IONIZATION OF HYDROGEN ATOM BY ELECTRON IMPACT IN THE THREE-BODY APPROXIMATION OF CLASSICAL MECHANICS

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It is shown that complete allowance for all interaction greatly improves both the form of the ionization function and the absolute values of the cross sections. The remaining discrepancy can be regarded as a measure of the error of the classical description. The ionization cross sections of an arbitrarily excited atom can be obtained with the aid of the calculated cross sections by simply changing the scale.

CALCULATIONS of the probability of excitation and ionization of atoms by electron impact, based on the use of classical mechanics, have recently received wide circulation. It becomes of interest in this connection to consider the question of the accuracy of the classical description of problems of this kind. Unfortunately, the available papers do not answer this question, since they make essential use of a number of supplementary simplifications, of which the most important is the use of the two-body approximation. There is only one paper [1] where the three-body problem is considered fully and where the ionization and charge-exchange probabilities are calculated for collisions of protons with hydrogen atoms. We report in this paper the results of a similar calculation of the ionization of the hydrogen atom by electron impact.

The calculations were made for an atom in the ground state, but the results can be readily recalculated for the ionization of an arbitrarily excited atom. The feasibility of such a recalculation is of particular interest, for when an electron collides with an excited atom the classical description, by virtue of the correspondence principle, should be valid with an accuracy that increases with the excitation of the initial state. On the other hand, there are no experimental data on processes of this kind, and the need for information on their cross sections is particularly great.

We assume the model of the hydrogen atom as a classical particle with charge 1 at. un., moving in the Coulomb field of the nucleus. The hydrogen atom is in a bound state if its energy is $E_a < 0$, and in an ionized state if $E_a > 0$. The ground state is defined as the state with $E_a = -0.5$ at. un. Finally, we assume that the random character of the results of the collision is due to the following two independent causes. First, the incident electron has at the instant of its emergence from the electron gun ($t = 0$) random coordinates x and y, which are uniformly distributed in the XY plane. Second, at the same instant of time the atomic electron can be situated at an arbitrary point on the energy surface

$$H_a(\mathbf{p}_a, \mathbf{r}_a) = {}^1/_2 p_a^2 - 1/r_a = E_a, \tag{1}$$

and with this the probability of that point belonging to a certain set S is given, as usual, by the formula

$$P(S) = \int_S |\nabla H_a|^{-1} d\omega \Big/ \int_{H_a = E_a} |\nabla H_a|^{-1} d\omega, \tag{2}$$

i.e., it is proportional to the volume of phase space between the energy surface $H_a = E_a$ and the neighboring surface $H_a = E_a + \Delta E_a$, having the area S as a base. We note that this definition leads to the same momentum distribution as in quantum mechanics [2].

We can now formulate in terms of the classical mechanics the questions involved in the collision between an electron and a hydrogen atom in the ground state, and obtain for them probabilistic answers. Namely, we determine the conditional probability $w(S|x, y)$ of some particular result of the collision as a measure of that set of initial data for the atomic electrons, which lead by virtue of Newton's equations to the same result if the incident electron has at the instant $t = 0$ the coordinates x, y, z ($z \gg 1$) and momenta $p_x = p_y = 0$, $p_z = \sqrt{2E}$. Then the total probability W, which corresponds to the cross section with allowance for the axial symmetry of the problem, is equal to

$$W = 2\pi \int_0^\infty w(S|\rho)\rho d\rho, \qquad \rho^2 = x^2 + y^2.$$

The solution of such problems is best obtained by the Monte Carlo method. This method was used to calculate $w(S|\rho)$ for several values of ρ at fixed E, after which the integral was estimated.

The only nontrivial part of the computational problem is to obtain random points that are uniformly distributed relative to the introduced measure. To this end it is convenient to go over to a parametric form of the energy surface. Let the parameters η, β_1, β_2, γ_1, and γ_2 be connected with x_a, y_a, z_a, p_{ax}, p_{ay}, and p_{yz} by the following relations:

$$\begin{aligned} x_a &= 2|E_a|^{-1}\cos^2\alpha(\eta)\sqrt{\beta_1(1-\beta_1)}\cos 2\pi\gamma_1, \\ y_a &= 2|E_a|^{-1}\cos^2\alpha(\eta)\sqrt{\beta_1(1-\beta_1)}\sin 2\pi\gamma_1, \\ z_a &= 2|E_a|^{-1}\cos^2\alpha(\eta)(1-2\beta_1), \end{aligned}$$

$$\begin{aligned} p_{ax} &= \sqrt{2|E_a|}\,\mathrm{tg}\,\alpha(\eta)\sqrt{\beta_2(1-\beta_2)}\cos 2\pi\gamma_2, \\ p_{ay} &= \sqrt{2|E_a|}\,\mathrm{tg}\,\alpha(\eta)\sqrt{\beta_2(1-\beta_2)}\sin 2\pi\gamma_2, \\ p_{az} &= \sqrt{2|E_a|}\,\mathrm{tg}\,\alpha(\eta)(1-2\beta_2), \end{aligned} \qquad (3)$$

where α is the root of the equation

$$\mu = 2\pi^{-1}(\alpha - {}^1/_4\sin 4\alpha + {}^1/_3\sin^3 2\alpha).$$

Elementary calculations show that when the parameters vary from zero to unity, the points of phase space defined by formulas (3) fill the energy surface (1) and

