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Elastic scattering of electrons by Ne at intermediate energies using the Schwinger variational principle with plane wave as a trial basis set

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We report a application of the Schwinger variational principle with plane waves as a trial basis set. Differential cross sections are obtained for e^-–Ne collisions from 130 to 500 eV. Our differential cross sections are found to be in reasonable agreement with existing measurements.

Keywords: Schwinger; electron; plane waves; scattering.

Se analiza una aplicación del principio variacional de Schwinger desde la perspectiva de ondas planas para un cunjunto base. El propósito de este trabajo es mostrar la sección eficaz diferencial para e^-–Ne en el intervalo de 130–500 eV. Los resultados obtenidos se comparan con los experimentos.

Descriptores: Schwinger; electrón; ondas planas; dispersión.

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1. Introduction

Elastic cross sections for intermediate-energy electron-atom scattering play an important role in a number of fields. For example, these cross sections arise in the modelling of swarm and plasma-etching systems [1], gas lasers and planetary atmospheres [2]. In spite of these needs, the availability of experimental data and of theoretical techniques for studing these cross sections is very important. For the system e^-–Ne most theoretical studies have been carriet out. For example Jhanwar and Khare [3] have employed the plane-wave approximation (PWA) and has been shown that even at 300 eV the PWA does not yield satisfactory for a target like neon in the intermediate energy range. Fink and Yates [4] have solved the Dirac equation in the static-field approximation and their results are satisfactory only at very high energies. Calculation also were presented by Fon and Berrington [5] using the R-matrix (RM) method with polarization effects and obtained good results for electron-Ne atom elastic scattering. Dewangan and Walters [6] have extended the earlier work of Buckley and Walters [7] by treating the e^-–Ne scattering using variants of the second Born approximation (SBA) and allowing for distortion due to the static atomic field. Byron and Joachain have used an *ab initio* optical model which is especially suitable for atoms [8]. The same authors have, in addition, studied $e^\pm$–Ne which involves a comparison of the terms in the Eikonal and Born series of the scattering amplitudes (EBS) [8]. Since several approximations for scattering amplitude involves the evaluation closure methods, the range of applications of methods as, for example, EBS, and PWA is retricted to relatively simple atoms. In fact, the available experimental data of differential cross sections do not provide a definitive test capable of juding the efficience of the theoretical methods. Obtaining accurate differential cross sections (DCS) for e^-–Ne collisions still remains an important endeavour. As a step toward addressing this need, we have recently described the Schwinger variational principle with plane waves as a trial basis set [9]. As an extension of our previous work [9] differential cross sections for e^-–Ne are obtained and we have used the Born-Ochkur approximation to include the effect of electron exchange. The present study has several goals: first, to our knowledge, no study theoretical using Schwinger variational principle (SVP) have yet been published for e^-–Ne; second, to test the relevance of the exchange effects at intermediate-energies and large scattering angles; and third, the present work serves in addition as a necessary prelude to studies planned at low energy scattering. Since the static and static-exchange level of theory is not sufficient to give highly quantitative predictions (in present paper polarization effects are not considered), we compare our results with other theoretical developments using polarization effetcs which is important to check if the SVP using plane waves is capable of describing correctly the structures in the DCS for e^-–Ne collisions at intermediate-energies. Here after, we will refer the SVP using plane waves as 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. Formalism

Details of the SVP have been discussed extensively elsewhere [10]. Here we will review a few steps in the development which are essential to the present discussion.

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

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

Here $|S_{\vec{k}_i}\rangle$ is the input channel state represented by the product of a plane wave $\vec{k}_i$ times $|\Phi_0\rangle$, the initial (ground) target state. $|S_{\vec{k}_f}\rangle$ has analogous definition, except that the plane wave points to $\vec{k}_f$, V is the interaction between the incident electron with the target, $G_o^{(+)}$ is the projected Green's function, writen as in the SMC method [10] as

$$G_o^{(+)} = \int d^3k \, \frac{|\Phi_0\vec{k}\rangle\langle\vec{k}\Phi_0|}{E - H_0 + i\epsilon}, \tag{2}$$

where H_o is the Hamiltonian for the N electrons of the target plus the kinectic energy of the incident electron and E is total energy of the system (target+electron). The scattering states $|\Psi_{\vec{k}_i}^{(+)}\rangle$ and $\langle\Psi_{\vec{k}_f}^{(-)}|$ are products of the target wave function $|\Phi_0\rangle$ and one-particle scattering wave function. The initial step in our SVP 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

$$|\Psi_{\vec{k}_i}^{(+)}\rangle = \sum_m a_m(\vec{k}_m)|\Phi_0\vec{k}_m\rangle, \tag{3}$$

