Coherent effects in the loss of electrons by channeled ions

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A theory is developed of inelastic collisions of ions with a crystal. Analytic expressions are obtained for the probabilities of electron excitation in an ion and for the loss of electrons by an ion when the ion is scattered by a chain of atoms, with account taken of the thermal vibrations of the lattice. It is shown that the probability of these processes in a crystal can vary significantly in comparison with an amorphous medium, because of the incoherent action of the various crystal atoms on the ion.

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1. INTRODUCTION

The theory of inelastic collisions of fast heavy ions with isolated atoms of matter was developed in the classical papers of Bethe[1] and Bloch.[2] The probability $w(\rho)$ of the formation of vacancies in the electron shells of ions and atoms depends on the distance ρ between the ion trajectory, which can be regarded as a straight line, and the nucleus of the target atom. The observed probability is obtained by averaging $w(\rho)$ over all possible impact parameters.

If the target is a crystal, then the formation of vacancies in the electron shells can lead to a number of effects that are directly or indirectly connected with the ordered arrangement of the atoms in the crystal. One such effect arises when the ion is channeled in the crystal (see, e.g., Ref. 3) along a crystallographic axis or plane. Under these conditions the ion trajectories pass at relatively large distances from the crystal nuclei, and this can lead to a decrease of the vacancy-formation probability both in the ion and in the target atoms, compared with an amorphous medium. A detailed discussion of this effect is contained, for example, in the paper of Appleton, Eginsoy, and Gibson.[4]

An effect of a different type should arise when the ion traverses in the crystal a sufficiently large distance at constant velocity along a near-linear trajectory. This, in particular, is the condition that obtains for a channeled ion. In this case the individual collisions of the ion with the target atoms are correlated in time. This correlation, as will be shown below, can lead to a substantial change of the probability of electron loss by the ion. Okorokov[5] has previously called attention to the possibility of coherent excitation of optical electron levels in an ion that passes through a crystal. The theory of the coherent excitation effect was considered later by Kalashnikov and Pankratov,[6] who used a perturbation method, and by Shindo and Ohtsuka[7] in the two-level approximation. The coherence effect arises, according to Refs. 5–7, when the characteristic frequencies of the successive collisions of the ion with the crystal atoms are close to the frequency of the transition between discrete electron levels.

The electron level of the transition can decay within the time of flight of the ion through the crystal by transition of the electron to the continuous spectrum. In this case, as was recently observed by Datz *et al.*[8] a relative increase of the probability of the electron loss by the ion is observed under conditions close to resonance. The theory of this phenomenon will be considered in the present paper. Within the framework of the general approach we shall consider also the effects of coherent excitation and coherent ionization. The major role played by thermal vibrations of the crystal atoms in processes of coherent ionization and excitation will be demonstrated, and the probabilities of these processes in a crystal and in an amorphous medium will be compared.

2. POTENTIAL OF ELECTRON-CRYSTAL INTERACTION

Assume that an ion with a nuclear charge eZ_1 moves along a channeled trajectory in the direction of a definite crystallographic axis. We assume that this axis consists of indentical atoms of matter with nuclear charge eZ_2 spaced a distance d apart. In a cylindrical coordinate system with z axis along the atom chain, the electrostatic potential of the chain can be represented in the form of a one-dimensional Fourier integral

$$U(\rho, z)=\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(-iK_z z)\, V(K_z, \rho) S(K_z)\, dK_z. \tag{1}$$

We have introduced here the notation

$$V(K_z, \rho)=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} \mathscr{V}(\mathbf{K}) \exp(-i\mathbf{K}_\perp \boldsymbol{\rho})\, d^2K_\perp,$$
$$\mathscr{V}(\mathbf{K})=4\pi e K^{-2}[Z_2-F(\mathbf{K})], \tag{2}$$

$F(\mathbf{K})$ is the form factor of the crystal atom, ρ is the radius vector and is perpendicular to the chain axis,

$$S(K_z)=\sum_m \exp[iK_z(md+z_m)] \tag{3}$$

is the structure factor of the chain, and z_m is the longitudinal displacement of the mth atom of the chain from its eqiilibrium position.

We approximate the potential of an individual atom of the chain by the Moliere potential

$$v(\mathbf{r})=\frac{eZ_2}{r}\sum_{i=1}^{3} \alpha_i \exp\left(-\frac{\beta_i r}{a}\right),$$

where $a=0.885Z_2^{-1/3}a_0$ is the Thomas–Fermi radius of the atom, and $a_0=\hbar^2/me^2$; $\alpha_i=\{0.1; 0.55; 0.35\}$, and $\beta_i=\{6.0; 1.2; 0.3\}$ are the Moliere constants. In this case, according to (2)

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$$V(K_z,\rho)=2eZ_2\sum_{i=1}^{3}\alpha_iK_0(\varkappa_i\rho), \tag{4}$$

where $K_0(\varkappa_i\rho)$ is a Macdonald function, and

$$\varkappa_i=[K_z^2+(\beta_i/a)^2]^{1/2}. \tag{5}$$

The processes considered here take place mainly at relatively close distances between the ion and one of the chains, and we can therefore neglect for simplicity the influence of the neighboring chains, and assume that the ion moves in the field of one chain.[1)] In the laboratory frame, the channeled ion moves mainly along a chain with velocity v and executes slow (compared with the frequency of the passage between the atoms) oscillations in the transverse plane.[3] In a coordinate system where the ion is on the average at rest and a chain of atoms is incident on it with velocity v, the four-potential of the chain is given by

$$U'(\rho,z')=\frac{\gamma}{2\pi}\int_{-\infty}^{\infty}\exp[-iK_z\gamma(z'+vt')]V(K_z,\rho)S(K_z)dK_z, \tag{6}$$

$$A_z'(\rho,z')=\gamma\frac{v}{c}U'(\rho,z'),\qquad A_x'=A_y'=0,$$

where $\gamma=(1-v^2/c^2)^{-1/2}$. In this coordinate frame the potential depends on the time t'. Since even the most tightly bound electrons move in the ion with nonrelativistic velocities, the appearance of a magnetic field in this coordinate system can be neglected.

