POSITION OF THE MAXIMUM OF THE CROSS SECTION FOR INELASTIC SCATTERING OF AN ION WITH AN ATOM

G. F. DRUKAREV

Leningrad State University

Submitted to JETP editor July 22, 1966

J. Exptl. Theoret. Phys. (U.S.S.R.) **52**, 498–501 (February, 1967)

An expression is derived for the velocity v_0 at which the cross section of inelastic collision between an ion and an atom is a maximum. In the case when the energy transfer ΔE is a small fraction of the binding energy of the electron in the target atom, we get $v_0 \sim \Delta E$. But if ΔE is close to the binding energy of the electron in the target atom, then $v_0 \sim \Delta E^{1/2}$.

THE purpose of this communication is to derive an expression for the velocity at which the cross section for inelastic collisions between an ion and an atom, at a fixed energy transfer, reaches a maximum value. We shall show that the well known Massey rule, according to which the aforementioned velocity is proportional to the energy transfer ΔE, is valid only under certain conditions, and that a case is possible when this velocity is proportional to $\Delta E^{1/2}$. We shall use the Born approximation for the derivation.

Let us consider first the excitation of an atom by an ion. The effective cross section in the Born approximation is

$$\sigma_{if} = \frac{M^2}{2\pi\hbar^4}\frac{v_f}{v_i}\int_0^\pi |W|^2 \sin\theta d\theta, \quad (1)$$

where M is the reduced mass, and v_i and v_f are the initial and final velocities of the ion. The matrix element W is of the form

$$W = \int d\mathbf{r} d\mathbf{R} \psi_i^*(\mathbf{r})\psi_f(\mathbf{r}) e^{i\mathbf{qR}} V(\mathbf{r}, \mathbf{R}), \quad (2)$$

$\hbar q$ is the momentum transfer, $\mathbf{R}$ the radius vector of the ion relative to the center of the atom, $\mathbf{r}$ the radius vector of the electron undergoing the transition, and V the energy of interaction of the electron with the ion. Assuming the ion to be a point charge, we get

$$V = Ze^2|\mathbf{r} - \mathbf{R}|^{-1},$$

so that

$$W = \frac{4\pi Ze^2}{q^2}\int d\mathbf{r}\psi_i^*(\mathbf{r})\psi_f(\mathbf{r}) e^{i\mathbf{qr}}. \quad (3)$$

Going over in (1) from integration over the angle to integration over the momentum transfer, in accordance with the relation

$$\hbar^2 q\, dq = M^2 v_i v_f \sin\theta\, d\theta,$$

we obtain (we omit the index i from the velocity symbol)

$$\sigma_{if} = 8\pi\left(\frac{Ze^2}{\hbar v}\right)^2 \int_{q_{min}}^{q_{max}} |W|^2 q dq. \quad (4)$$

In collisions of heavy particles it can be assumed that $q_{max} = \infty$,

$$q_{min} = |\varepsilon_i - \varepsilon_f|/\hbar v; \quad (5)$$

where ϵ_i and ϵ_f are the electron binding energies before and after the collision (expression (5) is valid accurate to a quantity of the order of $|\epsilon_i - \epsilon_f|/Mv^2$).

Let us consider in greater detail the matrix element W. Representing ψ in the form $\psi = R(r)\Theta(\theta, \varphi)$, and using the approximate analytic expressions for radial functions $R(r)$ according to Slater:

$$R(r) = Ar^{\nu-1}e^{-\alpha r}, \quad (6)$$

where ν is the effective quantum number and $\alpha = (2m\epsilon/\hbar^2)^{1/2}$, we obtain in (3) an integral in the form

$$I = \int d\Omega\Theta_i\Theta_f \int_0^\infty dr\, r^{\nu_i+\nu_f} \exp\{i\mathbf{qr} - (\alpha_i + \alpha_f)r\}. \quad (7)$$

We introduce new variables

$$\boldsymbol{\rho} = (\alpha_i + \alpha_f)\mathbf{r}, \quad (8)$$

$$\mathbf{s} = \frac{1}{\alpha_i + \alpha_f}\mathbf{q}. \quad (9)$$

Then

$$I = (\alpha_i + \alpha_f)^{-\nu_i-\nu_f-1}\int d\Omega\Theta_i\Theta_f \int_0^\infty d\rho\, \rho^{\nu_i+\nu_f} \exp\{i\mathbf{s}\boldsymbol{\rho} - \rho\}. \quad (10)$$

Thus, the dependence of I, and with it also of W, on the momentum transfer is expressed in terms of the parameter s. We can therefore change over in (4) from integration with respect to q to integration with respect to s. Putting

$$\xi = \frac{|\varepsilon_i - \varepsilon_f|}{\hbar v (\alpha_i + \alpha_f)}, \tag{11}$$

we can reduce (4) to the form

$$\sigma_{if} = \xi^2 \int_{\xi}^{\infty} F_{if}(s)\, ds. \tag{12}$$

This expression, regarded as a function of ξ, has a maximum at a certain value ξ_0. Inasmuch as the functions F_{if} in (12) depend on the quantum numbers of the initial and final states, ξ_0 also depends on them. However, for different estimates, for example for comparison of transitions of the same type for a number of targets, we can assume for ξ_0 a certain mean value. As a rule, the mean value of ξ_0 is not far from unity.

