Coulomb ionization of an atom by a fast multiply charged ion

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A theory of sudden perturbations, valid at high collision velocities v in the range $Ze^2/\hbar v \lesssim 1$ (Z is the charge of the incident particle), is used to obtain formulas for the probabilities of the Coulomb excitation of arbitrary states in the discrete and continous spectra of a hydrogenic atom and a negative ion with an outer S electron by a fast bare multiply charged ion. The total probabilities of electron detachment are investigated in detail throughout the whole range of the impact parameters and for various values of $Ze^2/\hbar v$. The angular and energy distributions of fast secondary electrons ($\hbar k \gtrsim mv$), which do not satisfy the suddenness condition, are analyzed by a method similar to the usual impulse approximation.

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1. INTRODUCTION. GENERAL RELATIONSHIPS

Collisions involving multiply charged ions have recently become the object of intensive experimental and theoretical investigations in connection with analysis of the role of impurities in thermonuclear fusion plasma, development of ion implantation processes, determination of the energy spectra of nuclear fission fragments, design and use of accelerators of heavy high-energy ions, and need to interpret correctly the data on ultraheavy cosmic rays.

The progress in generation of beams of fast bare ions makes it reasonable to expect, in the near future, precision experimental studies of the Coulomb excitation of single atoms by fast multiply charged ions employing the already available method of excitation by protons and alpha particles. In the simplest case one has to determine the cross sections of the individual excitation or ionization channels, weheras in more complex situations one needs to determine the probabilities of transitions for various impact parameters by a method developed in the last few years.

Investigations of this kind are undoubtedly of scientific interest because, from the theoretical point of view, we have here one of the few problems in atomic collisions that can be solved in a consistent manner when a strong field is introduced from outside into a system and its influence cannot be allowed in any order of the conventional perturbation theory.

The problem of the dependence of the probabilities of individual transitions on the impact parameter in the theory of the Coulomb excitation by fast protons has become urgent only because of the development of new experimental techniques and a deeper analysis of the channeling effect. Calculation of cross sections in this problem is mch easier and adequate mathematical methods are generally familiar. However, in the theory dealing with multiply charged ions the problem of the dependence of the probabilities on the impact parameter is introduced organically, in contrast to the case of protons, because the correct answer is obtained for different trajectories of telative motion by using qualitatively different theoretical approaches.[1]

The two central parameters in the theory of the Coulomb excitation are the ratio of the electron velocity in a target atom to the velocity of the incident particle

$$\xi=\hbar/mav=Z_ae^2/\hbar v \tag{1}$$

(m is the electron mass) and the quantity

$$\eta=Ze^2/\hbar v=\xi(Z/Z_a), \tag{2}$$

which determines—in the case of small impact parameters—the intensity of the interaction of this electron with a moving force center of charge Z.

In a majority of the experiments on the stripping of atomic shells, in order to obtain partly or totally bare nuclei, the velocities of ion beams are such that

$$v\gg e^2/\hbar, \quad Ze^2/\hbar v\lesssim 1.$$

A detailed investigation of the processes of the Coulomb excitation and ionization under these conditions is reported below.

In the case of fast protons and multiply charged ions when $v \ll e^2/\hbar$, the whole range of target parameters of interest to us $b \gtrsim a_0 = \hbar^2/me^2$ can be considered as follows. Electrons in inner shells of the target atom ($\xi \lesssim 1$) experience a weak external interaction because the characteristics quantity for such electrons in the dipole range $b \gtrsim a_0 \gg a = a_0/Z_a$ is of the order of $\eta_{eff} \sim \eta a/b \gg 1$. Therefore, the probabilities of the Coulomb excitation involving these electrons are found using the conventional perturbation theory[2,3] in the lowest order in η.

A general approach to the solution of this problem in the case of outer-shell electrons ($Z_a \sim 1$, $\xi \ll 1$) is given in Ref. 1. In the case of small impact parameters ($b \lesssim a_0$) the Coulomb excitation of states in the discrete spectrum should be described using the theory of sudden perturbations[4] and in the dipole range ($b \gg a_0$), it should be described by the conventional theory. Matching of the results obtained in these two cases [which can be made more accurately the better the condition $\eta\xi \ll \gamma$ is satisfied, where $\gamma = (1 - v^2/c^2)^{-1/2}$ is the Lorentz factor] makes it possible to calculate correctly also the excitations cross sections.

In addition to separate discussion of the dipole and nondipole ranges in the ionization process,[5,6] one should also distinguish between channels involving de-

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tachment of fast ($ka_0 \gg 1$) and slow ($ka_0 \lesssim 1$) weakly bound ($\xi \ll 1$) electrons ($\hbar\mathbf{k}$ is the momentum of the knocked-out electron). The theory of sudden perturbations can be applied in the range $b \lesssim a_0$ right up to the values of k corresponding to the condition $\hbar k/mv \ll 1$. However, if $\hbar k \gtrsim mv$, the situation simplifies in a different sense, because we can then use a method similar to the conventional impulse approximation (for details see Appendix B).