We confine ourselves to the case when the closest-approach distance $\rho_{\min}$ between the moving ion nucleus and the chain axis greatly exceeds the radius of the initial orbit of the electron whose transitions will be considered. The minimum distance $\rho_{\min}$ depends on the chaneeling conditions. At ion incident angles to the axis close to critical,[3]

$$\rho_{\min}\approx0.885(\hbar^2/me^2)(Z_1^{1/2}+Z_2^{1/2})^{-2/3}$$

and the condition $\rho_{\min}\gg r_e$ is satisfied at least for the inner shells, where $r_e=a_0Z_1^{-1}$. For electrons of the outer shells this condition is satisfied at incidence angles $\psi\ll\psi_{cr}$, when part of the ions move near the center of the channel and therefore $\rho_{\min}$ can be comparable with the channel diameter. Putting in (6) $\rho=|\rho_n+\rho_{en}|$ and $z'=z'_{en}$, where $\rho_n=0$ and $z'_n=0$ are the coordinates of the ion nucleus and ρ_{en} and z'_{en} are the coordinates of the electron relative to the ion nucleus, we can expand $U'(\rho,z')$ in a Taylor series and retain the first nonvanishing terms:

$$\exp(-iK_z\gamma z')\dot{V}(K_z,\rho)\approx V(K_z,\rho_n)-iK_z\gamma V(K_z,\rho_n)z'+\frac{\partial V(K_z,\rho_n)}{\partial\rho_n}\mathbf{n}\boldsymbol{\rho}_{en}. \tag{7}$$

Here n is a unit vector normal to the z axis.

The quantity $V(K_z,\rho_n)$ in (7) does not depend on the electron coordinates and does not lead to any transitions whatever. The Hamiltonian of the interaction of the electron with the field of the chain is of the form

$$U^{(int)}(t')=\frac{\gamma}{2\pi}\int_{-\infty}^{\infty}\exp(-iK_z\gamma vt')\Big[-iK_z\gamma^{-1}V(K_z,\rho)z'+\frac{\partial V(K_z,\rho_n)}{\partial\rho_n}\mathbf{n}\boldsymbol{\rho}_{en}\Big]S(K_z)dK_z. \tag{8}$$

Because of the transverse oscillations of the ion in the channel, ρ_n depends on t'. However, this dependence can be neglected because, as already noted above, the frequencies of these oscillations are much lower than the frequencies of the passage between the neighboring atoms of the chain.

3. COHERENT IONIZATION AND ELECTRON EXCITATION

We consider first electron transitions from the quasidiscrete level i in an ion to an excited state f, which can be quasidiscrete (excitation) or belong to the energy continuum (direct ionization). Using a time-dependent perturbation method, we calculate the transition probability $w_{if}(\rho_n)$ over the entire time of interaction of the ion with the chain at a given ion trajectory ρ_n. The limits of applicability of such a calculation will be analyzed later on. In first-order perturbation theory (see, e.g., Ref. 9, Sec. 41) we obtain for the probability of the electron transition during the entire interaction time

$$w_{if}(\rho_n)=\hbar^{-2}\left|\int_{-\infty}^{\infty}\exp(i\omega_{if}t')U_{if}^{(int)}(t')dt'\right|^2, \tag{9}$$

where $\hbar\omega_{if}=\varepsilon_f-\varepsilon_i$ is the energy difference between the final and initial states of the electron, and $U_{if}^{(int)}(t')$ is a matrix element of the interaction Hamiltonian (8). Integration in (9) yields

$$w_{if}(\rho_n)=\frac{|d_{if}|^2}{(\hbar v)^2}\Big[\Big|\frac{\omega_{if}}{v\gamma^2}V\Big(\frac{\omega_{if}}{\gamma v},\rho_n\Big)\Big|^2+\Big|\frac{\partial}{\partial\rho_n}V\Big(\frac{\omega_{if}}{\gamma v},\rho_n\Big)\Big|^2\Big]\overline{\Big|S\Big(\frac{\omega_{if}}{\gamma v}\Big)\Big|^2}.$$

The square of the modulus of the structure factor, averaged over the longitudinal thermal vibrations, is

$$\overline{\Big|S\Big(\frac{\omega_{if}}{\gamma v}\Big)\Big|^2}=N\Big[1-\exp\Big(-\frac{\omega_{if}^2u^2}{\gamma^2v^2}\Big)\Big]+\sin^2\frac{\omega_{if}Nd}{2\gamma v}\sin^{-2}\frac{\omega_{if}d}{2\gamma v}\exp\Big(-\frac{\omega_{if}^2u^2}{\gamma^2v^2}\Big). \tag{10}$$

Here N is the number of atoms in the chain and u^2 is the mean squared amplitude of the thermal oscillations. It is known that in the Debye approximation the temperature dependence of u^2 is given by

$$u^2=\frac{3\hbar^2}{4Mk_B\Theta_D}\Big[1+4\Big(\frac{T}{\Theta_D}\Big)^2\int_0^{\Theta_D/T}\frac{ydy}{e^y-1}\Big],$$

where M is the mass of the atom of the chain, Θ_D is the Debye temperature, and k_B is the Boltzmann constant.

