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Theoretical Tests Of Scattering Potential Models For Electron-Atom System : An Alternative Separation Of Exchange and Correlation with Correct Long-Range Asymptotic behavior in Density-Functional Theory

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Abstract:

The effects of scattering potentials are tested by using the partial wave method for low-energy elastic scattering of electrons from helium atom . Roothaan- Hartree-Fock atomic wave functions are used to performing these calculations. In this paper three modern models for correlation potentials I derive from Armiento-Mattsson (2003) and Baer-Neuhauser (2005) correlation energy functions respectively ,these three models used separately to constructing the optical (full) scattering potentials that used to performing my calculations and this can serve as new addition in this field where the results I get are discussed . These optical scattering potential models consists of the sum of the energy dependent electron gas exchange potential (Hara version) plus the energy independent electron gas correlation potential (one of the models I derive in this work) plus the long range polarization potential (Ali version) plus the well known static potential .I present a modify results for differential, total elastic and momentum transfer cross sections. My models and corresponding my results can serve as a new addition in this field. The results obtained in this paper are in good agreement with the other theoretical results of other investigators and with experimental measurements.

Keywords: Density Functional Theory ;Scattering Potentials ;Electron-Atom system

1.Introduction:

The study of electron-atom scattering has grown considerably during the last years. This field has received increasable attention within the last twenty five years. The aim of this paper is to apply my models of correlation potentials I derive from density functional theory to construct my scattering potential models that consist of a static, exchange, correlation and polarization effects and to apply at low impact energies for electron-atom collision processes .The purpose of choosing helium atom has twofold ;firstly, for its relatively simple structure ,and secondly it becomes the subject of extensive investigation to compare the results obtained by using my scattering potential models with the other theoretical and expermintal results of other investigators in order to examine degree of success of my models.

2.Introductory Remarks:

The theoretical complexity of the electronic structure or electron-scattering dynamics of atoms is due to electron exchange and correlation effects [1,2]. Electron exchange effects are due to the Pauli exclusion principle and the consequence that the total wave function of the system must be antisymmetric with respect to the interchange of the coordinates (spatial and spin) of any two electrons[3] . Thus a variety of exchange approximations has been devised to permit the study of large atoms and molecules and other forms of condensed matter[4,5].On the other hand ,in the static-exchange approximation ,the theory takes into account only the static and exchange interactions of the electron with an unperturbed ground electronic state of the target .There is no allowance for polarization or other correlation effects. Where exchange effects preventing two electrons of like spin from being found near one another because of Each bound electron is surrounded by a Fermi hole where the repulsive Coulomb interaction between two electrons of like spin vanishes[5]. In

the Hartree -Fock approach each electron is assumed to move in the average self-consistent field of the other electrons, taking into account only the Coulomb energy and the Pauli exclusion principle .Thus ,correlation is the correction of this average interaction to allow electrons to avoid one another ,not only "on the average" but in every region of configuration space .Thus, in addition to the "Fermi hole" each electron surrounds itself with a "Coulomb hole" from which other electrons are excluded[3]. The polarization is an important correlation effect found to be particularly important in low energy electron scattering .When an electron slowly approaches the target atom, the bound electrons are influenced by the electric field of the external charge, and an adiabatic redistribution of bound electronic density occurs, resulting in an (indused) dipole moment on the target atom .The adiabatic change in energy due to the slow approach of the electron exhibits the asymptotic form[5]:

$$V_{pol.}(r) \xrightarrow[r\longrightarrow\infty]{} -\frac{\alpha_d}{2r^4} \qquad \text{----------(1)}$$

where α_d is the electric dipole polarizability of the inner charge distribution depends on the direction of the external electric field and hence the position vector of the electron. Equation (1) represents a dipole approximation and breaks down as the electron closely approaches the target .Moreover ,the adiabatic effect breaks down at high energies and near the nuclei, where the electron has a large local kinetic energy[5].

