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ELASTIC CROSS SECTIONS FOR e^+ - He SCATTERING

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ABSTRACT

We report an application of the Schwinger variational principle with plane waves as a trial basis set. Differential cross sections are found for positron-He collisions from 100 to 300 eV. Differential cross sections are found to be in reasonable agreement with theoretical methods and experimental data.

1. INTRODUCTION

The process of scattering of low, intermediate and high-energy positrons by atoms (and molecules) plays an important role in the description of cold plasmas and astrophysical area, and are currently used in technological applications [1,2]. It follows that the knowledge of elastic and inelastic cross sections for a wide range of atomic and molecular systems is a very important subject. For cross sections some *ab initio* calculations have been developed as the Schwinger multichannel method (SMC) [3], the Kohn variational method [3] and R-Matrix [3] for positron scattering. Positron interactions with atoms or molecules can cause a variety of intriguing phenomena different from electrons 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. Most of calculations used are for elastic cross sections and are made with model polarizations potentials (e.g., Jain [4], Gibson [5] and Gianturco [6]). 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 the resonances. Although substantial progress has been made for some systems, the further drawback in model potentials is the need for parameters which are usually obtained by "tuning" so as to reproduce known features in the cross sections. A series of experiments involving positron impact with target atomic or molecular has been done recently so that the theoretical calculations are extremely important for an adequate comparison. In the present paper, we apply the Schwinger variational principle using plane waves as a trial basis set (SVP-PW) for the study of positron-He scattering. Our SVP-PW, for instance, does not incorporate positronium formation and the polarization potential can be here approximated by meams of the Buckingham model with a phenomenological cutoff parameter [7]. The present study has several objectives. First, test the relevance of the polarization effects used in our formalism; second, the original Schwinger multichannel method (SMC) [8] was introduced before to study scattering problems at low energies of incident electron and Germano and Lima [8] adapted the SMC for positron scattering [8]. The main limitation of the SMC method resides on 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 potential. 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 experimentalists to look these cross sections at higher energies.

An outline of this paper is as follows. The next section we briefly discuss our SVP-PW for positron scattering by He. In Sect. 3 we will show our results and conclusions.

2. FORMALISM

Details of the Schwinger variational principle have been discussed extensively elsewhere [9,10]. Here we will review a few steps in the development, which are essential to the present discussion. In the SVP for positron-target elastic scattering, the bilinear form of the scattering is

$$f(\mathbf{k}_f, \mathbf{k}_i) = -(1/2\pi)\{< S_{\mathbf{kf}} \mid V \mid \Psi^{(+)} > + <\Psi^{(-)} \mid V \mid S_{\mathbf{kf}}> - <\Psi^{(-)} \mid V - VG_oV \mid \Psi^{(+)} >\} \quad (1)$$

Here $|S_{\mathbf{ki}}>$ is the input channel state represented by the product of a plane wave k_i time, the initial (ground) target state. $|S_{\mathbf{kf}}>$ has analogous definition. The inclusion of plane waves in Eq. (1), gives the working form of the scattering amplitude [9,10]:

$$f(\mathbf{k}_f, \mathbf{k}_i) = -(1/2\pi)\{< S_{\mathbf{kf}} \mid V \mid \Phi k_m > \text{x} \; (d^{-1})_{mn} < k_n\Phi) \mid V \mid S_{\mathbf{ki}}>$$

where

$$d_{mn} = < k_n\Phi \mid V - VGV \mid \Phi k_m > \quad (2)$$

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We have implemented a set of computational programs to evaluate all matrix elements of Eq. (1). The numerical calculation of the matrix elements from VGV represents the more expensive step in the SVP-PW code and demand almost the entire computational time of the scattering calculation. When the positrons so far from the atom, the polarization energy can be approximated by Buckingham potential [11],

$$V_{pol} = - \alpha / [r^2 + r_c^2] \quad (3)$$

where "α" is the dipole polarizability of the atom and " r_c '' represents an phenomenological cutoff parameter, which serves to prevent the polarization from diverging at r = 0. Following Salvat [11], we write