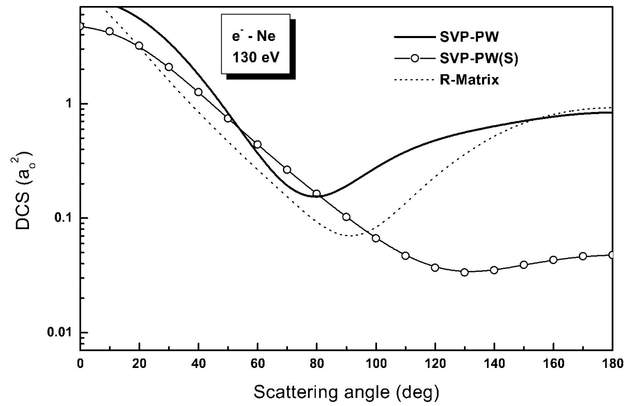

FIGURE 1. Elastic differential cross sections for e^-–Ne scattering at 130 eV. (——) is our SVP-PW, (—○—) is our SVP-PW(S), and (- - -) is the R-matrix [5].

and

$$|\Psi_{\vec{k}_f}^{(-)}\rangle = \sum_n b_n(\vec{k}_n)|\Phi_0\vec{k}_n\rangle. \tag{4}$$

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

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

where

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

We have implemented a set of computational programs to evaluate all matrix elements of Eq. (5) and when exchange effects are to be considered in electron scattering the first Born approximation (FBA) used in Eq. (4) is replaced by

$$f_{\rm FBA}^{(\rm E)} = f_{\rm FBA} + f_{\rm OB} \tag{7}$$

where $f^{(\rm E)}$ is the exchange amplitude ($f_{\rm OB}$ is the exchange amplitude in the Ochkur-Bonham (OB) approximation [11]). The Green's function given in Eq. (5) and its associated discontinuities have been examined and treated in a similar way as in the subtraction method [12–15]. 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).

3. Results and discussion

We have calculated elastic differential cross sections at a number of energies for e^-–Ne. 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 also are compared.

For the ground state of Ne we have used a self-consistent-field (SCF) wave function obtained with Cartesian Gaussian basis [16]. With this basis we obtain a SCF energy of -128.5242 au to be compared with -128.5405 au (configuration interaction calculation [17]).

In Fig. 1 we shows elastic differential cross sections (DCS) for e^-–Ne scattering at 130 eV. Our results using Born-Ochkur approximation approximation are compared with R-matrix (using exchange plus polarization) [5]. As noted, although the SVP-PW do not include polarization, our results are in general quite satisfactory with R-matrix [5]. For comparison we have also included in Fig. 1 the SVP results in the static field only (without exchange and we refer to this case as SVP-PW(S)). As noted the exchange effects plays a special role at 130 eV.

In Fig. 2 we shows elastic differential cross sections (DCS) for e^-–Ne scattering at 150 eV. Our results are also compared with R-matrix (using exchange plus polarization) [5] and experimental data [19]. Again, the comparison between our SVP-PW and experimental data and theoretical results are in general quite satisfactory. For comparison we have also included in Fig. 2 the SVP-PW(S) results in the static field only. As noted the exchange effects plays a special role for large scattering angle at 150 eV.

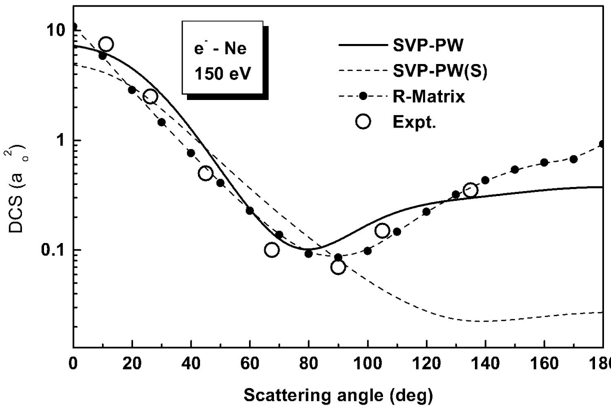

FIGURE 2. Elastic differential cross sections for e^-–Ne scattering at 150 eV. (—–) is our SVP-PW, (- - -) is R-matrix [5], (- -○- -) is our SVP-PW(S), and (○) are the experimental data [19].

