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SCATTERING OF LOW-ENERGY ELECTRONS AND MODEL OF HELIUM ATOM

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Angular distribution of slow electrons scattered from helium and momentum transfer cross sections for three variants of the free-fall atomic model have been calculated (in each considered case the free-fall electron orbits formed different spatial configurations). The obtained results show that the nucleus and two electrons in the helium atom form linear (or almost linear) configuration firmly (or almost firmly) oriented in space.

1. Introduction

It is an obvious matter that results of atomic collisions are determined by the structure of colliding atoms and that the experimental data contain, although in the hidden form, information about the structure of colliding atoms. Theoretical interpretation of atomic collision experiments with appropriately developed mathematical method is, therefore, one of the ways to deciphering the structure of atoms and molecules. In this way at the beginnings of atomic physics Thomson[1], Rutherford[2], Williams[3] and Thomas[4], have shown that atom represents a collection of point particles being in dynamic equilibrium. Modern atomic collision investigations threw some light upon the form of the electron orbits in the atom and have led to the free-fall (FF) atomic model concept (Gryziński[5-7]). In turn, the free-fall atomic model enabled us to describe in a consistent way a large variety of atomic collision experiments: ionization of hydrogen atom by an electron (Gryziński et al.[8]), inner shell ionization by low-energy protons (Gryziński and Kunc[9]), ejection from helium by protons (Gryziński and Okopińska[10]) and small-angle scattering of low-energy electrons from atoms and molecules (Gryziński[11]).

Not long ago two variants of the free-fall atomic model, that is the synchronous (symmetrical) and the asynchronous (asymmetrical) models, were applied to describe e — He scattering (Dimitrijević et al. [12]). Recently the free-fall atomic model was, with a some success, applied to description of e± — H (1s) scattering (Grujić et al.[13]).

The works mentioned above and some other works in this field (Abrines and Percival[14], Abrines et al.[15], Bates[16], Percival[17] and Gryziński[18]) show that possibilities of deterministic description of atomic processes are not small. One can suppose that the atomic model with electrons moving along well specified orbits is a good representation of reality. Free-fall model of the hydrogen atom seems to describe this reality quite precisely. In the case of many electron atoms, however, the situation is not so good. The simple free-fall atomic model neglecting spin (gyromagnetic) properties of the electron responsible for the behaviour of electrons in the close vicinity of nucleus, leaves many problems open for discussion. In the incomplete spinless model of the helium atom we meet, for instance, the following difficulty: is the *ff*-radial trajectory firmly oriented in space or is it subjected to regular or stochastic changes of orientation, as it was discussed by Grujić et al.[13].

Since the scattering of slow electrons is in the first instance determined by the time averaged distribution of the electric charge in the atom (Gryziński[11]) and the latter is determined by changes of radial (quasi-radial) orbit orientation around the nucleus, we shall try to shed some light on the problem, comparing results of theoretical calculations with the experimental data.

2. *The physical model and method of solving the scattering problem*

Scattering of low-energy electrons from atoms, if considered in the collective field approximation which neglects deformations of atomic shells during the collision, is from mathematical point of view, a rather trivial problem. We must simply solve equations of motion for the electron moving in the given electric field.

So formulated scattering problem was (in the so-called small angle approximation and for the atomic field being expanded into series and approximated by some electric multipoles) solved some time ago by one uf us (Gryziński[11]). Now, performing numerical calculations of equations of motion we shall give exact, within the collective field approximation of course, solution of the scattering problem. In the particular case of helium-like atom the equation to be solved has the form:

$$m\frac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} = -\frac{Ze^2}{r^2}\hat{r} + \frac{e^2}{|\vec{r}-\vec{r}_e(t)|^3}(\vec{r}-\vec{r}_e(t)) + \frac{e^2}{|\vec{r}+\vec{r}_e(t)|^3}(\vec{r}+\vec{r}_e(t)), \qquad (1)$$

where Ze is the charge of nucleus, m is the mass of the scattered particle (electron) and $\vec{r}_e(t)$ describes the motion of the electron in an isolated atom. For the considered atomic model the latter is given by:

$$\vec{r}_e(t) = \frac{1}{2} r_0 (1 - \cos\xi(t))\hat{r}(t), \qquad (2)$$

$$t = \frac{T_0}{2\pi} (\xi - \sin \xi), \tag{3}$$

where

$$r_0 = \frac{\left(Z - \frac{1}{4}\right) e^2,}{W} \tag{4}$$

$$T_0 = 2\pi \left(Z - \frac{1}{4}\right) e^2 \sqrt{\frac{m}{W^3}} \tag{5}$$

and W is the binding energy of the electron in the given atomic shell. The unit vector $\hat{r}^{ff}$, defining orientation of the free-fall orbit may in general have different direction at each reflection of electrons from nucleus. One can suppose, however, that the atom has a regular structure and, therefore, $\hat{r}^{ff}$ is a periodic function of time: $\hat{r}_1^{ff}(t) = \hat{r}_n^{ff}(t + nT)$. Since in the spinless approximation the product $\hat{r}_{n=1}^{ff} \cdot \hat{r}_n^{ff}$ remains undefined we have decided to investigate three extremal cases corresponding to three various models of helium atom:

— linear model: electrons are exactly reflected back,

— planar model: electrons are scattered at 90° remaining all the time in the same plane,

— spatial model: electrons are scattered at 90°, but they move successively along the three axes of Cartesian system of coordinates.

Solving the equation of motion for the given value of the impact parameter D, for given $\vec{r}_e(t)$, one finds the experimentally measurable value of the scattering angle ϑ. Unfortunately, the obtained relation $\vartheta = f_\vartheta(D)$ cannot be directly checked, as in the atomic world the individual history of atomic particle is not admissible to direct observation, and the impact parameter D is not experimentally determined quantity. In macroscopic experiments we can observe only statistical links, arising among others from accidental value of D in the separate event, between initial and final states of atomic systems and the cross section is the quantity which represents this statistics.

To obtain the considered cross section one must, according to the procedure given by Gryziński[5], calculate the following integral.

$$\sigma_{\cos\vartheta} = \frac{d\sigma}{d\cos\vartheta} = 2\pi \int \delta\, [\cos\vartheta - f_{\cos\vartheta}(D; \alpha, \beta, \gamma; t_0)]\, D \, d D, \tag{6}$$

where δ is Dirac delta function and

$$\cos\vartheta = f_{\cos\vartheta}(D; \alpha, \beta, \gamma; t_0)$$

is the relation between the scattering angle ϑ and the impact parameter D obtained from equations of motion integrated at the given orientation of the atom (specified by three Euler angles α, β, γ) and the at given phase of motion (t_0) of atomic electrons.

Since the phase of the motion of electrons in the atomic system is the unobservable quantity the averaging over t_0 must be carried out

$$\sigma_{\cos\vartheta} = \frac{1}{T} \int_0^T \sigma_{\cos\vartheta}(t_0)\, \mathrm{d}\, t_0, \tag{7}$$

where T is period of motion of atomic electrons, to obtain the effectively measured cross section.

In the case of gaseous targets, atoms are randomly oriented in space and averaging procedure over three Euler angles describing orientation of the atom in space is necessary:

$$\sigma_{\cos\vartheta} = \frac{1}{8\pi^2} \int\int\int \sigma_{\cos\vartheta}(\alpha, \beta, \gamma) \sin\alpha\, \mathrm{d}\alpha\, \mathrm{d}\beta\, \mathrm{d}\gamma. \tag{8}$$

As a result we obtain the quantity which can be compared with experimental results.

3. Numerical calculations

The most convenient way of evaluation of the cross section within the classical trajectory method is the Monte Carlo method. Since the general procedure of the Monte Carlo method was described elsewhere (Percival[17]) we will not discuss this point here, except the point concerned with a proper choice of the integration limit for the impact parameter D_{max}. This is the important practical problem, since the computer consumption time depends highly on the value of D_{max}.

It is an obvious matter that for impact parameters larger than dimensions of the atom the scattering angle ϑ is a continuously decreasing function of the impact parameter. It is reasonable, therefore, to relate the upper limit of the impact parameter D to the lowest experimentally measured value of the scattering angle ϑ_{min}.

To estimate the value of D_{max} one can use the small angle scattering formulas given by Gryziński[11]. In the first approximation D_{max} may be calculated from

$$D_{max} \simeq \left(\frac{Q_n}{E \cdot \mathrm{tg}\, \vartheta_{min}} \right)^{\frac{1}{n+1}}, \tag{9}$$

where Q_n is the leading term of the expansion into electric multipoles of the electric field of considered system.

The estimated value of D_{max} may be, of course, a posteriori checked from the graph $\vartheta = f(D)$, obtained from some relatively small number of collision events — see Figs. 1 and 2.

