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Elastic Scattering of a Positron on Ne Atoms at Intermediate Energies

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We report on an application of the Schwinger multichannel method with plane waves as a trial basis set [Phys. Scr. **76**, 521 (2007)] to intermediate and high energy positron collisions with a Ne atom. Differential cross sections (DCSs) are obtained from 50 to 500 eV. In this study we focus our method for investigation by means of the Buckingham model on positron-Ne scattering, with polarization effects only. Our DCSs are found to be in reasonable agreement with existing theoretical studies.

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I. INTRODUCTION

Investigations of the scattering of positrons by atomic and molecular gases have gained significant importance because the positron, being a positively-charged probe, offers a more sensitive test of our ability to understand atomic interactions than the electron does. With the appearance of reliable magnetic traps, studies on matter-antimatter have gained attention in the last few years [1]. Positron interactions with atoms can cause a variety of intriguing phenomena different from those of the electron case. 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. The polarization potentials are always attractive, drawing positrons and electrons together. A description of the polarization interaction is very sensible because the static potential has the opposite sign to that of the polarization potential. Therefore the positron-atom problem is indeed more difficult to solve than the electron case, making the theoretical task of describing the phenomena very challenging (this is especially true when one is dealing with more complicated molecules, made up of several different atoms and a large number of bound electrons, which tremendously increase, with their higher density of internal states, the complexity of treating as correctly as possible the dynamical couplings between the impinging positron and the bound electronuclear molecular network) [2]. In this study we present a development of the wave function description of the Schwinger multichannel (SMC) method for the positron-molecule scattering proposed by Germano and Lima [3]. In particular, the main limitation of the SMC method resides in what makes it a general method: the expansion of the scattering functions is very effective only for short range potentials. An important development of the method would be to allow

the inclusion of plane waves (PW) in the scattering basis set [4], and this is the motivation of the present paper. We will describe some developments of the SMC method which we believe can provide a practical approach to addressing such problems in positron-target collisions.

The SMC method for positrons has been used to study the elastic cross sections of H_2 [3, 5, 6], CH_4 [3], C_2H_4 [7], and the inelastic cross sections of H_2 [8]. Here the plane waves as a trial basis set is used for the SMC, and in order to do this we developed reliable computer codes (numerically stable) to evaluate the second Born approximation (SBA) without restriction on the molecular geometries [4]. At intermediate and high energies ($E_0 \geq 10$ eV), almost all inelastic channels (positronium formation, dissociation, rotational, excitation, ionization, etc.) are open, which makes an *ab initio* calculation almost impossible. It is thus quite obvious that most of the exact calculations carried out on the positron atom (or molecule) systems have been restricted to low energies (below 10 eV). Therefore, a simpler approximation approach for positron-atom scattering systems at the intermediate-and high-energy region is very necessary. Most of the calculations used are for elastic processes and are made with model polarization potentials (e.g., Byron and Joachain [9] and Salvat [10]). The study presented here using the SMC-PW examines the elastic cross sections for e^+-Ne. For positron scattering the real part of the interaction is presented as into the static, correlation-polarization and also the imaginary (or absorption) which takes into account various inelastic processes. In our work we focus on the SMC-PW for studying the elastic scattering of positron-Ne with polarization effects only (the full treatment of the e^+-Ne problem requires the inclusion of various other effects; we will assume the polarization effect only. This study establishes benchmark calculations for the static plus polarization effects, which is indispensable in the development of a more complete SMC-PW formalism using the system e^+-Ne). The present investigation can adequately study the relevance of the polarization effects using a Buckingham potential with an empirical energy dependent cutoff parameter [10].

An outline of the paper is as follows. In the next section we briefly discuss our SMC-PW for positron scattering by Ne. In Sect. 3 we will show our procedure and calculations, and in Sect. 4 we summarize our conclusions.

II. THE SCHWINGER MULTICHANNEL METHOD: FORMALISM

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

$$H = (H_N + T_{N+1}) + V = Ho + V, \tag{1}$$

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

$$A^{(+)}\Psi^{(+)}_{\vec{k}_f} = VS_{\vec{k}_f}, \tag{2}$$

where

$$A^{(+)} = V - VG_p^{(+)}V \tag{3}$$

and $S_{\vec{k}_f}$ are solutions of the unperturbed Hamiltonian Ho, and $G_p^{(+)}$ is the projected outgoing-wave Green's function [11].

