ATOMIC IONIZATION AS A SUDDEN PERTURBATION OF AN ELECTRON BY THE CHARGE OF A PROJECTILE

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It is proposed to consider the atomic ionization as a sudden perturbation of an atomic electron at the passage of a charged particle near the atom ("shake-off" approximation). The ionization process is presented as a quantum-mechanical transition of the electron from the bound atomic state to the continuum due to the perturbation acting during a very short time interval. It is described with the help of the corresponding formulas of quantum mechanics (shake-off effect formulas). A formula for the determination of the electron energy distribution in the continuum of the final state is obtained. The integral electron spectrum depending on the energy of the charged particle is calculated. It is noted that the formula used for the determination of the transition probability W for an immobile charge must be supplemented with the dependence on the velocity of the charged particle $W \sim \nu^{-1}$.

1. Introduction

A charged particle moving through a substance looses energy for the deceleration and the ionization of atoms. The theory of inelastic collisions was developed by Bohr and Bethe. In particular, mean bremsstrahlung losses of charged particles per unit path length are till now determined using the formulas given in [1]. After that, the theory was developed in [2], and these processes are referred now to the kinetic electron emission (KEE) under the assumption that electrons are excited inside a solid body due to the direct transfer of kinetic energy from an exciting particle [3,4,5]. In this case, the main attention is paid to the energy losses of a charged particle under its flight near the atom rather than to the process of transition of bound electrons beyond the atomic limits.

However, considering a transition of bound atomic electrons to the continuous spectral range under the action of a charge suddenly arising in the neighborhood of the atom, it is also necessary to take the "shake-off" effect into account. The phenomenon of atomic ionization under the β-decay was first studied theoretically by Feinberg [6] and Migdal [7]. It consists in that the spontaneous change of the nucleus charge under the action of a sudden perturbation can result in a transition of a bound atomic electron to the continuous spectrum, i.e., the atomic ionization. This phenomenon is known in the literature as the "shake-off". However, the shake-off of electron shells takes place not only under nuclear transformations but also under transitions in atomic electron shells. Without taking the shake-off effect into account, it is impossible to give a complete description of final states of a system and processes resulting in the excitation of electron shells [8]. These problems were studied in numerous theoretical and experimental works including reviews [9, 10].

One can consider two stages of the shake-off phenomenon. On the first stage, the sudden perturbation of the system takes place in the case where the duration of this stage τ is much less than the period of low-frequency motion $2\pi\omega_{fi}^{-1}$ of the second stage following the first one. On the second stage of the process, the system passes from state i to state f, which is accompanied by the ejection of an electron. Though this second stage is impossible in the absence of the first one, its amplitude does not depend on the physical nature of the first stage.

In this work, we consider the atomic ionization under the action of a sudden perturbation of an atomic electron by a charged particle moving near the atom, calculate the energy spectrum of ionization electrons, and analyze the peculiarities of this phenomenon. Our case differs from the generally accepted conception of the shake-off at the point that the perturbation source moves rather than rests. But in [9] and the subsequent studies, such a perturbation of a system is already considered as the "shock-off" phenomenon. Taking the suddenness of a perturbation into account, we neglect, at first, the influence of the particle's motion at the time moment of interaction and consider the immobile charge.

2. Description of the Electron Transition Probability from the Bound State to the Continuum at Shaking-Off

Moving past an atomic electron, the particle with charge Z_pe produces a perturbation $V = \frac{Z_p e^2}{r}$ at the time moment of the closest approach to the atom at a distance r.

