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OPTICAL-POTENTIAL APPROACH TO HIGH-ENERGY ELECTRON-ATOM SCATTERING. APPLICATION TO e-He AND e-O COLLISIONS

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Abstract: Starting from the scattering amplitude in the second Born approximation an optical potential for elastic scattering of electrons on complex atoms is obtained. Proposed optical model gives the possibility of direct determination of the high-energy elastic scattering cross-section in the second Born approximation.
General theoretical results are applied to the e-He and e-O collisions. Results of the calculations are compared with the experimental data as well as with the more exact calculations.

1. Introduction

In the theoretical treatment of the scattering of electrons on atoms at high energies, the atomic field as seen by the incident electron can be satisfactorily approximated by an effective potential represented by an electron-atom interaction averaged over the wave function of the atom. At low energies the atomic structure begins to manifest itself in the scattering (distortion and exchange effects) and such an averaging becomes ineffective. While the exchange effects can be taken into account by antisymmetrizing the total wave function, this is not so simple to perform with the distortion. It is well known that in the adiabatic approximation the description of the distortion effects is not complete[1]. Variational[2] and Temkin's nonadiabatic methods[3] are more successful, but their application is rather restricted. In the close-coupling method some polarization effects are included, but the results are strongly dependent on the number of states retained in the expansion.

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Another way of taking into account these effects is to introduce an one--body non-local potential operator $\mathcal{U}$ into the scattering equation, known in the nuclear scattering problems as optical-potential method. To the atomic case this approach was applied by Mittleman and Watson and others[1]. Kelly[5] and Pu and Chang[6] used Coldstone diagrammatic technique to obtain optical potentials for e-H and e-He low-energy elastic scattering, with remarkably good results.

In the high-energy electron-atom scattering the optical potential method was first applied by Massey and Mohr[7], using the second Born amplitude as the starting point. They obtained the asymptotic behaviour of the potential only. Following their idea, Ob'edkov[8] constructed a complex potential for the elastic scattering of the electrons from the hydrogen atom. At $k \geqslant 1.2$ his cross-section is identical with that of Kingston and Skinner[9], calculated in the second Born approximation, taking into account the $1s$, $2s$ and $2p$ atomic states. Recently Amus'ya[10] gave a theoretical field version of the optical-potential method for high energy electron-atom collisions. However, his final results contain parameters which must be determined from the experimental data. The generalization of the method of ref.[8] to the case of elastic electron scattering from an arbitrary atom is made in Section 2. In Section 3. as examples of application of the method we calculated the zero angle scattering intensity, and the cross sections for elastic e-He and e-O collisions, calculating the first order quantities in the Hartree--Fock approximation for the atomic field.

2. *Optical potential for elastic electron-atom scattering*

Let us consider the scattering of an electron on the atom A in his ground state. Let $\vec{r}_1$ and $\vec{r}$ be the coordinates of the incident electron and all atomic electrons, respectively. If the Hamiltonian of the (e + A) system is H, then the total wave function $\Psi(\vec{r}_1, \vec{r})$ satisfies the equation

$$(H - E)\,\Psi(\vec{r}_1, \vec{r}) = 0, \tag{1}$$

$$H = H_A + T_1 + V = H_0 + V, \tag{2}$$

where E is the total energy, H_A the atomic Hamiltonian, T_1 is the kinetic energy operator of the incident electron, and V represents the electron-atom electrostatic interaction. Equation (1) is usually solved by expanding the total

wave function Ψ in terms of the eigen-functions $|n>$ of the atomic Hamiltonian, i. e. as $\Psi = \Sigma F_n |n>$, where the coefficients $F_n(\vec{r}_1) = <n|\Psi>$ describe the motion of the scattered electron and have standard asymptotic behaviour:

$$F_n(\vec{r}_1) \underset{\vec{r}_1 \to \infty}{\sim} |\vec{k}_n \vec{r}_1> \delta_{on} + f_n \exp(ik_n r_1)/r_1 \tag{3}$$

(k_n is the relevant wave number of the $\vec{r}_1$ electron).

