INTERFERENCE EFFECTS IN THE IONIZATION OF HYDROGEN ATOMS BY ELECTRON IMPACT

R. K. PETERKOP

Physics Institute, Academy of Sciences, Latvian S.S.R.

Submitted to JETP editor July 13, 1961

J. Exptl. Theoret. Phys. (U.S.S.R.) 41, 1938-1939 (December, 1961)

The cross section for ionization of hydrogen atoms by electrons is calculated in the Born approximation, taking interference effects into account.

It has been shown that in the ionization of hydrogen atoms by electrons exchange effects can be considered as an interference between parts of the wave function.[1] This is a purely quantum mechanical effect and can be described by saying that when the wave function is symmetrized in accordance with Pauli's principle, interference occurs between scattering events that differ by an exchange of electrons in the initial or final states. The ionization cross section, taking exchange into account, can be written in the form

$$Q = Q' - Q_{int}, \tag{1}$$

where Q' is the cross section without exchange and Q_{int} is the interference term

$$Q_{int} = \int_0^{E/2} \frac{kc}{q}\, d\varepsilon \iint \mathrm{Re}\,[f(\mathbf{k}, \mathbf{c})\, g^*(\mathbf{k}, \mathbf{c})]\, d\mathbf{k} d\mathbf{c}. \tag{2}$$

In this formula, q is the momentum of the incident electron, $\epsilon = k^2/2$, $E = E_q - 1/2$, $E_q = q^2/2$ is the energy of the incident electron, and $f(\mathbf{k}, \mathbf{c})$ is the probability amplitude for the electron being scattered with momentum $\mathbf{c}$ and the atom to have final momentum $\mathbf{k}$; $g(\mathbf{k}, \mathbf{c})$ is the corresponding exchange amplitude. All quantities are measured in atomic units.

We now calculate the interference term in the Born approximation. In this approximation[2]

$$f(\mathbf{k}, \mathbf{c}) = -\frac{2}{x^2}\int \psi_1(\mathbf{r})\, e^{i\mathbf{x}\mathbf{r}} \psi_{\mathbf{k}}^*(\mathbf{r})\, d\mathbf{r};$$

$$\mathbf{x} = \mathbf{q} - \mathbf{c}, \quad x^2 = q^2 + c^2 - 2qc\cos(\mathbf{q}, \mathbf{c}), \tag{3}$$

where ψ_1 and ψ_2 are atomic wave functions for the initial and final states. The result of the integration is

$$f(\mathbf{k}, \mathbf{c}) = \frac{16\exp(i\delta(k))\,[(1-ik)^2 + x^2]^{n-1}\,[(1-n)\,\mathbf{k}\mathbf{x} - x^2]}{\{\pi k\,(1-\exp(-2\pi/k))\}^{1/2} x^2\,[1 + (\mathbf{x}-\mathbf{k})^2]^{n+2}};$$

$$\delta(k) = \arg\Gamma(1 - i/k), \quad n = 1/ik. \tag{4}$$

According to [1], the phase shift η of the wave function of the scattered electron can be chosen so that

$$g(\mathbf{k}, \mathbf{c}) = f(\mathbf{c}, \mathbf{k}). \tag{5}$$

In general, for an arbitrary phase shift $\eta' = \eta - \Delta(\mathbf{k}, \mathbf{c})$, Eq. (5) is to be replaced by

$$g(\mathbf{k}, \mathbf{c}) = f(\mathbf{c}, \mathbf{k}) \exp[i\Delta(\mathbf{k}, \mathbf{c}) - i\Delta(\mathbf{c}, \mathbf{k})], \tag{6}$$

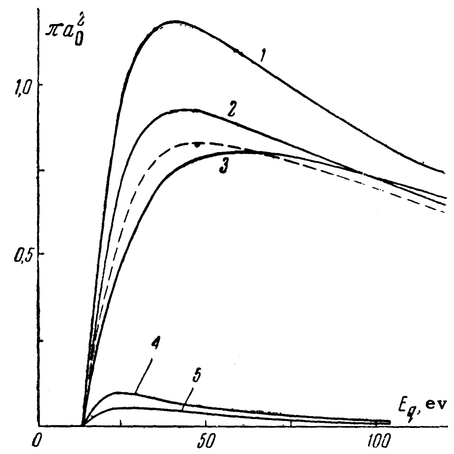
and the interference term then becomes

$$Q_{int} = \int_0^{E/2} \frac{kc}{q}\, d\varepsilon \iint \mathrm{Re}\,\{f(\mathbf{k}, \mathbf{c}) f^*(\mathbf{c}, \mathbf{k}) \times \exp[i\Delta(\mathbf{c}, \mathbf{k}) - i\Delta(\mathbf{k}, \mathbf{c})]\}\, d\mathbf{k} d\mathbf{c}. \tag{7}$$

The magnitude of Δ in the Born approximation is not known. However, calculations in the Born-Oppenheimer approximation for incident s-waves[3], and also by Geltman[4], show that near the threshold for ionization the direct and exchange amplitudes do not differ by a rapidly oscillating factor. In the Born approximation this corresponds to the relation $\Delta(\mathbf{k}, \mathbf{c}) = \delta(k)$, and this is the choice which was made in the work being reported upon here. This implies that the factor $\exp\{i\delta(k)\}$ in (4) should be dropped if (5) is used.

The integration over one of the four angles in (7) can be carried out analytically. The remaining integrals were determined with the BÉSM-2 computer. The cross section Q given by formula (1) is then as shown in the figure, with the Born cross section without exchange having been taken from [5].

Since we did not determine Δ rigorously, we also calculated the integral (2) with the amplitudes replaced by moduli, so as to find the maximum possible amount of interference. This corresponds to the choice $\Delta(\mathbf{k}, \mathbf{c}) = \arg f(\mathbf{k}, \mathbf{c})$. The partial cross section for S-wave scattering has also been



1, 2 – the Born cross section without taking interference into account, and with this effect included; 3 – experimental cross section[6]; dashed line – Born cross section assuming the maximum possible amount of interference; 4, 5 – Born cross sections for S-wave scattering without taking interference into account and with this effect included.

calculated in the Born approximation and the results are shown in the figure. The S-wave partial cross section, which corresponds to both electrons being in s-states after ionization, constitutes only a small part of the total cross section.

The results shown in the figure indicate that by taking interference effects into account the agreement between theory and experiment can be markedly improved.

[1] R. Peterkop, Izv. Akad. Nauk Latv. S.S.R. **12**, 57 (1960); Proc. Phys. Soc. (London) **A77**, 1220 (1961).

[2] N. F. Mott and H. S. W. Massey, Theory of Atomic Collisions, Oxford University Press, London, 1952.

[3] R. Peterkop, Dissertation, Physics Institute, Acad. Sci. Latv. S.S.R., Riga, 1960.

[4] S. Geltman, Phys. Rev. **102**, 171 (1956).

[5] R. McCarroll, Proc. Phys. Soc. (London) **A70**, 460 (1957).

[6] W. Fite and R. Brackman, Phys. Rev. **112**, 1141 (1958).

Translated by R. Krotkov
326