization energy of the target atom.

## V. COMPUTATIONAL DETAILS

The calculation of the Ps-formation differential cross sections has now been reduced to the evaluation of six-dimensional integrals, one for each value of $E$ and $\theta$, as given in Eq. (23), plus a supplementary integration on $\theta$ in order to obtain the integral cross sections. We adopted for this purpose the standard Gauss-Legendre quadrature method. It is useful to remember here the input parameters of the code:

(1) the atomic polarizability coefficients;

(2) the ionization and the first atomic excitation levels;

(3) the ground-state orbitals of the target.

The polarizability series has been truncated at the octupole term and the adopted Hartree-Fock atomic orbitals used are tabulated in Ref. [25]. It is interesting to observe that, although the dynamics is dominated by the excited states of the target (and for this reason the close-coupling calculations need a large number of atomic and positronic states to converge), the present approach does not require an explicit knowledge of such states. The direct integration has the advantage of producing the differential cross sections automatically, but it is indeed more demanding than an expansion in partial waves, owing to the high degree of nesting of the DO loops. The computational time, in fact, grows as $N^d$, where $N$ is the number of integration points and $d$ is the dimension of the integral. The number of steps to reach convergence depends mainly on the oscillatory part of the integrand function that is on the energy of the plane waves in Eq. (23). We report a useful empirical law to estimate this number: $N\simeq R\sqrt{2mE}/\hbar$, where $R$ is the maximum radius of the integration domains (16–20 atomic units in the present work) referred to the $e^+$ and $e^-$ coordinates.

All calculations have been performed on a RISC 6000 workstation, with about 30 h of CPU time consumed for each atomic system. In concluding this section we wish to point out that the CC methods, the results of which are reported for comparison against our calculations, are (owing to the large number of coupled integro-differential equations to solve) about two orders of magnitude more demanding in computational time than the present approach.

## VI. DISCUSSION OF RESULTS

Some preliminary remarks are the following.

(1) The required analyticity of the polarization potential on the complex $E$ plane cancels the information on the optical potential poles. It follows that Feshbach's resonances are not considered within this application and the calculated curves are expected to be smooth.

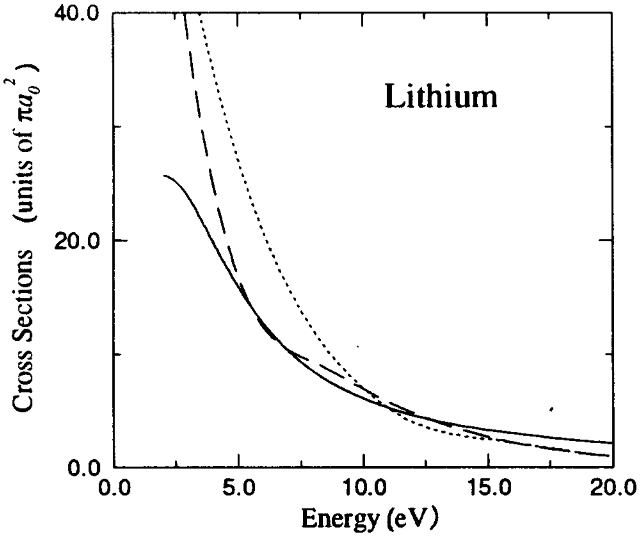

FIG. 2. Ps-formation channel cross sections as function of collision energy for the lithium target. The state considered is the Ps ground state. Solid line: present calculations. Dashed line: from Ref. [6]. Dotted line, from Ref. [10].

(2) The imaginary part of $V^{\text{opt}}$ is not defined below the excitation energy $\mathscr{E}_1$, so the calculations start above this limit at about 2 eV.

(3) In the high-energy region the present method reproduces the mathematical form as described in the first Born approximation. This can be seen by just observing the high-energy behavior, in Eqs. (11) and (13), of the real and imaginary parts of $V^{\text{opt}}$ and remembering that the cross sections are related to $|T|^2$.

(4) Experimental data are available for sodium and potassium targets, but they do not discriminate between the Ps ground-state formation and the electron capture in other excited states, so that a homogeneous comparison with our theoretical Ps($1s$) cross sections cannot be done.

Figure 2 shows the present computed Ps($1s$) integral cross sections (solid lines) together with two earlier calculations, namely, the Hewitt-Noble-Bransden CC data [6] (dashed lines) and the McAlinden-Kernoghan-Walters results [10] (dotted lines). It is interesting to note that the CC curves are comparable in shape and size with the outcomes of the present calculations, thereby showing a good convergence of the present model for impact energies larger than 5 eV.

This general trend of the present calculation is indeed confirmed by the results which we have obtained for more complicated systems like sodium and potassium. Figure 3, for instance, presents our calculations for the Ps-formation cross sections in the ground state of the compound during $e^+$-Na collisions. They are given by a solid line while the earlier coupled-channel results are given by a dashed line (from Ref. [16]) and by a dotted line (from Ref. [10]).

