Inelastic processes in collisions of relativistic multicharged ions with atoms

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Inelastic atomic collisions of relativistic multicharged ions are studied, in which the ions have charge numbers $Z \gg 1$ and relative collision velocities $v \gg 1$, such that the condition $Z/v \sim 1$ holds (in atomic units). The Born approximation cannot be used for parameter values in this region. The result of such a collision reduces to a sudden transfer of momentum to the atomic electrons. The cross sections for ionization of hydrogen atoms are calculated. Cases of the collisions of multicharged ions with complex atoms are studied.

1. INTRODUCTION

Inelastic processes which occur in the course of collisions of fast multicharged ions with atoms have rather large cross sections. Calculations on these processes are of interest primarily from the standpoint of applications. Because of the strong ion field, one cannot use the Born approximation. As a result, the calculations become very complicated, even for nonrelativistic collisions of fast multicharged ions with hydrogen atoms.[1–5] Relativistic collision velocities make the calculations even more complicated.[6] The reason is that the corresponding experiments (see Refs. 7 and 8 and the papers cited there) often use heavy ions of such a large charge that the Born approximation, $Z/v \ll 1$ (Z is the charge of the incident ion, v is the relative collision velocity, and atomic units are being used here and below), does not become applicable even at relativistic velocities $v \sim c \approx 137$. Primarily because of experimental requirements, there is a need for simple estimates of the cross sections for inelastic processes accompanying collisions of fast multiply charged ions with atoms—an approach has been proposed[9] according to which the result of the inelastic collision of the fast, nonrelativistic multicharged ion (under the condition $Z/v \sim 1$) with the atom reduces to a sudden transfer of momentum to atomic electrons. The cross sections for inelastic processes in Refs. 9–12 calculated by this simple approach agree well with experiment.

In the present paper we propose a generalization of the method of Ref. 9 (for calculating the cross sections for inelastic processes accompanying collisions of multiply charged ions and atoms) to the range of relativistic collision velocities, for ion charges $Z \gg 1$ and for relative collision velocities $v \gg 1$ such that the condition $Z/v \sim 1$ holds, with $v \lesssim c$. We estimate the cross sections for ionization of the hydrogen atom, and we consider collisions of multicharged ions with complex atoms. This new approach proves particularly convenient for the case of multiple ionization and excitation of complex atoms.

2. GENERAL FORMALISM

We use the approximation of sudden perturbations, according to which the amplitude for a transition of an atom from the state $|0\rangle$ to the $|n\rangle$ state due to a sudden perturbation $V(t)$ is[1,3,13]

$$M_n = \left\langle n \left| \exp\left\{ -i \int_{-\infty}^{\infty} V(t)\,dt \right\} \right| 0 \right\rangle. \quad (1)$$

We first consider a collision between a multicharged ion moving at a relativistic velocity and a hydrogen atom. We assume that the hydrogen atom is at rest at the origin of coordinates, while the ion is moving along a rectilinear trajectory $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t$, where $\mathbf{b}$ is the impact parameter, and $\mathbf{v}$ is the ion velocity. In this case the approximation of sudden perturbations can be justified in the following way: The collision time can be estimated to be $\tau \sim b\sqrt{1-\beta^2}/v$, where $\beta = v/c$ [in the nonrelativistic case we would have $\tau \sim b/v$; the factor $\sqrt{1-\beta^2}$ appears because of the relativistic "flattening" of the field of the ion;[14] see also Eq. (11) below]. In a collision, the electron of the hydrogen atom is moving under the influence of the field of the ion with an acceleration $a \sim Z/(b^2\sqrt{1-\beta^2})$, and it is displaced a distance $l \sim a\tau^2 \sim Z\sqrt{1-\beta^2}/v^2$. The following conditions must therefore hold:

1) The effect of the perturbation is sudden: $\tau \ll 1$ is on the order of the time scale of the motion of the electron in the hydrogen atom; $b \ll v/\sqrt{1-\beta^2}$. This condition imposes a restriction on the region of impact parameters.

2. The distortion of the square of the absolute value of the wave function of the atomic electron is small: $l \ll 1$. In other words, we have $v^2/\sqrt{1-\beta^2} \gg Z$. (In the nonrelativistic case, conditions 1 and 2 become $b \ll v$ and $v \gg \sqrt{Z}$.)