The purpose of this paper is to report a simple and accurate models of scattering potential for electron-atom system .The approach represents a hybridization of free-electron-gas (FEG) theory and the long range polarization interaction theory , some what along the lines of Armiento-Mattsson[6] and Baer-Neuhauser[7] of the short range correlation interaction theory .My approach is to adopt the static potential plus Hara's modification [8] of the free-electron-gas exchang potential plus the short range correlation potential (one of the models I derive in this work from Armiento-Mattsson (2003) and Baer-Neuhauser (2005) correlation energy functions respectively) plus the long range polarization potential of Ali [9] where the short range correlation potential becomes equal to the long range polarization potential at the crossing point r_o when $r = r_o$ .Thus requires only the electron density and polarizabilities of the target .I report here applications to elastic scattering of electrons from the helium atom ,since this atom provide a range of electron densities and corresponding electron-gas characteristics .This atom seemed to be the best choice to use in testing models that I hope it will be useful in describing more complex systems in future works ,because of its relatively simple structure and there are lots of theoretical and experimental results which are available for comparison and for the examine of successful of my models used here. The approach described in this paper is similar to that used by O,Connell and Lane[3].However, the choice of correlation potentials and the full models used to perform the calculations is quite different. In sec.3 ,the forms of exchange and correlation potentials used in this paper are described .In sec.4,the computational method used in present work is discussed. While sec.5 deals with the results obtained from application of elastic electron scattering from helium atom and the comparisons given with other theoretical and experimental results of other investigators ,the conclusions are given in sec.6 .

3. Exchange and Correlation Potentials:

3.1: Hara-Free-Electron-Gas (HFEG) Exchange potential:

The free electron gas exchange potential form used is [5]:

$$V_{FEG}^{ex}(r) = -\frac{2}{\pi} k_F(r) F[\eta(r)] \qquad \text{----------(2)}$$

Where $k_F(r)$ is related to the charge density of the target atom $n(r)$ by :

$$k_F(r) = [3\pi^2 n(r)]^{1/3} \qquad \text{----------(3)}$$

and $F[\eta(r)]$ is given by :

$$F[\eta(r)] = \frac{1}{2} + \frac{1-\eta^2}{4\eta} \ln\left|\frac{1+\eta}{1-\eta}\right| \qquad \text{----------(4)}$$

with:

$\eta(r)$ =k(r)/k$_F$ (r) ----------(5)

defined in terms of the "local momentum" k(r) of the projectile electron and the "local fermi momentum" k$_F$ (r) . In equation (5) , Hara[5] , suggested that the momentum k(r) of the scattered electron should be referred to the same energy base as that of the bound electrons in the gas .Thus the variation of k(r) with r arises from k$_F$ (r) according to:

k^2 (r)= k$_F^2$ (r)+2I+ k^2 ----------(6)

where I is the ionization potential of the target atom and $k^2/2$ is the incident kinetic energy of the projectile electron. In the present study the Hara free electron gas (HFEG)exchange potential of equation (2) with the help of equation (6) has been adopted.

For correlation potentials in density functional theory, there are three models used to perform my calculations:

3.2:Armiento–Mattsson correlation functions:

Armiento and Mattsson[6] have shown that the local values of the conventional exchange energy per particle cannot be described by an analytic expansion in the density variation . They construct an alternative separation in which the exchange part is made well behaved by screening its long-ranged contributions,and the correlation part is adjusted accordingly .They demonstrate functional development based on this approach by creating and deploying a local-density-approximation-type xc functional .Armiento and Mattsson[6] present results by separating the xc energy in an alternative way and show this results to hold for systems of generic effective potentials by introduces $\bar{K}_y$ as the Yakawa wave vector which effectively is an inverse screening length for the coulomb potential that may dependent on r. Acorresponing correlation like term E$_{cor.-y}$ is defined by the relation E$_{ex.+y}$+E$_{cor.-y}$ =E$_{xc}$ [6],where E$_{xc}$ is the total exchange-correlation energy per particle.This can be seen as moving a term E$_y$ from correlation to exchange[6]. So,

E$_{ex.+y}$=E$_{ex.}$ +E$_y$ ----------(7)

And,

E$_{cor.-y}$ =E$_{cor.}$ –E$_y$ ----------(8)

This is an alternative way of partitioning E$_{xc}$ without introducing any new approximations .This approach is fundamentally different from other previous approaches in that the screening of the exchange is compensated for by redefining correlation to keep the total E$_{xc}$ constant[6].In the present work, the exchange part of the alternative separation is neglected after the correlation part is adjusted accordingly(i.e I used only the correlation part).Thus ,there are two correction models of Armiento-Mattsson correlation energy function for local density approximation in density functional theory [6] used to performing my calculations, these are:

3.2.1:Correlation energy function (Model 1):