One clearly sees that, from about 5 up to 20 eV, our model reproduces remarkably well the CC calculations, while the latter also agree with each other within the same range of energies. As the collision energy decreases, however, we see that the three sets of calculations begin to differ

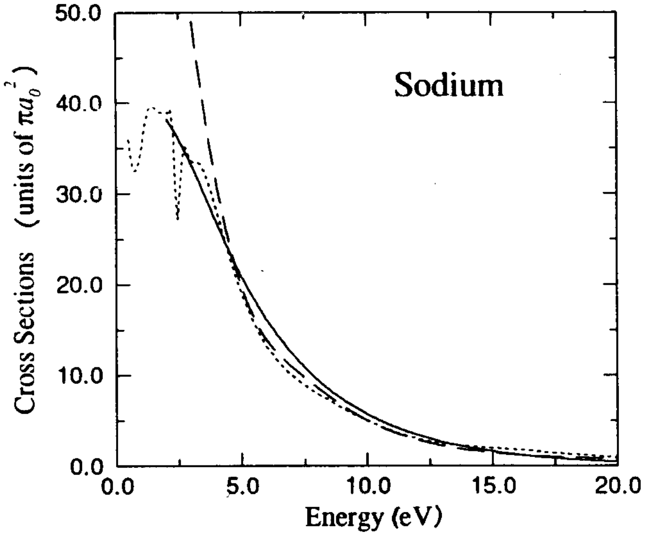

FIG. 3. Same as in Fig. 2 but for the case of the sodium target. Solid line: present calculations. Dashed line: from Ref. [16]. Dotted line, from Ref. [10].

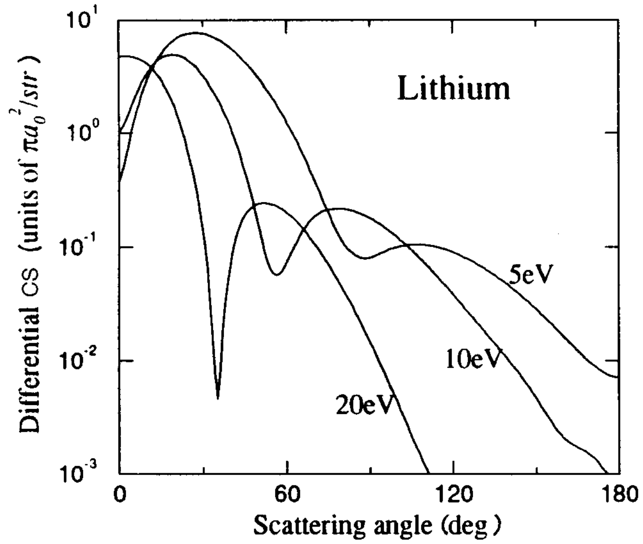

FIG. 5. Computed angular distributions for the Ps(1*s*)-formation channel in the case of Li atoms. The calculations refer to three different collision energies. (CS denotes cross section.)

from each other: the two CC results are markedly different in magnitude and the present model appears to follow the predictions of the results from Ref. [10]. It should be kept in mind, however, that the present use of a model optical potential and the physical assumptions outlined in the previous sections appear to handle very well the size and energy dependence of the reactive process we are describing here and afford a tremendous reduction of the required computational times, especially when compared with the earlier CC calculations.

If we now move to an even more complicated system, the potassium target, we see in Fig. 4 that the general behavior indicated by the previous results is indeed confirmed. From about 5 eV of collision energy and up to 20 eV our model calculations follow remarkably closely the energy behavior of the same cross sections produced in the CC calculations given by the dashed [16] and the dotted [17] lines. Below that energy the CC results agree with each other only in part and differ markedly below 4 eV. As in the previous Na case, our calculations appear to favor the results from McAlinden, Kernoghan, and Walters [17]. Considering the good agreement of its outcomes with those from the more complicated CC computations, it seems possible to say that the present optical potential is including all the relevant physical ingredients and that both the dispersion relation and the global damping functions do a very good job in describing the correct final states of the scattering process.

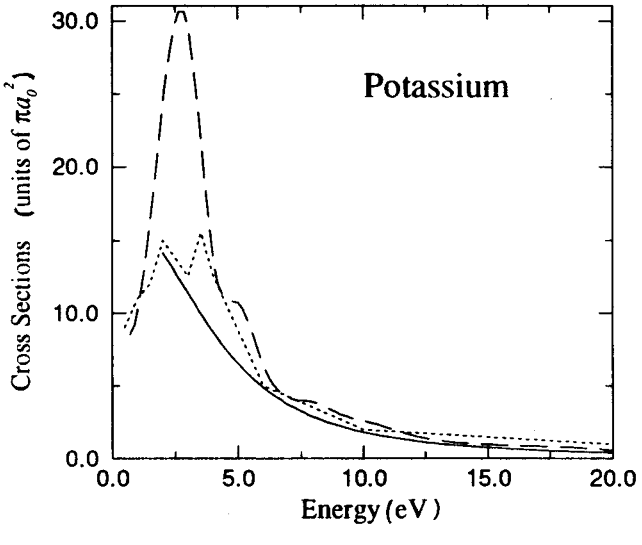

FIG. 4. Same as in Fig. 2 but for the case of the K atom as target. Solid line: present calculations. Dashed line: from Ref. [16]. Dotted line, from Ref. [17].