The expression for the transition probability must generally speaking be averaged also over the transverse thermal vibrations of the chain atoms. This averaging, however, hardly changes the result in the practical case when the distance ρ_n between the channeled ion and the chain axis exceeds the amplitude u of the transverse thermal vibrations. At the same time, allowance for the longitudinal thermal vibrations is essential, since it leads to the appearance of an incoherent background in the probability (see below).

After summing the transition probability over the final states of the electron in the ion, we get

$$w(\rho_n)=\sum_f w_{if}(\rho_n)=\int_0^\infty \sigma(\omega)n(\omega)\,d\omega. \tag{11}$$

The quantity

$$\frac{v}{Nd}n(\omega)=\frac{c}{(2\pi)^2\hbar vN\omega d}\left[\left|\frac{\omega}{v\gamma^2}V\left(\frac{\omega}{\gamma v},\rho_n\right)\right|^2 + \left|\frac{\partial}{\partial\rho_n}V\left(\frac{\omega}{\gamma v},\rho_n\right)\right|^2\right]\overline{\left|S\left(\frac{\omega}{\gamma v}\right)\right|}^2 \tag{12}$$

can be interpreted here as the flux density of photons with frequency ω, whose action on the electron is equivalent to the action of the field of the chain of crystal atoms, and $\sigma(\omega)$ is the cross section for photoabsorption on the electrons of the ions in the state i. As a function of ω, this cross section has sharp maxima near the discrete absorption lines corresponding to electron excitation, and a rather smooth maximum above the photoabsorption edge; this maximum corresponds to the transition of the electron into the continuum.

Corresponding to the amorphous medium in (12) is either the case of sufficiently large amplitude of thermal vibrations ($u^2\rightarrow\infty$), or the case of sufficiently large lattice constant ($d\rightarrow\infty, Nd=L$, where L is the length of the chain), when there are no coherent effects. For a Moliere potential, $V(\omega/\gamma v,\rho_n)$ is determined by expression (4). In this case

$$\frac{\partial}{\partial\rho_n}V\left(\frac{\omega}{\gamma v},\rho_n\right)=2eZ_2\sum_{i=1}^{3}\alpha_i\varkappa_iK_1(\varkappa_i\rho_n), \tag{13}$$

$$\varkappa_i=[(\omega/\gamma v)^2+(\beta_i/a)^2]^{1/2}.$$

If we neglect next the screening of the field by the target atom ($a=\infty$) and the relativistic effects ($\gamma=1$), we can obtain for an amorphous medium ($u^2\rightarrow\infty$) with the aid of expressions (10)–(13) and (4) the result of Datz *et al.*[10] for the average ionization losses, as well as the classical results of Bethe and Bloch.

According to results the (10)–(12), the transition probability consists of an incoherent part, which is always present because of the thermal vibrations of the atoms in the crystal and is proportional to the number of atoms in the chain, and a coherent part, which is determined by the second term of (10).

We consider first the case of electron excitation. In this case $\sigma(\omega)$ in (11) is determined by the resonant absorption of the equivalent photons:

$$\sigma(\omega)=g\frac{2\pi^2c^2}{\omega_0^2}\Gamma_R\delta(\omega-\omega_0).$$

Here $\hbar\omega_0$ is the difference between the energies of the levels between which the transition takes place; Γ_R is the partial radiative width of the excited level, and g is a factor that takes into account the level degeneracy with respect to the projections of the angular momentum of the ion.

At conditions far from resonance, i.e., if

$$|2\pi k\gamma v/d-\omega_0|\gg v/Nd,$$

the coherent part makes a negligibly small contribution to the total probability of the excitation. Therefore the probability is determined mainly by the incoherent part:

$$w_{ex}(\rho_n)\approx w_{ex}^{(0)}(\rho_n)N[1-\exp(-\omega_0^2u^2/\gamma^2v^2)], \tag{14}$$

where

$$w_{ex}^{(0)}(\rho_n)=\frac{2}{3}g\frac{|d_{if}|^2}{(\hbar v)^2}\left[\left|\frac{\omega_0}{\gamma^2v}V\left(\frac{\omega_0}{\gamma v},\rho_n\right)\right|^2+\left|\frac{\partial}{\partial\rho_n}V\left(\frac{\omega_0}{\gamma v},\rho_n\right)\right|^2\right]$$

is the electron excitation probability by interaction with an isolated atom of the chain. It is easily seen with the aid of (14) that if the amplitude of the thermal vibrations is small enough, then the excitation probability $w_{ex}(\rho_n)$ can be in this case much smaller than in an amorphous medium. The excitation-probability suppression factor is determined by the quantity

$$f(v)=1-\exp(-\omega^2u^2/\gamma^2v^2).$$

On the contrary, when the resonance condition $\omega_0=2\pi k\gamma vd^{-1}$ is satisfied the excitation probability takes the form

$$w_{ex}(\rho_n)=w_{ex}^{(0)}(\rho_n)\left\{N\left[1-\exp\left(-\frac{\omega_0^2u^2}{\gamma^2v^2}\right)\right] + \sin^2\frac{\omega_0Nd}{2\gamma\nu}\sin^{-2}\frac{\omega_0d}{2\gamma v}\exp\left(-\frac{\omega_0^2u^2}{\gamma^2v^2}\right)\right\}. \tag{15}$$

If the number k of the resonant harmonic is not too large ($k\lesssim 8$–10), the coherent part of the excitation probability is approximately N times larger than the incoherent part.[5,6] Therefore the total excitation probability (15) is also substantially larger than in an amorphous medium.