The function F_0 describes the elastic scattering and it should be determined. The general methods of determining F_n are well known[11]. Here, we are interested in F_0 only, and for this funotion substitution of the expansion $\Sigma F_n |n>$ in (1) gives

$$\left(T_1 - \frac{k_0^2}{2} + U\right) F_0 = 0 \tag{4}$$

where $k_0/2$ is the kinetic energy of the incident electron, and the potential operator U is defined as

$$U F_0 = <0|V|\Psi>. \tag{5}$$

The equation (4) describes the motion of a particle in the field U, and thus if k_0' is the momentum of the scattered electron, elastic scattering amplitude has the form

$$f = -\frac{1}{2\pi} <\vec{k}_0' \vec{r}_1 | U F_0(\vec{r}_1)> \tag{6}$$

The first approximation for f can be obtained if for Ψ we take the eigenfunctions of the noninteracting system operator H_0, i. e. $\Psi^{(0)} = \Phi = |\vec{k}_0 \vec{r}_1> |0>$. This is just the first Born approximation $f_{B_1} = -\frac{1}{2\pi} <\vec{k}_0 \vec{r}_1 | V_{00} | \vec{k}_0 \vec{r}_1>$, $V_{00} = <0|V|0>$. To obtain the second approximation for f, we should calculate $U F_0$ with the first order wave function,

$$\Psi^{(1)} = (1 + g^{(-)} V)\Phi, \tag{7}$$

and we obtain the second Born amplitude,

$$f_{B_2} = -\frac{1}{2\pi} <\vec{k}_0' \vec{r}_1 | (U F_0)^{(1)}> \tag{8}$$

The resolvent operator $g^{(-)}$ in the coordinate representation is expressed by the Green's function (ref.[11], p. 331)

$$G^{(-)}(\vec{r}_1 \vec{r} \,|\, \vec{r}_1' \vec{r}') = \Sigma' \,|\, n > G_n^{(-)}(\vec{r}_1 \,|\, \vec{r}_1') < n' \,|\,, \tag{9}$$

where

$$G_n^{(-)} = -\frac{1}{4\pi} \frac{\exp(-k_n |\vec{r}_1 - \vec{r}_1'|)}{|\vec{r}_1 - \vec{r}_1'|} .$$

The »prime« indicates that in the sum the $n = 0$ term is omitted. With (7) and (9) for $(\mathcal{U} F_0)^{(1)}$ one obtains

$$(\mathcal{U} F_0)^{(1)} = (V_{00} + V_{0s}) \,|\, \vec{k}_0 \vec{r}_1 >, \tag{10}$$

where $\mathcal{U}_{0s}$ is the operator

$$V_{0s} \,|\, \vec{k}_0 \vec{r}_1 > = \sum_n{}' V_{0n} < G_n^{(+)}(\vec{r}_1 \,|\, \vec{r}_1') V_{n0}(\vec{r}_1') \,|\, \vec{k}_0 r_1' > . \tag{11}$$

The second term in (10) represents the correction term of the second Born approximation, and all the above considerations are exact in frame of this approximation.

Now we shall take into account that the incident electron energy is high $(k_0^2 \gg 1)$, and assume that in the sum (11) the main contribution gives the terms with n close to zero. This approximation was suggested by Massey and Mohr,[7] and its physical meaning is that in an electron-atom collision only the first few higher states have effect on elastic scattering. Taking this into account, from (11) for V_{0s} we obtain

$$V_{0s} = <0 \,|\, V \,|\, s>, \tag{12}$$

$$|\, s > \vec{k}_0 \vec{r}_1 > = |\, 0 > < G_0^{(+)} \vec{r}_1 \,|\, \vec{r}_1') \,|\, V(\vec{r}_1 \vec{r}_1') \,|\, k_0 r_1' > . \tag{13}$$

Following the procedure of ref.[8], the integral in (13) can be estimated by expanding it in terms of k_0^{-1} retaining the first term only. The result is

$$|\, s > = -i \frac{\varkappa}{k_0} \,|\, 0 > . \tag{14}$$

With $\varkappa$ in (14) we designate a slowly varying function (a sum of logarithmic terms), which at $k_0^2 \gg 1$ does not depend on energy, and for which we shall take to be constant. Now, using (14), (12) and (10) we obtain

$$(\mathcal{U} F_0)^{(1)} = \widetilde{V} \,|\, \vec{k}_0 \vec{r}_1 > \quad , \quad \widetilde{V} = \left(1 - i \frac{\varkappa}{k_0} \right) V_{00} \, . \tag{15}$$

The expressions for the amplitude and the elastic cross-section in this optical-potential model have the form

$$f_V = - \frac{1}{2\pi} < \vec{k}'_0 \vec{r}_1 \,|\, \widetilde{V} \,|\, \vec{k}_0 \vec{r}_1 >$$

$$= \left(1 - i \frac{\varkappa}{k_0} \right) f_{B1} \, , \tag{16}$$

$$\sigma_V = \left(1 + \frac{\varkappa^2}{k_0^2} \right) \sigma_{B1} \, , \tag{17}$$

i. e. they are expressed in terms of corresponding quantities in the first Born approximation.

