

RADIATIVE ELECTRON CAPTURE IN HEAVY-ION COLLISIONS

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Abstract: The cross section for radiative capture of bound electrons (REC) by fast heavy ions is calculated in (i) the impulse approximation, (ii) the impact parameter approximation and (iii) the first Born approximation. The last two methods yield the same result. It agrees with the result given by the impulse approximation in the case of small perturbation of the initial electronic state during the collision. The question how REC may be utilized to measure electronic momentum densities is investigated. For this purpose higher order effects are calculated.

1. Introduction

In the X-ray emission accompanying the passage of highly stripped, heavy ions through gases or metal foils one can distinguish between three types of radiation:

- (a) characteristic X-ray lines;
- (b) a broad X-ray band due to radiative electron capture¹⁻³) (REC) of the bound target electrons;
- (c) high-energy radiation observed mainly in medium and heavy targets.

In process (b) the target electrons are captured directly into the K-shell of the projectile. Process (c) is the result of several effects: nuclear and electronic bremsstrahlung and, at low beam velocities, it includes radiative electronic transitions during the temporary formation of a quasimolecule made up of the target atom and the heavy ion.

In this paper we shall concentrate on the REC and to a lesser extent on molecular orbital (MO) phenomena³⁻⁷). The REC cross section turns out²) to be proportional to the Compton profile⁸) and therefore in principle may be used to measure electronic momentum distributions. This will be shown in sect. 2 by means of the impulse approximation. In sect. 3 we calculate the dependence of the REC on the impact parameter. In sect. 4 we show that the first Born approximation is equivalent to the impact parameter method. We investigate second order Feynman diagrams as a first correction for off-energy-shell effects, i.e. for MO phenomena. In sect. 5 we discuss the relationship between REC and MO radiation.

2. Impulse approximation

Consider the radiative capture of a free electron into the ground state of a completely stripped nucleus with charge Z . This effect is known as radiative recombina-

tion and the corresponding cross section is ^{9,10})

$$\frac{d\sigma_{rec}}{d\Omega} = \sigma_{rec} \frac{3}{8\pi} \sin^2 \vartheta, \quad (1)$$

$$\sigma_{rec} = 9.1 \left(\frac{\eta^3}{1+\eta^2} \right)^2 \frac{\exp(-4\eta \arctan(1/\eta))}{1 - \exp(-2\pi\eta)} 10^{-21} \text{ cm}^2. \quad (2)$$

Here $\eta = Ze^2/\hbar v$ is the Sommerfeld parameter (or Coulomb parameter) and v is the original relative velocity between electron and nucleus. The angle ϑ denotes the angle between v and the direction of the emitted photon. The energy of the emitted photon is

$$\hbar\omega = \frac{1}{2}mv^2(1+\eta^2), \quad (3)$$

where m is the mass of the electron.

In fig. 1 we show σ_{rec} as a function of Z for different values of v . The non-relativistic high-energy limit ($\eta \ll 1$) of eq. (2) reads

$$\sigma_{rec} = 1.4 \eta^5 10^{-21} \text{ cm}^2. \quad (2a)$$

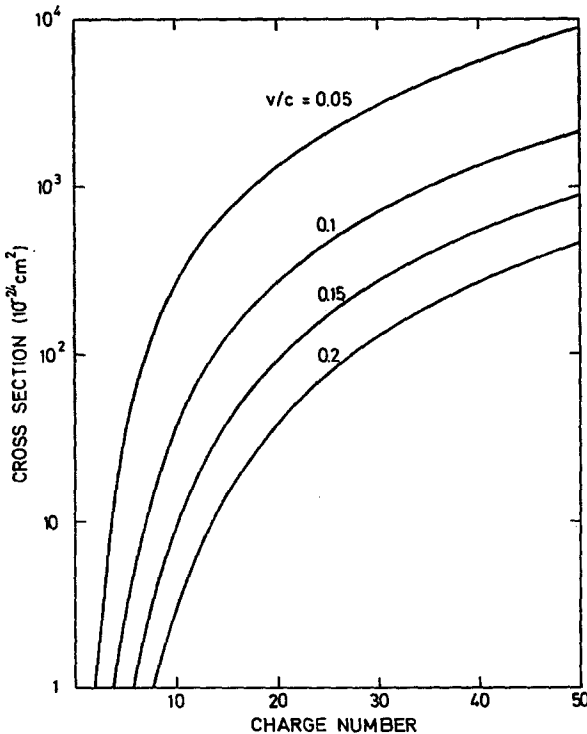


Fig. 1. Cross section σ_{rec} [eq. (2)] for the radiative recombination of a free electron into the K-shell of a bare nucleus of charge Z for various relative velocities v (in units of c).

