Estimates of cross sections for excitation and ionization of an atom in collision with a fast multiply charged ion

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A simple method is proposed for estimating cross sections for excitation and ionization in collision of atoms with fast multiply charged ions in cases in which the Born approximation is inapplicable. This method is analogous to the approximation of sudden excitations and permits direct generalization to collisions that lead to simultaneous excitation or ionization of two or more electrons.

Usually cross sections for inelastic processes in collision of an atom with a fast charged particle are calculated in the Born approximation (see for example the review by Inokuti[1]), which is valid if $Z/v \ll 1$, where Z is the charge of the particle and v is the relative velocity of the collision (in atomic units). However, in a collision with fast multiply charged ions this inequality is violated (as a result of the large values of $Z \gg 1$, in spite of the fact that $v \gg 1$), so that one frequently has $Z/v \sim 1$. Under these conditions it is suggested to use either the Glauber approximation[2] or the sudden-excitation approximation.[3,4] The relation between these approximations is discussed by Eichler.[3] However, the expressions obtained in these approximations for the amplitudes of inelastic processes are cumbersome, and therefore it is difficult to use them for estimates, whereas it is necessary to have simple estimates of cross sections for experiments involving fast multiply charged ions. A method of just that type is presented below.

Let us consider for simplicity the collision of a hydrogen atom with a fast ($v \sim Z$) heavy particle of charge $Z \gg 1$. For convenience we shall consider the ion to be stationary and placed at the origin, and the hydrogen atom to be moving with velocity $\mathbf{v}$ along a straight trajectory

$$\mathbf{R}_0(t) = \mathbf{b} + \mathbf{v}t,$$

where $\mathbf{b}$ is the impact-parameter vector. Then before the collision the wave function of the hydrogen atom has the form (Ref. 5, p. 77)

$$\Phi(\mathbf{r}, t) = \varphi(\mathbf{r} - \mathbf{R}_0(t)) \exp(i\mathbf{v}\mathbf{r} - i\varepsilon t - {}^1/_2 i v^2 t), \qquad (1)$$

where $\varphi(\mathbf{r})$ is the wave function of the ground state of the stationary hydrogen atom and ε is the energy of this state.

Let us surround the ion by a sphere of radius d such that when the hydrogen atom moves inside this sphere the interaction of the electron of the hydrogen atom with the proton (the nucleus of the atom) is much smaller than the interaction of the electron with the ion, i.e., $d \ll Z$. Then when the atom moves along trajectories with impact parameters $b \leqslant d$ it is possible (during the time of the collision $t_0 \sim d/v \ll 1$) to neglect the field of the proton and to assume that a free electron whose wave function is represented by the packet (1) is scattered by a heavy particle of charge Z. The characteristic time of spreading of this packet is ~ 1, and therefore in a time t_0 one can assume that it is nonspreading. However, one can then assume (with the exception of trajectories with very small $b < 1$, which make a very small contribution to the cross section) that the packet (1) moves as a whole along the classical Coulomb trajectory $\mathbf{R}_C(t)$ in the field of a charge Z (we assume that, even though $d \ll Z$ we can consider that $Z \gg 1$ because $d \gg 1$). Therefore after the scattering the electron wave function will have the form

$$\psi(\mathbf{r}, t) = \varphi(\mathbf{r} - \mathbf{R}_C(t)) \exp(i\mathbf{v}_C\mathbf{r} - i\varepsilon t - {}^1/_2 i v^2 t), \qquad (2)$$

where $\mathbf{v}_C = v\mathbf{R}_C(t)/R_C(t)$ is simply the velocity vector rotated by the scattering angle χ, in the Coulomb field, and $b^2 = (Z^2/v^4)ctg^2(\chi/2)$ (Ref. 6, p. 70). However, the proton in the considered region of impact parameters continues during the entire time to move along a straight trajectory $\mathbf{R}_0(t)$. Therefore the amplitude of the transition during the collision time t_0 to some state g_n of the hydrogen atom with energy ε_n has the form

$$A_n = \int d^3r\, \varphi(\mathbf{r}) g_n^*(\mathbf{r} + \Delta\mathbf{R}) \exp\{i\Delta\mathbf{v}(\mathbf{r} + \mathbf{R}_C(t_0)) + i(\varepsilon_n - \varepsilon)t_0\}, \qquad (3)$$

where (Ref. 6, p. 53)

$$\Delta\mathbf{v} = \mathbf{v}_C - \mathbf{v}, \quad \Delta\mathbf{R} = \mathbf{R}_C(t_0) - \mathbf{R}_0(t_0) \approx t_0\Delta\mathbf{v},$$

and

$$\Delta v = 2v \sin(\chi/2) \sim v\chi \sim 2Z/vb,$$

so that

$$t_0\Delta v \sim (2Z/v^2)(d/b) \ll 1, \quad 1 < b < d.$$

Since in Eq. (3) $r \sim 1$, the quantity $\Delta R \approx t_0\Delta v \ll 1$ can be neglected and, dropping an unimportant time-dependent phase factor, we obtain an expression for the amplitude

$$A_n = \int d^3r g_n^*(\mathbf{r}) \varphi(\mathbf{r}) \exp(i\Delta\mathbf{v}\mathbf{r}). \qquad (4)$$