The relative trajectory of the incident heavy particle will be regarded as rectilinear $\mathbf{R}(t)=\mathbf{b}+\mathbf{v}t$, and the interaction potential with an electron in an atom as of the retarded Coulomb type:

$$\hat{V}(t)=\frac{Ze^2}{2\pi^2}\int\frac{d^3q}{q^2-(\mathbf{qv}/c)^2}\exp(-i\mathbf{qb}-i\mathbf{qv}t)(1-e^{i\mathbf{qr}}). \tag{3}$$

The scattering operator includes a quantity proportional to the Fourier component of the potential (3):

$$\hat{V}_\Omega=-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\exp(i\Omega t)\hat{V}(t)$$
$$=2i\eta\left[\exp\left(i\frac{\Omega\mathbf{rv}}{v^2}\right)K_0\left(\varkappa\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|\right)-K_0(\varkappa)\right], \tag{4}$$

where

$$\varkappa=\Omega b/v\gamma,\quad \mathbf{s}=\mathbf{r}-\frac{\mathbf{v}}{v}\left(\mathbf{r}\frac{\mathbf{v}}{v}\right), \tag{5}$$

$K_\nu(z)$ is a modified Bessel function, and $\mathbf{s}$ is the projection of the vector $\mathbf{r}$ on the plane of the impact parameter. In the conventional perturbation theory the excitation amplitude includes a Fourier component at the frequency of a transition in the target, $\Omega=\omega_f-\omega_i$, and in the lowest order theory of sudden perturbations[4] it is expressed in terms of the Fourier component (4) at zero frequency:

$$\mathfrak{M}_{fi}(\mathbf{b})=\langle f|\exp(\hat{V}_0)|i\rangle=\langle f|\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|^{-2i\eta}|i\rangle. \tag{6}$$

2. IONIZATION OF A HYDROGENIC ATOM

The probability of the Coulomb ionization

$$\frac{dW(\mathbf{b})}{d(ka)do_e}=\frac{(ka)^2}{(2\pi)^3}|\mathfrak{M}_{1S}(\mathbf{k})|^2 \tag{7}$$

is calculated in the suddenness approximation using the amplitude

$$\mathfrak{M}_{1S}(\mathbf{k})=a^{-3/2}\int d^3r\,\psi_{\mathbf{k}}^{(-)*}(\mathbf{r})\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|^{-2i\eta}\psi_{1S}(\mathbf{r}), \tag{8}$$

where do_e is an element of the solid angle within which the momentum $\hbar\mathbf{k}$ of the knocked-out electron is located The wave function of the final state in Eq. (8) is normalized to unit volume:

$$\psi_{\mathbf{k}}^{(-)}(\mathbf{r})=4\pi e^{\pi/2ka}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}^*\left(\frac{\mathbf{k}}{k}\right)Y_{lm}\left(\frac{\mathbf{r}}{r}\right)$$
$$\times\frac{\Gamma(l+1-i/ka)}{\Gamma(2l+2)}(2ikr)^l e^{-ikr}F\left(l+1+\frac{i}{ka};\ 2l+2;\ 2ikr\right). \tag{9}$$

The ionization amplitude was calculated in the first work cited under Ref. 5 by a method representing essentially a development of the methods in Ref. 7 (see also Ref. 8). We shall obtain a different, simpler, expression and also show that the amplitudes of any transitions in a hydrogenic atom can be found in a unified manner using a function $M_{lm}(\alpha;\beta)$ calculated in the Appendix A. Moreover, as shown below, our method makes it possible to find all the more important asymptotes for the ionization channel and for the bound-bound transitions.

The amplitude (8) is described by a series containing the functions $M_{lm}(\alpha;\beta)$:

$$\mathfrak{M}_{1S}(\mathbf{k})=4\sqrt{\pi}\,e^{\pi/2ka}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\mathbf{k}/k)\Gamma(l+1+i/ka)$$
$$\times\sum_{\sigma=0}^{\infty}\frac{(l+1-i/ka)_\sigma}{\sigma!(2l+\sigma+1)!}(-2ika)^{l+\sigma}M_{lm}(l+\sigma;\ 1-ika). \tag{10}$$

Its asymptote in the range $b\ll a$ for any value of ka is

$$\mathfrak{M}_{1S}(\mathbf{k})\approx 4\pi\left(\frac{b}{a}\right)^{2i\eta}e^{\pi/2ka}\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}(1-ika)^{2i\eta-3}$$
$$\times\sum_{l=0}\sum_{m=-l}(-1)^{(m+|m|)/2}i^{|m|}Y_{lm}(\mathbf{k}/k)S_{lm}\left(\frac{2ka}{ika-1}\right)^l\left[(2l+1)\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}$$
$$\times\Gamma\left(i\eta+\frac{|m|}{2}\right)\Gamma\left(l+1+\frac{i}{ka}\right)\frac{\Gamma(3+l-2i\eta)}{\Gamma(2l+2)}$$
$$\times F\left(l+1-\frac{i}{ka},\ 3+l-2i\eta;\ 2l+2;\ \frac{2ika}{ika-1}\right). \tag{11}$$

