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A CLASSICAL MODEL FOR e — He $(2s^2)$ ELASTIC SCATTERING

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Two variants of the *free fall model* for helium in the first autoionizational state have been proposed for calculating differential cross section for e — He $(2s^2)$ elastic scattering. At $E = 7$ eV impact energy the cross sections are evaluated numerically, making use of the classical trajectory method and are found sistematically higher for the case of the asynchronous atomic electrons motion than for the synchronous one.

1. Introduction

Owing to their physical transparency and mathematical simplicity, classical models continue to attract attention in the theory of atomic collisions. One can distinguish three main areas where the classical picture of atomic particle scattering may be employed: (i) Colliding particles inteact *via* pure Coulomb force (e. g. Rutherford scattering), when in the case of distinguishable particles quantum mechanical and classical theories provide essentially the same results (correspondence identities[1]); (ii) Scattering of charged particles on highly excited atomic systems, when the correspondence principle ensures a reasonably good accuracy of the classical method; (iii) Scattering when ground-state atoms are involved. In the latter case there exists no general principle which could justify an application of the classical picture and validity of a classical model can be proved only *a posteriori*.

In this work we continue investigations of classical atomic systems and their behaviour in collisions with low-energy electrons[2]. First doubly excited state of helium atom has been chosen for two different set-ups for the electron distribution[3], when the electrons »oscillate« either in phase or out of phase near the nucleus and we wanted to see what difference it makes within the classical approach. Secondly, there are at present no experimental data for the electron scattering on these autoionizing states, which are very short-lived and therefore experimentally difficult to deal with.

Unlike the previous models for ground-state atoms[2], where a sort of stochasticity in the electron motion was introduced, the present arrangements of the electron motion is strictly deterministic. This choice has been dictated by the asynchronous model, where the line of electron motion must be fixed in space. We have, therefore, adopted the same feature for the symmetric electron motion, so as to be able to compare effects steming from different types of correlations within the target. Further, we have not taken into account the adiabatic distorsion effects, as different from the ground-state targets[2], since polarizabilities of doubly excited states are not known at present, to our knowledge.

In Section 2 we set up the He $(2s^2)$ classical models and quote some of their properties, whereas in Section 3 the classical trajectory method calculations of e — He $(2s^2)$ elastic scattering are presented. Finally, we discuss the model proposed and its possible improvements, in the last section.

2. He $(2s^2)$ classical models

Since atoms are essentially quantal systems, no *ab initio* classical model can be complete and a number of phenomenological parameters must be introduced. At the beginning we specify, therefore, the following properties of two-electron atomic systems: (a) the energy levels are given by Bohr's formula: $E_n = -Z_{eff}/n^2$, with the effective nuclear charge: $Z_{eff} = Z - 1/4$, where Z is the charge of the nucleus*; (b) spin of electrons and related effects are ignored.

We distinguish two cases, according to types of interelectron correlation: synchronous (symmetric) and asynchronous (asymmetric) models.

2.1. Synchronous motion model

This is a straightforward generalization of the hydrogenic *free fall model*, as used by Gryzinski[4]. Both electrons move along a common straight line in a strictly symmetric fashion: $\vec{r}_1 = -\vec{r}_2$, $\vec{v}_1 = -\vec{v}_2$, as shown in Fig. 1 (a). Each electron »sees« an effective charge $Z_{eff} = Z - 1/4$. Major axis of (degenerate) Kepler orbit $(\varepsilon = 1)$ is given by: $r_A = 2n^2/Z_{eff}$, what in our case yields: $r_A = 4.57\, a_0$, and should be compared with a quantum mechanical estimate[5]. The energy calculated by Bohr's formula is: $E_B(2s^2) = -20.825$ eV (-0.766 au), as compared with experimental value[6]: $E_{exp} = -20.046$ eV (see also Ref. 7). The system is periodic with period: $T = 2\pi n^3/Z_{eff}^2$, what provides for the case at hand: $T = 16.40$ au.

*Atomic units are used throughout, unless otherwise stated.