Thus, the coherent action of the crystal-chain atoms on an electron in a moving ion can either increase or decrease the electron excitation probability compared with an amorphous medium.

Let the channeling conditions be such that the Massey criterion for the nonadiabaticity of the collisions ($\omega_0\rho\lesssim\gamma v$) is satisfied. Then the excitation cross section (15) as a whole decreases like $v^{-4}f(v)$ with increasing ion velocity v. Against the background of this general decrease there should be observed probability maxima at velocities $v=v_k=\omega_0d/2\pi k\gamma$ corresponding to the resonance conditions.

The criterion for the applicability of perturbation theory is that the excitation probability $w_{ex}(\rho_n)$ be small. Under resonance conditions, according to (15), this criterion may be violated in sufficiently thick crystals. We shall return to this case later.

We now investigate the process of electron loss by the ion. In this case the electron goes over from a discrete energy level into the continuous spectrum, and $\sigma(\omega)$ in (11) is now the cross section $\sigma_{ph}(\omega)$ of the photoeffect on one of the electron subshells of the ion. In accordance with the character of the behavior of the photoeffect cross section,[11] we obtain the following result.

Let the equivalent-photon energy $\hbar\omega_{min}=\hbar 2\pi v\gamma d^{-1}$ corresponding to the first harmonic greatly exceed the binding energy I of the electron in the ion. Then the coherent part of the electron-loss probability

$$w_{\text{loss}}^{(\text{coh})}(\rho_n)=\frac{cN}{(2\pi v)^2\hbar}\sum_{k=1}^{\infty}k^{-1}\exp\left(-\frac{4\pi^2k^2u^2}{d^2}\right)\sigma_\Phi\left(\frac{2\pi kv\gamma}{d}\right)$$

$$\times\left[\left|\frac{2\pi k}{d\gamma}V\left(\frac{2\pi k}{d},\rho_n\right)\right|^2+\left|\frac{\partial}{\partial\rho_n}V\left(\frac{2\pi k}{d},\rho_n\right)\right|^2\right] \tag{16}$$

become negligibly small compared with the incoherent part

$$w_{\text{loss}}^{(\text{inc})}(\rho_n)=\frac{cN}{(2\pi v)^2\hbar}\int_0^{\infty}\left[1-\exp\left(-\frac{\omega^2w^2}{\gamma^2v^2}\right)\right]\frac{\sigma_\Phi(\omega)}{\omega}$$

$$\times\left[\left|\frac{\omega}{\gamma^2v}V\left(\frac{\omega}{\gamma v},\rho_n\right)\right|^2+\left|\frac{\partial}{\partial\rho_n}V\left(\frac{\omega}{\gamma v},\rho_n\right)\right|^2\right]d\omega\,. \tag{17}$$

In turn, the incoherent part of the probability can in this case be substantially smaller than in an amorphous medium. Thus, the total electron-loss probability w_{loss} turns out in this case to be smaller by a factor $(\hbar\gamma v/Iu)^2$ than in an amorphous medium.

On the other hand if the first-harmonic energy $\hbar\omega_{\min}$ is smaller than or comparable with the binding energy, then the energy loss probability $w_{\text{loss}}(\rho_n)$ can differ only by a numerical factor of the order of unity from the corresponding probability in an amorphous medium. Coherent effects cannot lead in this case, in contrast to excitation, to a substantial increase of the probability. The reason is the relatively large width of the photoeffect spectrum compared with the width of the excitation spectrum. The conditions for the applicability of the perturbation method to the calculation of $w_{\text{loss}}(\rho_n)$ therefore remain generally speaking the same as in an amorphous medium.

Assume that a multiply charged channeled ion has more than two bound electrons on its shells. Assume furthermore that for one of the inner shells (say, the K shell) the quantity $\hbar\omega_{\min}$ is of the order of the ionization threshold I_K of this shell, with $\hbar\omega_{\min}$ much higher than the ionization threshold I_L of the next shell (say, the L shell). Then, according to (16) and (17) at sufficiently low thermal-vibration amplitude $(I_Lu\ll\gamma v)$ the probability of formation of a vacancy in the K shell can become mugh higher than the probability of the L vacancy. If at the same time the Massey criterion $I\rho\lesssim\gamma v$ is satisfied for both shells, than the ion beam will contain, as a result of collision with a sufficiently thin crystal, an appreciable number of ions with vacancies in the inner shell.

