BORN CROSS SECTION FOR THE $n-n'$ TRANSITION IN THE HYDROGEN ATOM ON ELECTRON IMPACT

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By means of the Coulomb Green function an analytic expression is obtained for the composite (over l and l') squared Born amplitude for the $n-n'$ transition. The formula is essentially simplified in the limiting case of large values of n and n′. At high external electron energies an expression is obtained for the transition cross section in an approximation analogous to the Kramers approximation for oscillator strengths ($1 \ll \Delta n \ll n$).

BORN cross sections for excitation of atoms by electrons are usually determined by numerical methods. Results in analytic form have been obtained only for the excitation amplitudes of states nl with $n \lesssim 5$ (cf., e.g.,[1]). Application of the methods used in such calculations is practically impossible in the case of states with large values of the principal quantum number n. Calculation of the $n-n'$ transition cross section summed over the orbital quantum numbers l and l' is all the more unrealistic. In[2,3] analytic expressions were obtained for the amplitudes of transitions between states describable by parabolic quantum numbers. In this case too, because of the unwieldiness of the formulas obtained, it is in practice impossible to perform the indicated summation. At the same time, it is precisely these cross sections that are of fundamental interest both in a number of experimental problems and in certain theoretical questions.

In the present paper an analytic expression for the square of the $n-n'$ transition amplitude totalled over l and l', is obtained by means of the Green function for the Coulomb field. In the case of large values of n and n′, the formula is essentially simplified and for small momentum transfers leads to an expression for the oscillator strength coinciding with the quasi-classical formula.

Throughout we use the atomic system of units with the Rydberg as the unit of energy.

1. In the Born approximation the $n-n'$ transition cross section has the form

$$\sigma_{nn'} = \frac{8\pi}{k^2}\int_{k-k'}^{k+k'} f(q)\frac{dq}{q^3} \qquad (1)$$

$$f(q) = \frac{1}{n^2}\sum_{l,m,l',m'} |\langle nlm|e^{i\mathbf{qr}}|n'l'm'\rangle|^2, \qquad (2)$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the wave vectors of the external electron before and after the collision and n, l, and m are the quantum numbers of the electron in the atom. We shall sum over the quantum numbers l and m in (2). To do this we shall extend the sum (2) over all the quantum numbers

$$\sum_{l,m,l',m'} \langle nlm|e^{-i\mathbf{qr}}|n'l'm'\rangle\langle n'l'm'|e^{i\mathbf{qr}}|nlm\rangle$$

$$= \lim_{\substack{E\to E_n\\ E'\to E_{n'}}} (E-E_n)(E'-E_{n'}) \mathop{S}_{\gamma,\gamma'} \frac{\langle\gamma|e^{-i\mathbf{qr}}|\gamma'\rangle\langle\gamma'|e^{i\mathbf{qr}}|\gamma\rangle}{(E-E_\gamma)(E'-E_{\gamma'})}; \qquad (3)$$

where γ is the set of quantum numbers n, l, and m, and S includes summation over the states of the discrete spectrum and integration over the continuum states. Using the spectral expansion of the Green function

$$G_E(\mathbf{r},\mathbf{r}') = \mathop{S}_{\gamma}\frac{|\gamma\rangle\langle\gamma|}{E-E_\gamma}, \qquad (4)$$

we obtain

$$f(q) = \frac{1}{n^2}\lim_{\substack{E\to E_n\\ E'\to E_{n'}}}(E-E_n)(E'-E_{n'})\int G_E(\mathbf{r},\mathbf{r}')e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')}G_{E'}(\mathbf{r}',\mathbf{r})\,d\mathbf{r}\,d\mathbf{r}'. \qquad (5)$$

The Green function for the Coulomb field has the form[4]

$$G_E(\mathbf{r},\mathbf{r}') = \frac{\Gamma(1-\nu)}{2\pi(x-y)}\nu\hat{L}\left[W_{\nu,\frac{1}{2}}\left(\frac{x}{\nu}\right)M_{\nu,\frac{1}{2}}\left(\frac{y}{\nu}\right)\right], \qquad (6)$$

where

$$\hat{L} = \frac{\partial}{\partial x}-\frac{\partial}{\partial y},\quad x = r+r'+|\mathbf{r}-\mathbf{r}'|,\quad y = r+r'-|\mathbf{r}-\mathbf{r}'|,\quad \nu = (-E)^{-1/2},$$

W(x) and M(x) are Whittaker functions of the first and second kinds.