As a further application of our calculated $T$ matrix elements, we see that Eq. (24) allows us to produce easily the corresponding angular distributions at any of the required collision energies. Although such quantities are still not available from experiments, one could envisage a time when even the angular distributions for partial channels of positron scattering will become accessible. This is especially true when the rapid, recent increase of the availability of intense positron sources is considered [26–28]. Within this context it therefore will become useful to have available the general behavior of angular distributions for several systems and at several collision energies.

Figures 5, 6, and 7 therefore report our calculations for Li, Na, and K targets and for three of the collision energies in the range where our model was the most successful in reproducing the CC results. The three systems behave, as expected, rather differently from each other although all of them show rather marked forward scattering, especially at the higher collision energies. Furthermore, the Li and K targets indicate the presence of very marked oscillations and large dips in the cross sections as the scattering angle increases, while the Na target exhibits smoother differential cross sections (DCS's) and much less marked oscillations. In sum, however, one sees from our DCS calculations that the intensity of the scattered Ps is strongest within a rather narrow cone in the forward direction and that cone gets narrower with increasing energy of the projectile.

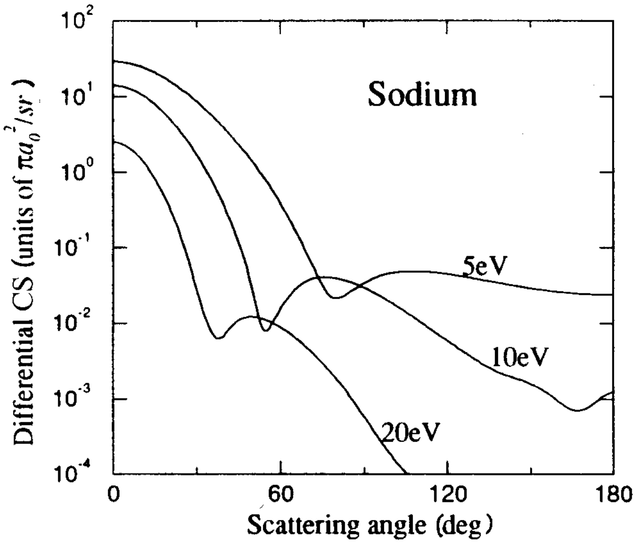

FIG. 6. Same as in Fig. 5 but for the case of the Na atom (CS denotes cross section).

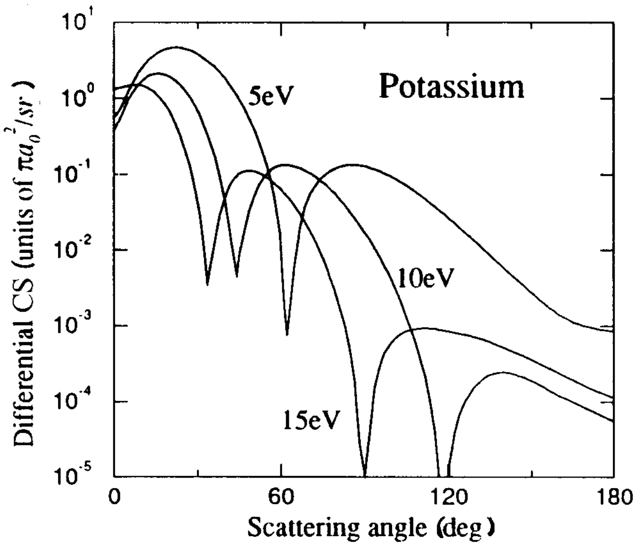

FIG. 7. Same as in Fig. 5 but for the case of the potassium atom (CS denotes cross section).

## VII. CONCLUSIONS

We have discussed in the previous sections the formulation of a model treatment of the Ps-formation channel in positron-atom scattering and found that the use of an optical potential based on this model allows us to obtain the relevant scattering attributes of the process rather directly and by performing fairly straightforward numerical quadratures. In comparison with the more conventional, and computationally more demanding, close-coupled expansion over a large number of states, the present method turns out to produce rather good results and to follow closely the CC outcomes even for very complicated atomic targets.

One could therefore conclude from this analysis, and from what we have found with the much more popular H and He targets [18], that the present model can constitute an easy and simple starting point for extending the predictive value of calculations in the search for the most efficient targets for Ps formation at low collision energies. Furthermore, since we have also shown that angular distributions could also be obtained rather directly with the present method, we can expect that such calculations for a broad variety of atomic targets would provide indications and suggestions for the new generation of experiments which are currently in preparation.

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