The relevant parameter for recombination is η which measures how strongly the Coulomb interaction will distort the asymptotic wave function of the electron during the collision. For $\eta \lesssim 1$ the distortion is small and recombination may be calculated in first Born approximation. If $\eta > 1$ the distortion is strong enough to change the electronic wave function considerably during the collision.

Bound electrons are characterized by their momentum distribution. If the velocity of the ion is considerably greater than the orbital velocity of the electron to be captured, then the cross section can be written as

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \int d^3\mathbf{p} \frac{d\sigma_{\text{rec}}}{d\Omega} |\psi_i(\mathbf{p}-\mathbf{p}_0)|^2 \delta(E_f - E_i). \quad (4)$$

This is the impulse approximation⁸). The δ -function guarantees energy conservation and $|\psi_i(\mathbf{p})|^2$ is the initial electronic momentum distribution, which now is peaked around $\mathbf{p}_0 = m\mathbf{v}$ because the electron is moving with this average momentum towards the projectile considered at rest. For the type of collision specified above the initial electronic potential V_i remains constant during the capture process and we may write

$$E_i = \frac{(\mathbf{p}_0 + \mathbf{p}_i)^2}{2m} + V_i = -\varepsilon_i + \frac{p_0^2}{2m} + \mathbf{v} \cdot \mathbf{p}_i, \quad (5)$$

where we have introduced the initial electronic binding energy ε_i . Furthermore,

$$E_f = -\varepsilon_f + \hbar\omega, \quad (6)$$

so that

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \int d^3\mathbf{p}_i \left(\frac{d\sigma_{\text{rec}}}{d\Omega} \right)_{\mathbf{p}=\mathbf{p}_0+\mathbf{p}_i} |\psi_i(\mathbf{p}_i)|^2 \delta \left(\hbar\omega - \varepsilon_f + \varepsilon_i - \frac{p_0^2}{2m} - \mathbf{v} \cdot \mathbf{p}_i \right). \quad (7)$$

The cross section shows a Doppler broadening: the energy of the emitted photon depends on the electronic momentum component, p_{iz} say, parallel to \mathbf{v} .

If REC goes into the K-shell of an ion heavier than the target then the cross section is peaked around $\mathbf{p}_i = 0$. In this region the recombination cross section varies slowly and may be taken out of the integral

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \left(\frac{d\sigma_{\text{rec}}}{d\Omega} \right)_{\mathbf{p}=\mathbf{p}_0+\mathbf{p}_{iz}} \int d^3\mathbf{p}_i |\psi_i(\mathbf{p}_i)|^2 \delta \left(\hbar\omega - \varepsilon_f + \varepsilon_i - \frac{p_0^2}{2m} - v p_{iz} \right). \quad (8)$$

Introducing the Compton profile

$$\mathcal{J}_i(p_{iz}) = \int dp_{ix} dp_{iy} |\psi_i(\mathbf{p}_i)|^2, \quad (9)$$

which is the probability of finding the electron with momentum p_{iz} , the cross section reads

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \frac{1}{v} \left(\frac{d\sigma_{rec}}{d\Omega} \right)_{p=p_0+p_{iz}} \mathcal{J}_i(p_{iz}), \quad (10)$$

$$\hbar\omega = \varepsilon_f - \varepsilon_i + \frac{p_0^2}{2m} + vp_{iz}.$$

When integrated over the energies of the emitted photon, the cross section is seen to be approximately the recombination cross section for a *free* electron.

If $\eta \lesssim 1$, the recombination cross section may be replaced by its Born value σ_{rec}^B ,

$$\frac{1}{v} \left(\frac{d\sigma_{rec}^B}{d\Omega} \right)_p = \frac{e^2}{\hbar c} \left(\frac{2\pi\hbar}{c} \right)^2 \hbar\omega \left(\frac{p \sin \vartheta}{mv} \right)^2 \rho_f(\mathbf{p}), \quad (11)$$

where $\rho_f(\mathbf{p})$ is the electronic momentum density in the final target state.

