It is obvious that the matrix $X^{(r)}_{ai,\alpha}$ must be proportional to $\Theta^{(r)}_{ai,\alpha}$. We determine the proportionality coefficient and show that it does not depend on the representation r of the scalar fields which enter into the Lagrangian (A.1) but is completely determined by the representations r_L and r_R to which the fermions belong.

The matrix $X^{(r)}_{ai,\alpha}$ can be identically rewritten in the form

$$X^{(r)}_{ai,\alpha}={}^1/_2[(F_{ab}{}^n\Theta_{bj,\alpha}-\Theta_{ak,\alpha}F_{kj}{}^n)F_{ji}{}^n$$
$$+\Theta_{ak,\alpha}(F^nF^n)_{ki}]+{}^1/_2[F_{ab}{}^n(\Theta_{bj,\alpha}F_{ji}{}^n-F_{bc}{}^n\Theta_{ci,\alpha})$$
$$+(F^nF^n)_{ac}\Theta_{ci,\alpha}]+{}^1/_2\Theta_{ai,\beta}(F^nF^n)_{\beta\alpha}.$$

We make use of the commutation relation (A.2) and of the fact that $(F^nF^n)_{xy}=C_2(r)\,\delta_{xy'}$, where $C_2(r)$ is the eigenvalue of the Casimir operator in the given representation. We have

$$X^{(r)}_{ai,\alpha}={}^1/_2\Theta_{ai,\alpha}[C_2(r_L)+C_2(r_R)+C_2(r)]$$
$$+{}^1/_2(\Theta_{aj,\gamma}F_{ji}{}^n-F_{ab}{}^n\Theta_{bi,\gamma})F_{\gamma\alpha}{}^n.$$

Using Eq. (A.2) once again, we obtain

$$X^{(r)}_{ai,\alpha}={}^1/_2[C_2(r_L)+C_2(r_R)]\Theta^{(r)}_{ai,\alpha}.$$

We see that the explicit dependence on the representation r of the scalar particles has disappeared. Thus

$$\beta_r=-\frac{3h_rg^2}{8\pi^2}\frac{C_2(r_L)+C_2(r_R)}{2}$$

in agreement with the calculations of Sec. 3.

1)The fact that the large-field limit corresponds to a passage to short distances follows from the circumstance that the field-dependence of the effective coupling constants in the effective Lagrangian duplicates the dependence of these constants on the momentum (for some definition of the renormalized charges). Moreover, it can be seen from the Feynman diagrams that large values of the external scalar fields as well as large external momenta cut off the region of integration with respect to small momenta, i.e., the contribution of large distances.

2)For switched off sources we shall assume that simultaneously $\Phi_r\to v_r$ and $\Phi'_r\to v_r$, which reduces to the normalization $\zeta_r(\Phi'_s)=1$ condition for ζ_r with all $\Phi'_s=v_s$. This implies some change of the normalization and will be discussed in detail below.

3)We note that the constants defined according to (37) and (36) differ by quantities of the order g^2.

4)One can verify that this is the situation which arises in the renormalization of the coupling constants in a $\lambda\phi^4$ coupling. If one requires chiral invariance of these interactions by imposing relations on the coupling constants λ, then these relations will be violated already in first order in g^2, so that in this sense the Yukawa couplings are unique.

[1]H. Georgi and S. L. Glashow, Phys. Rev. D7, 2457 (1973).
[2]G. Jona-Lasinio, Nuovo Cimento 34, 1790 (1964).
[3]S. Coleman and E. Weinberg, Phys. Rev. D7, 1888 (1973).
[4]A. A. Ansel'm and D. I. D'yakonov, Zh. Eksp. Teor. Fiz. 68, 1614 (1975) [Sov. Phys. JETP 41, 809 (1975)].

Translated by M. E. Mayer

Nonadiabatic transitions between decaying states

V. A. Bazylev, N. K. Zhevago, and M. I. Chibisov

I. V. Kurchatov Atomic Energy Institute

(Submitted February 24, 1976; resubmitted May 24, 1976)
Zh. Eksp. Teor. Fiz. 71, 1285–1298 (October 1976)

Processes of the charge exchange type between multiply charged ions and atoms are investigated taking into account the decay of states due to Auger ionization. It is shown that for sufficiently slow collisions with a small resonance defect the decay of states can significantly alter the probability of elastic collisions and the probability of charge exchange. It is also shown that along with the traditional charge exchange scheme a stepwise charge exchange is possible as a result of coherent interaction of states, between which electron transitions occur, via virtual states of the continuous spectrum. The probability of stepwise charge exchange is calculated taking into account the interference between two channels.

PACS numbers: 34.60.+z, 32.10.Qy

INTRODUCTION

In many problems of the physics of atomic collisions one has to consider transitions between states which decay into the continuous spectrum in the course of the collision. Transitions occurring in collisions of multiply charged ions and atoms,[1,2] in collisions of many-electron atoms with the formation of vacancies in the inner shells[3,4] and in many other cases[5,6] are of such a nature. All the aforementioned processes are characterized by the fact that the lifetime of quasimolecular states between which the transition occurs can be comparable with the time of their interaction in the act of collision.

In investigating the effect of the interactions between states decaying into a common continuum on the probability of a transition it is necessary to distinguish two cases, which practically can be realized in the case of atomic collisions and which in a certain sense are limiting cases. In the first case only the direct interaction between two states and, consequently, only the usual channel for the transition from the initial state to the final state is essential, while the interaction between

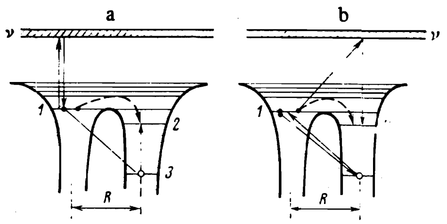

FIG. 1. Possible channels for charge exchange in the case of a collision of a multiply charged ion with a neutral atom.

states and the continuous spectrum leads only to their decay. In the second case the coherent interaction between two states via the intermediate virtual (but close to real) states of the discrete and the continuous spectrum is essential. Therefore a stepwise transition from the initial state into the final state can be realized, and also the interference of this transition with the direct one.

Specifically we consider charge exchange in a collision of a multiply charged ion with a neutral atom. In the initial state $|1\rangle$ let both electrons be situated in the atom, while the final state $|2\rangle$ is formed as a result of the transition of one of the electrons into the excited state of the multiply charged ion closest is energy. If the transition from the state $|2\rangle$ into the ground state $|3\rangle$ is allowed, then in addition to the usual channel for charge exchange brought about by the exchange interaction and shown in Fig. 1a by the broken line another channel is opened up shown in the diagram by solid lines. The role played by the second electron which is virtually Auger-emitted and absorbed by the atom reduces to satisfying the law of conservation of energy, or in fact to guaranteeing the coherent interaction of the states $|1\rangle$ and $|2\rangle$ via the intermediate resonance state. In this case the problem consists of determining the probability of stepwise charge exchange and of its interference with the direct charge exchange. The necessary investigation is carried out in §3 of the present paper.

If the transition from the excited state of the ion into the ground state is forbidden (Fig. 1b), then, in principle, a charge exchange channel is possible in which the electron undergoing the transition is emitted by the atom, and is absorbed by the ion. An anologous situation is also possible in the case of a two-electron charge exchange. As will be shown below, in this case for the process under consideration, just as for a majority of the problems of atomic collisions with a distant crossover of terms, the stepwise charge exchange can be neglected, since the de Broglie wavelength for the electron in the continuous spectrum is considerably smaller than the internuclear distances R, which are effective for charge exchange. Then the problem consists of investigating the effect of the decay of the states on the probability of direct charge exchange. The corresponding results are given in §2.