Using the relationship [Eq. (13) in §2.3.2 of Ref. 9] for the hypergeometric function in Eq. (11), and omitting unimportant phase factors, we find that if $b\ll a$ and $ka\ll 1$, then

$$\mathfrak{M}_{1S}(\mathbf{k})\approx 8\pi\left(\frac{2}{ka}\right)^{1/2}\Gamma(1-i\eta)\Gamma(2-i\eta)F(3-2i\eta;\ 2;\ -2). \tag{12}$$

Similarly, the amplitude of arbitrary bound-bound transitions can be calculated in the nondipole range:

$$\mathfrak{M}_{nlm}(\mathbf{b})=\langle nlm|\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|^{-2i\eta}|1S\rangle=\frac{2/\sqrt{\pi}}{n^2(2l+1)!}\left(\frac{(n+l)!}{(n-l-1)!}\right)^{1/2}$$
$$\times\sum_{\sigma=0}^{n-l-1}\frac{(l+1-n)_\sigma}{(2l+2)_\sigma\sigma!}(2/n)^{l+\sigma}M_{lm}\left(l+\sigma;\ \frac{n+1}{n}\right). \tag{13}$$

The result (13) simplifies greatly if we investigate the excitation of high-lying levels ($n\gg 1$). In the range of parameters $n\gg l+1$, $n^2\gg r/a$, of interest to us, the wave function is

$$\psi_{nlm}(\mathbf{r})\approx\left(\frac{4}{n^3a^3}\right)^{1/2}\frac{J_{2l+1}[(8r/a)^{1/2}]}{(2r/a)^{1/2}}Y_{lm}(\theta,\varphi) \tag{14}$$

and instead of Eq. (13) we have

$$\mathfrak{M}_{nlm}(\mathbf{b})\approx\frac{2^{l+1}}{\sqrt{\pi n^3}}\sum_{\sigma=0}^{\infty}\frac{(-2)^\sigma}{(2l+\sigma+1)!\sigma!}M_{lm}(l+\sigma;\ 1). \tag{15}$$

In the limit $b\ll a$, we then find

$$\mathfrak{M}_{nlm}(\mathbf{b})\approx\left(\frac{b}{a}\right)^{2i\eta}2^{l+1}(-1)^{(m-|m|)/2}(-i)^{l+|m|}\left[\frac{2l+1}{n^3}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}S_{lm}$$
$$\times\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}\Gamma\left(i\eta+\frac{|m|}{2}\right)\frac{\Gamma(l+3-2i\eta)}{\Gamma(2l+2)}F(l+3-2i\eta;\ 2l+2;\ -2). \tag{16}$$

We shall give, by way of example, the asymptotes of the amplitudes of the $1S\to nS$ transitions in the $b\ll a$ case:

$$\mathfrak{M}_{1S\to nS}(\mathbf{b})\approx\Gamma(1-i\eta)\Gamma(2-i\eta)\left(\frac{2\sqrt{n}}{n+1}\right)^3F\left(1-n,\ 3-2i\eta;\ 2;\ \frac{2}{n+1}\right) \tag{17}$$

{the phase factor $[b(n+1)/2an]^{2i\eta}$ is omitted here}, and their values in the $n\gg 1$ case:

$$\mathfrak{M}_{1s\to ns}(\mathbf{b})\approx\left(\frac{4}{n}\right)^{1/2}\Gamma(1-i\eta)\Gamma(2-i\eta)F(3-2i\eta;\;2;\;-2). \qquad (18)$$

3. DETACHMENT OF AN ELECTRON FROM A NEGATIVE ION

The results obtained in Sec. 2 using the hydrogenic model can also be employed in calculations relating to the excitation and ionization of neutral atoms and of positively charged ions. In the case of negative ions, we have here fundamental differences associated with a basically different behavior of the wave functions of a weakly bound electron in the ground state and in the continuous spectrum. Thus, the problem of the Coulomb detachment of an electron from a negative ion should be discussed separately.

The states of an outer S electron in a negative atomic ion can be represented well by the states of a particle in the field of a point potential. If this model is adopted there is only one bound state and its wave function is

$$\psi_0(\mathbf{r})=(2\pi a)^{-1/2}\exp(-r/a)/r \qquad (19)$$

and its energy is $E_0=-\hbar^2/2ma^2$; the probability of detachment is simply the sum of the probabilities of the inelastic excitation channels.

