

clei lighter than Au will increase, while for energies for which $y_{\max} \sim y_{cr}$, the fission cross section will actually coincide with the total reaction cross section. Since the value of z will be greater than 0.3 for target nuclei lighter than Au, expression (8) will contain a large error, so we can only approximately give the region of ion energies for which the fission cross section will equal the total cross section. Thus, for example, for Yb and Dy, this region is around 150 Mev. The fission cross section, naturally, also increases with increasing mass of the bombarding particles.

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¹Druin, Polikanov, and Flerov, *J. Exptl. Theoret. Phys. (U.S.S.R.)* **32**, 1298 (1957), *Soviet Phys. JETP* **5**, 1059 (1957).

²W. Heisenberg, *Nuclear Physics*, London, Methuen, 1953.

³H. A. Bethe, *Revs. Mod. Phys.* **9**, 69 (1937).

⁴A. Bohr, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **26**, #14 (1952).

⁵Y. Fujimoto and Y. Yamaguchi, *Progr. Theoret. Phys. (Japan)* **5**, 76 (1950).

⁶Baraboshkin, Karamian, and Flerov, *J. Exptl. Theoret. Phys. (U.S.S.R.)* **32**, 1294 (1957), *Soviet Phys. JETP* **5**, 1055 (1957).

⁷D. Hill and J. Wheeler, *Phys. Rev.* **89**, 1102 (1953).

⁸W. J. Swiatecki, *Phys. Rev.* **104**, 993 (1956).

⁹D. J. Hughes and R. B. Schwartz, *Neutron Cross Sections*, Suppl. 1, 1957.

¹⁰*Experimental Nuclear Physics*, ed. E. Segre, Vol. 1, article by K. T. Bainbridge, "Atomic Masses," Wiley, New York, 1953.

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ON THE THEORY OF THERMAL EXCITATION OF POLARONS

V. A. MOSKALENKO

Kishinev State University

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The probability of a quantum transition of a polaron from the 1s to the 2p state caused by thermal vibrations of the lattice is computed. The adiabatic form of perturbation theory is used in the calculations. At room and higher temperatures transition to the 2p state occurs during $10^{-8} - 10^{-9}$ sec.

1. INTRODUCTION

POLARONS are the principal carriers of current in ionic crystals.¹ As is well known, in crystals which have large cohesive energies polarons are characterized by large effective masses, and also by the existence of a fluctuation movement of the electron with respect to the center of gravity of the polaron. There exists a series of bound states, between which quantum transitions are possible. In this paper we shall consider such a transition between a 1s ground state and a 2p final state.

During the transition, the momentum of the po-

laron is conserved and changes in its kinetic energy occur at the expense of changes in its effective mass. The process under consideration turns out to be a multiphonon process. Frenkel² was the first to show that such transitions are possible in crystals. He pointed out that the equilibrium configuration of the field oscillators changes during such a transition. A quantitative theory of non-radiative transitions at F centers, based on this idea, was presented by a number of authors.³⁻⁶ Another mechanism for thermal transitions was suggested by Kubo.⁷

In this paper the basic idea and method of the

theory of nonradiative transitions at F centers, proposed by Lax,⁴ is used.

In the present work by a thermal transition is meant a transition induced by thermal vibrations of the lattice, and described by the terms in the initial Hamiltonian for the quantitative description of the polaron as proposed by Bogoliubov and Tiablikov. These terms are caused by departures from adiabaticity, and equal weight is given to all terms, which have the same order of smallness (ϵ^3). By formulating the problem in this way, we shall obtain information about the duration of the ground state (1s).

Anticipating the results somewhat, it can be said, that in the case under consideration the most important part of the transition matrix element is that part which is related to the dependence of the electronic wave function on the oscillator coordinates. This agrees with previously cited work.³⁻⁶

Finally it should be noted, that for a more consistent treatment, in the theory of F centers there must arise a question about changes of frequency of the field oscillators in the presence of an electron. This question is considered in Sec. 2 of this paper.

