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THE CORRESPONDENCE PRINCIPLE IN INELASTIC SCATTERING

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Abstract

Ionization of hydrogen by electrons is examined for the case of high incident electron energies. The Born quantum cross section is found to approach the classical expression in the limit of large principal quantum numbers. The energy dependence of the cross section at high energy is discussed; it is expected that the cross sections go smoothly from $\frac{\log E}{E}$ to $\frac{1}{E}$ behavior as n becomes large.

I. INTRODUCTION

There have been a number of recent papers[1-6] dealing with classical models for inelastic collisions; most of these concern the Gryzinski[1] binary encounter model. Though it is often stated that the quantum and classical cross sections differ in their high energy behavior, the nature of the relationship has not been carefully explored. That they should be intimately related is suggested by the equality of the quantum and classical elastic coulomb cross section. Section II shows that the classical differential cross section and the quantum cross section for ionization in the binary encounter approximation are related simply. Section III illustrates the correspondence between the two expressions in the limit of large principal quantum numbers. Some consequences of this correspondence are discussed.

II. HIGH ENERGY CROSS SECTIONS

We consider the ionizing collision of an electron with a hydrogen atom. In a classical analysis of the problem, the binary encounter model of Gryzinski proceeds by finding first the cross section for energy exchange in the laboratory frame between two moving charged particles. We quote the result[7] for the differential cross section for energy exchange ΔE and momentum transfer K, averaged over an isotropic distribution of target electron directions

$$d\sigma = \frac{2\pi dK}{E_1 K^4} \frac{d\Delta E}{v_2} \quad . \tag{1}$$

(Atomic units are used throughout.) This expression is then integrated over all allowable momentum transfers and all ΔE from the ionization energy up to the incident energy E_1. The model thus assumes that the collision is such that only the interaction between the two electrons is important in determining the cross section. The resultant total cross section[3,4] is proportional to $\frac{1}{E_1}$ for large E_1.

The corresponding quantum mechanical result for high energy incident electrons can be obtained by considering the Born approximation. In this limit the scattering amplitude for ionization is[8]

$$f_{0\mathcal{K}} = -\frac{1}{4\pi}\int U(r_{12})e^{i\vec{K}\cdot\vec{r}_{12}}\,d^3r_{12}\int e^{i\vec{K}\cdot\vec{r}_2}\psi_o(r_2)\psi^*_{\mathcal{K}}(r_2)d^3r_2 \qquad (2)$$

where 1 is the scattered electron, 2 is the ejected electron, $\vec{K} = \vec{k}_o - \vec{k}'$ is the momentum transfer vector, $\vec{k}_o$ the initial, $\vec{k}'$ the final incident electron momentum. $\mathcal{K}$ is the ejected electron's momentum, whose initial and final state are described by ψ_o, $\psi_{\mathcal{K}}$, respectively. This amplitude, in the case of hydrogen where $U = \frac{1}{r_{12}}$, is seen to be merely a free particle coulomb amplitude multiplied by a "form factor" associated with the bound state description. In Eq. (2) it is presumed (so as to correspond to the classical presumption) that the electrons are distinguishable, i.e., the wave function has not been antisymmetrized.

The differential cross section is (assuming -- as will generally be the case -- that after integrating over $d\Omega_2$, the expression will not depend on azimuth of $\vec{k}'$ relative to $\vec{k}_o$)

$$d\sigma = \frac{4\pi}{E_1}\frac{dK}{K^3}\,|\varepsilon_{0\mathcal{K}}(K)|^2\,\mathcal{K}^2 d\mathcal{K}\,d\Omega_2 \qquad (3)$$

where $$|\varepsilon_{0\mathcal{K}}(K)|^2 = \frac{1}{(2\pi)^3}\left|\int e^{i\vec{K}\cdot\vec{r}}\psi_o(r)\psi^*_{\mathcal{K}}(r)d^3r\right|^2 \quad . \qquad (4)$$

It is now easy to see that the classical value is identical to (3) in the limit that

$$|\varepsilon_{0\mathcal{H}}(K)|^2 = \frac{1}{4\pi v_2^2}\,\delta(|\vec{K} - \vec{\mathcal{H}}| - v_2)$$

$$= \frac{1}{4\pi v_2^2}\,\delta(\sqrt{K^2 + \mathcal{H}^2 - 2K\mathcal{H}\cos\beta} - v_2)\ . \qquad (5)$$

