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Core-Model Calculations of Triple-Differential Cross Sections for Electron Impact Ionization of Helium

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The triple-differential cross sections for electron impact ionization of helium have been calculated in the distorted wave Born approximation using a frozen core model. The wave functions used are obtained by the method of Herman-Skillman. The results calculated show considerable agreement with the experimental data.

KEY WORDS: Electron impact/ Helium ionization/ Triple-differential Cross sections/ DWBA calculations/ Frozen core model/

I. INTRODUCTION

The triple-differential cross section $d^3\sigma/d\Omega_f\, d\Omega_s\, dE_s$ for electron impact ionization is a measure of the probability of the phenomena that an electron impact will produce two free electrons: a faster electron of energy E_f into the differential element of solid angle at Ω_f and a slower electron of energy E_s into the differential element of solid angle at Ω_s. The value of E_s can be calculated from those of E_f, the energy of incident electron E_i and the ionization potential using energy conservation and is not an independent variable. The triple-differential cross section is the most detailed value of electron impact ionization except that related to the spin and is used most seriously to test the ability of any theory for ionization. Double- and single-differential cross sections are derived by integration which obscure details of the results of a theory.

The triple-differential cross sections of helium have been obtained experimentally by Ehrhardt *et al.*[1] and others[2~6] and compared with the results of many theories.[7~14] Sufficiently good agreements have not been obtained between the calculated results and the experimental ones for all cases. Two factors are considered to affect the theoretical results. One of them is the degree of approximation of a theory to the ionization phenomena and the other one is the suitability of the wave functions used.

In this work, a frozen-core model is proposed to obtain the triple-differential cross section of helium using the distorted wave Born approximation. The wave functions used are obtained for four quantum states by the method of Herman-Skillman.[15] The calculated results are compared with the experimental ones.

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II. THEORY

II. 1 *A core model*

In order to obtain the triple-differential cross section for electron impact ionization, a frozen core model has been assumed. In the model, an atom is considered to be composed of an core and an electron (No 2) which is ejected from the atom by the atom by the impact of incoming electron (No 1). The core is made of a nucleus and the residual electrons except the No 2 electron and is assumed not to change its state before and after the ionization. A potential which acts on the No 2 electron in the atom is denoted by $V(\boldsymbol{r}_2)$. Then the Hamiltonian for the No 2 electron is given by

$$H_2 = -(\hbar^2/2m)\nabla_2^2 + V(\boldsymbol{r}_2), \qquad (1)$$

where ∇_2 expresses the differentiation on the coordinate r_2 and m the electron mass. The incoming No 1 electron is considered to interact with core by the potential $V(\boldsymbol{r}_1)$ and with the No 2 electron by the Coulomb potential e^2/r_{12}, where r_{12} is a distance between two electrons. Then the total Hamiltonian is given by

$$H = [-(\hbar^2/2m)\nabla_1^2 + V(\boldsymbol{r}_1)] + [-(\hbar^2/2m)\nabla_2^2 + V(\boldsymbol{r}_2)] + e^2/r_{12}. \qquad (2)$$

Here, the distorted wave Born approximation is used. The triple-differential cross section is obtained as follows

$$d^3\sigma/d\Omega_f\, d\Omega_s\, dE_s = N_0(2\pi)^4/E_i \cdot [3/4 \cdot |T^D - T^E|^2 + 1/4 \cdot |T^D + T^E|^2] \qquad (3)$$

where

$$T^D = \langle \phi(\boldsymbol{r}_1, \boldsymbol{k}_f) \cdot \phi(\boldsymbol{r}_2, \boldsymbol{k}_s) \,|\, 1/r_{12} \,|\, \phi(\boldsymbol{r}_1, \boldsymbol{k}_i)\phi^B(\boldsymbol{r}_2) \rangle, \qquad (4)$$

$$T^E = \langle \phi(\boldsymbol{r}_2, \boldsymbol{k}_f)\phi(\boldsymbol{r}_1, \boldsymbol{k}_s) \,|\, 1/r_{12} \,|\, \phi(\boldsymbol{r}_1, \boldsymbol{k}_i)\phi^B(\boldsymbol{r}_2) \rangle \qquad (5)$$

and N_0 is the number of electron in an electronic shell of the atom. The symbols T^D and T^E are a T matrix for the direct and exchange reactions, respectively. The wave function ϕ for the continuum state is the wave distorted by the potential $V(\boldsymbol{r})$ and satisfies the following Schrödinger equation

$$[-(\hbar^2/2m)\nabla_2^2 + V(\boldsymbol{r})]\phi(\boldsymbol{r}, \boldsymbol{k}) = \hbar^2 k^2/2m. \qquad (6)$$

