Theoretical study of e^- - He scattering using the Schwinger variational principle with plane waves as a trial basis set

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We report an application of the Schwinger variational principle with plane waves as a trial basis set. Differential cross sections are obtained for e$^-$ - He from 15 to 100 eV. Our differential cross is found to be in reasonable agreement with experimental data.

Keywords: Schwinger; electron.

Se analiza una aplicación del principio variacional de Schwinger desde la perspectiva de ondas planas para un cunjunto base. El proposito de este trabajo es mostrar la sección eficaz deferencial para e$^-$ - He en el intervalo de 15 to 100 eV. Los resultados se comparam com los experimentos.

Descriptores: Schwinger; electrón.

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1. Introduction

In the last few years, there have been several theoretical activities concerning the electron-atom at low, intermediate and high impact energies [1–3]. As we know, with the increase of the kinetic energy, the penetration power of the incident electron into the atom will too increase. Therefore, the convergence of the partial-wave expansion for continuum scattering wavefunction will become more difficult to achieve. Although several alternative theoretical approaches have been proposed for studying electron-atom scattering at several energies, available experimental data of differential cross sections (DCS) do not provide a definitive test capable of judging the efficiency of the theoretical methods for several targets. For example, obtaining an accurate differential cross sections for e$^-$ - He collisions still remains an important test for several new formalisms. As a step toward addressing this need, we have recently described the Schwinger variational principle with plane waves (SVP-PW) as a trial basis set [4–6]. The main propose of the present work is to study the elastic electron-He scattering at several energies using the SVP-PW, where the exchange effects are treated by a Born-Ochkur approximation [7–10] and polarization effects by Buckingham polarization potential [11] using a "r$_c$" cut-off parameter and polarizability α of the atom. The present study has several goals: first, to our knowledge, no theoretical study using the Schwinger variational principle with plane waves as a trial basis set has yet been published for e$^-$ - He over the present energy range; second, to test the relevance of Born-Ochkur plus Buckingham polarization potential combined with the SVP-PW; and third, the present work also serves in addition as a necessary prelude to new studies using the SVP-PW.

The organization of this paper is the following: in Sec. 2 the theory is briefly described. Our calculated results and discussions are presented in Sec. 3. Section 4 summarizes our conclusions.

2. The Schwinger variational principle

In the SVP for electron-molecule elastic scattering, the bilinear variational form of the scattering is

$$[f(\vec{k}_f,\vec{k}_i)] = -\frac{1}{2\pi}\{\langle S_{\vec{k}_f}|V|\Psi^{(+)}_{\vec{k}_i}\rangle + \langle\Psi^{(-)}_{\vec{k}_f}|V|S_{\vec{k}_i}\rangle - \langle\Psi^{(-)}_{\vec{k}_f} \mid V - VG_0^{(+)}V \mid \Psi^{(+)}_{\vec{k}_i}\rangle\} \quad (1)$$

Here $\mid S_{\vec{k}_i}\rangle$ is the input channel state represented by the product of a plane wave $\vec{k}_i$ times $\mid \Phi_0\rangle$, the initial (ground) target state. $\mid S_{\vec{k}_f}\rangle$ has an analogous definition, except that the plane wave points to $\vec{k}_f$, V is the interaction between the incident electron with the target, $G_0^{(+)}$ is the projected Green's function, written as in the Schwinger multichannel method (SMC) as

$$G_0^{(+)} = \int d^3k \frac{\mid \Phi_0\vec{k}\rangle\langle\vec{k}\Phi_0 \mid}{(E - H_0 + i\epsilon)} \quad (2)$$

H_0 is the Hamiltonian for the N electrons of the target, plus the kinectic energy of the incident electron, and E is the total energy of the system (target + electron). The scattering states $\mid \Psi^{(+)}_{\vec{k}_i}\rangle$ and $\langle\Psi^{(-)}_{\vec{k}_f} \mid$ are products of the target wave function $\mid \Phi_o\rangle$ and one-particle scattering wave function. The initial step in our SVP calculations is to expand the one-particle scattering wave function as a combination of plane waves. So, for elastic scattering, the expansion of the scattering wave function is done in a discrete form as

$$\mid \Psi^{(+)}_{\vec{k}_i}\rangle = \sum_m a_m(\vec{k}_m) \mid \Phi_0\vec{k}_m\rangle \quad (3)$$

$$\mid \Psi^{(-)}_{\vec{k}_f}\rangle = \sum_n b_n(\vec{k}_n) \mid \Phi_0\vec{k}_n\rangle \quad (4)$$

