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# ANGULAR DISTRIBUTION OF ELECTRONS EJECTED BY CHARGED PARTICLES

## II. THE BINARY-ENCOUNTER POLARIZED-ORBITAL METHOD

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**Synopsis**

Cross sections for ejection of electrons from helium by 100 to 300 keV protons have been calculated with a combined binary-encounter polarized-orbital method. The resulting cross sections are shown to be in better agreement with experiment than those obtained with the binary-encounter theory alone. Remaining discrepancies are discussed in some detail.

1. *Introduction*. In ref. 1, differential binary-encounter cross sections were calculated for electron ejection from He and $H_2$ by 100 to 2000 keV protons. Comparison with the experimental cross sections of Rudd *et al.*[2]) showed good agreement for intermediate ejection angles and not too small ejection energies. In the forward direction, however, the calculated cross sections were found to be much smaller than the experimental ones.

Bonsen and Banks[3]) used the classical three-body computer programme developed by Percival and coworkers[4]) to calculate the differential electron-ejection cross sections. Very good agreement with experiment was obtained for forward electron ejection.

Salin[5]) and Macek[6]) also calculated differential cross sections for electron ejection from $H_2$ and He by protons. Salin generalized the theory of Rudge and Seaton[7]) for incident electrons to incident heavy particles and Macek used the first term of the Neumann expansion of Faddeev's equations. The approximations of Salin and Macek are superior to the binary-encounter and Born approximations in that they give a forward peaking of the cross sections, as found experimentally. The peak at larger angles (the binary peak), however, is not reproduced very well. Salin's theory for ejection of, for example, 150 eV electrons from $H_2$ by 300 keV protons, reproduces the maximum of this peak well but gives a width, that is only 50% of the experimental one. Macek's theory reproduces the width but overestimates the magnitude of the cross sections by 70%.

Our theory differs from Salin's and Macek's theories in that we only take account of the initial-state distortion (prior interaction, polarization) while Salin and Macek only include the final-state distortion (post interaction) in their calculations.

2. *Polarized wavefunctions and velocity distributions.* The polarization of the target atom by the slow proton is included using Temkin's[8]) polarized orbital method. The Schrödinger equation for the undistorted He atom is

$$(\nabla_3^2 + \nabla_2^2 + 4/r_2 + 4/r_3 - 2/r_{23} + \Gamma)\,\psi(\boldsymbol{r}_2; \boldsymbol{r}_3) = 0, \tag{1}$$

where $\boldsymbol{r}_2$ and $\boldsymbol{r}_3$ stand for the position coordinates of the atomic electrons with respect to the nucleus, $r_{23} = |\boldsymbol{r}_2 - \boldsymbol{r}_3|$ and $\Gamma$ is the energy of the He atom. The coordinates are given in atomic units. We now make first the hydrogenic approximation, hence $4/r_2 + 4/r_3 - 2/r_{23}$ is replaced by $2Z/r_2 + 2Z/r_3$, $Z$ being the effective nuclear charge and $\psi(\boldsymbol{r}_2; \boldsymbol{r}_3)$ is replaced by $\psi(\boldsymbol{r}_2)\cdot\psi(\boldsymbol{r}_3)$. Next we follow Temkin's convention to take the polarization potential equal to zero if the internuclear distance $r_1$ is smaller than $r_2$, $r_3$ and to include only the dipole polarization potential

$$(2r_2/r_1^2)\cos\theta_{12} + (2r_3/r_1^2)\cos\theta_{13} \qquad \text{for} \qquad r_1 > r_2, r_3.$$

