Elastic Scattering of Electrons by Atomic Helium

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Abstract:

We have calculated the phase shifts and DCS's for electrons scattered elastically from Helium atom by combining the exchange potential of Hara to Perdew and Wang correlation potential together with a parameter free polarisation potential, and the static potential. This model shows , a good agreement with the previous theoretical and in accord with the a vailable experimental values for many investigators.

1. INTRODUCTION

During recent years a growing interest has arisen in the study of elastic scattering of electrons by atoms. In particular, because of its relatively simple structure, helium has become the subject of extensive investigation and is quite frequently used as a testing tool for various theoretical schemes to predict differential cross sections. The experimental measurements of absolute cross sections made over the last decade for the scattering of electrons by helium have provided a further stimulation to this study; for example, by Bromberg [1,2] , Sethuraman et al [3] , McConkey and Preston [4], Kurepa and Voskovic [5], Gupta and Rees [6], Jansen et al [7] Register et al [8]. The theoretical approaches in the literature can be broadly grouped into three categories depending on the energy range over which they are applicable [9, 10, 11, 12], on the low energy side, there are methods like close-coupling approximation and its variants (correlation approximation, polarised pseudostate approximation), secondly, the R-matrix methods, ..etc which have been shown to give very good results, and thirdly, scattering phase shifts have been extracted from experimental measurements of the angular distribution of the scattered electrons by Andrick and Bitsch [13], Newell et al [14] and Williams [15]. Unlike the heavier noble gases, there has been also a fair number of theoretical calculations of electrons scattering from helium. Nesbet [16] has reported a matrix variational calculation for helium while O'Malley et al [17] and Fon et al [18] have carried out R-matrix calculation for this atom.

There has been a number of polarised orbital type calculations by LaBahn and Callaway [19-20], Callaway et at. [21], Duxler et at. [22] and Yau et al [23]. In the work of Yau et al. [23, 24] an adiabatic exchange approximation was used to calculate low-energy electron scattering from the noble gases. McEachran and Stauffer [25] treated exchange within the adiabatic exchange approximation and also studied. The effect of higher multipole moments in the polarisation potential. A reasonable agreement has been achieved between the experimental investigation and phase shift analysis by Andrick and Bitsch [13] and a number of theoretical methods, Including those based on many-body theory and the method of polarised orbitals. Pu and Chang [26] employed many body perturbation theory to construct an energy-dependent optical potential and calculated S- and P-wave phaseshifts, this work was later extended by Knowles and McDowell [27] who also included the d-wave phaseshift. Good agreement with these results has also been obtained in the many body Green's function scheme introduced by Schneider et at [28] and applied to electron-helium collisions by Yarlagadda et al [29]. In fact the perturbation form of many-body theory used by Pu and Chang [26] and Knowles and McDowell [27] can be derived from the many body Scheme of

Schneider a at [28] as shown by Csanak and Taylor [30]. Other theoretical models employed include the extended polarisation potential approach of Callaway et al [21] as applied by Labahn and Callaway [31,20] and also that of Duxler et al [22] based on the polarised orbital method introduced by Temken [32]. Both of these polarised orbital treatments have provided results in good agreement with the many body calculations and with the phase shift analysis of Andrick and Bitsch [13]. Further, since they are not restricted to this energy region alone, additional results at higher energies have readily been obtained.

In this work, we adopt the local density approximations for exchange- correlation potential, where we have employed an exchange potential of Hara [33] plus correlation potential of Perdew-Wang [34] model (HPW),
combined together to parameter-free polarisation potential [35]. In addition to the static potential in our calculations. This work shows a good agreement with previous theoretical and experimental values for many investigators.

2. THEORY

In the static-exchange approximation, the scattering theory starts with solving the Hartree-Fock equation (in atomic units: $e^2 = \hbar = m = 1$):

$$[-\frac{\nabla_1^2}{2} - \frac{Z}{r_1} + \sum_j \int \frac{U_j^*(2)U_j(2)}{r_{12}} dv_2 - \frac{\sum_j \int \delta_{ij} \int U_i^*(1)U_j^*(2)U_i(1)U_i(2)/r_{12}}{U_i^*(1)U_i(1)}]U_i(1) = E_i U_i(1)$$

where the third term on the left represents is the Hartree potential, while the last term on the left is the exchange term which is due to the pauli exclusion principle. In this exchange term there is no real allowence for correlation or polarization effect except partially the parameter α in the $X\alpha$ potential.

