

EJECTION OF ELECTRONS FROM HELIUM BY PROTONS AND THE ATOMIC MODEL

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Various assumptions about the form of the collective motion of atomic electrons in the helium atom are made and energy spectra of electrons ejected by protons within the binary encounter (b. e.) approximation have been calculated. The result of theoretical calculations carried out for some class of collective orbits are compared with the experimental data and the class of orbits which may represent the helium atom is determined. The conclusion is drawn that motion of electrons in the helium atom is almost strictly radial and the real electron orbit cannot be much different from the free-fall orbit.

1. Introduction

It has been shown some time ago, that energy spectra of electrons ejected from atoms depend essentially upon the atomic model used in calculations¹⁾ and that results of various other calculations for the free-fall atomic model are in a fairly good agreement with the experimental data — see, for instance Gryziński and Kunc²⁾. Since the free-fall atomic model seems to describe the reality rather approximately, there have been undertaken efforts towards the construction of the more advanced model of the atom. Trying to solve this problem, a more sophisticated collective motion of electrons in the field of nucleus was recently investigated and a set of orbits which may represent the atomic shell was determined³⁾.

It is the aim of the present paper, using the atomic collision technique, to estimate the class of collective orbits, which from the point of view of the ejection process may represent the helium atom.

2. Model of the atom in the b. e. atomic collision theory

In the atomic collision theory formulated within the binary encounter approximation (b. e. a.) the atomic cross section in the isotropic case, that is for atoms randomly oriented in space, is given by:

$$\sigma_t^{at} = \int_0^{\infty} \sigma_t^{b.e.}(v_p, v_e) f^{at}(v_e) dv_e, \quad (2.1)$$

where $\sigma^{b.e.}$ is the b. e. cross section for a collision between the projectile of velocity v_p and the atomic electron of velocity v_e , in which the given transfer of energy, or momentum, or their combination (ζ stands for one of them) takes place, and $f^{at}(v_e)$ is the electron velocity distribution function, which describes the behaviour of electrons in the atom.

According to the shell structure of the atom and according to the classical concept of the shell, which assumes that all electrons of the shell move in identical way, the atomic velocity distribution function $f^{at}(v_e)$ can be written in the following way:

$$f^{at}(v_e) = \sum_s N_s^e \frac{1}{v_s} p_s(v_e), \quad (2.2)$$

where s is the shell index in the considered atom, N_s^e is the number of electron in the given atomic shell, $p_s(v_e)$ is the probability that at given moment of time velocity of the s -shell electron is in the interval v_e and $v_e + dv_e$ and v_s is the velocity corresponding to the binding energy of the electron in the given atomic shell

$$W_s = \frac{m_e v_s^2}{2}. \quad (2.3)$$

It is clearly seen from the all above, that in the b. e. theory the electron velocity distribution function $f^{at}(v_e)$ is the quantity which represents the atom and determines the atomic cross section. In a consistently formulated atomic collision theory the both terms defining the atomic cross section, that is the binary encounter cross section $\sigma^{b.e.}$ and the velocity distribution function $f^{at}(v_e)$, must have an identical underlying physical basis. The concept of a point-electron forms the essence of the classical approach and it was within this concept that the binary encounter cross section was derived. The classical model of the atom with a well defined orbital motion of atomic electron must, therefore, form the inherent part of any consistently formulated classical atomic collision theory. A correct model of the atom (actually one witnesses an increase of number of papers devoted to the construction of atomic models — see for instance Refs. 4–6) is the key to a successful description of atomic collision experiments.

If only the atomic model is defined and electron coordinates as a function of time are known (and, therefore, $v_e(t)$ is known), the electron velocity distribution function $p_s(v_e)$ can be easily calculated. It is simply given by:

$$p_s(v_e) = \frac{v_s}{T_s} \frac{1}{(dv_e/dt)} \Big|_{t = f^{-1}(v_e)} \tag{2.4}$$

where T_s is the period of the electron motion on the given orbit.

Usually in classical atomic calculations the microcanonical velocity distribution function was used⁷⁻¹⁰⁾. But, as we have shown recently¹¹⁾, this distribution represents the whole ensemble of Kepler orbits, with the square of angular momentum uniformly distributed from zero to unity and, therefore, it cannot represent the ground state atom, the angular momentum of which has a well defined value (it is precisely equal to zero).