For hydrogen-like atoms the spherically averaged electron density in a shell with principal quantum number n is

$$\rho_f(p) = \frac{1}{n^2} \sum_{l=0}^{n-1} \sum_{m=-l}^l |\psi_{nlm}(\mathbf{p})|^2 = \frac{8\kappa_f^5}{\pi^2(p^2 + \kappa_f^2)^4}, \quad (12)$$

where the momentum κ depends on the screened charge Z_{sc} through $\kappa = Z_{sc}me^2/\hbar n$. The Compton profile then reads

$$\mathcal{J}_i(p_z) = 2\pi \int_{p_z}^{\infty} \rho_i(p) p dp = \frac{8\kappa_i^5}{3\pi(p_z^2 + \kappa_i^2)^3}. \quad (13)$$

From eqs. (10) and (13) it follows that the full width w of the REC peak is given by

$$w \approx v\kappa_i. \quad (14)$$

The total REC peak is obtained by adding the contributions of all target electrons incoherently.

It should be noted that the impulse approximation (7) or (10) is restricted to an intrinsic momentum p_{iz} not exceeding the relative momentum p_0 . It is also not applicable to large negative values of p_{iz} ($p_{iz} \lesssim -p_0$).

3. Impact parameter method

We apply the straight line version of the impact parameter method because REC takes place at distances where the Coulomb repulsion of the two nuclei is not important. Furthermore, if $\eta \lesssim 1$, we may use unperturbed electronic wave functions in target and projectile. We introduce (fig. 2) the separation R between target

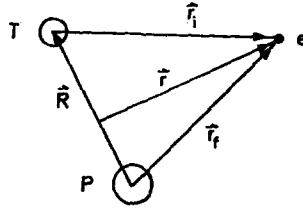


Fig. 2. Coordinates for the system of projectile P, residual target T (target minus electron) and electron e. The electron coordinate r is measured from the c.m. of P and T.

T (mass m_T) and projectile P (mass m_P) together with the electron coordinate r measured from the c.m., so that

$$r_i = r - \frac{m_P}{m_T + m_P} R, \quad r_f = r + \frac{m_T}{m_T + m_P} R, \quad (15)$$

and small corrections \dagger from the electronic mass are neglected. The wave function of the electron in the target is given by

$$\varphi_i(r, R, t) = \varphi_i(r_i) \exp \left[ik_i \cdot r - i \left(\frac{\hbar^2 k_i^2}{2m} - \varepsilon_i \right) \frac{t}{\hbar} \right], \quad (16)$$

and in the final state of the projectile by

$$\varphi_f(r, R, t) = \varphi_f(r_f) \exp \left[ik_f \cdot r - i \left(\frac{\hbar^2 k_f^2}{2m} - \varepsilon_f \right) \frac{t}{\hbar} \right], \quad (17)$$

with $\varphi_i(r_i)$, $\varphi_f(r_f)$, ε_i and ε_f being the undisturbed time-independent wave functions and binding energies of the electron in target and projectile. The phase factors in eq. (16) and (17) reflect the motion of the electron with respect to the c.m. The corresponding momenta are

$$k_i = \frac{m_P}{m_T + m_P} k, \quad k_f = - \frac{m_T}{m_T + m_P} k, \quad (18)$$

where $k = mv/\hbar = p_0/\hbar$.

REC is caused by the transition operator

$$W = - \frac{e}{c} A \cdot v_e, \quad (19)$$

where v_e is the electronic velocity with respect to the projectile. One may decompose v_e into a part v_r parallel to r and into one parallel to R ,

$$v_e = v_r + \frac{m_T}{m_T + m_P} v. \quad (20)$$

\dagger These recoil corrections are important in the time-independent treatment.

The impact parameter method treats \mathbf{R} and \mathbf{v} as parameters

$$\mathbf{R} = \mathbf{b} + \mathbf{v}t, \quad \mathbf{b} \cdot \mathbf{v} = 0. \quad (21)$$

However, \mathbf{v} , still acts as an operator.

