Elastic Scattering of Electrons by Helium Atoms at Intermediate Energies

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The unitarised Eikonal Born series (UEBS) method has been used successfully by Byron et al. for elastic scattering of electrons and positrons by hydrogen atoms. Here an attempt is made to apply the UEBS method in the case of elastic scattering of electrons by helium atoms. The total and differential cross sections are calculated for the energy range 100–700 eV. The results are compared with experimental and other theoretical results. It is found that the results obtained with the UEBS method agree best with the experimental results.

There is no simple yet satisfactory method for computing the scattering of electrons by helium atoms in the intermediate energy region. After the introduction of the Eikonal approximation in the potential scattering theory by Molière [1], Glauber [2] extended it by using a frozen target approximation to convert the many body scattering problem into a potential scattering problem in which the potential depends on the coordinates of the target. However this could not be free from some drawbacks (Byron et al. [3]). To eliminate the deficiencies of the eikonal approximation and the Glauber many body generalization, Byron and Joachain [4] formulated the Eikonal-Born series (EBS) method. But the EBS method was not unitarised. On the other and, Wallace [5, 6] introduced a systematic correction to the Eikonal phase that did not account, however, for long range polarization effects at small angles and represented absorption inadequately. To eliminate these difficulties, Byron et al. [7] suggested to remove the second order Wallace term f_{W2} from the Wallace amplitude f_W and to replace it by the second Born term f_{B2}. The direct amplitude thus obtained was called the Unitarised Eikonal Born series (UEBS) amplitude. They applied the UEBS method successfully to the elastic scattering of electrons and positrons by hydrogen atoms in the energy range 100 to 400 eV [7] and obtained better results than those obtained with the other methods. In the present investigation the UEBS method is applied to the elastic scattering of electrons by He atoms in the intermediate energy range.

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The interaction potential between the electron and the helium atom in the direct arrangement channel can be expressed as (in atomic units)

$$V(\boldsymbol{r}, \boldsymbol{r}_1, \boldsymbol{r}_2) = \left(\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_1|} + \frac{1}{|\boldsymbol{r}-\boldsymbol{r}_2|} - \frac{2}{|\boldsymbol{r}|} \right), \quad (1)$$

where $\boldsymbol{r}$, $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the position vectors of the incident electron and target electrons, respectively, with respect to the target nucleus. In the cylindrical coordinate system, $\boldsymbol{r} = \boldsymbol{b} + z\hat{\eta}$, $\boldsymbol{r}_1 = \boldsymbol{b}_1 + z_1\hat{\eta}$ and $\boldsymbol{r}_2 = \boldsymbol{b}_2 + z_2\hat{\eta}$, where $\hat{\eta}$ is chosen perpendicular to the momentum transfer $\boldsymbol{k}$. If $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ are the initial and final wave vectors, then $\boldsymbol{k} = \boldsymbol{k}_i - \boldsymbol{k}_f$.

The Eikonal phase $\chi_0(\boldsymbol{b}, \boldsymbol{b}_1 \cdot \boldsymbol{b}_2)$ is given by

$$\chi_0(\boldsymbol{b}, \boldsymbol{b}_1, \boldsymbol{b}_2) = \int_{-\infty}^{\infty} V(\boldsymbol{b}, z, \boldsymbol{r}_1, \boldsymbol{r}_2)\, \mathrm{d}z\,. \quad (2)$$

Substituting V from (1) into (2), χ_0 is obtained as

$$\chi_0(\boldsymbol{b}, \boldsymbol{b}_1, \boldsymbol{b}_2) = \ln\left(\frac{\beta_1^2\, \beta_2^2}{b^2}\right) \quad (3)$$

with $\boldsymbol{\beta}_1 = \boldsymbol{b} - \boldsymbol{b}_1$ and $\boldsymbol{\beta}_2 = \boldsymbol{b} - \boldsymbol{b}_2$.