In the nondipole range the amplitude of the elastic channel calculated from the theory of abrupt perturbations is

$$\mathfrak{M}_{\rm el}(\mathbf{b})=\pi^{-1/2}M_{00}(-2;\,2). \qquad (20)$$

Hence, in particular, we can easily obtain expressions for the total probability of detachment of an electron in the $b\ll a$ case

$$W_{\rm inel}(\mathbf{b})=1-W_{\rm el}(b)\approx1-\left(\frac{\pi\eta}{\operatorname{sh}\pi\eta}\right)^2\Big/(1+4\eta^2) \qquad (21)$$

and in the case when $b\gg a$:

$$W_{\rm inel}(\mathbf{b})\approx2(\eta a/b)^2/3. \qquad (22)$$

The amplitude of detachment accompanied by the emission of an electron with a momentum $\hbar\mathbf{q}$ is found from the general formula (8) after the substitution of

$$\psi_{\mathbf{q}}^{(-)}(\mathbf{r})=e^{i\mathbf{q}\mathbf{r}}-\frac{1}{1-iqa}\frac{e^{-iqr}}{r/a}. \qquad (23)$$

This amplitude can be described by

$$\mathfrak{M}(\mathbf{q})=M(\mathbf{q})-\frac{\sqrt{2}}{1+iqa}M_{00}(-2;\,1-iqa). \qquad (24)$$

Here,

$$M(\mathbf{q})=a^{-3/2}\int d^3r\,e^{-i\mathbf{q}\mathbf{r}}\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|^{-2i\eta}\psi_0(\mathbf{r})$$
$$=2\sqrt{2\pi}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(-2iqa)^lY_{lm}(\mathbf{q}/q)$$
$$\times\sum_{\sigma=0}^{\infty}\frac{(-1)^\sigma(\sigma+l)!}{\sigma!(2\sigma+2l+1)!}(qa)^{2\sigma}M_{lm}(2\sigma+l-1;\,1). \qquad (25)$$

If $b\ll a$ and $qa\ll1$, then

$$M(\mathbf{q})\approx2\sqrt{2\pi}(b/2a)^{2i\eta}[\Gamma(1-i\eta)]^2. \qquad (26)$$

In the limit $b\ll a$, Eq. (25) can be made more flexible in respect of the parameter qa, in the same way as has been done in the derivation of formula (11). Reducing the sum over k before integration with respect to r in Eq. (A7) to a Bessel function of half-integer order, bearing in mind that if $b\ll a$, then practically throughout the whole of space we have

$$B_\lambda(r)\approx(b/r)^{2i\eta-\lambda-1/2}/\Gamma\left(\lambda+\frac{|m|+3}{2}-i\eta\right), \qquad (27)$$

we obtain

$$M(\mathbf{q})\approx\frac{\sqrt{2\pi^3}}{1+q^2a^2}\left[\frac{b^2}{a^2}(1+q^2a^2)\right]^{i\eta}\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}$$
$$\times\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\mathbf{q}/q)\left(-\frac{1}{2}\right)^l(-1)^{(m-|m|)/2}(-i)^{|m|}S_{lm}$$
$$\times\left[(2l+1)\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}\Gamma\left(i\eta+\frac{|m|}{2}\right)\left(\frac{q^2a^2}{1+q^2a^2}\right)^{l/2}\frac{\Gamma(l+2-2i\eta)}{\Gamma(l+3/2)}$$
$$\times F\left(1-i\eta+l/2,\;i\eta+l/2;\;l+3/2;\;\frac{q^2a^2}{1+q^2a^2}\right). \qquad (28)$$

For any value of qa in the limit $b\ll a$, we have

$$M_{00}(-2;\,1-iqa)\approx\frac{2\sqrt{\pi}}{1-iqa}\frac{[\Gamma(1-i\eta)]^2}{1-2i\eta}\left(\frac{b}{a}\frac{1-iqa}{2}\right)^{2i\eta}. \qquad (29)$$

4. DISCUSSION OF RESULTS

The differential probability of ionization of a hydrogenic atom in the nondipole range can be determined if, bearing in mind the orthonormalization properties of the spherical functions, we integrate directly the square of the modulus of the amplitude (8) along the directions of momentum of the knocked out electron. However, in calculating the total ionization probability there is no need to carry out separately the very complex numerical calculations of the type reported in Ref. 5. The probability is found much more easily and sufficiently accurately by subtracting from the total probability of all the inelastic channels $W_{\rm inel}(\mathbf{b})=1-W_{1s\to1s}(\mathbf{b})$ the probabilities of the first few excitation channels and the sum of all the others, whose contribution is estimated from the above asymptotic expressions in the $n\gg1$ case.