The function ϕ is expanded into the partial waves:

$$\phi(\boldsymbol{r}, \boldsymbol{k}) = (k\pi)^{-1/2}(1/r)\sum_{lm} i^l \beta_l(r, k) Y_{lm}^*(\hat{\boldsymbol{k}}) Y_{lm}(\hat{\boldsymbol{r}}). \qquad (7)$$

The wave function ϕ^B for the bound state is a solution of eq. (6) with the negative energy and is expressed by

$$\phi^B(\boldsymbol{r}_2) = i^{l_0}(1/r_2)\beta_{l_0}(r_2) Y_{l_0 m_0}(\hat{\boldsymbol{r}}_2). \qquad (8)$$

These wave functions are orthogonal with each other and substituted into Eqs. (4) or (5) with the following multipole expansion,

$$1/r_{12}=\sum_{lm}(4\pi/(4l+1)\cdot(r_2^l/r_1^{l+1})Y^*_{lm}(\hat{\boldsymbol{r}}_1)\cdot Y_{lm}(\hat{\boldsymbol{r}}_2), \tag{9}$$

then the T matrices are obtained in the same way as in Ref. 12, so that

$$T^D=(4\pi^3)^{-1}(k_ik_sk_f)^{-1/2}\times\sum_{l_2m_2}D^{l_0m_0}_{l_2m_2}(\theta_f)P^{|m_2|}_{l_2}(\cos\theta_s)\exp(im_2\phi_s) \tag{10}$$

where

$$D^{l_0m_0}_{l_2m_2}(\theta_f)=\sum_{l_1ll_i}G^{m_1m_2}_{l_0l_il_1l_2l}\cdot I^{k_ik_sk_f}_{l_0l_il_1l_2l}\cdot P^{|m_1|}_{l_1}(\cos\theta_f), \tag{11}$$

$$\begin{aligned} G^{m_1m_2}_{l_0l_il_1l_2l}=&(2l_i+1)(2l_1+1)(2l_0+1)^{1/2}(2l+1)^{-1}\\ &\times i^{(l_0+l_i-l_1-l_2)}\\ &\times(-1)^{(m_i+m_1+m_2+|m_i|+|m_1|+|m_2|)/2}\\ &\times C(l_il_1l,\ m_im_1m)\cdot C(l_0l\,l_2,\ m_0m\,m_2)\\ &\times C(l_il_1l,\ 000)\cdot C(l_0l\,l_2,\ 000)\\ &\times R^{|m_1|}_{l_1}\cdot R^{|m_2|}_{l_2}\cdot R^{|m_i|}_{l_i}, \end{aligned} \tag{12}$$

$$R^{|m|}_l=\left[\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}, \tag{13}$$

$$I^{k_ik_sk_f}_{l_0l_il_1l_2l}=\int_0^\infty\beta_{l_1}(R,\ k_f)\cdot\beta_{l_i}(R,\ k_i)F^{k_s}_{l_0ll_2}(R)\,dR, \tag{14}$$

$$F^{k_s}_{l_0ll_2}(R)=\int_0^\infty\beta_{l_2}(r,\ k_s)\beta_{l_0}(r)(r^l_</r^{l+1}_>)\,dr. \tag{15}$$

Here $P^{|m|}_l$ is the associated Legendre function, θ_f and θ_s are the polar angles of the direction of motion for the faster and slower electrons respectively, l_i, l_1 and l_2 are the orbital angular momenta of partial waves in Eq. (7) for the incoming, No 1 and No 2 electrons respectively, $C(l_1l_2l_3,\ m_1m_2m_3)$ is the Clebsh-Gordan coefficient and $r_<$ is the lesser of r or R.