§1. FORMULATION OF THE PROBLEM

From a formal point of view in the phenomena under investigation two quadiscrete states interact within a given time interval both with each other and with the states of an unbounded continuous spectrum.[1)] For the slow collisions of atomic particles considered in this paper the states of the continuous spectrum can be excluded from the time-dependent Schrödinger equation in a manner analogous to the way this was done in the paper by Lisitsa and Yakovlenko[7] and under the same assumptions. As a result a system of equations is obtained for the amplitudes of only the quasidiscrete states $|1\rangle$ and $|2\rangle$, while the effect of the continuous spectrum in this system is taken into account by introducing the widths and shifts of the states $|1\rangle$ and $|2\rangle$ under consideration and their effective interaction through the intermediate virtual states of the continuous spectrum

$$i\dot a_1=[E_1(t)-i\Gamma_1(t)]a_1+V(t)a_2,\qquad\qquad (1)$$
$$i\dot a_2=[E_2(t)-i\Gamma_2(t)]a_2+V(t)a_1,$$

where

$$E_n(t)=H_{nn}(t)+\Delta_{nn}(t),\qquad n=1,2.$$
$$V(t)=H_{12}(t)+\Delta_{12}(t)-i\Gamma_{12}(t).$$

The expansion coefficients of the total wave function in the diabatic basis $a_1(t)$, $a_2(t)$ as $t\to\pm\infty$ can be interpreted as probability amplitudes for finding the system in some particular state. The matrix elements of the electron Hamiltonian $H_{nm}(t)$ depend implicitly on the time through the internuclear distance $R(t)$. The widths $2\Gamma_n(t)$ and the shifts $\Delta_{nn}(t)$ of the states can be expressed in terms of the matrix elements $H_{nk}(t)$ which connect the state $|n\rangle$ under consideration with one of the states of the continuous spectrum $|k\rangle$, and the density of the final states $\rho(k)$ in the following manner

$$\Gamma_n(t)=\pi\int\delta[(H_{11}+H_{22})/2-k^2/2]H_{nk}^2(t)\rho(k)\,dk\,d\Omega_k,\qquad (2)$$
$$\Delta_{nn}(t)=\int d\Omega_k\int_0^\infty\frac{H_{nk}^2(t)\rho(k)\,dk}{(H_{11}+H_{22})/2-k^2/2},$$

$\delta(x)$ is the Dirac delta-function. The quantities Γ_{12}, Γ_{21}, Δ_{12}, Δ_{21} describing the interaction of the decaying states via the continuous spectrum are equal to

$$\Gamma_{nm}(t)=\pi\int H_{nk}(t)H_{km}(t)\delta[(H_{11}+H_{22})/2-k^2/2]\,dk\,d\Omega_k.\qquad (3)$$
$$\Delta_{nm}(t)=\int d\Omega_k\int_0^\infty\frac{H_{nk}(t)H_{km}(t)\rho(k)}{(H_{11}+H_{22})/2-k^2/2}dk,\quad (n,m=1,2;\ n\neq m).$$

The system of equations (1) is non-Hermitian, the derivative $d(|a_1|^2+|a_2|^2)/dt$ is equal to the total rate of decay of both states $|1\rangle$ and $|2\rangle$.

Analysis shows that the interaction of the states $|1\rangle$ and $|2\rangle$ via the intermediate states of the continuous spectrum depends on the different physical parameters for two different channels of stepwise charge exchange (cf., Figs. 1a, b). The interaction leading to channel a which is characterized by the emission and absorption of an electron by the same atom can be expressed only in terms of the decay parameters $\Gamma_1(t)$ and $\Gamma_2(t)$

$$\Gamma_{12}(t)=(\Gamma_1(t)\Gamma_2(t))^{1/2}.\qquad (4)$$

As the atoms move apart this interaction is "switched off" simply because the states become stable as $t \to \pm\infty$.

The interaction leading to the channel b which is characterized by the emission and absorption of an electron by different atoms is, generally speaking, considerably more complicated. Under the fairly realistic assumption that all directions of emission of the electron are equally probable, while the widths do not depend on the energy, it has the form

$$\Gamma_{12}=(\Gamma_1\Gamma_2)^{1/2}\sin k_eR/k_eR. \quad (5)$$

The presence of the factor $\sin k_eR/k_eR$ is quite essential. It guarantees the "switching off" of the interaction via the virtual states of the continuous spectrum even in the case when $H_{nk}(R) \to \text{const}$ as $R \to \infty$. (Such behavior of the matrix element means that if the electron is situated in the field of each isolated atom, then this atom decays.) For the majority of problems of the type under consideration the parameter k_eR is large ($k_eR \gg 1$), and therefore one can neglect the interaction between states via the continuous spectrum. If at the same time one neglects the shifts Δ, treating them as quantities which are numerically even smaller, then from the system (1) we will arrive at the system of equations investigated earlier.[6] In this system only the widths $2\Gamma_1$ and $2\Gamma_2$ are contributed by the states of the continuous spectrum.

§2. THE EFFECT OF THE DECAY OF STATES ON THE PROBABILITY OF CHARGE EXCHANGE

In this section we investigate the effect of the decay of states on the probability of charge exchange in the case when one can neglect the interaction between these states via the continuous spectrum. Such a problem had been investigated earlier within the framework of the Landau–Zener model[6] and, in particular, the limitation of this model was demonstrated associated with the fact that as the difference in the decay constants $\Delta\Gamma$ is increased the rapidly growing region of essential interaction between the terms can include those ranges of internuclear distances within which the terms are practically parallel, and do not diverge linearly. Therefore for a complete solution of the formulated problem the model selected must describe in a sufficiently realistic manner the behavior of the terms and the exchange interaction far from the point of quasi-intersection.

With this aim in mind we approximate the dependence of the matrix elements of the Hamiltonian of the system (1) in the following manner;

$$[E_2(t)-i\Gamma_2]-[E_1(t)-i\Gamma_1]=\Delta E(1-\beta e^{2\alpha t})-i\Delta\Gamma, \quad V(t)=Ve^{\alpha t}, \quad (6)$$

where ΔE is the difference in the energies of the terms at a sufficiently great distance between the nuclei (the resonance defect); $V>0$ is a characteristic value of the energy of the exchange interaction; α is the rate of change of the interaction; β is a parameter characterizing the behavior of the terms in the neighborhood of the point of intersection. For $t \geq 0$ the values of the matrix elements in (6) vary in inverse order ($\alpha \to -\alpha$), and this corresponds to a symmetric (with respect to the instant of minimum distance between the nuclei $t=0$) trajectory of relative motion.

