

ON THE DIFFERENCE BETWEEN "CLASSICAL" AND QUANTUM MECHANICAL COLLISION THEORIES

L. VRIENS

Physical Laboratory of the University, Utrecht, Netherlands

Received 4 May 1964

When calculating cross sections for ionisation (or excitation) of atoms by electrons, it is possible to make use of two types of collision theories. First the so called "classical" theories 1), in which the ionisation process is described as a collision between two free electrons, and second the well known quantum theories, for example the Born approximation.

For high energies E_1 of the impinging electron there is an important discrepancy between these theories. Namely, the two particle collision theory predicts 2) the ionisation and excitation cross sections Q to be proportional to E_1^{-1} , whereas the quantum theories predict 3) the Q 's to be proportional to $E_1^{-1} \ln E_1$. Seaton pointed out 4) that in quantum theory one obtains finite contributions from impact parameters which are much larger than those which contribute in "classical" theories. How fully this indicates the cause of the difference in behaviour of the cross section formulae, is discussed in this letter in terms of differential cross sections.

In the two particle collision theory Gryzinsky derived 5) a differential cross section $\sigma_{\Delta E, \theta} d\Delta E d\theta$ for an energy loss ΔE of the impinging electron to the atomic electron, and a simultaneous scattering of the impinging electron by an angle θ . We transformed this cross section to a differential cross section dependent on ΔE and K , where $\hbar K$ is the magnitude of the momentum change of the incident electron. The result is:

$$\sigma_{\Delta E, K} dK d\Delta E = \frac{4m^3 \pi e^4}{\hbar^6 k_2 k_1^2} \frac{|k_1 - K|}{k_1} \frac{dK}{K^4} d\Delta E, \quad (1)$$

where $\hbar k_1$ and $\hbar k_2$ are the initial momenta of the impinging and the atomic electron respectively. Eq. (1) is valid if: k_2 is constant, $K_{\min} < K < K_{\max}$, and $\Delta E < E_1 - E_2$. Here E_2 is the kinetic energy of the atomic electron and

$$K_{\min, \max} = \frac{(2m)^{\frac{1}{2}}}{\hbar} \{ \sqrt{\Delta E + E_2} \pm \sqrt{E_2} \}. \quad (2)$$

We restrict ΔE to positive values, corresponding in our formulae to an energy loss of the impinging electron. We assume that the atomic electrons have an isotropic velocity-direction distribution. For $E_1 \gg \Delta E$ is $k_1 \gg K$ and eq. (1) simplifies to:

$$\sigma_{\Delta E, K} dK d\Delta E \approx \frac{4m^3 \pi e^4}{\hbar^6 k_2 k_1^2} \frac{dK}{K^4} d\Delta E. \quad (3)$$

Integration of eq. (3) over K will result in the differential cross section $\sigma_{\Delta E} d\Delta E$, which was given in a previous letter 2). From eq. (2) it follows that $K = K_{\min} = K_{\max}$ for $E_2 = 0$. Then only one momentum change of the impinging electron is possible for one ΔE .

Now we compare eqs. (1), (2) and (3) with the corresponding quantum formulae. For simplicity we give the quantum formula for excitation of an atom from the ground state 0 to an excited state n , in the case that the transition is optically allowed. The cross sections Q are known to be proportional to $E_1^{-1} \ln E_1$ for large E_1 both for ionisation and for an optically allowed excitation.

The differential cross section for momentum change $\hbar K$ in excitation of an atom to state n is 3):

$$I_{0n}(K) dK = \frac{8m^2 \pi e^4}{\hbar^4 k_1^2} \frac{dK}{K^3} |\epsilon_{0n}(K)|^2, \quad (4)$$

where $\epsilon_{0n}(K)$ is given by Massey 3). For high E_1 quantum theory (Born approximation) gives

$$K_{\min} \approx \frac{m\Delta E}{\hbar^2 k_1} \quad \text{and} \quad K_{\max} \approx 2k_1. \quad (5)$$

For sufficiently small K , the matrix element $\epsilon_{0n}(K)$ can be expanded such that $\epsilon_{0n}(K) \approx iKz_{0n}$, where z_{0n} is a constant for $Ka_0 \ll 1$ (a_0 = radius of first Bohr orbit). Then eq. (4) simplifies to

$$I_{0n}(K) dK \approx \frac{8m^2 \pi e^4}{\hbar^4 k_1^2} \frac{dK}{K} |z_{0n}|^2. \quad (6)$$

