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Radiative Charge Transfer from H Atoms by Fast Ions

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The cross section for radiative electron transfer from H atoms to bound states of an incident ion is calculated for velocities much greater than the orbital velocity of the captured electron. It is shown to dominate over the Coulomb–charge-exchange cross section for $E > 9$ MeV per incident nucleon.

The process of charge transfer from a target atom to an incident ion by the Coulomb interaction has been the subject of considerable theoretical effort, particularly with regard to the asymptotic behavior of the cross section at high velocity.[1] It has been recognized from the outset[2] that the transfer of charge by a radiative process will provide a competing channel although its contribution was estimated to be small at high velocity. Since that time attention has been mostly directed towards the evaluation of cross sections for this process at very low velocity, in the region of thermal encounters.[3] For relativistic projectile energies the radiative capture of free electrons has been discussed with the theory of the relativistic photoeffect.[4] It has been pointed out that charge exchange in metal foils for sufficiently high incident energies is due predominantly to radiative electron capture. Recent observations[5,6] of the radiation emitted in collisions of fast charged ions with gases have indicated a broad x-ray band which has been attributed to the process of radiative charge transfer of bound electrons. It is our purpose in this Letter to examine the nonrelativistic limiting behavior of the cross section for this process under conditions where the velocity of the incident ion is much greater than the initial and final orbital velocity of the electron which is captured. Throughout we will work in atomic units.

The probability for transferring an electron from a hydrogen atom 2 to an incident ion 1 in a collision at impact parameter $\vec{b}$ and velocity $\vec{v}$ (see Fig. 1), with concomitant emission of a photon of frequency ω, is

$$d^3P(\omega, \vec{b})/d^3k = |f|^2, \tag{1}$$

where $\vec{k}$ is the photon propagation vector and $d^3k = k^2\, dk\, d\Omega$ with $k = \omega/c$. As we will subsequently restrict discussion to high velocities, we will adopt the impact-parameter formalism[1] to describe the ion-atom collision. In addition we will consider only the first-order interaction with the radiation field and assume the dipole approximation of replacing the factor $\exp(i\vec{k}\cdot\vec{r})$ occurring in this interaction by unity. So long as the impact

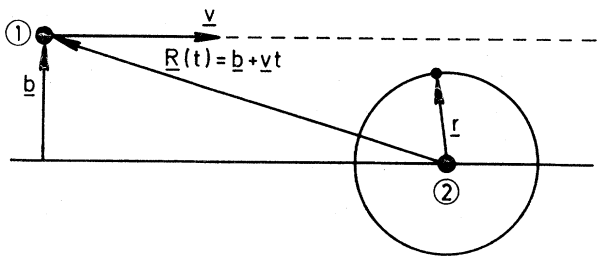

FIG. 1. An ion 1 moving in a straight line is incident on a hydrogen atom 2.

velocities do not approach the velocity of light this approximation alters only the frequency spectrum and not the integrated cross section of interest here. Treating the interaction with the radiation field as small compared with the Coulomb interactions between the electron and the colliding nuclei and proceeding in a manner similar to the derivation of the distorted-wave Born approximation,[7] we find for the amplitude f for radiative charge transfer the expression

$$f=(2\pi\sqrt{\omega})^{-1}\int dt\, e^{i\omega t}\langle\Psi^{-}(t)|\vec{p}\cdot\vec{e}|\Psi^{+}(t)\rangle\,, \qquad (2)$$

where $\vec{p}$ is the momentum operator of the transferred electron and $\vec{e}$ is the polarization vector of the emitted photon. Here, $\Psi^{+}(t)$ and $\Psi^{-}(t)$ are full solutions of the scattering problem

$$H\Psi^{\pm}=i\dot{\Psi}^{\pm}\,, \qquad (3)$$

satisfying boundary conditions appropriate to the initial and final states of the transferred electron, respectively. The Hamiltonian H is the electronic time-dependent Hamiltonian of the impact-parameter formalism,

$$H=-\tfrac{1}{2}\nabla^2+V_2(r)+V_1(\vec{r}-\vec{R}(t))\,, \qquad (4)$$

with $\vec{R}(t)=\vec{b}+\vec{v}t$ and where V_1, V_2 are the Coulomb interactions of the electron with nuclei 1 and 2, respectively. For high velocities we expand the exact wave functions $\Psi^{\pm}$ in atomic states centered at each nucleus and retain only the initial and final atomic states in this expansion; i.e.,