An analogous dependence was utilized in the paper by Vitlina *et al.*[8] in calculating the charge exchange cross section in the field of an intense electromagnetic wave. In contrast to the aforementioned paper we take into account the decay of the states in the course of the reaction: $\Delta\Gamma=\Gamma_2-\Gamma_1$ is the difference in the decay constants of the terms which is assumed to be constant within the domain of the interaction. It must be noted that, as follows from the results of the work of Vitlina *et al.*,[8] the use of the relations (6) in the absence of decay does not lead to a result for the probability of charge exchange which would not be well described by the well-known Nitkitin model.[9] The difference consists only of the fact that in passing through the region of closest approach of nuclei (in the absence of decay real transitions do not occur in this region) a different phase difference of wave functions is accumulated. In averaging over this phase, which is large in both cases, the difference disappears entirely. But when decay of the states is taken into account the model (6) has a greater degree of generality than the Nikitin model. Indeed, in the Nikitin model the case when the principal contribution to the probability of charge exchange comes from the region where the terms are parallel corresponds to the situation in which terms become significantly mixed in the region of closest approach of the nuclei; i.e., the system developing according to the collective terms decays according to half the sum of the decay constants Γ_1 and Γ_2. The model utilized in the present work enables us to describe both the case referred to above ($\beta=0$) and also another one when in the region of closest approach the system develops according to isolated terms each of which decays with its own decay constant.

The particular solution of the system (1) with the model dependences (6) satisfying the initial conditions

$$|a_1(t_0)|=1, \quad t_0\to-\infty, \qquad |a_2(t_0)|=0, \quad t_0\to-\infty \quad (7)$$

can be written in the form

$$a_1(t)=\exp\left[-i\int_{t_0}^{t}\varepsilon(t')\,dt'-\Delta\Gamma t_0/2+\alpha qt-z/2\right]\Phi(-p, {}^1/_2+q, z),$$
$$a_2(t)=\exp\left[-i\int_{t_0}^{t}\varepsilon(t')\,dt'-\Delta\Gamma t_0/2+\alpha qt-z/2\right]\frac{(-pz)^{1/2}}{{}^1/_2+q}\Phi(1-p, {}^3/_2+q, z), \quad (8)$$
$$\varepsilon(t)=[E_2(t)-i\Gamma_2+E_1(t)-i\Gamma_1]/2,$$

$p=-iV^2/2\Delta E\alpha\beta$ is the Landau–Zener parameter,[10,11] $q=(\Delta E/2\alpha)[i+(\Delta\Gamma/\Delta E)]$; $\Delta E/2\alpha$ is the Rosen–Zener parameter,[14] $z=i\Delta E\exp(2\alpha t)/2\alpha$, $\Phi(a, c, z)$ is the confluent hypergeometric function. The asymptotic values of expressions (8) for the amplitudes $a_1(t)$ and $a_2(t)$ enables us to obtain the probability of the electron remaining in the atom $w_{11}(t)$, and also the probability of the transition of the electron to the ion $w_{12}(t)$ after a single passage through the essential charge exchange region, i.e., when the nuclei approach each other ($t\sim0$):

$$w_{11}(t)=\exp[2\Gamma_1 t_0]\left|\frac{\Gamma(1/2+q)}{\Gamma(1/2+q+p)}\right|^2 \exp[-i\pi p\,\mathrm{sgn}(\Delta E\beta)]\exp[-2\Gamma_1 t],$$
$$w_{12}(t)=\exp[2\Gamma_1 t_0]\left|\frac{\Delta E\beta}{2\alpha}\right|^{-\Delta\Gamma/\alpha} \qquad (9)$$
$$\times\frac{|\Gamma(1/2+q)|^2[1-\exp\{-2i\pi p\,\mathrm{sgn}(\Delta E\beta)\}]}{2\pi\exp(-\pi|\Delta E|\mathrm{sgn}\,\beta/2\alpha)}\exp[-2\Gamma_2 t].$$

where $\mathrm{sgn}\,x = x/|x|$; $\Gamma(x)$ is the Gamma function of x. We emphasize that the formulas (9) describe the charge exchange process in which within the region of closest approach of the nuclei the terms are isolated and each decays with its own decay constant. We consider two limiting cases of expressions (9) which enable us to investigate in detail the effect of the decay of intersecting terms and also of terms parallel within the effective region of interaction on the probability of transition between them.

1. Let the principal contribution to the probability of these processes be given by the immediate neighborhood of the point of intersection which occurs at relatively large values of the resonance defect

$$|\Delta E/\alpha| \gg \max\,(1,\ |V^2/\Delta E\alpha\beta|). \qquad (10)$$

Utilizing the asymptotic representation of the Γ-functions in (9) for large values of the parameter q we obtain

$$w_{11}(t)=\gamma_1(t',t_0)\exp\left[-\frac{\pi V^2}{|\Delta E|\alpha\beta}\left(1-\frac{1}{\pi}\,\mathrm{arctg}\frac{\Delta\Gamma}{|\Delta E|}\right)\right]\gamma_1(t,t'),$$
$$w_{12}(t)=\gamma_1(t',t_0)\left[1-\exp\left(-\frac{\pi V^2}{|\Delta E|\alpha\beta}\right)\right]\exp\left(\frac{\Delta E}{\alpha}\,\mathrm{arctg}\frac{\Delta\Gamma}{\Delta E}-\frac{\Delta\Gamma}{\alpha}\right)\gamma_2(t,t'), \qquad (11)$$
$$\gamma_i(t_1,\ t_2)=\exp[-2\Gamma_i(t_1-t_2)], \quad i=1,\ 2.$$

In expressions for the probabilities (11), exponential factors of the form $e^{-2\Gamma_k\tau}$ have been separated out. These factors can be taken into account in advance, as has been done by Kishinevskiĭ and Parilis,[1] by assuming that the transition between terms occurs at the point of "intersection" of the complex terms $t' = -(1/2\alpha)\ln[\beta(1+(\Delta\Gamma/\Delta E)^2)]$, and neglecting the finite size of the region of interaction between the terms. The remaining dependence of the probabilities (11) on the difference between the decay constants of the terms is associated with the effect of decay in the region of interaction of the terms. If one neglects this dependence by considering such impact parameters when the following inequalities are satisfied

$$|\Delta\Gamma/\Delta E| \ll \min\,(1,\ |\Delta E\alpha\beta|/V^2),$$
$$7|\Delta\Gamma|^3/12\alpha\Delta E^2 \ll \min\,(1,\ \exp[-\pi V^2/|\Delta E\alpha\beta|]), \qquad (12)$$

then with an accuracy up to trivial factors we shall obtain a result which agrees with the result obtained earlier[6] and which consists of the fact that the decay of the terms does not affect the process of charge exchange (apart from the appearance of trivial multiplying factors), if from the very beginning we restrict ourselves to a linear dependence of the difference between the energies of the terms on the distance to the point of intersection of the terms.

Thus, in taking into account the decay of the terms, the use of the Landau–Zener model is justified if the resonance defect is so great that in addition to the inequality (10) condition (12) is also satisfied.

It should be noted that the division of the effect of the decay of the terms into a "trivial" effect and an effect occurring in the "process of transition" is, generally speaking, arbitrary. Thus, for example, the probability of a transition of an electron to an ion when the nuclei approach each other extrapolated to the point of intersection of the terms (for $t = t'$) can for a sufficiently large value of Γ_2 exceed not only the transition probability according to Landau–Zener[10,11] but also can exceed unity. However, the population of the state of the electrons in the ion at the instant of interaction t' is an unobservable quantity. In order to measure the population of this state it is necessary that a time should elapse greater than the duration of the interaction. It is just at such times that the asymptotic expressions (9) and (11) are valid, and the probability $w_{12}(t)$ is less than unity. The example cited above demonstrates the arbitrary nature of splitting up the effect of decay, however, such a splitting up turns out to be convenient in comparing and interpreting results.