Figure 1 shows the dependence of the total probability of ionization $W_{\rm ion}(\mathbf{b})$ on the parameter η in the limit $b\ll a$. For comparison, this figure includes the probabilities of the elastic channel, several inelastic channels, and the total probability $W_{\rm inel}(\mathbf{b})$. It should be pointed out that in the nondipole range the proba-

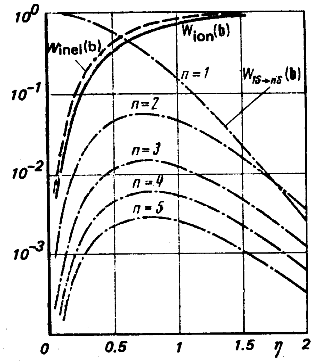

FIG. 1. Probabilities of individual excitation and ionization channels of a hydrogenic atom in the limit $b\ll a$.

bilities of excitation of the S states in the discrete spectrum vary nonmonotonically with η. For example, of $b \ll a$, all of them have maxima in the region of $\eta \approx 0.75$ (which is shifted slightly to the right on increase in n). The point is this: a further increase in η makes the Coulomb ionization the dominant process and in this range it is more important than the probability of the elastic channel. In view of this nonmonotonic behavior, we can also expect nonmonotonic dependences of the other channels $1S \rightarrow nS$ on the impact parameter in the case when $\eta > 0.75$, because an increase in b/a reduces continuously the effective interaction $\eta_{eff} \sim \eta a/b$ and moving effectively to the left of the $W_{1S \rightarrow nS}(\eta_{eff})$ curves, we again pass the probability peak at $\eta_{eff} \approx 0.75$.

The situation is different in the case of ionization. For any value of η, the dependence $W_{ion}(b)$ is monotonic, as shown in Fig. 2. It is also worth noting that, according to the theory of sudden perturbations, the relationships between the probabilities of electron detachment from a negative ion differ considerably from the probabilities of detachment from a neutral atom (or a negative ion). This is mainly due to the qualitatively different behavior of the wave functions of the ground state, which results in very different values of the probabilities of the elastic channel. In the limit $b \ll a$, the total probability of all the inelastic processes is much greater in the case of a negative ion when the state of an electron is largely localized (see the dependences of η in Figs. 1 and 3). Moreover, in the case of a hydrogenic atom there are additional excitation channels that do not cause ionization. Conversely, at high impact parameters, when the probability of electron detachment decreases in either case in accordance with practically the same law [see the asymptote (22)], an additional power-law reduction in the electron density in a negative ion [see Eq. (19)] reduces also the role of inelastic channels for this ion.

The considerable difference between the ionization probabilities calculated by two different methods is demonstrated in Fig. 4. In the nondipole range for $\eta \ll 1$ (and in Fig. 4 also even for $\eta = 0.5$) the results of the theory of sudden perturbations are close to those given by the conventional theory, but the difference between them rises rapidly on increase in η so that the ionization probabilities are calculated using the conventional theory lose their physical meaning. The conclusions of the theory of sudden perturbations become qualitatively incorrect for high impact parameters when the suddenness condition is no longer obeyed. Matching of the correct results in the two regions solves the problem of the dependence of the probability of ionization of a target atom by a fast multiply charged ion on the impact parameter. In the case of cross sections the theory of sudden perturbations changes the results only slightly compared with the usual method of renormalization of the probabilities in the nondipole range[6] because if $\xi \ll 1$, the main contribution to the ionization comes from the dipole approaches in the theory of Coulomb detachment of an electron from a negative ion is basically the same as in the case of ionization of a neutral atom. However, it should be noted that, other conditions (charges and velocities of the incident particles) being constant, the matching is much more accurate because the inequality $\eta\xi \ll \gamma$ is satisfied by a larger margin.

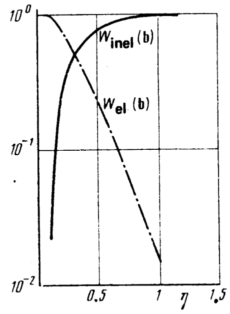

FIG. 3. Probabilities of the elastic channel in the case of Coulomb detachment of an electron from a negative ion in the limit $b \ll a$.

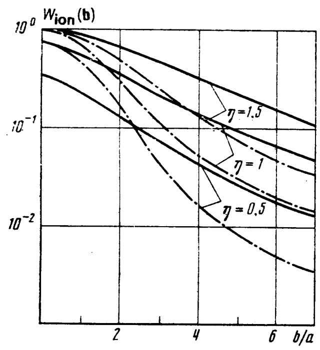

FIG. 2. Probabilities of ionization of a hydrogenic atom (continuous curves) and of Coulomb detachment of an electron from a negative ion (dash-dot curves), calculated using the theory of sudden perturbations.

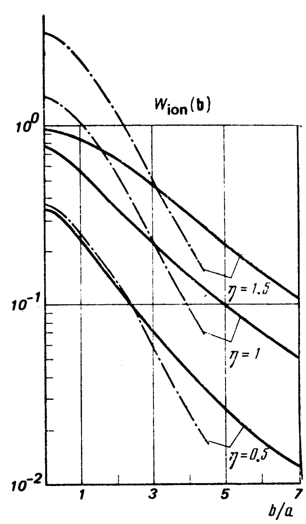

FIG. 4. Probabilities of Coulomb ionization of a hydrogenic atom calculated using the theory of sudden perturbations (continuous curves) and by the conventional method assuming that $1^*/10$ and $\gamma = 1$ (dash-dot curves).