An ion in uniform rectilinear motion creates a field[14] described by the following scalar potential φ and vector potential $\mathbf{A}$:

$$\varphi = \frac{Z}{R^*}, \quad \mathbf{A} = \frac{\mathbf{v}}{c}\varphi,$$

$$R^* = \sqrt{(x-vt)^2 + (1-\beta^2)(\mathbf{s}-\mathbf{b})^2}, \quad \beta = v/c, \quad (2)$$

where $(x,y,z) = (x,\mathbf{s}) = \mathbf{r}$ are the coordinates of the observation point, the x axis is directed along $\mathbf{v}$, and $\mathbf{s}$ is the projection of $\mathbf{r}$ onto the plane of the impact parameter. Accordingly, the behavior of an electron of a nonrelativistic hydrogen atom is described by the Schrödinger equation

$$i\frac{\partial\Psi}{\partial t} = [H_0 + V(t)]\Psi, \quad (3)$$

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where H_0 is the unperturbed Hamiltonian of the hydrogen atom, and the perturbation $V(t)$ is (the electron charge is -1)

$$V(t)=\frac{1}{2c}(\mathbf{pA}+\mathbf{Ap})+\frac{1}{2c^2}\mathbf{A}^2-\varphi. \tag{4}$$

In (1), $\mathbf{r}=(x,\mathbf{s})$ are the coordinates the electron of the hydrogen atom with the atom at the origin of coordinates. The size of the hydrogen atom is ~ 1, so we have $s\sim 1$; for large impact parameters $b\gg 1$ we find from (2)

$$\varphi\approx\frac{Z}{R_0(t)}+\frac{Z(1-\beta^2)\mathbf{bs}}{R_0^3(t)}, \quad \mathbf{A}=\frac{\mathbf{v}}{c}\varphi, \tag{5}$$

where

$$R_0(t)=\sqrt{(x-vt)^2+(1-\beta^2)b^2}. \tag{6}$$

The expansion (5) corresponds to transverse (with respect to $\mathbf{v}$) uniformity of the field of the ion (at $b\gg 1$) over the extent of the hydrogen atom. Since the hydrogen atom is a nonrelativistic system, it is clear in principle that the interaction of the electron of the hydrogen atom with a multicharged ion can be chosen in the form of a retarded scalar Coulomb potential: $V(t)\approx-\varphi$. However, this point can also be verified directly. To do this, we write a gauge transformation of the potentials (5):

$$\varphi'=\varphi-\frac{1}{c}\frac{\partial f}{\partial t}, \quad \mathbf{A}'=\mathbf{A}+\nabla f, \tag{7}$$

where

$$f=-\frac{Zv}{c}\ln|(x-vt)+R_0(t)|.$$

As a result we find

$$\varphi'=\frac{(1-\beta^2)Z}{R_0(t)}+\frac{Z(1-\beta^2)\mathbf{bs}}{R_0^3(t)}, \qquad \mathbf{A}'=\frac{\mathbf{v}}{c}\frac{Z(1-\beta^2)\mathbf{bs}}{R_0^3(t)}. \tag{8}$$

However, the linear terms (linear in terms of the dimensions of the hydrogen) in the perturbation (4) are then contained only in the scalar potential φ'. We can thus set $V(t)\approx-\varphi'$.

For this choice of perturbation we have

$$\int_{-\infty}^{\infty}V(t)dt=-Z\int_{-\infty}^{\infty}\frac{(1-\beta^2)dt}{R_0(t)} -Z\int_{-\infty}^{\infty}\frac{(1-\beta^2)\mathbf{bs}}{R_0^3(t)}dt. \tag{9}$$

When we substitute this integral into (1), the first term on the right side of (9) gives rise to a constant phase factor, which is independent of the coordinates of the atomic electron. Although this phase factor is infinite, it does not affect the probability for transitions, so it can be discarded. Without any loss of generality, in the approximation of sudden perturbations, we can thus replace (4) by the perturbation

$$V(t)=\frac{Z(1-\beta^2)\mathbf{bs}}{\sqrt{[(x-vt)^2+(1-\beta^2)b^2]^3}}. \tag{10}$$