Going over to the limit in (5) reduces to calculation of the residue of the gamma function. As a result we obtain

$$f(q) = \frac{1}{\pi^2 n^3 n'}\int e^{-i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\frac{1}{(x-y)^2}P_nP_{n'}\,d\mathbf{r}\,d\mathbf{r}', \qquad (7)$$

$$P_n = \hat{L}\left[M_{n,\frac{1}{2}}\left(\frac{x}{n}\right)M_{n,\frac{1}{2}}\left(\frac{y}{n}\right)\right]. \qquad (8)$$

The integral in (7) can be reduced to a double integral over the variables x and y; to calculate this it is convenient to introduce the quantity A(q):

$$f(q) = \frac{1}{n^2 q}\int_0^q A(q)\,dq. \qquad (9)$$

Then, taking account of the symmetry of P_n with respect to x and y, we shall have

$$A(q) = \frac{1}{48nn'}\iint_0^\infty e^{-iq(x-y)/2}P_nP_{n'}\,dx\,dy. \qquad (10)$$

With this, the cross section $\sigma_{nn'}$ is equal to

$$\sigma_{nn'}=\frac{8\pi}{3k^2n^2}\left\{\int\limits_{q_-}^{q_+}\left(\frac{1}{q^3}-\frac{1}{q_+^3}\right)A(q)\,dq+\left(\frac{1}{q_-^3}-\frac{1}{q_+^3}\right)\int\limits_0^{q_-}A(q)\,dq\right\},\quad(11)$$

where $q_\pm = k \pm k'$.

Expressing P_n in terms of degenerate hypergeometric functions and using the known integral (cf., e.g.,[5])

$$I_\lambda(\alpha,\alpha')=\int\limits_0^\infty e^{-\lambda x}F(\alpha,1,px)F(\alpha',1,p'x)\,dx$$
$$=\lambda^{\alpha+\alpha'-1}(\lambda-p)^{-\alpha}(\lambda-p')^{-\alpha'}F\left(\alpha,\alpha',1;\frac{pp'}{(\lambda-p)(\lambda-p')}\right),\quad(12)$$

we write A(q) in terms of I and $I' \equiv dI/dq$ (the line over the I denotes the complex conjugate):

$$A(q)=(nn')^{-2}\,\mathrm{Re}\Big\{{}^1/_4[I_\lambda'(-n+1,-n'+1)\bar I_\lambda'(-n,-n')$$
$$-I_\lambda'(-n+1,-n')\bar I_\lambda'(-n,-n'+1)]$$
$$-{}^1/_6\frac{d^2}{dq^2}[I_\lambda(-n+1,-n'+1)\bar I_\lambda(-n,-n')$$
$$-I_\lambda(-n+1,-n')\bar I_\lambda(-n,-n'+1)]\Big\};\quad(13)$$

where $p = 1/n$, $p' = 1/n'$ and $\lambda = (p + p' + iq)/2$.

The expression for A(q) in terms of hypergeometric functions is extremely cumbersome and will not be given here.

2. The case of most interest for physical applications is that when $n \gg 1$ and $\Delta n \ll n$. According to (12) and (13), the quantity A(q) is determined by the value of the argument z of the hypergeometric function, which in our case is equal to

$$z=-\frac{4}{nn'[(1/n-1/n')^2+q^2]}\approx-\frac{4}{n^2[(\Delta n/n)^2+q^2]}.$$

If q is finite and $n \to \infty$, then $z \sim 1/n^2$. However, as n increases the region of q making the main contribution to the cross section is displaced in the direction of lower values and, therefore, in going over to the limit $n \to \infty$ in (13) it is necessary to make q go simultaneously to zero. It is easy to see that here the behaviour of z as $n \to \infty$ is determined by the law by which q decreases. Detailed analysis shows that if we put $q \sim 1/n^2$, the asymptotic series for A(q) in powers of 1/n is found to be uniform with respect to $\kappa = n^2q$ in the region giving the main contribution to the cross section; then $z \sim n^2$.

Using the relation

$$\lim_{n,\,n'\to\infty}\left[\frac{4nn'}{x^2}\right]^{-(n+n')/2}F\left(-n,-n',1;-\frac{4nn'}{x^2}\right)=(-1)^nJ_{\Delta n}(x),\quad(14)$$

for the first term of the asymptotic series for A(q) in powers of 1/n, we find

$$A(q)=\frac{2}{3}\frac{n^2}{\Delta n}[A_1(\varepsilon)+A_2(\varepsilon)],$$
$$A_1(\varepsilon)=\frac{\varepsilon^2-1}{\varepsilon^3}\left(\frac{4}{\varepsilon^2}-1\right)J_{\Delta n}(\varepsilon\Delta n)J_{\Delta n}'(\varepsilon\Delta n),$$
$$A_2(\varepsilon)=\Delta n\frac{(\varepsilon^2-1)^2}{\varepsilon^4}\left[\left(1+\frac{8}{\varepsilon^2}-\frac{6}{\varepsilon^4}\right)J_{\Delta n}^2(\varepsilon\Delta n)\right.$$
$$\left.-\left(1-\frac{12}{\varepsilon^2}\right)(J_{\Delta n}'(\varepsilon\Delta n))^2\right],\quad(15)$$
$$\varepsilon=[1+(\kappa/\Delta n)^2]^{1/2},\quad q=\kappa/n^2,\quad \Delta n\ll n.$$