Thus, a comparison of the probability w_{11} of an elastic process as the nuclei are made to approach each other (cf., (11) without the trivial factors) with the corresponding probability according to Landau–Zener (cf., (11) for $\Gamma_1 = \Gamma_2 = 0$) shows that these quantities differ by a factor of $\exp[V^2\tan^{-1}(\Delta\Gamma/\Delta E)/\Delta E\,\alpha\beta]$. For relative velocities $v \sim 10^6$ cm/sec the Landau–Zener parameter $V^2/|\Delta E\,\alpha\beta|$ can attain values of ≈ 10. For a resonance defect $|\Delta E| \approx 10^{-15}$ sec^{-1} and for decay constants $\Gamma_2 \approx 10^{14}$ sec^{-1} ($\Gamma_1 \ll \Gamma_2$), which is characteristic for collisions of multiply charged ions with neutral atoms, the probability of an elastic process, according to our results, is reduced by a factor of e compared with the usual theory which does not take decay into account.

The ratio of R_1, the probability of charge exchange as the nuclei approach each other, to the corresponding probability according to Landau–Zener is illustrated by a graph (Fig. 2). Along the vertical axis we plot the logarithm of this ratio, and along the horizontal axis we plot the Rozen–Zener parameter $x = |\Delta E|/2\alpha$. The different curves correspond to different ratios of the difference between the decay constants to the resonance defect ($\delta = \Delta\Gamma/|\Delta E|$). It can be seen that for a fixed

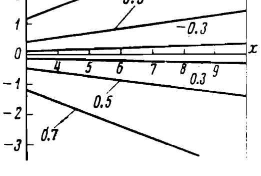

FIG. 2. The logarithm of the ratio of the probability of charge exchange taking the decay of terms into account to the probability of charge exchange according to Landau–Zener as a function of x—the ratio of the resonance defect $|\Delta E|$ to the quantity $2\alpha = 2v(2\varepsilon)^{1/2}$ (ε is the greatest of the electron binding energies in the atom and the ion, v is the relative velocity of the nuclei) for different parameters $\delta = \Delta\Gamma/|\Delta E|$ ($\Delta\Gamma$—is the difference between the decay constants for the states of the electron in an ion and in an atom).

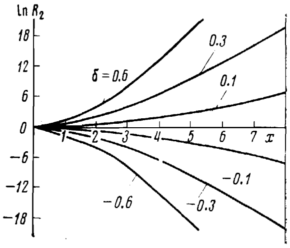

FIG. 3. The logarithm of the ratio of the probability of charge exchange (elastic collision) taking the decay of the terms into account to the probability of charge exchange (elastic collision) according to Rozen–Zener as a function of the parameter $|\Delta E|/2\alpha$ for different values of $\delta = \Delta\Gamma/|\Delta E|$.

resonance defect the deviation of the theory which takes into account the decay of terms from the usual theory is the greater, the greater is the difference between the decay constants of the terms and the smaller is the relative velocity of the nuclei ($v \sim \alpha$).

2. Further, let the principal contribution to the probability of the processes be given by the region in which the terms are parallel, and this is satisfied for relatively small values of the resonance defect

$$|V^2/\Delta E\alpha\beta| \gg \max(1, |\Delta E|/\alpha). \tag{13}$$

Then the expressions for the probabilities (9) can be represented in the form

$$\begin{aligned} w_{11}(t) &= \gamma_1(t_1, t_0)\frac{|\Gamma(^1/_2+q)|^2}{2\pi\exp(\pi|\Delta E|/2\alpha)}\gamma_{12}(t_2, t_1)\gamma_1(t, t_2),\\ w_{12}(t) &= \gamma_1(t_1, t_0)\frac{|\Gamma(^1/_2+q)|^2}{2\pi\exp(-\pi|\Delta E|/2\alpha)}\gamma_{12}(t_2, t_1)\gamma_2(t, t_2),\\ \gamma_{12} &= (\gamma_1\gamma_2)^{1/2},\quad t_2=(1/\alpha)\ln(V/|\Delta E\beta|),\quad t_1=(1/\alpha)\ln(2\alpha/V). \end{aligned} \tag{14}$$

Factors of the form $\gamma_{12}(t_2, t_1)$ and $\gamma_i(t, t_1)$ can be foreseen in advance, assuming that in the interval of time from t_1 to t_2 the electron exists in the molecular state which decays with a constant equal to half the sum of the decay constants of the atomic states, while at other times it decays with the constants Γ_1 or Γ_2 which correspond to the electron being situated in the atom or in the ion. The remaining dependence of the probability on the difference between the decay constants can be regarded as the effect of decay in the region of the transition. The ratio of the probability (14) (without "trivial" factors) to the corresponding probabilities obtained without taking into account the decay of the state, is determined by the factor $R_2 = |\Gamma(\frac{1}{2}+q)|^2/\pi\cos(\pi\Delta E/2\alpha)$. The logarithm of this ratio is graphically shown in Fig. 3 as a function of the Rozen–Zener parameter $x = |\Delta E|/2\alpha$ for different values of $\delta = \Delta\Gamma/|\Delta E|$. Just as in the case of intersecting terms the effect of the decay is the greater the greater is the ratio δ and the smaller is the relative velocity of the nuclei, with the decay effect in the case under consideration being more sensitive to a change in the parameters δ and x than in the case of intersecting terms.

The probability of charge exchange after two transitions through the interaction region can be obtained after joining the solutions of the system of equations (1) at the point of closest approach of the nuclei. The result appears to be fairly awkward, but the prescription for writing it is simple due to the fact that in the region of closest approach the terms diverge without interacting. Therefore we shall not exhibit the corresponding expressions.

3. The other limiting case which we consider also corresponds to transitions between parallel terms—but with the essential difference that in the region of closest approach of nuclei the terms are strongly "mixed" and, consequently, decay with the collective decay constant. This limit describes a weak variation of the difference in the energies of the terms during a time in the course of which the magnitude of the interaction varies from values smaller than $|\Delta E|$ to values considerably exceeding $|\Delta E|$ within the region of closest approach of the nuclei $t \approx 0$ ($\beta = 0$ in expressions (8)). Then the probability of the elastic process W_{11} and the probability of charge exchange W_{12} in the collision of an atom with an ion can be represented in the form

$$\begin{aligned} W_{11} &= \gamma_1(t_1, t_0)\pi^{-1}|\Gamma(^1/_2+q)|^2|\cos(V/\alpha-\pi q)|^2\gamma_{12}(-t_1, t_1)\,\gamma_1(t, -t_1),\\ W_{12} &= \gamma_1(t_1, t_0)|\cos\pi q|^{-2}\sin^2(2V/\alpha)\gamma_{12}(-t_1, t_1)\gamma_2(t, -t_1), \end{aligned} \tag{15}$$

where $t_1 = -(1/\alpha)\ln(V/2\alpha)$—is the "instant of transition" of the electron from an atomic state into a molecular one. As a result of the symmetry of the trajectory with respect to $t=0$ for $t=-t_1$ the wave function for the electron again becomes close to an atomic one. If we assume that the transitions from an atomic state into a molecular one and in the opposite direction take place "instantaneously" respectively at the points t_1 and $-t_1$, then the appearance in (15) of factors of the form $\gamma_{12}(-t_1, t_1)$ and $\gamma_i(t, t_1)$ becomes understandable.