If the velocity of the particle ν_p is large, the perturbation acts during a short time interval τ, when the particle passes the distance $\triangle L \sim r$. This perturbation appears sudden for an atomic electron, which results in its transition to the continuous spectral range with kinetic energy E. This quantum-mechanical process can be described with the help of the theoretical conceptions stated in [11]. In our case of a sudden perturbation, the transition probability of the electron from a bound state to the continuous spectrum can be written in the form

$$dW = \frac{|\int \psi_f^* \frac{Z_p e^2}{r} \psi_i^{(0)} dq\,|^2}{(E+E_{\rm B})^2} d\nu = W_{fi} d\nu, \tag{1}$$

where dW is the transition probability of the bound atomic electron from state i to state f in the energy range between E and $E{+}dE$, W_{fi} is the transition probability from state i to one of the states f of the continuous spectrum, $d\nu$ is the number of electron states in the energy range between E and $E{+}dE$, E_B is the electron binding energy that is assumed to be positive in all formulas, $\psi_i^{(0)}$ is the coordinate part of the wave function in the initial state of the system, $\psi_f^*(q)$ is the coordinate part of the wave function in its final state after the formation of a vacancy at one of the atomic subshells (after ionization), and q are the coordinates of the wave function.

The perturbation $\frac{Z_p e^2}{r}$ arises suddenly, i.e. during the time interval τ that is small as compared to the period $2\pi\omega_{fi}^{-1}$ of the transition from state i to state f, so that the wave function $\psi_i^{(0)}$ of the initial state of the system "has no time" to change and remains the same as it was before the perturbation. The formula is valid only at the time moment of the sudden switch-on of a perturbation. A contribution to the transition probability will be made only during the time moment of switching-on this interaction, i.e. at the time moment of the closest approach of the particle to the electron. Since the perturbation changes slowly (adiabatically) before and after the approach, it will not contribute to the transition probability W [12].

The transition probability W_{fi} can be also determined from the overlap integral of the wave functions

$$W_{fi} = \left| \int \psi_f^* \psi_i^{(0)} dq \right|^2. \tag{2}$$

The both wave functions are related to the Hamiltonians $\hat{H}_0$ and $\hat{H}$, respectively, and are stationary. That is, they have the form $\Psi = \psi(q) e^{\frac{-iEt}{\hbar}}$, where $\psi(q)$ is the wave function depending only on the coordinates. Therefore, the transition probability W_{fi} does not depend on the energy. During the time of transition, the wave function of the system "has no time" to change and remains the same as it was before the perturbation. Still it will not any more be the characteristic function of the new Hamiltonian of the system $\hat{H}$, that is the state $\psi_i^{(0)}$ will not be stationary [11]. Comparing formulas (1) and (2), we conclude that the equality always holds true under the condition

$$\frac{Z_p e^2}{r} = E + E_{\rm B}. \tag{3}$$

In other words, this condition means that the potential energy acquired by the atomic electron from the charge Z_pe, which has suddenly appeared at the distance r from the former, overcomes the binding energy and is completely converted to the kinetic energy of the free electron. This process is similar to the photoelectric effect, where an electron, having suddenly absorbed a photon and overcoming the binding energy, appears in the continuous spectral range [9]. Another consequence of the sudden-perturbation approximation is the independence of the probability of the transition $i \to f$ on the imparted energy, as it follows from formula (2) or from formula (1) with regard for (3). Moving at different distances from the electron, the charged particle provides equal probabilities of the transition W_{fi} regardless of the imparted energy.

Considering the phase volume for the electrons able to pass to vacuum, the level density of the final state is expressed by the following formula:

$$\frac{d\nu}{dE} = a\sqrt{E}, \quad a = \frac{\sqrt{2} m^{3/2} V}{\pi^2 \hbar^3}. \tag{4}$$

Here, m is the electron mass, and V is the volume occupied by one electron in the final state. With regard for formula (1), the energy distribution of electrons after their transition to vacuum is described as follows:

$$\frac{dN}{dE} = \frac{a\sqrt{E}}{(E+E_{\rm B})^2}. \qquad (5)$$

3. Differential and Integral Probabilities of Transition of Ionization Electrons to Continuum

Figure 1 presents the dependence of the energy distribution of electrons ejected from the atom $\frac{1}{a}\frac{dN}{dE}$ at the binding energy $E_{\rm B} = 70$ eV. This binding energy approximately corresponds to the observed Auger structures: 63 eV MVV Cu, 63.2 eV LMM Al, 69.8 keV, N_7VV Au, and others [3]. In [13], we also obtained an estimate of the binding energy ~ 70 eV. That is why we assume that the binding energy of the ionization electron amounts to 70 eV. Starting from zero, the intensity of the electron distribution rapidly grows with increase in the energy and reaches a maximum $\frac{1}{a}\frac{dN}{dE} = 0.325\,(E_{\rm B})^{-3/2} = 5.5\times10^{-4}$ at $E = \frac{E_{\rm B}}{3}$. After that, the intensity diminishes, so that it decreases twice at $E \simeq 2E_{\rm B}$ and, at $E \to \infty$, $\frac{dN}{dE} \to 0$. The comparison of an experimental electron energy distribution with formula (5) could serve as an evidence of the applicability of the sudden-perturbation approximation when considering the atomic ionization phenomenon. Unfortunately, no information on such experiments is available except for the emission of e_0-electrons that obey this distribution [13].

The substitution of (5) into (1) provides the probability of the electron transition from the bound state to vacuum with the kinetic energy $E = \frac{Z_pe^2}{r} - E_B$ or, which is the same, in the case where the particle moves past the electron at the distance r:

$$dW = \left(\frac{Z_pe^2}{r}\right)^2 \left|\int \psi_f^*\psi_i^{(0)}dq\right|^2 \frac{a\sqrt{E}}{(E+E_{\rm B})^2}dE. \qquad (6)$$

After that, we perform the integration over all possible states of the electron in the continuous spectral range from the energy $E = 0 = \frac{Ze^2}{r_{\max}} - E_{\rm B}$ to $E = E_{\max} = \frac{Ze^2}{r_{\min}} - E_{\rm B}$. In this case, the closest approach distance changes from $r_{\max} = \frac{Z_pe^2}{E_{\rm B}}$ to $r_{\min} = \frac{Z_pe^2}{E_{\max}}$. In addition, it is assumed that, moving past the atom, the charged particle appears in the region of this approach with the probability $W = 1$. We have

$$W_1 = \left(\frac{Z_pe^2}{r_{\min}}\right)^2 \left|\int \psi_f^*\psi_i^{(0)}dq\right|^2 aF(E_{\max}), \qquad (7)$$

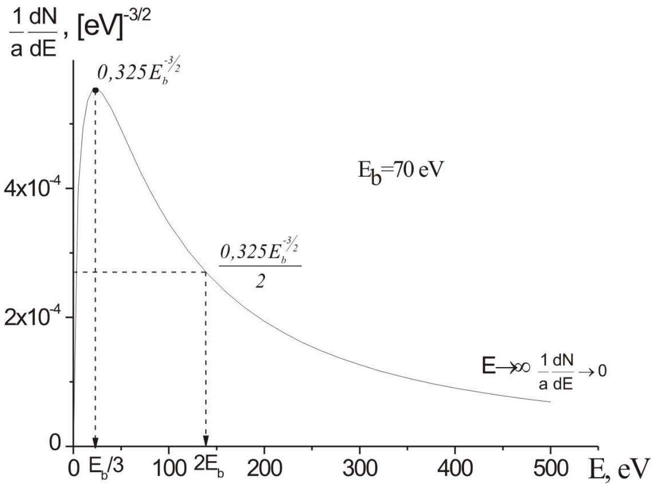

Fig. 1. Dependence of the energy distribution of ejected electrons at the binding energy $E_{\rm B} = 70$ eV

where

$$F(E) = \frac{1}{\sqrt{E_{\rm B}}}\arctan\sqrt{\frac{E}{E_{\rm B}}} - \frac{\sqrt{E}}{E+E_{\rm B}}, \quad F(0) = 0. \qquad (8)$$

Let the charged particle move past an atomic electron with the probability $W = 1$ equiprobably appearing at different points of the circle, whose center coincides with the electron, and the radius is equal to the atomic radius r_a. The probability for the charged particle to appear in the region between $r_{\max}$ and $r_{\min}$ from the circle center is determined as $W_r = \frac{r_{\max}^2 - r_{\min}^2}{r_a^2}$. With regard for the relation $F(0) = 0$ at $r = r_{\max}$, we obtain a formula describing the atomic ionization under a sudden perturbation of the electron by the charged particle at the moment of its flight near the electron. In this case, we neglect the influence of the particle's motion at the time moment of interaction, i.e. the particle's charge is considered immobile. We have

$$W_a = \left(\frac{Z_pe^2}{r_a}\right)^2 \left|\int \psi_f^*\psi_i^{(0)}dq\right|^2 aF(E_{\max}). \qquad (9)$$

