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Translated by G. M. Volkoff
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SOVIET PHYSICS JETP

VOLUME 5, NUMBER 6

DECEMBER 15, 1957

Interaction between Current Carriers and *F*-centers and the Acoustic Vibrations of the Lattice in Ionic Crystals

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(Submitted to JETP editor July 7, 1956)

J. Exptl. Theoret. Phys. (U.S.S.R.) **32**, 1382-1392 (June, 1957)

Interaction between an "excess" electron in an ionic crystal with optical and acoustical vibrations of the lattice is considered. Account of interaction with acoustical vibrations leads to a reduction of the energy of the system and to a change in the effective mass of the current carrier in comparison with the polaron. The wave functions, the energies of the ground and excited states of the *F*-centers and the parameters of the *F*-absorption band are computed with account of the "condenson" interaction. A comparison of the polaron and condenson effects in ionic crystals is given.

THE INTERACTION of the "excess" electron with optical vibrations in an ionic dielectric leads to the appearance of "polaron" states.¹ The effective mass of the current carrier in such crystals—the polarons—can differ appreciably from the effective mass of the "band" electron. In polaron theory the interaction with acoustical vibrations was not excluded in the zeroth approximation, but was considered as a reason for the scattering of polaron waves.² As an excitation potential, use was made of the micropotential assumed by Bloch, Brillouin and Bethe.³ Such a consideration is valid for those crystals in which the corrections to the energy (as a result of consideration of the interaction with the acoustical vibrations of the lattice) are significantly smaller than the spacing of the energy levels of the polaron. However, the effect of the interaction with acoustical vibrations of the lattice is not small in a whole series of ionic crystals with strong homopolar coupling. Hence, considera-

tion of this interaction in the zeroth approximation of the theory is a necessity.

Such a consideration is given below. We chose a potential of the deformation type as the interaction potential for the electron with the acoustical vibrations of the lattice. This potential was hypothesized by Pekar and one of the authors of this paper,⁴ and is the condenson potential.* The energy terms and wave functions of the system were computed by the variational method and by an adiabatic approximation. The effective mass of the current carrier was computed; it differs from the effective mass of the polaron. In this same approximation, the quantum states of the *F*-center were considered and the parameters of the *F*-absorption band were obtained. A comparison of the magnitude of the condenson and polaron effects in ionic crystals is given.

* This potential was proposed independently by Bardeen and Shockley.¹⁰

1. HAMILTONIAN OF THE SYSTEM. GROUND STATES OF THE CRYSTAL WITH AN "EXCESS" ELECTRON (VARIATIONAL METHOD)

Making use of the results of Refs. 1, 4, 5, the Hamiltonian of the crystal - "excess" electron system can be written in the following fashion:

$$\hat{H} = -\frac{\hbar^2}{2\mu_0} \Delta + V_p(\mathbf{r}) + V_k(\mathbf{r}) + \hat{H}_{\text{op}\parallel} + \hat{H}_{\text{ac}}, \quad (1)$$

$$V_p(\mathbf{r}) = e \int \frac{\mathbf{P}(\mathbf{r}') \cdot (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\tau' \quad (2)$$

$\mathbf{P}(\mathbf{r})$ is the inertial part of the separate polarization of the dielectric by the field of the electron:

$$V_k(\mathbf{r}) = a(u_{11} + u_{22} + u_{33}), \quad (3)$$

u_{kk} are the diagonal components of the deformation tensor of the dielectric; a is the coupling constant of the electron with the acoustical vibrations of the lattice; $\hat{H}_{\text{op}\parallel}$ and \hat{H}_{ac} are the Hamiltonians of the longitudinal optical and acoustical vibrations, respectively, of the lattice; μ_0 is the effective mass of the band electron. In Eq. (1) we have omitted the Hamiltonian of the transverse optical vibrations of the lattice, since, in the macroscopic approximation used here, the electron is not excited by these vibrations.¹

The Hamiltonian (1), after substitution of (2) and (3), can be transformed to

$$\begin{aligned} \hat{H} = & -\frac{\hbar^2}{2\mu_0} \Delta + e \int \frac{\mathbf{P}(\mathbf{r}_1) \cdot (\mathbf{r} - \mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|^3} d\tau_1 + a(u_{11} + u_{22} + u_{33}) \\ & + \frac{\hbar\omega}{2} \sum_k (q_k^2 - \partial^2 / \partial q_k^2) + \frac{1}{2} \sum_{\kappa\alpha} \hbar\omega_{\kappa\alpha} (q_{\kappa\alpha}^2 - \partial^2 / \partial q_{\kappa\alpha}^2), \end{aligned} \quad (4)$$

where q_k , $q_{\kappa\alpha}$ are the generalized coordinates of the normal vibrations, k and κ are the number of the optical and acoustical vibrations; ω is the limiting frequency of the optical vibrations; $\omega_{\kappa\alpha}$ are the frequencies of the corresponding acoustical vibrations, α is the number of the acoustical branch of the vibrations.