In the particular case of the collective motion of atomic electrons, when all electrons move along identical free-fall Kepler orbits, the velocity distribution function can be effectively calculated. It is simply given by:

$$p_s''(v_e) = \frac{4}{\pi} \left(\frac{v_s^2}{v_s^2 + v_e^2} \right)^2 \tag{2.5}$$

In general, however, when electrons move along the more complicated orbits, velocity distribution cannot be obtained in analytical form. For the particular collective orbits it can be calculated numerically. The calculation procedure is as follows.

According to results of Ref. 3, equation describing the collective motion of electrons in the Coulomb field of nucleus is given by:

$$m_e \frac{d^2 \vec{r}}{dt^2} = \nabla \left[\frac{(Z - \sigma(\hat{r})) \cdot e^2}{r} \right], \tag{2.6}$$

where $\sigma(\hat{r})$ is the screening factor which represents electrostatic interaction of electrons. Solving Eq. (2.6) for the given initial conditions $(r_0, \dot{r}_0, \Theta_0, \dot{\Theta}_0)$, specifying the type of the closed orbit, one finds

$$v_e(i) \equiv v_e(t_i = t_0 + \sum_{j=1}^i \Delta t_j), \tag{2.7}$$

where Δt_j is the variable step of numerical integration. Now, according to Eq. (2.4), we can calculate the considered distribution function in the finite number of time intervals

$$p_s(t_i) = \frac{v_s}{T_s} \frac{1}{\frac{v_e(i+1) - v_e(i-1)}{\Delta t_{i+1} + \Delta t_i}} \rightarrow p_s[v_e(i)], \tag{2.8}$$

The discrete set of points obtained in this way, when plotted in (p_s, v_e) coordinates, forms the curve, which in general case may have more than one value of p_s for specified value of v_e (electron may have the same velocity but its acceleration may be different in a few points along the trajectory). The true value of p_s for particular v_e can be obtained by simple summing:

$$p_s(v_e) = \sum_{j=1}^k \delta[v_e(j) - v_e] \cdot p_s[v_e(j)] \tag{2.9}$$

where

$$\begin{aligned} \delta[v_e(j) - v_e] &= 0 && \text{for } v_e(j) \neq v_e \\ \delta[v_e(j) - v_e] &= 1 && \text{for } v_e(j) = v_e. \end{aligned}$$

If the values of p_s for arbitrary v_e are to be found, it is necessary to perform some interpolation between points $p_s[v_e(i)]$ and $p_s[v_e(i + 1)]$.

For the few simplest two-electron collective orbits that have been recently found, see Fig. 1, numerical calculations were carried out and the respective distributions were determined. The calculated distributions are shown in Fig. 2.

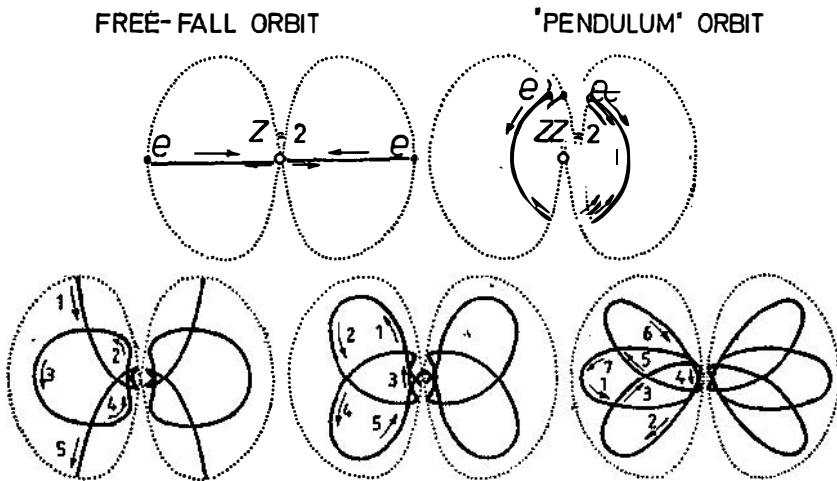


Fig. 1. Various forms of collective motion of two electrons in the field of nucleus, as used in the present analysis of the ejection process.

Having the electron velocity distribution found, any of the binary encounter cross sections can be calculated. In the present paper we use them to calculate the energy spectra of secondary electrons produced by protons.