These correlation effects take account of the tendency of electrons to avoid each other in the configuration space. The exchange term is non-local, so it is important to replace the exchange kernels in the scattering equation by an equivalent local density potential:

$$V_{ex}^{Hara}(r) = -\frac{2}{\pi} K_F(r) F(\xi)$$

$$where K_F(r) = [3\pi^2 p(r)]^{1/3}$$

$$F(\xi) = \frac{1}{2} + \frac{1-\xi^2}{4\xi} \ln\left|\frac{1+\xi}{1-\xi}\right|; \xi = \frac{k(r)}{K_F(r)}$$

and $K_2(r) = 2(E+I) + K_F^2(r)$

where E is the incident energy and I is the ionisation potential.
For the correlation potential, which we use, is that of O'Connell and Lane [36] as:

$$V_{cor}(r) = \begin{bmatrix} V_{cor}^{SR}(r) & r \le r_0 \\ V_{POL}^{LR}(r) & r > r_0 \end{bmatrix} \qquad \text{…….. (1)}$$

where r is the crossing point between $V_{cor}^{SR}(r)$ and $V_{POL}^{LR}(r)$, $V_{cor}^{SR}(r)$ is the correlation potential at short distance and $V_{POL}^{LR}(r)$ is the polarisation potential at long range distance which is usually taken as [35]:-

$$V_{POL}^{LR}(r) = -\frac{1}{2}\sum \frac{\alpha_{2L}(0) r^{2L}}{(r^2 + d^2)^{2L+1}} \qquad \text{……..(2)}$$

where $\alpha_{2L}(0)$ is the static multipole polarisabilities of the target and d is the cut-off distance of the order of atomic size. For the correlation potential, we have employed the formula of Perdew and Wang [34]:-

$$V_{cor}^{SR}(r) = \begin{bmatrix} 0.031091 \ln r_s - 0.0570076 + 0.0044266\, r_s \ln r_s - 0.009166\, r_s ; \; small & r_s \\ -0.578 r_s^{-1} + 2.1612\, r_s^{-3/2}; & \text{large} \quad r_s \end{bmatrix} \ldots.(3)$$

where $r_s = [3/4\pi\ \rho(r)]^{1/3}$. Then, there are two parameters that should be correctly defined, these are r_0 and d.

According to eqs. (1) and (2) the value of d is usually used to determine r this makes the the value r_0 dependent on the number of terms included in eqs. (2), which in turns has its effect on the calculations and as the result the total interaction of a projectile electron with a target atom can be represented by a local and energy dependent optical potential:-

$$V_{opt}(r, E_i) = V_{St}(r) + V_{ex}^{Hara}(r, E_i) + V_{cor}^{SR}(r) + V_{POL}^{LR}(r) \qquad \ldots\ldots\ldots\ldots (4)$$

where r and E_i are the position coordinates and the energy (in a.u.) respectively, of the projectile electron. The static potential is given by

$$V_s(r) = -\int \frac{\rho(r')}{|r - r'|} d^3 r' \qquad \ldots\ldots\ldots\ldots\ldots (5)$$

where $\rho(r')$, is the total electronic charge density of the target atom. This potential $V_s(r)$ is usually obtained through the atomic charge density calculated from the Hartree-Fock wave functions given by Clementi and Roetti [37], while the correlation potential is usually obtained as a function of the atomic charge density.

In section 3 , we present a model calculation using above stated potential and in section 4, we apply the partial wave method by using CAVLEED program [38] to study low energy elastic electron scattering from He atom (closed shell system).

3. MODEL CALCULATION:

We make use of the recent correlation potential $V_{cor}^{SR}(r)$ Perdew and Wang [34]. Fig. (1a), we have ploted the calculated $V_{cor}^{SR}(r)$ as a function of the radial distance r, it is shown that the $V_{cor}^{SR}(r)$ to be a rapidly varying function of r at very short region (core region), and increasing r makes this variation more moderate until a region of r lies outside the ionic radius where the variation of $V_{cor}^{SR}(r)$ is very slow. Inside the later region, our function behaves linearly with r, accordingly the function $rV_{cor}^{SR}(r)$ has a minimum defined by,

$$r_0 = -\left[\frac{V_{cor}^{SR}(r_0)}{\frac{d}{dr} V_{cor}^{SR}(r_0)} \right] \qquad \ldots\ldots\ldots\ldots\ldots (6)$$

Fig (1b) shows this point of minima, r_0 , where we plot $V_{cor}^{SR}(r)$ as a function of r it is clear that the point r_0 always falls in the low density region ($r_s(r_0 > 1$), and where for larger than r_0 where the $V_{cor}^{SR}(r)$ is unimportant. In our calculation, we choose the r_0 point to be the point of aminima for the function $V_{cor}^{SR}(r)$ as evaluated by eq. (6).