The ground state of the system is determined from the absolute minimum of the functional

$$\bar{H} = \int \Psi^*(\mathbf{r} \dots q_k \dots q_{\kappa\alpha}) \hat{H} \Psi(\mathbf{r} \dots q_k \dots q_{\kappa\alpha} \dots) d\tau dq_1 dq_2, \quad dq_1 = \prod_k dq_k; \quad dq_2 = \prod_{\alpha} \prod_{\kappa} dq_{\kappa\alpha} \quad (5)$$

with the additional normalization condition

$$\int |\Psi|^2 d\tau dq_1 dq_2 = 1.$$

The minimized function is put in product form:

$$\Psi(\mathbf{r} \dots q_k \dots q_{\kappa\alpha} \dots) = \psi(\mathbf{r}) \Phi(\dots q_k \dots) \prod_{\alpha} F_{\alpha}(\dots q_{\kappa\alpha} \dots). \quad (6)$$

Substitution of (6) in (5), and variation with respect to Φ and to F_{α} lead to a system of equations for Φ and F_{α}

$$\begin{aligned} \left(\sum_k H_k \right) \Phi &= \lambda \Phi; \quad \left(\sum_{\kappa} H_{\kappa\alpha} \right) F_{\alpha} = \lambda_{\alpha} F_{\alpha}, \\ H_k &= \frac{1}{2} \hbar\omega [(q_k - q_k^0)^2 - \partial^2 / \partial q_k^2] - \frac{c}{8\pi} D_k^2[\psi], \\ H_{\kappa\alpha} &= \frac{1}{2} \hbar\omega_{\kappa\alpha} [(q_{\kappa\alpha} - q_{\kappa\alpha}^0)^2 - \partial^2 / \partial q_{\kappa\alpha}^2] - \frac{a^2}{2\rho} K_{-\kappa}^2[\psi] \cos^2 \theta_{\alpha} / f_{\alpha}^2, \\ q_k^0 &= (c / 4\pi\hbar\omega)^{1/2} D_k[\psi], \quad q_{\kappa\alpha}^0 = (\rho\hbar\omega_{\kappa\alpha})^{-1/2} aK_{-\kappa}[\psi] \cos \theta_{\alpha} / f_{\alpha}, \end{aligned} \quad (7)$$

$c = 1/n^2 - 1/\epsilon$; ϵ is the dielectric constant of the crystal, n = optical index of refraction; $f_{\alpha} = \omega_{\kappa\alpha}/|\kappa|$; ρ = density of the crystal, θ_{α} is the angle between the vectors κ and $q_{\kappa\alpha}$:

$$D_k[\psi] = e \int |\psi(\mathbf{r})|^2 \frac{(\mathbf{r}_1 - \mathbf{r})}{|\mathbf{r}_1 - \mathbf{r}|^3} \chi_k(\mathbf{r}_1) d\tau d\tau_1, \quad K_{-x}[\psi] = - \int |\psi(\mathbf{r})|^2 \chi_{-x}(\mathbf{r}) d\tau, \quad (8)$$

χ_k and χ_x are basic functions to which the expansion of the vectors of the specific polarization of the dielectric $\mathbf{P}(\mathbf{r})$ and the displacement of the medium $\mathbf{u}(\mathbf{r})$ reduce.¹

The eigenfunctions and the eigenvalues of Eq. (7) have the form

$$\begin{aligned} \Phi &= \prod_k \exp \left\{ -\frac{1}{2} (q_k - q_k^0)^2 \right\} H_{n_k}(q_k - q_k^0), \quad E = \hbar\omega \sum_k \left(n_k + \frac{1}{2} \right) - \frac{c}{8\pi} D_k^2[\psi], \\ F_\alpha &= \prod_{x\alpha} \exp \left\{ -\frac{1}{2} (q_{x\alpha} - q_{x\alpha}^0)^2 \right\} H_{n_{x\alpha}}(q_{x\alpha} - q_{x\alpha}^0) \\ E_\alpha &= \sum_x \hbar\omega_{x\alpha} \left(n_x + \frac{1}{2} \right) - \frac{a^2}{2\rho} K_{-x}^2[\psi] \frac{\cos^2 \theta_\alpha}{f_\alpha^2}, \end{aligned} \quad (9)$$

n_k and n_x are the quantum numbers of the oscillators, H_n are the Tschebycheff-Hermite polynomials of order n .

Use of Eqs. (9) allows us to represent the functions \bar{H} in the form

$$\bar{H} = J[\psi] + \hbar\omega \sum_k \left(n_k + \frac{1}{2} \right) + \sum_{x\alpha} \hbar\omega_{x\alpha} \left(n_x + \frac{1}{2} \right), \quad (10)$$

where $J[\psi]$ is a function depending only on $\psi(\mathbf{r})$:

$$J[\psi] = \frac{\hbar^2}{2\mu_0} \int |\nabla\psi|^2 d\tau - \frac{c}{8\pi} \sum_k D_k^2[\psi] - \frac{a^2}{2\rho} \sum_{x\alpha} f_\alpha^{-2} \cos^2 \theta_\alpha K_{-x}^2[\psi]. \quad (11)$$

The procedure for further calculations requires a knowledge of the explicit form of the dependence of the quantities $\cos \theta_\alpha$ and f_α on x . For crystals with a lattice of the type NaCl, these dependencies can be found by making use of the results of Tolpygo.⁶ It follows from his work that

$$\cos^2 \theta_\alpha = \frac{[(k_1 + k_2 s_\alpha)z - (k_3 + k_4 s_\alpha)]^2}{Y_\alpha (k_1 + k_2 s_\alpha)^2 + (k_3 + k_4 s_\alpha)^2 - 2z(k_1 + k_2 s_\alpha)(k_3 + k_4 s_\alpha)}.$$

Here k_1, k_2, \dots, z are constants depending on the parameters of the crystal,

$$Y_\alpha = n_x^2 / (n_x^2 - s_\alpha)^2 + n_y^2 / (n_y^2 - s_\alpha)^2 + n_z^2 / (n_z^2 - s_\alpha)^2, \quad \mathbf{n} = \mathbf{x} / |\mathbf{x}|,$$

s_α is a root of the cubic equation:

$$\begin{aligned} n_x^2 / (n_x^2 - s) + n_y^2 / (n_y^2 - s) \\ + n_z^2 / (n_z^2 - s) + z = 0. \end{aligned}$$