Let us now determine the constant $\varkappa$. For a complex potential $\widetilde{V}$ as in (15), the generalized optical theorem (see, e. g. ref.[12], p. 255) gives

$$4\pi \operatorname{Im} f_V (0) = k_0 \sigma_V + \frac{\varkappa}{k_0} 2\pi f_{B1} (0) \, . \tag{18}$$

Using the expressions (16) and (17) (at $k_0^2 \gg 1$) for f_V and σ_V, from (18) one obtains

$$\varkappa = - \frac{k_0^2 \sigma_{B1}}{2\pi f_{B1} (0)} \, , \tag{19}$$

where from it can be seen that at high energies $\varkappa$ is really constant.

3. Calculation of the elastic e-He and e-O scattering cross-sections

In the existing literature several very accurate calculations of e-He and e-O elastic scattering in the low energy region[1, 6, 13, 14] are given. At high energies calculations exist only in the first Born approximation (see, e. g., ref.[11]). In this Section we shall calculate the cross-sections for these processes in the high-energy region using the optical-potential method of Section 2.

As it can be seen from (17) and (19), the problem of the elastic scattering cross-section calculation in our optical model is transfered to the calculation of this quantity in the first Born aproximation, i. e. to the determination of the static field V_{00} of the atom. In the calculations of σ_{B_1} and $\varkappa$ for e-He and e-O elastic collisions, for the static field V_{00} of the He and O atoms we used the Hartree-Fock expressions of Strand and Bonham[15]. The calculation of the scattering intensity $|f_{B_1}|^2$ is trivial. However, the result is fairly extensive to be done here (see, e. g., ref.[16]) there are two, probably typographical, errors which can be easily noted). The cross-section for e-He scattering we calculated also with one parameter variational wave function of the helium atom: $|0\rangle^{(0)} = (\alpha^3/\pi)^{1/2}$. exp. $[-\alpha(r_1 + r_2)]$, $\alpha = 27/16$ (the curve σ_V in Fig. 2). Comparison of σ_V^0 and σ_V^{HF} shows great sensitivity of the optical model results as regards the choise of the atomic wave function. It is interesting to note that σ_{B1}^0 and σ_{B1}^{HF} are different in the second decimal place only. The corresponding $\varkappa^2$ constants for $V_{00}^{(0)}$ and V_{00}^{HF} have the values: $[\varkappa^2]^{(0)} = 5.44$ and $[\varkappa^2]^{HF} = 3{,}98$.

In Fig. 1 the curves are given (versus incident electron energy) of the e-He scattering intensity in the forward direction, calculated in the first Born approximation (B1), and in the optical model (V). Curve DR represents

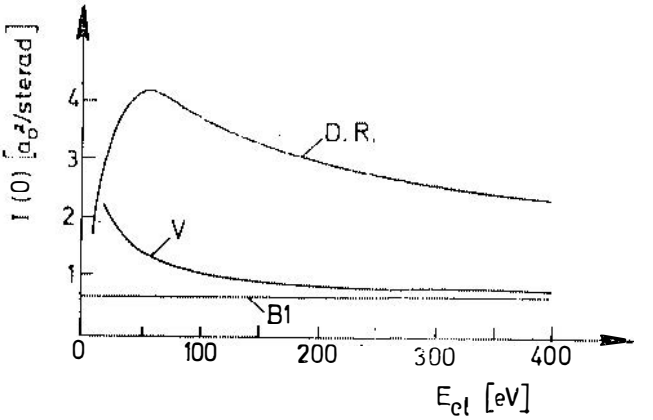

Fig. 1. Zero-angle intensity of e-He elastic scattering. B1-the first Born approximation, D. R. – dispersion relations result of ref.[17] and V – the optical-potential result of this paper.

the results of Lawson, Massey and Wallace[17] obtained from the dispersion relations. At electron energies in the range of 350 eV to 700 eV, the observed average value of $I(0)$ is about 0.75 (see ref. [18]), in accordance with the optical model result. The Hartree-Fock value of 0.655 was taken for $I_{B_1}(0)$.