2. TRANSFORMATION OF THE HAMILTONIAN OF THE SYSTEM

The Hamiltonian of the polaron problem has the form

$$H = \frac{p^2}{2m} + \sum_{\mathbf{f}} A_{\mathbf{f}} e^{i\mathbf{f}\mathbf{r}} q_{\mathbf{f}} + \frac{1}{2} \sum_{\mathbf{f}} E(\mathbf{f}) (q_{\mathbf{f}} q_{-\mathbf{f}} + \epsilon^4 p_{\mathbf{f}} p_{-\mathbf{f}}). \quad (1)$$

Here p and r are the momentum and coordinate of the electron; $p_{\mathbf{f}}$ and $q_{\mathbf{f}}$ are analogous quantities for the field oscillators; $E(\mathbf{f}) = \hbar\omega_{\mathbf{f}}$ with $\omega_{\mathbf{f}} \approx \omega$, the limiting frequency of optical vibrations,

$$A_{\mathbf{f}} = -(e/f) (4\pi\hbar\omega c/V)^{1/2},$$

where $c = 1/n^2 - 1/\epsilon_0$, n^2 and ϵ_0 are the square of the index of refraction and the dielectric constant of the material respectively, and V is the volume of the crystal.

According to Bogoliubov and Tiablikov,⁸⁻¹⁰ to separate the translational invariance of Eq. (1) one must write

$$\mathbf{r} = \boldsymbol{\lambda} + \mathbf{q}, \quad q_{\mathbf{f}} = (r_{\mathbf{f}} + \epsilon Q_{\mathbf{f}}) e^{-i\mathbf{f}\mathbf{q}}; \quad (2)$$

$\boldsymbol{\lambda}$ and \mathbf{q} describe the fluctuational and translational motion of the electron, respectively.

For nonspherically symmetrical states, the limitations on the new coordinates $Q_{\mathbf{f}}$ should be written thus

$$\sum_{\alpha} \int_{\mathbf{f}} \hat{f}^{\alpha} v_{\alpha\beta}^*(\mathbf{f}) Q_{\mathbf{f}} = 0, \quad \beta = 1, 2, 3, \quad (3)$$

where

$$\sum_{\beta} \sum_{\mathbf{f}} \hat{f}^{\alpha} f^{\beta} v_{\alpha\beta}^*(\mathbf{f}) r_{\mathbf{f}} = \delta_{\alpha\gamma}. \quad (4)$$

In terms of the new variables the Hamiltonian (1) takes the form

$$H = H_0 + \epsilon H_1 + \epsilon^2 H_2 \quad (5)$$

where

$$\begin{aligned} H_0 &= \frac{p_{\boldsymbol{\lambda}}^2}{2m} + \sum_{\mathbf{f}} A_{\mathbf{f}} e^{i\mathbf{f}\boldsymbol{\lambda}} r_{\mathbf{f}} + \frac{1}{2} \sum_{\mathbf{f}} E(\mathbf{f}) |r_{\mathbf{f}}|^2, \\ H_1 &= \sum_{\mathbf{f}} \{A_{\mathbf{f}} e^{i\mathbf{f}\boldsymbol{\lambda}} + E(\mathbf{f}) r_{-\mathbf{f}}\} Q_{\mathbf{f}}; \\ H_2 &= \frac{1}{2} \sum_{\mathbf{f}} E(\mathbf{f}) Q_{\mathbf{f}} Q_{-\mathbf{f}} + \frac{1}{2} \sum_{\mathbf{f}} E(\mathbf{f}) \left\{ P'_{-\mathbf{f}} - \frac{i}{\hbar} v_{\alpha\beta}(\mathbf{f}) f^{\beta} J_{\alpha} \right\} \\ &\quad \times \left\{ P'_{\mathbf{f}} + \frac{i}{\hbar} v_{\alpha\beta}^*(\mathbf{f}) f^{\beta} J_{\alpha} \right\}; \\ H_3 &= -\frac{1}{2} \sum_{\mathbf{f}} E(\mathbf{f}) \left\{ P'_{-\mathbf{f}} - \frac{i v_{\alpha\beta}(\mathbf{f})}{\hbar} f^{\beta} J_{\alpha} \right\} v_{\gamma\delta}^*(\mathbf{f}) \{ f^{\delta} \partial / \partial \lambda_{\gamma} \\ &\quad + \sum_{\mathbf{k}} k^{\delta} f^{\gamma} Q_{\mathbf{k}} P'_{\mathbf{k}} + \frac{i}{\hbar} \sum_{\mathbf{k}} f^{\delta} k^{\gamma} k^{\sigma} J_{\sigma} v_{\sigma\alpha}^*(\mathbf{k}) Q_{\mathbf{k}} \} - \\ &\quad - \frac{1}{2} \sum_{\mathbf{f}} E(\mathbf{f}) v_{\alpha\beta}^*(\mathbf{f}) \left\{ f^{\beta} \partial / \partial \lambda_{\alpha} + \frac{1}{\hbar} \sum_{\mathbf{k}} f^{\beta} k^{\alpha} k^{\sigma} J_{\sigma} v_{\sigma\alpha}^*(\mathbf{k}) Q_{\mathbf{k}} \right. \\ &\quad \left. + \sum_{\mathbf{k}} k^{\alpha} f^{\beta} Q_{\mathbf{k}} P'_{\mathbf{k}} \right\} \left\{ P'_{-\mathbf{k}} - \frac{i}{\hbar} v_{\epsilon\delta}(\mathbf{f}) f^{\epsilon} J_{\delta} \right\}. \end{aligned} \quad (6)$$