This is the first term of the multipole expansion of the complete distortion potential $-4/r_1 + 2/r_{12} + 2/r_{13}$. Here $\boldsymbol{r}_1$ is the position vector of the proton and $\theta_{1i}$ the angle between $\boldsymbol{r}_1$ and $\boldsymbol{r}_i$. Inclusion of the polarization potential and addition of polarization terms to the undistorted wavefunctions $\psi(\boldsymbol{r}_2)$ and $\psi(\boldsymbol{r}_3)$ yields:

$$\left[\nabla_2^2 + \frac{2Z}{r_2} + \frac{2r_2\cos\theta_{12}}{r_1^2} + \nabla_3^2 + \frac{2Z}{r_3} + \frac{2r_3\cos\theta_{13}}{r_1^2} + \Gamma\right] \times [\psi(\boldsymbol{r}_2) + \psi^{\text{pol}}(\boldsymbol{r}_2; \boldsymbol{r}_1)][\psi(\boldsymbol{r}_3) + \psi^{\text{pol}}(\boldsymbol{r}_3; \boldsymbol{r}_1)] = 0. \tag{2}$$

Separation of variables and substitution of $\Gamma = -2Z^2$ gives in first-order approximation

$$\psi(\boldsymbol{r}_i) + \psi^{\text{pol}}(\boldsymbol{r}_i; \boldsymbol{r}_1) = \left(\frac{Z^3}{\pi}\right)^{\frac{1}{2}} e^{-Zr_i}\left\{1 + \frac{\varepsilon(r_1; r_i)}{(Zr_1)^2}(r_i + Zr_i^2/2)\cos\theta_{1i}\right\}, \tag{3}$$

where suffix $i$ stands for 2 or 3 and $\varepsilon(r_1; r_i)$ is equal to unity for $r_1 > r_i$ and equal to zero for $r_1 < r_i$. Transformation of eq. (3) to velocity (momentum) space leads to the velocity-space wavefunction and thus to the velocity distribution of the atomic electrons. After averaging over the azimuth of the incident proton the resulting expression is:

$$f(v_2, \chi) = N[f_0(v_2) + (\cos^2\theta \cos^2\chi + \tfrac{1}{2} \sin^2\theta \sin^2\chi)\, f^{\mathrm{pol}}(v_2; r_1)], \tag{4}$$

in which the undistorted velocity distribution

$$f_0(v_2) = \frac{16Z^5}{\pi(v_2^2 + Z^2)^4}, \tag{5}$$

and the radial part of the distortion is given by

$$\begin{aligned} f^{\mathrm{pol}}(v_2; r_1) = \frac{4Z}{\pi r_1^4} \Bigg\{ & \frac{4(v_2^3 + v_2 Z^2)}{(v_2^2 + Z^2)^4} + \mathrm{e}^{-Zr_1} \cos(v_2 r_1) \\ & \times \left[ \frac{-4(v_2^3 + v_2 Z^2)}{(v_2^2 + Z^2)^4} + \frac{r_1(-3v_2^4 - 13v_2^2 Z^2 + 2Z^4)}{(v_2^2 + Z^2)^3} \right. \\ & \left. + \frac{r_1(2Z^2 - v_2^2)}{(v_2^2 + Z^2)^2} + \frac{Zr_1^3}{(v_2^2 + Z^2)} \right] + \mathrm{e}^{-Zr_1} \sin(v_2 r_1) \\ & \times \left[ \frac{(3v_2^6 + 12v_2^2 Z^4 - 17v_2^4 Z^2 - 2Z^6)}{Zv_2^2(v_2^2 + Z^2)^4} + \frac{r_1(-v_2^4 - 15v_2^2 Z^2 - 2Z^4)}{v_2^2(v_2^2 + Z^2)^3} \right. \\ & \left. + \frac{r_1^2(-2v_2^4 - 9v_2^2 Z^2 - Z^4)}{2Zv_2^2(v_2^2 + Z^2)^2} - \frac{r_1^3}{2(v_2^2 + Z^2)} \right] \Bigg\}^2 . \end{aligned}$$

In these expressions $v_2$ is given in atomic units $(e^2/\hbar)$, $\cos\theta = (\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{v}}_1)$ and $\cos\chi = (\hat{\boldsymbol{v}}_1, \hat{\boldsymbol{v}}_2)$. The normalization constant, given by

$$\begin{aligned} N^{-1} = 1 + \frac{43}{8Z^6 r_1^4} \{ & 1 - \mathrm{e}^{-2Zr_1}[1 + 2Zr_1 + 2(Zr_1)^2 + \tfrac{4}{3}(Zr_1)^3 \\ & + \tfrac{2}{3}(Zr_1)^4 + \tfrac{28}{129}(Zr_1)^5 + \tfrac{4}{129}(Zr_1)^6]\}, \end{aligned} \tag{7}$$

ensures that

$$\int f(\boldsymbol{v}_2)\, \mathrm{d}\boldsymbol{v}_2 = 1, \tag{8}$$

as required for each atomic electron. In eqs. (4) and (7), $r_1$ and $\theta$ are still unspecified parameters.