APPENDIX A

We shall consider an integral of the type

$$M_{lm}(\alpha;\beta)=\left(\frac{1}{a}\right)^{\alpha+3}\int d^3r r^\alpha e^{-\beta r/a}Y_{lm}^*(\mathbf{r}/r)\,|(\mathbf{b}-\mathbf{s})/b|^{-2i\eta}, \tag{A1}$$

$$\operatorname{Re}\alpha>-3,\qquad \operatorname{Re}\beta>0,$$

$$Y_{lm}(\mathbf{r}/r)=(-1)^{(m+|m|)/2}i^l\left[\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}P_l^{|m|}(\cos\theta)e^{im\varphi}, \tag{A2}$$

$$\cos\theta=\mathbf{rv}/rv,\qquad \cos\varphi=\mathbf{rb}/rb. \tag{A3}$$

The associated Legendre polynomial, which occurs in the spherical function (A2), is a product of $\sin^{|m|}\theta$ and a polynomial of degree $(l-|m|)$ and parity $(-1)^{l-|m|}$ on $\cos\theta$:

$$P_l^{|m|}(\cos\theta)=\sin^{|m|}\theta\sum_{\lambda=0}^{(l-|m|)/2}A_\lambda\cos^{2\lambda}\theta. \tag{A4}$$

It follows from the theory of Bessel functions (see also Refs. 7 and 10) that

$$\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|^{-2i\eta}=2^{1-2i\eta}\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}\int_0^\infty dp\,p^{2i\eta-1+\varepsilon}J_0\left(p\left|\frac{\mathbf{b}-\mathbf{s}}{b}\right|\right)$$
$$=\frac{2^{-2i\eta}}{\pi}\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}\int d^2p\,p^{2i\eta-2+\varepsilon}\exp[-i\mathbf{p}(\mathbf{b}-\mathbf{s})/b], \tag{A5}$$
$$\mathbf{pv}=0,\qquad \varepsilon\to+0.$$

If the above relationships are used to integrate Eq. (A1) with respect to the angles φ and θ and the vectors $\mathbf{p}$, we obtain

$$M_{lm}(\alpha;\beta)=(-1)^{(m-|m|)/2}(-i)^{l+|m|}\left[\pi(2l+1)\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}$$
$$\times\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}\Gamma\left(i\eta+\frac{|m|}{2}\right)\sum_{\lambda=0}^{(l-|m|)/2}A_\lambda\Gamma\left(\lambda+\frac{1}{2}\right)M_\lambda(b), \tag{A6}$$

$$M_\lambda(b)=\left(\frac{b}{a}\right)^{\lambda+1/2}\int_0^\infty d\left(\frac{r}{a}\right)\left(\frac{r}{a}\right)^{\alpha-\lambda+3/2}e^{-\beta r/a}B_\lambda(r). \tag{A7}$$

The function $B_\lambda(r)$ can be expressed in terms of a discontinuous Weber–Schafheitlin integral and, in the ranges of parameters of interest to us, this function is given by

$$B_\lambda(r<b)=\frac{(r/b)^{\lambda+|m|+1/2}}{\Gamma(1-|m|/2-i\eta)\Gamma(\lambda+|m|+3/2)}F\left(i\eta+\frac{|m|}{2},i\eta+\frac{|m|}{2};\lambda\right.$$
$$\left.+|m|+\frac{3}{2};\frac{r^2}{b^2}\right)=\sum_{s=0}^\infty C_s(r/b)^{2s+\lambda+|m|+1/2}, \tag{A8}$$

$$B_\lambda(r>b)=\left[\left(\frac{b}{r}\right)^{2i\eta-\lambda-1/2}\Big/\Gamma\left(\lambda+\frac{|m|+3}{2}-i\eta\right)\right]$$
$$\times F\left(i\eta+\frac{|m|}{2},i\eta-\lambda-\frac{|m|+1}{2};1;\frac{b^2}{r^2}\right)=\sum_{s=0}^\infty D_s(b/r)^{2s+2i\eta-\lambda-1/2}. \tag{A9}$$

Integration of Eq. (A7) gives finally

$$M_\lambda(b)=\sum_{s=0}^\infty\{C_s(a/b)^{2s+|m|}\beta^{-\nu}\gamma(\nu,\beta b/a)+D_s(b/a)^{2s+2i\eta}\beta^{-\mu}\Gamma(\mu,\beta b/a)\}, \tag{A10}$$

$$\nu=3+\alpha+|m|+2s,\qquad \mu=3+\alpha-2i\eta-2s, \tag{A11}$$

where $\gamma(\nu,x)$ and $\Gamma(\mu,x)$ are incomplete gamma functions.