In order to calculate the transition amplitude

$$f = \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt \int d^3r \varphi_f^*(\mathbf{r}, \mathbf{R}, t) W \varphi_i(\mathbf{r}, \mathbf{R}, t), \quad (22)$$

it is convenient to introduce wave functions in momentum space,

$$\varphi_i(\mathbf{r}_i) = (2\pi\hbar)^{-\frac{3}{2}} \int d^3p_i \psi_i(\mathbf{p}_i) \exp(i\mathbf{p}_i \cdot \mathbf{r}_i/\hbar), \quad (23)$$

together with a similar relation for the final configuration. The emission of a photon with wave number $s = \omega/c$, energy $\hbar\omega$ and polarization vector \mathbf{u}_λ ($\lambda = 1, 2$) is due to the field

$$A_\lambda(s, \hbar\omega) = \left(\frac{2\pi\hbar c^2}{V\omega} \right)^{\frac{1}{2}} \exp[-i(\mathbf{s} \cdot \mathbf{r}_f - \omega t)] \mathbf{u}_\lambda. \quad (24)$$

Here V stands for the periodicity volume of the electromagnetic field. We neglect the phase factor $\exp(-i\mathbf{s} \cdot \mathbf{r}_f)$ because $\mathbf{s} \cdot \mathbf{r}_f \ll 1$ is normally satisfied if we identify \mathbf{r}_f with the electronic K-shell radius in the heavy ion. It is straightforward to cast eq. (22) into the form

$$f = f_\lambda(\mathbf{b}) = 2\pi i \frac{e}{m} \left(\frac{2\pi\hbar}{V\omega} \right)^{\frac{1}{2}} \mathbf{u}_\lambda \int d^3p_i (\mathbf{p}_i + \mathbf{p}_0) \psi_f^*(\mathbf{p}_i + \mathbf{p}_0) \\ \times \psi_i(\mathbf{p}_i) \exp(-i\mathbf{p}_i \cdot \mathbf{b}/\hbar) \delta \left(\hbar\omega - \varepsilon_f + \varepsilon_i - \frac{p_0^2}{2m} - \mathbf{v} \cdot \mathbf{p}_i \right). \quad (25)$$

If we take \mathbf{v} to be in the z -direction the cross section for the emission of a photon is given by

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \frac{V(\hbar\omega)^2}{(2\pi\hbar c)^3} \int db_x db_y \sum_{\lambda=1,2} |a_\lambda(b)|^2. \quad (26)$$

The factor in front of the integral is the number of photon states per unit energy and unit solid angle. The summation over the two polarization directions is easily performed because the wave function $\psi_i(\mathbf{p}_i)$ is significantly different from zero only for values of \mathbf{p}_i much smaller than \mathbf{p}_0 ,

$$\sum_{\lambda=1,2} |\mathbf{u}_\lambda(\mathbf{p}_i + \mathbf{p}_0)|^2 \approx \sin^2 \vartheta (p_{iz} + p_0)^2, \quad (27)$$

and ϑ is the angle between beam direction and direction of the emitted photon. After some calculation we arrive at

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \frac{e^2}{\hbar c} \left(\frac{2\pi\hbar}{c} \right)^2 \hbar\omega \left(\sin \vartheta \frac{p_0 + p_{iz}}{p_0} \right)^2 \int dp_{ix} dp_{iy} |\psi_i(\mathbf{p}_i) \psi_f(\mathbf{p}_i + \mathbf{p}_0)|^2, \quad (28)$$

where p_{iz} is linked to $\hbar\omega$ by eq. (10). By comparing the Born version (11) of the impulse approximation (7) with the result ^{2,11} (28) of the impact parameter method we find the two expressions to be identical.

In this section we formulated the REC with respect to the c.m. The result eq. (28) does not, however, depend on this choice as long as for an arbitrary origin the velocity v_e in eq. (19) is taken as the velocity between electron and projectile.

We are now in a position to investigate the contributions to the REC cross section as a function of the impact parameter. The integrand on the right hand side of eq. (25) is peaked around $\mathbf{p}_i = 0$ if REC goes into the K-shell of a heavy ion. Then the transition amplitude is proportional to

$$f(\mathbf{b}) \sim \int dp_{ix} dp_{iy} \psi_i(\mathbf{p}_i) \exp(-i\mathbf{p}_i \cdot \mathbf{b}/\hbar). \quad (29)$$

For an electron in a hydrogenic 1s state $f(\mathbf{b})$ can be calculated analytically. The relative contribution P to the REC cross section as a function of the impact parameter turns out to be

$$P(x) = \frac{3}{2}x^3(K_1(x))^2, \quad (30)$$

$$x = \frac{b}{a} \left[1 + \left(\frac{ap_{iz}}{\hbar} \right)^2 \right]^{\frac{1}{2}}.$$

Here $K_1(x)$ denotes the modified Bessel function of the second kind and of order one and a is the Bohr radius of the initial 1s state. The function $P(x)$ is plotted in fig. 3;