3. *Cross-section formulae.* The nonisotropic velocity distribution given by eq. (4) can now be used in the binary-encounter theory to obtain the differential cross section $\sigma(E, \hat{\boldsymbol{v}}_e)$ for transfer of energy $E$ and for ejection of an atomic electron in the direction $\hat{\boldsymbol{v}}_e$. For isotropic velocity distributions, $\sigma(E, \hat{\boldsymbol{v}}_e)$ has been calculated in ref. 1 [see eqs. (1) to (10)].

Substitution of any nonisotropic velocity distribution $f(v_2, \chi)$ in eq. (7) of ref. 1 leads to

$$\sigma(E, S, v_2) = \int_{\chi_{\min}}^{\chi_{\max}} \sigma(E, S, v_2, \chi)\, f(v_2, \chi)\, \tfrac{1}{2} \sin\chi\, d\chi, \tag{9}$$

where $\sigma(E, S, v_2, \chi)$ is the cross section for energy transfer $E$, "exchange momentum transfer" $\boldsymbol{S}(\boldsymbol{S} = \boldsymbol{p}_2' - \boldsymbol{p}_1)$ and for ejection of an atomic electron with velocity $v_2$ through an angle $\chi$ with respect to the incident proton. In eq. (9), $\chi_{\min}$ and $\chi_{\max}$ are determined by the condition that $\sigma(E, S, v_2, \chi)$ be real. The angular integration in eq. (9) can be performed by expanding $f(v_2, \chi)$ in the form

$$f(v_2, \chi) = \sum_{n=0}^{\infty} c_n(v_2) \cos^{2n} \chi. \tag{10}$$

This is justified by the symmetry properties of the momentum-space wavefunctions. In our case, for heavy incident particles, $\sigma(E, \hat{\boldsymbol{v}}_e, v_2)$ simplifies to

$$\sigma(E, \boldsymbol{v}_e, \hat{\boldsymbol{v}}_2) = \sigma_0(E, \hat{\boldsymbol{v}}_e, v_2) \sum_{n=0}^{\infty} c_n(v_2) \left(\frac{v_2'}{v_2}\cos\theta - \frac{E}{m_2 v_1 v_2}\right)^{2n}, \tag{11}$$

where $\sigma_0(E, \hat{\boldsymbol{v}}_e, v_2)$ is the cross section for isotropic velocity distributions $(n = 0)$ as given by eq. (9) of ref. 1; $v_2'$ is the velocity of the atomic electron after the collision, $\theta$ is the ejection angle and $v_1$ is the velocity of the incident proton.

For the velocity distribution of eq. (4) only the $n = 0$ and $n = 1$ terms differ from zero, owing to the dipole character of the polarized-orbital method. From eqs. (4) and (10) it follows that

$$c_0(v_2) = N\{f_0(v_2) + \tfrac{1}{2} f^{\text{pol}}(v_2; r_1) \sin^2\theta\}, \tag{12}$$

and

$$c_1(v_2) = N(\tfrac{3}{2} \cos^2\theta - \tfrac{1}{2})\, f^{\text{pol}}(v_2; r_1). \tag{13}$$

4. *Results.* In fig. 1 we present the energy distribution of electrons ejected in the forward direction from He by 300 keV protons. The ejection angle is 10 degrees. The figure illustrates that the combined polarized-orbital binary-encounter theory gives an improvement over the binary-encounter theory alone. The parameters were chosen to be $r_1 = 1$ a.u. and $\cos\theta = -1$. Other values of these parameters did not improve the results; however, for each value of $r_1$ and $\theta$ there is an improvement over the undistorted binary-encounter theory.