Based on the inhomogeneous Eq. (2), the bilinear variational form of the scattering is given by

$$[f(\vec{k}_f,\vec{k}_i)] = -\frac{1}{2\pi}\{< S_{\vec{k}_f}|V|\Psi^{(+)}_{\vec{k}_i} > + < \Psi^{(-)}_{\vec{k}_f}|V|S_{\vec{k}_i} > - < \Psi^{(-)}_{\vec{k}_f}|V - VG_0^{(+)}V|\Psi^{(+)}_{\vec{k}_i} >\}. \tag{4}$$

The scattering states $|\Psi^{(+)}_{\vec{k}_i} >$ and $< \Psi^{(-)}_{\vec{k}_f}|$ are products of the target wave function $|\Phi_o >$ and the one-particle scattering wave function. The initial step in our SMC-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 [11]

$$|\Psi^{(+)}_{\vec{k}_i} > = \sum_m a_m(\vec{k}_m)|\Phi_0\vec{k}_m >, \tag{5}$$

$$|\Psi^{(-)}_{\vec{k}_f} > = \sum_n b_n(\vec{k}_n)|\Phi_0\vec{k}_n > . \tag{6}$$

Inclusion of these definitions in Eq. (4), and the application of a stationarity condition [11] with respect to the coefficients, gives the working form of the scattering amplitude:

$$[f(\vec{k}_f,\vec{k}_i)] = -\frac{1}{2\pi}(\sum_{mn} < S_{\vec{k}_f}|V|\Phi_0\vec{k}_m > (d^{-1})_{mn} < \vec{k}_n\Phi_0|V|S_{\vec{k}_i} >), \tag{7}$$

where

$$d_{mn} = < \Phi_0\vec{k}_m|V - VG_p^{(+)}V|\Phi_0\vec{k}_n > . \tag{8}$$

We have implemented a set of computational programs to evaluate all matrix elements of Eq. (7). The numerical calculation of the matrix elements from $VG_p^{(+)}V$ represents the more expensive step in the SMC-PW code and demands almost the entire computational time of the scattering calculation. The Green's function given in Eq. (8) and its associated discontinuities have been examined and treated in a similar way as in the subtraction method [12]. 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 θ and ϕ.

III. POLARIZATION POTENTIAL

Slow positrons cause the polarization of the charge cloud of the atom and, in turn, the induced dipole moment acts back on the projectile. Considerable effort has therefore been expended in the past three decades to try to include correlations and the distortion of the target as accurately as possible. In order to devise simpler ways of handling the polarization forces, various approaches have been tried in recent years, as discussed in Ref. [10]. When the positron is far from the atom, the polarization potential energy can be approximated by means of the Buckingham potential [10],

$$V_{pol}(\vec{r}) = -\alpha/[(r^2 + r_c^2)]^2, \tag{9}$$

where α is the dipole polarizability of the atom and "r_c" represent a phenomenological cutoff parameter, which serves to prevent the polarization potential from diverging at $r = 0$. Following Salvat [10], we write

$$r_c^4 = (1/2)\alpha a_o Z^{-1/3} b_{pol}^2 \tag{10}$$

and consider b_{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_{pol}), reflecting the fact that atomic electrons do not react instantaneously to external electric fields. Some studies shown by Salvat [10] and also by Lino [13] suggested a empirical formula as a test:

$$b_{pol}^2 = (E - 50\ eV)/(16\ eV). \tag{11}$$

In our calculations the Born scattering amplitude used is now formed as

$$f^{Born-Closure} = f^{static} + f^{Born-pol}, \tag{12}$$

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

$$f^{Born-pol} = (-2/q^2) \int e^{i\vec{q}.\vec{r}} V_{pol}(\vec{r}) d\vec{r}, \tag{13}$$

where $\vec{q}$ is the elastic momentum transfer vector. By combining Equations (8), (13), and (14) we obtain the differential cross sections for e^+-Ne scattering (without correlation and absorption).