The roots s_α ($\alpha = 1, 2, 3$) correspond to the three branches of acoustic vibrations:

$$f_\alpha = v_\alpha e l / \sqrt{\mu d},$$

μ is the reduced mass of the two ions of opposite sign, d is the shortest distance between them;

$$l = (\mu_1 + \mu_2) / [0,69557 - 4(a_{11} + a_{22})],$$

$\mu_i = m_i / \mu$ ($i = 1, 2$), m_i is the mass of the ion, a_{11} and a_{22} are functions of the parameters of the crystal;

$$v_\alpha^2 = 1 + 2z s_\alpha.$$

It is appropriate to approximate the quantity

$$B = \sum_\alpha B_\alpha = \sum_\alpha v_\alpha^{-2} \cos^2 \theta_\alpha \quad (12)$$

by the expression

$$B = (c_0 + c_4 Y_4 + c_6 Y_6 + c_8 Y_8 + c_{10} Y_{10})^2, \quad (13)$$

where Y_i is a spherical function which is invariant

relative to a rotation about the coordinate axes by $\pi/2$, and reflection from the coordinate planes.⁹

The coefficients c_i were determined by comparison of Eqs. (12) and (13) at five different points. The smoothness of the approximation is verified at seven other points.

The chosen approximation gives an error of the order of 10%. Changing from summation to integration in Eq. (11), we can write

$$J[\psi] = \frac{\hbar^2}{2\mu_0} \int |\nabla\psi|^2 d\tau - \frac{e^2 c}{2} \int \frac{\psi^2(1)\psi^2(2)}{r_1 - r_2} d\tau_1 d\tau_2 - \frac{a^2 L^3}{2\rho 8\pi^3} \int_0^\infty K_{-\kappa}^2[\psi] \kappa^2 d\kappa \int_0^{\pi/2} \sin\vartheta d\vartheta \int_0^{2\pi} B(\vartheta, \varphi) d\varphi,$$

L^3 is the volume of the fundamental cell of the crystal. $J[\psi]$ is minimized with respect to $\psi(r)$ by means of the approximating function

$$\psi_0(r) = (\alpha^3/7\pi)^{1/2} (1 + \alpha r) e^{-\alpha r}. \quad (14)$$

Use of (14) and (8) and rather tedious calculations permit us to determine $J[\psi]$ as a function of the parameter α of the approximation:

$$J_0[\alpha] = \frac{1}{14} \left\{ \frac{3\hbar^2}{\mu_0} \alpha^2 - 3e^2 c \alpha - a^2 \frac{\mu l Q_0 d}{\rho e^2} \frac{437}{2^9 \cdot 7\pi^2} \alpha^3 \right\},$$

$$Q_0 = \int_0^{\pi/2} \sin\vartheta d\vartheta \int_0^{2\pi} B(\vartheta, \varphi) d\varphi. \quad (15)$$

The extremum condition $dJ_0/d\alpha = 0$ allows us to find the expression α corresponding to a minimum of the functional α_m :

$$\alpha_m = \hbar^2 e^2 g_0 (1 - \sqrt{1 - \mu_0 c / \hbar^4 g_0}), \quad (16)$$

$$g_0 = (2^9 \cdot 7\pi^2 / 437) \rho / \mu a^2 \mu_0 Q_0 l d. \quad (17)$$

Expressions (15)–(17) determine the minimal value of the functional.

The above calculation can be carried as far as numerical results only for certain crystals, for which the dependence of f_α and $\cos\vartheta_\alpha$ on κ is known. Therefore, the approximate consideration of the ground state of the current carrier in polar crystals is of interest, under the assumption that the crystal is isotropic. In this case, using the results of Refs. 1 and 5, we can write the function $J[\psi]$ in the form

$$J[\psi] = \frac{\hbar^2}{2\mu_0} \int |\nabla\psi|^2 d\tau \quad (18)$$

$$- \frac{e^2 c}{2} \int \frac{\psi^2(1)\psi^2(2)}{r_1 - r_2} d\tau_1 d\tau_2 - \frac{a^2}{2(K + 4\mu/3)} \int \psi^4 d\tau.$$

Here K and μ are the moduli of uniform compression and shear, respectively.

Using Eq. (14) as an approximating function, we get

$$J_0[\alpha] = \frac{3}{14} \frac{\hbar^2}{\mu_0} \alpha^2 - \frac{3}{14} e^2 c \alpha - \frac{437 a^2}{49 \cdot 2^9 \pi (K + 4\mu/3)} \alpha^3. \quad (19)$$

The condition $dJ_0/d\alpha = 0$ leads in this case to an expression for α_m analogous to Eq. (16), but with a value of g_0 different from Eq. (17):

$$g_0 = (2^8 \cdot 7\pi/437) (K + 4\mu/3) / \mu_0 a^2 e^2. \quad (20)$$

2. ENERGY OF THE FUNDAMENTAL STATE AND THE WAVE FUNCTION OF A SYSTEM IN THE ADIABATIC APPROXIMATION. EFFECTIVE MASS OF THE CURRENT CARRIER.

In the adiabatic approximation the energy of the system is computed in two ways: first, the configuration of the ions is fixed by giving the totality of the normal coordinates P_k ; u_k or q_k , q_κ . The state of the conduction electron corresponding to this configuration is determined by the equation

$$\left[-\frac{\hbar^2}{2\mu_0} \Delta + V_p(\mathbf{r}) + V_k(\mathbf{r}) \right] \psi(\mathbf{r}) = E_0 \psi(\mathbf{r}). \quad (21)$$

Here $V_p(\mathbf{r})$ and $V_k(\mathbf{r})$ are expressed by Eqs. (2) and (3). The value of E_0 which is found enters as a component part in the energy of the "heavy" subsystem.