Inclusion of these definitions in Eq. (1), and application of a stationarity condition [4] with respect to the coefficients, gives the working form of the scattering amplitude

$$[f(\vec{k}_f,\vec{k}_i)]=-\frac{1}{2\pi}$$
$$\times\left(\sum_{mn}\langle S_{\vec{k}_f}|V|\Phi_0\vec{k}_m\rangle(d^{-1})_{mn}\langle\vec{k}_n\Phi_0|V|S_{\vec{k}_i}\rangle\right) \quad (5)$$

where

$$d_{mn} = \langle\Phi_0\vec{k}_m \mid V - VG_0^{(+)}V \mid \Phi_0\vec{k}_n\rangle \quad (6)$$

We have implemented a set of computational programs to evaluate all matrix elements of Eq. (5). The Green's function given in Eq. (2), and its associated discontinuities have been examined and treated in a similar way as in the subtraction method [4]. Our discrete representation of the scattering wave function [given by Eqs. (3) and (4)] is made only in two dimensional space (spherical coordinates, using Gaussian quadratures for θ and ϕ and the on-shell k value for the radial coordinate). When exchange effects are to be considered in electron scattering the first Born approximation used in the SVP-PW is replaced by

$$f^{Born-Ochkur} = f^{Born} + g \quad (7)$$

where "g" is the exchange amplitude in the Born-Ochkur approximation (we will refer to this formalism as SVP-PW(BO)). The long-range effects can also to be represented by a polarization potential

$$V_{pol}(\vec{r}) = -\alpha/[(r^2+r_c^2)]^2 \quad (8)$$

where "r_c" represents an adjustable cut-off parameter [11]. The Born scattering amplitude used is now formed by two parts, namely:

$$f^{Born-Closure} = f^{Born-Ochkur} + f^{Born-pol} \quad (9)$$

where $f^{Born-pol}$ is the polarization part of the scattering amplitude and, in the body frame, is calculated as follows:

$$f^{Bornpol} = -2/q^2\int e^{i\vec{q}.\vec{r}}V_{pol}(\vec{r})d\vec{r} \quad (10)$$

where $\vec{q}$ is the elastic momentum transfer vector. If the atomic wavefunction is expressed in a Cartesian Gaussian basis function, the $f^{Born-Closure}$ scattering amplitude can be obtained analytically and evaluated in closed form [12]. By combining Eqs. (9), (10), and (5) we obtain the differential cross sections for e^- - He scattering.

3. Results

We have calculated elastic differential cross sections at a number of energies for e^- - He. We present representative results, enphasizing cases where experimental data is available for comparison. Other theoretical cross sections using static-exchange plus polarization level of approximation are also compared. For the ground state of He we have used a self-consistend-field (SCF) wave function obtained with Cartesian basis [13]. With this basis we obtain a SCF energy of -2.8616 a.u. to be compared with -2.8615 a.u. [13]. In all figures we have used r_c= 1.460 as in Ref. [11]. In Figs. 1-5 we show differential cross sections at 15 eV, 20 eV, 30 eV, 50 eV, and 100 eV, respectively. We have compared our SVP-PW using Born-Ochkur plus polarization effects, with the Schwinger variational principle using Born-Ochkur only (we will refer to this second case as SVP-PW(BO)), the R-matrix method [14], the static-exchange simplified second Born approximation [15], and experimental data [16–20]. In Fig. 1 we show elastic differential cross sections (DCS) for e^- - He scattering at 15 eV. Our results using the SVP-PW are compared with experimental data of Shyn [19]. For comparison we have also included in Fig. 1 the SVP-PW without polarization (SVP-PW(BO)). As noted, our SVP-PW describes correctly the shape of the experimental data with some discrepancies at intermediate angle. Our polarization model is the so called Buckingham polarization potential and has been widely used in the dscription of elastic scattering of electron by atoms [1]. The discrepancy between our results and experimental data at intermediate angle can possibly be attributed to the inadequacy of the cut-off parameter (r_c) in the polarization potential. The DCS for electron-atom scattering at the low-energy ($\leq$ 40 eV) is very sensitive to this cut-off parameter [11] (the authors in Ref. 11 have tested the sensitivity of r_c for some energies. Their studies show that the best value of r_c was found at 1.460, and although not shown here, our results using different values of r_c were little affected at intermediate energies). Another important consideration may be the use of effects as multichannel and/or correlation of the target, which are not included in our calculations (for comparison we have included in Fig. 2 theoretical studies of Saha [2] using 35 states coupled and correlation of the target).