Figure 2 presents the function $F(E)$ for the electron passing from the bound state with $E_{\rm B}$=70 eV to the continuous spectral range E. The function is divided into two parts with the kinetic energy from 0 to 200 eV and from 0 to 2×10^5 eV. With increase in the energy of the charged particle, $F(E_{\max})$ grows until $E_{\max}$ remains comparable to $E_{\rm B}$. Starting from $E_{\max} \sim 21$ keV, which corresponds to $\frac{E_{\max}}{E_{\rm B}} \sim 300$ and the distance of the closest approach to the electron $r = 7\times10^{-12}$ cm

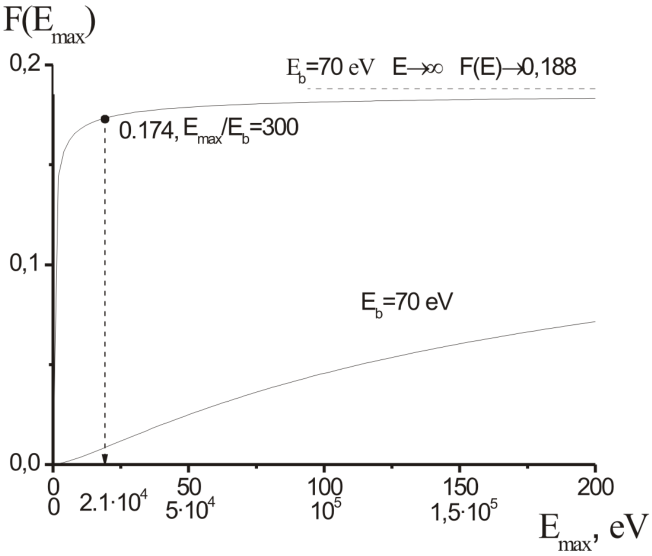

Fig. 2. Function $F(E)$ for an electron passing from the bound state with $E_B = 70$ eV to the continuum with E. The energy on the X-axis is presented on two scales of units. The upper and lower curves $F(E_{\max})$ correspond to the energy scales from 0 to 2×10^5 eV and from 0 to 200 eV, respectively

if $Z_p = 1$, the function $F(E)$ remains practically constant and does not considerably change the transition probability.

In order to estimate the values of $r_{\max}$ and $r_{\min}$, we suppose that the average energy of β-particles under radioactive decay is close to 1 MeV, whereas that of α-particles is close to 6 MeV. Then, at $E_B = 70$ eV, $r_{\max}$ are equal to 2.05×10^{-9} cm and 4.1×10^{-9} cm, respectively. If the particle moves at a larger distance from the circle center, it is not able to impart the necessary binding energy to the electron. If a β-particle moves at the distance $r_{\min} = 1.4 \times 10^{-13}$ cm and an α-particle – at the distance $r_{\min} = 4.8 \times 10^{-13}$ cm, then the charged particle completely imparts its kinetic energy E_p to the electron. In the case of the further approach ($r < r_{\min}$), the imparted energy must be higher than the actually available kinetic energy of the charged particle, and these transitions cannot be realized due to the violation of the energy conservation law. Moreover, this imparted energy is too large from the viewpoint of the applicability of perturbation theory and requires the involvement of other mechanisms of interaction (escort electrons, binary collisions, and others) [14]. It is evident that the maximal perturbation transferred, when considering the ionization as a shake-off, is approximately equal to 10^4 keV, which corresponds to the distance $r_{\min} = 3 \times 10^{-11}$ cm for an α-particle and $F(E_{\max}) = 0.17$ at $E_B = 70$ eV.