It is appropriate to replace Eq. (21) by the equivalent variational principle

$$E_0(\dots P_k \dots u_\kappa \dots) = \min_\psi \left\{ \frac{\hbar^2}{2\mu_0} \int |\nabla\psi|^2 d\tau + \int V_p(\mathbf{r}) |\psi|^2 d\tau + \int V_k(\mathbf{r}) |\psi|^2 d\tau \right\}.$$

The total energy of the conduction electron in the longitudinal acoustic and optical vibrations is equal to

$$H = E_0(\dots P_k \dots u_x \dots) + H_{\text{op}} + H_{\text{ac}}. \quad (22)$$

Solution of the Schrödinger equation with Hamiltonian (22) is very difficult in the general case. However, it is possible to find the solution for the equilibrium configuration of the ions, for which the potential energy of the ions is a minimum. This potential energy can be written in the form

$$F(\psi \dots P_k \dots u_x \dots) = E_0(\dots P_x \dots u_x \dots) + \sum_k \frac{2\pi}{c_k} P_k^2 + \frac{\rho}{2} \sum_x \omega_x^2 u_x^2.$$

Here the second and third terms are the potential energies of the optical and acoustical vibrations of the ions. Let us assume that the crystal is isotropic.

Minimizing F with respect to P_k and u_x , we get

$$P_k = c_k D_k / 4\pi; \quad u_x = -aK_{-x} / |x| (K + 4\mu/3). \quad (23)$$

Substitution of (23) reduces F to the functional $J[\psi]$ [Eq. (18)] which depends only on $\psi(\mathbf{r})$. Minimizing $J[\psi]$ was carried out above. The solutions obtained refer to an electron in a polaron-condenson well,* the center of which is at the origin of the coordinates. However, the current carrier can be localized at any point of the crystal. For a polaron-condenson with center at the point ξ , the equilibrium solution is obtained by a translation of the quantities $\psi_0(\mathbf{r})$, $\mathbf{P}_0(\mathbf{r})$, $\mathbf{u}_0(\mathbf{r})$, $V_{p_0}(\mathbf{r})$ and $V_{k_0}(\mathbf{r})$ through the vector ξ . In complete analogy with Ref. 1, we represent the polarization \mathbf{P} and the displacement \mathbf{u} at an arbitrary point in the crystal in the form

$$\mathbf{P}(\mathbf{r}) = \mathbf{P}_0(\mathbf{r} - \xi) + \mathbf{P}'(\mathbf{r}); \quad \mathbf{u}(\mathbf{r}) = \mathbf{u}_0(\mathbf{r} - \xi) + \mathbf{u}'(\mathbf{r}),$$

where $\mathbf{P}'(\mathbf{r})$ and $\mathbf{u}'(\mathbf{r})$ can be regarded as small perturbations of the polarization and displacement, respectively, at those places in space where the polaro-condenson is localized, and where the terms $\mathbf{P}_0(\mathbf{r} - \xi)$ and $\mathbf{u}_0(\mathbf{r} - \xi)$ are large. In the rest of space, far from the polaro-condenson, $\mathbf{P}_0(\mathbf{r} - \xi)$ and $\mathbf{u}_0(\mathbf{r} - \xi)$ are small and the polarization and the displacement are defined by the vectors $\mathbf{P}'(\mathbf{r})$ and $\mathbf{u}'(\mathbf{r})$. In the zeroth approximations, the terms $\mathbf{P}'(\mathbf{r})$ and $\mathbf{u}'(\mathbf{r})$ are omitted; then the solution of Eq. (21) will be $\psi_0(\mathbf{r} - \xi)$. Introducing the terms $\mathbf{P}'(\mathbf{r})$ and $\mathbf{u}(\mathbf{r})$ as small perturbations, and making use of perturbation theory, we compute the energy of the electron in the first approximation. It is shown to be equal to

$$E(\dots P_k \dots u_x \dots) = \frac{\hbar^2}{2\mu_0} \int |\nabla\psi|^2 d\tau - \int \mathbf{P}(\mathbf{r}) D_0(\mathbf{r} - \xi) d\tau + a \sum_x u_x |x| K_{-x}(\xi), \quad (24)$$

$$K_{-x}(\xi) = - \int [\psi_0(r - \xi)]^2 \chi_{-x}(r) d\tau.$$

Substituting Eqs. (23) and (24) in Eq. (22), and making use of the relation

$$\omega_x^2 = (K + 4\mu/3) x^2 / \rho,$$

we get

$$H = J[\psi] + \sum_k \frac{2\pi}{c_k} P_k^2 + \sum_k \frac{2\pi}{c_k \omega_k^2} P_k^2 + \frac{1}{2} (K + 4\mu/3) \sum_x u_x'^2 x^2 + \frac{\rho}{2} \sum_x \dot{u}_x'^2. \quad (25)$$

Introducing the notation

$$2\pi P_k^2 / c_k \omega_k^2 = \varphi_{1k}^2; \quad \rho u_x'^2 / 2 = \varphi_{2k}^2; \quad 2\pi P_{k\xi}^2 / c_k \omega_k^2 = \varphi_{1k\xi}^2; \quad \rho u_{x\xi}'^2 / 2 = \varphi_{2k\xi}^2, \quad (26)$$

* Such a development will be called hereinafter a polaro-condenson.

we can rewrite Eq. (25) in the form

$$H = J[\psi] + \sum_{\alpha=1}^2 \sum_k [\dot{\varphi}_{\alpha k}^2 + (\varphi_{\alpha k} - \varphi_{\alpha k \xi})^2 \omega_{\alpha k}^2].$$