Symmetric model is, in fact, a quasihydrogenic case, with Z substituted by Z_{eff}. As is well known, equation of motion in the latter case cannot be obtained in a closed form, but can be expressed as an infinite series in terms of Bessel functions.

On the other hand, $r(t)$ can easily be evaluated from equations:

$$t = T(\omega - \varepsilon \sin \omega), \quad r = a(1 - \varepsilon \cos \omega) \tag{1}$$

where ε is the eccentricity, a is the major semiaxis and ω is the so called eccentric anomaly. If a solution for a particular energy of the atom is $r = f(t)$, equation of motion is easily obtained for other energies making use of the so called scaling laws[8]:

$$r' = \lambda f(\lambda^{3/2} t), \quad \lambda = E/E'. \tag{2}$$

From the numerical results for He $(1s^2)$ we have thus calculated a number of relevant quantities, which are shown in Table 1.

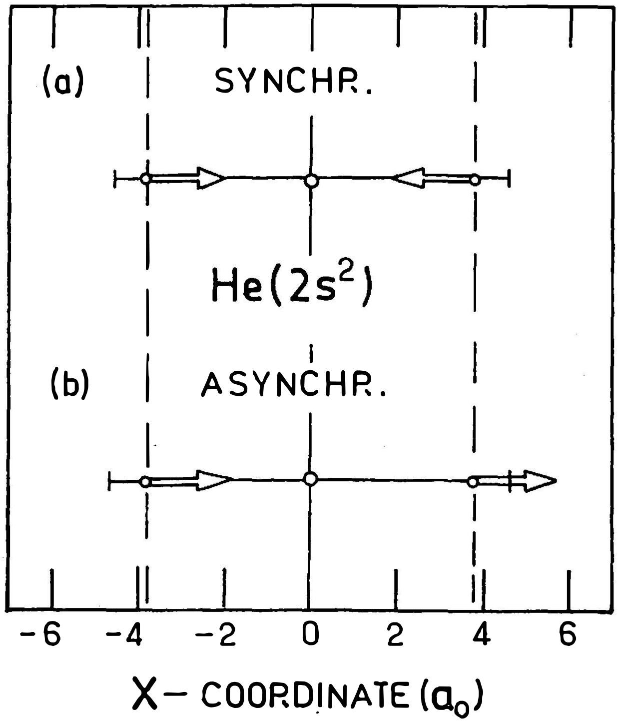

Fig. 1. Free fall configuration for He $(2s^2)$ at $t = T/4$: (a) synchronous (symmetrical) motion; (b) asynchronous (asymmetrical) motion.

2.2. Asynchronous motion model

The model must satisfy two requirements: (i) total energy must be the same as for the synchronous case; (ii) electron motion should be out of phase: $r_1(t = 0) = 0$, $r_2(t = 0) = r_A$, or *vice versa* (see Fig. 1 (b)).

If the system has a period T, then from simple kinematic considerations follows: $r_1(t) = r_2(t + T/4)$. Let the line of motion be along Ox axis, then (relativistic) equations of motion are[9]:

$$\left\{1 - \left|\frac{\mathrm{d}x_i}{\mathrm{d}t}\right|^2 / c^2\right\}^{-3/2} \frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = -\frac{Z}{x_i^2} + \frac{1}{(x_i - x_j)^2}, \; i, j = 1, 2 \qquad (3)$$

with initial conditions:

$$r_1(\delta t) = r_0, \; \dot{r}_1(\delta t) = [E + 2Z/r_0]^{1/2}, \; r_2(\delta t) = 2(1 - Z)/E,$$

$$\dot{r}_2(\delta t) \cong 0 \qquad (4)$$

where E is the total energy, r_0 is a small quantity of the order of the classical radius of electron and t may be set to zero. Equations (3) are solved numerically, for $Z = 2$. For that purpose the computer code for e-He classical collisions[10] has been used, appropriately modified. Some relevant results are shown in Table 1, where they are compared with corresponding values for the synchronous model. As can be seen in Table 1, numerical results reveal