Here the following notation is used:

$$P_{\boldsymbol{\lambda}} = -i\hbar\partial/\partial\boldsymbol{\lambda}, \quad P_{\mathbf{f}} = -i\partial/\partial Q_{\mathbf{f}}, \quad \mathbf{J} = -i\hbar\partial/\partial\mathbf{q},$$

$$P'_{\mathbf{f}} = P_{\mathbf{f}} - \sum_{\sigma\beta} v_{\alpha\beta}^*(\mathbf{f}) f^{\alpha} \sum_{\mathbf{k}} k^{\beta} r_{\mathbf{k}} P_{\mathbf{k}}. \quad (7)$$

The quantity \mathbf{J} is the momentum of the whole system, and is an integral of the motion.

In the first approximation in ϵ , we obtain for the electronic function the expression

$$\varphi_n(\boldsymbol{\lambda}, \dots, Q_{\mathbf{f}} \dots) = \varphi_n(\boldsymbol{\lambda}) + \epsilon \sum_m' \frac{(H_1)_{mn}}{W_n^0 - W_m^0} \varphi_m(\boldsymbol{\lambda}), \quad (8)$$

where $\varphi_n(\boldsymbol{\lambda})$ and W_n^0 are non-self-consistent quantities of the zeroth approximation. The symbols $\psi_n(\boldsymbol{\lambda})$ and G_n will be used to denote self-consistent quantities.

The energy of the electron $W_n(\dots, Q_{\mathbf{f}} \dots)$ depends on $Q_{\mathbf{f}}$ through perturbation theory corrections of the first, second, and third order, i.e., through ϵ , ϵ^2 , and ϵ^3 , it being obvious that the first-order correction $\epsilon(H_1)_{nn}$ vanishes. This leads to the definition

$$r_{\mathbf{f}} = -\frac{A_{\mathbf{f}}}{E(\mathbf{f})} J_{\mathbf{f}}^{nn}, \quad (9)$$

where

$$J_{\mathbf{f}}^{nm} = (\varphi_n(\boldsymbol{\lambda}), e^{i\mathbf{f}\boldsymbol{\lambda}} \varphi_m(\boldsymbol{\lambda})).$$

The motion of the oscillators is described by the equation

$$[\varepsilon^2 \tilde{H}_2 + \varepsilon^3 \tilde{H}_3 - (E'_{nN} - G_n)] \Phi'_{nN} = 0, \quad (10)$$

where

$$\tilde{H}_2 = (H_2)_{nn} + \sum_m \frac{(H_1)_{nm} (H_1)_{mn}}{G_n - W_m^0}, \quad (11)$$

$$\tilde{H}_3 = (H_3)_{nn} + \sum_p \sum_m \frac{(H_1)_{nm} (H_1)_{mp} (H_1)_{pn}}{(G_n - W_m^0)(G_n - W_p^0)}. \quad (12)$$

The last terms in (11) and (12) we denote by

$$\sum B_{fg} Q_f Q_g \text{ and } \sum B_{fgh} Q_f Q_g Q_h.$$

respectively.

In determining the energy E'_{nN} of the whole system and the corresponding wave function, we shall neglect the term of order ε^3 , considering it to be one of the causes of quantum transitions between the states that are obtained. In this way we obtain

$$\varepsilon^2 H_2 \Phi_{nN} (\dots Q_f \dots) = (E_{nN} - G_n) \Phi_{nN} (\dots Q_f \dots), \quad (13)$$

where N is the set of quantum numbers of the oscillators. The first index in Φ_{nN} indicates that the motion of the oscillators occurs under the action of average field of an electron in the state n .