Also, we use the following formula for $V_{POL}^{LR}(r)$ as given by Ali [35]:-

$$V_{POL}^{LR}(r) = -\frac{1}{2}\sum \frac{\alpha_{2L}(0) r^{2L}}{(r^2 + d_n^2)^{2L+1}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (7)$$

whereby, the values of d_n (n = 1, 2,...) are different by including any desired number of multipoles. These values of d_n are obtained in our caluclation according to the condition .

$$V_{POL}^{LR}(r_0) = V_{cor}^{SR}(r_0) \qquad \ldots\ldots\ldots\ldots\ldots\ldots (8)$$

This treatment insures that one can consider any number of terms and many (multipoles) in the series and at the same time cancelling the effect of increasing (n) by choosing a new value of d_n obtained from eq. (5).

For the calculation of the static and the exchange-correlation potential we have used the Roothaan-Hartree-Fock wave function given by Clementi- Roetti [37].

4. RESULTS AND DISCUSSION

The ionization energy which we use for Helium atom is I= 24.58 eV as given by Kittel [39], For the dipole , the quadrupole and the octopole polarisabilities, we take $\alpha_2(0)$= 1.39 as given by M. Lal and Srivastava [40], $\alpha_4(0)$= 2.43 and $\alpha_6(0)$= 10.48 as given by Luyckx et al [41]. Where we use (L=3) in eq. (7) also, the crossing point between $V_{cor}^{SR}(r)$ and $V_{POL}^{LR}(r)$. is r_0= 2.038 which give $r_s(r_0)$= 3.9275 and r$V_{cor}^{SR}(r)$ = -0.07569 (all quantities in a.u., $a_0 = \hbar$ = m= e= 1).

Phase shifts are calculated using the CAVLEED Programme (Titterington and Kinniburgh) [38] modified to optimise step sizes. In calculating differential cross sections up to (8), phaseshifts are used as required.

We have computed s-, p-, and d-waves phase-shifts of elastic scattering of electrons from free helium atom at ground state in the energy range (1- 20) eV.

Table (1) contains the calculated S-, P-, and d-waves phase-shifts of helium, using the eq. (4), these results are compared to the experimental values of Williams [15], and the theoretical values of Fon et al [18] and McEachran-Stauffer [25]. These results are shown in Figure (2). Our present values are in a good agreement with other theoretical and experimental data. The difference between them does not exceed 5% .

Also, we have calculate the differential cross section for elastic scattering of electrons from Heluim atom for incident energies 5, 12, 18, 30, 50 and 100 eV. For these energies we compare our results with the experimental values of Sethuraman et al [3], Jansen et al [7], Andriec and Bitsch [13,42], McConkey and Preston [4], T.W. Shyn [43] and Register et at [8], and the theoretical data of Scott and Taylor [44], Fon et at [18], Mohanlal-Srivastava [40], and McEachran-Stauffer [25].

These results are shown in figure (3), our results using eq. (4) give a good correspondence with experimental and theoretical data.

To sum up, it is clear that the study presented here suggests that highly satisfactory effective Scattering potential can be derived using the local density approximation also, the theoretical model of eq. (4) can repesents the ideal theoretical model for studying the elastic scattering of electrons from free atoms in general.

Table : (1): Elastic secattering Phase-shifts(δ_l) (in rad.) for S-, P- and d- waves for elastic scattening of electrons by helium atom in the energy range (1-20) eV.

Waves	E(eV.)	P. W.	a	b	c
S	1	-04350	---	---	-0.5056
	5	-0.8847	---	---	1.0559
	8	-1/0088	-1.008	-0.9848	---
	10	-1.1068	-1.1068	-1.0772	-1.3615
	16	-1.2858	-1.2790	-1.2790	---
	18	-1.3278	-1.3278	-1.3293	---
	20	----	---	---	-1.6679
P	1	---	---	---	-1.6679
	5	---	---	---	0.2435
	8	0.1860	0.1860	0.766	---
	10	0.2160	0.216	0.2080	0.3529
	16	0.2890	0.2890	0.2756	---
	18	0.3050	0.3050	0.2917	---
	20	---	---	---	0.4144
d	1	---	---	---	0.4144
	5	---	---	---	0.0333
	8	0.0228	0.0228	0.0232	---
	10	0.0302	0.0302	0.0290	0.0658
	16	0.0501	0.0501	0.0468	---
	18	0.0556	0.0556	0.0526	---
	20	---	---	---	0.1120

P. W. : Present Work.

(a) reference [15].