Then we shall have for the cross section

$$\sigma_{nn'}=\frac{8\pi}{k^2}\frac{n^4}{(\Delta n)^3}\frac{2}{9}\left\{\int\limits_1^{\varepsilon_-}\frac{A_1(\varepsilon)+A_2(\varepsilon)}{(\varepsilon_-^2-1)^{3/2}(\varepsilon^2-1)^{1/2}}\varepsilon\,d\varepsilon\right.$$
$$\left.+\int\limits_{\varepsilon_-}^{\varepsilon_+}\frac{A_1(\varepsilon)+A_2(\varepsilon)}{(\varepsilon^2-1)^2}\varepsilon\,d\varepsilon\right\},\quad(16)$$
$$\varepsilon_\pm=\left[1+\left[\frac{(k\pm k')n^2}{\Delta n}\right]^2\right]^{1/2}.$$

We note that for $\kappa \to 0$ (i.e., $q \to 0$ faster than $1/n^2$) it follows from (15) that the oscillator strength is

$$f_{nn'}=(E_{n'}-E_n)\lim_{q\to0}\frac{f(q)}{q^2}$$
$$=\frac{32}{3}\frac{1}{(\Delta n)^2n^2}\left(\frac{nn'}{n+n'}\right)^3J_{\Delta n}(\Delta n)J_{\Delta n}'(\Delta n).\quad(17)$$

The formula (17) is the same as the expression for the oscillator strength obtained with quasi-classical functions in the paper[6].

For a number of problems, the total amplitude for inelastic transitions from a level n to all the levels $n' \neq n$ is of interest. This amplitude can be expressed in terms of the total amplitude of all transitions with no change in the principal quantum number. Using (15) and (9), we find

$$A(q)\Big|_{\Delta n=0}=-\frac{2}{3}n^2\left[J_0^2(\kappa)-J_1^2(\kappa)+\frac{J_0(\kappa)J_1(\kappa)}{\kappa}\right],\quad(18)$$

and, consequently,

$$\frac{1}{n^2}\sum_{\substack{n'\neq n\\ l,m,l',m'}}|\langle nlm|e^{i\mathbf{qr}}|n'l'm'\rangle|^2$$
$$=1-\frac{1}{n^2}\sum_{l,m,l',m'}|\langle nlm|e^{i\mathbf{qr}}|nl'm'\rangle|^2$$
$$=1+\frac{2}{3}\left[\frac{1}{\kappa}J_0(\kappa)J_1(\kappa)-2(J_0^2(\kappa)+J_1^2(\kappa))\right].\quad(19)$$

3. We shall consider the behavior at high external electron energies of the cross section determined by the formulas (15) and (16). For $k \gg 1/n$, the upper limit ϵ_+ can be put equal to infinity. Then integrating $A_1(\epsilon)$ gives a logarithmic function of k, since $\epsilon_- \to 1$ as $k \to \infty$. The remaining integrals converge and, in general, are functions only of Δn. Thus, at high energies the cross section is a sum of two terms:

$$\sigma=C_1(\Delta n)\frac{\ln k}{k^2}+\frac{C_2(\Delta n)}{k^2}.\quad(20)$$

The first term corresponds to the usual dipole approximation and, as can be shown, is proportional to the oscillator strength (17). It is difficult to find the dependence of the second term on Δn in the general case.

With the additional assumption that $\Delta n \gg 1$, the functions C_1 and C_2 have a simple form. In fact, using the asymptotic expansions of the Bessel function $J_m(mx)$ as $m \to \infty$, we shall obtain for the cross section

$$\sigma_{nn'}=\frac{8\pi}{k^2}\frac{n^4}{(\Delta n)^3}\left\{\frac{2}{3\pi\sqrt{3}(\Delta n)}\ln\frac{2Ckn}{(\Delta n)^{1/3}}+\frac{\sqrt{2}}{9\pi}a\right\},$$
$$a=\int\limits_1^\infty\frac{d\varepsilon}{\varepsilon^3}\frac{1}{[\varepsilon(\varepsilon-1)]^{1/2}}\left[1+\frac{8}{\varepsilon^2}-\frac{6}{\varepsilon^4}-\frac{2}{9}\left(2+\frac{1}{\varepsilon}\right)^2\right.$$
$$\left.\times\left(1-\frac{1}{\varepsilon}\right)\left(1-\frac{12}{\varepsilon^2}\right)\right]=5.5,\quad(21)$$

where the constant $C \approx 1$.

In conclusion, we note that the conditions of applicability of this formula ($1 \ll \Delta n \ll n$) are the same as those for the Kramers approximation for the oscillator strength. In particular, the coefficient of the logarithm in (21) is equal to $(4\pi n^3/k^2\Delta n)f^c$ (f^c is the oscillator strength in the Kramers approximation).

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