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INELASTIC ELECTRON COLLISIONS WITH RYDBERG ATOMS

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The standard classical method of computer simulation is used for evaluation of the inelastic cross section in electron collisions with a highly excited (Rydberg) atom. In the course of collision, the incident and bound electrons move along classical trajectories in the Coulomb field of the nucleus, and the scattering parameters are averaged over many initial conditions. The reduced ionization cross section of a Rydberg atom by an electron impact approximately corresponds to that of atoms in the ground states with valence s-electrons and coincides with the results of the previous Monte Carlo calculations. The cross section of an atom transition between Rydberg atom states as a result of electron impact is used for finding the stepwise ionization rate constant of atoms in collisions with electrons or the rate constant of three-body electron–ion recombination in a dense ionized gas because these processes are determined by kinetics of highly excited atom states. Surprising, the limit of low electron temperatures is realized when the electron thermal energy is lower than the atom ionization potential by about three orders of magnitude, as follows from the kinetics of excited atom states.

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1. INTRODUCTION

From the theoretical standpoint, an electron–atom collision at velocities compared to typical valence electron velocities is a many-electron problem, because the exchange between electrons gives the same contribution to the scattering cross section as the electrostatic interaction between incident and atomic electrons. The contribution of the exchange interaction becomes small when velocities of an incident electron are small compared to those of valence electrons. This leads to the Born approximation [1–3], which can be extended to lower collision energies in appropriate models for the cross section of inelastic electron–atom collisions [4–6]. At collision energies that are comparable to the transition energy, classical models are used starting from the Thomson model for atom ionization by electron impact [7]. Although the classical approach for electron–atom collisions is expected to be invalidated by the quantum nature of the atom, classical models are useful because of the identity of the classical and quantum mechanical Coulomb cross sections for elastic scattering [3]. Therefore, classical models for inelastic electron–atom scattering were attractive and were developed (see, e.g., [7–9] for atom ionization by electron impact) until 1930, when Bethe proved [10] that at large collision energies, the logarithmic factor must be included in the expression for the atom ionization cross section by electron impact, whereas this factor is absent in the classical expression for the ionization cross section.

This statement was of principal importance and changed the relation to classical models of electron–atom collisions. As was shown in [11], the logarithmic energy dependence of the quantum cross section is determined by large impact parameters of collision when the atom ionization probability is small or zero in the classical consideration. One can expect the validity of the classical approach to ionization of excited atoms, and the bridge between the classical and quantum approaches was broken by Kingston [12], who proved on the basis of numerical calculations that the cross sections of ionization of excited atoms by electron impact are quite close for the calculation at large collision energies in the quantum (Born approximation) and classical approaches. This means that the different energy dependences in the classical and quantum ionization cross sections are not of principal importance. Nevertheless, because an atom is a quantum system of electrons, caution is required in applying classical methods to electron–atom scattering.

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We consider inelastic electron collisions with highly excited or Rydberg atoms when the classical approach is applicable in principle. The results have a two-fold use. First, the results can be extended to the cases where atom excitation is not high and the results for Rydberg atoms can be used as model ones for various atom transitions. Of course, this requires an additional analysis and grounds. Second, these results are necessary for the analysis of stepwise atom ionization in a plasma or three-body recombination of electrons and ions in a low-temperature plasma. In these cases, the process results from many inelastic electron–atom collisions and is described by the BKW (Bates, Kingston, and McWhirter) scheme [13–15]. For low temperatures and dense plasma, the rates of resultant processes of stepwise atom ionization or three-body electron–ion recombination are determined by inelastic collisions involving electrons and Rydberg atoms [16], and the cross sections for the processes under consideration are important in these problems. Thus, the goal of this paper is to evaluate the cross sections for collisions involving electrons and Rydberg atoms and to use these results in appropriate problems.

2. COMPUTER CODE FOR INELASTIC COLLISIONS INVOLVING ELECTRONS AND RYDBERG ATOMS

Although highly excited or Rydberg atoms have specifics as a quantum object [17–20], we consider inelastic electron collisions with Rydberg atoms as a result of scattering of an incident and valence electrons assuming the motion of electrons in the course of these transitions to be classical. We use our experience in other problems of Rydberg atom collisions, e.g., the resonant charge exchange [21] and Penning process [22] involving Rydberg atoms. Therefore, our goal is to evaluate the cross sections for electron-excited atom inelastic collisions on the basis of computer simulation; these cross sections then give appropriate rate constants. Initially, a colliding atom is in a highly excited state, and the transition process results from collision of two classical electrons in the field of a Coulomb center. We are based on the standard classical Monte Carlo method for collisions involving Rydberg atoms [21, 22] with general peculiarities of this approach taken into account [23, 24]. In these evaluations, we analyze the process for a certain impact parameter of the electron–atom collision that varies from zero to ρ_{max} in a definitive manner.