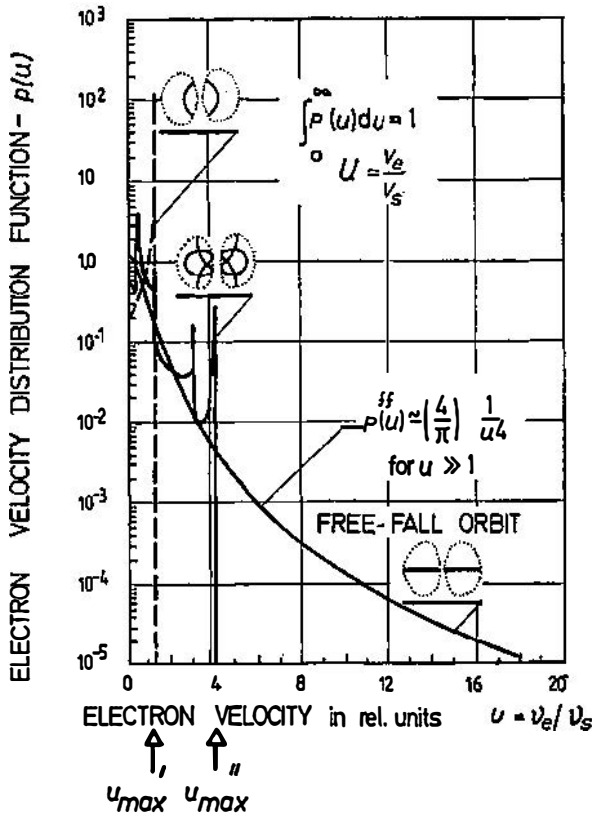


Fig. 2. Electron velocity distribution for various collective orbits.

3. Recoiled electrons energy spectra

The binary encounter cross section describing energy spectrum of secondary electrons produced by heavy particles ($m_p \gg m_e$), which for the first time was exactly derived by one of us — see Eq. (15) of the paper by Gryziński^{1,2}), has the form:

$$\sigma_{\Delta E} = Z_p^2 \frac{\sigma_0}{(\Delta E)^3} \left(\frac{v_e}{v_p} \right)^2 \times \left\{ \begin{array}{l} \frac{4}{3} + \frac{\Delta E}{E_e} \quad , \text{ if } \frac{\Delta E}{2m_e v_p^2} < \left(1 - \frac{v_e}{v_p} \right) \\ \frac{4}{3} \left(\frac{v_p}{v_e} \right)^3 - \frac{1}{6} \left(\sqrt{1 + \frac{\Delta E}{E_e}} - 1 \right)^3 \quad , \text{ if } \left(1 - \frac{v_e}{v_p} \right) < \frac{\Delta E}{2m_e v_p^2} < \left(1 + \frac{v_e}{v_p} \right) \end{array} \right\} \quad (3.1)$$

where ΔE is the transfer of energy between the massive projectile of velocity v_p and the electron of velocity v_e (of energy E_e).

Having in view the above and introducing the notation:

$$u = \frac{v_e}{v_s} \tag{3.2}$$

$$\lambda = \frac{v_p}{v_s} \tag{3.3}$$

$$\varepsilon = \frac{\Delta E}{W_s} \tag{3.4}$$

the atomic cross section can be written in the following way:

$$\sigma^{at} = \sum_s N_s^2 \cdot \frac{\sigma_0}{W_s^2} \cdot \frac{1}{\lambda_s^2} \times$$

$$\times \left[\begin{array}{l} \int_0^{\lambda_s - \frac{\varepsilon_s}{4\lambda_s}} \left(\frac{4}{3} u_s^2 + \varepsilon_s \right) p_s(u_s) du_s + \int_{\lambda_s - \frac{\varepsilon_s}{4\lambda_s}}^{\infty} [8\lambda_s^3 - (\sqrt{u_s^2 + \varepsilon_s} - u_s)^3] \frac{1}{u_s} p_s(u_s) du_s, & \text{if } \varepsilon_s < 4\lambda_s^2 \\ \int_{\lambda_s + \frac{\varepsilon_s}{4\lambda_s}}^{\infty} [8\lambda_s^3 - (\sqrt{u_s^2 + \varepsilon_s} - u_s)^3] \frac{1}{u_s} p_s(u_s) du_s, & \text{if } \varepsilon_s > 4\lambda_s^2 \end{array} \right] \tag{3.5}$$

Since the individual collision process takes place inside the atom, the energy of the ejected electron as measured outside the atom, is by the amount of the binding energy less than just after collision inside the atom, and therefore:

$$\varepsilon_s^\infty = \varepsilon_s - 1.$$

The energy spectrum of ejected electrons is, therefore, given by Eq. (3.5) with ε_s being replaced by $\varepsilon_s^\infty + 1$.