Transforming to canonically conjugate coordinates,

$$g_{\alpha k} = \dot{\varphi}_{\alpha k} \sqrt{2/\hbar\omega_{\alpha k}}; \quad q_{\alpha k} = \varphi_{\alpha k} \sqrt{2\omega_{\alpha k}/\hbar}$$

and replacing $g_{\alpha k}$ by the operator $-i\partial/\partial q_{\alpha k}$, we get

$$H = J[\psi] + \frac{1}{2} \sum_{\alpha=1}^2 \sum_k \hbar\omega_{\alpha k} [(q_{\alpha k} - q_{\alpha k \xi})^2 - \partial^2/\partial q_{\alpha k}^2]. \tag{27}$$

We can determine the quantity ξ , which enters into Eq. (27), from the condition

$$\partial E(\dots P_k \dots u_x \dots \xi) / \partial \xi_i = 0 \quad (i = 1, 2, 3),$$

which, with the use of the notation (26) and Eq. (23), can be written in the following form:

$$\sum_{\alpha} \sum_k \varphi_{\alpha k} \omega_{\alpha k}^2 \partial \varphi_{\alpha k \xi} / \partial \xi_i = 0. \tag{28}$$

We can determine ξ in another manner; let us approximate φ_{α} by the function $\varphi_{\alpha \xi}$ by means of the method of least squares, and so choose ξ_i that the integral $\sum_{\alpha} \int (\varphi_{\alpha} - \varphi_{\alpha \xi})^2 d\tau$ will be a minimum. In this case, in place of the condition (28), we get

$$\sum_{\alpha} \sum_k \varphi_{\alpha k} \partial \varphi_{\alpha k \xi} / \partial \xi_i = 0. \tag{29}$$

In a way similar to that used by Pekar,⁷ we select (for the determination of ξ) an equation intermediate to (28) and (29):

$$\sum_{\alpha} \sum_k \varphi_{\alpha k} \omega_{\alpha k} \partial \varphi_{\alpha k \xi} / \partial \xi_i = 0$$

or, in normal coordinates

$$\sum_{\alpha} \sum_k q_{\alpha k} \partial q_{\alpha k \xi} / \partial \xi_i = 0. \tag{30}$$

By use of the method developed by Pekar, we can obtain a series of auxiliary relations which are necessary for what follows.

Defining the operators $\hat{\omega}_{1k}$ and $\hat{\omega}_{2k}$ by means of the relation

$$\hat{\omega}_{1k} \chi_k(r) = (\omega_0 + k^2 \omega_1) \chi_k(r), \quad \hat{\omega}_{2k} \chi_k(r) = -k \chi_{-k}(r),$$

we can show that

$$\sum_{\alpha} \int [\hat{\omega}_{\alpha}^{n_1} \varphi_{\alpha}(r - \xi)] [\hat{\omega}_{\alpha}^{n_2} \varphi_{\alpha}(r - \xi)] d\tau = \sum_{\alpha} \int \varphi_{\alpha}(r) \hat{\omega}_{\alpha}^{n_1} \varphi_{\alpha}(r) d\tau.$$

We differentiate this equation with respect to ξ_i , recalling that $n_1 = n_2 = n/2$:

$$\sum_{\alpha} \int \frac{\partial \varphi_{\alpha}(r - \xi)}{\partial \xi_i} \hat{\omega}_{\alpha}^{n/2} \varphi_{\alpha}(r - \xi) d\tau = 0,$$

and then differentiate with respect to ξ_j :

$$\sum_{\alpha} \int \frac{\partial \varphi_{\alpha}(r - \xi)}{\partial \xi_i} \frac{\partial \hat{\omega}_{\alpha}^{n/2} \varphi_{\alpha}(r - \xi)}{\partial \xi_j} = - \sum_{\alpha} \int \frac{\partial^2 \varphi_{\alpha}(r - \xi)}{\partial \xi_i \partial \xi_j} \hat{\omega}_{\alpha}^{n/2} \varphi_{\alpha}(r - \xi) d\tau = O_{ij}^{(n)}.$$

Thanks to the spherical symmetry of the functions $\varphi_{\alpha}(r)$ and $\hat{\omega}_{\alpha}^{n/2} \varphi_{\alpha}(r)$, $O_{ij}^{(n)} = \delta_{ij} O^{(n)}$. The total differential of Eq. (30) is then

$$\sum_{\alpha k} dq_{\alpha k} \partial q_{\alpha k \xi} / \partial \xi_i + \sum_{\alpha k} \sum_{j=1}^3 q_{\alpha k} (\partial^2 q_{\alpha k \xi} / \partial \xi_i \partial \xi_j) d\xi_j = 0. \tag{31}$$

It is easy to show that

$$\sum_{\alpha k} \sum_j q_{\alpha k} \partial^2 q_{\alpha k \xi} / \partial \xi_i \partial \xi_j = - \frac{2}{\hbar} \delta_{ij} O^{(1)}.$$

Here we can transform Eq. (31) to the form

$$\frac{\partial q_{\alpha k \xi}}{\partial \xi_i} = \frac{2}{\hbar} O^{(1)} \frac{\partial \xi_i}{\partial q_{\alpha k}} \quad \text{or} \quad \frac{\partial \xi_i}{\partial q_{\alpha k}} = \frac{\hbar}{2O^{(1)}} \frac{\partial q_{\alpha k \xi}}{\partial \xi_i}.$$

These formulas allow us to establish the validity of the following equations:

$$\sum_{\alpha k} \sum_{j=1}^3 \hbar \omega_{\alpha k} \frac{\partial \xi_i}{\partial q_{\alpha k}} \frac{\partial \xi_j}{\partial q_{\alpha k}} \frac{\partial^2}{\partial \xi_i \partial \xi_j} = \frac{\hbar^2 O^{(2)}}{2(O^{(1)})^2} \sum_{j=1}^3 \frac{\partial^2}{\partial \xi_j^2}, \quad (32a)$$

$$\begin{aligned} & \sum_{\alpha k} \sum_{ij} \hbar \omega_{\alpha k} \frac{\partial \xi_j}{\partial q_{\alpha k}} \left(\frac{\partial}{\partial \xi_j} \frac{\partial \xi_i}{\partial q_{\alpha k}} \right) \frac{\partial}{\partial \xi_i} \\ &= \frac{\hbar^3}{4(O^{(1)})^2} \sum_{\alpha k ij} \omega_{\alpha k} \frac{\partial q_{\alpha k \xi}}{\partial \xi_j} \frac{\partial^2 q_{\alpha k \xi}}{\partial \xi_i \partial \xi_j} \frac{\partial}{\partial \xi_j}. \end{aligned} \quad (32b)$$

In the case of spherical symmetry of the function φ_{α} , Eq. (32b) will vanish.