4. ENERGY LOSS BY AN ION UNDER CONDITIONS OF RESONANT INTERACTION WITH THE CRYSTAL

Let one of the characteristic frequencies $\omega_k=2\pi k\gamma vd^{-1}$ of the field of the atom chain (a) be close to the frequency $\omega_0=(\varepsilon_2-\varepsilon_1)\hbar^{-1}$, where ε_1 is the energy of the initial electron level in the ion, and ε_2 is the energy of the excited level. We consider the case when the lifetime on the excited level can be comparable with or even smaller than the time of passage τ_p of the ion through the crystal.

When solving the Schrödinger equation for the wave function of the electron in the ion we confine ourselves to two states $\psi_1(\mathbf{r}')$ and $\psi_2(\mathbf{r}')$ and one preferred harmonic ω_k of the interaction potential. Then the wave function of the electron at an arbitrary instant of the proper time $t'<\gamma\tau_p$ can be represented in the form

$$\Psi(\mathbf{r}',t')=c_1(t')\psi_1(\mathbf{r}')+c_2(t')\psi_2(\mathbf{r}').$$

The probability amplitudes $c_1(t')$ and $c_2(t')$ of observing an electron at the instant $t'=\gamma t$ in one state or another satisfy the system of equations

$$i\hbar\dot{c}_1=\left(\varepsilon_1-i\hbar\frac{\Gamma_1}{2}\right)c_1+V_{12}\exp(i\omega_kt'),$$

$$i\hbar\dot{c}_2=\left(\varepsilon_2-i\hbar\frac{\Gamma_2}{2}\right)c_2+V_{12}^*\exp(-i\omega_kt'). \tag{18}$$

The matrix element of the interaction energy of the electron with the field of the chain is determined here by the expression

$$|V_{12}|^2=\exp\left(-\frac{4\pi^2k^2u^2}{d^2}\right)\frac{\gamma^2|d_{if}|^2}{d^2}\left[\left|\frac{\omega_0}{\gamma^2v}V\left(\frac{\omega_0}{\gamma v},\rho_n\right)\right|^2\right.$$

$$\left.+\left|\frac{\partial}{\partial\rho_n}V\left(\frac{\omega_0}{\gamma v},\rho_n\right)\right|^2\right], \tag{19}$$

and a dot over a symbol means differentiation with respect to the proper time t'. We assume also that the level widths Γ_1 and Γ_2 are determined mainly by the processes of the transition of the electron to the continuous spectrum under the influence of the field of the chain. Then Γ_1 and Γ_2 coincide with the probabilities of electron loss per unit proper time [see (16) and (17)] from the corresponding levels.[2)]

It should be noted that the ionization widths Γ decrease with increasing charge Z_1. Therefore at sufficiently high charges the width of the excited level too can be determined by the radiative lifetime, inasmuch as $\Gamma_R\sim Z_1^4$.

Thus, the problem reduces formally to the system of equations for two levels acted upon by a resonant field. In contrast to Ohtsuka and Shindo[7] we take into account, by means of the quantities Γ_1 and Γ_2, the possibility of the interaction of the levels with the continuous spectrum; this interaction, as will be shown below, can substantially alter the picture of the considered coherent effects. It should also be noted that an analogous problem of resonant interaction of two damped levels arises in the investigation of such problems as the decay of atomic levels in an intense field of resonant electromagnetic radiation,[12] the collective spontaneous emission of close almost identical atoms,[13] transitions between decaying electron terms in slow ion–atom collisions,[14] and in other problems.[15,16]

A solution of Eqs. (18) that satisfies the initial conditions $c_1(0)=1$ and $c_2(0)=0$ is

$$c_1(t')=\exp\left[\left(-i\frac{\varepsilon_1+\varepsilon_2}{2}-\frac{\Gamma_1+\Gamma_2}{4}\right)t'\right]\frac{1}{2\Omega}(\alpha_1e^{i\Omega t'}-\alpha_2e^{-i\Omega t'}),$$

$$c_2(t')=\exp\left[\left(-i\frac{\varepsilon_1+\varepsilon_2+\hbar\omega_k}{2}-\frac{\Gamma_1+\Gamma_2}{2}\right)t'\right]\frac{V_{12}i}{\Omega}\sin\Omega t'. \tag{20}$$

We have introduced here the notation

$$\Omega=\frac{1}{2}\left[\left(\delta-i\frac{\Delta\Gamma}{2}\right)^2+\frac{4|V_{12}|^2}{\hbar^2}\right]^{1/2},$$

$$\alpha_1=\frac{1}{2}\left(\delta-i\frac{\Delta\Gamma}{2}\right)+\Omega,\quad \alpha_2=\frac{1}{2}\left(\delta-i\frac{\Delta\Gamma}{2}\right)-\Omega,$$

$$\delta=\omega_k-(\varepsilon_2-\varepsilon_1)/\hbar,\ \Delta\Gamma=\Gamma_1-\Gamma_2.$$

As a rule, the width of the initial level is much less than the width of the excited level $(\Gamma_1\ll\Gamma_2)$. Let the channeling conditions be such that the interaction energy $|V_{12}(\rho_n)|$ is much less than the resonance defect $|\hbar\delta|$ or the energy uncertainty $\hbar\Gamma_2/2$ of the excited level. We then obtain for the probability of observing an electron in an excited state at the instant of laboratory time t

$$w_2(t)=\frac{|V_{12}|^2}{\hbar^2[\delta^2+(\Gamma_2/2)^2]}. \tag{21}$$

It follows therefore that at resonance ($\delta=0$) the probability of observing an electron in an excited state at the instant when the ion emerges from the crystal is proportional to the square of the number of atoms of the chain over the length traversed by the ion during the time of decay of the excited state.

