Classical approximation for the ionization of a negative ion by electron impact near the threshold

E. A. Solov'ev

Leningrad State University
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A classical model of the ionization of a negative ion by electron impact is considered. The interaction between the weakly-bound electron of the negative ion and the neutral core of the ion is simulated by a short-range potential. An analytic solution is obtained for incident-electron velocities lower than the velocity of the weakly-bound electron in the short-range potential. The results are compared with experimental data and with the theoretical predictions reported by other authors for the case of ionization of H^- by electron impact. The model is valid for this reaction at incident-electron energies of 4–20 eV.

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1. The ionization of a negative ion by electron impact has been investigated in a number of experimental and theoretical papers (see, for example, Smirnov and Chibisov,[1] Walton *et al.*,[2] and Narain and Jain[3]). Interest in this reaction is due to the fact that it has a large cross section and plays an important role in the understanding of the processes occurring in stellar atmospheres. Satisfactory agreement between theoretical and experimental results has now been obtained, but this agreement is achieved at the expense of relatively complicated computer calculations. No simple analytic expressions are available for the ionization cross section.

Another approach to this problem involves the study of exactly soluble models. The natural quantum-mechanical model of this reaction is the three-particle model (incident electron, outer electron of negative ion, neutral core of negative ion) in which the interaction between the electrons and the neutral core is taken into account in the approximation of the zero-range potential (Veselova[4] and Demkov and Ostrovskiĭ[5]). This model involves both Coulomb and short-range two-particle potentials. Three-particle models are currently used most extensively in relation to the case where all the two-particle potentials are of the short range type. (Baz' and Merkur'ev[6]). The presence of Coulomb two-particle potentials gives rise to a considerable complication, and the Faddeev equations must be modified. This modification has been effected by several workers (Veselova[4] and Merkur'ev[7]), but the behavior of the ionization cross section near the threshold has not as yet been investigated for the above model.

The classical approach to problems in collision theory has been widely used and leads to adequate results. The classical approximation has been developed for the region of the ionization threshold by Wannier[8] (see also Peterkop[9]) in relation to the ionization of atoms and positive ions by charged particles. The essential point of the method used by Wannier[8] is that all the two-particle potentials are Coulomb potentials. The case in which we are interested here has two features: firstly, the interaction between the electrons and the neutral core is of the short-range type (this means that the Wannier method[8] cannot be used) and, secondly, the exact form of this interaction is not known. Short-range potentials are usually simulated in quantum mechanics by the zero-range potential[5] but, in the classical formulation of the problem, the zero-range potential loses its meaning. This is immediately clear from the fact that, in the zero-range potential, the electron is confined to the classically forbidden region (if we are concerned with a bound state).

2. In this paper, we consider the classical model of the ionization of a negative ion by electron impact near the threshold. We shall base our discussion on the same representation of the interaction between the electron and the neutral core as in the method of zero-range potential,[5] i.e., we shall take the potential well to be spherical, narrow, and deep, and will suppose that the energy of the bound state in the well is small. Moreover, we shall confine our attention to the s-state of the bound electron. The classical orbit of an electron in this state is a segment of a straight line passing through the center of the potential well. The electron is reflected by the walls of the potential well and oscillates between them. We shall see later that the frequency of these oscillations is high. Since the binding energy ε is small, the energy E of the incident electron near the threshold is also small. This means that we can isolate slowly-varying and rapidly-varying subsystems (incident electron and bound electron, respectively). In addition to the frequency ω, there is another large parameter near the threshold, namely, the distance of closest approach R_0 between the electrons. The latter parameter is large because, at low energies, the Coulomb repulsion prevents the electrons from approaching each other too closely. In the approximation in which these two parameters can be regarded as being, respectively, small and large, the problem can be solved analytically in a closed form.

3. In the classical formulation, the problem can be split into two parts: (a) solution of the equations of motion and (b) statistical analysis of the results obtained.