Armiento–Mattsson [6] gives an explicit expression to model E$^{LDA1}_{cor.-y}$,(all equations used in the following in mRy. atomic units),

$$E^{LDA1}_{cor.-y}(r_s)=\frac{b_1\sqrt{r_s}+b_2}{r_s^{3/2}+b_3 r_s+b_4\sqrt{r_s}} \quad \text{----------(9)}$$

of the four free parameters, b_1-b_4 where, $r_s=[3/4\pi n(r)]^{1/3}$ (a.u.) is the charge density parameter, $b_1=-1.71478, b_2=-7.57697, b_3=5.13452$ *and* $b_4=10.7168$.Where these free parameters is compared with the Ceperley and Alder [10] data and other xc parametrizations currently in use [11].Then I extract the correlation potential V$_{cor.}$(r) from the flowing relation [11]:

$$V_{cor.}(r)=E_{cor.}(r_s)-\frac{r_s}{3}\frac{\partial E_{cor.}(r_s)}{\partial r_s} \quad \text{----------(10)}$$

Thus ,the result from equations (9) and (10) is:

$$V_{cor.}^{LDA1}(r)=E_{cor.-y}^{LDA1}(r_s)-\frac{r_s}{3}\left[\frac{\left(r_s^{3/2}+b_3 r_s+b_4\sqrt{r_s}\right)\left(\frac{b_1}{2\sqrt{r_s}}\right)-\left(b_1\sqrt{r_s}+b_2\right)\left(\frac{3}{2}\sqrt{r_s}+b_3+\frac{b_4}{2\sqrt{r_s}}\right)}{\left(r_s^{3/2}+b_3 r_s+b_4\sqrt{r_s}\right)^2}\right]$$ --

(11)

3.2.2:Correlation energy function (Model 2) :

An improved is given by adding two parameters to the $E_{cor.-y}^{LDA}$ part ,the result is [6]:

$$E_{cor.-y}^{LDA2}(r_s)=\frac{e_1 r_s+e_2\sqrt{r_s}+e_3}{r_s^{\,2}+e_4 r_s^{3/2}+e_5 r_s+e_6\sqrt{r_s}} \qquad \text{----------(12)}$$

With

$e_1=-1.81942, e_2=2.74122, e_3=-14.4288, e_4=0.537230, e_5=1.28184$ *and* $e_6=20.4048$.A rmiento & Mattsson[6]make sure that there is no major difference between these correlation energy functionals and the other LDA correlation functionals. i.e. Perdew–Zunger[12],Vosko–Wilk–Nusair[13],Perdew–Wang[11],LDA1 and LDA2 [6]give essentially equal values.And again by using equations (10) and (12) I get expression for correlation potential as followed:

$$V_{cor.}^{LDA2}(r)=E_{cor.-y}^{LDA2}(r_s)-\frac{r_s}{3}\left(\frac{c_1.c_2-c_3.c_4}{c_5}\right) \qquad \text{----------(13)}$$

where,

$$c_1=r_s^{\,2}+e_4 r_s^{3/2}+e_5 r_s+e_6\sqrt{r_s} \qquad \text{----------(14)}$$

$$c_2=e_1+\frac{e_2}{2\sqrt{r_s}} \qquad \text{----------(15)}$$

$$c_3=e_1 r_s+e_2\sqrt{r_s}+e_3 \qquad \text{----------(16)}$$

$$c_4=2r_s+\frac{3e_4\sqrt{r_s}}{2}+e_5+\frac{e_6}{2\sqrt{r_s}} \qquad \text{----------(17)}$$

$$c_5=\left(r_s^{\,2}+e_4 r_s^{3/2}+e_5 r_s+e_6\sqrt{r_s}\right)^2 \qquad \text{----------(18)}$$

where e_1-e_6 as given previously ,in the present study the correlation potentials represent by equations (11) and (13) are adopted in order to construct my scattering potential models to perform the calculations of this work.

3.3:Baer – Neuhauser correlation function:

Recently,Baer and Neuhauser[7]derive an exact representation of the exchange-correlation energy within density functional theory which spawns a class of approximations leading to correct long-range asymptotic behavior .Using a simple approximation ,they developed an electronic structure theory that combines a new local correlation energy (based on Monte Carlo calculations applied to the homogeneous electron gas) and combination of local and explicit long range exchange . For convenience, they write exchange-correlation energy per particle for homogeneous electron gas as[7,14]:

$$E_{xc}(n)=E_{ex.}(n)+E_{cor.}(n) \qquad \text{----------(19)}$$

where $E_{xc}(n)$ is the analytical local screened exchange in a homogeneous electron gas. as before ,in the present work ,the exchange part of equation (19) is neglected, thus ,the function $E_{cor.}(n)$ was evaluated numerically for homogeneous electron gas using the shifted-contour auxiliary field Monte Carlo (SCAFMC) method [15,16],performed with plane waves .For convenience of application , the results are[7]:

$$E_{cor.}(r_s)=\left[\frac{d}{d_o+d_1 r_s+r_s^{\,2}}\right].E_{cor.}^{LDA}(r_s) \qquad \text{----------(20)}$$

where $E_{cor.}^{LDA}(r_s)$ is the usual correlation energy for the homogeneous electron gas (parameterized in any DFT code.)[7], $d=3.4602, d_o=3.2$ and $d_1=-0.9$ .For $E_{cor.}^{LDA}(r_s)$ of equation (20) I use equation (12),therefore by using equations (20) and (12) with the help of equation (10), I get another expression of the correlation potential as followed:

$$\mathrm{V}_{cor.}(\mathrm{r})=\left[\frac{d}{d_o+d_1 r_s+r_s^{\,2}}\right]\cdot\left[\frac{c_3}{\sqrt{c_5}}\right]-$$

$$\frac{r_s}{3}\left[\left\{\frac{d}{d_o+d_1 r_s+r_s^{\,2}}\right\}\cdot\left\{\frac{c_1\cdot c_2-c_3\cdot c_4}{c_5}\right\}-\left\{\frac{d(d_o+2r_s)}{(d_o+d_1 r_s+r_s^{\,2})^2}\right\}\cdot\left\{\frac{c_3}{\sqrt{c_5}}\right\}\right] \qquad \text{----------(21)}$$

where c_1-c_5 represented by equations (14)–(18) respectively .This model is adopted in my calculations , where I refer to it as (model 3) correlation potential .On the other hand , the long range polarization potential is defined by the relation(Ali version)[9]:

$$V_{pol}^{LR}(r)=-\frac{1}{2}\sum_{L=1}^{n}\frac{\alpha_{2L}(0)\cdot r^{2L}}{(r^2+d_n^2)^{2L+1}} \qquad \text{----------(22)}$$

where $2L$ represent order of multipole, $\alpha_{2L}(0)$ is electric multipole polarizability of the target atom and d_n is a cut-off parameter which is important in which it gives correction for correlation effects at low distance from the atom .The full correlation potential ,then ,is obtained by continuously joining of the short-and long-range forms at the crossing point r_o where $V_{cor.}^{SR}(r)$ and $V_{pol}^{LR}(r)$ are cross at the crossing point r_o ,thus obtaining :

$$\mathrm{V}_{cor.}(r)=\begin{Bmatrix}V_{cor.}^{SR}(r) & ,r\le r_o\\ V_{pol}^{LR}(r) & ,r>r_o\end{Bmatrix} \qquad \text{----------(23)}$$

This is the simplest prescription for joining the correlation and polarization potential. This treatment similar to that used by O'Connell–Lane[3] in the local density functional theory .However , the choice of correlation and polarization potentials is quite different.

4. Computational method:

In this section ,the elastic scattering of electrons by helium atom is described. Atomic unit will be used throughout but unless otherwise stated , I will assume the target nucleus to be infinitely heavy compared with the electrons so that we may work in the center of mass frame with the origin of coordinates fixed at the nucleus.

The Z-axis will be defined as the direction of the incoming electron .I had chosen to illustrate the method of solution by using partial wave method by calculating phase shifts ,differential ,total elastic and momentum transfer cross sections for the elastic scattering of electrons by helium atom .For the spherically symmetric atomic targets, the radial partial wave functions satisfy the radial equation [17]:

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{l(l+1)}{r^2}-2V(r)\right]R_{kl}(r)=0 \qquad \text{----------(24)}$$

where $V(r)$ is the full electron–atom potential energy ,including the static potential $V_s(r)$,the exchange $V_{FEG}^{ex}(r)$ and correlation–polarization $V_{cor.}(r)$ potentials described by the following expression:

$$V(r)=V_s(r)+V_{FEG}^{ex}(r)+V_{cor.}(r) \qquad \text{----------(25)}$$

where $V_{cor.}(r)$ represent the correlation–polarization potential which is given by equation (23) with the help of equation (22).Therefore ,the correlation potential $V_{cor.}(r)$ which I had been adopted in precent work ,can be represent by three models:

$$V_{cor.}^{model\,1}(r)=\begin{Bmatrix} V_{cor.}^{SR}(r) & ,r\le r_o & of\ equation\ (11) \\ V_{pol}^{LR}(r) & ,r>r_o & of\ equation\ (22) \end{Bmatrix} \qquad \text{----------(26)}$$

$$V_{cor.}^{model\,2}(r)=\begin{Bmatrix} V_{cor.}^{SR}(r) & ,r\le r_o & of\ equation\ (13) \\ V_{pol}^{LR}(r) & ,r>r_o & of\ equation\ (22) \end{Bmatrix} \qquad \text{----------(27)}$$

$$V_{cor.}^{model\,3}(r)=\begin{Bmatrix} V_{cor.}^{SR}(r) & ,r\le r_o & of\ equation\ (21) \\ V_{pol}^{LR}(r) & ,r>r_o & of\ equation\ (22) \end{Bmatrix} \qquad \text{----------(28)}$$