The unknown quantities, $v_{\alpha\beta}$ are determined from the following relationship:^{9,10}

$$\sum_{\alpha} k^{\alpha} v_{\alpha\beta} (k) = \hbar^2 r_k k^{\beta} / E(k) \mu^{\beta}, \quad (14)$$

where μ is the diagonalized effective mass tensor of the polaron

$$\mu^{\alpha} = \hbar^2 \sum k^{2\alpha} |r_k|^2 / E(k). \quad (15)$$

Taking (14) and (15) into account, we have

$$\begin{aligned} \tilde{H}_2 = & 1/2 \sum_{\alpha} J_{\alpha}^2 / \mu^{\alpha} + 1/2 \sum_f E(f) (Q_f Q_{-f} \\ & + P'_f P'_{-f}) + \sum_{f,g} B_{fg} Q_f Q_g, \end{aligned} \quad (16)$$

$$\begin{aligned} \tilde{H}_3 = & i\hbar (V\partial/\partial\lambda)_{nn} - \sum_f (Vf) v_{\alpha\beta}^*(f) f^{\alpha} J_{\beta} Q_f \\ & + i\hbar \sum_f (fV) Q_f P'_f + \sum_{fgh} B_{fgh} Q_f Q_g Q_h, \end{aligned} \quad (17)$$

where

$$V^{\alpha} = J_{\alpha} / \mu^{\alpha}.$$

According to Tiablikov,¹⁰ diagonalization of Eq. (16) is accomplished by a single orthogonal transformation by the matrix $a_{f,\nu}$:

$$Q_f = \sqrt{E(f)} \sum_{\nu} a_{f\nu} q_{\nu}, \quad P_f = \frac{1}{\sqrt{E(f)}} \sum_{\nu} a_{f\nu}^* P_{\nu}; \quad (18)$$

$$p_{\nu} = -i\partial/\partial q_{\nu}.$$

The matrix $a_{f,\nu}$ is determined from the condition

$$E^2(f) a_{f\nu} + \sum_g \bar{B}_{-f,g} a_{g\nu} = \lambda_{\nu}^2 a_{f\nu}, \quad (19)$$

where

$$\bar{B}_{fg} = \sqrt{E(f)E(g)} (B_{fg} + B_{gf});$$

q_{ν} and λ_{ν} are the new coordinates and frequencies of the field oscillators. Equation (19) has three eigenvalues λ_{α} ($\alpha = 1, 2, 3$) which are equal to zero; thus

$$a_{f\alpha} = -i\hbar f^{\alpha} r_f / \sqrt{E(f)} \mu^{\alpha}. \quad (20)$$

It should be noted that the coordinates q_{α} corresponding to λ_{α} , are equal to zero. This means, that as a result of condition (3), three degrees of freedom of the field are transferred to the polaron and they are found in the translational motion of the latter.

After diagonalization, \tilde{H}_2 has the form

$$\tilde{H}_2 = 1/2 \sum_{\alpha} J_{\alpha}^2 / \mu^{\alpha} + 1/2 \sum_{\nu} (p_{\nu} p_{\nu} + \lambda_{\nu}^2 q_{\nu} q_{-\nu}). \quad (21)$$

The primes on the summation sign signify that terms with $\nu = \alpha$ are to be left out of the sum. It should be noted that μ^{α} , λ_{ν} and q_{ν} depend on the state of the electron and therefore should bear indices which correspond to the appropriate electronic state. We shall introduce the Bose operators ζ_{ν} and ζ_{ν}^+ as follows:

$$q_{\nu} = \frac{1}{\sqrt{2\lambda_{\nu}}} (\zeta_{\nu} + \zeta_{-\nu}^+), \quad p_{\nu} = -i \sqrt{\frac{\lambda_{\nu}}{2}} (\zeta_{-\nu} - \zeta_{\nu}^+). \quad (22)$$

Then

$$\tilde{H}_2 = 1/2 \sum_{\alpha} J_{\alpha}^2 / \mu^{\alpha} + \sum_{\nu} \lambda_{\nu} (\zeta_{\nu}^+ \zeta_{\nu} + 1/2) \quad (23)$$

The eigenfunctions and eigenvalues of Eq. (13) assume the form:

$$\Phi_{nNJ} = V^{-1/2} e^{iJq/\hbar} \prod_{\nu \neq \alpha} \Phi_{n\nu}(q_{\nu}), \quad (24)$$

$$E_{nNJ} = G_n + \varepsilon^2 \sum_{\alpha} J_{\alpha}^2 / 2\mu_{\alpha}^2 + \varepsilon^2 \sum_{\nu} \lambda_{\nu}^2 (n_{\nu} + 1/2). \quad (25)$$

For the wave function of the complete system we have

$$\psi_{nNJ} = \psi_n(\dots, q_{\nu} \dots) \Phi_{nNJ}. \quad (25')$$

3. PROBABILITY OF A NONRADIATIVE TRANSITION

Quantum transitions will occur between the states given by Eq. (25'). These transitions come about because of the inaccuracy of the function (25') and omission of the terms $\epsilon^3 \tilde{H}_3$ from the Hamiltonian.