TABLE 1

He ($2s^2$)	symmetric model	asymmetric model
total energy	-0.766	-0.766
period T	16.40	17.2
$r_{1,2}(T/4)$	3.80	3.9
r_A	4.57	4.62
$\bar{r}_{1,2}$	3.39	3.39
$\bar{r}^2_{1,2}$	13.0	13.6
$E_1(T/4), E_2(T/4)$	-0.383, $-0,383$	-0.380, -0.385
$E_1(0), E_2(0)$	-0.383, -0.383	-0.325, -0.441

Numerical results for symmetric and asymmetric He ($2s^2$) classical models (atomic units).

a number of striking similarities between two models. Differences in numerical values, except for single-electron energies, may be ascribed to the insufficient accuracy in solving Eq. (3), because of the highly singular behaviour of the interaction potential near the origin. From our calculations we are pretty sure that, except $r_i(t)$ and $E_i(t)$, other quantities shown in Table 1 should appear identical in both cases, had Eqs. (3) been solved analytically. Unlike the synchronous case, asynchronous motion yields a (changeable) dipole moment of the system, with zero mean value. In Fig. 2 dipole moment: $D = x_1 + x_2$, is plotted as function of time.

This dipole moment makes the asynchronous model much like the hydrogen *free fall* model from Ref. 2 (except for the stochastic effects), and determines the long-range e — He ($2s^2$) interaction to be of monopole — dipole character.

As for the single-electron energies, they are shown in Fig. 2, too. Evidently, these are not constant in time, but are interchanged during a single period T. As can be seen from Table 1, maximum relative asymmetry in energy is: $(E_1(0) - E_1(T/4))/E_1(T/4) = 0.15$. This is an interesting result, indicating that it makes sense to ascribe an energy to a single electron as a mean value only. Consequently, in fast inelastic collisions of charged particles with atoms, it is an instantaneous energy value that matters, whereas in slow collisions the mean energy of an electron is relevant.

On the other hand, for energetic collision differences instantaneous energies are supressed by large impact energies, and this masks the interelectron energy transfer during collisions.

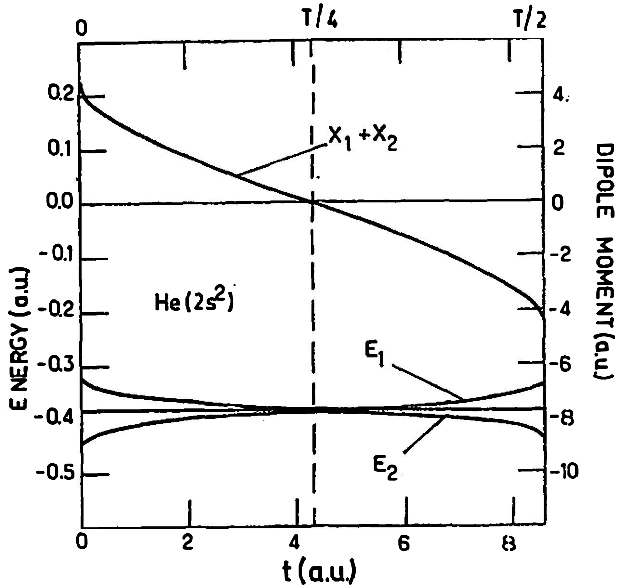

Fig. 2. Dipole moment and single-electron energies of He $(2s^2)$ as function of time, within a half of period T.

It is interesting to note that there exists a moment ($t = T/4$) when corresponding configurations of two models, in phase space, differ only in sign of velocity of one of electrons. It is exactly this configuration that has been shown in Fig. 1. Obviously, it is the most suitable initial state for starting numerical calculations. The quasisymmetry found in respect to this point deserves an analytical investigation, at least a qualitative one.

3. *Elastic e-He$(2s^2)$ scattering calculations*

Even if equations of motion of the atomic electrons were known, an analytical derivation of differential cross section for the electron scattering on a time-dependent nonspherical potential would be beyond our present mathematical capabilities.