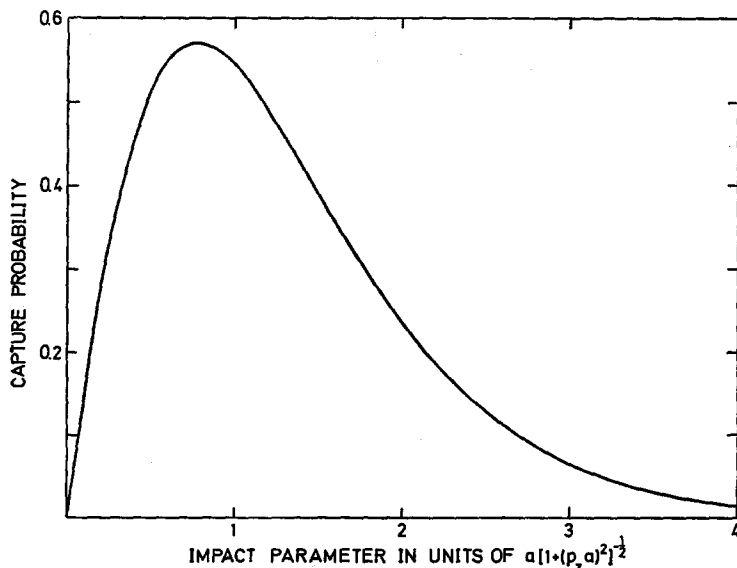


Fig. 3. Relative contribution [eq. (30)] to the REC as a function of the impact parameter measured in units of $a[1+(p_z a)^2]^{-\frac{1}{2}}$.

its integral over all positive values of x is, of course, normalized to unity. The main contribution to REC occurs at $x \approx 1$. This means that the wings of the radiation peak come from close collisions.

4. Born series

In the time-independent formulation the cross section for REC is

$$\frac{d^2\sigma}{d\Omega d\hbar\omega} = \rho_{ph} \frac{\mu_i \mu_f}{(2\pi\hbar^2)^2} \frac{k_f}{k_i} \int d\Omega' |T_{if}|^2. \quad (31)$$

The quantities μ_i , μ_f , k_i and k_f are the reduced masses and total relative momenta in the entrance and in the exit channel, respectively. The number of photon states per unit energy and unit solid angle is denoted by ρ_{ph} . As usual eq. (31) contains an integration over all directions of the outgoing heavy-ion beam. It is well known that the second and higher order Born approximations for the exact T -matrix are not uniquely defined for rearrangement collisions. One possible expansion is ¹²⁾

$$T_{if} = T_{if}^B + \langle \psi_f | V_f G_i^\dagger V_i | \psi_i \rangle + \dots, \quad (32)$$

where G_i^\dagger is the initial state Green function and V_i and V_f stand for initial and final state interactions. Therefore, V_i consists of the radiation field plus the Coulomb interaction between projectile and electron whereas V_f is the sum of radiation field and the Coulomb interaction between target and electron. In the case of REC

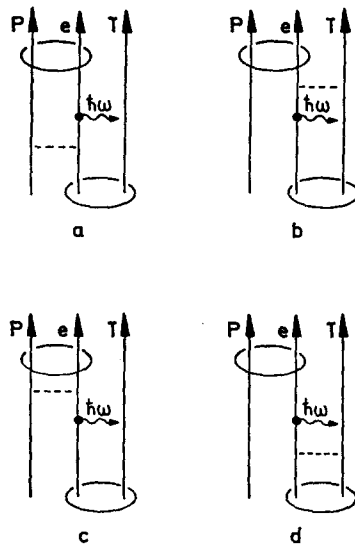


Fig. 4. Second order Feynman diagrams for the REC. The dotted line stands for a Coulomb interaction; the wavy line means the emission of a photon. The loops indicate to which system (either projectile or target) the electron is bound. Note that diagrams 4c and 4d do *not* contribute to the second order Born approximation.

there are two second order Born terms. Their corresponding Feynman graphs are shown in figs. 4a and 4b. It has to be noted that the second order Feynman graphs 4c and 4b do *not* contribute to the second order Born approximation. In fact, it can be shown by a straightforward but lengthy calculation that graph 4c *alone* gives the REC cross section which we derived in the foregoing sections.