For the T matrix of the exchange reaction,

$$\begin{aligned} T^E=&(4\pi^3)^{-1}(k_ik_sk_f)^{-1/2}\\ &\times\sum_{l_1m_1}E^{l_0m_0}_{l_1m_1}(\theta_f)\cdot P^{|m_1|}_{l_1}(\cos\theta_s)\cdot\exp(i\,m_1\phi_s) \end{aligned} \tag{16}$$

where

$$E^{l_0m_0}_{l_1m_1}(\theta_f)=\sum_{l_2ll_i}G^{m_1m_2}_{l_0l_il_1l_2l}I^{k_ik_fk_s}_{l_0l_il_1l_2l}P^{|m_2|}_{l_2}(\cos\theta_f), \tag{17}$$

and k_s and k_f are interchanged for I in Eq. (17).

II. 2 Numerical procedure

Numerical calculations were performed for the incoming energy of 256.6 eV and the slower electron energy of 3 eV for the comarison with the experimental results of Ehrhardt *et al.*[1)]

The wave function ($l_0=0$) of the bound state in helium atom was calculated by the method of Herman and Skillman[15] and the central atomic potential $V(r)$ was also obtained.

Integrations in Eqs. (14) and (15) were carried out up to a radius of 72 a_0 where a_0 is the Bohr radius. The maximum values of l used in the calculation were as follows: $l_i=39$, $l_1=39$, $l_2=9$ and $l=10$. The values of I of Eq. (14) decrease for large values of l_1 and l_i. Those in the case of $l_1=l_i=39$ were less than one-hundredth of those for small values of them. The values of F of Eq. (15) for large values of l and l_2 were also less than one-hundredth of those for small ones. From the variations of the values of F with R and those of I with l_1 and l_i, the errors of the numerical calculations were estimated approximately to be less than a few percents and considered to be sufficient for the comparison with the experimental results.

III. RESULTS AND DISCUSSION

The triple-differential cross sections were obtained for the incoming electron of 256.6 eV, the ejected slower electron of 3 eV and the scattering angles of the faster electron θ_f of 4°, 6°, 8°, 60°, 90°, 120° and 150°. The results are shown in Figs. 1 to 7. Experimental data of Ehrhardt *et al.*[1] are also shown in Figs. 1, 2 and 3 for the comparison with the calculated results. The dots in the figures express the representative mean values of experimental points. The peak experimental values in the forward angle of θ_s were normalized to the calculated ones. The angles of the peak nearly agree with each other all in three figures. The calculated values of lobe in the backward angle

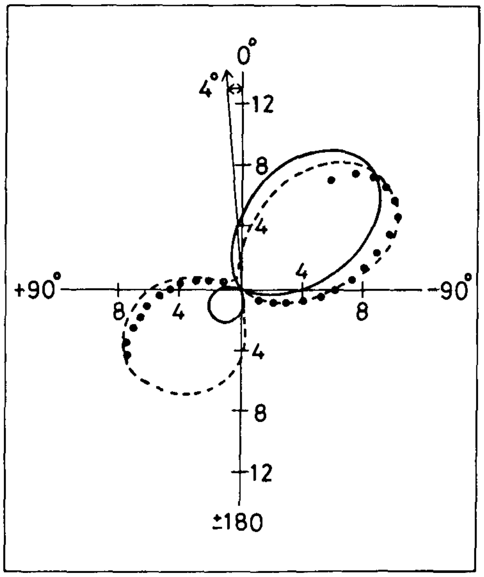

Fig. 1 Triple-differential cross section for 256.6 eV electron-impact ionization of helium in units of 10^{-3} a_0^2/sr^2 Ry. The angle of observation for the faster electron θ_f is 4° and the energy of the slower electron E_s is 3 eV. The solid curve is the present calculations. The dashed curve is the results calculated by Madison *et al.* The closed circles are the experimental data of Ehrhardt *et al.*

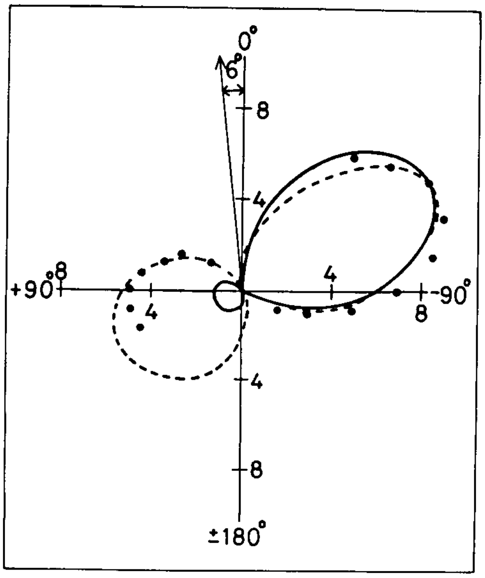

Fig. 2 Triple-differential cross section for 256.6 eV electron-impact ionization of helium in units of 10^{-3} a_0^2/sr^2 Ry. The angle of observation for the faster electron θ_f is 6° and the energy of the slower electron E_s is 3 eV. Symbols are the same as in Fig. 1.