The interpretation is as follows: during the collision of the atom with the multiply charged ion, the atomic electron acquires relative to the nucleus of the atom a momentum Δv, but does not succeed in changing appreciably its position relative to the nucleus of the atom (of course, the change in the position of the electron relative to the ion is large). A

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similar expression was used by Migdal (Ref. 7, pp. 89–91) to calculate the probability of ionization of an atom in impact of a neutron by a nucleus. The cross section for transition of the hydrogen atom from the state φ to g_n is obtained by multiplying $|A_n|^2$ by the Rutherford scattering cross section $d\sigma_R$ of the packet (1) in the field of the ion: $d\sigma_n = |A_n|^2$ and by integrating over the impact parameter or over the scattering angle. Introducing instead of the scattering angle the momentum transfer q, we obtain

$$\sigma_n = 8\pi \frac{Z^2}{v^2} \int_{q_0}^{q_1} \frac{dq}{q^3} |A_n|^2, \quad q = \Delta v = 2v \sin\frac{\chi}{2}, \tag{5}$$

where the integration limits $q_1 = 2Z/v$ and $q_0 = 2/v$ are determined from the conditions of applicability of the approach. The upper limit corresponds to small impact parameters $b_1 \sim 1$ of the order of the size of the state φ up to which it is still possible to speak of motion of the packet (1) as a whole in the field of the ion, or corresponds to large momentum transfers $q \sim 2Z/v$; for such values of q the inelastic form factor (4) is small (see Ref. 1), and therefore the integral (5) will depend only weakly on the upper limit and consequently we can assume that $q_1 = 2Z/v$. The lower limit corresponds to small momentum transfers or to large impact parameters b_0, up to which it is still possible to neglect the proton field in comparison with the ion field; here, since the square of the modulus of the inelastic form factor (4) for small q behaves as q^2 (Ref. 1), the integral (5) will depend on the lower limit logarithmically, i.e., weakly. Therefore we can assume that $b_0 \sim Z$, since at just such distances from the ion the field of the ion becomes equal to the field of the proton (at a distance of 1 amu from the proton); therefore $q_0 = 2/v$.

A similar method of cutting off the integral over momentum transfer is used in the theory of scattering of fast charged particles by an atom in the dipole approximation (Ref. 5, p. 710). In principle it is necessary to add to the cross section (5) contributions from trajectories with impact parameters $b < 1$ and $b > Z$. In the region $b < 1$ (i.e., for impact parameters smaller than the size of the packet (1)), breakup of the packet occurs in the collision, and therefore ionization is highly probable (this is confirmed also by the calculations of Yudin[4]). Thus, the contribution of this region to the cross section is $\Delta\sigma \approx \pi\xi$, where $\xi = 1$ for ionization and $\xi = 0$ for excitation. In the region of large impact parameters the Born approximation is applicable (Eq. (23) of Ref. 8). However, the additions from the regions $b < 1$ and $b > Z$ are small in view of the inequality $Z \gg 1$, and can be neglected.

Note that the approximations made by us in derivation of Eq. (4) or Eq. (5) are not specific. For example, in use of the Glauber approximation it is assumed that the atomic electron does not change its position with respect to the nucleus of the atom during the entire collision time. This, of course, requires separation of the region where the action of the potential of the multiply charged ion is substantial and where the time of dwell of the hydrogen atom is short. Essentially similar assumptions must be made in use of the sudden-excitation approximation. Generally speaking, both approximations are applicable only for potentials with a finite range or which fall off sufficiently rapidly with distance.

A natural generalization of the amplitude (4) to the case of collision of a fast multiply charged ion with a complex atom, as a result of which the atom goes over from an initial state $\Phi_0(\mathbf{r}_1,...,\mathbf{r}_n)$, where $\mathbf{r}_i$ are the coordinates of the atomic electrons, to a state $\Phi_n(\mathbf{r}_1,...,\mathbf{r}_n)$, has the form

$$A_n = \int d^3r_1 \ldots d^3r_n \Phi_n^*(\mathbf{r}_1, \ldots, \mathbf{r}_n)\Phi_0(\mathbf{r}_1, \ldots, \mathbf{r}_n) \times \exp\left(i\Delta\mathbf{v}\sum_{i=1}^{n}\mathbf{r}_i\right). \tag{6}$$

Here Φ_n can correspond to ionization or excitation of one or several electrons. Equation (6) is valid if the relative velocity of the collision $v \gg v_a$—the characteristic velocities of the atomic electrons, if $Z \gg Z_a$—the charge of the nucleus of the atom, and $Z/v \sim 1$, and also if during the collision time t_0 it is possible to neglect the interelectron interaction in comparison with the interaction of the atomic electrons with the multiply charged ion. In this case $\Delta\mathbf{v}$ in Eq. (6) is the same as in Eq. (4). In other words, the result of scattering of a fast multiply charged ion by an atom reduces to a sudden transfer of a momentum $\Delta\mathbf{v}$ to each of the atomic electrons.