IV. RESULTS

In this section we test the SMC-PW by applying it to the elastic positron scattering by Ne. For the ground state of Ne we have used a self-consistent-field (SCF) wave function obtained with the Cartesian basis. With this basis we obtain a SCF energy of -128 a.u., to be compared with the -128 a.u. of Ref. [9]. As we know, the polarization and absorption

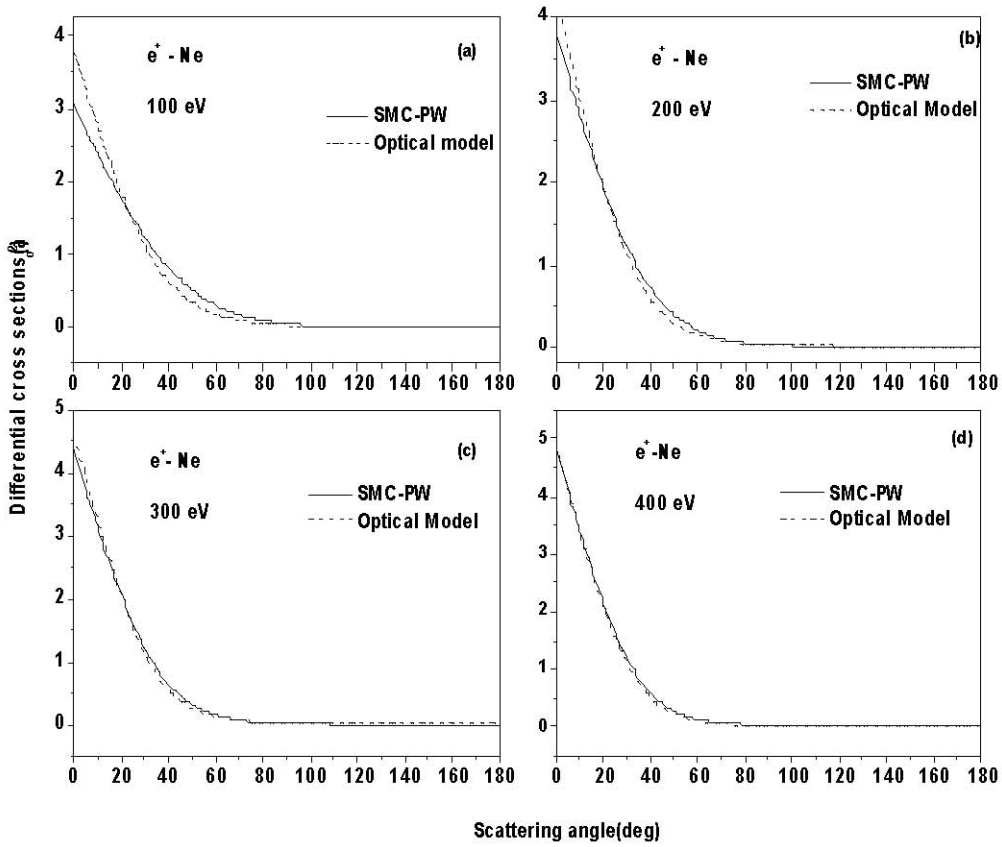

FIG. 1: Differential cross sections for e^+ - Ne scattering at 100 eV (a), 200 eV (b), 300 eV (c), and 400 eV (d). Our SMC-PW : solid line ; Optical model: dashed dot line.

potential demonstrate a strong effect on cross sections. In order to observe the effect of including absorption and correlation-polarization in the calculations, we show in Figure 1(a-d) differential cross sections (DCSs) for the scattering of positron-Ne at 100, 200, 300, and 400 eV, and these results are compared with theoretical studies [9]. In Figure 1(a), at 100 eV, a comparison with the theoretical results of Ref. [9] reveals a poor agreement at small angles and a good agreement at large angles. In Figure 1(b), at 200 eV, our results agrees well in shape and magnitude with Ref. [9], and, as noted, the discrepancies at small angles now is not extreme. In Figure 1(c) at 300 eV and 1(d) at 400 eV the results compared with Ref. [9] are encouraging. These results suggests that correlation and absorption have small influence on the differential cross sections.

V. CONCLUSIONS

We have carried out calculations of the elastic cross sections of e^+-Ne using the Schwinger multichannel method with plane waves as a trial basis set. Differential cross sections were obtained and were compared with theoretical studies. The present results suggests that our formalism can be effective in the study of collisions of intermediate-energy.

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