We note that the condition $|V_{12}|\ll\max\{\hbar|\delta|, \hbar\Gamma_2/2\}$ is the condition for the validity of perturbation theory in the treatment of coherent excitation of an ion in a channel in sufficiently thick crystals $Ndv^{-1}\gg\Gamma_2^{-1}$. Therefore the result (21) agrees with the corresponding result obtained within the framework of perturbation theory in the case when the time of passage through the crystal is shorter than the lifetime of the excited state (see formula (15) and the text that follows).

In the general case, when $|V_{12}|\gtrsim\hbar|\delta|+\hbar\Gamma_2/2$, we shall describe the energy lost by the ion in terms of the electron-dragging probability:

$$w(t)=|c_1(t')|^2+|c_2(t')|^2.$$

The relaxation of this probability with time is determined according to (20) by the expression

$$w(t)=\exp\left[-\frac{\Gamma_1+\Gamma_2}{2}t'\right]\frac{1}{|2\Omega|^2}\left\{\left(|\alpha_1|^2+\frac{|V_{12}|^2}{\hbar^2}\right)e^{2\Omega''t'}\right.$$
$$\left.+\left(|\alpha_2|^2+\frac{|V_{12}|^2}{\hbar^2}\right)e^{-2\Omega''t'}-2\,\mathrm{Re}\left[e^{2i\Omega't'}\left(\alpha_1\alpha_2^*+\frac{|V_{12}|^2}{\hbar^2}\right)\right]\right\}. \tag{22}$$

Here $\Omega'=\mathrm{Re}\Omega$, $\Omega''=\mathrm{Im}\Omega$, and $t'=\gamma t$.

The relaxation of the electron-dragging probability (22) is accompanied in the general case by oscillations, this being a characteristic effect in the decay from resonantly interacting levels (cf. the results of Refs. 12–14). The frequency Ω' of the modulation of the dragging probability increases, and the modulation depth decreases, both with increasing resonance defect $\hbar\delta$ and with increasing level splitting $|2V_{12}|$ by the resonant field of the crystal chain.

The expression for the electron-dragging probability (22) can be presented in a more illustrative form when the level-uncertainty energy difference $|\hbar\Delta\Gamma/2|$ is much less than the level splitting $|2V_{12}|$ or the resonance defect $|\hbar\delta|$:

$$w(t)=\exp\left(-\frac{\Gamma_1+\Gamma_2}{2}t'\right)\left[\mathrm{ch}\frac{\Delta\Gamma t'}{2(1+\xi^2)^{1/2}}-(1+\xi^2)^{-1/2}\,\mathrm{sh}\frac{\Delta\Gamma t'}{2(1+\xi^2)^{1/2}}\right]. \tag{23}$$

Here $\xi=2|V_{12}|/\hbar\delta$ is the ratio of the level splitting to the resonance defect and can be arbitrary. It is seen that in this limiting case the probability does not oscillate with time (with the crystal thickness), but the state-decay law, generally speaking, does not reduce to a sum of exponentials with corresponding damping constants. This is the result of the substantial interference between the decay and the level interaction via the resonant field of the chain.

In the limit of small ξ we obtain the results of perturbation theory. At large ξ,

$$w(t)=\exp(-(\Gamma_1+\Gamma_2)t\gamma/2).$$

The decay of the initial state of the electron in an ion is exponential, but the argument of the exponential contains now the rate of decay of the excited level. In particular, if the initial state of the electron was metastable ($\Gamma_1\ll\Gamma_2$), then under the influence of the strong ($\xi\gg1$) resonant field of the chain it begins to decay at a rate equal to half the rate of decay of the excited virtual level. We also note that if the level damping is completely neglected ($\Gamma_1=\Gamma_2=0$) the probability of absorbing an electron in an excited state in this limiting case ($\xi\gg1$) contains only terms that oscillate with time. Thus, if we neglect the electron level decay in the course of interaction with the crystal, then only periodic transfer of an electron from one state to another takes place. In this case we obtain the result of Ohtsuka and Shindo[7] (see also Ref. 9, problem of Sec. 40). This result, however, does not lead to any conclusions concerning the probability of electron loss by the ion.

5. LIMITS OF APPLICABILITY OF THE THEORY AND FINE STRUCTURE OF RESONANCES

An analysis of expression (23) shows also that coherent effects in the process of electron loss by an ion should be observed not only in the case when the resonance defect is smaller than the width of the quasi-discrete levels. If the level splitting due to the resonant periodic field in the chain is large enough, it suffices to have the resonance defect smaller than the value of this level splitting ($|\hbar\delta|\lesssim2|V_{12}|$).

The resonance width $2|V_{12}|$ can exceed under certain conditions the energy difference of two neighboring harmonics of the periodic potential of the crystal chain. In that case we cannot confine ourselves in the analysis to the action of only one harmonic on the electron. Thus, the necessary condition for the applicability of the developed method is

$$4|V_{12}|^2/(\hbar\Delta\omega)^2\ll1. \tag{24}$$

We substitute in this condition the matrix element of the interaction energy (19) and the value $\hbar\Delta\omega=2\pi\gamma v\hbar d^{-1}$, and then compare the ratio in the left-hand side of inequality (24) with the probability $w_{ex}^{(0)}(\rho_n)$ of the excitation of the electron in interaction with an isolated atom of the crystal [see (14)]. It is then easily seen that the condition (24) is equivalent to the condition that $w_{ex}^{(0)}(\rho_n)$ be small. On the other hand, the condition $w_{ex}^{(0)}(\rho_n)\ll1$ is necessary for the entire approach as a whole, which presupposes smallness of the field of the chain atoms at the location of the electron compared with the field of the nucleus of the ion [see (7) and the corresponding text].