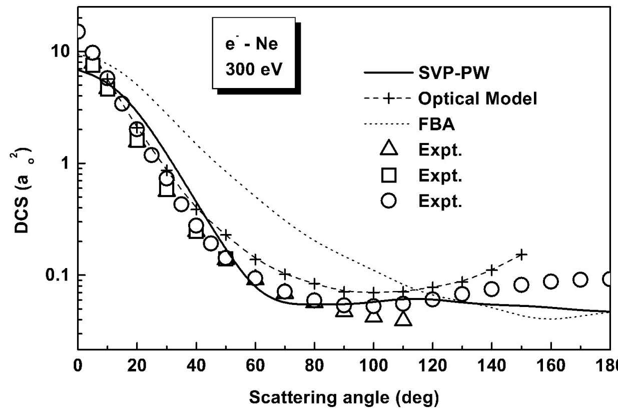

FIGURE 4. Elastic differential cross sections for e^-–Ne scattering at 300 eV. (—–) is our SVP-PW, (- - + - -) is optical model [8], (· · · ·) are FBA results [8], (□) are experimental data [18], (△) are experimental data [19], and (○) are experimental data [20].

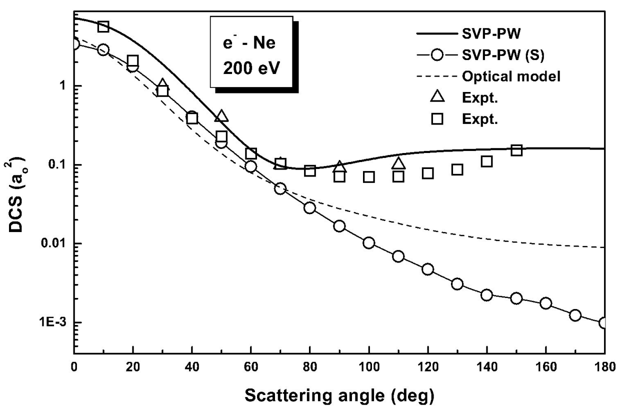

FIGURE 3. Elastic differential cross sections for e^-–Ne scattering at 200 eV. (—–) is our SVP-PW, (- -○- -) is our SVP-PW(S), (- - + - -) is the optical model [8], (□) are experimental data [19], and (△) are experimental data [20].

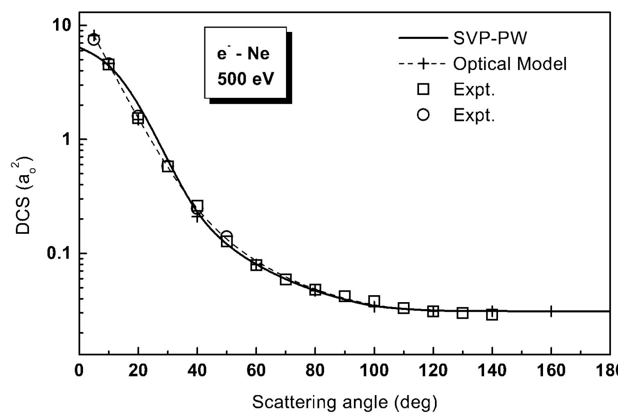

FIGURE 5. Elastic differential cross sections for e^-–Ne scattering at 500 eV. (—–) is our SVP-PW, (- - + - -) is the optical model [8], (□) are experimental data [18], (△) are experimental data [19].

In Fig. 3 we shows elastic differential cross sections (DCS) for e^-–Ne scattering at 200 eV. Our results are compared with optical model (using exchange plus polarization) [8], and experimental data [19, 20]. Our results agrees well in shape and magnitude with experimental and theoretical results. As in Figs. 1 and 2 we have included the SVP-PW(S) results in the static field only.

In Fig. 4 we shows elastic DCS for e^-–Ne scattering at 300 eV. Our results are compared with optical model (using exchange plus polarization) [8], first Born approximation (FBA) [8] and experimental data [18–20]. The agreement between our results and experimental and theoretical results are encouraging.

In Fig. 5 we shows elastic DCS for e^-–Ne scattering at 500 eV. Our results are compared with optical model (using exchange plus polarization) [8], and experimental data [18, 19]. As Fig. 4 the agreement between our results and experimental and theoretical results are encouraging.

4. Conclusions

We have carried out calculations of the elastic cross sections of e^-–Ne using the Schwinger variational principle with plane waves as a trial basis set. Differential cross sections were obtained and were compared with other theoretical developments using exchange plus polarization effects and good agreement was found in the region of intermediate energies. The present results suggests that the SVP-PW can be effective in the study of collisions of intermediate-energy electron-Ne.

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