4. Consideration of the Motion of a Charged Particle at the Time Moment of Its Interaction with the Electron at Ionization

Investigating the shake-off of near-zero-energy electrons from the target surface due to the sudden appearance of a charge resulting from the passage of a charged particle through the surface, we have established that the probability of the electron transition to vacuum $W \sim \frac{(Z_p e^2)^2}{\nu_p}$ is not only proportional to the squared charge of the particle but also is inversely proportional to its velocity [15–17]. This dependence was determined for electrons and α-particles; in [14], it was obtained for α-particles and heavy ions as a generalization of experimental works. The initial cause of the sudden appearance of a charge lies in the process of ionization of atomic electrons at the passage of a charged particle through the target. That is why the probability of the atomic ionization must be inversely proportional to the velocity of the incident charged particle. This dependence was observed in a wide range of velocities of charged particles. In particular, the dependence $W \sim \nu^{-1}$ was observed for β-particles at mean velocities below $\nu_\beta = 2.7 \times 10^{10}$ cm s^{-1}. The approaching to the light velocity c does not change the character of this relation. That is why the probability of the shake-off at the light velocity can be obtained extrapolating the dependence $W(\nu_\beta)$ to the value at $\nu_\beta = c$ and assuming it to be the standard of the ionization probability under a sudden perturbation as it is the shortest perturbation process. With decrease in the velocity of particles, the range of interaction times widens and the transition probability grows. For example, if the velocity decreases twice, the transition probability also rises twice. However, this widening of the interaction time must not conflict with the basic sudden-perturbation approximation $w_{fi}\frac{\Delta L}{\nu_p} \leq 1$, where w_{fi} is the transition frequency, $\Delta L \simeq r_{\max}$, while $\frac{\Delta L}{\nu_p}$ is the time of flight of the charged particle near the atomic electron. Substituting the values $\hbar w = 70$ eV, $r_{\max} = 4.1 \times 10^{-9}$ cm, and $\nu_p \sim 3.4 \times 10^9$ cm s^{-1} for an α-particle at $E_\alpha = 6$ MeV, we obtain $w_{fi}\frac{\Delta L}{\nu_p} = 0.13$. This value does not contradict the applicability of the sudden-perturbation approximation for an α-particle and, all the more, for a β-particle, where $\nu_p \sim 10^{10}$ cm s^{-1}. That is why, with regard for the influence of the particle's motion, formula (9) must be written down in the following form:

$$W(E) = \mathrm{const}\frac{C}{\nu_p}\left(\frac{Z_p e^2}{r_a}\right)^2 \left|\int \psi_f^* \psi_i^{(0)} dq\right|^2 aF(E), \qquad (10)$$

where $\frac{c}{\nu_p}$ determines the factor by which the transition probability at the velocity of a charged particle ν_p exceeds that at the velocity of light.

The probability of the ionization of an atom is proportional to the duration of its sudden excitation by a projectile, its squared charge, the transition probability of the atom from the neutral state to an excited one accompanied by the appearance of a vacancy in one of its subshells (electron-hole transition), and the transition probability of the electron to the continuous spectral range. Formula (10) allows one to compare the probabilities of the atomic ionization under various experimental conditions in the case of a sudden perturbation of an electron due to the bombardment by charged particles of different sorts.

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ІОНІЗАЦІЯ АТОМА ЯК РАПТОВЕ ЗБУРЕННЯ ЕЛЕКТРОНА ЗАРЯДОМ ПРОЛІТАЮЧОЇ ЧАСТИНКИ

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Р е з ю м е

Іонізацію атома розглянуто в наближенні раптового збурення електрона атома в момент проходження зарядженої частинки повз нього (в наближенні "струсу"). Її представлено як квантово-механічний перехід системи з початкового стану в кінцевий з випромінюванням електрона із зв'язаного стану в атомі в стан неперервного спектра під дією збурення, що діє впродовж дуже короткого проміжку часу, і для його опису використовуються відповідні формули квантової механіки (формули ефекту струсу). Отримано формулу для визначення розподілу електронів за енергіями в неперервному спектрі кінцевого стану, а також обчислено інтегральний спектр електронів залежно від енергії зарядженої частинки. Зазначено, що формула для визначення ймовірності переходу W від нерухомого заряду має бути доповнена залежністю від швидкості зарядженої частинки $W \sim \nu^{-1}$.