SOVIET PHYSICS JETP VOLUME 31, NUMBER 6 DECEMBER, 1970

ON THE THEORY OF THE FORMATION OF EXCITED HYDROGEN ATOMS IN COLLISIONS BETWEEN NEGATIVE HYDROGEN IONS AND NEUTRAL ATOMS

G. F. DRUKAREV

Leningrad State University

Submitted January 20, 1970

Zh. Eksp. Teor. Fiz. 58, 2210–2212 (June, 1970)

Collision between a neutral atom and a negative hydrogen ion, leading to detachment of one of the electrons from the negative ion and the formation of an excited hydrogen atom, is considered. It is shown that, in a certain approximation, this process can be considered as the expulsion of a strongly bound electron from the negative ion followed by adaptation of the remaining electron to the modified field. It follows from this idea that the energy dependence of the yield of hydrogen atoms in excited s-states in this process must be the same as for ionization of hydrogen atoms.

WE shall consider the process

$$H^- + X \rightarrow H + X + e, \tag{1}$$

where X is some neutral atom, the state of which is not changed in the collision, and H is a hydrogen atom, which can, in general, be in an excited state.

At high energies we can apply the Born approximation to give an account of the process (1). The detachment of an electron from H^- in the case when a helium atom plays the part of atom X was treated in the Born approximation by Sida[1]. We shall not write out in full the formula derived in[1] for the cross section, but shall cite only the expression for the matrix element will be the subject of the discussion below:

$$N = \int \Psi_i(\mathbf{r}_1, \mathbf{r}_2) e^{-i\mathbf{K}\mathbf{r}_2} \Psi_f(\mathbf{r}_1, \mathbf{r}_2)\, d\mathbf{r}_1\, d\mathbf{r}_2. \tag{2}$$

Here **K** is the difference between the momentum of H^- before the collision and that of H after the collision, Ψ_i is the wave function of H^-, and Ψ_f is the wave function of the hydrogen atom + electron system.

Sida limited the treatment to the case when the atom H is found to be in the ground state after the collision. Apart from this, he used the expression $e^{-\alpha(r_1+r_2)}$ for Ψ_i. However, as is known[2], this expression is too poor an approximation to the true wave function of a negative hydrogen ion (it gives no bound state at all for H^- and has an obviously incorrect asymptotic form).

A much more satisfactory approximation is the expression proposed by Chandresekar (cf.[2]),

$$\Psi_i(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{a}} \{\varphi(\mathbf{r}_1)\eta(\mathbf{r}_2) + \varphi(\mathbf{r}_2)\eta(\mathbf{r}_1)\}, \tag{3}$$

where φ and η are hydrogen-like wave functions

$$\varphi = \alpha_1^{3/2}\pi^{-1/2}e^{-\alpha_1 r}, \qquad \eta = \alpha_2^{3/2}\pi^{-1/2}e^{-\alpha_2 r}, \tag{4}$$

a, α_1 and α_2 are (in the atomic system of units)

$$a = 2.6, \qquad \alpha_1 = 1.039, \qquad \alpha_2 = 0.283. \tag{5}$$

Since α_1 is close to unity, φ practically coincides with the wave function of the ground state of the hydrogen atom. However, $\alpha_2 \ll 1$. It is in this sense that we shall speak of weakly bound and strongly bound electrons in H^-.

Here we shall consider the matrix element N for the case when the hydrogen atom is found to be excited after the collision and shall make use of a more accurate wave function $\Psi_i(\mathbf{r}_1, \mathbf{r}_2)$ in the form (3). We shall represent the function Ψ_f approximately in the form

$$\Psi_f = \frac{1}{\sqrt{2}} \{\varphi_n(\mathbf{r}_1) f(\mathbf{r}_2) + \varphi_n(\mathbf{r}_2) f(\mathbf{r}_1)\}, \tag{6}$$

where φ_n is the wave function of an excited state of H, and f is the continuous-spectrum wave function of an electron in the field of the atom H.