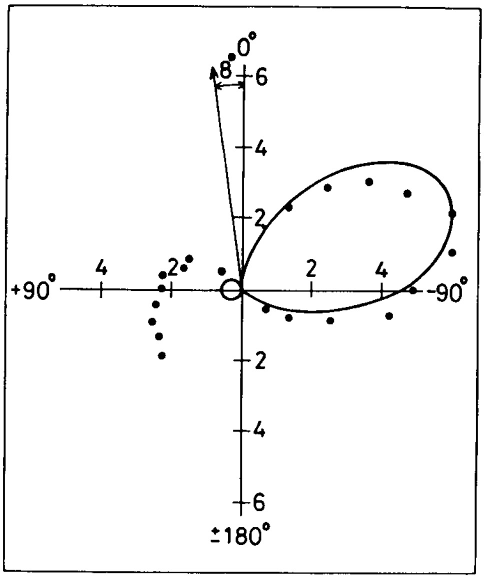

Fig. 3 Triple-differential cross section for 256.6 eV electron-impact ionization of helium in units of 10^{-3} a_0^2/sr^2 Ry. The angle of observation for the faster electron θ_f is 8° and the energy of the slower electron E_s is 3 eV. Symbols are the same as in Fig. 1.

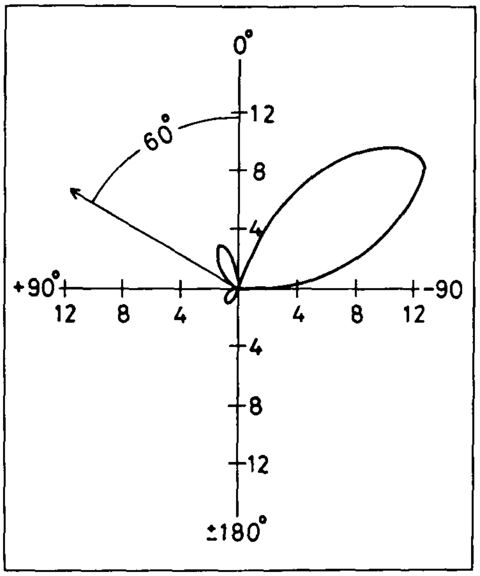

Fig. 4 Triple-differential cross section for 256.6 eV electron-impact ionization of helium in units of 10^{-8} a_0^2/sr^2 Ry. The angle of observaion for the faster electron θ_f is 60° and the energy of the slower electron E_s is 3 eV. The solid curve is the present calculation.

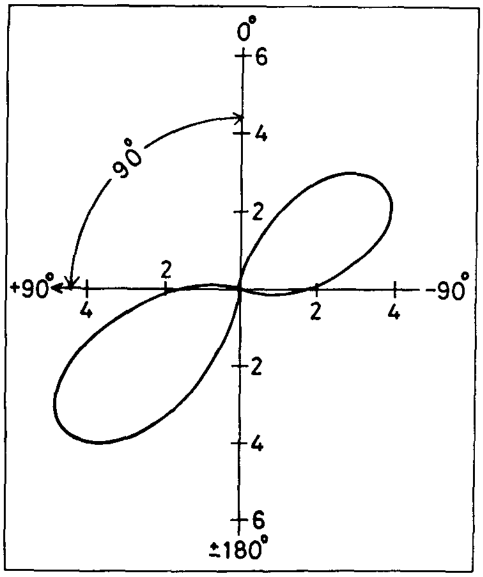

Fig. 5 Triple-differential cross section for 256.6 eV electron-impact ionization of helium in units of 10^{-8} a_0^2/sr^2 Ry. The angle of observation for the faster electron θ_f is 90° and the energy of the slower electron E_s is 3 eV. The solid curve is the present calculation.