Let us begin by considering the motion of an incident electron in the field of an oscillating bound electron (since R_0 is large, there is not interaction between the incident electron and the neutral core). The mass of

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the neutral core is much greater than the mass of the bound and incident electrons, and we shall therefore consider that the center of inertia and the origin of coordinates lie at the center of the potential well. The equation of motion of the incident electron ($m = e = 1$) is:

$$\ddot{\mathbf{r}}_1 = \frac{\mathbf{r}_{12}}{r_{12}^3}, \tag{1}$$

where $\mathbf{r}_1$ is the position vector of the incident particle, $\mathbf{r}_2$ is the position vector of the bound electron, and $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$. Since $r_2 \leq d$ (d is the width of the potential well) and $r_{12} \geq R_0$, we can expand the right-hand side of (1) over the sequence of multipoles. For our purposes, it is sufficient to consider the dipole approximation

$$\ddot{\mathbf{r}}_1 = \frac{\mathbf{r}_1}{r_1^3} - \frac{\mathbf{r}_2}{r_1^3} + \frac{3(\mathbf{r}_1 \cdot \mathbf{r}_2)\mathbf{r}_1}{r_1^5} \tag{2}$$

The first term on the right-hand side of (2) describes the interaction with the constant Coulomb field, and the second and third represent the rapidly oscillating force. Kapitsa[10] (see also Landau and Lifshitz,[11] §30) has developed an approximate method for this situation. Following Kapitsa,[10] we write $\mathbf{r}_1$ in the form $\mathbf{R}+\eta$, where $\mathbf{R}$ is a smoothly-varying function and η is the rapidly oscillating part of the position vector of the incident electron, where the mean value of η over a period $2\pi/\omega$ is zero. The pseudopotential method leads to the following expressions for $\mathbf{R}$ and η:

$$\frac{1}{2}\dot{R}^2 + \frac{L^2}{2R^2} + \frac{1}{R} = E, \tag{3}$$

$$\eta = \frac{1}{\omega^2}\left(\frac{\mathbf{r}^2}{R^3} - 3\frac{(\mathbf{r}_2 \cdot \mathbf{R})\mathbf{R}}{R^5}\right), \tag{4}$$

where $L = (2E)^{1/2}\rho$ is the angular momentum and ρ is the impact parameter. It follows that the slowly-varying component of $\mathbf{R}$ behaves as if the incident electron were in the field of a unit Coulomb charge placed at the origin. The oscillating component is small and satisfies the following inequality:

$$\eta < \frac{4d}{\omega^2 R_0^3}. \tag{5}$$

The condition for ionization is that the bound electron leaves the potential well. The interaction with the incident electron is such that the bound electron is slowed down as it moves toward it, but if it moves in the opposite direction, it is accelerated. Ionization will therefore occur in such a way that the bound electron will leave the potential well on the side opposite to that facing the incident electron and, having once left the potential well, it will not reenter it.

Ionization occurs when the work done by the incident electron becomes equal to the binding energy, i.e.,

$$A = \int \frac{\mathbf{r}_{12} \cdot d\mathbf{r}_2}{r_{12}^3} = \varepsilon. \tag{6}$$

It is easily verified with the aid of (3) and (4) that the work done by the incident electron is an oscillating function whose mean is zero, and the amplitude of the oscillations increases in the course of the collision. Consequently, the energy necessary for ionization is not accumulated gradually in the collision process, but is transferred in a quarter of the period while the bound electron moves from the center of the potential well in the direction opposite to that of the incident electrons, and the amplitude of the oscillations in work done becomes equal to the binding energy:

$$\frac{d\cos\vartheta}{R^2} = \varepsilon. \tag{7}$$

where ϑ is the angle between $R(t)$ and the straight path of the bound electron.

4. Condition (7) is the ionization condition for given trajectories of the bound and incident electrons. To calculate the ionization cross section, the trajectories of the bound electron corresponding to the bound state of the negative ion must be subjected to statistical analysis. The trajectory of the bound electron is a segment of a straight line passing through the origin, and can be specified by a point on the surface of a unit sphere with center at the origin. The bound s-state corresponds to an ensemble of such trajectories (points on the sphere) and, since the bound state is spherically symmetric, the density of points on the sphere is uniform, i.e., all the directions of the trajectories are of equal probability.

The ionization probability $W(\rho)$ for a given incident-electron trajectory is the ratio of the area S on the sphere corresponding to the bound-electron trajectories for which (7) is satisfied to the area of the complete sphere. For the sake of simplicity, we let R in (7) be equal to the distance of closest approach:

$$R_0 = \frac{1}{2E}[1 + (1 + 4E^2\rho^2)^{1/2}]. \tag{8}$$

This approximation will result in a slight underestimate of the ionization probability since (7) may be satisfied for certain trajectories only for $R > R_0$ because $\cos\vartheta(R) > \cos\vartheta(R_0)$. However, the correction for such trajectories is small, especially near the threshold. If we accept this approximation, the area S on the sphere bounded by a circle of angular size ϑ_0 can be obtained from the formula

$$\cos\vartheta_0 = \frac{\varepsilon}{4dE^2}[1 + (1 + 4E^2\rho^2)^{1/2}]^2, \tag{9}$$

which follows from (7) and (8).