Neglecting the decay of the states ($\Gamma_1 = \Gamma_2 = 0$) in expressions (15) we obtain for the probability of charge exchange

$$W_{12} = \mathrm{sech}^2(\pi\Delta E/2\alpha)\sin^2(2V/\alpha), \tag{16}$$

and this agrees with the result of Demkov.[12] The quantity V/α, which is usually large, varies rapidly corresponding to a small alteration in the impact parameter.[13] Therefore, averaging (15) over a small integral of impact parameters and considering the probability of an elastic collision in the case when the initial state of the electron in the atom has a sufficiently long lifetime ($\Gamma_1 \to 0$), we obtain the following result:

$$W_{12} = \left(\frac{V}{2\alpha}\right)^{-2\Gamma_2/\alpha}\frac{|\Gamma(^1/_2+\Delta\Gamma/2\alpha+i\Delta E/2\alpha)|^2}{\pi\,\mathrm{ch}^2(\pi\Delta E/2\alpha)}W_{11}^{(R-Z)}, \tag{17}$$

where $W_{11}^{(R-Z)} = 1 - [2\mathrm{ch}^2(\pi\Delta E/2\alpha)]^{-1}$ is the probability of an elastic collision averaged over the oscillations and calculated without taking into account the decay of the state of the electron.[14]

As has been noted already, the first factor in (17) arises as a result of the "transfer" of the decay from the second term to the first term in the case of an intense "mixing" of the terms over a fairly wide time interval $\tau \sim 2|t_1|$. The dependence of the second factor in (17) on the Rozen–Zener parameter ($x = |\Delta E|/2\alpha$) is shown in Fig. 3. This factor takes into account the "nontrivial" effect of decay in a "transition region" between the terms.

In follows from (17) that the decay of the state of the electron in an ion reduces the probability for an elastic process. If we substitute into (17) the values $V/2\alpha = 10$, $\Gamma_2 = 10^{13}$ sec^{-1} $(\Gamma_2/|\Delta E|) = 10^{-1}$, $|\Delta E|/2\alpha = 1$, and this is quite realistic for not too rapid collisions ($v \lesssim 10^7$ cm/sec), then W_{11} turns out to be smaller by a factor of 2.8 than the probability according to Rozen–Zener $W_{11}^{(R-Z)}$.

4. The discussion given above confirms the qualitative considerations states in the Introduction concerning the necessity of taking into account the decay of the states in processes of the type of charge exchange between a multiply charges ion and an atom. According to the results obtained, as the nuclei move along a given trajectory one can arbitrarily distinguish several regions of relative distances between the nuclei depending on the mechanism by which the decay of the terms exerts its effect. In the range of distances where the overlapping of atomic wave functions is small $V(t) \ll [E_2(t) - E_1(t)]$, the decay reduces the population of the states in a trivial manner (as $\exp[-2\Gamma_k\tau]$). Generally speaking, there also exists a range of distances over which the overlap of atomic wave functions is great, but in the absence of decay real transitions between terms do not occur since the Massey criterion[15] required for the transitions is not satisfied. Taking decay into account within this range of relative distances leads to a "transfer" of the decay from the one term to the other one. Thus, for example, if the state within the atom is stable, then for appropriate distances between the nuclei it can decay with a constant equal to half of the decay constant of the state in the ion. This effect has an analogy in the problem of the destruction of the metastable $2S_{1/2}$ level of a hydrogen atom by an external field.[5] The role of the external field in this case is played by the relative motion of the nuclei. The parameter which determines this effect is the quantity $(\Gamma_1+\Gamma_2)\tau_{12}$, where τ_{12} is the effective time for the "mixing" of the terms.

On the other hand the decay of states can manifest itself for those relative distances between the nuclei for which the overlap of the atomic wave functions is great and at the same time the Massey criterion is satisfied $(V^2/|\Delta E|\,\alpha\beta \sim 1,\ |\Delta E|/\alpha \sim 1)$, i.e., in the region where real transitions between terms take place even in the absence of decay. In this case the decay of the states affects in a quite nontrivial manner the probability of transition between them.

§3. COHERENT INTERACTION IN THE PROCESS OF CHARGE EXCHANGE

We consider a stepwise channel for the charge exchange between a multiply charged ion and an atom in the case when the interaction of the states $|1\rangle$ and $|2\rangle$ through an intermediate stage is significant, and also the interference of this channel with the direct charge exchange channel.

The model utilized in §2 in order to obtain the probability of charge exchange is no longer able to describe adequately the effects being investigated, since for them it is essential that the terms begin to decay only during the process of interaction. In such a case the exponentially decreasing exchange matrix element appears both in the real interaction Re $V(t)$, and in the widths of both terms $\Gamma_1(t)$, $\Gamma_2(t)$ and, consequently, it turns out to be possible to describe the dependence of all the coefficients in equations (1) by a single exponential dependence. In this case of the exactly soluble models only the Nikitin model[9] with complex parameters enables one to formalize the problem in a noncontradictory and most general manner (cf., also the text following formulas (22)):

$$[E_2(t)-i\Gamma_2(t)]-[E_1(t)-i\Gamma_1(t)]=\Delta E(1-be^{\alpha t}),\qquad V(t)=(V-iU)e^{\alpha t},\ -\infty<t\leqslant 0, \tag{18}$$

where the quantities $b=\beta(1+i\Delta\Gamma/\Delta E)$ and $V(t)$ are complex. In this case $U=(\Gamma_1\Gamma_2)^{1/2}$ for channel a (Fig. 1) and $U=(\Gamma_1\Gamma_2)^{1/2}\sin k_e R_0/k_e R_0$ for channel b.

To obtain the probability of charge exchange it is necessary to solve equations (1) with model dependences of the form (18) and initial conditions (7), and then to connect these solutions with solutions valid for $t\geq 0$, and to examine the asymptotic expressions for the amplitudes, the square of whose modulus determines the desired probability.

1. We first investigate the processes occurring when the nuclei are brought closer together. The solution which describes the evoluation of the amplitudes of the states as the nuclei are brought closer together has the form

$$a_1(t)=\left(i\frac{\varkappa}{\alpha}\right)^{-\tilde q} M_{\lambda,\tilde q-1/2}(z)\exp\left[-i\int_{-\infty}^{t}\varepsilon(t')\,dt'\right],$$
$$a_2(t)=\left(i\frac{\varkappa}{\alpha}\right)^{-\tilde q}\frac{(\lambda/\tilde q-1)(\lambda/2\tilde q+1/2)\varkappa}{2(2\tilde q+1)(V-iU)}M_{\lambda,\tilde q+1/2}(z)\times\exp\left[-i\int_{-\infty}^{t}\varepsilon(t')\,dt'\right], \tag{19}$$

where

$$\tilde q=i\Delta E/2\alpha,\quad \lambda=i\Delta E^2 b/2\alpha\varkappa,$$

$\varkappa=[4(V-iU)^2+(\Delta E b)^2]^{1/2}$, $z=i\varkappa\exp(\alpha t)/\alpha$, and $M_{\lambda,\mu}(z)$ is a Whittaker function.

