COLLISION THEORY OF IONISATION OF ATOMS BY ELECTRONS

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Gryzinski developed a theory [1,2] of atomic collisions which is applied by several authors in its first form [1,3,4] as well as in its revised form [2,5]. The principal idea of the theory is that the ionisation of an atom can be described approximately as a two particle collision, in which the impinging electron "hits" one atomic electron. The atom is ionised when the energy transfer to the atomic electron is greater than its binding energy U. This way of approximating the ionisation process is only "fully correct" when both the kinetic energy E_1 of the impinging electron and the energy transfer ΔE to the atomic electron are large compared to U. As ionising collisions with low ΔE (comparable to U) are the most important ones (even for high E_1), Gryzinski's theory is not very well founded. But this theory is very practical as it enables us to calculate in a simpler manner ionisation functions, even for complicated atoms. In this letter we discuss two points in Gryzinski's theory. Next we derive with the exact cross section formula for electron-electron collisions inexact cross section formulae for ionisation of atoms by electrons. Finally we compare classical cross section formulae with quantum formulae.

a. To calculate ionisation cross sections, Gryzinski and other authors [1-5] took the average kinetic energies $\bar{E}_2$ of the atomic electrons equal to their binding energies U. This was done for all atoms and molecules with exception of He in ref. 1 and 3. For the hydrogen atom is $\bar{E}_2 = U$, for He is $\bar{E}_2 = 1.6\ U$ (which is easy to derive from the virial theorem). For other atoms with two or more electrons in one shell $\bar{E}_2 > 1.6\ U$. So the approximation $\bar{E}_2 = U$ is in most cases somewhat crude. We remark that there is a better agreement between experiment and theory as applied in its first form [1,3,4] (for high energies E_1) if we take $\bar{E}_2 = 1.6\ U$ and not $\bar{E}_2 = U$. This is not justified for hydrogen-like atoms, in which case $\bar{E}_2 = U$ is (in general) a better choice.

b. First [1] Gryzinski took a δ-function for the kinetic energy distribution of the atomic electrons. This will result in too low ionisation cross sections [1,3,4] (compared with experiment) for high energies E_1. For these high energies Gryzinski's theory predicts $Q \sim E_1^{-1}$ in contradiction to quantum theory [6] which gives a dependence of $Q \sim E_1^{-1} \ln E_1$. In his recent reports [2] Gryzinski introduced the following kinetic energy distribution for the atomic electrons:

$$f(E_2)\mathrm{d}E_2 = \frac{\bar{E}_2}{2E_2^2} \exp -\left(\frac{\bar{E}_2}{E_2}\right)^{\frac{1}{2}} \mathrm{d}E_2 \qquad (1)$$

This will result in ionisation cross sections in better agreement [2,5] with experiment for high energies E_1 and a dependence of $Q \sim E_1^{-1} \ln E_1$. But this distribution function is not correct because:

$$\bar{E}_2 \neq \int_0^\infty E_2 f(E_2)\mathrm{d}E_2$$

if we take eq. (1) for $f(E_2)\mathrm{d}E_2$. Moreover, by comparison with the momentum distribution functions for the electron in the hydrogen atom [7], we see that there is no exponential factor in these functions. Using the correct momentum distributions, we do not get a logarithmical factor for high energies E_1 (see section c). Therefore Gryzinski's resulting formulae, as given in references 2 and 5, have to be considered as semi-empirical.

c. Assuming that the atomic electrons have an isotropic velocity-direction distribution, with one kinetic energy E_2, the cross section for an energy transfer $\Delta E (< E_1 - E_2)$ from the impinging to the atomic electron is [3,8].