For larger ejection angles, the energy distribution calculated with the polarized velocity distribution tends to the undistorted binary-encounter energy distribution. In order to obtain an estimate of the of the influence of higher-order distortions on the cross sections, we calculated the velocity distribution of the atomic electrons in the ground state of the He $H^+$-molecular ion. For small velocities of the incident proton, when such an

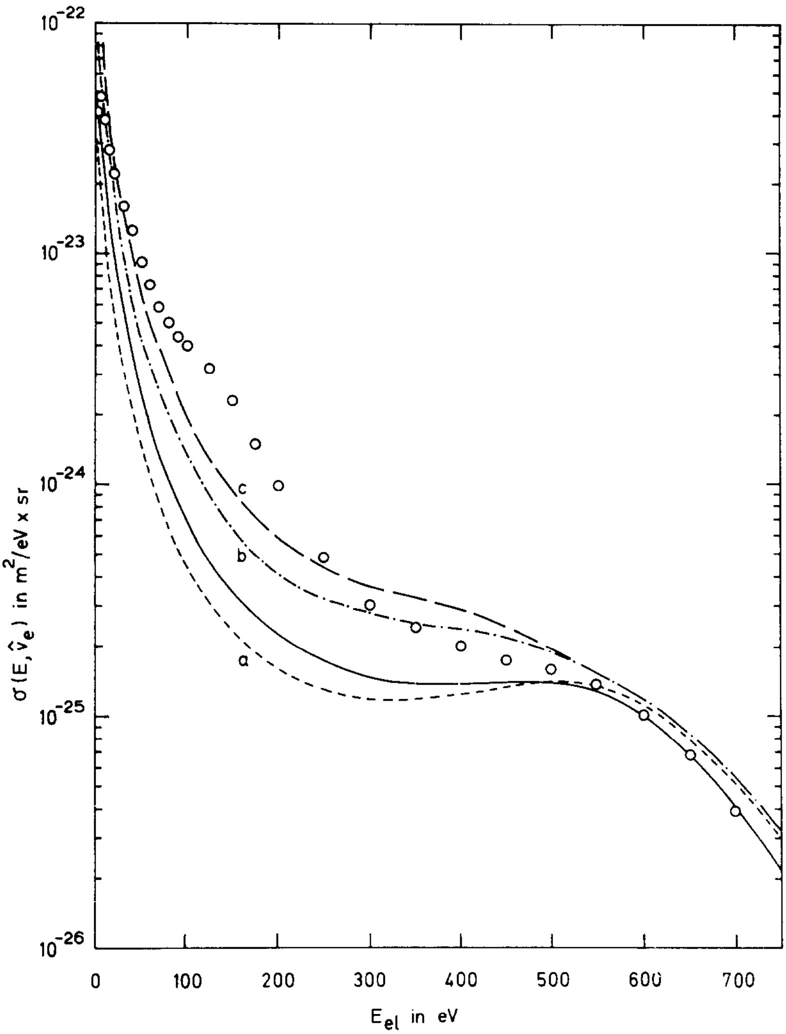


Fig. 1. Energy distribution of electrons ejected by 300 keV protons from He. The ejection angle is 10 degrees. Full curve: combined polarized-orbital binary-encounter cross section with $r_1 = 1$ a.u. and $\cos\theta = -1$; a, b and c: binary-encounter cross sections with $\cos^0$, $\cos^2$ and $\cos^4$ velocity distributions, in that order; open circles: experiment.

intermediate molecular ion is formed, the resulting velocity distribution of the atomic electron can be written as:

$$f(v_2, \chi) = c_0(v_2) + d_1(v_2)\cos(v_2 R\cos\chi) + d_2(v_2)\cos\chi\sin(v_2 R\cos\chi),$$

in which $R$ is the internuclear distance and $c_0$, $d_1$ and $d_2$ are complicated functions of $v_2$ and $R$. Expansion of $f(v_2, \chi)$ in terms of $\cos^{2n}\chi$ results in nonzero contribution of terms with $n = 2$, and higher powers of $\cos^2\chi$.