This potential can be considered to be acting for a finite time τ, so we have

$$\int_{-\infty}^{\infty}V(t)dt=\frac{2Z}{v}\frac{\mathbf{bs}}{b^2}=\mathbf{qs}=2V(t=x/v)\tau, \qquad \mathbf{q}=\frac{2Z\mathbf{b}}{vb^2}, \quad \tau=b\sqrt{1-\beta^2}/v, \tag{11}$$

where τ has the meaning of the time over which potential (10) acts, and $\mathbf{q}$ is the momentum transferred to the atomic electron. It is this procedure (involving the omission of a constant phase factor and making it possible to introduce a collision time τ) which justifies the application of the sudden-perturbation approximation to a long-range Coulomb field (cf. the corresponding computational procedure in Ref. 1). Accordingly, under the condition of a sudden perturbation, i.e., with $\tau\ll 1$ on the order of the time scale for the motion of an electron in the hydrogen atom, the amplitude for the transition (1) takes the form

$$M_n=\langle n|\exp(-i\mathbf{qr})|0\rangle. \tag{12}$$

Here, according to (11), we have $\mathbf{qr}=\mathbf{qs}$, where $\mathbf{s}$ is the projection of $\mathbf{r}$ onto the impact-parameter plane. The result of the collision of the multicharged relativistic ion with the atom thus reduces to a sudden transfer of momentum to the atomic electron. This interpretation is valid for impact parameters for which expansion (5) is valid, i.e., $b\gg 1$, and for which the inequality $\tau\ll 1$ holds (hence $b\ll v/\sqrt{1-\beta^2}\sim Z/\sqrt{1-\beta^2}$ at $v\sim Z$) or for impact parameters b such that

$$1=b_1\ll b\ll b_0=Z/\sqrt{1-\beta^2}. \tag{13}$$

The cross section for the transition of the hydrogen atom from the state $|0\rangle$ to the state $|n\rangle$ is found by multiplying the square of the absolute value of the amplitude for the transition from $|0\rangle$ to $|n\rangle$ by $2\pi bdb$ and by integrating over all impact parameters b. For the same reasons as in the nonrelativistic case [which is discussed in detail after the derivation of Eq. (5) in Ref. 9], we can ignore the contributions from the regions $b<b_1$ and $b>b_0$, and we can assume

$$\sigma_n\approx\int_{b_1}^{b_0}2\pi bdb|M_n|^2=8\pi\frac{Z^2}{v^2}\int_{q_0}^{q_1}|M_n|^2\frac{dq}{q^3}. \tag{14}$$

From (11) we have $q=2Z/vb$ and, correspondingly,

$$q_0=2Z/vb_0=2\sqrt{1-\beta^2}/v, \qquad q_1=2Z/vb_1=2Z/v. \tag{15}$$

According to (15), the momentum transfer q is small in comparison with mc ($m=1$ is the mass of an electron). This implies that for $b_1\leqslant b\leqslant b_0$ (the impact parameters which basically determine the cross section) the hydrogen atom can be assumed nonrelativistic, even in the final state (even in the continuum).

TABLE I. Cross sections for ionization of the hydrogen atom as a function of the relative collision velocity.

β	Ion energy, MeV/nucleon	σ_B/Z^2, 10^3 a.u. [Eq. (17)]	σ/Z^2, 10^3 a.u. [Eq. (16)]
0.10	4.72	183.00	133.00
0.20	19.30	52.30	40.10
0.30	45.30	25.00	19.90
0.40	85.40	14.70	12.00
0.50	145.00	9.79	8.14
0.60	234.00	7.02	5.94
0.70	375.00	5.31	4.59
0.80	615.00	4.20	3.70
0.90	1213.00	3.49	3.14
0.91	1323.00	3.43	3.10
0.92	1454.00	3.39	3.07
0.93	1613.00	3.34	3.04
0.94	1810.00	3.30	3.01
0.95	2064.00	3.27	2.99
0.96	2410.00	3.25	2.98
0.97	2918.00	3.24	3.00
0.98	3773.00	3.25	3.03
0.99	5707.00	3.32	3.10

