THRESHOLD BEHAVIOR OF THE CROSS SECTION FOR THE IONIZATION OF ATOMS BY ELECTRONS

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According to the theory of Wannier, the dimensionality of the regions of ionization in the space of the initial conditions reduces to unity at threshold. For a verification of the threshold law it is therefore sufficient to investigate the variation in linear sizes, i.e., to solve problems with a single variable parameter in the initial conditions. Numerical calculations of the classical ionization cross section are carried out for a model of this type. The results obtained confirm the Wannier formula ($\sigma \sim E^{1.127}$). It is found that this formula is also valid for total orbital angular momentum $L > 0$. The present-day experimental data are discussed.

1. INTRODUCTION

THE cross section for the ionization of a neutral atom by electrons near the ionization threshold can be written in the form

$$\sigma \sim E^{\gamma}, \tag{1}$$

where E is the energy of the system "atom + incident electron," $E = E_1 - I$, E_1 is the energy of the incident electron, and I is the ionization potential.

The question of the exact value of γ has attracted considerable attention in recent years. In several experimental works[1-3] a nonlinear behavior with an exponent γ close to, but somewhat larger, than that predicted theoretically by Wannier ($\gamma = 1.127$)[4] has been found. On the other hand, Zapesochniĭ and Aleksakhin[5] concluded on the basis of the experimental data that the threshold behavior is linear ($\gamma = 1$).

In Born approximation one finds $\gamma = 1.5$. In the Coulomb-Born approximation proposed by Geltman,[6] $\gamma = 1$. A linear threshold law was also obtained by Rudge and Seaton[7] and Kang and Foland[8] via a limiting transition under the integral for the ionization amplitude. However, it can be shown[9] that this limiting transition under the integral for the ionization amplitude is not generally permitted, since it leads to an ambiguous result. Recently a method[10] has been proposed for the determination of the threshold behavior of the ionization cross section by extrapolating from the properties of the doubly excited states of the H^- ion. However, so far it has yielded only very uncertain results.

From the theoretical point of view, the paper of Wannier[4] should be regarded as the most rigorous work in this area; Wannier finds $\gamma = 1.127$ by the methods of classical mechanics. Some new results have been obtained by Vinkaln and Gaĭlitis[11] through a development of the work of Wannier. The result of Wannier should be valid in the classical as well as the quantal ionization problems, since the threshold properties of the cross section are determined by the behavior of the wave function at large distances, where classical mechanics is applicable. It can be shown[12] that the more usual (from the point of view of quantum mechanics) formalism of the quasiclassical (WKB) approximation also leads to the result of Wannier.

The cross section for the ionization of the hydrogen atom by electrons has been obtained by several authors[13,14] by numerical methods of classical mechanics, i.e., by determining the trajectory by integrating Newton's equations. On the basis of an analysis of the results of the numerical calculations Burgess and Percival[15] arrived at the conclusion that the threshold behavior of the ionization cross section in classical mechanics follows a linear law. This has been advanced as one of the arguments against the Wannier theory.[10]

The purpose of the present paper is a more detailed numerical investigation of the threshold behavior of the classical ionization cross section.

2. METHOD OF CALCULATION

The initial conditions in the classical ionization problem form a 6-dimensional hyperspace. The effective ionization cross section is proportional to the volume of those regions of the hyperspace in which the initial conditions generate the trajectories of motion corresponding to the emission of two electrons (if the coordinates are chosen such that the distribution function can be regarded as constant, which is always the case for sufficiently small regions). Near the threshold the regions of ionization tend to zero. When the Monte Carlo method is used for the choice of the initial conditions[13,14] the volumes of the small regions are determined with large relative error. An exact determination of the volumes of the regions of ionization in the 6-dimensional space for energies near the threshold of ionization requires excessive demands on computing time. Moreover, it should be taken into account that for small energies of the emitted electrons that interval of each trajectory in which the interaction of the particles is important, i.e., over which the numerical integration must be carried out, is increased.