Since

$$M_\lambda(b\ll a)\approx\left(\frac{b}{a}\right)^{2i\eta}\beta^{2i\eta-\alpha-3}\frac{\Gamma(3+\alpha-2i\eta)}{\Gamma[\lambda+(|m|+3)/2-i\eta]}, \tag{A12}$$

the asymptote of the integral (A1) in the $b\ll a$ case is

$$M_{lm}(\alpha,\beta)\approx\left(\frac{\beta b}{a}\right)^{2i\eta}\left(\frac{1}{\beta}\right)^{\alpha+3}\frac{\Gamma(1-i\eta)}{\Gamma(i\eta)}\Gamma(\alpha+3-2i\eta)$$
$$\times(-1)^{(m-|m|)/2}(-i)^{l+|m|}\left[\pi(2l+1)\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2}\Gamma\left(i\eta+\frac{|m|}{2}\right)S_{lm}. \tag{A13}$$

Here,

$$S_{lm}=\sum_{\lambda=0}^{(l-|m|)/2}A_\lambda\frac{\Gamma(\lambda+1/2)}{\Gamma[\lambda+(|m|+3)/2-i\eta]}. \tag{A14}$$

It follows from the results of Ref. 1 and the definition of $M_{lm}(\alpha;\beta)$ that the function $M_{00}(\alpha;\beta)$ can be written in the form of the following rapidly converging series:

$$M_{00}(\alpha;\beta)=2\sqrt{\pi}\left(-\frac{b}{2a}\right)^{\alpha+3}\frac{\partial^{\alpha+1}}{\partial x^{\alpha+1}}J_S(x)\big|_{x=\beta b/2a}, \tag{A15}$$

$$J_S(x)=\left(\frac{\Gamma(1-i\eta)}{x^{1-i\eta}}\right)^2I_0(2x)-\sum_{k=0}^\infty\left(\frac{x^k}{(1-i\eta)_{k+1}}\right)^2, \tag{A16}$$

$$J_S^{\text{dip}}(x)=(\eta^2+x^2)^{-1}. \tag{A17}$$

If $\alpha=-2$, we have to use $\partial^{-1}/\partial x^{-1}\equiv\int_\infty^x dx; I_0(z)$ in Eq. (A15); $I_0(z)$ is a cylindrical function with an imaginary argument.

APPENDIX B. ANGULAR AND ENERGY DISTRIBUTIONS OF FAST SECONDARY ELECTRONS

We recall first the method of calculation of the amplitudes of transitions in situations when the suddenness conditions are satisfied not by the complete Hamiltonian of the unperturbed system $\hat{H}=\hat{H}_0+\hat{H}'$, but only by its "small" part $\hat{H}'$, which we shall call the distortion of the Hamiltonian $\hat{H}_0$. It is shown in Ref. 4 that in the most general case the problem reduces to finding the time evolution operator $\hat{S}(t,t')$ in the case of scattering of the shake-up type, when an external perturbation $\hat{V}(t)$ acts for a short time interval τ near a certain moment t_0. This applies also to the weakly distorted quantum systems ($\omega\tau\ll 1$, where $\hbar\omega$ are typical eigenvalues of $\hat{H}'$). In this case we can effectively retain the usual scheme of the theory of sudden perturbations and in zeroth order in respect to $\omega\tau$ we find that $\hat{S}(t,t')$ is identical with the evolution operator $\hat{S}_0(t,t')$ in the absence of distortion.

Use of the Magnus of Fer expansions[4] makes it possible to identify whole classes of systems that permit compact representations of the evolution operators $\hat{S}_0(t,t')$. For example, in the case of arbitrary quadratic Hamiltonians

$$\hat{H}_0=E+\alpha\hat{\mathbf{p}}^2+\beta\hat{\mathbf{p}}+\gamma r^2+\delta\mathbf{r}$$

and interaction potentials of the type

$$\hat{V}(t)=h(t)-\mathbf{f}(t)\mathbf{r}-\mathbf{g}(t)\hat{\mathbf{p}},$$

we find, to within an unimportant phase factor

$$\left.\begin{aligned}&\hat{S}_0(t,t')=\exp(i\mathbf{qr}+i\boldsymbol{\lambda}\hat{\mathbf{p}}/\hbar),\\&\mathbf{q}=(1/\hbar)\int_{t'}^t dt[\mathbf{f}(t)\cos\varphi-(\gamma/\alpha)^{1/2}\mathbf{g}(t)\sin\varphi],\\&\boldsymbol{\lambda}=\int_{t'}^t dt[(\alpha/\gamma)^{1/2}\mathbf{f}(t)\sin\varphi-\mathbf{g}(t)\cos\varphi],\quad\varphi=2t(\alpha\gamma)^{1/2}.\end{aligned}\right\} \tag{B1}$$

If, for example, $\hat{H}_0$ is the Hamiltonian of a free particle, $H_0=\hat{\mathbf{p}}^2/2m$ and $\hat{V}(t)=-\mathbf{f}(t)\mathbf{r}$, the amplitude of a transition between stationary states of $\hat{H}$ in the zeroth order with respect to $\omega\tau$ is

$$\mathfrak{M}_{fi}=\left\langle f\left|\exp\left\{\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\,\mathbf{f}(t)\left[\mathbf{r}+t\hat{\mathbf{p}}/m\right]\right\}\right|i\right\rangle. \quad \text{(B2)}$$

The second term in the exponential function of (B2) is missing in the usual formulation of the theory of sudden perturbations, but in the case of large momenta transferred to a target it does indeed play the decisive role. We shall show how this occurs in the process of Coulomb ionization of an atom by a fast multiply charged ion.