Further calculations based on Eq. (14) are possible only by numerical methods. However, in the case of the ionization of the hydrogen atom we can propose, by analogy with Ref. 9, the following approximate formula for the total cross section for ionization by impact by a multicharged ion moving at a relativistic velocity v satisfying $Z/v\sim 1$:

$$\sigma=8\pi\frac{Z^2}{v^2}\,0.3\ln\frac{2v}{\sqrt{1-\beta^2}}\,. \qquad (16)$$

Table I shows the results of a calculation of the cross section for the ionization of the hydrogen atom through impact with a relativistic multicharged ion. The third column shows the Born approximation (or the Bethe asymptotic expression)[15]

$$\sigma_B=4\pi\frac{Z^2}{v^2}\left[0.283\left(\ln\frac{\beta^2}{1-\beta^2}-\beta^2\right)+4.0364\right]. \qquad (17)$$

This approximation systematically overestimates the cross section by $\approx$30–10% because, as in Ref. 9, the Born approximation is not unitary. This small difference between our result, (16) and the Born approximation is possible only for one-electron transitions; for multielectron transitions in complex atoms, the situation is completely different.

3. EXCITATION AND IONIZATION OF A COMPLEX ATOM

A natural generalization of Eq. (14) to the case of the collision of a fast, relativistic multiply charged ion with a complex N-electron nonrelativistic atom can be carried out directly by replacing $V(t)$ in (4) by the operator representing the interaction of the multicharged ion with atomic electrons, with the subsequent obvious repetition of calculations which led us to Eq. (14). As a result the cross section for the transition of an atom from state $|0\rangle$ to state $|n\rangle$ in a collision with a multicharged ion moving at a relativistic velocity takes the form

$$\sigma_n=8\pi\frac{Z^2}{v^2}\int_{q_0}^{q_1}\frac{dq}{q^3}\left|\left\langle 0\left|\exp\left\{-i\mathbf{q}\sum_{a=1}^{N}\mathbf{r}_a\right\}\right|n\right\rangle\right|^2, \qquad (18)$$

where the state $|n\rangle$ may correspond to the excitation or ionization of one or several electrons, and $\mathbf{r}_a$ are the coordinates of the atomic electrons. Equation (18) is valid if the relative collision velocity satisfies $v\gg v_a$ (v_a are characteristic atomic velocities), if the ion charge satisfies $Z\gg Z_a$ (Z_a is the charge of the atomic nucleus, and $Z/v\sim 1$ and $v\lesssim c$), and also if, over the time τ, we can ignore interelectron interactions in comparison with interactions of the atomic electrons with the multicharged ions. The scattering of a fast multicharged ion by an atom thus reduces to a sudden transfer of momentum $\mathbf{q}$ to each of the atomic electrons. The range of the integration over the momentum transfer $q=2Z/vb$ in (18) is found, as in the case of the hydrogen atom, from the limits on the applicability of the approach. According to (15) it is sufficient to redefine b_0 and b_1 here. The values of b_0 are found from the equality $\tau=\tau_a$ (τ is an atomic time scale), and b_1 is found from the equality $b_1=r_a$ (r_a is an atomic length scale).

As an example we consider the K shell. We introduce Z_a, the effective charge of the nucleus for the K shell. We then have $b_1=1/Z_a$ and, correspondingly, $q_1=2ZZ_a/v$. We then find $\tau_a\sim 1/Z_a^2$ and $\tau=b\sqrt{1-\beta^2}/v$. From the equality $\tau=\tau_a$ we find $b_0\sqrt{1-\beta^2}/v=1/Z_a^2$ or $b_0=v/(Z_a^2\sqrt{1-\beta^2})$. Correspondingly, for $v\sim Z$ we have $b_0=Z/(Z_a^2\sqrt{1-\beta^2})$; we then find $q_0=2Z/vb_0=2\sqrt{1-\beta^2}Z_a^2/v$ (cf. Ref. 9).