According to (11), the velocity v_0 at which σ_{if} is maximal is

$$v_0 = \frac{|\varepsilon_i - \varepsilon_f|}{\xi_0 \hbar (\alpha_i + \alpha_f)} \tag{13}$$

or, what is the same,

$$v_0 = \frac{1}{(2m)^{1/2}\xi_0} |\varepsilon_i^{1/2} - \varepsilon_f^{1/2}|. \tag{14}$$

In the case when $|\alpha_i - \alpha_f| \ll \alpha_i$, expression (13) reduces to the well known Massey rule

$$v_0 = \Delta E a/\hbar, \tag{15}$$

where the constant a does not depend on ΔE. From (13) we get the following expression for a:

$$a = 1 / 2\xi_0 \alpha_i = \hbar / 2\xi_0 (2m\varepsilon_i)^{1/2}. \tag{16}$$

If $\alpha_i \gg \alpha_f$, we obtain from (13)

$$v_0 = \varepsilon_i / \xi_0 \alpha_i \hbar = \varepsilon_i^{1/2} / \xi_0 (2m)^{1/2}. \tag{17}$$

Since in our case $\epsilon_i \approx \Delta E$, it turns out, unlike (15), that

$$v_0 = \Delta E^{1/2} / \xi_0 (2m)^{1/2}. \tag{18}$$

We now turn to the charge-exchange process, in which an electron goes over from the atom a to the ion b. The matrix element determining the charge-exchange cross section, neglecting quantities of the order of the ratio of electron mass to the atom mass, is

$$W = \int d\mathbf{r}_a \psi_i(\mathbf{r}_a) e^{i\mathbf{q}\mathbf{r}_a} V(\mathbf{r}_a) \quad \int d\mathbf{r}_b \psi_f(\mathbf{r}_b) e^{-i\mathbf{q}\mathbf{r}_b}. \tag{19}$$

Here $\mathbf{r}_a$ and $\mathbf{r}_b$ are the electron radius vectors relative to the centers a and b. The expression for q_{min} coincides with (5) at the same accuracy.

With the aid of a transformation similar to (8) and (9), the first integral in (19) can be expressed in terms of the dimensionless parameter q/α_i and the second integral in terms of the parameter q/α_f. Thus, instead of one parameter $s = q/(\alpha_i + \alpha_f)$, as above, the matrix element for the charge exchange contains two parameters $s_i = q/\alpha_i$ and $s_f = q/\alpha_f$.

In two cases, however, W depends in practice only on one parameter s_i: (a) when $|\alpha_i - \alpha_f| \ll \alpha_i$ and (b) when $\alpha_i \gg \alpha_f$. (In case b the quantity α_f enters only in the coefficient preceding of the integral for W, in analogy with (10). This coefficient expresses only the absolute value of the cross section and does not influence the position of the maximum.) With this, the entire analysis becomes similar to that given above and leads respectively to formulas (15) and (18). The correction to (19) for the finite mass of the electron reduces to the following substitution [1]:

$$\mathbf{q}\mathbf{r}_a \to \left(\mathbf{q} - \frac{mM_b}{M_a + M_b + m}\mathbf{v}_i\right)\mathbf{r}_a,$$
$$\mathbf{q}\mathbf{r}_b \to \left(\mathbf{q} + \frac{mM_a}{M_a + M_b + m}\mathbf{v}_f\right)\mathbf{r}_b. \tag{20}$$

In this case W depends already not only on the momentum transfer, but also on the momenta of the initial and final states separately.

The velocity at which σ_{if} has a maximum can be determined only after actual calculation of σ_{if}. However, in view of the smallness of the ratio of the electron mass to the masses of the colliding particles, we can expect the position of the maximum, with allowance for the correction (20), not to differ much from that determined by formulas (15) and (18) (all the more since ξ_0 is determined only tentatively and is essentially an empirical parameter).

In conclusion we note that although the entire reasoning is based on the Born formula, the region of applicability of the results is actually broader than the region of applicability of the Born approximation itself. This is confirmed, in particular, by the fact that in a paper by Demkov [2], devoted to charge exchange with a small resonance defect, he obtained for the constant a in (15) an expression similar to our (16). Yet, in this region of energies, to which Demkov's paper pertains [2], the Born approximation is not valid and the entire analysis is carried out by an entirely different method.

Experimental investigations of charge exchange in a highly excited state [3] at which the case $\alpha_i \gg \alpha_f$ is realized leads to the conclusion that $v_0 \sim \Delta E^{1/2}$. This agrees with (18).

I am grateful to V. A. Oparin, E. G. Solov'ev, and R. N. Il'in for a discussion and a communication of the results of [3]. I am also grateful to Yu. N. Demkov for a discussion.

[1] D. Bates, in: Atomic and Molecular Processes, D. Bates, ed., (Russ. Transl.) Mir, 1964, Ch. 14, Sec. 1c.

[2] Yu. N. Demkov, JETP 45, 195 (1963), Soviet Phys. JETP 18, 138 (1964).

[3] V. A. Oparin, R. N. Il'in and E. Solov'ev, JETP 52, 369 (1967), this issue p. 000.

Translated by J. G. Adashko
63