A Calculation of $e^+$ - He Collisions Using the Schwinger Variational Principle with Plane Waves as a Trial Basis Set

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We report on an application of the Schwinger variational principle with plane waves as a trial basis set. Differential cross sections are obtained for $e^+$ - He collisions from 100 to 300 eV at the static plus polarization interaction level. Our differential cross sections are found to be in reasonable agreement with existing theoretical methods and experimental data.

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I. INTRODUCTION

Investigations of the scattering of positrons by atomic (molecular) gases have gained significant importance because positrons, being a positively charged probe, offer a more sensitive test of our ability to understand atomic interactions than electrons do [1]. An additional importance of positron scattering derives from the fact that it involves interactions of matter with antimatter, which have possible applications in the astrophysical area [2]. Some investigations are in part motivated by the possible analytical applications of positrons, which include surface analysis [3] and medical tomography [4]. The fundamental motivation for studying positron scattering from targets is to compare the scattering cross sections to those of the corresponding electron scattering process. The reason is that positrons can annihilate with an electron of the target during the process. The Coulombic attraction between positrons and electrons makes an enormous difference from the always repulsive interaction between electrons. Most of the calculations used are for elastic processes and are made with model polarization potentials (e.g., Jain and Gianturco [5], Gibson [6] and Gianturco et al. [7]). In these cases the polarization interaction has a significant effect on the overall shape and magnitude of the scattering cross section as well as on the width and position of resonances. The major difference between electron and positron scattering is that in the later case there is the possibility of positronium (Ps) formation. Substantial progress has been made for some systems using model potentials with the need for parameters which are usually obtained by “tuning”, so as to reproduce known features in the cross sections. A suitable method should be capable of dealing with several important aspects of the problem such as polarization effects, resonances, electronically inelastic scattering [8–10] with several open and closed channels, and, of considerable importance,
nonlinear targets. A series of experiments involving positron impacts with atomic or molecular targets has been done recently (see, Refs. [11, 12]), so that theoretical calculations are extremely important for an adequate comparison. In particular for the system analysed here, e\(^+\) - He scattering, some methods, such as the second Born approximation [13], close coupling approximation [13], the distributed positron model [6], and the Schwinger multichannel (SMC) method [14], have been used to calculate elastic cross sections (accurate elastic differential cross sections still remain an important and challenging endeavor). An adequate model for positron-target scattering consists of the static field, correlation, polarization, and an absorptive imaginary potential (which describes the loss of flux due to the coupling with inelastic channels). In this paper, we apply the Schwinger variational principle using plane waves as a trial basis set (SVP-PW) [15] to study high-energy positron-He scattering, and do not incorporate correlation effects and positronium formation. The polarization potential can here be approximated by means of the Buckingham potential with a phenomenological cutoff parameter [16]. To our knowledge this level of study is the first for positron-He scattering using the SVP-PW, and represents a natural step towards a more complex situation involving multichannel effects. Results at this level are extremely important in the development of new methodologies. The present study has several objectives. First: to test the relevance of the polarization effects used in our formalism. Second: the original Schwinger multichannel (SMC) method was introduced some time ago to study scattering problems at low energies of electron incidence, and later Germano and Lima [17] adapted the SMC for positron scattering (the main limitation of the SMC method resides in what makes it a general method: the expansion of the scattering function is done in a \(L^2\) basis only and this is adequate only for short-range potentials). Our implementation of plane waves as a trial basis set can be desirable to adequately represent, for example, the long range regions. Third: our results can motivate experimenters to look at these cross sections at high energies. Summarizing, our SVP-PW for positrons used the static plus polarization potential, and we have performed a comparison of e\(^+\) - He elastic differential cross sections with the optical model used by Byron and Joachain [20], the theoretical results of Reid and Wadehra [19] using correlation-polarization plus absorption effects, and the experimental data of Smith [22].

II. FORMULATION

The Hamiltonian for the \((N + 1)\)-positron collision system can be written as

\[
H = (H_N + T_{N+1}) + V = H_0 + V ,
\]

where \(H_N\) is the target Hamiltonian, \(T_{N+1}\) is the kinetic energy operator for the incident positron, and \(V\) is the interaction between the scattering positron and the nuclei and electrons of the target. The complete scattering wave function can be shown to satisfy a modified Lippmann-Schwinger equation [18],

\[
A^{(+)} \Psi^{(+)}_{k_f} = V S_{k_f} ,
\]
where
\[ A^{(+)} = V - VG_p^{(+)}V, \] (3)

\( S_{k_f} \) are solutions of the unperturbed Hamiltonian \( H_0 \), and \( G_p^{(+)} \) is the projected outgoing-wave Greens function \([15]\).