Many studies have recently been carried out on the multiple ionization of complex atoms in collisions with fast multicharged ions (see, for example, Ref. 8 and the papers cited there). Most of the studies have used ions of high charge $Z \gg 1$, moving at velocities $v \gg 1$, with $Z/v \sim 1$. In calculations on such processes, the multielectron ionization of the complex atom should be explained on the basis of the so-called direct excitation of the atom by the strong field of the multicharged ion.[16] Phenomenologically, this approach corresponds to the independent-electron model[17] which is customarily used in such cases. The mechanism of direct excitation also corresponds to our approach, according to which the excitation of a complex atom in a collision with a fast multicharged ion results from a sudden transfer of momentum to atomic electrons. It is thus a simple matter to derive the formulas of the model of independent electrons directly from (18) (see also Ref. 12). It follows from the arguments which led us to Eq. (18) that the probability for the transition of a complex atom from an initial state $\Phi_0(\mathbf{r}_1,...,\mathbf{r}_N)$ to a final state $\Phi_n(\mathbf{r}_1,...,\mathbf{r}_N)$ as the result of a collision with a fast multicharged ion is

$$W(\mathbf{q}) = \left| \int \prod_{i=1}^{N} d^3r_i \Phi_n^*(\mathbf{r}_1,...,\mathbf{r}_N) \times \exp\left\{ -i\mathbf{q} \sum_a \mathbf{r}_a \right\} \Phi_0(\mathbf{r}_1,...,\mathbf{r}_N) \right|^2. \quad (19)$$

To calculate this probability we write the wave functions in the Hartree approximation:

$$\Phi_0(\mathbf{r}_1,...,\mathbf{r}_N) = \prod_{i=1}^{N} \varphi_i(\mathbf{r}_i); \quad \Phi_n(\mathbf{r}_1,...,\mathbf{r}_N) = \prod_{i=1}^{N} \psi_i(\mathbf{r}_i). \quad (20)$$

Hence the total probability for M-fold ionization of an N-electron atom corresponding to the transition of some M electrons into continuum states, while the other N-M electrons go into arbitrary states of the discrete spectrum, is as follows, where we are taking account of the unitarity of the probability (19):

$$W(\mathbf{q}) = \frac{N!}{(N-M)!M!} \prod_{s=1}^{M} P_s(\mathbf{q}) \prod_{j=M+1}^{N} [1 - P_j(\mathbf{q})], \quad (21)$$

where

$$P_s(\mathbf{q}) = \int d^3k_s \left| \int d^3r_s \psi_{\mathbf{k}_s}^*(\mathbf{r}_s) \exp(-i\mathbf{q}\mathbf{r}_s) \varphi_s(\mathbf{r}_s) \right|^2$$

is a one-electron inelastic form factor, and $\mathbf{k}_s$ is the momentum of an electron in the continuum. In addition, in the case $M=N$ we should set $\Pi_{j=M+1}^{N}[1-P_j(\mathbf{q})]=1$ in (21). We note that the probability (21) depends on the vector $\mathbf{q}$. However, after an average is taken over the projections of the total orbital angular momentum of the initial state of the atom, the probability is a function only of $|\mathbf{q}|$.

For simplicity we will discuss the ionization of only the outer shell below; then N is the number of electrons in the shell. We introduce the average value, over the orbital angular momentum l and its projection m, of the one-electron inelastic form factor for each electron of the shell:

$$P(q) = \frac{1}{S_n} \sum_{l,m} \int d^3k \left| \int d^3r \psi_{\mathbf{k}}^*(\mathbf{r}) \exp(-i\mathbf{q}\mathbf{r}) \varphi_{nlm}(\mathbf{r}) \right|^2, \quad (22)$$

where the summation is over all possible values of l and m for the given n shell, S_n is the number of such values, and n is the principal quantum number. Obviously, $P(q) \equiv P(|\mathbf{q}|)$ is independent of the angles of the vector $\mathbf{q}$. Since we have $q=2Z/(vb)$, $P=P(b)$ is a function of the impact parameter b. This function has the obvious meaning of the average probability for the ionization of one electron. Replacing each one-electron form factor in (21) by the average in (22), we then find the following expression for the probability for M-fold ionization (this is the usual expression for the independent-electron approximation):[8]

$$W(q) = \frac{N!}{(N-M)!M!} P(q)^N [1 - P(q)]^{N-M}. \quad (23)$$

The widely used independent-electron model thus follows directly from our approach under natural simplifications.

5. CONCLUSION

The simple approach proposed here completely replaces complicated numerical calculations of the cross sections for ionization and excitation of atoms by fast, relativistic multicharged ions in the case in which the Born approximation cannot be used ($Z \sim v, Z \gg 1, v < c$). The calculation method proposed here proves particularly convenient for estimating cross sections for the simultaneous excitation or ionization of two or more electrons when complex atoms collide with fast multicharged ions.

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