The probability $P_{nn'}$ of a quantum transition per unit time between the initial state of the system nN and its final state $n'N'$ has the form:

$$P_{nn'} = \frac{2\pi}{\hbar} A_{VN} \sum_{N'} \int d\Gamma | \langle n'N' | H - E_{nN} | nN \rangle |^2 \delta(E_{n'N'} - E_{nN}), \quad (26)$$

Here $d\Gamma$ is the number of states, in the energy interval $dE_{n'N'}$ of the final states. Summation over N' is performed over all final oscillator states. A_{VN} denotes an average over the initial quantum states of the oscillators, N . The matrix element in (26), to an accuracy of quantities of the order ϵ^3 , has the form:

$$\begin{aligned} & \langle n', \dots, n'_v, \dots | H - E_{nN} | n, \dots, n_v, \dots \rangle \\ &= \epsilon^3 \int \prod_{\sigma} \Phi_{n'n'_\sigma} \left\{ \sum_{\nu} \lambda_{\nu}^{n'n} M_{\nu}^{n'n} (\zeta_{-\nu}^+ - \zeta_{\nu}) \right. \\ & \quad \left. + N^{nn'} \tilde{H}_3 \right\} \prod_{\sigma} \Phi_{n'n_\sigma} \prod_{\sigma} dq_{\sigma}, \end{aligned} \quad (27)$$

$$\begin{aligned} M_{\nu}^{n'n} &= \int \psi_{n'}^*(\lambda) L_{\nu}^n(\lambda) d\lambda, \\ L_{\nu}^n(\lambda) &= \sum_p \sum_f \frac{a_{\nu} A_f V \overline{E(f)} J_f^{pn}}{V 2\lambda_{\nu}^n (G_n - W_p^0)} \varphi_p(\lambda), \end{aligned} \quad (28)$$

where λ_{ν}^n is the lattice vibration frequency, $N^{nn'} = (\psi_{n'}, \psi_n)$ is the non-orthogonality integral of the self-consistent functions. To evaluate the sum (26) over all final oscillator states we make use of the integral form of the Dirac δ -function.

To simplify the calculation, let us change $a_{\mathbf{f}\nu}$ into $\delta_{\mathbf{f}\nu}$ and λ_{ν} into $\hbar\omega$. Let us also take it into account that in our case $N^{nn'} = 0$. Then after a series of simple transformations, we obtain:

$$\begin{aligned} P_{nn'} &= -\frac{\epsilon^6}{\hbar^2} \int d\Gamma \int_{-\infty}^{\infty} \exp\{(2\pi i \nu_0 + i\omega_a)u\} du A_{VN} (N | V^{-1/2} \\ & \times \sum_f (m_f^{n'n} \zeta_f^+ - m_f^{n'n'} \zeta_f) \prod_r \exp_{[-]} \left\{ \frac{i}{\hbar V \sqrt{V}} \int_0^u (R_r \zeta_r e^{-i\omega s} \right. \\ & \quad \left. + R_{-r} \zeta_{-r}^+ e^{i\omega s}) ds \right\} \times V^{-1/2} \sum_g (m_g^{n'n} \zeta_g^+ e^{i\omega u} \\ & \quad \left. - m_g^{n'n'} \zeta_g e^{-i\omega u}) | N \rangle, \end{aligned} \quad (29)$$

where

$$\begin{aligned} m_f^{n'n} / \sqrt{V} &= \frac{1}{\sqrt{2}} A_f E(f) (G_n - W_p^0)_{\text{av}}^{-1} J_f^{n'n}, \\ R_f / \sqrt{V} &= \frac{E(f)}{\sqrt{2}} (r_{-f}^n - r_{-f}^{n'}), \\ \hbar\omega_a &= 1/2 \sum_f E(f) |r_f^n - r_f^{n'}|^2, \\ \hbar\nu_0 &= G_{n'} - G_n + 1/2 \sum_{\alpha} J_{\alpha}^2 (1/\mu_{n'}^{\alpha} - 1/\mu_n^{\alpha}). \end{aligned} \quad (30)$$

A quantity with the index "av" is a certain average value of the denominator in Eq. (28). The sign [-] indicates a reordering of the operators in the product, so that they are arranged, reckoning from right to left, in order of decreasing value of the index s .^{4,11} In computing the average over the initial states N , the only terms retained in Eq. (29) are those which remain finite as $V \rightarrow \infty$.