In the particular case of the free-fall velocity distribution integration over v_e (over u_s) can be effectively carried out and the cross section can be given in the analytical form (for the Bohr atomic model cross section is simply given by Eq. (3.5) where E_e should be replaced by W_s). The result can be written in the following way:

$$\sigma_s'' = \frac{\sigma_0}{W_s^2} g_s''(\lambda), \tag{3.6}$$

where:

$$\begin{aligned}
 g''_0(\lambda) = & \frac{4}{\pi} \frac{1}{\varepsilon^2 \lambda^2} \left(-\frac{2}{3} \left(\frac{\lambda}{\varepsilon} \right) + \left(\frac{1}{4} + \frac{1}{3\varepsilon} \right) \text{arc ctg} \left(\frac{\varepsilon}{4\lambda} - \lambda \right) + \right. \\
 & \frac{2}{3} \frac{\lambda^3}{\varepsilon} \ln \frac{\left(\lambda - \frac{\varepsilon}{4\lambda} \right)^2}{1 + \left(\lambda - \frac{\varepsilon}{4\lambda} \right)^2} - \frac{\sqrt{\varepsilon}}{6} \text{arcth} \frac{\left(\lambda + \frac{\varepsilon}{4\lambda} \right)}{\sqrt{\varepsilon}} \left. + \right. \\
 & \left. + \frac{1}{6 \cdot \varepsilon} \frac{\varepsilon^2 - \frac{1}{2}\varepsilon - 2}{\sqrt{|\varepsilon - 1|}} \cdot \left[\begin{array}{l} \text{arcth} \frac{\left(\lambda + \frac{\varepsilon}{4\lambda} \right)}{\sqrt{\varepsilon - 1}}, \text{ if } \varepsilon > 1 \\ \text{arc ctg} \frac{\left(\lambda + \frac{\varepsilon}{4\lambda} \right)}{\sqrt{1 - \varepsilon}}, \text{ if } \varepsilon < 1. \end{array} \right] \right. \quad (3.7)
 \end{aligned}$$

To show some characteristic features of the obtained distribution (which is presented in Fig. 3), it is useful to have some asymptotic relations for the function $g''_0(\lambda)$.

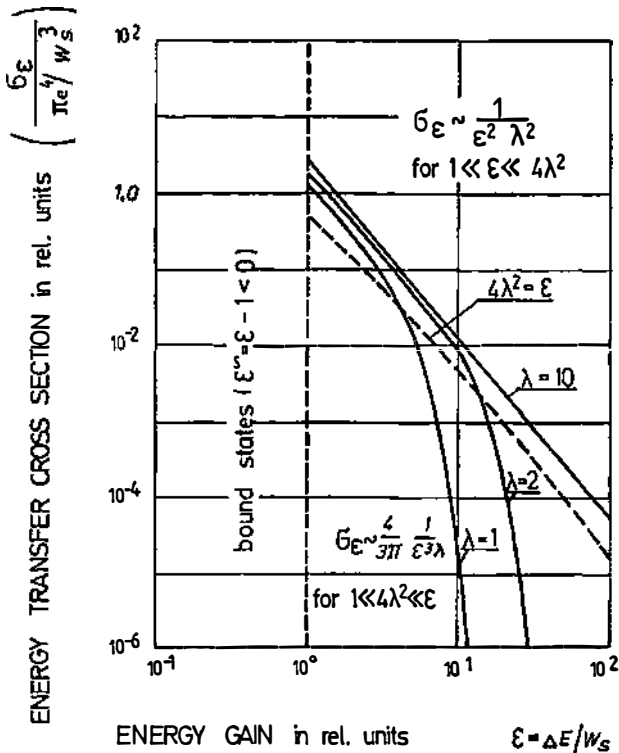


Fig. 3. Cross section for producing the recoiled electrons in binary collisions with heavy projectiles (protons) for the free-fall electron orbit, for some values of parameter λ .