Based on the inhomogeneous Eq. (2), the bilinear variational form of the scattering is given by
\[
[f(k_f, k_i)] = -\frac{1}{2\pi} \left\{ <S_{k_f} | V | \Psi_{k_i}^{(+)}> + <\Psi_{k_f}^{(-)} | V | S_{k_i}> \\
- <\Psi_{k_f}^{(-)} | V - VG_0^{(+)}V | \Psi_{k_i}^{(+)}> \right\}. \] (4)

The scattering states \( |\Psi_{k_i}^{(+)}> \) and \( <\Psi_{k_f}^{(-)}> \) are products of the target wave function \( |\Phi_0> \) and the one-particle scattering wave function. The initial step in our SVP-PW calculations is to expand the one-particle scattering wave functions as a combination of plane waves. So, for elastic scattering, the expansion of the scattering wave function is done in a discrete form as
\[
|\Psi_{k_i}^{(+)}> = \sum_m a_m(k_m) |\Phi_0 k_m>, \] (5)
\[
<\Psi_{k_f}^{(-)}> = \sum_n b_n(k_n) |\Phi_0 k_n>. \] (6)

Inclusion of these definitions in Eq. (4) and an application of a stationarity condition \([15]\) with respect to the coefficients gives the working form of the scattering amplitude,
\[
[f(k_f, k_i)] = -\frac{1}{2\pi} \left( \sum_{mn} <S_{k_f} | V | \Phi_0 k_m> (d^{-1})_{mn} <k_n | V | S_{k_i}> \right), \] (7)

where
\[
d_{mn} = <\Phi_0 k_m | V - VG_p^{(+)}V | \Phi_0 k_n>. \] (8)

We have implemented a set of computational codes to evaluate all matrix elements of Eq. (7). The \( G_p^{(+)} \) is the projected outgoing-wave Green’s function and \( P \) is the target-space unit operator,
\[
P = \sum_\ell |\Phi_\ell>c<\Phi_\ell| = 1, \] (9)

where \( P \) is truncated and carries only energetically open bound state channels. The calculation of the VGV term presents the more expensive step in the SVP-PW code and demands almost the entire computational time of the scattering calculation. With the help of the linear momentum representation of the one-particle unit operator, the matrix element
\[
<\Phi_0 k_m | VG_p^{(+)}V | \Phi_0 k_n> \] (10)
used in Eq. (8) is done by direct numerical quadrature and can be rewritten as

\[ \sum_{\ell}^{\text{open}} \int_0^\infty dk \frac{2k^2}{k^2_\ell - k^2} g_{k_m,k_n}(k), \]  

(11)

where

\[ g_{k_m,k_n}(k) = \int d\Omega_k < \Phi_0 k_m | V | \Phi_0 k > < k \Phi_0 | V | \Phi_0 k_n >, \]  

(12)

and the function \( g_{k_m,k_n}(k) \) is essentially an angular integration of first Born terms with different magnitude of \( k \)'s (off-shell terms). The difficulty in evaluating Eq. (10) associated with possible discontinuities has been examined and treated in a similar way as in the subtraction method. We just add and subtract the expression \( \frac{2k^2}{k^2_\ell - k^2} g_{k_m,k_n}(k) \) to Eq. (11), where the subtracted term makes the integration smoother (since the numerator and the denominator of the composed expression will vanish simultaneously for \( k \)'s around \( k_\ell \)) and the added term is evaluated analytically. In our implementation we use two different quadratures for \( k_m \) and \( k_n \) to avoid situations where \( |k_m - k_n| \) is too small. For example, to obtain differential cross section we just evaluate the square modulus of this amplitude, summing over all \( k_m \) directions and averaging over the \( k_n \)'s. Our discrete representation of the scattering wave function given by Eqs. (5) and (6) is made only in two dimensional space (spherical coordinates, using Gaussian quadratures for \( \theta \) and \( \phi \) and the on-shell \( k \) value for the radial coordinate). The present formulation allows us to calculate an analytical approximation to the body-frame fixed nuclei scattering amplitude for molecules of arbitrary geometry. We then expand \( f(k_m, k_n) \) in a partial-wave series and make the requisite transformation into the laboratory frame. After accounting for the random orientation of the target, the differential cross section is obtained in the usual manner by performing the appropriate average over initial spin states and sum over final spin states. The calculation is carried out via a Gauss-Legendre quadrature. As known, in positron-atom (molecule) scattering polarization effects and positronium formation play very important roles. The positron-target scattering can be classified first for the long range polarization potential, i.e, the positron creates a temporary dipole on the target by attracting the electronic atomic (or molecular) cloud towards itself (this is the known, always attractive, \( 1/r^4 \) potential). Second, for the short range polarization the positron reaches the inner region of the electronic charge, loses its energy by causing virtual or real electronic excitation of the target (it may also participate in the formation of a temporary composite system \( e^+ \cdot \text{target} \)). In our study we have used the traditional model of the Buckingham potential \[16],

\[ V_{\text{pol}}(r) = -\alpha/\left[(r^2 + r_c^2)^2\right], \]  