$$\sigma_{\Delta E}\mathrm{d}\Delta E = \frac{\sigma_0}{E_1}\left(\frac{1}{\Delta E^2} + \frac{4E_2}{3\Delta E^3}\right)\mathrm{d}\Delta E \qquad (2)$$

where $\sigma_0 = \pi e^4$. Eq. (2) is exact if the atomic electrons may be considered as free. For $\Delta E > E_1 - E_2$, the exact solution of $\sigma_{\Delta E}$ is a complicated function [3] of E_1, E_2 and ΔE. To get the cross section Q for detachment of one electron from the atom, we have to integrate over ΔE

from U to ΔE_{max} (given in ref. 1, 2 and 8). For $\Delta E < E_1 - E_2$ exact integrating is possible, for $\Delta E > E_1 - E_2$ we make use of the same approximations as Gryzinski has used [2] for the whole integration region $(U, \Delta E_{max})$. The result is (for $E_1 - E_2 > U$):

$$Q = Q_I + Q_{II}$$

where

$$Q_I = \frac{\sigma_0}{E_1}\left[\left\{\frac{1}{U} - \frac{1}{E_1 - E_2}\right\} + \frac{2E_2}{3U}\left\{\frac{1}{U} - \frac{U}{(E_1-E_2)^2}\right\}\right] \quad (3)$$

and

$$Q_{II} = \frac{\sigma_0}{(E_1-E_2)^2}\left(\frac{E_1}{E_1+E_2}\right)^{\frac{3}{2}}\left[1 - \frac{2E_2}{3E_1} + \frac{E_2^2}{3E_1^2}\right]\left(\frac{E_2}{E_1}\right)\frac{E_1+E_2}{E_1}$$

For $E_1 > 10\,U$ and $E_2 \approx U$ is $Q_I > 100\,Q_{II}$. Then a very good approximation of Q is:

$$Q = \frac{\sigma_0}{E_1}\left[\left(\frac{1}{U} - \frac{1}{E_1}\right) + \frac{2E_2}{3U}\left(\frac{1}{U} - \frac{U}{E_1^2}\right)\right] \quad (4)$$

Eqs. (2), (3) and (4) are derived for one kinetic energy of the atomic electron. We now have to average over the energy distribution of that electron.

For $E_1 \gg \bar{E}_2$ exact averaging in eqs. (2) and (4) is possible by substituting $\bar{E}_2$ for E_2, because these equations are linear in E_2 and because every E_2 of the distribution of E_2 is smaller than $E_1 - U$. By taking $\bar{E}_2 = 0$ in eqs. (2), (3) and (4) we get Thomson's formulae [9]. From eq. (4) it follows that neglection of the initial kinetic energies of the atomic electrons, for $E_1 \gg U$, leads to large errors. For high energies E_1, $Q \sim E_1^{-1}$ (according to eq. 4) and not $\sim E_1^{-1}$ ln E_1.

For low energies E_1, but $E_1 > \bar{E}_2 + U$, we must use eq. (3) instead of eq. (4). Then we can not simple average over E_2 by replacing E_2 by $\bar{E}_2$, because of the possibility that E_2 is greater than $E_1 - U$ at these low energies E_1, and because eq. (3) is not linear in E_2. In order to get simple formulae we have to approximate and this can be done by substituting $\bar{E}_2$ for E_2; this results in too high cross sections.

For $U < E_1 < \bar{E}_2 + U$, eqs. (2), (3) and (4) are not valid.

d. The two particle collision problem can be described with classical theory and with quantum theory. For Coulomb interaction the scattering formulae are essentially the same in classical and quantum theory (Rutherford formula) [10]. There is one exception namely the scattering of identical particles; only the quantum theory takes proper account of the indistinguishability of the particles [10]. This means that for ionisation of atoms by protons, Gryzinski's theory is not only a classical theory but a general theory, whereas for ionisation of atoms by electrons classical theory gives too high cross sections [8] for low energies E_1. For high energies E_1, classical theory and quantum theory give the same results [8], and will give $Q \sim E_1^{-1}$. This is not in accordance with the Bethe formula [6] which gives $Q \sim E_1^{-1}$ ln E_1. Therefore if $Q \sim E_1^{-1}$ is not correct, this means that the error is not due to the classical treatment of the problem, but to the approximate description of the ionisation process, namely as a collision between two free electrons.

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