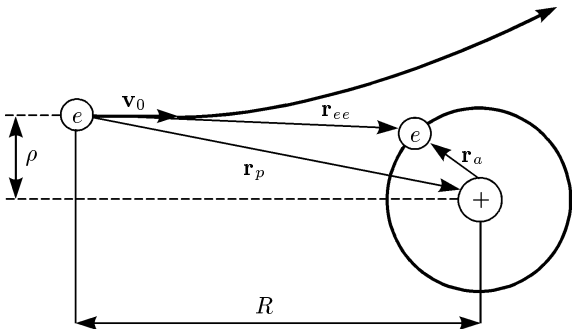

Fig. 1. Positions of the Coulomb center, the incident electron, and the bound electron in a collision of an electron and a Rydberg atom

In considering the problem of the interaction of classical electrons in the field of a Coulomb center, we take a certain value of the electron momentum of the bound electron characterized by the momentum quantum number l. The boundary condition is taken such that the radial electron velocity at the initial instant is zero, the electron distance $r_a(0)$ from the Coulomb center at zero time is $r_a(0) = r_0$, and $v_r(r_0) = 0$. The motion of electrons is described by the Newton equations

$$m\frac{d^2x_i}{dt^2} = -\frac{\partial U}{\partial x_i}, \quad U = \frac{e^2}{|\mathbf{r}_{ee}|} - \frac{e^2}{|\mathbf{r}_p|} - \frac{e^2}{|\mathbf{r}_a|}, \qquad (2.1)$$

where $x_i \equiv x, y, z$, the origin coincides with the nucleus location, r_{ee} is the distance between the incident and bound electrons, and r_p and r_a are distances between the nucleus and the incident or the bound atomic electron, as is shown in Fig. 1.

Because of the overall rotational symmetry of the system, the incident electron starts from a fixed plane with a predetermined velocity $\mathbf{v}_0$ oriented along a fixed direction. The initial distance between the incident electron and the ion is taken to be $R \approx 200r_0$ to take target polarization effects into account. The impact parameter ρ ranges from zero to ρ_{max}, which is equal to few r_0. If the momentum of a bound electron is zero, it is initially located on a sphere of the radius $r_0 = e^2/J$, where J is atom ionization potential. The initial coordinates for a bound electron with the origin at the nucleus are given in terms of the spherical coordinates r_0, θ, and φ:

$$r_0^x = r_0 \sin\theta\cos\varphi, \quad r_0^y = r_0 \sin\theta\sin\varphi, \quad r_0^z = r_0\cos\theta, \qquad (2.2)$$

but due to the electron angular momentum, the spatial distribution of a bound electron becomes more com-

plex. Following [23, 24], we determine the initial position of a bound electron as

$$\begin{aligned} &r_0^x = R_e \sin\theta\cos\varphi, \quad r_0^y = R_e^y \sin\theta\sin\varphi,\\ &r_0^z = R_e^z \cos\theta,\\ &P_0^x = -P_e(\sin\varphi\cos\theta + \cos\varphi\cos\theta\sin\eta),\\ &P_0^y = P_e(\cos\varphi\cos\eta + \sin\varphi\cos\theta\sin\eta),\\ &P_0^z = P_e \sin\theta\sin\eta, \end{aligned} \tag{2.3}$$

where R_e is the distance between a bound electron and the parent Coulomb center and P_e is the electron momentum with respect to its nucleus. Superscripts "x", "y", and "z" denote projections on the respective axis. Taking a random relative direction between initial momenta of the incident and bound electron, we solve the Kepler equation

$$\theta_n = u - \epsilon \sin u, \tag{2.4}$$

where u is the eccentric angle and ϵ is the orbit eccentricity (the ratio of the quantum numbers l and n). The angle θ_n is chosen randomly. At given values of θ_n and ϵ, we find the angle u from Eq. (2.4). Next, knowning the values of ϵ and θ_n, we can calculate R_e and P_e as

$$\begin{aligned} R_e &= \frac{1}{2J}(1 - \epsilon\cos u),\\ P_e &= \sqrt{2J}\,\frac{\sqrt{1-\epsilon^2\cos^2 u}}{1-\epsilon\cos u}, \end{aligned} \tag{2.5}$$

where the atom ionization potential J and other electron parameters are expressed in atomic units.