However, the problem can be considerably simplified. In the Wannier theory the important point is that it was shown that such coordinates $C_1, C_2, \ldots$ can be introduced in phase space for which the volume of phase space corresponding to ionization varies only in a single coordinate for $E \to 0$ and remains constant in all others. This

means that the dimensionality of the region of ionization in the space of the initial conditions reduces to unity for $E \to 0$. Hence the linear dimensions (i.e., the distances between the boundaries of the regions of ionization) near threshold decrease according to the same law which governs the variation of the volume of the region of ionization. An exception to this are those directions along which $C_2 = \text{const}$. But in the general case, for an arbitrary choice of the linear dimensions, the probability for choosing $C_2 = \text{const}$ is infinitely small. Thus the investigation of the regions of ionization may be replaced by a study of the intervals of ionization.

Wannier[4] has considered the ionization with total orbital angular momentum of the electrons L = 0. However, at large distances one can neglect the centrifugal forces compared with the Coulomb forces. Therefore, the threshold law of Wannier should be valid for arbitrary values of L, but the larger the value of L, the smaller will be the energy region in which it is valid.[11] As will be seen, this conclusion is confirmed by the numerical results of the present paper.

In the investigation of the intervals of ionization one must consider cases in which only one of the six parameters of the initial conditions is variable. We have carried out detailed numerical calculations for a model of this type. We assumed that the atomic electron at the initial instant has a velocity of one atomic unit and is located on a circular orbit with a radius of one atomic unit (i.e., on the first Bohr orbit). The incident electron moves in the same plane and has fixed impact parameter ρ and a distance from the nucleus d at t = 0. The mass of the nucleus is regarded as infinite. The only variable parameter of the initial conditions is the angle φ which determines the position of the atomic electron on its circular orbit at t = 0.

By numerical integration of Newton's equations of motion, we found the energy of the incident electron ϵ for $t \to \infty$. The calculations were carried out on an electronic computer by the Runge-Kutta-Merson method. As a criterion for the accuracy of the calculation one may regard the conservation of the integrals of motion (the energy of the system and the total angular momentum). These quantities differed by no more than 10^{-5} atomic units when evaluated at the beginning and the end of the trajectory. The initial distance and the corresponding final distances were chosen such that the interaction energy of the interaction between the electron and the atom or between all particles (in the case of ionization) was less than 1 to 3% of the total energy of the system E.

3. RESULTS AND DISCUSSION

For the main calculation we considered two cases. In the first case we set $\rho = 0$, which corresponds to L = 1. In the second case we chose ρ such that the total angular momentum of the system was L = 0. In Fig. 1 we show a typical dependence of ϵ on φ for L = 1 and two values of E. One of these energies is comparatively large, the other is close to the threshold. It is seen that the form of the curve shows almost no change with varying E.

The intervals of the angle φ in which $\epsilon > E$ correspond to a direct excitation of the atom; the intervals

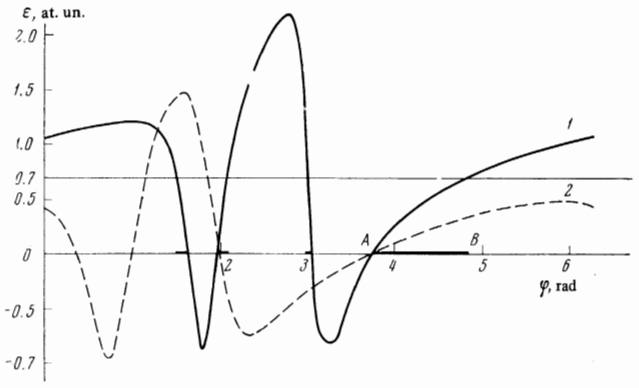

FIG. 1. Dependence of the final energy of the incident electron on the initial polar angle of the atomic electron at the energies E = 0.7 at. units (curve 1) and E = 0.05 at. units (curve 2) for L = 1. The intervals of ionization for E = 0.7 at. units are indicated by heavy lines.

where $\epsilon < 0$ correspond to exchange excitation, and the intervals where $0 \le \epsilon \le E$, to the emission of two electrons, i.e., to ionization. The four intervals of ionization are indicated by heavy lines in Fig. 1. We have investigated one of these (AB). The points A and B were determined with the help of the method of chords. The length of the interval of ionization $S_\varphi = A - B$ was determined with an error of 10^{-5} radians. The case L = 0 was investigated in a similar manner. The form of the curve $\epsilon(\varphi)$ for L = 0 differs little from that for the case L = 1.