The solution to Schrödinger's equation with operator \hat{H} is sought in the form

$$\begin{aligned} & \Psi(\dots q_{\alpha k} \dots) \\ &= U(\xi_1, \xi_2, \xi_3) \exp \left\{ -\frac{1}{2} \sum_{\alpha k} (q_{\alpha k} - q_{\alpha k \xi})^2 \right\}, \end{aligned}$$

the $q_{\alpha k}$ enter directly into Ψ , and are also contained in the ξ_i . We denote by $\frac{\partial}{\partial^* q_{\alpha k}}$ differentiation only with respect to the $q_{\alpha k}$ which do not enter into the ξ_i . In this case,

$$\begin{aligned} \frac{\partial^2}{\partial q_{\alpha k}^2} &= \frac{\partial^2}{\partial^* q_{\alpha k}^2} + \frac{\partial \xi_i}{\partial q_{\alpha k}} \frac{\partial \xi_j}{\partial q_{\alpha k}} \frac{\partial^2}{\partial \xi_i \partial \xi_j} \\ &+ \frac{\partial \xi_j}{\partial q_{\alpha k}} \left(\frac{\partial}{\partial \xi_j} \frac{\partial \xi_i}{\partial q_{\alpha k}} \right) \frac{\partial^2}{\partial \xi_i} + \frac{\partial \xi_i}{\partial q_{\alpha k}} \frac{\partial^2}{\partial \xi_i \partial^* q_{\alpha k}} + \frac{\partial \xi_i}{\partial q_{\alpha k}} \frac{\partial^2}{\partial^* q_{\alpha k} \partial \xi_i}. \end{aligned} \quad (33)$$

Taking (30) into account, we can show that

$$\partial^2 \Psi / \partial \xi_i \partial^* q_{\alpha k} = 0,$$

$$\partial^2 \Psi / \partial^* q_{\alpha k} \partial \xi_i = \Psi \partial q_{\alpha k \xi} / \partial \xi_i. \quad (34)$$

Considering Eqs. (27), (32a), (32b), (33) and (34), we get

$$\begin{aligned} H\Psi &= \left\{ J[\Psi] + \frac{1}{2} \sum_{\alpha k} \hbar \omega_{\alpha k} - \frac{3}{2} \hbar \frac{O^{(2)}}{O^{(1)}} - \frac{\hbar^2}{2M} \Delta_{\xi} \right\} \Psi, \\ M &= 2(O^{(1)})^2 / O^{(2)}. \end{aligned}$$

Thus the energy of the ground state of the polaron condensation is

$$H = J[\psi_0] + \frac{1}{2} \sum_{\alpha k} \hbar \omega_{\alpha k} - \frac{3}{2} \hbar (O^{(2)} / O^{(1)}). \quad (35)$$

It is easy to verify that for the polaron in the absence of dispersion of the optical frequencies, Eq. (35) takes the form

$$H = J[\psi_0] + \frac{\nu - 3}{2} \hbar \omega_0,$$

which coincides with the result of Ref. 1. Here ν is the general number of polarized longitudinal normal vibrations of the crystal in the volume L^3 .

Computation of the integrals $O^{(1)}$ and $O^{(2)}$ permits us to express the effective mass of the polaron condensation explicitly in terms of the parameters of the crystal. The integrals pertaining to the optical vibrations were computed earlier. Computation of the integrals pertaining to the acoustical vibrations lead to the following expression for the effective mass of the current carrier in an ionic crystal:

$$M = \frac{[437.70 \pi^2 c e^2 E^2 + 183.128 a^2 \sqrt{E_p} \omega \alpha]^2 \alpha^3}{147.64 \pi^3 \omega^2 E^3 [49.437 \pi c e^2 E + 43.147 a^2 \alpha^2]} 10^{-2},$$

where α is determined by Eqs. (16) and (20), $E = K + 4\mu/3$.

3. INTERACTION OF THE ELECTRON OF THE *F*-CENTER WITH THE ACOUSTICAL VIBRATIONS OF THE LATTICE. COMPARATIVE ESTIMATE OF THE POLARON AND CONDENSATION EFFECTS IN IONIC CRYSTALS.

The Hamiltonian of the *F*-centers – crystal system, analogous to Eq. (4), can be written in the form

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2\mu_0} \Delta + e \int \frac{\mathbf{P}(\mathbf{r}_1)(\mathbf{r} - \mathbf{r}_1)}{|\mathbf{r} - \mathbf{r}_1|^3} d\tau_1 + a(u_{11} + u_{22} + u_{33}) - \frac{ze^2}{\epsilon r} \\ &+ \frac{\hbar \omega}{2} \sum_k (q_k^2 - \partial^2 / \partial q_k^2) + \sum_{\alpha x} \frac{\hbar \omega_{\alpha x}}{2} (q_{\alpha x} - \partial^2 / \partial q_{\alpha x}^2). \end{aligned}$$

The result differs from Eq. (4) by the term $-ze^2/\epsilon r$, which represents the energy of interaction of the electron with the Coulomb field of the defect.