Respectively ,it has been noted that r_o from equation (26)–(28) vary from potential model to another .Therefore ,the three full electron–atom potential energy models have been adopted to perform my calculations described by:

$$V^{model\,1}(r)=V_s(r)+V_{FEG}^{ex}(r)+V_{cor.}^{model\,1}(r) \qquad \text{----------(29)}$$

$$V^{model\,2}(r)=V_s(r)+V_{FEG}^{ex}(r)+V_{cor.}^{model\,2}(r) \qquad \text{----------(30)}$$

$$V^{model\,3}(r)=V_s(r)+V_{FEG}^{ex}(r)+V_{cor.}^{model\,3}(r) \qquad \text{----------(31)}$$

respectively ,where $V_{FEG}^{ex}(r)$ is Hara's modification of FEG exchange potential (HFEG) [8] represented by equation (2) with the help of equation (6) I had been adopted for all calculations reported in this paper and $V_s(r)$ is the static coulomb potential is simply given by [9]:

$$V_s(r)=-\int\frac{n(r')}{|r-r'|}d^3r' \qquad \text{----------(32)}$$

The bound atomic orbital function $\Phi_i(r)$ are taken to be the analytic Hartree–Fock functions of Clementi–Roetti [18].Thus the radial electron density is given in terms of these orbitals by [3]:

$$n(r)=\frac{1}{4\pi r^2}\sum_{i=1}^{N}\Phi_i^2(r) \qquad \text{----------(33)}$$

where N represent an electrons of target atom ,therefore ,in order to compute the phase shifts $\delta_l(k)$,where $k^2/2$ is the incident electron energy ,the radial equation (24) where solved numerically in the internal region $(r<a)$ by using Numerov's algorithm [19] where a is called the matching radius at which the continuously occur between the solutions in the internal $(r<a)$ and external $(r>a)$ regions by matching the internal solution to the external ones at $(r=a)$ [It must note that the matching radius a differ from the crossing point r_o where a is related with the solution of the radial equation represent by equation (24) while r_o is the point at which $V_{cor.}^{SR}(r)=V_{pol.}^{LR}(r)$,also the parameter $r_s=[3/4\pi n(r)]^{1/3}$ (a.u.) is the charge density parameter which is related to the charge density of the target atom $n(r)$].Therefore, the asymptotic boundary conditions at $(r>a)$ [17]:

$$R_{kl}(r)=B_l(k)\left[j_l(kr)-\tan\delta_l(k)\cdot n_l(kr)\right] \qquad \text{----------(34)}$$

where $B_l(k)$ is real constant equal to one which is independent of r while $j_l(kr)$, $n_l(kr)$ are the spherical Bessel and spherical Neumann functions respectively .Thus,
by using the solutions in the internal $(r < a)$ and external $(r > a)$ regions at $(r = a)$ I get the result of phase shifts $\delta_l(k)$ [3].Thus, the scattering amplitude is given by the expression [17]:

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\exp(2i\delta_l(k)-1)P_l(\cos\theta) \qquad \text{----------(35)}$$

where $P_l(\cos\theta)$ are the Legendre polynomials and θ is the scattering angle .The elastic differential scattering cross section (DCS's) is given by [20]:

$$\frac{d\sigma}{d\Omega} = \left|f(\theta)\right|^2 \qquad \text{----------(36)}$$

and the total scattering cross section (TCS's), Q_T is given by [17]:

$$Q_T = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)Sin^2\delta_l(k) \qquad \text{----------(37)}$$

while the momentum transfer cross-section (MTCS's), Q_M is given by [9]:

$$Q_M = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(l+1)Sin^2(\delta_l(k)-\delta_{l+1}(k)) \qquad \text{----------(38)}$$

5.Result and Discussion :