So, for energy transfers much greater than the mean kinetic energy of the electron on the orbit, i. e. for $\varepsilon \gg 1$, the above formula assumes the form:

$$g'' \approx \frac{4}{\pi} \frac{1}{\varepsilon^2 \lambda^2} \left\{ \frac{1}{4} \operatorname{arc\,tg} \left(\frac{\varepsilon}{4\lambda} - \lambda \right) - \frac{2}{3} \left(\frac{\lambda}{\varepsilon} \right) \left[1 + \lambda^2 \ln \frac{\left(\frac{\varepsilon}{4\lambda} - \lambda \right)^2}{1 + \left(\frac{\varepsilon}{4\lambda} - \lambda \right)^2} \right] \right\}. \quad (3.8)$$

If, moreover, $\varepsilon \ll 4\lambda^2$ then we have approximately:

$$g'' \approx \frac{1}{2} \frac{1}{\varepsilon^2 \lambda^2}. \quad (3.9)$$

In the opposite case, i. e. for $\varepsilon \gg 4\lambda^2$ the asymptotic dependence has the form:

$$g'' \approx \frac{4}{3\pi} \frac{1}{\varepsilon^3 \lambda}. \quad (3.10)$$

In the particular case $\varepsilon = 4\lambda^2$ we have:

$$g'' = \frac{2}{3\pi \lambda^2} \left\{ \pi (1 + 3\lambda^2) - 4\lambda [1 + 2\lambda^2 \ln (2\lambda)] - \sqrt{|4\lambda^2 - 1|} \left[\begin{array}{l} \operatorname{arc\,tg} \frac{2\lambda}{\sqrt{1 - 4\lambda^2}}, \text{ if } \lambda < \frac{1}{2} \\ \operatorname{ar\,cth} \frac{2\lambda}{\sqrt{4\lambda^2 - 1}}, \text{ if } \lambda > \frac{1}{2} \end{array} \right] \right\}. \quad (3.11)$$

It is important to note that in the case of the Bohr atomic model the energy of ejected electrons is limited and this limit is given by:

$$\varepsilon_{\max} = 4\lambda (1 + \lambda), \quad (3.12)$$

while in the case of the free-fall atomic model such a limit does not exist (there is only a trivial limit resulting from the energy conservation law $-\varepsilon_{\max} = E_p/W_s$).

To get energy spectra of recoils for some other forms of collective motion of electrons, numerical integration must be carried out. Results of integration for some particular electron velocity distributions found previously — as shown in Fig. 2 — are presented in Fig. 4.

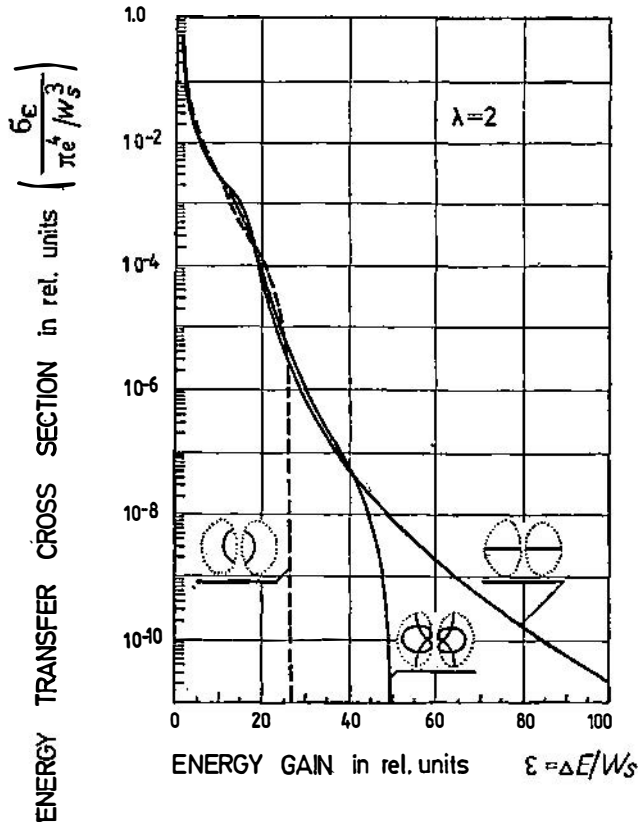


Fig. 4. Energy spectra of recoiled electrons for various velocity distributions (various forms of collective orbits) and for the given value of the parameter λ (given value of the ratio v_p/v_d).