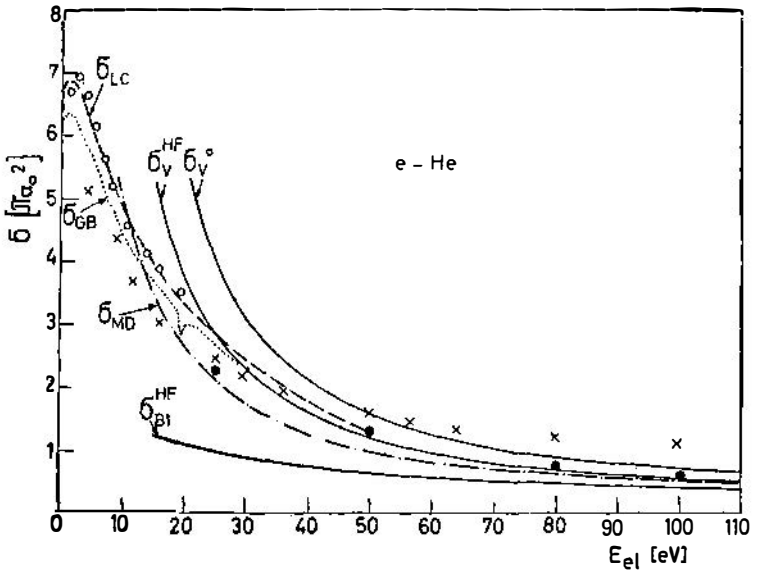

Fig. 2. Elastic e-He scattering cross-section. Full lines are the results of this paper. σ_{LC} and σ_{GB} are the calculations of La Bahn and Callaway[20] and experimental data of Golden and Bandel[23], respectively. The open circles and crosses are the total cross-sections of Ramsauer and Kolath[21] and Normand[22]. The full circles are »experimental« results obtained in the manner explained in the text.

The curves σ_{B1}^{HF}, $\sigma_V^{(0)}$ and σ_V^{HF} in Fig. 2 represent our cross sections for helium. The dash-dotted σ_{MD} curve in this figure is obtained from the partial wave formula using the numerically calculated phase shifts of McDougall[19]. In the same figure the results of LaBahn and Callaway[20] (curve LC) are plotted. They calculated the first three phase shifts for e-He in the adiabatic-polarization + dynamic-exchange approximation (including some velocity-dependent terms in the distortion potential). Very close to their results are those of Pu and Chang[6] (in the region 1,22 to 16,4 eV) in the modified optical-potential method. The open circles and crosses represent the experimentally obtained total cross-sections by Ramsauer and Kollath[21] and Normand[22], respectively. The curve σ_{GB} represents the experimental results of Golden and Bandel[23], and at high energies it approaches Normand's data In order to make possible a comparison of our calculations with the experimental cross-sections, we substracted the ionization cross-section of Smith[24] and the sum of the excitation cross-sections of the first nineteen singlet and triplet states of Moussa[25] from the total cross-section values of Normand at 25 eV, 50 eV, 80 eV and 100 eV incident electron energies.

So deduced »experimental« elastic cross-section values are represented in Fig. 2 by full circles. The close proximity of the σ_V^{HF} curve to these elastic cross-section points and to the McDougall's curve shows that optical model gives a possibility of relatively simple and very effective elastic cross-section calculations, whenever σ_{B_1} can be calculated with reasonable accuracy.