We have, therefore, resorted to numerical integrations of corresponding Newton's equations (classical trajectory method) and have computed probabilities for scattering into a solid angle by counting those orbits finishing in a prescribed direction. This is acomplished by choosing relevant initial system parameters at random (Monte Carlo method[11]), i. e. by numerical simulation of a real scattering process. For this purpose use was made of the numerical code developed for e-H stochastic elastic scattering[2], with those features accounting for the stochasticity and target deformability suppressed (see Ref. 2 for numerical detailes).

The incoming electron is chosen to move initially parallel to Oz axis, in the Oyz plane, with the target nucleus (of infinite mass) situated at the origin.

Initial random parameters, generated by the computer, are: orientation angles of the atomic electrons orbits: $\varphi\,(0, 2\pi)$, $\Theta\,(0, \pi)$, time $t\,(0, T)$ and impact parameter $h\,(h_{min}, h_{max})$. In fact, it is the square of the impact parameter which is uniformly distributed and a biased sampling[11] in h^2 has been used in the present calculations, so as to promote those h-regions that contribute most to the scattering. Differential cross section for the scattering at the angle Θ is calculated by[12];

$$\frac{\mathrm{d}\sigma_i}{\mathrm{d}\Omega} = \frac{n_i(\Theta)}{2n_i \Delta\Theta \sin\Theta}\,(h_i^2 - h_{i-1}^2) \pm \delta(\Theta),\ \mathrm{d}\sigma/\mathrm{d}\Omega = \sum_{i=1}^{N} \mathrm{d}\sigma_i/\mathrm{d}\Omega \tag{5}$$

$$\delta(\Theta) = [\sum_{i=1}^{N} (\mathrm{d}\sigma_i/\mathrm{d}\Omega)^2/n_i(\Theta)]^{1/2} \tag{6}$$

where n_i is the total number of orbits between h_i and h_{i-1}, $n_i(\Theta)$ corresponding number of orbits finishing between $\Theta - \Delta\Theta/2$ and $\Theta + \Delta\Theta/2$, N is the total number of h-segments and $\delta(\Theta)$ is the statistical error. In the present work we put: $h_0 = 0.05\,a_0$, $h_N = 25\,a_0$ and $\Delta\Theta = 10^{\circ}$, with $N = 4$. The cut-off at h_N yielded only lower limits for $\mathrm{d}\sigma/\mathrm{d}\Omega\,(\Theta > 25^{\circ})$ (it should be noted that in this region Eq. (6) for the statistical error becomes inadequate[12], anyway).

Computations have been carried out at $E = 7$ eV and results are shown in Fig. 3. Both differential cross sections appear similar in shape, with that for the asynchronous model consistently higher than for the synchronous one. This was to be expected, since at medium distances from the target it is the dipole potential which the impact electron *sees* from the asymmetric configuration, whereas in the case of completely symmetric motion the quadrupole component dominates. As can be seen from Fig. 3 both cross sections have minima approximately at $\Theta =$ $= 130^{\circ}$. Statistical errors appear rather large for $\Theta < 90^{\circ}$, but since there exist no experimental data to be compared with, a better accuracy would not be compelling at present. Generally, thousand orbits for one cross section are needed, with a typical computing time one second per orbit. Besides the statistical error, another limiting factor appears: nonconservation of the impact electron energy. This error is inherent in the model employed and is generally larger for small impact parameters (close collisions), that lead to large scattering angles. Thus, large-angle scattering has been presumably underestimated in our calculations, since all orbits with $|\Delta E|/E < 0.3$ have been discarded.

No other theoretical investigations of e-He$\,(2s^2)$ elastic scattering, either by quantum mechanical approaches or within the classical picture, have been reported up to now, to our knowledge.