Since the ionization condition is satisfied simultaneously for diametrically opposite points on the sphere, the ionization probability is given by

$$W(\rho) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \int_0^{\vartheta_0} \sin\vartheta\, d\vartheta = 1 - \cos\vartheta_0. \tag{10}$$

The total ionization cross section is

$$\sigma = 2\pi \int_0^{\rho_m} W(\rho)\rho\, d\rho = \frac{\pi}{2E^4E_p^2}\left(E^4 - \frac{4}{3}E^3E_p + \frac{1}{3}E_p^4\right), \tag{11}$$

where $E_p = (\varepsilon/d)^{1/2}$ and the upper limit of the integral can be obtained from the condition

$$\frac{d}{R_0^2(\rho_m)} = \varepsilon.$$

There is no ionization for impact parameters $\rho > \rho_m$.

Equation (11) can be rewritten in the form

$$\sigma = \frac{\pi}{2E^4E_p^2}(E-E_p)^2\left(E^2+\frac{2}{3}EE_p+\frac{1}{3}E_p^2\right). \quad (12)$$

Hence, it is clear that E_p is the threshold energy for the ionization reaction. This is easily verified directly from (7). At the threshold, condition (7) is satisfied only for $\rho = 0$, $\vartheta = 0$, and, consequently, the distance to which the electrons must approach for ionization to occur is

$$R_p = \left(\frac{d}{\varepsilon}\right)^{1/2}. \quad (13)$$

The minimum energy of the incident electron for which this will occur is

$$E_p = \frac{1}{R_p} = \left(\frac{\varepsilon}{d}\right)^{1/2},$$

and is equal to the energy necessary to overcome the Coulomb repulsion. It differs from the exact value of the threshold energy ε. For $\varepsilon < E < E_p$, the ionization mechanism is purely quantum-mechanical and is connected with tunneling by the bound electron. Since the Coulomb barrier is very broad at low energies, the ionization cross section in this interval is small and varies as $\exp[-2^{3/2}\pi/(E-\varepsilon)^{1/2}]$.[1]

5. At high incident-electron energies, the model that we have investigated is no longer valid because the incident electron can no longer be regarded as a slow subsystem. Formal continuation into the high-energy region takes the cross section given by (11) toward a constant value, and this can be used to estimate the maximum value of the ionization cross section:

$$\sigma_{max} \approx \frac{\pi}{2E_p^2}. \quad (14)$$

The condition for the validity of the pseudopotential method is that the velocity of the incident electron must be small in comparison with the velocity of the bound electron. This leads to the following inequality (we use the atomic system of units in the derivation of the validity conditions):

$$E < \frac{\pi^2}{d^2}. \quad (15)$$

Moreover, expansion over the multipoles in (1) is valid provided $R_p > d$ or, if we use (13),

$$(\varepsilon d)^{1/2} < 1. \quad (16)$$

It was assumed in the derivation of the ionization condition (7) that the trajectory of the bound electron is a segment of a straight line but, in fact, the interaction with the incident electron for $\vartheta \neq 0$ leads to a curvature of the bound-electron trajectory. The maximum deviation Δ of the trajectory from the undisturbed position is $\Delta < d^3\varepsilon\pi^{-2}$. The corresponding result for the angle $\delta = \Delta/d$ is $\delta < d^2\varepsilon\pi^{-2}$. The trajectory of the bound electron may be looked upon as rectilinear if $\delta \ll 1$, and this leads to one further condition for the validity of the above model, namely,

$$\frac{d^2\varepsilon}{\pi^2} \ll 1. \quad (17)$$

Classical description of the incident electron is valid provided $[v = (2E)^{1/2}]$:

$$l \equiv \rho_m v \approx (2Ed/\varepsilon)^{1/2} > 1. \quad (18)$$

The inequalities given by (15)–(18) are the most important restrictions in this model. On the other hand, we have the question of the validity of the model itself, i.e., the extent to which the classical description can be used for a weakly bound electron. It is commonly accepted that the outer electron of a negative ion is confined to a region which is classically forbiddent (see, for example, Demkov[5]). However, this not always the case. For example, the use of the Hulthén orbitals for H^- leads to the following result: the probability of finding the electron in the classically allowed and classically forbidden regions is 0.6 and 0.4, respectively (if the parameters of the Hulthén potential are chosen on the basis of correct behavior at the origin). If the parameters of the potential are determined from the scattering length, the probability of finding the electron in the classically allowed and classically forbidden regions is 0.7 and 0.3, respectively. We thus have the reverse situation in the case of H^-. However, even if the weakly bound electron is confined largely to the classically forbidden region, it does not follow that the above result is invalid. In this paper, we have, in fact, considered the classically allowed electron-detachment mechanism. If the motion of the electron in the classically forbidden region is to be included, this means that, insofar as the detachment process is concerned, we must also introduce subbarrier tunneling. Since the barrier is relatively thick and the collision time relatively long even in the threshold region (the incident particle is light), it is difficult to see how the tunnel effect can produce a substantial increase in the detachment cross section.

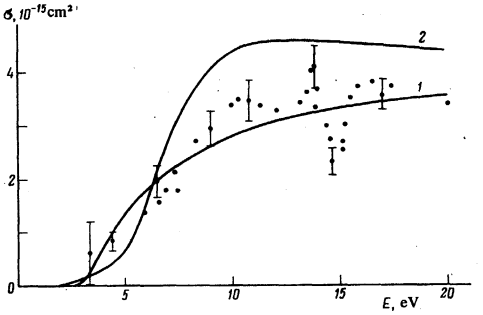

FIG. 1. Detachment cross section of H^- under electron impact: 1–ionization cross section calculated from (11), 2–results taken from the paper by Narain and Jain.[3] Points represent experimental data taken from Walton *et al.*[2] The experimental uncertainty is indicated for some of the points.

6. Figure 1 shows the total cross section for the breakup of the negative ion of hydrogen, calculated from (11), together with the experimental and theoretical results obtained by other authors. The parameters for H^- were taken from the book by Demkov and Ostrovskiĭ[5] (§1.4). They were: $d = 2.7$ a.u., $\varkappa = 0.231$ a.u. ($\varepsilon = \varkappa^2/2$). The classical model is valid, in this case, for incident electron energies of 4.20 eV.

It is important to note that no adjustable parameters are used when the cross section is calculated from (11), whereas the data reported by Narain and Jain,[3] which are at present in better agreement with experimental results than any other calculations, were obtained as a result of a very complicated semiempirical calculation. Nevertheless, near the threshold, our simple model of ionization provides good agreement with experiment. Unfortunately, there are no experimental data for other negative ions near the ionization threshold, so that it is difficult to establish the validity of this conclusion.

The reason why the simple classical calculation gives roughly the same result as the relatively sophisticated quantum-mechanical analysis is probably that, as noted by Smirnov,[1] Narain and Jain,[3] and others, the ionization cross section near the threshold depends critically on the choice of the trajectory of the incident electron. In the quantum-mechanical calculation, it is difficult to take the Coulomb interaction rigorously into account, whereas, in the classical approach, this can be done simply and naturally.

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Excitation of autoionization states by electrons near the threshold

V. N. Ostrovskiĭ

Leningrad State University
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The theory of the interaction of a slow quantum particle with a system having an autoionization state is considered. The theory is used to describe a recently observed phenomenon [P. J. Hicks *et al.*, Vacuum **24**, 573 (1974)], namely "interaction after the collision" in the excitation of an autoionization state of an atom by an electron. The roles of various quantum effects in the formation of the resonant structure and in the spectra of the electrons and in the excitation functions of the Rydberg states of the atom are investigated. The possibility of further refining the theory is discussed.

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1. INTRODUCTION

Hicks *et al.* have observed in 1974[1] a new phenomenon, which occurs when electrons with energy E_i somewhat higher than the energy E_a of excitation of the autoionization states (AS) of an atom are scattered by the atom. An AS manifests itself as a resonant contour in the energy distribution (spectrum) of the electrons knocked out of the atom. It has turned out that the contour shifts towards higher energies with decreasing E_i. Therefore the AS begins to be excited effectively not at $E_i = E_a$, but at a higher incident-electron energy. This new effect was therefore called the "shift of the threshold" in the excitation of AS. Of course, the position of the threshold can be determined only accurate to the level width Γ, but the observed threshold shifts greatly exceed this value.

In the cited paper, this phenomenon was attributed to energy exchange that occurs between the slow scattered electron which has excited the AS and the atomic electron when the two particles move apart. If the lifetime[1)]

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