The ionization potential used for helium atom is I=24.58 eV[21],and the electric dipole ,quadrapole and octapole polarizabilities used in these calculations are $\alpha_2(0) = 1.39a_o^3$[22], $\alpha_4(0) = 2.43a_o^3$[23]and $\alpha_6(0) = 10.48a_o^3$[23] respectively ,where I used three terms (L=3) in polarization potential represent by equation (22) ,while the crossing point r_o (in a.u.) are depend on the correlation potential models used, where it vary between (1.5-2.0) for the three models adopted here . Figure (1) shows the variation $r*V_{cor}(r)$ (a.u.) of correlation potential models used with the radial distance r (a.u.) for helium atom .I note that these curves vary with distance r in similar way with each other especially for long distance $(r > r_o)$ where polarization potential dominant . Where In my calculations I always choose the r_o point to be the point of a minimum for the function $r*V_{cor}(r)$. While figure(2) explains the curves of $r*$ potentials (a.u.) for my models as a function of r (a.u.) . Figure(3) gives results for DCS's for elastic scattering of electrons from helium for incident energies 5,12,18 and 30 eV ,for these energies I compare my results with the available results of other investigators, for example , the theoretical values of Fon et.al.[24], McEachran and Stauffer[25] and the absolute experimental values of Register et.al.[26] , Andrick and Bitsch[27] and Shyn[28].From these results I note that there is agreement between the results of my models with each other ,while there is a slightly difference between my results and the results of others as shown in figures (3a–c) for small and large angles because these angles is dominated by the long range polarization and the short range static potential respectively .As the impact energy increases the results slightly agree with the results of others especially at large angles ,as shown in figure (3–d),because the effects of the polarization and the exchange effects at large angles become negligible at high energies ,since my scattering potential models used are much sensitive to the incident electron energy. I represent my results for the total elastic scattering (TCS's) and momentum transfer cross-sections (MTCS's) for helium atom .Where figure(4) shows the results of total cross sections for energy region (1-20 eV) by using the models adopted in present work. I compare my data of TCS's with the available experimental results of Kennerly and Bonham[29] and Stein et.al.[30].And with the theoretical results of McEachran and Stauffer[25].For small impact energy model1 and model2 results agree well with the experimental and theoretical results of other investigators than model3 results after which it lie slightly lower .As the impact energy increases the results of my models agree well with each other ,but it lie slightly higher ,This behavior depend on scattering potential models used where at small impact energies these models become much sensitive than at large energies .Similarly figure (5) shows the results of the present data of the momentum transfer cross-sections for energy range (1-20eV) by using my three models , I compare the results of momentum transfer cross-sections for helium atom with the available

experimental values of Crompton et.al.[31] and Newell et.al.[32]as well as the theoretical calculations of McEachran and Stauffer[25],my results of MTCS's exhibit similar behavior to the total cross –sections and the reason is the same as discuss in figure (4).

6.Conclusions:

In this paper, I has used my models in electron-helium scattering .I take the exchange potential to include it in the total scattering potential model because of exchange effects are due to the Pauli exclusion principle ,consequently ,exchange potential prevent two electrons of like spin from being found near one another because it make each bound electron is surrounded by a "Fermi hole" where the repulsive Coulomb interaction between two electrons of like spin vanishes .Also ,I included the correlation potential in the total scattering potential model because each electron is assumed to move in the average self consistent field of other electron ,taking in to account only the Coulomb energy and the Pauli exclusion principle .Thus, the correlation potential is the correction of this average interaction to allow electrons to avoid one another ,not only "on the average' but in every region of configuration space .Thus in addition to the "Fermi hole" caused by the exchange potential ,the correlation potential make each electron surrounds itself with a "Coulomb hole" from which other electrons are excluded when a single electron is removed sufficiently far from the other electrons .These effects are important for all atomic system except for hydrogen atom where there is one electron in this atom .Therefore ,if these effects are neglected ,then the results obtained does not have any physical feature .However ,the theoretical complexity of the electron scattering dynamics of atoms is due to electron exchange and correlation effects. The comparision of my results of differential (DCS's),total (TCS's) and momentum transfer cross-sections (MTCS's) that preformed by using my scattering potentials models that derived in this paper with experimental measurements and other theoretical results of other investigator explain the success of my models .The present calculations test more stringently the features of these potentials and suggest that these potentials can produce reliable differential, total and momentum transfer cross sections for electron- helium scattering at impact energies above the region used to perform my calculations .Therefore I believe that my present models serve as a good starting point from which to construct a scattering potential model involve an relativistic effects . I intend to extend these calculations by including the absorption potential in these models in future