We note also that it may happen that the collision velocity is greater than the velocity of the outer electrons but less than the velocity of the inner electrons, or that Z is greater than the effective charge of the nucleus of the atom for the outer electrons but less than the effective charge of the nucleus for the inner electrons; in such cases the multiply charged ion "blows away" only the outer shells (compare with Ref. 7, p. 91). Therefore Eq. (5) with the amplitude (6) can be used for estimates of the cross sections for ionization and excitation in collision of fast multiply charged ions with a complex atom; it is necessary only to redefine the integration limits.

For simplicity we shall consider ionization or excitation of the K shell. We introduce Z_a—the effective charge of the nucleus of the atom for the K shell. Then $b_1 \sim 1/Z_a$, correspondingly $q_1 = 2ZZ_a/v$, and b_0 is determined from the equality of the field of the atomic nucleus (at a distance $1/Z_a$ from the nucleus) to the field of the multiply charged ion (at a distance b_0 from the ion), i.e., $b_0 \sim Z/Z_a^2$ and consequently $q_0 = 2Z_a^2/v$. We emphasize that Eq. (5), which differs formally in appearance from the first Born approximation (Ref. 5, p. 719) only in the limits of integration over the momentum transfer, has a completely different region of applicability than the Born approximation.

Using the data of Ref. 1 on the inelastic form factor of the hydrogen atom, we obtain from (5) an estimate of the cross section for ionization of the hydrogen atom from the $1s$ state by impact of a fast multiply charged ion (for $Z/v \gtrsim 1$)

$$\sigma \approx 8\pi \frac{Z^2}{v^2} \cdot 0{,}3 \ln(2v) \approx \frac{\ln(2v)}{\ln(9.1v)} \sigma_B, \tag{7}$$

where σ_B is the ionization cross section calculated in the first Born approximation; the Bethe asymptotic behavior is

$$\sigma_B \approx 4\pi \frac{Z^2}{v^2} \cdot 0.3 \ln\frac{v^2}{0.012}.$$

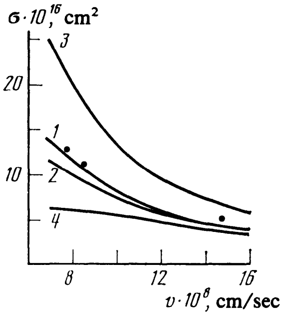

FIG. 1. Cross section for ionization of the hydrogen atom by C^{6+} ions as a function of the relative velocity of the collision.

We estimate also the cross section for ionization of a hydrogen-like ion (nuclear charge Z_a) from the 1s state by impact of a fast multiply charged ion (for $Z/v \gtrsim 1$)

$$\sigma \approx 8\pi \frac{1}{v^2}\left(\frac{Z}{Z_a}\right)^2 \cdot 0.3 \ln \frac{2v}{Z_a}.$$

The fact that the ionization cross section (7) in the velocity region of interest here is less than σ_B is due to our use of the unitary approach, whereas it is well known that the first Born approximation is not unitary. We note that the frequently used renormalized Born approximation,[9] which corresponds to unitarization of the Born approximation, was obtained on the basis of phenomenological considerations.

In the figure we have shown the cross section for ionization of the hydrogen atom by carbon ions with charge six: curve 1 is from Eq. (7), curve 2 is from a calculation[10] in the sudden-excitation approximation[3] (it is evident that the cross section according to Eq. (7) is only slightly greater than the result of Ref. 10), curve 3 gives σ_B, and curve 4 is the cross section calculated by the formula of Ref. 8,

$$\sigma_{\text{ion}} = 7{,}2 \frac{Z^2}{v^2} \ln\left(\frac{1{,}43}{Z} v^2\right),$$

which was obtained on the basis of the Born approximation; the points are from the experiments of Refs. 11 and 12. As can be seen from the figure, the agreement with experiment is good for such a simple method of calculation. The calculations with Eq. (7) are in the same agreement with the remaining experimental data[12] ($\sigma_{H2} \approx 2\sigma_H$).

Therefore the proposed simple approach completely replaces the complicated numerical calculations of the ionization and excitation cross setions of atoms by fast multiply charged ions in the case in which the Born approximation is inapplicable. The proposed scheme of calculation is specially convenient for estimates of the cross section for simultaneous excitation or ionization of two or more electrons in collision of complex atoms with fast multiply charged ions.

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