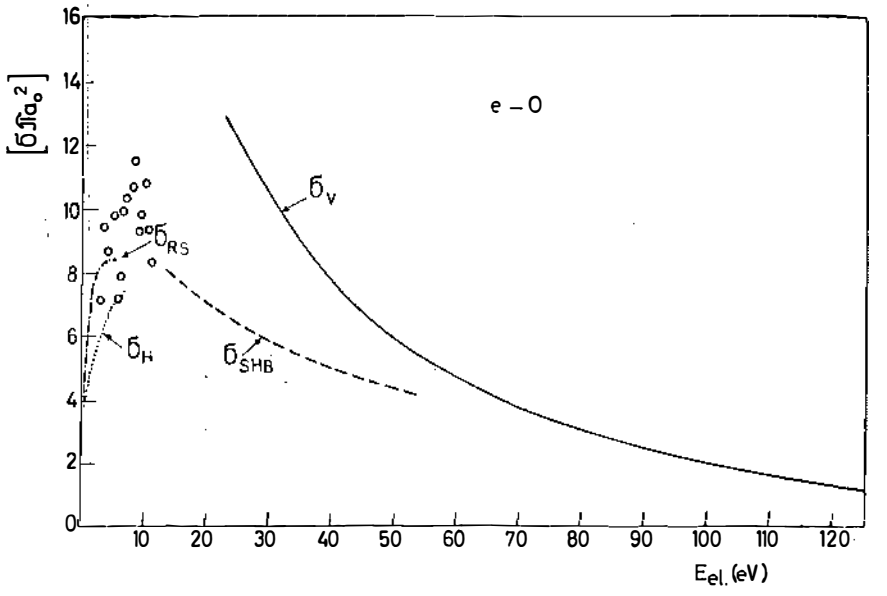

Fig. 3. Elastic e-O scattering cross-section. The full line represents the optical model results of this paper. The curves σ_{RG}, σ_H and σ_{SHB} are the theoretical results of refs.[26,27,28]. The open circles are experimental data of ref.[29].

The full line in Fig. 3 represents σ_V^{HF} cross-section for e-O elastic collision. In the low-energy region curves σ_{RG} and σ_H represent the calculations of Robinson and Geltman[26], and Henry[27] (Temkin's method), respectively. The σ_{SHB} curve are the results of the calculations of Smith, Henry and Burke[28] (numerical solution of the continuum Hartree-Fock equation without polarization). The open circles in this figure are the experimental results of Sunshine, Aubrey and Bederson[29]. The optical model result seems to be quite reasonable for this case also, since it is a satisfactory extrapolation of the fairly good calculations of Smith et al.[28]. This method also seems to be very useful in the estimation of high-energy elastic cross-sections of other electron-atom collisions important in the astrophysical laboratory plasmas because of its simplicity.

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ОПТИЧКО-ПОТЕНЦИАЛЕН ПРИСТАП КОН ВИСОКО-ЕНЕРГЕТСКОГО РАСЕЈУВАЊЕ НА ЕЛЕКТРОНИТЕ ОД АТОМИТЕ. ПРИМЕНА НА e-He и e-O СУДАРИ

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Содржина

При еластичното расејување на електроните од атомите во нивното основно состојание, другите атомски состојанија имаат значително влијание (разменски, поларизационни и др. ефекти) и при определувањето на амплитудата за расејување овоа влијание треба да се земе во предвид. При малите енергии на судирот постоат методи кои до извесен степен ги вклучуваат во теоријата овие ефекти: неадиабатски методи, метода на силното спрегнување на состојанијата итд. Друг начин да се земат во предвид овие ефекти и да се воведе во равенката за расејување еден едночестичен нелокален оператор чија природа е комплексна и кој е наречен оптички потенциал.

Во овој труд е изведен еден оптички потенциал за високо-енергетско еластично расејување на електроните од произволен атом во рамките на втората Борнова апроксимација (формулата [15] во текстот). Овој потенциал е изразен преку статичкото поле на атомот V_{00}, амплитудата за агол $\Theta = 0$ и асимптотиката на ефективниот пресек, пресметнати во првата Борнова апроксимација.

Амплитудата за расејување и ефективниот пресек во оптичкиот модел се изразени исто така преку соотвените количини во првата Борнова апроксимација (формулите [16] и [17] во текстот). Предложената метода за определување на еластичниот пресек при високите енергии е еквивалентна на втората Борнова апроксимација.

Како илустрација на методата пресметнати се ефективните пресеци за еластичното e-He и e-O расејување. Статичкото поле (значи и σ_{B1}) и константата $\varkappa$ (в. [19]) се определени во Хартри-Фоковската апроксимација. Резултатите се поредуваат со експерименталните мерења и премсетнувањата на другите автори, и при високите енергии, каде методата има важност, добиена е добра согласност.