The dependence of the intervals of ionization on the energy E for L = 0 and L = 1 is shown in Fig. 2. For greater clarity we have drawn the ratio S_φ/E. In the case of a linear threshold law $S_\varphi/E = \text{const}$. For a comparison we show the curves corresponding to the threshold law of Wannier ($S_\varphi = \text{const} \cdot E^{1.127}$). It is seen that for small energies the numerical points fall nicely on the Wannier curves. For L = 0 the Wannier formula is valid in the region $E < 0.08$ atomic units (2 eV), and for L = 1 it is valid in the region $E < 0.05$ atomic units (1.4 eV).

The interval of ionization can be written in the form

$$S_\varphi = \int_A^B d\varphi = \int_0^E \frac{d\varphi}{d\varepsilon}\, d\varepsilon. \qquad (2)$$

The derivative $d\varphi/d\epsilon$ has the meaning of a differential

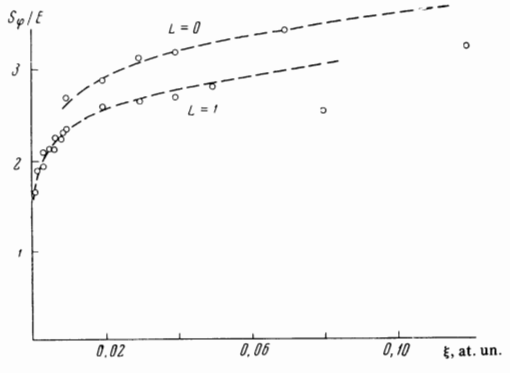

FIG. 2. Dependence of the intervals of ionization on energy for L = 0 and L = 1. Dashed curves: curves of the type const. $E^{0.127}$.

cross section for the ionization. If the curve of $\epsilon(\varphi)$ is smooth, as confirmed by our calculations (cf. Figs. 1 and 3), one can regard it as a straight line in a sufficiently small interval of ionization, i.e., regard the derivative $d\varphi/d\epsilon$ as independent of ϵ.[1)] Then

$$S_\varphi \approx E d\varphi / d\varepsilon. \tag{3}$$

We note that according to (3), the curves shown in Fig. 2 represent the differential cross section for ionization. Evidently, the linear threshold law would hold if the form of the curve $\epsilon(\varphi)$ were exactly conserved as E changes, i.e., if the derivative $d\varphi/d\epsilon$ were also independent of E as $E \to 0$. The presence of a small nonlinearity implies that $d\varphi/d\epsilon$ must decrease with decreasing E. The Wannier formula holds when

$$d\varphi / d\varepsilon \approx \text{const} \cdot E^{0.127} \tag{4}$$

Therefore, in the Wannier theory, the differential cross section for ionization is independent of ϵ near threshold but depends on E. On the other hand (cf. Fig. 3), $d\varphi/d\epsilon = \cot\alpha$. Therefore

$$\lim_{E\to 0} \alpha = \pi/2. \tag{5}$$

The curve $\epsilon(\varphi)$ must intersect the $\epsilon = 0$ axis at right angles at E = 0, i.e., must go through a bend, which should also be observable at energies E close to zero, as is indeed the case (cf. Fig. 3). The bend continues to show up also into neighboring regions corresponding to the excitation of highly-excited discrete states. Here we have for the cross section for the excitation of the n-th level

$$\sigma_n \sim \text{const} \cdot n^{-3} |E|^{0.127}. \tag{6}$$

When comparing the Wannier theory with the experimental data, several points must be considered. Fairly close to the threshold the ionization cross section is practically a straight line as a function of the energy. The Wannier formula also differs from a straight line law only at very small energies. Thus the region of nonlinearity, in which the special features of the Wannier theory show up appreciably, may be smaller than the region of applicability of the Wannier formula. For example, in the case of the ionization of helium atoms[2] the Wannier formula is in satisfactory agreement with the experimental data up to energies of 10 eV above threshold, but the region of nonlinearity extends only over a few eV.