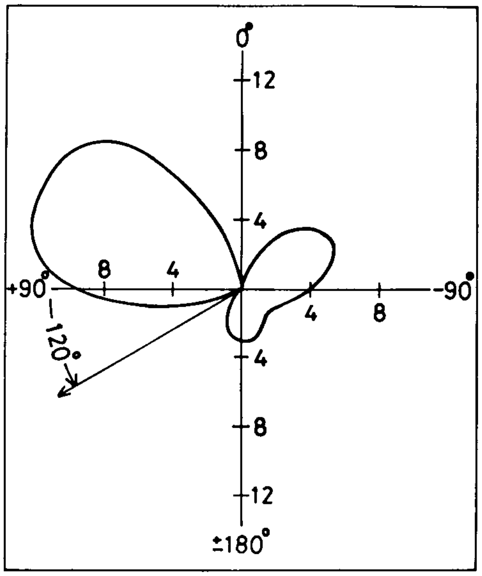

Fig. 6 Triple-differential cross section for 256.6 eV electron-impact ionization of helium in units of $10^{-7}\ a_0^2/sr^2\ Ry$. The angle of observation for the fatser electron θ_f is 120° and the energy of the slower electron E_s is 3 eV. The solid curve is the present calculation.

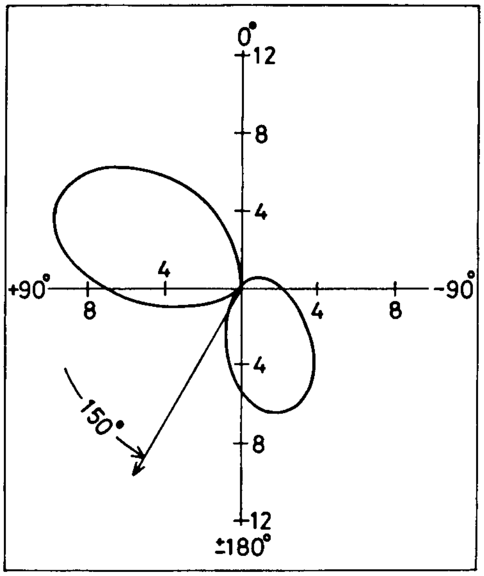

Fig. 7 Triple-differential cross section for 256. 6 eV electron-impact ionization of helium in units of $10^{-7}\ a_0^2/sr^2\ Ry$. The angle of observation for the faster electron θ_f is 150° and the energy of the slower electron E_s is 3 eV. The solid curve is the present calculation.

are about one-third of the experimental ones. The values calculated by Madison *et al.*[12] are shown by dotted lines in Figs. 1 and 2. The agreements of their values with the experimental data are better than those of the present work. They obtained the atomic potential using the Hartree-Fock program of Froes-Fischer.[16] The neutral potential was used to calculate the fast continuum electron wave function as in the present work, where all wave functions were obtained for the same potential. However, the ionic potential was used for the calculations of the bound-state wave function and the slow continuum electron wave function. These differences are considered to result in the diversity between two calculated results.

For other values of θ_f, there are no experimental data. The present results show the large variation of the pattern of the triple-differential cross section with the angle θ_f. Therefore it will be very interesting to compare the calculated with the exparimental ones for large value of θ_f, for which the value of the cross section is about 10^{-4} times as large as those for the small angle. It may be difficult to obtain them experimentally.

In the present work, the frozen core model has been used. In the case of helium atom two electrons in the atom are interacting before the electron impact ionization. After it happens one of them is ejected from the atom and the other one remains as a constituent of the core in the atom. The electronic wave funcion of this electron will change in a certain amount which can not be neglected. Therefore, the frozen core mobel may not be a good approximation for helium. This will be one of the causes of the insufficient agreement between the calculated and experimedtal data. For the further improvement of the model, the use of the ionic potential or the effective charge is considered to obtain the distorted waves. This use is, however, not logical in the present model. It will be desirable to make the core soft and to take into consideration the effect of the change of its state.

The frozen core model is considered to be most suitable for the ionization of sodium atom for example. The triple-differential cross sections of sodium are required to be measured to test the model.

IV. CONCLUSIONS

The triple-differential cross sections calculated for helium show considerable close agreement with the experimental data. The forzen core model used is considered to be modified somewhat for helium in order to obtain the better agreement with the experimental data. The similar measurements on the atom of the alkali metal are desirable to test the applicability of the core model to the electron impact ionzation.

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