(b) reference [18].

(c) reference [25].

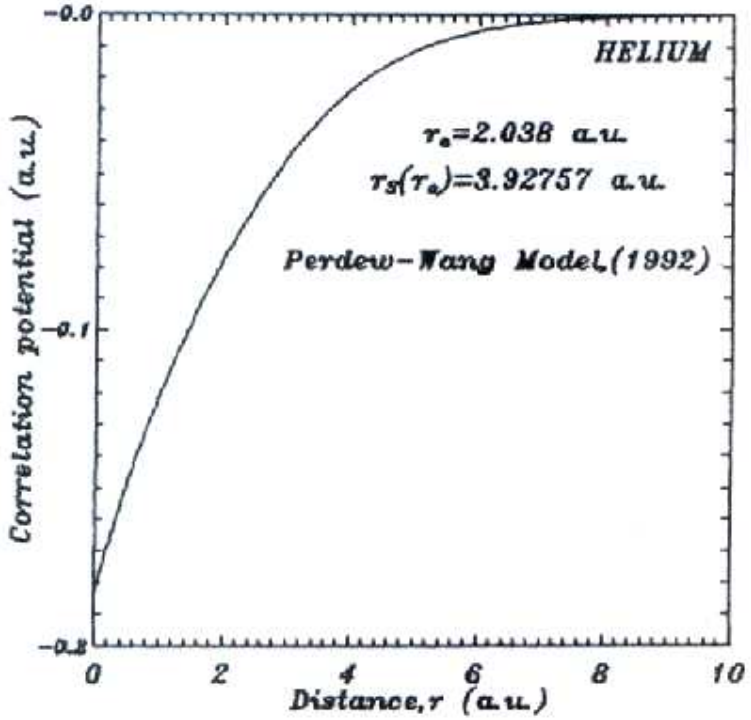

Figure (la): Correlation potentials of Perdew-Wang Model as a function of radial distance r for Helium atom.

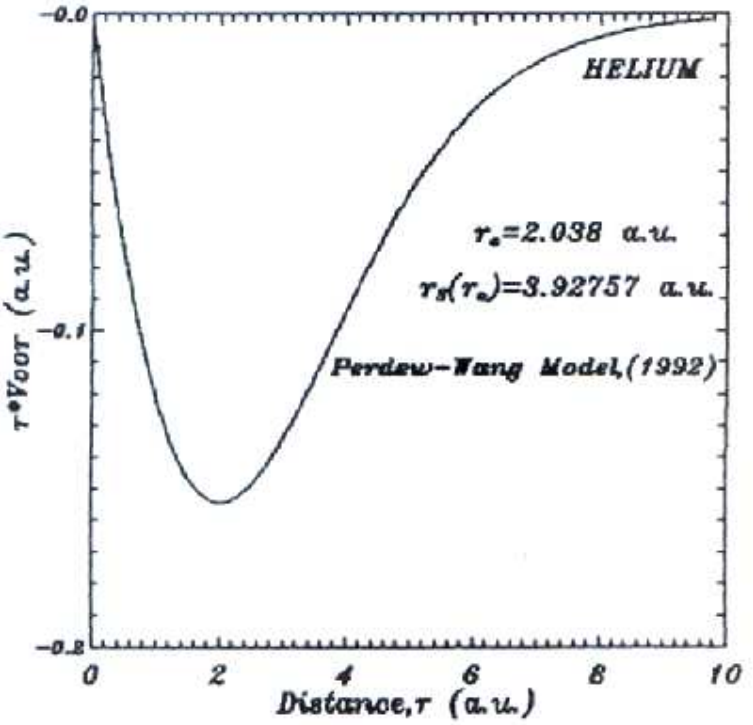

Figure (1b): Variation of r Vcor(r) as a function of radial distance r for Helium atom.

