THEORETICAL STUDY OF INTERMEDIATE-ENERGY ELECTRONS WITH
He USING THE SCHWINGER VARIATIONAL PRINCIPLE WITH
PLANE WAVES AS A TRIAL BASIS SET

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Abstract

We report elastic differential cross sections (DCS) for the scattering of electrons by He in the 50 to 200
eV energy range. These cross sections were obtained using the Schwinger variational principle (SVP). In
our procedures the scattering wave function is expanded as a combination of plane waves. We pay
particular attention is to the exchange effects based on na Born-Ochkur approximation and to include
polarization effects we use a model which contain only one adjustable parameter. Our calculated DCS
agree reasonably well with available experimental.

1. Introduction

In the last few years, there have been several theoretical activities concerning the electron-atom at
intermediate and high impact energies [1]. As we know, with the increase of the kinetic energy, the
penetration power of the incident electron into the atom will be increased. Therefore, the convergence of
the partial-wave expansion for continuum scattering wavefunction will become more difficult to be
achieved. Although several alternative theoretical approaches have been proposed for studying electron-
atom scattering at intermediate energy range, 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 accurate differential cross sections for electron-He collisions still
remains an important test for several new formalism. 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 [2].
The main propose of the present work is to study the elastic electron-He scattering at intermediate energy
using the SVP-PW where the exchange effects are treated by a Born-Ochkur approximation [3] and
polarization effects by Buckingham polarization potential [4] using a “rc” cutoff parameter and polarizability α of the atom (we will refer to this formalism using exchange plus polarization as SVP-
PW(BOP)). The present study has several goals: first, in just the last years, more results on the DCS have
become available for molecules using the Schwinger variational principle [2]. Below about first electronic
threshold (E < 20 eV), these cross sections can be compared with experimental data. Another reason for
more work in the low-energy regime being that the scattering cross sections full of structures due to strong
resonance, exchange, and polarization effects. However, the situation at intermediate energies is quit
different. In general, the scattering parameters in this region do not show any noticeable structure, rather
they smoothly with the increase in energy. To our knowledge, no investigations theoretical using the
Schwinger variational principle have yet been published for electron - He at intermediate energies; second,
to test the relevance of Born-Ochkur plus Buckingham polarization potential combined with the SVP-PW;
and third, the present work serves in addition as a necessary prelude to studies planned using the
Schwinger's method. 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
\[
\tilde{f}(k_f, k_i) = -\frac{1}{2\pi} \left[ -\left< S_{kf} | V | \Psi^{(+)} \right> + \left< \Psi^{(+)} | V | S_{ki} \right> - \left< \Psi^{(-)} | V - VG^{(+)} \right> \right]
\]
(1)

Here \(|S_{kf}\rangle\) is the input channel state represented by the product of a plane wave and the target (function).
\(<S_{kf}|\) has analogous definition, except that the plane wave points to , V is the interaction between the
incident electron with the target, \(G^{(+)}\) is the projected Green's function, written as in the Schwinger
multichannel method (SMC). 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
\[
\Psi^{(+)} = \sum a_m(k_m) | \Phi_o k_m \rangle
\]
\[
\Psi^{(-)} = \sum b_n(k_n) | \Phi_o k_n \rangle
\]
(2)

Inclusion of these definitions in Eq.(2) and application of a stationarity condition [2] with respect to the
coefficients,gives the working form of the scattering amplitude
\[
f[(k_f, k_i)] = -(1/2\pi) \left[ \sum <S_{kf}|V|\Phi_0 k_m \rangle (d^{-1})_{mn} <k_n\Phi_0 | V | S_{ki} \rangle \right]
\]
where
\[
d_{mn} = <k_m \Phi_0 | V - VG^{(+)} V | \Phi_0 k_n \rangle
\]
(3)

We have implemented a set of computational programs to evaluate all matrix elements of Eq.(3). The
Green's function \(G^{(+)}\) and its associated discontinuities have been examined and treated in a similar way
as in the subtraction method [2]. Our discrete representation of the scattering wave function (given by Eq.
(2) is made only in two dimensional space (spherical coordinates, using Gaussian quadratures for $\theta$ and $\varphi$ 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

$$f^{\text{Born-Ochkur}} = f^{\text{Born}} + g$$

(4)

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 be represented by a polarization potential

$$V_{\text{pol}}(r) = \frac{\alpha}{(r^2 + r_c^2)^2}$$

(5)

where `$r_c$' represents an adjustable cutoff parameter [4]. The Born scattering amplitude used is now formed by two parts, namely:

$$f^{\text{Born-Closure}} = f^{\text{Born-Ochkur}} + f^{\text{Born-pol}}$$

(6)

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

$$f^{\text{Born-pol}} = \frac{-2q^2}{E^2} \int e^{iqr^2} V_{\text{pol}}(r) \, dr$$

(7)

where $q$ is the elastic momentum transfer vector. If the atomic wavefunction is expressed in a Cartesian Gaussian basis function, the Born-Closure scattering amplitude can be obtained analytically as shown in previous works [5]. By combining equations (7), (5) and (4) we obtain the differential cross sections for electron - He scattering.

3. Results

We have calculated elastic differential cross sections at a number of energies for electron - He. We present representative results, emphasizing cases where experimental data is available for comparison. Other theoretical cross sections using static-exchange plus polarization level of approximation also are compared.

In figure 1(a), and (b) we show results obtained using the SVP-PW(BOP), and SVP-PW(BO) at 50 eV and 100 eV. We also show the available experimental data of Ref.[7] and theoretical results of Ref.[8] using R-matrix method (with exchange plus polarization effect). Comparison with the SVP-PW(BO) reveals that the polarization model used contributes mainly to the small-angle scattering. Figure 2 shows our DCS for electron - He at 200 eV. The comparison between our results and experimental data is in general satisfactory (in figures 1 and 2 we have used $r_c = 1.60$ as in Ref.[4]).
Figure 1(a)-(b): Elastic DCS for electron-\(\text{He}\) scattering at 50 eV (a) and 100 eV (b). Present results SVP-PW(BOP): solid line; Present results SVP-PW(BO): dashed line with open circle; R-Matrix method [8]: dashed line; Experimental results of Ref.[7].

Figure 2: Elastic DCS for electron-\(\text{He}\) scattering at 200 eV. Present results SVP-PW(BOP): solid line; Present results SVP-PW(BO): dashed line with open circle; R-Matrix method [8]: dashed line; Experimental results of Ref.[7].
4. Conclusions

We have shown that the SVP-PW(BOP) for electron - He scattering, can be used to the intermediate-energy range. Calculations of elastic electron scattering by H₂ are underway.

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References