$$\Psi^{\pm}\cong a_1^{\pm}(t)\chi_1(t)+a_2^{\pm}(t)\chi_2(t)\,. \qquad (5)$$

Here, $\chi_2(t)=\varphi_2(\vec{r})\exp(-i\epsilon_2 t)$ is the initial wave function of the electron in a stationary state of energy ϵ_2 about nucleus 2 and $\chi_1(t)$ is the final stationary state of energy ϵ_1 about nucleus 1, which is moving with a constant velocity $\vec{v}$ with respect to an origin fixed in 2; i.e.,

$$\chi_1(t)=\varphi_1(\vec{r}-\vec{R}(t))\exp(i\vec{v}\cdot\vec{r}-i\epsilon_1 t-\tfrac{1}{2}iv^2t)\,.$$

The substitution of the two-state expansion (5) in the expression (2) gives four terms of the form $a_i^{*}a_j\langle\chi_i|\vec{p}\cdot\vec{e}|\chi_j\rangle$. The term with $i=2$, $j=2$ has a vanishing dipole moment and does not contribute. In solving (3) with (4) and (5) we approximate the coefficients $a_i^{\pm}$ by their values taken to first order in the interactions V_1 or V_2. Then the term with $i=2$, $j=1$ is of second order and can be neglected. The term with $i=1$, $j=1$ is of first order and provides a dipole moment $\langle\chi_1|\vec{p}\cdot\vec{e}|\chi_1\rangle=\vec{v}\cdot\vec{e}$. The term with $i=1$, $j=2$ is of zeroth order so that the amplitude becomes

$$f\cong(2\pi\sqrt{\omega})^{-1}\int dt\, e^{i\omega t}(\langle\chi_1|\vec{p}\cdot\vec{e}|\chi_2\rangle+a_1^{+}\vec{v}\cdot\vec{e})\,, \qquad (6)$$

with

$$a_1^{+}=-i\int_{-\infty}^{t}\langle\chi_1(t')|V_1(t')|\chi_2(t')\rangle\,dt'$$

to first order. A partial integration with respect to time of the second term in (6) gives for $\omega>0$

$$f\cong(\vec{e}/2\pi\sqrt{\omega})\cdot\int dt\exp[i(\omega-\Delta\epsilon+\tfrac{1}{2}v^2)t]\langle\varphi_1(\vec{r}-\vec{R}(t))\exp(i\vec{v}\cdot\vec{r})|\vec{p}+(\vec{v}/\omega)V_1(t)|\varphi_2(\vec{r})\rangle\,, \qquad (7)$$

where we have put $\Delta\epsilon\equiv\epsilon_2-\epsilon_1$.

The first term in the matrix element of (7) is the Born approximation for radiative charge transfer, whereas the second term describes the radiation of the electron in the state χ_1 of the moving atom. The second term can be transformed by the substitution $V_1=H_1+\frac{1}{2}\nabla^2$, where H_1 is the electronic Hamiltonian for atom 1: i.e., $H_1\varphi_1=\epsilon_1\varphi_1$. Then, after Fourier transformation of the wave functions to the momentum representation, differential operations can be performed to yield

$$f\cong-[(2\pi)^3/\sqrt{\omega}]\vec{e}\cdot\int d^3q\,\delta(\omega-\Delta\epsilon-\tfrac{1}{2}v^2+\vec{q}\cdot\vec{v})\exp(i\vec{q}\cdot\vec{b})\varphi_1^{*}(\vec{q}-\vec{v})\varphi_2(\vec{q})\{\vec{q}-(\vec{v}/\omega)[\epsilon_1-\tfrac{1}{2}(\vec{q}-\vec{v})^2]\}\,. \qquad (8)$$

Since the momentum wave functions $\varphi_{1,2}(\vec{q})$ are peaked around $\vec{q}=0$ there are two regions where the integrand in (8) is large, namely at $\vec{q}=0$ and $\vec{q}=\vec{v}$. These regions give rise to two contributions to f, centered around $\omega=v^2/2+\Delta\epsilon$ and $\omega=-v^2/2+\Delta\epsilon$, respectively. Clearly, when $v^2/2>\Delta\epsilon$, the only physically important contribution is that which peaks around $\omega=v^2/2+\Delta\epsilon$. This contribution is supplied by $\vec{q}=0$, i.e., by the second term in the curly brackets of (8), which arises from the second term in the matrix element of (7). When $v^2/2\gg\Delta\epsilon$ we can further approximate f by putting $\omega\cong\frac{1}{2}v^2$ and $\varphi_1^{*}(\vec{q}-\vec{v})\cong\varphi_1^{*}(-\vec{v})$ for $\vec{q}\cong 0$ so that (8) reduces to

$$f\cong-[(2\pi)^3/\sqrt{\omega}]\vec{e}\cdot\vec{v}\varphi_1^{*}(-\vec{v})\int d^3q\,\delta(\omega-\Delta\epsilon-\tfrac{1}{2}v^2+\vec{q}\cdot\vec{v})\exp(i\vec{q}\cdot\vec{b})\varphi_2(\vec{q})\,. \qquad (9)$$