$$dP = d\eta\, d\beta_1\, d\beta_2\, d\gamma_1\, d\gamma_2.$$

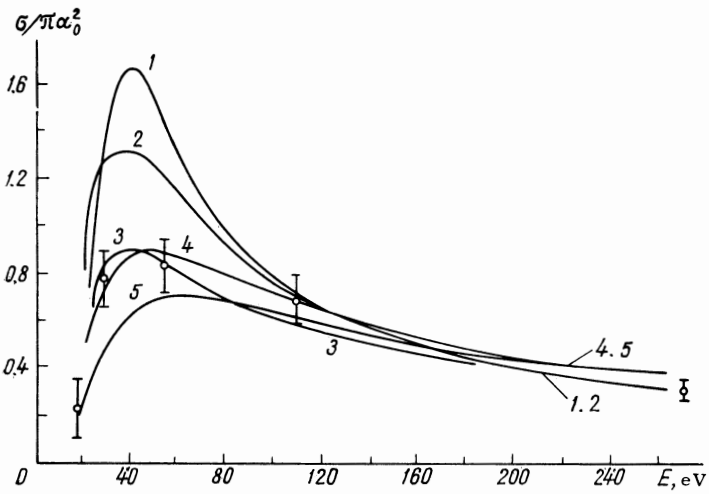
It is seen from the last equation that these points will be distributed on the energy surface with density (2), when each of the parameters is independent of the other and is uniformly distributed in the interval [0, 1].

The calculation was carried out with the BÉSM-2 computer. The parameters η, β_1, β_2, γ_1, and γ_2 were obtained with the aid of a random-number generator. Further, formulas (3) were used to calculate the initial data for the atomic electron. The initial data for the incoming electron were assumed, in the calculation of $w(S|\rho)$ to be $x = \rho$, $y = 0$, $z = 20$, $p_x = p_y = 0$, and $p_z = \sqrt{2E}$; ρ was assigned values between 0 and 3, since it turned out that there is practically no ionization at larger impact parameters.

Newton's equations based on these data were solved by the Runge-Kutta method with automatic choice of the integration steps in accordance with the accuracy of the conservation of the integrals of motion. The trajectories were classified in accord with the agreed-to assumptions. The calculations were made for five values of the energy of the incident electron: 0.6, 1.0, 2.0, 4.0, and 10 atomic units. For each value of E we counted a large number of trajectories (from 1 to 3 thousand). Since for each value of the parameter ρ there were not less than 2—3 dozen trajectories corresponding to ionization and making a noticeable contribution of the ionization cross section, the error in the sought cross section, which from the point of view of our computational scheme is a random quantity, can be estimated with the aid of the Gaussian distribution law.

The result, with the vertical bars showing the estimated statistical errors, are given in the figure. In estimating the error, the probability of the estimate itself was assumed to be 0.99. The same figure shows for comparison the experimental data (curve 5, taken from [3]), the results of the quantum-mechanical calculation [4] (curve 4), and also the results of certain variants of a classical calculation in the two-body approximation. Curve 1 was obtained under the assumption that the atomic electron has a velocity $v = \sqrt{2I}$, where I is the ionization potential [5,6]. Curve 2 shows an analogous calculation with averaging of the cross section over the quantum-mechanical distribution of the momenta of the atomic electron.

It is seen from the figure that near the region



Cross section for the ionization of a hydrogen atom by electron impact: 1—two-body approximation, atomic electron has a velocity $v = \sqrt{2I}$ (I = ionization potential), 2—two-body approximation with averaging over the quantum-mechanical distribution of the momenta of the atomic electron, 3—two-body approximation with allowance for the acceleration of the incoming electron in the field of the nucleus, 4—quantum mechanical calculation [4], 5—experiment of Boyd and Boxenberg (quoted in [3]); circles—results of present work, vertical lines indicate the statistical error, a_0 - Bohr radius of the atom.

of the maximum the results obtained in the three-body approximation of classical mechanics are quite close to the experimental data and agree with the latter much better than the results obtained in the aforementioned variants of the two-body approximation. It is interesting to note, incidentally, that if the incident-electron energy at infinity, E, is replaced in the formulas corresponding to the two-body approximation by $E + \Delta$, where Δ is the additional kinetic energy acquired in the field of the nucleus when penetrating to a depth on the order of the Bohr radius into the atom, then, by choosing Δ equal to 2I, it is possible to obtain a very satisfactory approximation[1)] (curve 3 in the figure). Perhaps not much importance should be attached to this result, since it is difficult to justify just this choice of ρ with sufficient rigor. At the same time, it is appropriate to recall that allowance for the acceleration effect has turned out to be quite useful for the construction of a classical model of exchange scattering.[7] One can therefore think that the correction Δ, when included in simple semi-empirical formulas, is not simply an additional parameter, but somehow corresponds to the essence of the matter.

As indicated at the beginning of the article, the most interesting feature of calculations based on the classical-mechanics scheme is, however, not the maximally accurate approximation of the experimental data for the ground state, but the possibility of renormalizing the obtained cross sections in such a way as to be able to use them to describe ionization from excited states. To this end it is merely necessary to change the scale along the coordinate axes, replacing E by n^2E and σ by $n^{-4}\sigma$, where n is the principal quantum number of the level from which the ionization under consideration proceeds. The possibility of such a renormalization is the consequence of the similarity principle of classical mechanics [8] and was already used in collision-theory problems [1,9]. As was already noted, when $n \to \infty$ the cross sections obtained in this manner go over asymptotically into the exact ones. It is assumed here, of course (formula (2)), that the excitation conditions guarantee equal populations of all sublevels corresponding to the given n. On the other hand, the good result already obtained with the classical calculation in the case of ionization of an unexcited atom indicates apparently that this transition proceeds quite rapidly.

[1)] This possibility was first called to our attention by O. B. Firsov.

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