The functions Ψ_i and Ψ_f should be orthogonal. Within the limits of the approximation (3) and (6), this orthogonality can be ensured by requring that

$$\int f\varphi\, d\mathbf{r} = 0, \qquad \int f\eta\, d\mathbf{r} = 0. \tag{7}$$

Substituting (3) and (6) into (2) and taking (7) into account, we obtain N in the form of a sum of two terms:

$$N = \frac{1}{\sqrt{2a}} \int \varphi_n\varphi\, d\mathbf{r}_1 \int f e^{-i\mathbf{K}\mathbf{r}_2} \eta\, d\mathbf{r}_2 + \frac{1}{\sqrt{2a}} \int \varphi_n\eta\, d\mathbf{r}_1 \int f e^{-i\mathbf{K}\mathbf{r}_2} \varphi\, d\mathbf{r}_2.$$

Since φ is close to the wave function of the hydrogen atom ground state, the integral $\int \varphi_n \varphi\, d\mathbf{r}_1$ is very small and we shall neglect this term below. Then N reduces to the expression:

$$N = \sqrt{\frac{2}{2.6}} \int \varphi_n\eta\, d\mathbf{r}_1 \, \frac{1}{2} \int f e^{-i\mathbf{K}\mathbf{r}_2} \varphi\, d\mathbf{r}_2. \tag{8}$$

The quantity

$$C_n = \sqrt{\frac{2}{2.6}} \int \varphi_n \eta\, d\mathbf{r}_1 \tag{9}$$

does not contain any of the parameters over which further integration of N is performed in[1]. Therefore, in the final expression for the effective cross section, the quantity C_n^2 occurs simply as a factor.

The expression (8) for N has a simple and intuitive meaning. On collision of H^- with atom X, the strongly bound electron is expelled (the integral $\frac{1}{2}\int \varphi e^{-i\mathbf{K}\cdot\mathbf{r}_2} f\, d\mathbf{r}_2$ is the matrix element for this process), and the weakly bound electron adapts to the suddenly altered field (C_n^2 gives the probability of finding the hydrogen atom in the state n).

If f is approximated by a plane wave in expression (8) and φ by the ground state wave function of the hydrogen atom, the integral $\frac{1}{2}\int \varphi e^{-i\mathbf{K}\cdot\mathbf{r}_2} f\, d\mathbf{r}_2$ will become the matrix element for the process of ionization of a hydrogen atom

$$H + X \rightarrow H^+ + X + e \tag{10}$$

in the Born approximation. Denoting the cross section of reaction (1) by σ and that of reaction (10) by σ', we obtain an approximate relationship between σ and σ' at high electron energies:

$$\sigma \approx C_n{}^2\sigma'. \tag{11}$$

It follows from this that at high energies we can expect that the energy dependence of the cross sections σ and σ' of the processes (1) and (10) will be the same and that the ratio σ/σ' will be equal to C_n^2. In particular, for the case when an atom H is formed in the 2s-state after the collision, we have $C_2^2 \approx 0.5$.

We note that, if we use expression (3) for Ψ_i, the only non-zero cross sections are found to be those for excitation of s-states. For all other states, with $l \neq 0$, the cross section vanishes in this approximation.

In order to obtain a non-zero cross section for excitation of states with $l \neq 0$, it is necessary to allow in the wave function for correlation between the electrons, i.e., to introduce terms containing $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ into the analytic expression for Ψ_i. But in this case, the matrix element N will no longer have the form of a product of two integrals of the type (8) and there is, therefore, no relation analogous to (11) for excitation of p- and d-states, etc.

In comparing the above considerations with experimental results, one must bear in mind the possibility of mixing of states with the same n and different l during the motion of the particles through different parts of the apparatus. This fact can change the relative yields of atoms in different excited states.

In conclusion I thank the authors of the experimental paper[1], E. P. Andreev, V. A. Ankudinov, V. M. Dukel'skiĭ and A. L. Orbeli, who drew my attention to the original and interesting results they have obtained. The present paper is the outcome of discussion of these results with the authors.

---

[1] D. W. Sida, Proc. Phys. Soc. A68, 240 (1955).

[2] H. A. Bethe and E. E. Salpeter, Sec. 34 in Quantum Mechanics of One- and Two-electron Atoms (in Encyclopedia of Physics, Vol. XXXV) Springer-Verlag, Berlin, 1957 (Russ. Transl. Fizmatgiz, 1960).

[3] A. L. Orbeli, E. P. Andreev, V. A. Ankudnikov and V. M. Dukel'skiĭ, Zh. Eksp. Teor. Fiz. 58, 1938 (1970) [this issue, p. 1043].

Translated by P. J. Shepherd
268