Let us introduce the symbols

$$S = 1/2 \sum_f A_f^2 |J_f^{nn} - J_f^{n'n'}|^2 / E^2(f); \quad (31)$$

$$Z^2 = [(G_n - W_p^0)_{\text{av}}^{-1}]^2 \sum_f A_f^2 E^2(f) J_f^{n'n} J_{-f}^{n'n'}; \quad (32)$$

$$Y = (G_n - W_p^0)_{\text{av}}^{-1} \sum_f A_f^2 J_{-f}^{n'n} (J_f^{n'n'} - J_f^{nn}). \quad (33)$$

The index n corresponds to the self-consistent state $1s$, n' to the self-consistent state $2p$.

In terms of these new symbols one is led to the following result of averaging:

$$\begin{aligned} P_{nn'} &= \left(\frac{2\pi\epsilon^6}{\hbar^2\omega} \right) \exp[-S(2\bar{n} + 1) + i\ell\varphi] \times \\ & \times \left\{ \frac{Z^2}{2} \sqrt{\bar{n}(\bar{n} + 1)} (I_{l-1}(z) + I_{l+1}(z)) + \frac{|Y|^2}{4} \bar{n}(\bar{n} + 1) \times \right. \\ & \times (I_{l+2}(z) + I_{l-2}(z)) + |Y|^2 [(\bar{n} + 1/2)^2 + 1/2\bar{n}(\bar{n} + 1)] I_l(z) \\ & \quad \left. - (\bar{n} + 1/2) \sqrt{\bar{n}(\bar{n} + 1)} |Y|^2 (I_{l-1}(z) + I_{l+1}(z)) \right\}, \end{aligned} \quad (34)$$

where

$$\begin{aligned} \bar{n} &= [\exp(\hbar\omega/kT) - 1]^{-1} l = 2\pi\nu_0/\omega, \\ \varphi &= \frac{i}{2} \ln \frac{\bar{n} + 1}{\bar{n}}, \quad z = 2s \sqrt{\bar{n}(\bar{n} + 1)}; \end{aligned} \quad (35)$$

$I_l(z)$ is Bessel's function with an imaginary argument. The probability depends on the momentum of the polaron through the quantity ℓ .

Polarons obey the Maxwellian velocity distribution law; therefore the probability, averaged over the initial kinetic energy of the polaron, can be calculated from the equation:

$$\bar{P}_{nn'} = (2\pi\mu_n kT)^{-3/2} \int P_{nn'} \exp(-J^2/2\mu_n kT) dJ. \quad (36)$$

It can be evaluated approximately at low and high temperatures.

It should be noted that for the transition considered here $Y = 0$, and therefore Eq. (34) is simplified. Furthermore, it turns out that in the

state 2p differences among components in the effective mass tensor of the polaron are not large. To simplify the calculation of the integral (36), we introduce an average effective mass of the polaron in the excited state, representing it by the symbol $\mu_{n'}$.

At low temperatures, $I_{l-1}(z)$ turns out to be the larger of the two Bessel functions in Eq. (34). A simple calculation leads to the following expression:

$$\bar{P}_{nn'} = \omega K \exp\left(-\frac{\Delta G}{kT}\right) \times \left\{1 + \frac{3}{2} \frac{kT}{\hbar\omega} \frac{\mu_n - \mu_{n'}}{\mu_n} [\ln S - \psi(\gamma - 1)] + \dots\right\}, \quad (37)$$

where

$$K = \frac{\pi}{(\hbar\omega)^2} Z^2 \frac{e^{-S} S^{\gamma-1}}{\Gamma(\gamma)} (\mu_{n'}/\mu_n)^{3/2};$$

$$\gamma = \frac{\Delta G}{\hbar\omega}; \quad \Delta G = G_{2p} - G_{1s}; \quad (38)$$

$\psi(\gamma)$ is the logarithmic derivative for Γ .