(13)

where \( \alpha \) is the dipole polarizability of the atom and \( "r_c" \) represent an phenomenological cutoff parameter, which serves to prevent the polarization potential from diverging at \( r = 0 \). Following Salvat \[16], we write

\[ r_c^4 = (1/2) \alpha a_0 Z^{-1/3} b_{\text{pol}}^2 \]  

(14)
and consider $b_{\text{pol}}$ as an adjustable energy-dependent parameter. It is found that the magnitude of the polarization effects decreases when the energy of the incident positron increases (i.e., $b_{\text{pol}}$ increases with $E$), reflecting the fact that atomic electrons do not react instantaneously to external electric fields. Some studies by Salvat suggested the following empirical formula [16]:

$$b_{\text{pol}}^2 = \frac{(E - 50 \text{ eV})}{(16 \text{ eV})}. \quad (15)$$

In our calculations the Born scattering used is now formed as

$$f_{\text{Born-Closure}} = f_{\text{static}} + f_{\text{Born-pol}}, \quad (16)$$

where the polarization part of the scattering amplitude is calculated as follows:

$$f_{\text{Born-pol}} = -2/q^2 \int e^{iq \cdot r} V_{\text{pol}}(r) dr, \quad (17)$$

where $q$ is the elastic momentum transfer vector [20].

**III. RESULTS**

In this section we test the SVP-PW by applying it to elastic positron scattering by He. We present also other theoretical results as proposed by Reid and Wadehra [19], using

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**FIG. 1:** Elastic DCS for $e^+$ - He scattering at 100 eV. Present results SVP-PW: solid line; present results SVP-PW(S) level static only: dotted line; optical model of Ref. [18]: dashed line.
FIG. 2: Elastic DCS for $e^+$ - He scattering at 200 eV. Present results SVP-PW: solid line; optical model of Ref. [18]: dashed line; theoretical studies of Reid and Wadehra [17]: dotted line; experimental data: star.

FIG. 3: Elastic DCS for $e^+$ - He scattering at 300 eV. Present results SVP-PW: solid line; optical model of Ref. [18]: dashed line.
absorption effects and the optical model [20]. For the ground state of He we have used a self-consistent-field (SCF) wave function obtained with a Cartesian basis [21]. With this basis we obtain a SCF energy of $-2.8616$ a.u., to be compared with $-2.8615$ a.u. [21]. Fig. 1 shows the differential cross sections (DCS) for the scattering of positron-He at 100 eV using the SVP-PW, and the optical model used by Byron and Joachain [20]. A comparison of the two formalism shows that the SVP-PW has substantial agreement with the optical model when the polarization effect is included, which demonstrates that the purely static SVP-PW (SVP-PW(S)) is insufficient at small angle scattering (see Fig. 1). Fig. 2 shows the differential cross sections (DCS) for the scattering of positron-He at 200 eV using the SVP-PW, the optical model used by Byron and Joachain [20], theoretical results of Reid and Wadehra [19], and the experimental data of Smith [22]. As noted, our SVP-PW has a good agreement with the optical model [20], the studies of Reid and Wadehra [19], and the relative experimental data of Smith [22]. Although our SVP-PW does not include absorption effects (and positronium formation) the present results show significant improvement. Fig. 3 shows the differential cross sections (DCS) for the scattering of positron-He at 300 eV using the SVP-PW and the optical model used by Byron and Joachain [20]. Again, the agreement between our results and the optical model [20] is encouraging.

IV. CONCLUSIONS

In this paper we have reported the first application of the Schwinger variational principle using plane waves as a trial basis set to positron impact collisions with an atom. Differential cross sections at the static plus polarization level of approximation have been obtained for $e^+ - \text{He}$ collisions from 100 to 300 eV. A very interesting feature of the small-angle differential cross sections is ascribed to polarizations effects. The present study helps to demonstrate the utility of this approach; a more complete study including correlation (and absorption) effects is underway.

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