The Wallace correction is

$$\chi_1(\boldsymbol{b}, \boldsymbol{r}_1, \boldsymbol{r}_2) = \tfrac{1}{2} \int_{-\infty}^{\infty} (\nabla\chi_+ \cdot \nabla\chi_-)\, \mathrm{d}z\,, \quad (4)$$

where

$$\chi_+(\boldsymbol{b}, z, \boldsymbol{r}_1, \boldsymbol{r}_2) = -\int_{-\infty}^{z} V(\boldsymbol{b}, z', \boldsymbol{r}_1, \boldsymbol{r}_2)\, \mathrm{d}z'\,, \quad (5)$$

$$\chi_-(\boldsymbol{b}, z, \boldsymbol{r}_1, \boldsymbol{r}_2) = -\int_{z}^{\infty} V(\boldsymbol{b}, z', \boldsymbol{r}_1, \boldsymbol{r}_2)\, \mathrm{d}z'\,. \quad (6)$$

Using (4), (5) and (6), χ_1 is obtained as

$$\chi_1(\boldsymbol{b}, \boldsymbol{r}_1, \boldsymbol{r}_2) = 2I_1 + 2I_2 - I_3\,, \quad (7)$$

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where

$$I_1=\left(\frac{\pi}{b\,\beta_1}\right)^{1/2}(P_{-1/2}(U_1)-\hat{b}\,\hat{\beta}_1\,P_{1/2}(U_1)),$$

$$I_2=\left(\frac{\pi}{b\,\beta_2}\right)^{1/2}(P_{-1/2}(U_2)-\hat{b}\,\hat{\beta}_2\,P_{1/2}(U_2)),$$

$$I_3=\left(\frac{\pi}{\beta_1\,\beta_2}\right)^{1/2}(P_{-1/2}(U_3)-\hat{\beta}_1\,\hat{\beta}_2\,P_{1/2}(U_3)),$$

$$U_1=\frac{b^2+\beta_1^2+z_1^2}{2b\,\beta_1},\quad U_2=\frac{b^2+\beta_2^2+z_2^2}{2b\,\beta_2},$$

$$U_3=\frac{\beta_1^2+\beta_2^2+(z_2-z_1)^2}{2\beta_1\,\beta_2}.$$

$P_{1/2}$ and $P_{-1/2}$ are Legendre functions and $\hat{\beta}_1=\boldsymbol{\beta}_1/|\boldsymbol{\beta}_1|$, $\hat{\beta}_2=\boldsymbol{\beta}_2/|\boldsymbol{\beta}_2|$, $\hat{b}=\boldsymbol{b}/|\boldsymbol{b}|$.

In the present calculations the Hartree-Fock wave function for the ground state of the helium atom has been used. It is given by (Byron and Joachain [4])

$$\psi_{13}(r_1,r_2)=\frac{1}{4\pi}\left((A\,e^{-y_1r_1}+B\,e^{-y_2r_1})\,(A\,e^{-y_1r_2}+B\,e^{-y_2r_2})\right). \tag{8}$$

The normalization constant and exponential parameter in (8) are given as follows:

$A=2.60505$, $B=2.08144$, $y_1=1.41$ and $y_2=2.61$.

According to the UEBS method, the scattering amplitude f_{UEBS} is given by (Byron et al. [7])

$$f_{\mathrm{UEBS}}=f_{\mathrm{W}}-\bar{f}_{\mathrm{W2}}+\bar{f}_{\mathrm{B2}}, \tag{9}$$

where f_{W}, $\bar{f}_{\mathrm{W2}}$, and $\bar{f}_{\mathrm{B2}}$ are the Wallace amplitude, second order Wallace term and second Born term, respectively.

For $\mathrm{S}\to\mathrm{S}$ transitions f_{W} and $\bar{f}_{\mathrm{W2}}$ can be written as (Byron et al. [7])

$$f_{\mathrm{W}}(\mathrm{S}\to\mathrm{S})=-i\,k_{\mathrm{i}}\int_0^\infty J_0(kb)\,\langle\psi_{\mathrm{m}}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\,[\exp i\{k_{\mathrm{i}}^{-1}\,\chi_0(\boldsymbol{b},\boldsymbol{r}_1,\boldsymbol{r}_2)+k_{\mathrm{i}}^{-3}\,\chi_1(\boldsymbol{b},\boldsymbol{r}_1,\boldsymbol{r}_2)\}-1]\,|\psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle\,b\,\mathrm{d}b, \tag{10}$$