Let the terms intersect within the effective region of interaction, so that the principal contribution to the probabilities of the processes comes from the immediate neighborhood of the point of intersection

$$|\Delta E/2\alpha|\gg\max(1,\ |(V-iU)^2/\Delta E\alpha b^2|). \tag{20}$$

In this approximation $\lambda=\tilde q+\tilde p$, where $\tilde p=-i(V-iU)^2/\Delta E\,\alpha b^2$ is the generalized Landau and Zener parameter, and for the probability to remain in the original state $|a_1(t)|^2$ and for the probability to make a transition to another term $|a_2(t)|^2$ in the case when

$$\exp(\alpha t)\gg|(\tilde q-\lambda)(\tilde q+\lambda+1)\alpha/\varkappa| \tag{21}$$

we obtain the following expressions:

$$
\begin{aligned}
&|a_1(t)|^2=D_1(-\infty,\ t')w_{11}D_1(t',\ t)\exp[2\alpha\,\mathrm{Re}\,\tilde{p}(t-t')],\\
&w_{11}=\exp[2\,\mathrm{Im}\,\tilde{p}(\pi\,\mathrm{sgn}\,\Delta E-\mathrm{arctg}\,\Delta\Gamma/\Delta E)],\\
&|a_2(t)|^2=D_1(-\infty,\ t')w_{12}D_2(t',\ t)\exp[-2\alpha\,\mathrm{Re}\,\tilde{p}(t-t')],\\
&w_{12}=\frac{2\pi\exp(4\,\mathrm{Im}\,\tilde{q}\,\mathrm{arctg}\,\Delta\Gamma/\Delta E)}{|\tilde{p}||2\tilde{\gamma}|^{2\,\mathrm{Re}\,\tilde{p}}|\Gamma(-\tilde{p})|^2}\exp\left[-\frac{2\Delta\Gamma}{\alpha}\left(1+\left(\frac{\Delta\Gamma}{\Delta E}\right)^2\right)^{1/2}\right]\\
&\quad\times\exp[\mathrm{Im}\,\tilde{p}(\pi\,\mathrm{sgn}\,\Delta E+2\,\mathrm{arctg}\,\Delta\Gamma/\Delta E)+4\,\mathrm{Re}\,\tilde{p}],\\
&D_i(t_1,t_2)=\exp\left[-\int_{t_1}^{t_2}\Gamma_i(t)\,dt\right],\qquad t'=(1/\alpha)\ln|b|.
\end{aligned}
\tag{22}
$$

The factors $\exp[\pm 2\alpha\,\mathrm{Re}\,\tilde{p}(t-t')]$ are determined by the interference of the two charge exchange channels which, apparently, does not disappear after passage through a point of quasi-intersection, and in the region between two consecutive points of quasi-intersection leads either to an increase or to a decrease in the rates of decay of these states.

We note that the quantities w_{11} and w_{12}, which should not be interpreted as the probabilities for remaining on a particular term or making a transition to another term, can also be greater than unity, which directly means merely a slowing down of the decay.

Expressions (22) represent a result of a limiting transition from the general case to the particular case of Landau–Zener. This result explicitly contains parameters of the general model α and ΔE: rate of growth of the interaction and the splitting of the terms for $t\to-\infty$, which do not play a role in the Landau–Zener model for decaying states (excluding, of course, the difference in the forces $\Delta F\equiv\Delta E\alpha\beta^2/v$). Therefore, we emphasize that expressions (22) cannot be obtained from an *a priori* Landau–Zener model. Moreover, if one takes into account the interference of the direct charge exchange channel with the stepwise one, then within the framework of this model it is not possible to specify correctly the initial conditions due to the insufficiently rapid "switching off" of the interaction and, consequently, in general to obtain a noncontradictory result capable of sensible interpretation.

But if we neglect the direct charge exchange ($V=0$), and also the difference in the widths of the terms ($\Delta\Gamma=0$), then the corresponding formulas for the probabilities of stepwise charge exchange as the nuclei are brought closer together, which now can be obtained within the framework of the Landau–Zener model, have the form

$$
\begin{aligned}
&|a_1(t)|^2=D_1(-\infty,t')\exp\left(\frac{2\pi V^2}{|\Delta E|\alpha\beta^2}\right)D_1(t',t),\\
&|a_2(t)|^2=D_1(-\infty,t')\left[\exp\left(\frac{2\pi V^2}{|\Delta E|\alpha\beta^2}\right)-1\right]D_2(t',t).
\end{aligned}
\tag{23}
$$

As a result of two passages through a point of quasi-intersection the desired probabilities for the elastic process W_{11} and for charge exchange W_{12} can be written in the following form:

$$
\begin{aligned}
&W_{11}=W_{11}^{(1)}+W_{11}^{(2)}+(W_{11}^{(1)}W_{11}^{(2)})^{1/2}\cos\varphi,\\
&W_{12}=W_{12}^{(1)}+W_{12}^{(2)}-(W_{12}^{(1)}W_{12}^{(2)})^{1/2}\cos\varphi,\\
&W_{11}^{(1)}=D_1(-\infty,t')w_{11}D_1(t',-t')\exp(-4\alpha\,\mathrm{Re}\,\tilde{p}t')\overline{w}_{11}D_1(-t',\infty),\\
&W_{11}^{(2)}=D_1(-\infty,t')w_{12}D_2(t',-t')\exp(4\alpha\,\mathrm{Re}\,\tilde{p}t')\overline{w}_{21}D_1(-t',\infty),\\
&W_{12}^{(1)}=D_1(-\infty,t')w_{12}D_2(t',-t')\exp(4\alpha\,\mathrm{Re}\,\tilde{p}t')\overline{w}_{22}D_2(-t',\infty),\\
&W_{12}^{(2)}=D_1(-\infty,t')w_{11}D_1(t',-t')\exp(4\alpha\,\mathrm{Re}\,\tilde{p}t')\overline{w}_{12}D_2(-t',\infty),
\end{aligned}
\tag{24}
$$

Here $\varphi=\int_{t'}^{-t'}[E_1(t)-E_2(t)]\,dt/2$ is the real phase arising as a result of interference of different paths of making the transition to the final state. The "probabilities" on separation $\overline{w}_{ik}(i,\ k=1,\ 2)$ can be expressed in terms of the "probabilities" w_{ik} as the nuclei are brought closer together (cf., (22)) in the following manner:

$$
\begin{aligned}
&\overline{w}_{11}\equiv w_{11},\quad \overline{w}_{22}=w_{11}(-\Delta E,\ -\Delta\Gamma),\\
&\overline{w}_{21}\equiv w_{12},\quad \overline{w}_{12}=w_{12}(-\Delta E,\ -\Delta\Gamma).
\end{aligned}
\tag{25}
$$

2. We further investigate the case when in the essential region of transition the unperturbed terms are in practice parallel, while the nondiagonal matrix element of the interaction varies rapidly from values considerably smaller than the difference in the energies of the unperturbed terms up to values considerably in excess of this quantity

$$
\left|\frac{(V-iU)^2}{\Delta E\alpha b^2}\right|\gg\max\left(1,\ \frac{|\Delta E|}{2\alpha}\right).
\tag{26}
$$

In this case for times t satisfying the inequality (21) it is convenient to go over from the states $|1\rangle$ and $|2\rangle$ to a collective symmetric $|s\rangle$ and antisymmetric $|a\rangle$ states

$$
a_s(t)=\frac{a_1(t)+a_2(t)}{2},\qquad a_a(t)=\frac{a_1(t)-a_2(t)}{2}.
$$

Then $a_s(t)$ will have the meaning of the amplitude of the probability to find the system in the symmetric state after passing through the effective region of the interaction, while $a_a(t)$ has the meaning of the amplitude of the probability to find the system in the antisymmetric state. When condition (26) is satisfied then from the asymptotic values of expressions (19) we obtain

$$
\begin{aligned}
&|a_{s,a}(t)|^2=D_1(-\infty,t_1)|A_{1s,a}|^2\exp\left\{-i\,\mathrm{Im}\int_{t_1}^{t}[\varepsilon(t)\pm V(t)]\,dt\right\},\\
&A_{1s,a}=\pi^{-1/2}\Gamma(1/2+\tilde{q})\exp\left[i\tilde{q}\left(\mathrm{arctg}\frac{U}{V}\pm\frac{\pi}{2}\right)+\frac{2U-\Delta\Gamma}{(V^2+U^2)^{1/2}}\right],
\end{aligned}
\tag{27}
$$

where $t_1=(-1/\alpha)\ln[(V^2+U^2)^{1/2}/2\alpha]$ is the instant of transition into the symmetric or the antisymmetric state.