With the aid of computations similar to those carried out in the first part of the work, we obtain for the energy of the ground state of the F -center in crystals of the type NaCl an expression similar to Eq. (10), in which $J[\psi]$ is equal to

$$J[\psi] = \frac{\hbar^2}{2\mu_0} \int |\nabla\psi|^2 d\tau - \frac{ze^2}{\epsilon} \int \frac{|\psi|^2}{r} d\tau - \frac{e^2 c}{2} \int \frac{\psi^2(1)\psi^2(2)}{(r_1 - r_2)} d\tau_1 d\tau_2 - \frac{a^2 L^3}{2\rho 8\pi^3} \int K_{-x}^2[\psi] x^2 dx B(\vartheta, \varphi) \sin \vartheta d\vartheta d\varphi.$$

Making use of the function (14), we obtain

$$J(\alpha) = \frac{1}{14} \left\{ \frac{3\hbar^2}{\mu_0} \alpha^2 - \frac{3e^2}{\epsilon} (3z + \epsilon c) \alpha - a^2 \frac{\mu l Q_0 d}{\rho e^2} \frac{437\alpha^3}{2^9 \cdot 7\pi^2} \right\}, \quad (36)$$

$$\alpha_m = \hbar^2 e^2 g_0 \left(1 - \sqrt{\frac{\mu_0 (3z + \epsilon c)}{\hbar^4 \epsilon g_0}} \right), \quad (37)$$

where g_0 is defined by Eq. (17).

Calculation of the $2p$ state of the F -center is performed in an entirely similar way; the approximating function was chosen in the form

$$\varphi_{2p}(r) = \beta^{3/2} \pi^{-1/2} e^{-\beta r} r \cos \vartheta.$$

The energy of the excited state is determined by the expression

$$H_1 = J[\beta] + \hbar\omega \sum_k \left(n'_k + \frac{1}{2} \right) + \sum_{\alpha x} \hbar\omega_{\alpha x} \left(n'_{\alpha x} + \frac{1}{2} \right),$$

where

$$J_1[\beta] = \frac{1}{2} \left\{ \frac{\hbar^2}{\mu_0} \beta^2 - \frac{e^2}{\epsilon} (z + 0,3914\epsilon c) \beta - a^2 \frac{\mu l d}{\rho e^2} \frac{1}{2^9 \pi^2} (14Q_0 - 42Q_2 + 45Q_4) \beta^3 \right\}, \quad (38)$$

$$\beta = \hbar^2 e^2 g_1 \left\{ 1 - \sqrt{1 - (\mu_0 / \epsilon \hbar^4) (z + 0,3914\epsilon c) / g_1} \right\},$$

$$Q_k = \int_0^{\pi/2} \cos^k \vartheta \sin \vartheta d\vartheta \int_0^{2\pi} B(\vartheta, \varphi) d\varphi, \quad g_1 = 2^9 \pi^2 \rho / 3\mu_0 a^2 \mu l d (14Q_0 - 42Q_2 + 45Q_4). \quad (39)$$

According to Ref. 8, the frequency of the maximum of the absorption band of the local centers is computed from the equation

$$\hbar\Omega_{\max} = |J_0 - J_1| + 1/2 a\hbar\omega + \hbar\sigma_1. \quad (40)$$

The half width of the corresponding absorption band, in the limiting cases of high and low temperatures, is determined by the expressions

$$\delta = 2 \sqrt{2 \ln 2} \sqrt{kT (a_0 \hbar\omega + 2\hbar\sigma_1)}, \quad \delta^0 = 2 \sqrt{2 \ln 2} \sqrt{1/2 (\hbar\omega)^2 a_0 + \hbar^2 \sigma_2}, \quad (41)$$

where

$$a_0 = \sum_k (q_{k1s}^0 - q_{k2p}^0)^2; \quad \sigma_1 = \frac{1}{2} \sum_{\kappa\alpha} (q_{\kappa\alpha 1s}^0 - q_{\kappa\alpha 2p}^0)^2 \omega_{\kappa\alpha}; \quad \sigma_2 = \frac{1}{2} \sum_{\kappa\alpha} (q_{\kappa\alpha 1s}^0 - q_{\kappa\alpha 2p}^0)^2 \omega_{\kappa\alpha}^2.$$

The quantity $a_0 \hbar \omega / 2$ was computed in Ref. 1; calculations that are cumbersome, but that present no difficulties in principle, let us determine $\hbar \sigma_1$ and $\hbar^2 \sigma_2$:

$$\begin{aligned} \hbar \sigma_1 = & \frac{a^2 \mu l d \alpha^3}{2\pi^2 \rho e^2} \left\{ \frac{437}{2^9 \cdot 49} Q_0 + \frac{1}{2^9} \frac{1}{v^3} (14Q_0 - 42Q_2 + 45Q_4) \right. \\ & \left. - \frac{1}{28(v+1)^7} [(7v^4 + 49v^3 + 66v^2 + 28v + 4) Q_0 - 3v^2 (7v^2 + 49v + 12) Q_2] \right\}, \end{aligned} \quad (42)$$

$$\begin{aligned} \hbar^2 \sigma_2 = & \frac{a^2 \hbar V l \mu d \alpha^4}{2\pi^3 \rho e} \left[\frac{183}{7^3 \cdot 10} Q'_0 + \frac{1}{70v^4} (7Q'_0 - 28Q'_2 + 36Q'_4) \right. \\ & - \frac{4}{7} \left\{ \frac{(21v^8 + 288v^6 - 270v^4 - 48v^2 + 9) Q'_0 - 12(7v^8 + 192v^6 + 165v^4 - 4v^2) Q'_2}{6(v^2 - 1)^6} \right. \\ & \left. \left. + \frac{6v^2 \ln v}{(v^2 - 1)^2} [(-9v^6 - 3v^4 + 13v^2 - 1) Q'_0 + (54v^6 + 150v^4 + 38v^2 - 2) Q'_2] \right\} \right], \end{aligned} \quad (43)$$

where

$$v = \alpha / \beta; \quad Q'_k = \int_0^{\pi/2} \cos^k \vartheta \sin \vartheta d\vartheta \int_0^{2\pi} \left(\sum_{\alpha} B_{\alpha} v_{\alpha} \right) d\varphi.$$