For the high temperature region, but at the same time with the restrictive condition:

$$1 \ll kT/\hbar\omega < S,$$

one can obtain an approximate expression for (36), by the method of steepest descent.¹² Let us take account of the fact that in this temperature range one can write

$$\bar{n} \approx kT/\hbar\omega, \quad z = 2S(\bar{n} + 1/2).$$

We then obtain

$$\bar{P}_{nn'} = \frac{V\pi}{\hbar^2\omega} Z^2 \sqrt{\frac{kT}{\hbar\omega}} \left(\frac{2\mu_{n'}}{\mu_n + \mu_{n'}}\right)^{3/2} S^{-1/2}$$

$$\times \exp\left[-\frac{\Delta G}{2kT} \left(1 + \frac{\gamma}{2S}\right)\right] \quad (37')$$

$$\times \cosh\left(\frac{\gamma\hbar\omega}{2SkT}\right) \sigma^{-3/2} \left(1 - \frac{15kT}{4\hbar\omega} \frac{1}{S} \left(\frac{\mu_n - \mu_{n'}}{\mu_n + \mu_{n'}}\right)^2 \sigma^{-2}\right),$$

where

$$\sigma = 1 + (\gamma/S) (\mu_n - \mu_{n'}) / (\mu_n + \mu_{n'}).$$

4. CALCULATION OF THE PARAMETERS OF THE THEORY AND EVALUATION OF THE TRANSITION PROBABILITIES

For the ground state of the polaron, following Ref. 1, we have

$$\psi_{1s} = \frac{\alpha_1^{3/2}}{\sqrt{7\pi}} (1 + \alpha_1 r) e^{-\alpha_1 r}, \quad \alpha_1 = me^2 c / 2\hbar^2,$$

$$G_{1s} = -0.0535 me^4 c^2 / \hbar^2, \quad (39)$$

$$\mu_{1s} = 5.8 \cdot 10^{-3} (me^2 c / \hbar^2)^3 e^2 c / \omega^2.$$

For the 2p state of the polaron, consistent with 1s, we have

$$\varphi_{2p} = (4!)^{-1/2} (2\alpha)^{3/2} (2\beta)^{1/2} (2\alpha r) e^{-2\beta r} Y_{10}(\theta),$$

where

$$\alpha = 0.6585 me^2 c / \hbar^2, \quad 2\beta = 0.5146. \quad W_{2p}^0 = 0.0153 me^4 c^2 / \hbar^2. \quad (40)$$

In the self-consistent 2p state, we have

$$\psi_{2p} = \frac{\alpha_2^{3/2}}{2\sqrt{6}} e^{-\alpha_2 r/2} (2\alpha_2 r) Y_{10}(\theta),$$

$$\alpha_2 = 0.3914 me^2 c / \hbar^2, \quad G_{2p} = -0.0191 me^4 c^2 / \hbar^2. \quad (41)$$

For the effective mass of the polaron in the excited states we can write:

$$\mu_{2p}^1 = \mu_{2p}^2 = 6.30 \cdot 2^{-10} (e^2 c / \omega^2) \alpha_2^3,$$

$$\mu_{2p}^3 = 2.69 \cdot 2^{-9} (e^2 c / \omega^2) \alpha_2^3. \quad (42)$$

In view of the above, the average effective mass of the polaron in this state is equal to:

$$\mu_{2p} = (2\mu_{2p}^1 + \mu_{2p}^3) / 3. \quad (42')$$

The ratio of the polaron effective masses in the two states is the same in all crystals and is equal to:

$$\mu_{1s} / \mu_{2p} = 16.51. \quad (43)$$

Calculations of Eqs. (31), (32), and (33) yield the following expressions:

$$S = \frac{e^2 c \alpha_1}{\hbar\omega} \left\{ 0.2142 + 0.1957\tau - \frac{\tau}{14} \left[\frac{7+9\tau}{(1+\tau)^2} + \frac{11\tau^2+5\tau}{(1+\tau)^4} + \frac{6\tau^2+16\tau^3}{(1+\tau)^6} + \frac{15\tau^3}{(1+\tau)^7} \right] \right\}, \quad (44)$$

$$Z^2 = \frac{4}{3} \frac{e^2 c \alpha_1 (\hbar\omega)^3}{(1+\tau)^7} \left[\left(\frac{1}{G_{1s} - W_p^0} \right)_{\text{av}} \right]^2$$

$$\times \left(1 + \frac{7}{1+\tau} + \frac{185}{14(1+\tau)^2} \right), \quad (45)$$

where $\tau = \alpha_2 / 2\alpha_1$.