$$r_c^4 = (1/2)\, \alpha\, Z^{-1/3}\, b_{pol}^2 \quad (4)$$

and consider b_{pol} as a adjustable energy-dependence parameter. It is found that the magnitude of the polarization effects decreases when the energy of the incident positron increases. Some studies showed by Salvat suggested the following empirical formula [11],

$$b_{pol}^2 = (E – 50\ eV) / (16\ eV) \quad (5)$$

3. RESULTS

In this section we test the SVP-PW by applying it to the elastic positron scattering by He. We present also other theoretical results as proposed by Reid and Wadehra [12] (using also absorption and polarization effects). Figure 1 shows the differential cross sections (DCS) for the scattering of positron-He at 100 eV using the SVP-PW (for comparison only we have used the Schwinger principle without polarization, SVP-PW(S), and optical model used by Byron and Joachain [13]. A comparison of the two formalism shows that the SVP-PW has a substantial agreement with the optical model when the polarization effect is included. Figure 2 shows the differential cross sections for the scattering of positron-He at 200 eV using the SVP-PW, optical model [13], theoretical results of Reid and Wadehra [12] and experimental data of Smith [14]. As noted our SVP-PW shows a good agreement with the optical model and relative experimental data of Smith [14]. Although our SVP-PW no includes absorption effect (and positronium formation) the presented results show significant improvement.

4. CONCLUSION

We have carried out calculations of the elastic cross sections of positron-He using the Schwinger variational principle with plane waves as a trial basis set. Differential cross sections were obtained and were compared with the optical model. Good agreement was found and the presented results suggest that our formalism can be effective in the study of collisions of positron-He.

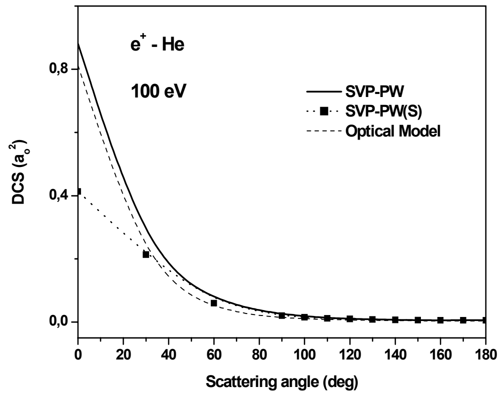

Figure 1 - Elastic DCS for e^+ - He at 100 eV. Solid line, SVP-PW. Dashed line with square, SVP-PW(S). Dott line, Optical model [13].

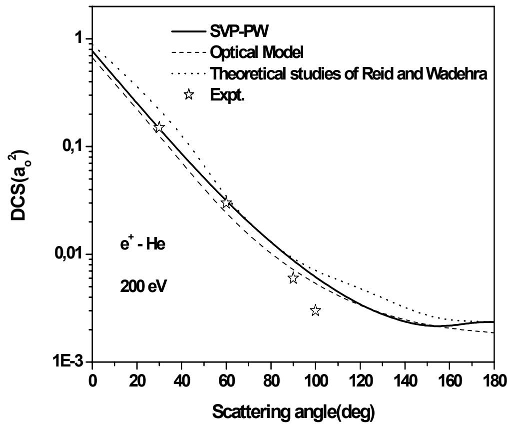

Figure 2 - Elastic DCS for e^+ - He at 200 eV. Solid line, SVP-PW. Dashed line, theoretical results [13]. Star, experimental data [14].

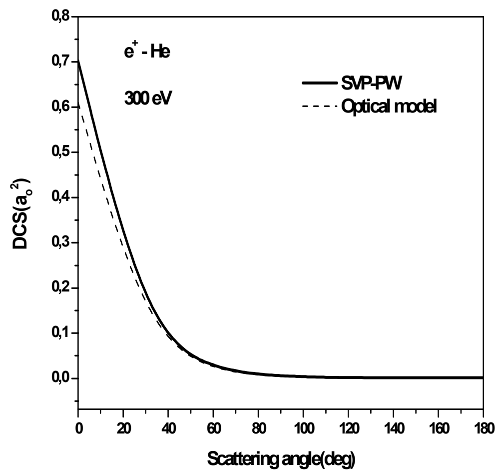

Figure 3 - Elastic DCS for e^+ - He at 300 eV. Solid line, SVP-PW. Dashed line with square, Optical model [13].

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