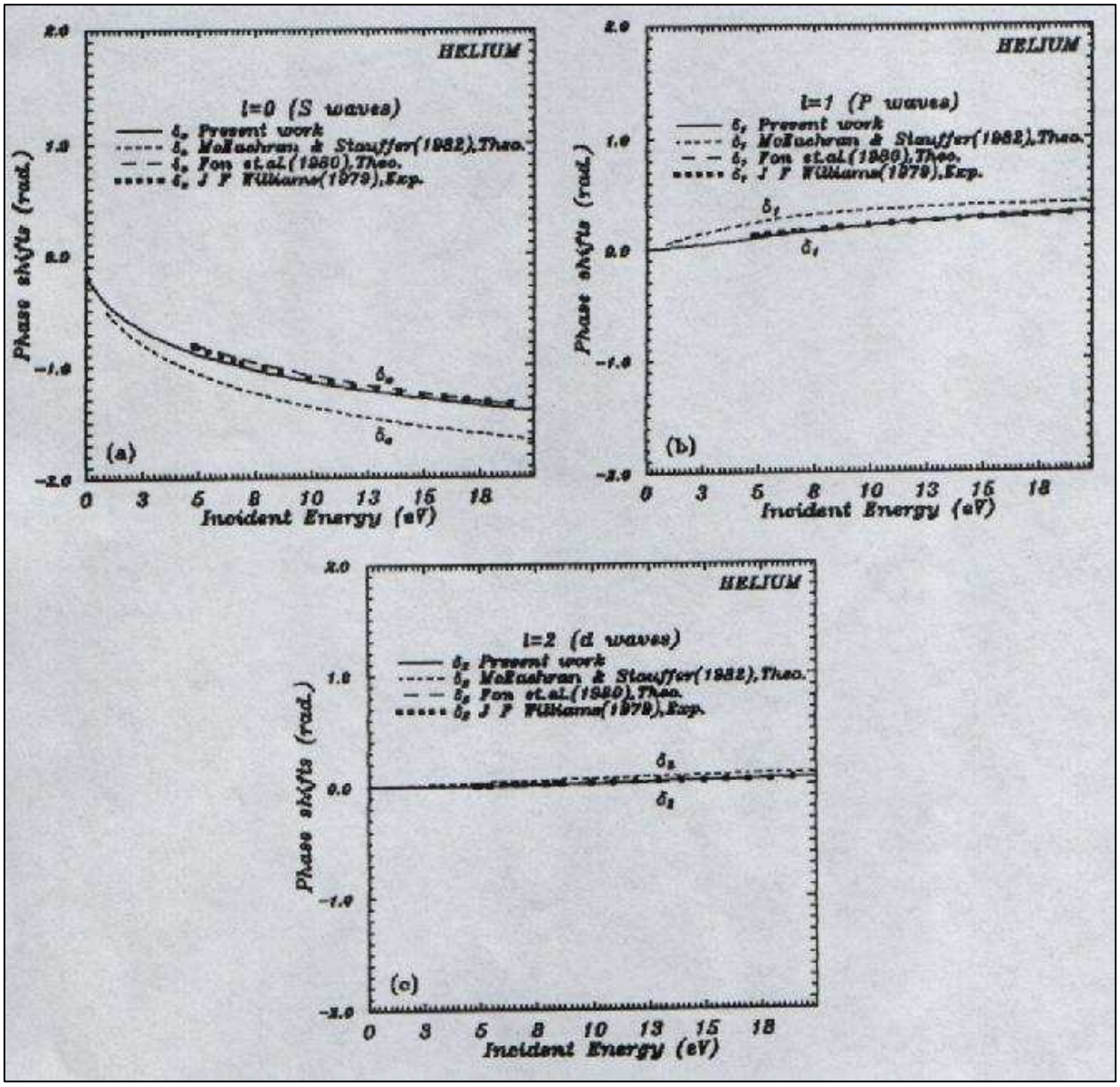

Figure (2): Phase shifts (in rad.) for elastic Scattering of electrons from Helium atom. (a) s- , (h) p- and (c) d- waves. Theory: —, Present results; .., McEachran Stauffer [25]; - --, Fon et al. [18]. Experiment: , Williams [15].