It follows that Eqs. (2.1)–(2.5) contain five initial parameters, φ, θ, η, ϵ, and θ_n, which are taken randomly for each given velocity of the incident electron and each given impact parameter of collision before numerically integrating equations of motion for electrons moving along classical trajectories. The six parameters, which are different for each trajectory, are given below together with their ranges:

$$\begin{aligned} &0 \le \varphi \le 2\pi, \quad 0 \le \theta \le \pi, \quad -\pi \le \eta \le \pi,\\ &0 \le \epsilon \le 1, \quad 0 \le \theta_n \le 2\pi, \quad 0 \le \rho \le \rho_{max}. \end{aligned} \tag{2.6}$$

Evidently, the classical approach is valid when the transition energy is large compared to the energy difference between neighboring levels, and we assume this criterion to be fulfilled. Moreover, in this analysis, we disregard inelastic collisions with a small energy change compared to the energy difference between neighboring levels because the classical description is not valid in this case. We also disregard large transition energies that are close to the energy of an incident electron because such transitions require a large number of trajectories compared to the used ones.

It is clear that the number of such trajectories has to be sufficiently large to obtain acceptable accuracy, and therefore the calculation stopping criterion must be chosen very carefully to save CPU time. We take this limit such that the interaction potential for an incident electron is small and check its validity by variation of the final time. Each trajectory has been numerically integrated using a predictor–corrector Adam's scheme, which is realized in the Mathematica software package as a built-in function. The total energy conservation was checked during simulation, and if the energy was not conserved, the trajectory was excluded from consideration.

The calculations were performed on the basis of classical formulas. Then the cross section σ_α of an inelastic process is given by

$$\sigma_\alpha = 2\pi \int_0^\infty \rho W_\alpha(\rho)\, d\rho, \tag{2.7}$$

where $W_\alpha(\rho)$ is the probability of this transition at an impact parameter ρ. The subscript "α" can be chosen as "ion", "ex", or "q", which corresponds to the processes of ionization, excitation, and quenching of a Rydberg atom by electron impact.

3. IONIZATION CROSS SECTIONS FOR ELECTRON – RYDBERG ATOM COLLISIONS

We first consider the ionization process in electron collision with a Rydberg atom A that proceeds according to the scheme

$$e(E) + \mathrm{A}(J) \to e(E') + e + \mathrm{A}^+, \tag{3.1}$$

where E and E' are the energies of the incident electron before and after the collision, the principal quantum number for a bound electron of a Rydberg atom is large, $n \gg 1$, and the ionization potential is $J = m_e e^4/2n^2\hbar^2$, where m_e is the electron mass and e is the electron charge. In atomic units $J = \gamma^2/2$, where $\gamma = 1/n$.

In evaluating the cross section of an inelastic collision, we verify the accuracy of the calculation by comparison of the results for different numbers of trajectories under consideration. This comparison is given in Fig. 2, where the ionization probability W_{ion} of a Rydberg atom by the electron impact is given as a function of the impact parameter ρ at a certain energy of the incident electron. The difference of the results for a

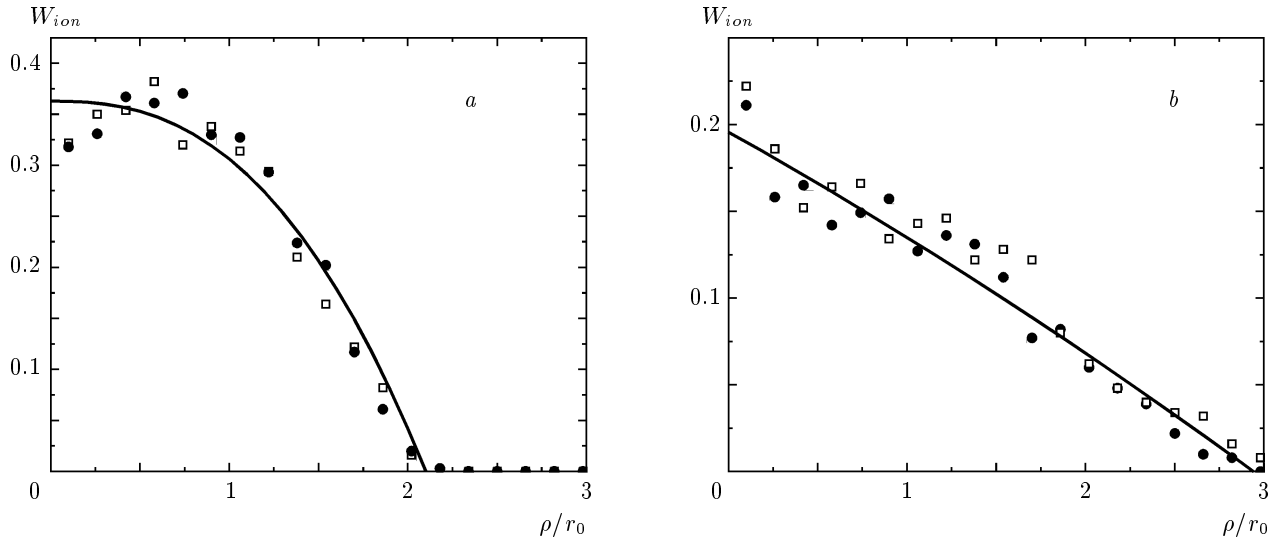

Fig. 2. Dependence of the probability W_{ion} of ionization of a Rydberg atom by electron impact on the impact collision parameter at the relative collision energy $E/J = 1.2$ (a) and $E/J = 5$ (b); $r_0 = e^2/J$

given impact parameter for 10000 and 20000 trajectories does not exceed 2 % and becomes small for the ionization cross section after integration over the impact parameters.