The Born term

$$T_{if}^B = \langle \psi_f | W | \psi_i \rangle, \quad (33)$$

where W is given by eq. (19), may be easily calculated and inserted into eq. (31). It turns out that the first Born approximation for REC is identical with the Born version of the impulse approximation and, thus, with the result of impact parameter method. This is not surprising because it is known that the first Born approximation and the impact parameter method yield equivalent results in case of the total non-radiative electron capture.

A calculation of the second order diagrams 4a and 4b shows that their effect is small if the collision is fast. Although these graphs are a first correction to the formation of quasimolecular states during the collision, the Born series is not suited for the calculation of MO radiation because it consists of terms with alternating signs.

5. Relation to molecular orbital X-rays

Radiative electronic transitions between bound states will also take place at low beam velocities. This radiation is the analogue to REC and it originates in a temporary formation of molecular orbitals (MO) during the collision. If the collision is fast with respect to the orbital velocity of the outer electrons but slow with respect to the inner electrons then REC and MO radiation will be observed simultaneously³⁾. Various MO phenomena have been discussed in the literature¹³⁻¹⁵⁾ so that we restrict our discussion to the close relationship between REC and MO radiation.

Consider an ion having a K-shell vacancy whose lifetime is much greater than the collision time. For slow collisions the unperturbed asymptotic wave functions of eqs. (16) and (17) must be replaced by time-dependent molecular wave functions

$$|i\rangle = \varphi_i(\mathbf{r}, \mathbf{R}(t)) \exp \left[\frac{i}{\hbar} \int_{-\infty}^t dt' \varepsilon_i(t') \right], \quad (34)$$

and a similar expression holds for the final electronic wave function. The electronic binding energies $\varepsilon_i(t)$ and $\varepsilon_f(t)$ now depend on time. The transition amplitude is

$$f = \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt \int d^3r \langle f | \frac{-e\hbar}{imc} \mathbf{A} \cdot \nabla_r | i \rangle. \quad (35)$$

Now the gradient operates on the electron coordinate \mathbf{r} which again is measured

from the c.m. of the quasimolecule. A similar calculation as in sect. 3 leads to

$$\frac{d\sigma}{d\hbar\omega} = \frac{4}{3} \frac{\hbar\omega}{(\hbar c)^2} \frac{e^2}{\hbar c} \int db_x db_y D_c^2(\omega), \quad (36)$$

where D_c is defined by

$$D_c(\omega) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} dt D(\mathbf{R}(t)) \exp \left[\frac{i}{\hbar} \int_{-\infty}^t dt' (\hbar\omega - \varepsilon_f(t') + \varepsilon_i(t')) \right], \quad (37)$$

$$D(\mathbf{R}(t)) = \frac{\varepsilon_f(t) - \varepsilon_i(t)}{\hbar} \int d^3r \varphi_f^*(\mathbf{r}, \mathbf{R}(t)) r \varphi_i(\mathbf{r}, \mathbf{R}(t)).$$

The REC can be considered as the limit of eqs. (36) and (37) when the collision is so fast that the binding energies of the electron do not change during the collision. For recent experiments and for a detailed discussion of the spectral shape of MO X-ray continua we refer to ref. ³).

6. Conclusion

We have established the main features which determine the spectral distribution of the non-relativistic REC. The REC phenomenon has been defined for sudden collisions and it is the analogue to MO radiation in adiabatic collisions. It is important to note that the Born version of the impulse approximation, the impact parameter method and the first order Born approximation are identical in case of REC. An important quantity is the Sommerfeld parameter $\eta = Z_{\text{eff}} e^2 / \hbar v$ which should be less than or approximately equal to unity. Here Z_{eff} is the effective charge of the ion. If η is much larger than unity both impact parameter method and Born approximation will fail because the Coulomb interaction between target electron and ion will excite or ionize the electron before REC takes place.

The charge state of fast heavy ions will be in many cases ¹⁶) such that $\eta \approx 1$ holds. Under this condition the high energy wing of the REC photon peak may be utilized by means of eq. (7) or (10) to measure electronic momentum distributions up to the relative kinetic momentum of the target electron with respect to the ion.

Except for very light targets the collision velocity will in general be fast only for the weakly bound outer electrons. On the other hand, the inner electrons, having a broad momentum distribution, will produce MO X-rays and bremsstrahlung ¹⁷) which is not suited to measure the underlying momentum distribution.

The REC into projectile states other than the K-shell is also not suited to measure electronic momentum distributions because the corresponding radiation peaks lie closer to the bremsstrahlung limit of weakly bound or free electrons than does the peak which originates from capture into the K-shell.

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