Calculations of scattering cross-sections were carried out according to the formula

$$\sigma_{\cos\vartheta} = \frac{n(\vartheta) \cdot \pi D_{max}^2}{N \cdot \Delta(\cos\vartheta)}, \tag{10}$$

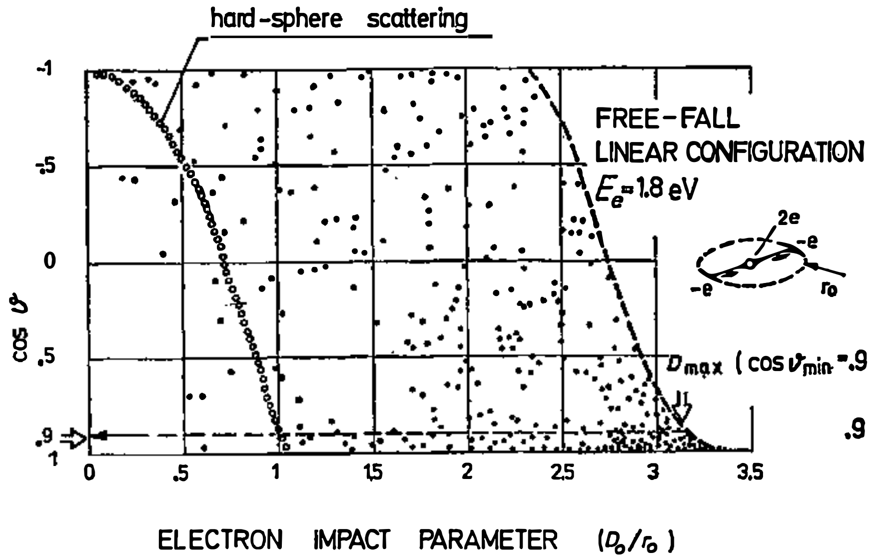

Fig. 1. Each point on the graph represents the single trajectory for the given value of the impact parameter D, for the given phase of motion of atomic electrons and for the given orientation of the atom in space. The dashed line marks the »effective« range of the atomic field (the term »effective range« in atomic collisions has no absolute meaning but depends upon the character of the collision process — in the considered case it depends on the angular resolving power of the measuring aparatus).

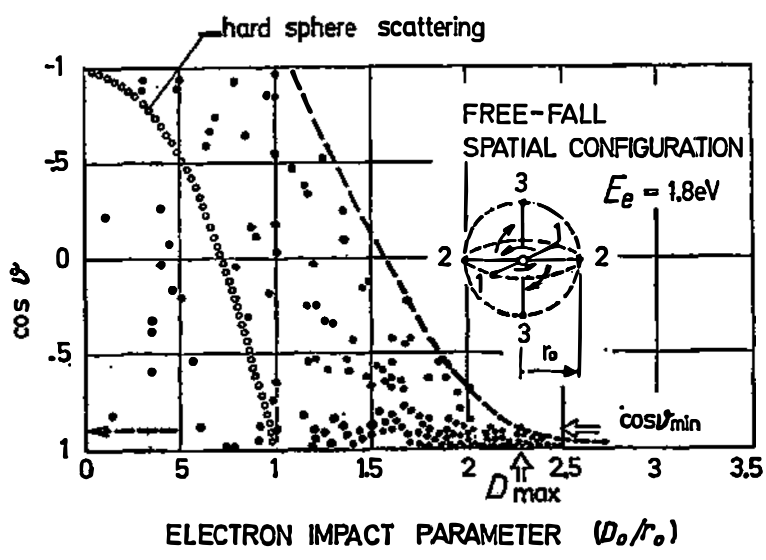

Fig. 2. The same as in Fig. 1 except for the atomic model. In the case of spatial *ff*-configuration the effective range is much smaller than in the case of linear free-fall configuration.

where $n(\vartheta)$ is the number of orbits finishing between $\vartheta - \left(\frac{\Delta\vartheta}{2}\right)$ and $\vartheta + \left(\frac{\Delta\vartheta}{2}\right)$ and N is the total number of collisions. Equations of motion were numerically integrated with the aid of Runge-Kutta procedure RKINIT at initial conditions determined by five random parameters: three Euler angles, the impact parameter D and the phase of motion t_0. The initial and final points of electron trajectories were located at the distance from nucleus 20 times larger than the dimension of the free-fall orbit. To keep the statistical error at sufficiently low level it was found satisfactory to calculate for each atomic model 1000 trajectories.