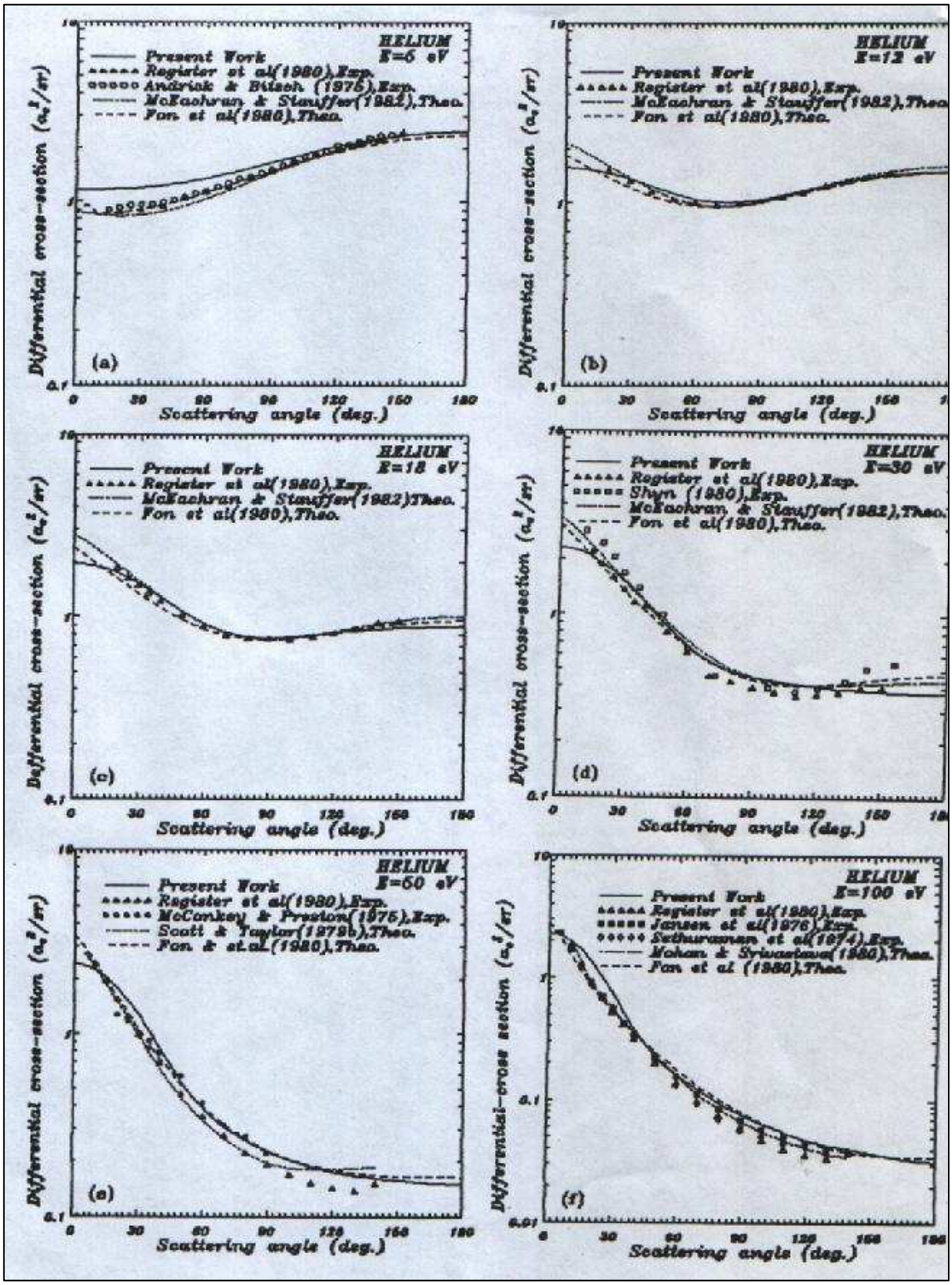

Figure (3): Low-energy differential cross sections ((a_0^2/sr) for the elastic scattering of electrons from Helium atom for an incident electron energy (a) 5eV, (b) 12eV, (c) 18eV, (d) 30eV, (e) 50eV, (f) 100eV.

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الاستطارة المرنة للالكترونات بوساطة ذرة الهيليوم

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بصرة – العراق

المستخلص

تم حساب ازاحات الطور و المقاطع العرضية التفاضلية (DCS's) للالكترونات المستطارة استطارة مرنة من ذرة الهيليوم الحرة وذلك بمزج جهد التبادل للباحث Hara مع جهد الترابط للباحثين Perdew-Wang وجهد الاستقطاب , فضلا عن الجهد المستقر . ان نتائج هذا النموذج النظري أعطت توافقاً جيداً عند مقارنتها مع قيم النظرية و العملية لباحثين اخرين .