Another limitation on the two-level approximation can arise in the presence of several close resonance frequencies $\omega_0^{(1)}, \omega_0^{(2)}, \ldots, \omega_0^{(n)}$, which occur, for example, when the initially degenerate levels 1 and 2 in a hydrogenlike ion are split under the influence of the timeindependent component of the field of the chain. This component corresponds to the continuous potential of the chain, which is defined by Eq. (4), where K_z must be set equal to zero. The expansion, similar to (7), of the continuous potential $U_0(\rho)$ of the chain in a Taylor series takes, accurate to the quadratic terms, the form

$$U_0(\rho)\approx U_0(\rho_n)+\frac{\partial U_0(\rho_n)}{\partial \rho_n}\mathbf{n}\rho_{en}+\frac{1}{2}\frac{\partial^2 U_0(\rho_n)}{\partial \rho_n^2}(\mathbf{n}\rho_{en})^2. \tag{25}$$

The dc component (25) of the chain-field potential splits the levels $2s_{1/2}$ and $2p_{1/2}$ in a hydrogenlike ion by an amount

$$\Delta_{2s_{1/2}2p_{1/2}}=\gamma|d_{2s2p}|\left|\frac{\partial U_0(\rho_n)}{\partial \rho_n}\right|, \tag{26}$$

where d_{2s2p} is the matrix element of the dipole moment of the electron. The splitting of the levels $2p_{1/2}$ and $2p_{3/2}$ is due mainly to the quadratic term in the expansion (25) and takes the form

$$\Delta_{2p_{1/2}2p_{3/2}}=\gamma|Q_{2p_{1/2}2p_{3/2}}|\left|\frac{\partial^2 U(\rho_n)}{\partial \rho_n^2}\right|, \tag{27}$$

where Q is the matrix element of the quadrupole moment of the electron. Since the matrix element of the dipole moment, which connects the states $2p_{1/2}2p_{3/2}$, is equal to zero, the splitting of these levels, which is connected with the second term in (25), arises only in second-order perturbation theory. Calculation shows that it is small compared with the quadrupole splitting (27) at $Z_1 \gg 1$.

Thus the transitions $1s_{1/2}\to 2p_{1/2}$ and $1s_{1/2}\to 2p_{3/2}$ will have close but unequal frequencies $\omega_0^{(1)}$ and $\omega_0^{(2)}$, such that $\omega^{(2)}-\omega_0^{(1)}=\Delta_{2p_{1/2}2p_{3/2}}$. These two resonances and the probabilities of the electron loss appear independently if the energy width $|V_{12}|$ of each resonance is smaller than the difference $\omega_0^{(2)}-\omega_0^{(1)}\equiv\Delta\omega_0$ of the resonance energies. The doublet structure of the resonance in the probability of the electron loss was observed in some cases by Datz *et al.*[8] In other cases, when $\Delta\omega_0 \ll |V_{12}|$, the two resonances merge into one. Since $\Delta\omega_0$ and $|V_{12}|$ have different dependences on the transverse coordinate ρ_n of the ion nucleus, their ratio can vary within certain limits, depending on the channeling conditions (the angle of indices of the ion beam on the crystal). It should be noted also that the resonant frequencies $\omega_0^{(2)}$ and $\omega_0^{(1)}$ are shifted relative to the frequency ω_0 which corresponds to the transition between the initial levels $1s_{1/2}$ and the degenerate levels $2s$ and $2p$. The shift turns out to be positive and is determined by the splitting of the levels $2s_{1/2}$ and $2p_{1/2}$:

$$\omega_0^{(1)}-\omega_0=\Delta_{2s_{1/2}2p_{1/2}}.$$

This shift was also observed in the cited experiments.[8]

In numerical calculations of the coherent ionization and of the excitation of multiply charged ions under channeling conditions, the single-chain approximation may not be sufficient. In this case the potential in the channel is determined by several closest chains and does not have axial symmetry. A generalization of the results in this case is attained by maiing the following substitutions in the final results [(12)-(19), (21), (26), (27)]:

$$\begin{aligned}&\left|\frac{\partial}{\partial\rho_n}V\left(\frac{\omega}{\gamma v},\rho_n\right)\right|^2+\left|\frac{\omega}{\gamma^2 v}V\left(\frac{\omega}{\gamma v},\rho_n\right)\right|^2\\ &\to\left|\frac{\partial}{\partial R}U\left(\frac{\omega}{\gamma v},R,\varphi\right)\right|^2+\left|\frac{1}{R}\frac{\partial}{\partial\varphi}U\left(\frac{\omega}{\gamma v},R,\varphi\right)\right|^2\\ &\quad+\left|\frac{\omega}{\gamma^2 v}U\left(\frac{\omega}{\gamma v},R,\varphi\right)\right|^2,\quad U\left(\frac{\omega}{\gamma v},R,\varphi\right)\\ &\quad=\sum_m V\left(\frac{\omega}{\gamma v},\ (R^2+\rho_m^2-2R\rho_m\cos(\varphi-\varphi_m))^{1/2}\right),\end{aligned} \tag{28}$$