From the dimensionality consideration, we can represent the ionization cross section σ_{ion} in the form

$$\sigma_{ion} = \frac{\pi e^4}{J^2} f\left(\frac{E}{J}\right), \tag{3.2}$$

and $f(x)$ is a universal function for various Rydberg states. The ionization cross section is evaluated by finding the ionization probability at a given collision energy and a given impact parameter and subsequently integrating over the impact parameters. Figure 3 gives the universal function $f(x)$ reconstructed from the ionization cross section. The results depend on the electron momentum and coincide with the results of the previous evaluation [25] of the ionization cross section of a Rydberg atom by electron impact within 1–2 %. The experimental data in Fig. 3 relate to atoms with valence s-electrons and demonstrate the possibility of using the classical approach beyond its applicability limits. The approximation of computer simulation gives the following approximate formula for ionization cross section (3.2) in the case of zero electron momentum:

$$f(x) = \frac{5.3(x-1)}{x(x+2)}. \tag{3.3}$$

It follows that the ionization cross section of a Rydberg atom by electron impact depends on the angular momentum of a bound electron. The ionization cross sections are given in Fig. 3 together with the Thomson cross section [7], the Born approximation [1–3] for the

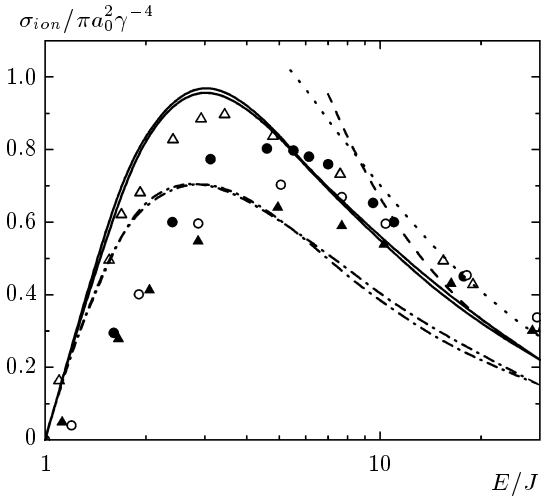

Fig. 3. Ionization cross section of a Rydberg atom by electron impact. Simbols are experimental values for atoms with one and two valence s-electrons, solid lines describe our calculations and calculations in Ref. [25] for zero angular momentum, dash-and-dotted lines are the same when angular and principal quantum numbers of a bound electron are equal, a dotted line corresponds to the tail of the Born approximation, and a dashed line relates to the tail of the Thomson model with the correction due to nonzero velocities of the bound electron [8, 9]; a_0 is the Bohr radius

hydrogen atom in the ground state, and some experimental data for ionization of atoms with one and two valence s-electrons. In addition, the modified Thomson theory with the velocity distribution of a weakly bound electron taken into account [8, 9] is represented in Fig. 3 for large collision energies. The comparison of these cross sections shows that the case of a highly excited atom can be used for estimation of the ionization cross sections for atoms with a weak excitation. The cross sections for a highly excited valence electron tends to an asymptote at very large collision energies.

We note that contemporary semiempirical models for evaluation of the cross section of atom ionization by electron impact start from the limit of large energies of the incident electrons; in this limit, these models amount to the Born approximation. This applies to the Deutsch–Märk [5, 6] and McQuire [4] models, which give an accuracy of the ionization cross section evaluation of approximately 20 % at its maximum, as follows from comparison of the results. The accuracy of such models is the better, the higher is the collision energy. On the contrary, the results of ionization of Rydberg atoms by electron impact, being used for a model of nonexcited or weakly excited atom ionization, are better for not large collision energies.