Proceeding to numerical calculations we have introduced the following units:
— the radius of the *ff*-orbit as a unit of length

$$l_1 = r_0, \tag{11}$$

— the period of motion on the Kepler orbit divided by 2π as a unit of time

$$t_1 = \frac{T_0}{2\pi}. \tag{12}$$

The binding energy of the electron in the shell has been calculated from experimentally measured successive ionization potentials of the shell

$$W = \frac{1}{N_e} \sum_{j=1}^{N_e} (U_i)_j. \tag{13}$$

In the case of helium atom the two succesive ionization potentials of the shell are:

$$U_{i1} = 24.59 \text{ eV},$$

$$U_{i2} = 54.42 \text{ eV}.$$

Therefore,

$$W^{He} = 39.5 \text{ eV},$$

and the unit of length has the value:

$$r_{max} = 1.2 \times 10^{-10} \text{ m}.$$

4. *Discussion and final conclusions*

One may be surprised but the only existing at the moment experimental data describing angular distribution of scattered electrons from helium at low energies, when all types of collisions (elastic and inelastic) are included, are those obtained half century ago by Ramsauer. During the passed time a lot of very sophisticated scattering experiments have been carried out, but the Ramsauer's[19] results have never been checked. Since in that time the atomic collision technique was not so well advanced as now, one should be very careful in drawing too detailed conclusions from Ramsauer's data. There are reasons to think that his data for scattering of low-energy electrons (1.8 eV) from helium at very small angles are underestimating. Such a conclusion can be drawn from the analysis of Golden and Bandel »total«

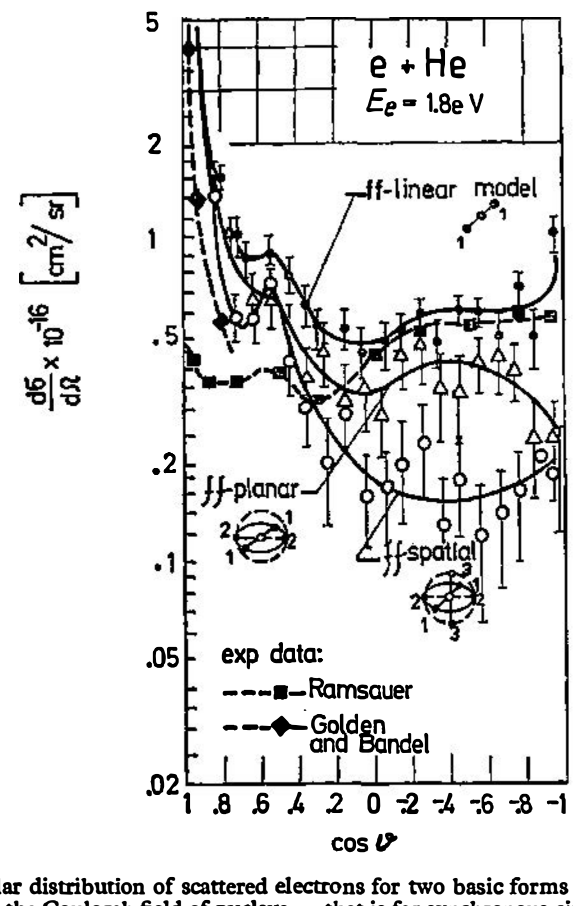

Fig. 3. The angular distribution of scattered electrons for two basic forms of collective motion of two electrons in the Coulomb field of nucleus — that is for synchronous circular motion of two electrons (Bohr's atomic model) and for synchronous strictly radial motion (free-fall atomic model).

scattering cross section measurements[20]. According to the small angle-angle scattering theory[11] the »total« scattering cross section $S(\vartheta_{min})$ and differential cross secrion $d\vartheta/d\Omega$ are related in the following way:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\vartheta=\vartheta_{min}} \simeq \frac{1}{2\pi} \frac{2(n+2)}{(n+1)} S(\vartheta_{min}), \tag{14}$$

where n is the order of the leading term of the expansion of the atomic field into multipoles and ϑ_{min} is determined by geometry of measuring system. Taking into account that for small values of the angle ϑ_{min} the following relation holds:

$$\left(\frac{\mathrm{d}\,\sigma}{\mathrm{d}\,\Omega}\right) \simeq \left(\frac{\mathrm{d}\,\sigma}{\mathrm{d}\,\Omega}\right)_{\vartheta=\vartheta_{min}} \cdot \left(\frac{\vartheta_{min}}{\vartheta}\right)^{\frac{n+3}{n+1}}, \tag{15}$$

one can estimate from experimentally measured value $S(\vartheta_{min})\,\mathrm{d}\sigma/\mathrm{d}\Omega$ in the whole range of small scattering angles. In this way differential cross section determined from the Golden and Bandel data appears to be at very small values of scattering angle distinctly above the Ramsauer's values — see Figs. 4 and 5.