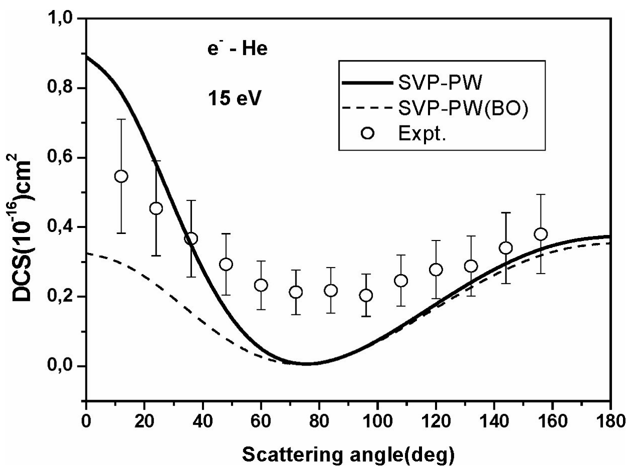

FIGURE 1. Elastic DCS for e^- - He scattering at 15 eV. Present results SVP-PW: solid line; dashed-line; SVP-PW(BO): Experimental results of Ref. 19: open circle..

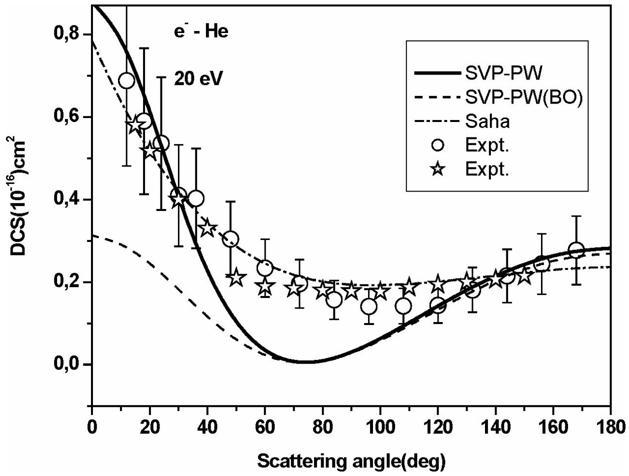

FIGURE 2. lastic DCS for e⁻ - He scattering at 20 eV. Present results SVP-PW: solid line; dashed-line; SVP-PW(BO): Experimental results of Ref. 19: open circle; theoretical results of Saha [2]: dashed dot; Experimental data of Register *et al.* 20; star.

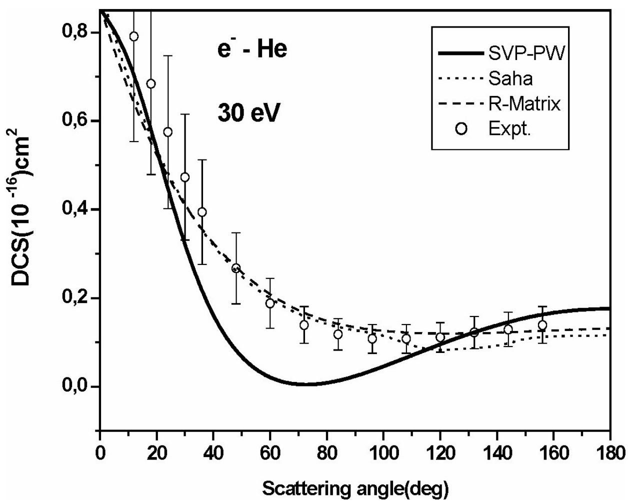

FIGURE 3. Elastic DCS for e⁻ - He scattering at 30 eV. Present results SVP-PW: solid line; Experimental results of Ref. 19: open circle; theoretical results of Saha [2]: dot line; R-matrix method [14]: dashed line.

In Fig. 2 we show elastic differential cross sections (DCS) for e⁻ - He scattering at 20 eV. Our results using the SVP-PW are compared with experimental data of Shyn [19], the experimental data of Register et al (we have not included the error bars of Register because these results are very close to those of Shyn) [20], and theoretical studies of Saha [2]. The theoretical results of Saha [2] include 35 states coupled, correlation, and a dynamical polarization of the target [2]. For comparison we have also included in Fig. 2 the SVP-PW without polarization (SVP-PW(BO)). As observed, our SVP-PW also describes correctly the shape of the experimental data with some discrepancies at intermediate angle(see text in Fig. 1).