$$\bar{f}_{\mathrm{W2}}(\mathrm{S}\to\mathrm{S})=\int_0^\infty J_0(kb)\,\langle\psi_{\mathrm{m}}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\,\{\tfrac{1}{2}\,i\,k_{\mathrm{i}}^{-1}\,\chi_0^2(b,\boldsymbol{r}_1,\boldsymbol{r}_2)+k_{\mathrm{i}}^{-2}\,\chi_1(\boldsymbol{b},\boldsymbol{r}_1,\boldsymbol{r}_2)\}\,|\psi_0(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle\,b\,\mathrm{d}b. \tag{11}$$

Here ψ_{m} and ψ_0 correpond to S-states.

We have replaced $\bar{f}_{\mathrm{B2}}$ by the simplified second Born term $\bar{f}_{\mathrm{SB2}}$ which is taken as (Joachain [8])

$$\bar{f}_{\mathrm{SB2}}=\frac{\left[\left(\frac{2}{\pi^2}\right)\mathrm{d}\boldsymbol{k}\,\langle 0|\sum_{i=1}^{z}\left\{(\exp(i\boldsymbol{k}_1\cdot\boldsymbol{r}_i)-1)\sum_{j=1}^{z}\exp(i\boldsymbol{k}_2\cdot\boldsymbol{r}_j)-1\right\}|0\rangle\right]}{k_1^2\,k_2^2(k^2-P^2-i\varepsilon)}, \tag{12}$$

where $\boldsymbol{k}_1=\boldsymbol{k}_{\mathrm{i}}-\boldsymbol{k}$, $\boldsymbol{k}_2=\boldsymbol{k}-\boldsymbol{k}_{\mathrm{f}}$, $P^2=k_{\mathrm{i}}^2-2\bar{W}$, $\bar{W}=$ mean excitation energy $=1\cdot 3$ a.u.

In this case we have used the first Born exchange amplitude $\bar{g}_{\mathrm{B1}}$, which is given by (Byron et al. [7])

$$\bar{g}_{\mathrm{B1}}=-(2\pi)^{-1}\,\langle\exp(i\boldsymbol{k}_{\mathrm{f}}\cdot\boldsymbol{r}_1)\,\psi_{13}(\boldsymbol{r}_1,\boldsymbol{r}_2)\,|V_{\mathrm{p}}|\,\exp(i\boldsymbol{k}_{\mathrm{i}}\cdot\boldsymbol{r})\,\psi_{13}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle. \tag{13}$$

The exchange potential for the $\bar{e}$-He collision is taken as

$$V_{\mathrm{p}}=\left(\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}|}+\frac{1}{|\boldsymbol{r}-\boldsymbol{r}_2|}-\frac{2}{|\boldsymbol{r}_1|}\right). \tag{14}$$

The differential cross section $I(\theta)$ and total cross section Q_{t} for the $\bar{e}$-He elastic collision are obtained by the relations

$$I(\theta)=|f_{\mathrm{UEBS}}-\bar{g}_{\mathrm{B1}}|^2,\quad Q_{\mathrm{t}}=\int I(\theta)\,\mathrm{d}\Omega. \tag{15), (16}$$

Table 1. Total cross sections (a^2) for the elastic scattering of electrons by helium atoms in the energy range 100–700 eV.

Energy (eV)	Theoretical values			Experimental values		
	Present UEBS	EBS	OM	Dalba et al. (1979)	Blaauw et al. (1980)	Kauppila et al. (1981)
100	4.135	4.57	6.16	4.15	3.97	3.96
200	2.751	2.89	3.37	2.73	2.58	2.55
300	1.993	2.14	2.38	2.02	1.98	1.95
400	1.664	1.71	1.86	1.61	1.64	1.61
500	1.398	1.44	1.54	1.35	1.35	1.36
700	1.015	1.10	1.16	1.01	1.04	–

Results and Discussions

The total cross sections (TCS) and differential cross sections (DCS) for the elastic scattering of electrons by helium atoms, calculated for incident energies ranging from 100 eV to 700 eV, are given in Tables 1 and 2, respectively. The TCS results are compared with the theoretical results calculated using the EBS method (Byron and Joachain [9]) and the optical potential model (OM) (Byron and Joachain [10]), and with the experimental results of Dalba et al. [11], Blaauw et al.