4. CROSS SECTIONS OF INELASTIC COLLISIONS BETWEEN ELECTRONS AND RYDBERG ATOMS

The process of transition between discrete levels of a Rydberg atom as a result of collision with an electron has a self-dependent meaning. We first consider processes of excitation and quenching of a Rydberg atom in the framework of the Thomson model, which allows highlighting the peculiarities of this process, which proceeds according to the scheme

$$e(E) + \mathrm{A}(J) \to e(E') + \mathrm{A}(J'), \tag{4.1}$$

where E and E' are the energies of the free electron before and after the collision, and J and J' are the binding energies of the initially bound electron before and after the collision. As above, the atom ionization potential is given by

$$J = \frac{\mathrm{Ry}}{n^2},$$

where $\mathrm{Ry} = m_e e^4/2\hbar^2$ is the Rydberg energy (i. e., the ionization potential of the hydrogen atom in the ground state), and we assume that $n \gg 1$, which allows using the classical description of this electron. Correspondingly, the final state is characterized by $J' > 0$ for a transition between discrete levels; introducing the principal number n' of the final state, we have

$$J' = -\frac{\mathrm{Ry}}{n'^2}.$$

It is interesting to compare the results of numerical simulation for an inelastic electron collision with a Rydberg atom and the results of the simple Thomson model, where the interaction of colliding electrons with a Coulomb center is ignored during a strong electron interaction. In the framework of the Thomson model, when the interaction of electrons with the Coulomb center is taken into account only before and after the collision, we characterize the collision process by a change $\Delta\varepsilon$ of the energy of the incident electron. According to the Rutherford formula for a motionless bound electron, we then have the cross section [26]

$$d\sigma = \frac{\pi e^4 d\Delta\varepsilon}{E\Delta\varepsilon^2} \tag{4.2}$$

if the exchange energy lies between $\Delta\varepsilon$ and $\Delta\varepsilon + d\Delta\varepsilon$. We note that because a bound electron has zero energy in the Thomson model, the quenching process is impossible in it.

On the basis of the Thomson model, we find the excitation cross section $\sigma_{ex}(E, \varepsilon_1 \to E - \Delta\varepsilon, \varepsilon_2)$ for the transition of a bound electron from the state with the energy $\varepsilon_1 = \mathrm{Ry}/n_1^2$ into a state with the energy $\varepsilon_2 = \mathrm{Ry}/n_2^2$ (the energy exchange between electrons is $\Delta\varepsilon = \varepsilon_2 - \varepsilon_1$). Correspondingly, the Thomson model gives the following excitation cross section for the transition from an initial highly excited state with the binding energy ε_1 into a group of highly excited states with the binding energy ε_2:

$$\sigma_{ex}(E, \varepsilon_1 \to E - \Delta\varepsilon, \varepsilon_2) = \frac{\pi e^4 \Delta_2}{E\varepsilon_1\varepsilon_2}, \tag{4.3}$$

where

$$\Delta_2 = \frac{\mathrm{Ry}}{(n_2 - 1/2)^2} - \frac{\mathrm{Ry}}{(n_2 + 1/2)^2} \approx \frac{2\mathrm{Ry}}{n_2^3}. \tag{4.4}$$

In terms of principal quantum numbers, expression (4.3) for the excitation cross section becomes

$$\sigma_{ex} = \frac{\pi e^4 \Delta_2}{E\varepsilon_1\varepsilon_2} = \frac{2\pi e^4 n_1^2}{n_2 E\mathrm{Ry}}, \tag{4.5}$$

where the transition proceeds into a group of states with the principal quantum number n_2. This expression also demonstrates the character of the scaling law for transitions between two bound atom states by electron impact.