Formulas (27) are easily interpreted. The adiabatic development of the initial state $|1\rangle$ (the factor $D_1(-\infty,t_1)$) at the point t_1 is replaced by the transition of the system into the collective symmetric and antisymmetric states (A_{1s}, A_{1a} are the amplitudes for the formation of these states). From formulas (27) it follows that the "probabilities" for the formation of collective states $|A_{1s}|^2$ and $|A_{1a}|^2$ depend in an essential manner both on the decay of the states $\Delta\Gamma$, and also on their interaction U via the continuum. After the instant t_1 the further development of the system according to the symmetric and the antisymmetric states is "marked" by the interference between the different decay channels which can lead to a significant decrease in the rate of the decay of the symmetric state, and, conversely, to an increase in the rate of decay of the antisymmetric state. Indeed, in the propagation amplitudes for these states in accordance with (27) the following factors appear

$$\exp\left[-\int_{t_0}^{t}\frac{\Gamma_1(t)\mp 2\,\mathrm{Im}\,V(t)+\Gamma_2(t)}{2}dt\right].$$

Therefore for $\mathrm{Im}\,V(t)=[\Gamma_1(t)\Gamma_2(t)]^{1/2}$, $\Gamma_1=\Gamma_2$ the symmetric state is stable, while the antisymmetric state decays twice as fast. This phenomenon is brought about by the coherent interaction of states via the continuum and is analogous to the Dicke problem[16] dealing with the collective spontaneous radiation from identical two-level systems situated within a volume whose linear dimensions are much smaller than a wavelength.

The result of two passages through the significant region of interaction obtained by joining together the solutions obtained for nuclei approaching and receding from each other we can write in the form

$$W_{11}=\exp\left[-\frac{2\Delta E}{\alpha}\mathrm{arctg}\frac{U}{V}-\frac{2(\Gamma_1+\Gamma_2)}{\alpha}\right]\frac{|\cos(2V/\alpha-i\pi\Delta E/2\alpha-i2U/\alpha)|^2}{\mathrm{ch}^2(\pi\Delta E/2\alpha)},$$
$$W_{12}=\exp\left[-\frac{2(\Gamma_1+\Gamma_2)}{\alpha}\right]\frac{|\sin(2V/\alpha-i2U/\alpha)|^2}{\mathrm{ch}^2(\pi\Delta E/2\alpha)}. \quad (28)$$

In the limiting case of the absence of decay ($\Gamma_1=\Gamma_2=U=0$) this result coincides with the results of Rozen-Zener[14] and of Demkov.[12]

If we neglect the direct charge exchange ($V=0$) we obtain the probability for the elastic process and the probability for the stepwise charge exchange

$$W_{11}=\exp\left[-\frac{\pi\Delta E}{\alpha}-\frac{2(\Gamma_1+\Gamma_2)}{\alpha}\right]\frac{\mathrm{ch}^2(\pi\Delta E/2\alpha+2U/\alpha)}{\mathrm{ch}^2(\pi\Delta E/2\alpha)},$$
$$W_{12}=\exp\left[-\frac{2(\Gamma_1+\Gamma_2)}{\alpha}\right]\frac{\mathrm{sh}^2(2U/\alpha)}{\mathrm{ch}^2(\pi\Delta E/2\alpha)}. \quad (29)$$

If in expressions (28) we average over the phase $2V/\alpha[\langle\sin^2(2V/\alpha)\rangle=\frac{1}{2}]$, then the general result is somewhat simplified:

$$W_{11}=\exp\left[-\frac{2\Delta E}{\alpha}\mathrm{arctg}\frac{U}{V}-\frac{2(\Gamma_1+\Gamma_2)}{\alpha}\right]\frac{\mathrm{ch}(4U/\alpha+\pi\Delta E/\alpha)}{2\,\mathrm{ch}^2(\pi\Delta E/2\alpha)},$$
$$W_{12}=\exp\left[-\frac{2(\Gamma_1+\Gamma_2)}{\alpha}\right]\frac{\mathrm{ch}(4U/\alpha)}{2\,\mathrm{ch}^2(\pi\Delta E/2\alpha)} \quad (30)$$

We note that in those cases when the interaction through the states of the continuous spectrum has the form $U=(\Gamma_1\Gamma_2)^{1/2}$, while the rates of decay are close to one another ($\Gamma_1=\Gamma_2$), then, as follows from (30), in the case of infinitely great decay ($\Gamma_{1,2}\to\infty$) the probability of the elastic process W_{11} and the probability of a transition W_{12} are finite

$$W_{11}=[4\,\mathrm{ch}^2(\pi\Delta E/2\alpha)]^{-1},\quad W_{12}=[4\,\mathrm{ch}^2(\pi\Delta E/2\alpha)]^{-1}. \quad (31)$$

This result also means that even in the case of infinitely slow motion of the nuclei the probability of "capturing" an Auger-electron differs from zero. Such an effect is associated with the fact that in a collision of atomic particles as a result of coherent interaction a metastable state arises in the stepwise channel which is symmetric (in terms of the initial stages). It is just along this nondecaying channel that the process of charge exchange is realized.

CONCLUSION

In conclusion we indicate one circumstance associated with the impossibility—in the general case—of excluding the continuous spectrum from the time-dependent Schrödinger equation. The possibility of such a procedure or, in other words, the possibility of diagonalizing the energy matrix, is closely associated with the independence of the Hamiltonian on the time.[17–19] But if the Hamiltonian is time-dependent—then the different states of the continuous spectrum are "mixed" as a result of the motion of the atoms (the matrix elements $(\partial/\partial t)_{kk'}$ or $H_{kk'}$ differ from zero). In the processes considered in this work which occur at large internuclear distances one can neglect the mixing of the states of the continuous spectrum. But if the matrix elements $(\partial/\partial t)_{kk'}$ are not small, then transitions take place between different states of the continuous spectrum (which are not excluded by a well-known procedure).[7,17–19] Their influence on the process of atomic collisions could be the object of a separate investigation, particularly when the problem is set of finding the spectrum of the Auger electrons which gives, in a definite respect, richer information concerning the collision process. (In a developed formalism the spectrum of Auger-electrons is in fact determined by taking the Fourier-components of the amplitudes $a_1(t)$ and $a_2(t)$ obtained in the present work.)

We note that the results obtained in this paper can be useful not only for the calculation of charge exchange of multiply charged ions with atoms. Other possible applications of the theory developed in this work can be processes of the transfer of excitation between metastable levels (in particular, the Penning ionization[20,21]), collisions of negatively charged ions with neutral atoms, and also processes of ionization of internal shells when many-electron atoms collide with ions, as has been mentioned in the Introduction.