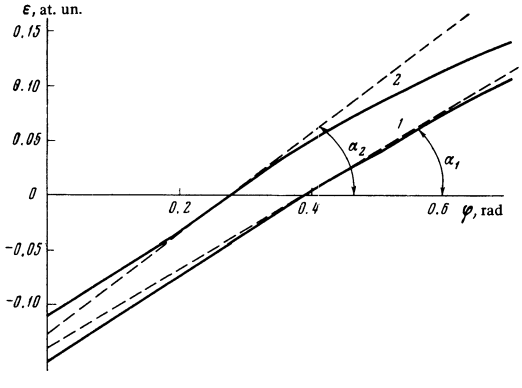

FIG. 3. Dependence of ϵ on φ in the neighborhood of the interval of ionization for L = 1 and E = 0.05 at. units (curve 1) and E = 0.005 at. units (curve 2); dashed curves: tangents to the curves at $\epsilon = 0$.

By the similarity principle we may conclude that for atoms with a smaller ionization potential the region of nonlinearity must be smaller. The nonlinearity is caused by the behavior of the wave function at large distances, where classical mechanics is applicable. At the boundary of the reaction zone and the region of classical motion the wave function (in the quantum case) or the distribution function (in the classical case) can be regarded as approximately constant. One may therefore expect that the regions of nonlinearity are approximately equal in the classical and quantum theories. For the classical ionization cross section the similarity principle holds;[15] this follows from the fact that the Coulomb interaction is a homogeneous function of the coordinates. According to this principle, the trajectories of motion remain similar when the energies of both electrons are changed in the same way. If $\sigma(w_1, E_1)$ is the classical cross section of ionization from an initial state of the atom with energy w_1, then the ionization from another initial state with energy w_2 (for the same energy E_1 of the incident electron) is given by the formula

$$\sigma(w_2, E_1) = a^2 \sigma(w_1, aE_1), \tag{7}$$

where $a = w_1/w_2$.

For excitations from higher levels the cross section is shifted towards smaller energies of the incident electron. Hence the region of nonlinearity shrinks. This is true when one considers ionization from different levels of the same atom but it will also hold approximately for different atoms.

This conclusion is confirmed by the experimental data. In the case of the ionization of hydrogen the region of nonlinearity is appreciably smaller (about 0.5 eV) than in the case of helium.[1,2] For the ionization of alkali metals, which has been considered by Zapesochnyĭ and Aleksakhin,[5] the region of nonlinearity must be even smaller. This may explain why these authors have not observed a nonlinear threshold behavior of the ionization cross section. The even stronger nonlinearity than predicted by Wannier, as found by Brian and Thomas,[2] can be explained partially by the circumstance that these authors have used the Wannier formula for a too wide region of energies (up to 10 eV above threshold). Moreover, as also noticed by other authors,[3] it is desirable to improve their data in the threshold region (up to 10 eV above threshold). Thus the present-day experimental data do not exclude the validity of the Wannier threshold law, but for a definite solution of this problem further experimental work is needed.

In conclusion we note the falseness of one particular argument which has recently been advanced against the Wannier theory. According to the similarity principle, the trajectories corresponding to the ionization from a given level do not go over into each other when only the energy of the incident electron is altered (the usual formulation of the problem in scattering theory). On the basis of this, Temkin et al.[10] arrived at the conclusion

[1)] This result has been obtained earlier with the help of the Wannier theory.[11]

that the use of the similarity principle in the Wannier theory is not allowed and hence the results of this theory are not justified. However, Wannier used the principle of similarity for the determination of the behavior of the entire manifold of trajectories of ionization (for all initial conditions). The trajectories of ionization from a fixed level are part of this manifold, which indeed does not change according to the similarity principle; i.e., the trajectory is shifted within the entire manifold. But at the same time, as part of the manifold, it tends to zero according to the same law.

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