If $ka\gg 1$, then in the range $b\sim a$ the operator of the interaction of an electron with a moving Coulomb center can be simply replaced with a dipole approximation, because the main contribution to the ionization amplitude is made by the range $r/a\lesssim 1/ka\ll 1$. The effective interaction occurring in q in Eqs. (B1) and (B2) is $\eta_{eff}\sim\eta r/b\sim\eta/ka\ll 1$, whereas the contribution of the second term—as shown below—is governed by the parameter $k\lambda\sim\eta\xi ka$, which easily reaches values of the order of unity. The ionization amplitude in Eq. (7) in the most interesting case of $k\lambda\gtrsim 1$ is

$$\mathfrak{M}(\mathbf{k})\approx a^{-3/2}\langle f|\exp\,(i\boldsymbol{\lambda}\hat{\mathbf{p}}/\hbar)\,|i\rangle. \quad \text{(B3)}$$

It is clear that the above formula has nothing in common with the results of the usual theory of sudden perturbations nor with the results of the conventional perturbation theory in the lowest order with respect to η.

Near a nucleus, where $r\lesssim 1/k$, if we substitute the condition $(ka)^2\gg Z/Z_a$, we find that the potential in the unperturbed system $Z_a e^2/r$ is much greater than the effective interaction potential of an electron with an incident particle Ze^2r/a^2, and the electron state is approximately the same as in the absence of an external perturbation. The wave function of the final state in the ionization amplitude (B3) should include the zeroth (plane wave) and the first Born approximation in respect to the potential of the target atom (the plane-wave approximation by itself is insufficient!). In the calculation of λ the integated with the long-range Coulomb potential should be truncated at $|t-t_0|\sim 1/\omega$, so that

$$\boldsymbol{\lambda}\approx\frac{1}{m}\int_{-\infty}^{\infty}dt\,e^{i\omega(t-t_0)}t\mathbf{f}(t)\approx 2\eta\frac{\hbar}{mv}\frac{\mathbf{v}}{v}\left[\ln\left(\frac{2v}{b\omega}\right)-C-1\right], \quad \text{(B4)}$$

where $C\approx 0.577$ is the Euler constant.

For comparison, we shall give the formula for the amplitude (B3) in the case of ionization of a hydrogenic atom

$$\mathfrak{M}_H(\mathbf{k})\approx\frac{8\pi}{(ka)^4}\left(\frac{2/ka}{1-\exp(-2\pi/ka)}\right)^{1/2}(e^{i\mathbf{k}\boldsymbol{\lambda}}-1) \quad \text{(B5)}$$

and the Coulomb detachment of an electron from a negative ion in the model of zero-radius potential

$$\mathfrak{M}_\delta(\mathbf{k})\approx\frac{(8\pi)^{1/2}}{(ka)^2}\left[e^{i\mathbf{k}\boldsymbol{\lambda}}+\frac{i}{k\lambda}(e^{i\mathbf{k}\boldsymbol{\lambda}}-1)\right]. \quad \text{(B6)}$$

The large difference between Eqs. (B5) and (B6) in respect of the fall expressed by the power of $1/ka$ is due to the fact that if $r\ll a$, the electron density in the ground state is considerably higher for the delta potential (we shall not deal with the real electron distribution in negative ions and, in particular, with the value of a in this or in any other system). Moreover, the angular distributions of the knocked-out electrons are very different. For example, a minimum in the probability of ionization of a hydrogenic atom

$$\frac{dW_H(\mathbf{b})}{d(ka)\,do_e}\approx\frac{32}{\pi(ka)^7}\frac{1-\cos\mathbf{k}\boldsymbol{\lambda}}{1-\exp(-2\pi/ka)} \quad \text{(B7)}$$

corresponds to the directions $\mathbf{k}\perp\mathbf{v}$ [it should be noted that if $k\lambda\ll 1$, the formulas for the amplitude and probability of ionization (B5) and (B7) become more complex expressions requiring numerical calculations and these follow from the general result (B2)]. In the case of a negative ion the extrema in the angular distribition

$$dW_\delta(\mathbf{b})/d(ka)\,do_e\approx(\pi ka)^{-2}\times\left[\left(\cos\mathbf{k}\boldsymbol{\lambda}-\frac{\sin k\lambda}{k\lambda}\right)^2+\left(\sin\mathbf{k}\boldsymbol{\lambda}-\frac{1-\cos k\lambda}{k\lambda}\right)^2\right] \quad \text{(B8)}$$

are located in cones defined by $\tan\mathbf{k}\cdot\boldsymbol{\lambda}=\tan(k\lambda/2)$.

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