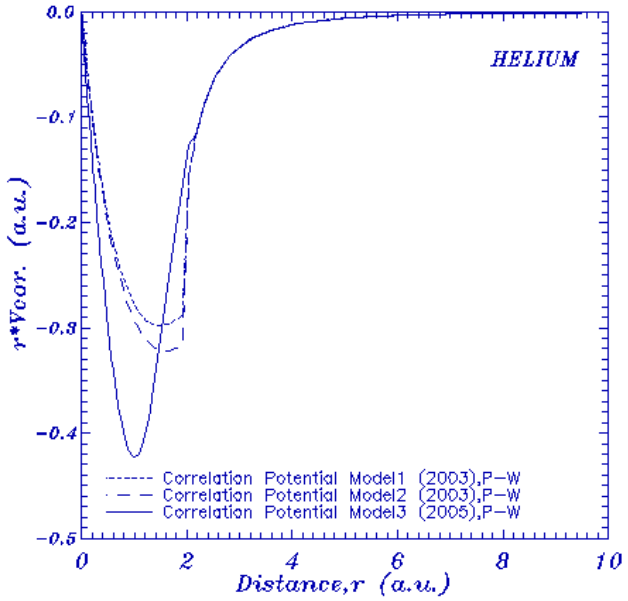

Figure (1):Variation of $r * V_{cor.}(r)$ for my correlation potential models with the radial distance r (a.u.) for helium atom .

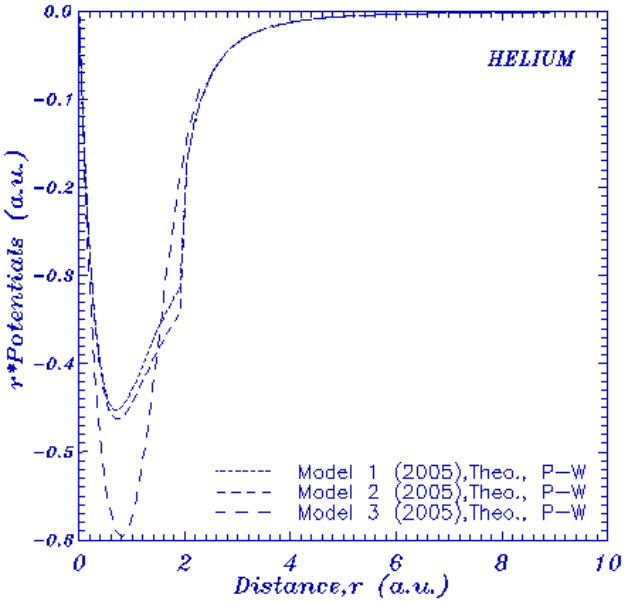

Figure (2): Variation of the my full potential models as a function of radial distance r (a.u.) for helium atom

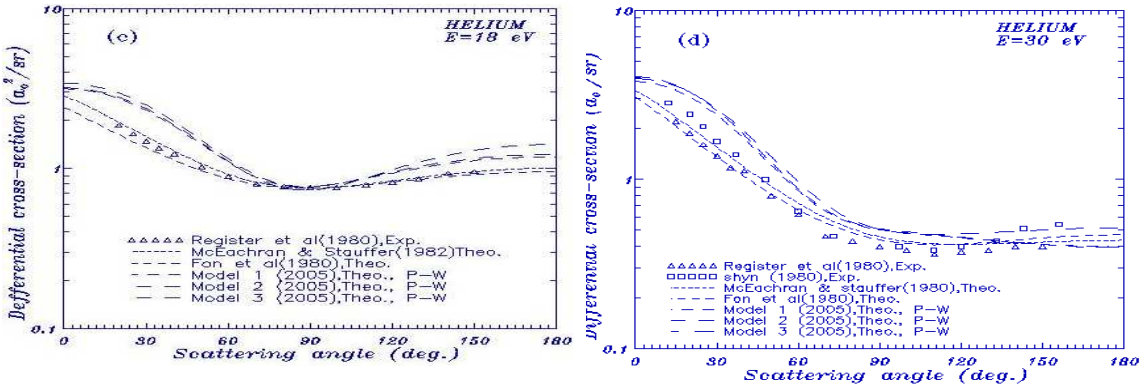

Figure (3):Differential cross-sections (a_o^2 / sr) for the elastic scattering of electrons from helium atoms for an incident electron energy (a) 5eV, (b) 12eV, (c) 18eV and (d) 30eV.