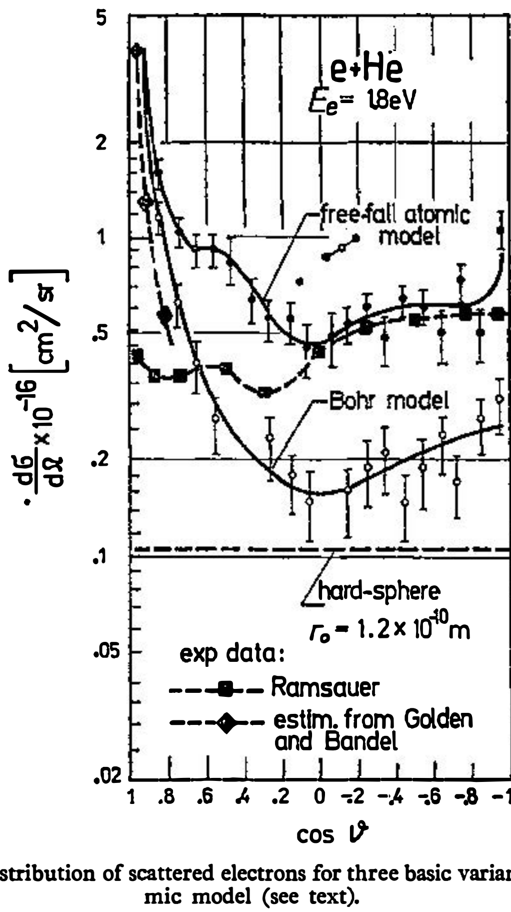

Fig. 4. The angular distribution of scattered electrons for three basic variants of the free-fall atomic model (see text).

Taking into account the above as well as the fact that the present theory neglects the polarisation effects as well as rotation of the atomic shell, which should be particularly important at large and moderate values of the impact parameter, scattering at small angles cannot form the basis for the present analysis of the atomic model.

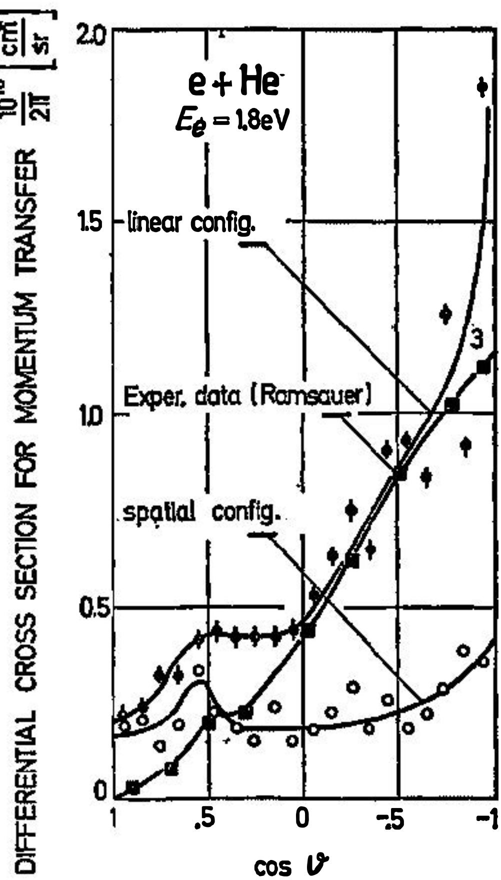

Fig. 5. The contribution of scatterings at various angles to the momentum transfer cross-section. It clearly follows from the figure that scattering at small angles, which are burdened with relatively large error, contribute negligibly to the total momentum transfer cross section.