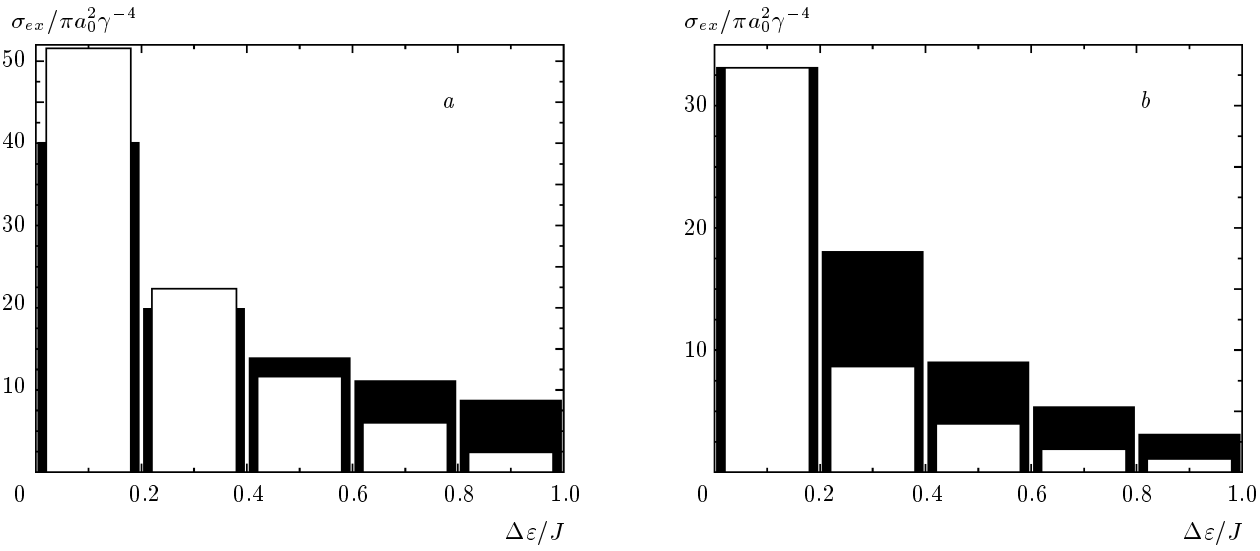

Fig. 4. Excitation cross sections of a Rydberg atom by electron impact at the relative collision energies $E/J = 1.2$ (a) and $E/J = 5$ (b); black histograms correspond to numerical evaluations and white histograms relate to the Thomson model

Figure 4 gives the histograms for computer simulation of the cross section of an inelastic collision between an electron and a Rydberg atom when the energy exchange is found in a given range. We note that the classical description restricts the exchange energy from below, and we exclude collisions with very small exchange energies from calculations. As can be seen from Fig. 4, the results correspond more or less to the Thomson model. By analogy with formula (4.5), using the scaling of the cross section for inelastic collisions, we represent the cross section of this transition in the form

$$\sigma_{ex} = \frac{2\pi e^4 n_1^2}{n_2 E \mathrm{Ry}} F\left(\frac{\Delta\varepsilon}{J},\ \frac{E}{J}\right). \tag{4.6}$$

For the Thomson model, $F(x,\ y) = 1$. According to the results of computer simulation, this function can be approximated as

$$F(x, y) = 1.9x + 0.15y. \tag{4.7}$$

We also separately analyzed quenching of a Rydberg atom in collision with an electron; histograms for such collisions are given in Fig. 5. We note that the Thomson model does not admit the quenching process in principle, because the problem of inelastic scattering of an electron on an atom is reduced there to scattering of the incident and valence motionless electrons. But the quenching cross section σ_q can be expressed through the excitation cross section σ_{ex} on the basis of the detailed balance principle [27] as

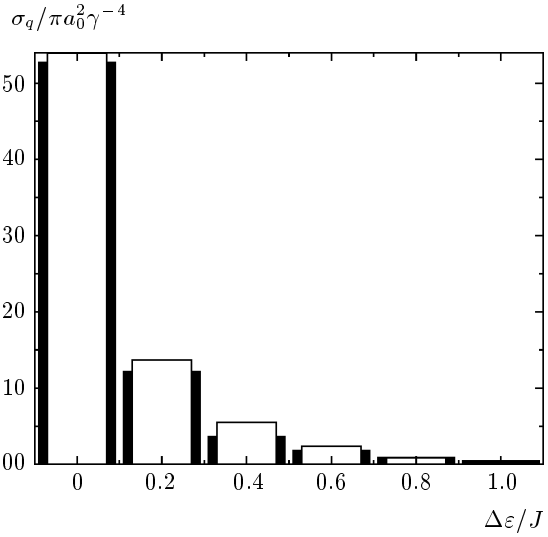

Fig. 5. Quenching cross sections of a Rydberg atom by electron impact at the relative collision energy $E/J = 1.2$; black histograms correspond to numerical evaluations, white histograms are obtained based on the principle of detailed balance from the excitation cross sections

$$\sigma_{ex}(E, \varepsilon_1 \to E - \Delta\varepsilon, \varepsilon_2) = \\ = \frac{g_2}{g_1}\frac{(E - \Delta\varepsilon)}{E}\sigma_q(E - \Delta\varepsilon, \varepsilon_2 \to E, \varepsilon_1), \tag{4.8}$$

where $g_1 \sim 1/\varepsilon_1$ and $g_2 \sim 1/\varepsilon_2$ are the statistical weights of the corresponding states. Formulas (4.5) and (4.6) give

$$\sigma_q = \frac{2\pi e^4 n_2^2}{n_1(E-\Delta\varepsilon)\mathrm{Ry}} F\left(\frac{\Delta\varepsilon}{J}, \frac{E-\Delta\varepsilon}{J}\right) \qquad (4.9)$$

for the quenching of a Rydberg atom state with the principal quantum number n_2 with the transition into a group of Rydberg states with the principal quantum number n_1.

Thus, we obtain classical expressions for the cross section of excitation and quenching of Rydberg atom states by electron impact when the final state is also a Rydberg one. The accuracy is worse for transitions with the energy change of the order of the ionization potential because it requires larger statistics. Nevertheless, the accuracy of the cross section evaluation is better than several percent. Of course, these results are not valid for transitions between neighboring levels because the classical approach is not applicable in this case. The results can be used for transitions between excited atom states as a result of collisions with electrons. They can be extended to the cases of the ground and low excited atom states, where the classical approach is taken as a model. But this requires a special analysis, and it is necessary to divide the cross sections of excitation (4.6), (4.7) and quenching (4.9) into partial cross sections with transitions between states with a given angular electron momentum. The above integral cross sections are used in what follows for the analysis of a stepwise atom ionization in a dense low-temperature plasma. This process, as well as the detailed opposite one, are determined by kinetics of transitions between excited atom states.