To obtain the total cross section for excitation we have to integrate eq. (4) from K_{\min} to K_{\max} . Since momentum transfers with $Ka_0 > 1$ are very improbable this integration will result in $Q \sim -k_1^{-2} \ln K_{\min} \sim E_1^{-1} \ln E_1$. So the factor $\ln E_1$ is due to the fact that K_{\min} is proportional to $E_1^{-1/2}$. But in the two particle collision theory K_{\min} is independent of E_1 (see eq. 2). On substituting the "classical" K_{\min} in the integration over K in eqs. (4) and (6) the result would be: $Q \sim E_1^{-1}$. This means that for large E_1 most ionising collisions or collisions resulting in excitation of the atom belong to very small momentum changes $\hbar K$ of the impinging electron, namely such, that $\hbar K \langle (2m\Delta E + 2mE_2)^{1/2} - (2mE_2)^{1/2} \rangle$. From comparison of eq. (3) with eq. (6) it follows that, for $Ka_0 \ll 1$, the corresponding differential cross sections are very different. As inelastic collisions with $Ka_0 < 1$ are more important for large E_1 than for small E_1 , this means that (for this reason) the application of the two particle collision theory is the more unjustifiable the higher the energy E_1 .

However, for small E_1 (for example $< 10U$, where U is the binding energy of the atomic electron) the K_{\min} , according to "classical" and to quantum mechanical collision theories, are not very different. Then application of eq. (6) is no longer possible because K_{\min} (eq. (5)) is too high, and quantum theories give results not yet very well in agreement with experiment. For these reasons it is understandable that the two particle collision theory can be applied successfully for these low E_1 .

We conclude (see also ref. 2) that the principal difference between "classical and quantum mechanical collision theories is not due to the classical treatment of the two particle collision theory, but to the fact that the law of conservation of momentum gives different values of K_{\min} for two particle (electron-electron) collisions as compared with more particle (electron-electron(s) + nucleus) collision, and to the special form of eq. (6).

Akerib and Borowitz ⁶) applied their "impulse approximation" on the ionisation and excitation of the hydrogen atom. In this impulse approxima-

tion, the interactions between the impinging electron and the nucleus and between the atomic electron and the nucleus are neglected during the collision. If this neglect means that the law of conservation of momentum is valid for the collision between the impinging and the atomic electron, then this impulse approximation will give erroneous results (compared with the Born approximation) for high E_1 . And if the law of conservation of momentum is not valid for the collision between the electrons (which is the case in ref. 6), then the electron-electron collision is not treated correctly. From eq. (32) of ref. 6, the differential cross section corresponding to eqs. (3) and (6), i.e. for large E_1 and small K , can be derived. This differential cross section is of the same type as eq. (3), which also shows that the continuous velocity-distribution of the atomic electron is not responsible for the logarithmical factor in the cross sections Q . We conclude: the impulse approximation is not reliable (compared with the Born approximation) for large E_1 .

The author wishes to express his gratitude to Professor Dr. B. R. A. Nijboer and Professor Dr. J. A. Smit for stimulating discussions, and to them and Dr. J. M. Fluit for reading the manuscript.

This investigation is part of the research program of the Foundation for Fundamental Research of Matter (F.O.M.), financially supported by the Netherlands Organisation for Pure Scientific Research (Z.W.O.).

References

- 1) M. Gryzinsky, Phys. Rev. 115 (1959) 374.
- 2) L. Vriens, Physics Letters 9 (1964) 295.
- 3) H. S. W. Massey, Handbuch der Physik (Springer-Verlag, Berlin, 1956) Vol. 36, p. 351-358.
- 4) M. J. Seaton, Atomic and Molecular Processes, ed. D. R. Bates (Academic Press, New York, 1962) p. 377.
- 5) M. Gryzinski, Reports No. 436 and 447/XVIII (1963), Institut for Nuclear Research, Swierk k/Otwocka, Poland.
- 6) R. Akerib and S. Borowitz, Phys. Rev. 122 (1961) 1177.

* * * * *