Confining, therefore, the discussion to large and medium scattering angles, where the collective field approximation should hold, the following conclusions can be drawn:

— scattering cross section is sensitive to the atomic model used for calculations,

— circular model as well as the spatial free-fall atomic model yield results which are in evident contradiction with the experimental data,

— the linear free-fall model, which in the considered range of angles describes quite accurately the experimental data, seems to be quite good description of the helium atom; however, a slight difference between calculated and measured values for the back scattered electrons, suggest a somewhat more complicated form of the electron orbits.

To verify above conclusions it is worthy to calculate (for the discussed forms of the collective motion of electrons) the momentum transfer cross section, in which relatively large-error scattering at small angles play a secondary role — see Fig. 6, i.e.

$$Q_d = 2\pi \int_0^{\pi} \sigma_{\cos\vartheta} \cdot (1 - \cos\vartheta) \cdot \sin\vartheta \, d\vartheta, \qquad (16)$$

and to compare it with experimentally measured one. Comparison of the theoretical and experimental values, see Fig. 6, supports conclusions drawn previously: free--fall atomic model, with eventual small modifications of the free-fall orbit, should be considered as a good picture of helium atom (it is worthy to note that the calculated momentum transfer cross section from Ramsauer's measurements is situated distinctly below the Crompton's et al. value[21]), what supports our doubts about the Ramsauer's data at small scattering angles).

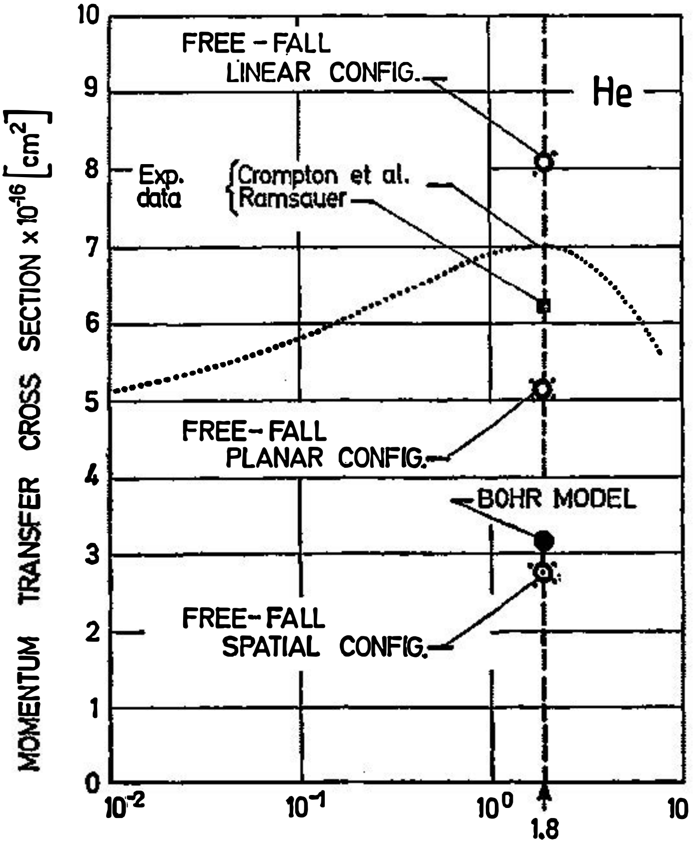

Fig. 6. The calculated momentum transfer cross sections depend strongly upon the atomic model used for calculations. Bohr's atomic model and free-fall spatial configuration give evidently wrong results and must be eliminated from further discussions.

The results obtained show that the collective field approximation may be a quite efficient way of investigation of the structure of atomic systems. The method applicable at small velocities of colliding systems seems to be very useful for investigation of the external parts of the atom and should be considered as a method complementary to the binary encounter approximation (which is a high-velocity approximation). Since in this approach distinction between elastic and inelastic collisions is meaningless, measurements of total differential cross sections of scattered electrons are necessary. On the other hand theoretical works, like the work of Grujić et al.[13], in which polarisation effects are being taken into account, are required.

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RASPRŠENJE NISKOENERGETSKIH ELEKTRONA I MODEL ATOMA He

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Računata je angularna distribucija sporih elektrona raspršenih na atomu He, kao i efikasni presjek za prenos momenta, za tri varijante atomskog modela slobodnog pada (u svakom razmatranom slučaju elektronske orbite obrazovale su različite prostorne konfiguracije). Dobijeni rezultati pokazuju da jezgra i oba elektrona obrazuju u atomu He linearnu (odnosno gotovo linearnu) konfiguraciju, čvrsto (ili skoro čvrsto) orijentiranu u prostoru.