4. Comparison with the experimental data and conclusions

Comparison of experimental data for 300 keV and 1 MeV protons¹³⁾ with results of calculations for various electron velocity distributions (for various forms of collective motion of electrons) is given in Figs. 5—7. In Fig. 6 the calculated cross sections and experimental data are presented in the normalized form (related to the free-fall spectrum). Inspecting Figs. 5—7 one arrives to the following conclusions:

1. Energy spectra of ejected electrons depend upon the form of the collective orbit (particularly in the high energy part of the spectrum).

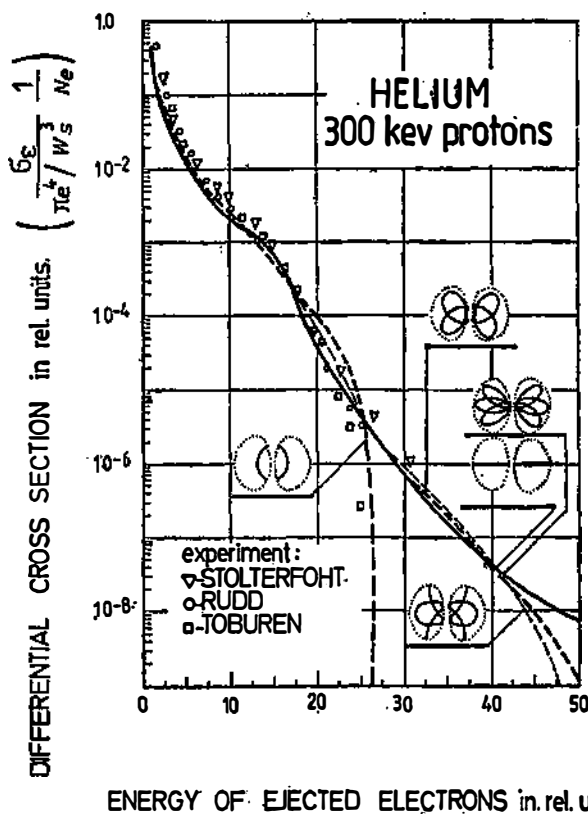


Fig. 5. Differential cross section for ejection of electrons from helium by 300 keV protons calculated for various collective orbits and experimental results of some authors^{1,3)}.

2. Existing experimental material and approximate character of calculations do not allow one to draw a final conclusion about the form of the electron orbit. Nevertheless, domination of the radial component of the electron velocity in the helium atom is evident — theoretical results for free-fall configuration are located very closely to the experimental values (see Fig. 5). Small deviations existing in the medium energy range of ejected electrons, particularly well seen if experimental data and theoretical results are presented in the normalized form, see Fig. 6, have probably the origin in not strictly radial motion of electrons.
3. Remarkable difference between the experimental data and theoretical results in the low energy range of the spectra has the origin in the approximate character of the whole analysis — binary encounter approximation works rather badly at small transfers of energy and modifications of the spectrum by electron-electron collisions inside the atom do not seem to be small.