Here β is the angle between $\vec{K}$ and $\vec{\mathcal{H}}$. (5) used in (3) and integrated over $d\Omega_2 = 2\pi\sin\beta d\beta$, together with energy conservation

$$\Delta E = 1/2\ k_o^2 - 1/2\ k'^2 = -\ E_2 + 1/2\ \mathcal{H}^2$$

or

$$d\Delta E = \mathcal{H} d\mathcal{H}$$

gives

$$d\sigma = \frac{2\pi}{E_1}\frac{dK}{K^4}\frac{d\Delta E}{v_2}$$

which is identical with (1). Gryzinski's classical approach requires full conservation of momentum and energy between the two electrons, whereas the quantum mechanical approximation insists only on energy conservation because the nucleus can take up momentum. However, in the limit when (5) is true, an averaged momentum conservation follows. That only the magnitude $|\vec{K} - \vec{\mathcal{H}}|$ is involved in the conservation of momentum is a consequence of the averaging over the atomic electron's angular distribution.

The high energy behavior is obtainable from (3) by noting that for very large E_1, K must be small; thus $e^{i\vec{K}\cdot\vec{r}} \sim 1 + i\vec{K}\cdot\vec{r}$ can be used in (4), yielding

$$|\varepsilon_{0\mathcal{H}}(K)|^2 \simeq K^2|\langle 0|z|\mathcal{H}\rangle|^2 \qquad .$$

This when used in (3) can be readily seen to lead to ℓn E/E behavior for the integrated ionization cross section.[8]

III. CORRESPONDENCE LIMIT

The genesis of Equation (5) can be most easily seen in the approximation that the ejected electron be describable by a plane wave rather than a coulomb wavefunction: $\psi_{\mathcal{H}} \sim e^{i\vec{\mathcal{H}}\cdot\vec{r}}$. In this approximation

$$|\varepsilon_{0\mathcal{H}}(K)|^2 = |\phi_0(\vec{K} - \vec{\mathcal{H}})|^2 \tag{6}$$

is just the square of the Fourier transform of the bound state wave function, evaluated at $\vec{q} = \vec{K} - \vec{\mathcal{H}}$. It can be seen that, aside from a constant term[9] which now arises because of the non-orthogonality of the bound and free wave functions, (6) also leads to a $\ln E/E$ behavior in the limit of small momentum transfer or high energy, where $e^{iK\cdot r} \simeq 1 + iK\cdot r$.

For the ground state this approximation gives:

$$|\varepsilon_{0\mathcal{H}}(K)|^2 \doteq \frac{8}{\pi^2} \frac{1}{[(\vec{K} - \vec{\mathcal{H}})^2 + 1]^4} \quad .$$

For excited states we would have additional complications because of the different angular momentum states. However, the normalized momentum space wave functions for a given principal quantum number <u>averaged</u> over all angular momenta have been shown by Fock[10] to be

$$|\phi_n(\vec{K} - \vec{\mathcal{H}})|^2 = \frac{8}{\pi^2} \frac{1}{n^5} \frac{1}{[(\vec{K} - \vec{\mathcal{H}})^2 + \frac{1}{n^2}]^4} \quad . \tag{7}$$

(7) is the correct expression to use for obtaining a classical correspondence. This function becomes sharply peaked as n increases, in fact acquires delta function behavior[11]:

$$\lim_{n\to\infty} \frac{1}{n^5} \frac{1}{[x^2 + \frac{1}{n^2}]^4} = 0 \qquad x \neq 0$$

$$\int |\phi_n(p)|^2 d^3p = \int_0^\infty 4\pi x^2 dx \{\frac{8}{\pi^2} \frac{1}{n^5} \frac{1}{(x^2 + \frac{1}{n^2})^4}\} = 1 \quad \text{for all } n \ . \tag{8}$$

Thus in the approximation implied by (6), the use of a delta function as in (5) is correct for large n.