We have shown that in a laboratory-fixed origin for high-velocity impacts, the dominant contribution to the radiative-charge-transfer spectrum is provided not by the Born approximation, but by the second term on the right-hand side of (6). However, with respect to a moving origin fixed on nucleus 1,

the Born approximation to the radiative-charge-transfer amplitude is

$$f' \cong (2\pi\sqrt{\omega})^{-1}\int dt \exp[i(\omega - \Delta\epsilon - \tfrac{1}{2}v^2)t]\langle \varphi_1(\vec{r}')|\vec{p}'\cdot\vec{e}|\varphi_2(\vec{r}'+\vec{R}(t))\exp(-i\vec{v}\cdot\vec{r})\rangle, \quad (10)$$

where primed quantities refer to the moving origin. After a Fourier transformation to the momentum representation followed by the same approximations as led from (8) to (9), the expression (10) for f' becomes identical to the expression (9) for f. Hence, since for high velocity the dominant contribution to the charge-transfer spectrum occurs near $\omega \cong \frac{1}{2}v^2$, the Born approximation is correct only when it is made with respect to the moving origin. In contrast, the two-state approximation obtained by substituting (5) in (2) is invariant under Galilean transformation.

The cross section for radiative charge transfer is obtained by integrating (1) over all impact parameters. Using the approximation (9) for f in (1), putting $d^3k = (\omega^2/c^3)d\omega\, d\Omega$, and averaging over polarizations, we find

$$d\sigma/d\omega\, d\Omega \cong [(2\pi)^8/c^3]v\omega\sin^2\theta|\varphi_1(-\vec{v})|^2\int d^3q|\varphi_2(\vec{q})|^2\delta(\omega - \Delta\epsilon - \tfrac{1}{2}v^2 + \vec{q}\cdot\vec{v}), \quad (11)$$

where θ is the angle of observation with respect to the fixed direction $\hat{v}$. The integral in (11) is the Compton profile[8] provided by the momentum distribution of the target electron.

The total cross section for radiative charge transfer is obtained by integrating the differential cross section (11) over ω and Ω and again neglecting $\Delta\epsilon$ compared with $v^2/2$ to obtain

$$\sigma \cong (2^7\pi^6v^3/3c^3)|\varphi_1(-\vec{v})|^2. \quad (12)$$

The only effect of the retention of the term $\exp(i\vec{k}\cdot\vec{r})$ in the interaction with the radiation field is to replace $\vec{q}\cdot\vec{v}$ in the δ function of (11) by $(\vec{q}+\vec{k})\cdot\vec{v}$. This alters the spectrum (11) but not the integrated cross section (12) so long as $v/c \ll 1$.

Considering the simplest example of radiative charge transfer to the hydrogenic ground state of a bare nucleus of charge Z_1, we find the cross section to be

$$\sigma \cong (2^7/3c^3)(Z_1/v)^5, \quad (13)$$

in units of $\pi a_B{}^2$, where a_B is the Bohr radius. In the same velocity region the cross section for Coulomb charge transfer from H atoms to the ground state has the approximate form[1]

$$\sigma_C \cong 0.3(2^{18}/5)Z_1{}^5/v^{12}$$

in units of $\pi a_B{}^2$. Hence, for sufficiently large v, the radiative-transfer cross section dominates over the Coulomb-transfer cross section. The two cross sections become of equal magnitude ($\cong 6\times10^{-12}Z_1{}^5\pi a_B{}^2$) when a velocity corresponding to an impact energy of ~9 MeV/nucleon is reached.

It should be noted that for a resonant process where $\Delta\epsilon = 0$, or when $v^2/2 \gg \Delta\epsilon$ for a nonresonant process, the photon energy is provided solely by the translational kinetic energy of the incident ion so that the radiative charge transfer provides a mechanism for the indirect conversion of ionic translational kinetic energy into electromagnetic energy. In such a radiative process the ion loses an energy v^2 (a.u.), which, on the average, is shared equally between the photon and the translational kinetic energy of the captured electron.

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