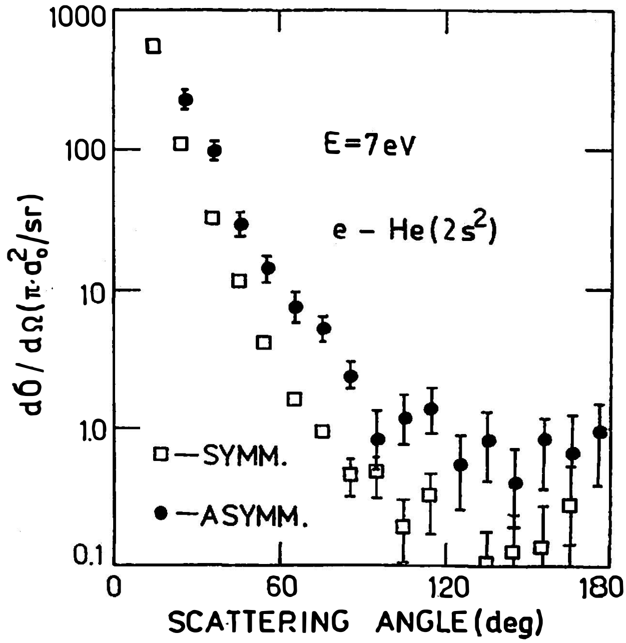

Fig. 3. Differential cross sections for e-He ($2s^2$) elastic scattering at $E = 7$ eV impact energy. □: symmetric model; ●: asymmetric model. Error bars indicate statistical errors.

4. Concluding remarks and discussions

Aim of the present calculations was twofold. First, we wanted to elaborate differences between two possible types of motion within the *free fall model,* in particular in view of the analogous quantum mechanical set-ups. Second, it is of interest to have at least some qualitative estimate of elastic scattering on helium metastable states, (cf. e. g. Ref. 13). These autoionizing states are generally formed *via* e — He ($1s^2$) collisions[6] and constitute a noticeable components in moderately hot plasmas. Though short-lived, with $\tau \cong 5 \cdot 10^{-15}$ s,[6,7] their mean life is still one order of magnitude larger than a typical collision time at $E = 7$ eV. Compared with corresponding cross section for e — He ($1s^2$) scattering, helium autoionizing states may exert stronger influence on the impact particles. For instance, comparing differential cross sections at 90° for e-He ($1s^2$) from Ref. 14 ($E = 5$ eV) with ours, the synchronous model provides only slightly larger value, but asynchronous case yields the cross section larger by factor 5 (note that at this angle classical calculations furnish a reasonably accurate cross sections, cf. Figs. 1, 2 in Ref. 2.)

Further possible improvements of the model proposed here fall into two categories. The first concerns inclusion of some effects analogous to Heisenberg and Pauli principles and are discussed in Ref. 2. Here belongs also a better fulfilment of the energy conservation requirement, which could appreciably affect large-angle scattering; investigations along these lines are in progress. Second class of further elaborations would be an explicite inclusion of the polarization effects, which dominate small-angle scattering. This requires calculation of He ($2s^2$) dipole polarizability and can be done, for example, making use of the variational-perturbational treatment, as used for He ($1s\,2s$) states[15]. One can also introduce stochastic feature into the symmetric model[2]. Spin-spin classical interaction may be accounted for, too[4] but is not expected to alter the overall picture of the scattering process.

As for the possible experimental investigations, they can be carried out within the crossed-beam set-up, with He ($1s^2$) first excited by an electron impact to $2s^2$ state and then bombarded by another electron beam. Another approach would be *via* beam-foil technique. Since $1s^2 \rightarrow 2s^2$ transition is optically forbidden, laser-assisted scattering could proceed only *via* intermediate states, like $2s\,2p$ and would seem hardly feasable.

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JEDAN KLASIČNI MODEL ZA *e*-He ($2s^2$) ELASTIČNO RASEJANJE

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Predložene su dve varijante modela helijuma u prvom autojonizacionom stanju u okviru konfiguracije *slobodnog pada* i primjene za izračunavanje diferencijalnog preseka za *e*-He ($2s^2$) elastično rasejanje. Pri upadnoj energiji $E = 7$ eV izračunat je efikasni presek numerički, pomoću metoda klasičnih trajektorija, za obe varijante. Nađeno je da je diferencijalni presek u slučaju asinhronog kretanja atomskih elektrona sistematski veći nego za sinhroni model.