Actually, for any state, no approximations need be made to obtain the exact $\varepsilon_{0\mathcal{K}}(K)$ in closed form.[8] The expression is not very transparent, but it can be argued that its behavior is at least qualitatively the same as that given by (7). For example, if we look at the ground state $\varepsilon_{0\mathcal{K}}(K)$ for nuclear charge $Z \neq 1$, this function also becomes sharply peaked as $\mu = Z/a_o$ decreases.[12] The expression for $\varepsilon_{n\mathcal{K}}(K)$ should go smoothly from its bound state form to the continuum form as n increases. Here by continuum form we mean that the nucleus is very far away so the collision will be ordinary elastic electron-electron scattering, for which the quantum mechanical (exact), Born, and classical cross sections are equal.

If we accept the validity of the Born approximation at sufficiently high energy, the above remarks imply that the cross section, at a given energy which is large compared to the binding energy, should go smoothly from ℓn E/E behavior to 1/E behavior as n increases. This follows since (1) produces a $\frac{1}{E}$ behavior, and also represents the limiting (fixed energy) behavior of (3) as n increases, whereas for low n and large enough E_1 (therefore small K) the cross section has log E_1/E_1 dependence. This can be seen to be verified by numerical calculations of Omidvar.[13] He plots both the Born approximation and Gryzinski ionization cross sections for n = 1 thru 5, and finds that for the higher n, the Born and classical agree at the higher energies calculated. Of course, since momentum transfer decreases with increasing energy, we can find an incident energy such that the logarithmic behavior of the Born approximation is valid for any given n. However, this energy will become increasingly larger,[14] and in the limit the logarithmic behavior no longer obtains.

These results also give some insight into the problem of averaging over velocity distributions which have been used[1,6] in connection with the Gryzinski model. In fact what is appropriate is a weighting of the differential cross section by $|\varepsilon_{n\ell}(K)|^2$. That is, the fact that the bound state momentum is uncertain requires a weighting of the probability of energy exchange at a given momentum transfer; the logarithmic dependence follows from this uncertainty. For highly excited states, however, the bound state momentum becomes sharply peaked, giving validity to the use of a delta function approximation for an averaged momentum conservation between the two electrons, as in the Gryzinski model. Restating this argument, the effect of the nucleus becomes unimportant for large n (the parameter, it should be kept in mind, is Z/n), and free particle descriptions become approximately valid.

Extension of these arguments to consideration of excitation cross sections is less straightforward.

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7. See equation (1) of Reference 3 or equation (66), page A332, of Reference 1. This latter equation becomes our equation (1) upon substitution $d(\cos\theta) = \frac{KdK}{m^2 v_2 v_2'}$, if we recognize that $v_2' = (2mE_2)^{1/2}(1 + \Delta E/E_2)^{1/2}$, and $E_2\xi = 1/2\ K^2$. In doing this we keep in mind that Gryzinski's incident electron is labelled 2. Our expression (1) has also been verified using the averaging procedures given in Reference 2.
8. N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions, Cambridge Univ. Press, Cambridge, England (1965), p. 335 and 489.
9. This constant term can be said to be due to the fact that this ejected electron wavefunction lacks knowledge of the nucleus. It vanishes if we orthogonalize the wave functions or even more simply by using the full interaction potential $U = \frac{1}{r_{12}} - \frac{1}{r_1}$ instead of the simple $\frac{1}{r_{12}}$ which is correct for orthogonal functions.
10. V. Fock, Z. fur Phys. 98, 145 (1935).
11. The function $4\pi p^2 |\phi_n(p)|^2$ given by (7) peaks at $p = \frac{1}{\sqrt{3}}\frac{1}{n}$, which differs slightly from the classical correspondence value for a circular orbit $v_2 = \frac{1}{n}$ (atomic units). This momentum distribution is very sharply peaked for large n.

12. That is, in expression XVI (97) of Reference 8, we can simulate the n behavior by letting $Z/a_o \to Z/na_o$. Then the limit $n \to \infty$ corresponds to $\mu \to 0$.

13. K. Omidvar, Phys. Rev. <u>140A</u>, 26 (1965).

14. A rough estimate of the required incident energy can be made by considering the expansion of (7) for small K. The $\ln E/E$ behavior then holds for $K^2 \lesssim 1/n^2$. If we now estimate K^2 by $K^2 = \frac{4\pi}{E_1^*} \ln \frac{E_1^*}{2I}$ (see Ref. 8, page 514) we obtain $E_1^* \sim 200\pi n^2 s$ electron volts, where s is a number of order of unity. Thus $E_1^*/E_n \sim 16\pi n^4 s$. Relativistic effects will begin to be important at these energies even for $n \sim 5$.