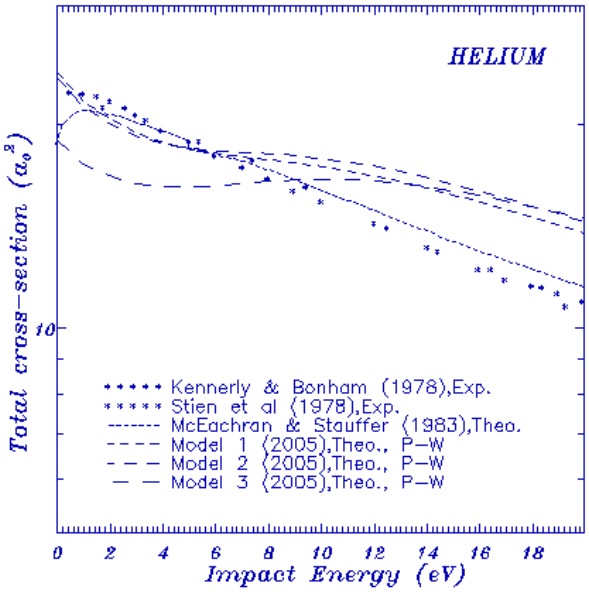

Figure (4): Total cross-sections (a_o^2) for an incident electron energy range (1-20eV) for helium atom.

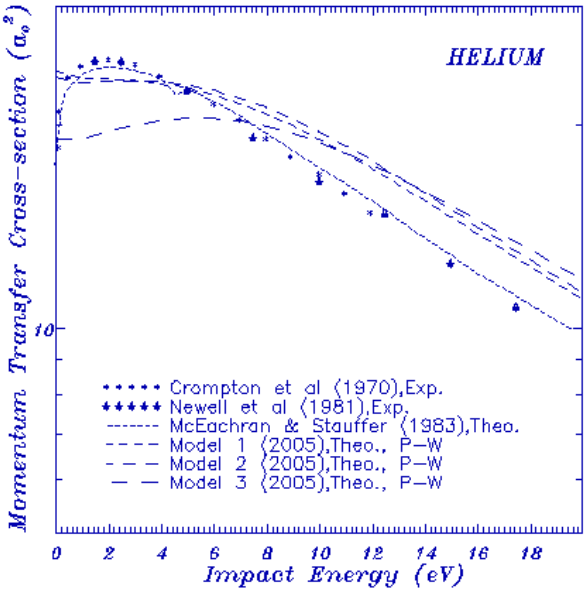

Figure (5): Momentum transfer cross-sections (a_o^2) for an incident electron energy region (1-20eV) for helium atom.

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اختبارات نظرية لنماذج جهد الاستطارة لنظام الكترون – ذرة : انفصال خياري للتبادل والترابط مع تصحيح السلوك المقارب للمدى الطويل في نظرية دوال الكثافة

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الملخص:

ان تاثيرات جهود الاستطارة تم اختبارها باستخدام طريقة الموجة المجزئة للاستطارة المرنة للالكترونات من ذرة الهيليوم عند الطاقة الواطئةواستخدمت الدوال الموجية الذرية للباحثين (روثان–هارتري–فوك) لانجاز هذة الحسابات.في هذا البحث تم اشتقاق ثلاثة نماذج حديثة لجهود الترابط من دوال طاقة الترابط للباحثين (ارمينتو–ماتسون)(2003) و (باير–نيوهاوسر)(2005) على التوالي.هذة النماذج الثلاث استخدمت بصورة منفصلة لتركيب جهود الاستطارة الكلية التي استخدمت لانجاز الحسابات,وهذا يمكن ان يعتبر كاضافة جديدة في هذا المجال حيث نوقشت النتائج التي تم الحصول عليها.هذه النماذج لجهد الاستطارة الكلي تتكون من مجموع جهد التبادل للغاز الالكتروني المعتمد على الطاقة (نموذج هارا) مضافا اليه جهد الترابط للغاز الالكتروني غير المعتمد على الطاقة (احد النماذج المشتقة في هذا العمل) مضافا اليه جهد الاستقطاب ذو المدى الطويل (نموذج علي) مضافا اليه الجهد المستقر (الاستاتيكي) المعروف.لقد تم الحصول على نتائج معدلة للمقاطع العرضية التفاضلية والكلية والمقاطع العرضية لزخم الانتقال على التوالي.ان النماذج والنتائج المقابلة المستخلصة يمكن ان تعتبر كاضافة جديدة في هذا المجال.ان النتائج التي تم الحصول عليها في هذا البحث في حالة اتفاق جيد مع النتائج العملية والقياسات المختبرية للباحثين الاخرين.