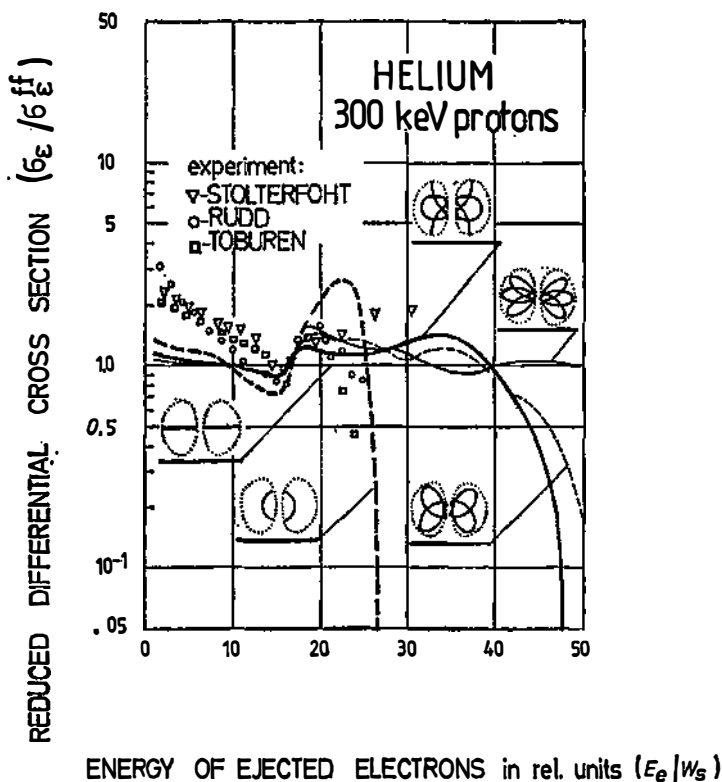


Fig. 6. Spectrum of ejected electrons from helium by 300 keV protons as measured experimentally and calculated theoretically for various collective orbits, both normalized to the free-fall spectrum.

Since the problem of deciphering the electronic structure of atoms seem to be of primary importance for atomic physics and ejection of electrons by heavy particles may give valuable informations on this subject, it would be helpful to have more accurate experimental data, particularly in the high energy part of the spectrum. Since in the case of high energy protons (see Fig. 7) the spectrum only slightly depends upon the atomic model and in the case of low energy protons the b. e. a. works rather badly, the most desired are measurements for 200—400 keV protons. It is worthy to note, that for checking the model, the absolute values are of secondary importance, what may simplify the experimental procedure. For precise verification of the helium atom model one should have more accurate results of theoretical calculations. Therefore, the three body numerical calculations, like those described by Olson and Salop¹⁴⁾ and Janev and Mc Dowell¹⁵⁾, based on the independent-particle model, or exact four-body numerical calculations, as reported by Zajfman and Maor¹⁶⁾ should be carried out.

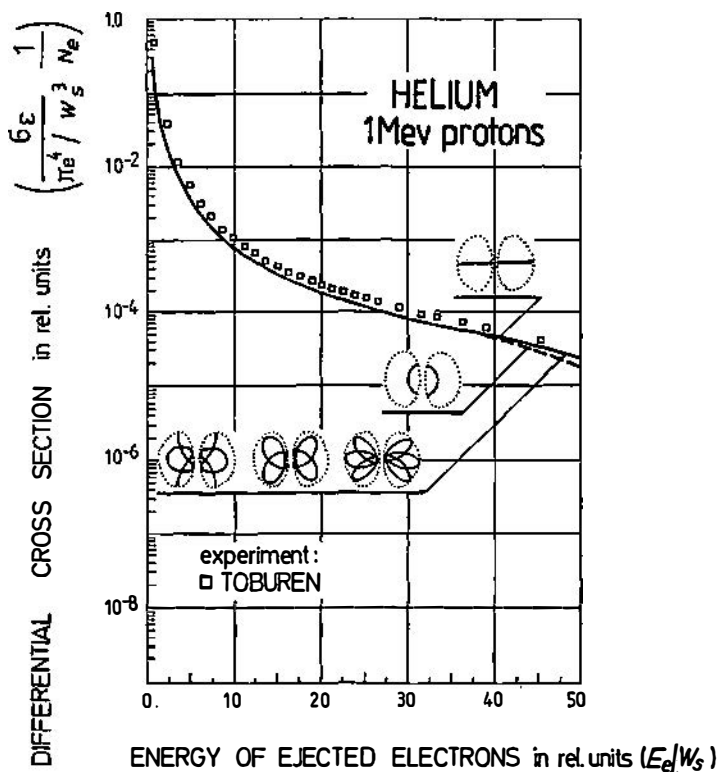


Fig. 7. The same as in Fig. 5, except for the proton energy.

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IZBACIVANJE ELEKTRONA IZ HELIJA PROTONIMA I ATOMSKI MODEL

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Ispitivano je nekoliko različitih pretpostavki o formi kolektivnog kretanja elektrona u atomu helija i izračunati su energetske spektri elektrona izbačenih protonima, u okviru aproksimacije binarnih sudara. Rezultati teorijskog izračunavanja, vršenog za jednu klasu kolektivnih orbita, komparirani su sa eksperimentalnim podacima i određena je vrsta orbita koja može da predstavlja atom helija. Izvučen je zaključak da je u helijevom atomu kretanje elektrona skoro isključivo radijalno i da stvarna elektronska orbita ne može biti mnogo različita od slučaja slobodnog pada.