5. STEPWISE ATOM IONIZATION AND THREE-BODY ELECTRON–ION RECOMBINATION IN LOW-TEMPERATURE PLASMA

We consider the process of a stepwise atom ionization in a dense ionized gas at low electron temperatures. Then the radiative processes involving excited atoms are not important, and atom ionization results from many successive transition between atom excited states in collisions with electrons. The rate constant of the ionization process in this limit is given by the asymptotic formula [28]

$$k_{step} = C\frac{g_i}{g_a}\frac{m_e e^{10}}{h^2 T_e}\exp\left(\frac{J}{T_e}\right), \qquad (5.1)$$

where g_i and g_a are the statistical weights of the ion and the atom and T_e is the electron temperature. The rate constant of the detailed opposite process of three-body electron–ion recombination

$$2e + \mathrm{A}^+ \to e + \mathrm{A} \qquad (5.2)$$

at low electron temperatures is given by [16]

$$K = A\frac{e^{10}}{m_e^{1/2} T_e^{9/2}}, \qquad (5.3)$$

The numerical coefficients in these formulas, as follows from various approximations, are [29]

$$C = 1.5\cdot 10^{\pm 0.2}, \quad A = 0.2\cdot 10^{\pm 0.2}. \qquad (5.4)$$

Below, we determine these coefficients on the basis of the above classical rate constants of inelastic collisions involving electrons and Rydberg atoms.

In analyzing stepwise ionization as the kinetics of excited atom states and the detailed opposite process of three-body electron–ion recombination, we are based on the BKW scheme [13–15]. Ignoring radiative transitions of excited atoms because they are located in a dense low-temperature plasma, we reduce the problem to the analysis of the kinetic equation in the space of excited energy levels. This equation for the distribution function f_n has the following form in the stationary case:

$$\frac{df_n}{dt} = 0 = N_e\sum_i k_{in} f_i - \\ - N_e f_n \sum_i k_{ni} - N_e f_n k_{ion}^n. \qquad (5.5)$$

Here, N_e is the number density of electrons, the distribution function f_n includes bound states denoted by n and i, k_{ni} (k_{in}) is the rate constant of transition between bound states n (i) and i (k) as a result of collisions with free electrons, and k_{ion}^n is the ionization rate constant by electron impact when an atom is found in a state n. We ignore opposite free–bound transitions because of a small number density of electrons in the ideal plasma under consideration.

We now determine the rate constant of stepwise atom ionization by electron impact and the rate constant of the opposite three-body process of electron–ion recombination in the framework of the above model. In considering this process in a dense low-temperature plasma, we neglect radiative processes involving excited atoms. As a result, the transitions under consideration result from the kinetics of transitions between excited atom states in electron–atom collisions. Thus, these rates follow from the analysis of the kinetic equation for the atom distribution function over states.

We find the rate constant k_{step} of the atom stepwise ionization in a plasma from the balance equation

$$\frac{dN_e}{dt} = N_0 N_e k_{step}, \qquad (5.6)$$

where N_0 is the number density of atoms in the ground state. Comparing equation (5.6) with that expressed through the atom distribution function, we have

$$N_0 N_e k_{step} = N_e \sum_n f_n k_{ion}^n. \tag{5.7}$$

It follows that the rate constant of stepwise atom ionization is expressed through the distribution function of atoms over excited states, f_n, that follows from a solution of BKW kinetic equation (5.5), and this equation is based on the rate constants of inelastic atom transitions due to electron impact that were evaluated above.

In solving kinetic equation (5.5), we note that the transitions between bound electron states establish thermodynamic equilibrium between states, whereas transitions from bound to free states violate thermodynamic equilibrium because of the absence of opposite processes. Hence, thermodynamic equilibrium occurs for bound atom states with large ionization potentials J ($J \gg T_e$). For these states, the distribution function f_n is given by the Boltzmann formula

$$f_n = g_n N_0 \exp\left(-\frac{E_n}{T_e}\right), \tag{5.8}$$

where E_n is the excitation energy for this state, g_n is the statistical weight of this state, and $g_n = n^2$ for an electron located in the Coulomb center. The ionization potential J_n for a state n is

$$J_n = J_0 - E_n, \tag{5.9}$$

where J_0 is the ionization potential for the ground atom state. Along with boundary condition (5.8) for states with a relatively high ionization potential, we have

$$f_n \to 0, \quad n \to \infty \tag{5.10}$$

for highly excited states because these states are destroyed as a result of ionization processes.