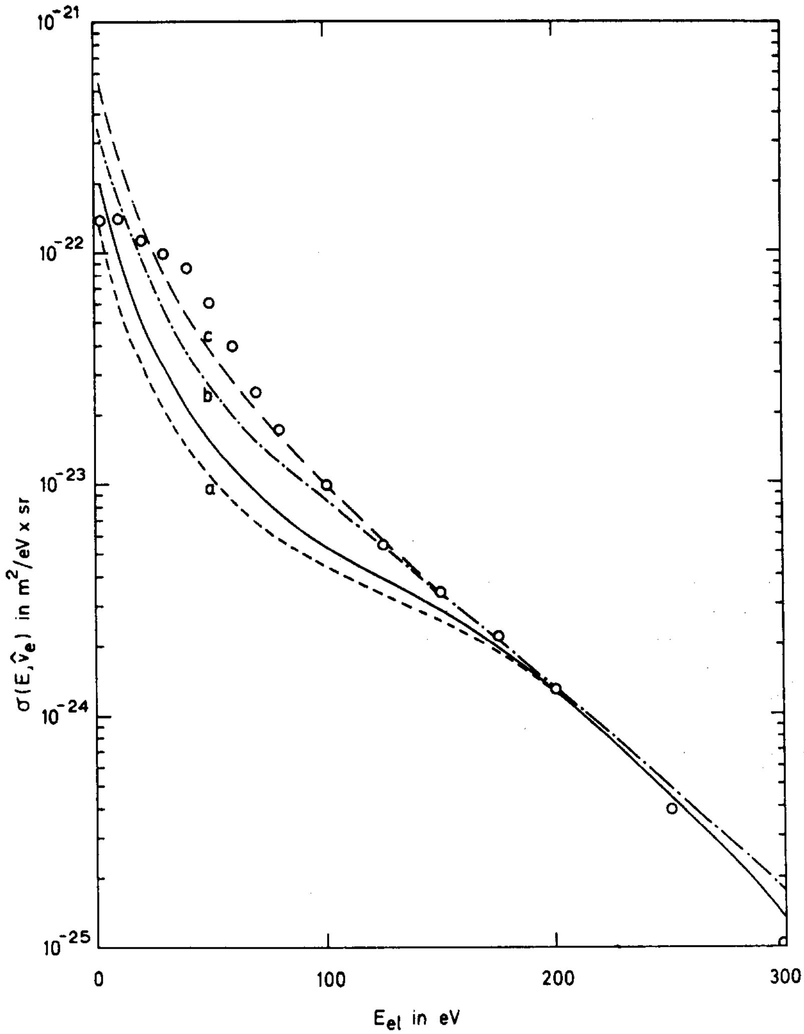


Fig. 2. As in fig. 1 for 100 keV proton impact.

In fig. 1 we also present the cross sections calculated with a pure $\cos^2$ and a pure $\cos^4$ velocity distribution. These peaked velocity distributions clearly improve the binary-encounter results to a large extent, indicating that inclusion of higher-order terms in the velocity distribution will lead to cross sections, which are in better agreement with experimental ones.

In fig. 2 we present our calculations for 100 keV protons. The improvement of the binary-encounter result by the first-order polarized-orbital method is somewhat less than for 300 keV proton impact, but the higher-order terms almost reproduce the experimental energy distribution. For larger ejection angles the cross sections of all peaked velocity distributions tend to the undistorted binary-encounter cross sections.

5. *Summary.* We calculated cross sections for ejection of electrons from helium by slow protons (100–300 keV) by taking account of the prior interaction of the colliding particles in the binary-encounter theory. Previously only undistorted velocity distributions of the atomic electron were considered. The combined polarized-orbital binary-encouter theory (a first-order approximation) gives a significant improvement over the undistorted binary-encounter theory. It has been argued that higher-order approximations for the velocity distribution of the atomic electron will lead to even better results.

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