The authors are grateful to O. B. Firsov for discussion of the results of the present work, and also to V. I. Glebov for numerical calculations on an electronic computer.

[1)]The discrete state $|3\rangle$ is included in the continuous spectrum.

[1]L. M. Kishinevskiĭ and É. S. Parilis, Zh. Eksp. Teor. Fiz. 55, 1932 (1968) [Sov. Phys. JETP 28, 1020 (1969)].
[2]É. S. Parilis, Effekt Ozhe (Auger Effect), FAN, Tashkent, 1969.
[3]V. V. Afrosimov, Yu. S. Gordeev, A. N. Zinov'ev, D. Kh. Rasulov, and A. P. Shergin, Sbornik trudov I Vsesoyuznogo seminara po avtoionizatsionnym yavleniyam (Collected Papers Presented at the I All-Union Seminar on Autoionization phenomena), MGU (Moscow State University), 1975.
[4]V. V. Afrosimov, G. A. Leiko, and M. I. Popov, Sbornik trudov I Vsesoyuznogo seminara po avtoionizatsionnym yavleniyam (Collected Papers Presented at the I All-Union Seminar on Autoionization Phenomena), MGU (Moscow State University), 1975.
[5]V. I. Kogan, V. S. Lisitsa, and A. D. Selidovkin, Zh. Eksp. Teor. Fiz. 65, 153 (1973); [Sov. Phys. JETP 38, 75 (1974)].

[6]V. A. Bazylev and N. K. Zhevago, Zh. Eksp. Teor. Fiz. 69, 853 (1975) [Sov. Phys. JETP 42, 436 (1976)].
[7]V. S. Lisitsa and S. I. Yakovlenko, Zh. Eksp. Teor. Fiz. 66, 1981 (1974) [Sov. Phys. JETP 39, 975 (1974)].
[8]R. Z. Vitlina, A. V. Chaplik, and M. V. Éntin, Zh. Eksp. Teor. Fiz. 67, 1667 (1974) [Sov. Phys. JETP 40, 829 (1975)].
[9]E. E. Nikitin, Teoriya élementarnykh atomno-molekulyarnykh reaktsiĭ (Theory of Elementary Atomic-Molecular Reactions), Novosibirsk (1971).
[10]L. D. Landau, Phys. Z. Sowjetunion 2, 41 (1932).
[11]C. Zener, Proc. R. Soc. Lond. A137, 696 (1932).
[12]Yu. N. Demkov, Zh. Eksp. Teor. Fiz. 45, 195 (1963) [Sov. Phys. JETP 18, 138 (1964)].
[13]B. M. Smirnov, Asimptoticheskie metody v teorii atomnykh stolknoveniĭ (Asymptotic Methods in the Theory of Atomic Collisions), Atomizdat, 1973.
[14]N. Rozen and C. Zener, Phys. Rev. 40, 502 (1932).
[15]N. Mott and G. Massey, Theory of Atomic Collisions (Russ. Transl., "Mir," M., 1969).
[16]R. H Dicke, Phys. Rev. 93, 99 (1954).
[17]R. Kh. Propin, Opt. Spektrosk. 8, 300 (1960); 10, 308 (1961).
[18]V. Fano, Phys. Rev. 124, 1866 (1961).
[19]Y. Pietenpol, Phys. Rev. 162, 1301 (1967).
[20]K. Katzuura, J. Chem. Phys. 42, 3771 (1965).
[21]B. M. Smirnov and O. B. Firsov, Pis'ma Zh. Eksp. Teor. Fiz. 2, 478 (1965) [JETP Lett. 2, 297 (1965)].

Translated by G. Volkoff

Decay and excitation of a quantum system following two successive sudden changes in the Hamiltonian

G. V. Golubkov, F. I. Dalidchik, and G. K. Ivanov

Institute of Chemical Physics, USSR Academy of Sciences
(Submitted March 3, 1976)
Zh. Eksp. Teor. Fiz. 71, 1299–1306 (October 1976)

The response of a quantum system to two successive sudden changes of the Hamiltonian is considered. The dependence of the probabilities for various processes on the dwell time τ of the system in the intermediate state is investigated, the interaction in the intermediate state being represented by a repulsive potential of the form γ/r^2. Analytic expressions are found for the limiting cases of large and small values of τ. The deviations of the spectra of the dissociation products of diatomic molecules from the Franck–Condon distribution for resonance scattering of electrons is investigated in detail. A possible isotope effect for hydrogen molecules is noted.

PACS numbers: 03.65.—w, 31.30.Gs, 34.70.Gm

1. The problem of the transitions of a quantum system described by a time dependent Hamiltonian arises in the treatment of various processes involving the interactions of atoms and molecules. Such problems do not admit of exact solution if the transitions in the continuous spectrum are to be taken into account, and most of the known results either relate to special model Hamiltonians or have been obtained within the limitations of time dependent perturbation theory. Here we examine the reaction of a quantum system to two successive sudden changes of the Hamiltonian $H(r, t)$[1]:

$$H(r,t)=\begin{cases}H_\alpha(r), & t<0\\ H_{int}(r), & 0<t<\tau.\\ H_\beta(r), & \tau<t\end{cases} \tag{1}$$

Here H_α and H_β are the initial and final Hamiltonian, and τ is the dwell time of the system in the intermediate state described by Hamiltonian H_{int}. Such a problem was first formulated for a zero-range potential model under the initiative of Yu. N. Demkov, and the ejection of a weakly bound electron in an atomic collision was treated by Bronfin and Ermolaev[2] as an example.

However, it is easy to exhibit a wide range of physical processes and systems involving successive fast changes in the character of the binding in which the interactions are of a more complicated type. As an example we might consider processes in which the outer electron shells of atoms are reconstituted as a result of a cascade of nuclear transformations (in which the nuclear charge or the effective charge of the core of tightly bound electrons suffers changes). Specifically, we might speak of a sequence of β^+ and β^- decays of a heavy nucleus, of the nuclear photoeffect $_ZA^N(\gamma, {}_1H^1)_{Z-1}A^{N-1}$ (with subsequent ejection of a K electron by a γ ray from the excited product nucleus $_{Z-1}A^{N-1}$), etc.

The resonance scattering of an electron by a diatomic molecule,

$$e^- + \mathrm{AB}(v) \to (\mathrm{AB})^- \begin{matrix} \nearrow e^- + \mathrm{AB}(v') \\ \searrow e^- + \mathrm{A} + \mathrm{B} \end{matrix}, \tag{2}$$

may serve as another example. As can be shown, the theoretical treatment of this process involves a stage in which the problem of the reaction of the nuclear subsystem to two successive sudden changes in the interatomic potential must be solved. In fact (see, e.g., [3–6]), the amplitude for process (2) has the form (except for a constant factor)

$$A_{if}=\sum_\mu\frac{\langle\varphi_f|\sqrt{\Gamma}|\chi_\mu\rangle\langle\chi_\mu|\sqrt{\Gamma}|\varphi_i\rangle}{\varepsilon-\varepsilon_\mu+i\Gamma_\mu/2}=\int d\mathbf{r}\,\varphi_f(\mathbf{r})\sqrt{\Gamma(r)}\,\zeta(\mathbf{r}). \tag{3}$$

Here $\varphi_{i(f)}$ and χ_μ are the wave functions for the initial (final) and intermediate states of the nuclear subsystem