To solve Eq. (5.5) for the distribution function f_n, we represent it in the form

$$f_n = \frac{\sum\limits_{i \neq n} k_{in} f_i}{k_{ion}^n + \sum\limits_{i \neq n} k_{ni}}. \tag{5.11}$$

This equation can be solved numerically by consecutive approximations. The resultant distribution function f_n with boundary conditions (5.8) and (5.10) is given in Fig. 6. We then use Eq. (5.7) we find the rate constant of stepwise ionization and the rate constant K of

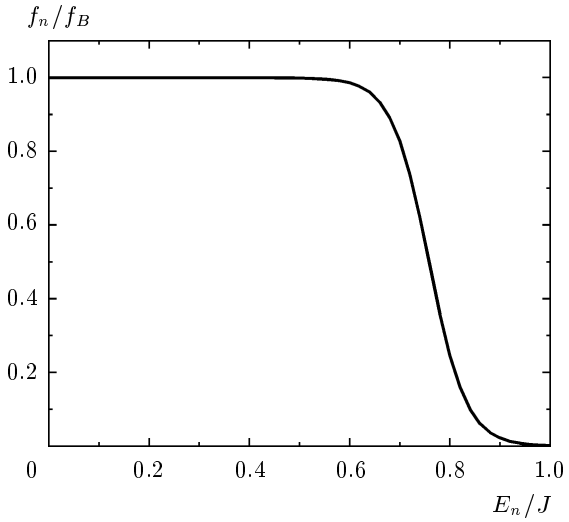

Fig. 6. Relation of the distribution function f_n for population of highly excited electron states of atoms to the Boltzmann distribution function f_B in the course of stepwise ionization or three-body electron–ion recombination

three-body electron–ion recombination on the basis of the principle of detailed balance. We represent the recombination rate constant in the form of relation (5.3),

$$K = \frac{A(T_e) e^{10}}{m_e^{1/2} T_e^{9/2}}. \tag{5.12}$$

In the limit of low electron temperatures T_e, the recombination rate constant depends on the temperature as $K \propto T_e^{-9/2}$ [16], and therefore the function $A(T_e)$ tends to a constant in the limit of low temperatures. Figure 7 gives the dependence $A(T_e)$ for the process

$$2e + \mathrm{H}^+ \to e + \mathrm{H}^*$$

with the evaluations [14, 15] for the hydrogen plasma and in the case where the hydrogen-atom states with $n = 2$ are used as the ground state in the electron kinetics along the excited levels. These evaluations use the classical rate constants by Gryzinski, which are based on some additional unrealistic assumptions. We note that, surprisingly, the limit of low electron temperatures $T_e/J \to 0$ starts from $T_e/J \sim 10^{-3}$.

6. CONCLUSION

The problem of electron–atom collisions is a many-electron problem because the exchange interaction involving electrons is of importance as well as the Coulomb and electrostatic interactions with participation of electrons and the core. Therefore, inelastic electron–atom collisions are studied on the basis

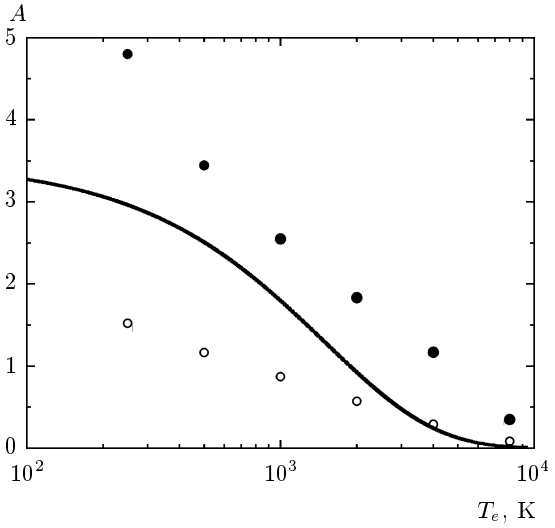

Fig. 7. Function $A(T_e)$ defined according to Eq. (5.12). Solid curve corresponds to present numerical evaluations in terms of the BKW scheme [14, 15] for a hydrogen plasma, filled circles relates to numerical evaluations for a hydrogen plasma, empty circles are numerical evaluations [14, 15] for an alkali metal plasma

of transparent models. This problem simplifies in the cases where the exchange interaction is not important, e.g., at large collision velocities when the Born approximation holds [1–3], or for transitions between states of a highly excited atom when the classical description of the collision problem applies. In this paper, we formulate the classical case of inelastic electron–atom collisions using the standard Monte Carlo method and integrating the equation of motion of electrons along trajectories.

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