In the approximation in which the crystal is considered isotropic, Eqs. (36), (38), (42), and (43) take the form

$$\begin{aligned} J[\alpha] = & \frac{3\hbar^2}{14\mu_0} \alpha^2 - \frac{3e^2}{14\epsilon} (3z + \epsilon c) \alpha - \frac{437}{49 \cdot 2^9 \pi} \frac{a^2}{(K + 4\mu/3)} \alpha^3, \\ J[\beta] = & \frac{\hbar^2}{2\mu_0} \beta^2 - \frac{e^2}{2\epsilon} (z + 0,3914\epsilon c) \beta - \frac{9}{2^9 \pi} \frac{a^2}{(K + 4\mu/3)} \beta^3, \\ \hbar \sigma_1 = & \frac{a^2 \alpha^3}{K + 4\mu/3} \left\{ 0,00555 - 0,0227 \frac{27v^2 + 14v + 2}{(v+1)^7} + \frac{1}{v^3} 0,00560 \right\}, \\ \hbar^2 \sigma_2 = & \frac{a^2 \alpha^4}{V \rho (K + 4\mu/3)} \left\{ 0,00540 + 0,00704 \frac{1}{v^4} + 0,00965 \frac{1}{(v^2 - 1)^7} [(v^2 - 1)(7v^8 \right. \\ & \left. + 480v^6 + 930v^4 + 32v^2 - 9) - 12v^2 \ln v (27v^6 + 141v^4 + 77v^2 - 5)] \right\}. \end{aligned} \quad (44)$$

Here α is determined from (37) and (20), and β from (39), but with a different value of g_1 :

$$g_1 = 2^8 \pi (K + 4\mu/3) / 27\mu_0 a^2 e^2.$$

The theory contains two parameters, a and μ_0 . Their determination is possible by comparison of the theoretically computed values of δ and $\hbar \Omega_{\max}$ with the corresponding experimental parameters of the *F*-band.

The best agreement of the theoretical and experimental data for the alkali halide crystals, consid-

ered in Ref. 1, is obtained if we set $a = 0$, which demonstrates the small value of the condensation effect in these crystals.

Unfortunately, the absence of a complete set of experimental data for other crystals compels us to limit ourselves only to estimates.

The most favorable of the crystals known to us in regard to the experimental data is Cu_2O . But even here information is lacking on the dispersion of the vibration frequencies of the lattice. For this reason, we restrict ourselves to a comparative estimate of the polaron and condensation effects in the approxima-

tion in which the crystal is regarded as isotropic. Availing ourselves of the data⁹ for F bands, and of the expressions (40) and (41), we can determine μ_0/m and a approximately:

$$\mu_0/m \approx 0.9; \quad |a| \approx 7 \text{ eV.}$$

From these parameters we estimated the polaron and condensation terms in (19) and (44). It turned out that for the polaron-condensation the magnitude of the condensation term amounted to about 10% of the total energy, while for the F -center, to about 25%.

The values of the effective masses of the bound electron and the current carrier change appreciably in comparison with the corresponding values obtained without regard to the condensation effect. Thus μ_0/m appeared to be two times smaller than the value in Ref. 1, while $M/m = 7.63$ instead of 9.69 as in Ref. 1.

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Translated by R. T. Beyer
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SOVIET PHYSICS JETP

VOLUME 5, NUMBER 6

DECEMBER 15, 1957

Dispersion Relations for Photoproduction of Pions on Nucleons*

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(Submitted to JETP editor July 24, 1956)

J. Exptl. Theoret. Phys. (U.S.S.R.) **32**, 1393-1403 (June, 1957)

Dispersion relations are derived for pion photoproduction reactions on nucleons. The spin and isotopic structure of the reaction amplitude is established, and the unobservable energy range is separated. It is shown that the dispersion relations are inhomogeneous.

FORMAL SCATTERING THEORY, based on the unitarity and asymmetry of the scattering matrix, leads to an expression for the amplitude in terms of phase shifts. The values of the phase shifts depend on the dynamics of the collision process. Since the character of the dynamics of the process is not taken into account in the formulation of the formal scattering theory, it is natural that the values of the phases remain unknown in such an analysis. The determination of phase shifts from experimental data is of great interest, for it permits a deeper study of the character of the meson-nucleon collisions. Using the charge-independence hypothesis in the s - and p -wave approximation it becomes possible to find several possible sets of phase

shifts for the meson-nucleon collisions. This ambiguity can be eliminated using the causality principle. In fact, Goldberger¹ has found the Hermitian and anti-Hermitian portions of the forward-scattering amplitude to be connected by dispersion relations that lead to a correct choice of phase shifts for the meson-nucleon collision processes.

N. N. Bogoliubov* developed general principles for the derivation of dispersion relations for a great variety of scattering processes. His method is essentially based on analyticity theorems that follow from the principle of causality.

In the present article we shall use the Bogoliubov method to derive dispersion relations for the photoproduction of mesons on nucleons.³

*Paper delivered at the All-Union Conference on Physics of High Energy Particles on May 15, 1956.

¹Reported by N. N. Bogoliubov to many seminars on theoretical physics in the V. A. Steklov Mathematics Institute in January 1956.