Table 2. Differential cross sections (a^2/sr) for the elastic scattering of electrons by helium atoms in the energy range 100–700 eV as obtained from the present UEBS theory.

Angle (degrees)	100	200	300	400	500	700
0	3.911	2.813	2.283	1.909	1.815	1.664
5	3.073	1.895	1.334	9.993 (−1)	9.123 (−1)	7.561 (−1)
10	2.210	1.108	8.109 (−1)	6.567 (−1)	5.592 (−1)	4.443 (−1)
20	1.121	5.394 (−1)	3.559 (−1)	2.751 (−1)	2.187 (−1)	1.507 (−1)
30	6.225 (−1)	2.591 (−1)	1.743 (−1)	1.191 (−1)	8.969 (−2)	5.438 (−2)
40	3.458 (−1)	1.470 (−1)	8.391 (−2)	5.611 (−2)	3.927 (−2)	2.199 (−2)
50	2.201 (−1)	8.650 (−2)	4.583 (−2)	2.899 (−2)	1.891 (−2)	1.071 (−2)
60	1.391 (−1)	5.291 (−2)	2.633 (−2)	1.639 (−2)	1.006 (−2)	5.756 (−3)
70	9.838 (−2)	3.390 (−2)	1.711 (−2)	9.887 (−3)	6.399 (−3)	3.577 (−3)
80	7.082 (−2)	2.359 (−2)	1.189 (−2)	6.653 (−3)	4.313 (−3)	2.308 (−3)
90	5.248 (−2)	1.708 (−2)	8.401 (−3)	4.918 (−3)	3.015 (−3)	1.626 (−3)
100	4.306 (−2)	1.363 (−2)	6.289 (−3)	3.717 (−3)	2.387 (−3)	1.208 (−3)
120	3.147 (−2)	9.924 (−3)	4.310 (−3)	2.451 (−3)	1.572 (−3)	7.893 (−4)
140	2.528 (−2)	8.197 (−3)	3.407 (−3)	1.852 (−3)	1.181 (−3)	6.033 (−4)
160	2.193 (−2)	7.266 (−3)	3.029 (−3)	1.572 (−3)	9.797 (−3)	5.009 (−4)
180	1.979 (−2)	6.519 (−3)	2.843 (−3)	1.489 (−3)	9.135 (−3)	4.612 (−4)

Table 3. Comparison of various theoretical and experimental differential cross sections for elastic electron-helium scattering at an incident electron energy of 200 eV. All results are in a^2/sr. Numbers in parenthesis are powers of ten.

Angle (degrees)	Theoretical values			Experimental values		
	Present UEBS	EBS	OM	Bromberg (1974)	Sethuraman et al. (1974)	Jansen et al. (1976)
0	2.813	3.16	2.99	–	–	–
5	1.895	2.12	1.98	1.73	–	1.68
10	1.108	1.34	1.25	1.12	–	1.08
20	5.394 (−1)	5.83 (−1)	5.75 (−1)	5.27 (−1)	–	5.28 (−1)
30	2.591 (−1)	2.88 (−1)	2.91 (−1)	2.76 (−1)	2.63 (−1)	2.81 (−1)
40	1.470 (−1)	1.54 (−1)	1.55 (−1)	1.52 (−1)	1.57 (−1)	1.51 (−1)
50	8.650 (−2)	8.81 (−2)	8.86 (−2)	8.91 (−2)	9.30 (−2)	8.85 (−2)
60	5.291 (−2)	5.44 (−2)	5.43 (−2)	5.57 (−2)	5.38 (−2)	–
70	3.390 (−2)	3.63 (−2)	3.57 (−2)	3.72 (−2)	3.57 (−2)	–
80	2.359 (−2)	2.59 (−2)	2.49 (−2)	2.63 (−2)	2.47 (−2)	–
90	1.708 (−2)	1.97 (−2)	1.84 (−2)	1.90 (−2)	1.77 (−2)	–
100	1.363 (−2)	1.57 (−2)	1.42 (−2)	1.45 (−2)	1.40 (−2)	–
120	9.924 (−3)	1.13 (−2)	9.51 (−3)	–	9.80 (−3)	–
140	8.197 (−3)	9.15 (−3)	7.28 (−3)	–	6.80 (−3)	–
160	7.266 (−3)	8.14 (−3)	6.24 (−3)	–	–	–
180	6.159 (−3)	7.84 (−3)	5.94 (−3)	–	–	–