In Fig. 3 we show elastic differential cross sections (DCS) for e⁻ - He scattering at 30 eV. Our results using the SVP-PW

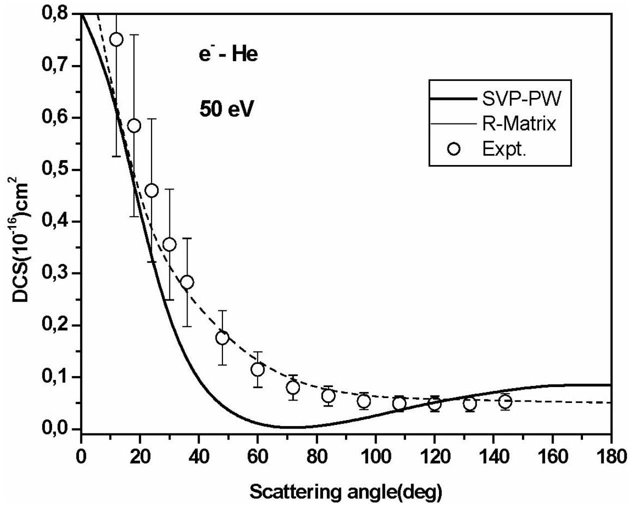

FIGURE 4. Elastic DCS for e⁻ - He scattering at 50 eV. Present results SVP-PW: solid line; Experimental results of Ref. 19: open circle; R-matrix method [14]: dashed line.

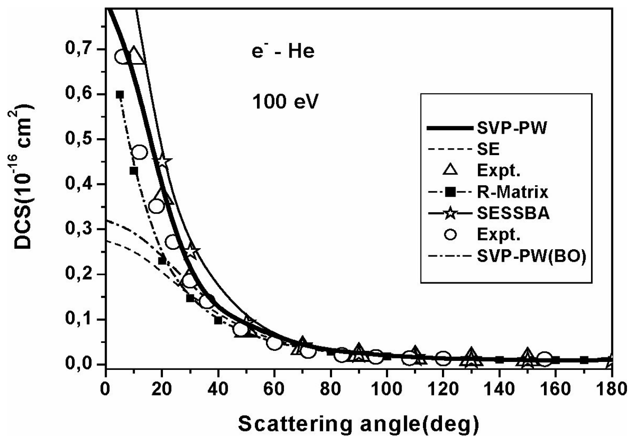

FIGURE 5. Elastic DCS for e⁻ - He scattering at 100 eV. Present results SVP-PW: solid line; dashed-dot line; SVP-PW(BO): Experimental results of Ref. 19; open circle; theoretical results of Saha [2]: star; Experimental data [16]: triangule; R-matrix method [14]: dashed line with square; theoretical results of Buckley and Walters using the SESSBA [15]: solid line with star; theoretical results static exchange [15]: dashed line.

are compared with experimental data of Shyn [19], theoretical studies of Saha [2], and results using R-Matrix [14]. As cited in Figs. 1, and 2 our results describe the shape of the experimental data and are encouraging.

In Fig. 4 we show elastic differential cross sections (DCS) for e⁻ - He scattering at 50 eV. Our results using the SVP-PW are compared with experimental data of Shyn [19], and theoretical studies by the R-Matrix method [14].

In Fig. 5 we show elastic differential cross sections (DCS) for e⁻ - He scattering at 100 eV. Our results using the SVP-PW are compared with experimental data of Shyn [19], experimental data of Bromberg [16], theoretical studies using the R-Mmatrix method [14], the static-exchange simplified second Born approximation [15], and the static-exchange studies by Walters [15]. For comparison we have also included in Fig. 5 the SVP-PW without polarization (SVP-PW(BO)). As noted, at 100 eV our DCS are reasonably close to the experimental and theoretical results (the difference at intermediate angle is less significant, which confirms the expectation cited in Fig. 1).

4. Conclusions

We have presented the Schwinger variational principle with plane waves as a trial basis set (SVP-PW) to electron-atom scattering. Our formulation can be used to calculate elastic cross section and the exchange and polarization effects have seen evaluated via Born amplitude. We have noted that the SVP-PW can be an efficient tool for the study of e^- - He collisions processes.

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