From Eqs. (44) and (45) we obtain

$$S = 0.0508 me^4 c^2 / \hbar^3 \omega, \quad (44')$$

$$Z^2 = 0.0156 (\hbar\omega)^3 e^2 c \alpha_1 [(G_{1s} - W_p^0)_{\text{av}}^{-1}]^2. \quad (45')$$

To calculate the average indicated here, one can make use of Kessler's method.¹³ This average value is of the order

$$(G_{1s} - W_{2p})^{-1},$$

if the energy of the states 2s, 2p, and 3s, consistent with 1s, are approximately equal to each other. Then one can write

$$Z^2 = 0.0567 (\hbar\omega)^2 / \gamma. \quad (45'')$$

For Eq. (37) we obtain

$$\bar{P}_{nn'} = \frac{1.917 \cdot 10^{-3} \omega}{\gamma V S} \sqrt{\frac{kT}{\hbar \omega}} \left(1 - \frac{1.148 kT}{S \hbar \omega}\right) \times \cosh\left(\frac{0.338 \hbar \omega}{kT}\right) \exp\left(-0.668 \frac{\Delta G}{kT}\right). \quad (37'')$$

Table I lists the values of the coefficient K of Eq. (38) for certain alkali-halide crystals.

Values of the probabilities of thermal excitation $\bar{P}_{nn'}$, arrived at from Eq. (37''), are presented in Table II (the probability is given in sec^{-1}).

TABLE I

	NaCl	KCl	KBr	KJ
K	$3.40 \cdot 10^{-5}$	$7.42 \cdot 10^{-5}$	$7.76 \cdot 10^{-5}$	$8.39 \cdot 10^{-5}$
$K\omega$	$1.66 \cdot 10^9$	$2.96 \cdot 10^9$	$2.37 \cdot 10^9$	$2.15 \cdot 10^9$

In Table II, the last two values ($T = 700^\circ \text{K}$) are less precise, since the criterion $kT/\hbar\omega < S$ does not hold very well.

TABLE II

$T \cdot \text{K}$	NaCl	KCl	KBr	KJ
293	$5.39 \cdot 10^7$	$3.38 \cdot 10^8$	$5.78 \cdot 10^8$	$7.60 \cdot 10^8$
500	$4.19 \cdot 10^8$	$1.22 \cdot 10^9$	$1.44 \cdot 10^9$	$1.45 \cdot 10^9$
700	$0.94 \cdot 10^9$	$1.91 \cdot 10^9$	$1.74 \cdot 10^9$	$1.40 \cdot 10^9$

These tables show that at room temperature and at higher temperatures, the probability of thermal excitation of the polaron $1s \rightarrow 2p$ is significant. The transition into an excited state oc-

curs approximately in a time $10^{-8} - 10^{-9}$ sec.

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¹S. I. Peкар, Исследования по электронной теории кристаллов (Investigations on the Electron Theory of Crystals), Moscow, 1951.

²J. Frenkel, Phys. Rev. **37**, 17; 1276 (1931).

³K. Huang and A. Rhys, Proc. Roy. Soc. **A204**, 406 (1950).

⁴M. Lax, Jour. Chem. Phys. **20**, 1752 (1952).

⁵M. A. Krivoglaz, J. Exptl. Theoret. Phys. (U.S.S.R.) **25**, 191 (1953).

⁶Yu. E. Perlin and M. M. Sharand, Уч. зап. Кишиневского ун-та (Science Notes, Kishinev State Univ.) **24**, 41 (1956).

⁷R. Kubo, Phys. Rev. **86**, 929 (1952).

⁸N. N. Bogoliubov, Укр. математич. журнал (Ukrainian Math. Jour.) **2**, 3 (1950).

⁹S. V. Tiablikov, J. Exptl. Theoret. Phys. (U.S.S.R.) **21**, 377 (1951).

¹⁰S. V. Tiablikov, Doctoral Dissertation, Moscow (1954).

¹¹R. P. Feynman, Phys. Rev. **84**, 108 (1951).

¹²V. I. Smirnov, Курс высшей математики (A Course in Higher Mathematics), Vol. 3, p. 286 (1955).

¹³P. Kessler, Compt. rend. **240**, 1058 (1955).

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