Table 4. Comparison of various theoretical and experimental differential cross sections for elastic electron-helium scattering at an incident electron energy of 500 eV. All results are in a^2/sr. Numbers in parenthesis are powers of ten.

Angle (degrees)	Theoretical values			Experimental values		
	Present UEBS	EBS	OM	Bromberg (1974)	Sethuraman et al. (1974)	Jansen et al. (1976)
0	1.815	2.03	1.98	–	–	–
5	9.123 (−1)	9.85 (−1)	9.34 (−1)	9.47 (−1)	–	9.06 (−1)
10	5.592 (−1)	5.80 (−1)	5.63 (−1)	5.77 (−1)	–	5.50 (−1)
20	2.187 (−1)	2.26 (−1)	2.23 (−1)	2.26 (−1)	–	2.24 (−1)
30	8.969 (−2)	9.08 (−2)	8.91 (−2)	9.15 (−2)	9.41 (−2)	9.33 (−2)
40	3.927 (−2)	4.02 (−2)	3.93 (−2)	4.10 (−2)	4.13 (−2)	4.12 (−2)
50	1.891 (−2)	2.20 (−2)	1.95 (−2)	2.02 (−2)	1.85 (−2)	2.03 (−2)
60	1.006 (−2)	1.14 (−2)	1.08 (−2)	1.13 (−2)	1.11 (−2)	–
70	6.399 (−3)	7.09 (−3)	6.58 (−3)	6.87 (−3)	6.10 (−3)	–
80	4.313 (−3)	4.79 (−3)	4.31 (−3)	4.48 (−3)	3.83 (−3)	–
90	3.015 (−3)	3.45 (−3)	3.01 (−3)	3.13 (−3)	2.54 (−3)	–
100	2.387 (−3)	2.63 (−3)	2.22 (−3)	2.30 (−3)	1.78 (−3)	–
120	1.572 (−3)	1.74 (−3)	1.38 (−3)	–	9.30 (−4)	–
140	1.181 (−3)	1.33 (−3)	1.01 (−3)	–	7.30 (−4)	–
160	9.797 (−4)	1.14 (−3)	8.38 (−4)	–	–	–
180	9.135 (−4)	1,08 (−3)	7.90 (−4)	–	–	–

[12], and Kauppila et al. [13]. Detailed comparisons of the present DCS values with the theoretical results calculated using the EBS and OM theories and experimental results of Bromberg [14], Sethuraman et al. [15] and Jansen et al. [16] for the energies 200 and 500 eV are shown in Tables 3 and 4, respectively. The present TCS values are smaller than those obtained from the EBS and OM methods. But they are in better agreement with the experimental results of Kauppila et al. [13]. The present DCS values are smaller than those obtained with the EBS method in the given angular and energy region, but they are found in better agreement with the experimental results than those from EBS method. This shows an improvement in the TCS and DCS values due to the unitarisation of the EBS method. Also, there is good agreement between the present results and OM results at small angles. At large angles there is poor agreement between the present results and the OM results, and also between the EBS and the OM results. At large angles the convergence of the perturbation theory is slow. Since the OM method treats the static potential, which is very important in large angle scattering, exactly to all orders of perturbation theory, the optical model is more accurate than the Eikonal-Born series method at large angles (Byron and Joachain [10]). However, at large angles some improvement is observed in the present results as compared to the EBS results. The present results can further be improved by using UEBS exchange amplitudes (Byron et al. [7]).

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