where ρ_m and φ_m are the polar coordinates of the mth chain, R and φ are the polar coordinates of the nucleus of the ion. The origin of the polar coordinates is chosen at the center of the channel, and the summation in (28) is over all the chain coordinates closest to the origin. The probability of inelastic transition depends in this case on the angle φ. For example, for a Moliere potential [see (4), (5), (13)] $U(\omega/\gamma v, R, \varphi)$ takes the form

$$U\left(\frac{\omega}{\gamma v},R,\varphi\right)=2eZ_2\sum_m\sum_{i=1}^{3}\alpha_i K_0(\varkappa_i[R^2+\rho_m^2-2R\rho_m\cos(\varphi-\varphi_m)]^{1/2}). \tag{29}$$

In the numerical calculations it may be convenient to represent the potential in the channel in the form of a Fourier series in φ:

$$U\left(\frac{\omega}{\gamma v},R,\varphi\right)=2eZ_2\sum_m\sum_{i=1}^{3}\sum_{l=-\infty}^{\infty}\alpha_i K_l(\varkappa_i\rho_m)I_l(\varkappa_i R)\exp(il(\varphi-\varphi_m)),$$
$$R<\rho_m. \tag{30}$$

We note that the axially asymmetrical field $U(0, R, \varphi)$ lifts the degeneracy of the $2p$ levels of the hydrogenlike multiply charged ions with respect to the projections of the angular momentum (in first-order perturbation theory). Therefore under certain conditions one can observe in the ionization probability a structure more complicated than the doublet structure.

CONCLUSION

The foregoing analysis shows that the rate of the ionization of an ion channeling in a crystal can differ substantially from with the ionization rate in an amorphous medium.

1. The increase of the probability of the electron loss by the ion via resonant excitation in channeling, which was considered theoretically, can be used to obtain fast multiply charged ions. An important factor is also that the ionization of the channeled ions is not accompanied by an increase of the angular divergence of the ion beam, as is the case in an amorphous medium.

2. The relative suppression of the probability of formation of a vacancy in a more exterior shell can be used as an effective means of obtaining vacancies in inner shells of many-electron ions. The discrete spectrum of the photons equivalent to the field of the chains, at ion velocities $v\sim 10^9$ cm/sec, lies in the x-ray region. Owing to the high flux density of the equivalent photons ($j\sim 10^{32}$–10^{33} cm^{-2}sec^{-1}) the rate of selective production of vacancies greatly exceeds the rate of production of such vacancies with the aid of the existing x-ray sources.

3. The dependence of the processes of loss and acquisition of charge by ions on the channeling conditions

can lead to a change in the magnitude and establishment time of an equilibrium charge in an oriented crystal target. The kinetic equations of the equilibrium-charge theory should take correct account of the elementary processes of ionization and recombination of ions in the channeling regime.

[1)] A generalization of the results to the case of several nearest chains will be presented in Sec. 4.

[2)] We neglect small shifts of the levels due to their interaction with the states of the continuous spectrum.

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The Kramers-Wannier transformation for spin systems

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The Kramers-Wannier transformation is constructed for spin systems on a plane lattice. Systems with discrete nonabelian groups are considered, including generalized Potts models. The existence of three different phases in these models is predicted.

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1. INTRODUCTION

In 1941 Kramers and Wannier[1] discovered a special symmetry which relates low-temperature and high-temperature expansions in the plane Ising model. The corresponding transformation, the Kramers-Wannier (KW) transformation, is a definite nonlocal substitution on the variables in the sum over states (partition function). After this substitution the statistical sum involves not the original "spin" variables $\sigma=\pm 1$, defined on the nodes of the lattice, but new "spin" variables $\mu=\pm 1$ defined on the faces of the lattice, or, equivalently, on the nodes of the "dual" lattice. Furthermore the new Hamiltonian, expressed in terms of μ, differ from the original one by the replacement $\sigma\to\mu$ and also a transformation of the temperature parameter:

$$\beta\to\beta^*=\operatorname{arth} e^{-2\beta}. \tag{1.1}$$

The transformation (1.1) establishes a connection between values of the statistical sum in high-temperature and low-temperature phases and, in particular, enables one to find the exact value of the critical temperature β_c^{-1}. In the phase in which the fluctuation of the order parameter σ are large, those of the variables μ are restricted, and conversely. For the "dual" variables μ we therefore use the name "disorder parameter."[2]

The existence of this sort of transformations is evidently a very general property of lattice statistical systems that possess a symmetry group. KW transformations have been constructed explicitly for a number of systems on a plane lattice. These include the N-position models of Potts (see Ref. 3) and generalized Ising models, systems with spins taking values in groups Z_N (Z_N Ising models),[4,5] and in the group $U(1)$ (XY model[6]). For Z_N systems the disorder parameter also takes a value in the group Z_N. Therefore the KW transformation reduces to a transformation of numerical parameters of the Hamiltonian, just as in the ordinary Ising model. In the case of the XY model the disorder parameter is an element of the group Z_N and the KW transformation relates to each other statistical sums of different spin systems.

KW transformations can also be carried out for some systems on many-dimensional lattices. Here new possibilities arise. For example, a KW transformation connects the three-dimensional Ising model with the gauge Ising model, and the four-dimensional gauge

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