

90 YEARS



EFFECTIVE MASS OF A POLARON

Translated and reprinted from *Zh. Eksp. Teor. Fiz.* **18**, No. 5, pp. 419–423 (1948)

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It is assumed that the current carrier in crystals with ionic lattice is a polaron rather than a conduction band electron. The conservative motion of a polaron as a whole is considered. The dependence of the system energy on the velocity of translational motion of a polaron and the equation of motion of a polaron in an external field are obtained.

Introduction

The available theory of the electron conduction in dielectrics and semiconductors assumes that the conduction electron moves within one of the “allowed” energy bands of a crystal, and the electron m -function is a wave, whose amplitude is constant over the whole crystal bulk. The presence of forbidden gaps in crystals is experimentally confirmed: this is testified by the fact of the dielectric existence itself, data on the temperature dependence of the electric conduction, data on the internal photoeffect and the photoeffect from a metal into a dielectric, etc. Other features of the theory mentioned above did not find any direct confirmation, and they even contradict sometimes the experimental facts.

But first of all (at least in the case of ionic crystals), it is worth to indicate that the available theory includes an internal contradiction, namely: while considering the quantum states of conduction electrons, it is assumed, as usual, that ions are fixed at lattice sites; in this case, an electron appears to be in a periodic field. However, in reality, ions are moving, and the electron state adiabatically follows the ion motion. S.I. Pekar already considered this motion [1] and showed that the conduction electron polarizes dielectrically the ionic crystal with the own electric field. It turns out that, already at the very beginning of the process of polarization, the polarized crystal represents a potential well with discrete spectrum for the electron. The electron having spent a part of its energy to polarize the crystal goes to a discrete level into the local state; then the

crystal polarization increases, and the electron level and the energy of the whole system are lowered. The equilibrium will be reached when the energy of the system reaches its minimum. In this case, the polaron is created, as was considered by one of the authors in the previous works [2, 3] in detail. Thus, the band state of a conduction electron does not correspond to an extremum of the system energy, i.e. it is unstable. Slow conduction electrons should constantly transfer into the polaron state. The decay time of a band state for the slow electron should be of the order of 10^{-13} s; hence, it is necessary to revise the foundations of the available conduction theory.

S.I. Pekar [1, 4] offered a new point of view concerning the electron conduction of ionic crystals. According to it, the current carrier is just a polaron, rather than a free electron in the conduction band. In an external electric field, the polaron should move like a negative charge. In this case, the local state should shift as a whole along the field direction (the inertial polarization of the crystal should follow the polaron movement). The calculated polaron mobility [4] is in good agreement, by the order of magnitude, with the mobility of a current carrier determined experimentally as a product of the electric conduction and the Hall constant.

In the present paper, we will calculate the effective mass of a polaron.

Effective Mass of a Polaron

The inertial and inertialess parts [2] may be separated within the dielectric polarization of ionic crystals. The inertialess part of the polarization is characterized by the square of the refraction index of light (within the range, where the dispersion curve has its plateau); it is assumed that it fully follows the movement of a conduction electron. As a result of the inertialess polarization of crystal sites by the field of the electron, it undergoes the action of a supplementary force modulated with

lattice periods; this force will be introduced into the total periodic potential of the electron in the crystal. To solve the coming tasks, we may use the known method of electron effective mass [5]. That is, we can ignore the periodic potential and simultaneously change the electron mass with its effective mass μ .

The assumption that the electron state $\psi(\mathbf{r}, t)$ adiabatically follows the ion motion and the radius of the ψ -state exceeds the lattice constant results in the following expression for the energy H of the system:

$$H = \frac{\hbar^2}{2\mu} \int |\nabla\psi|^2 d\tau - \int \mathbf{p}\mathbf{D}[\psi] d\tau + U_p. \quad (1)$$

Here, $\mathbf{p}(\mathbf{r}, t)$ is the inertial part of the specific polarization of a dielectric [2],

$$\mathbf{D}[\psi] = e \int |\psi(\mathbf{r}_1)|^2 \left\{ (\mathbf{r} - \mathbf{r}_1) / |\mathbf{r} - \mathbf{r}_1|^3 \right\} d\tau \quad (2)$$

is the quantum-mechanical mean of the electrostatic induction of the electron. In formula (1), the first and second terms stand, respectively, for the kinetic energy of an electron and the interaction energy of the electron with the polarized crystal, and U_p is the total energy of the crystal under the assumption that the electron is suddenly moved away (the potential and kinetic energies of ions).

In accordance with the variation principle of quantum mechanics (it replaces the Schrödinger equation), for every given polarization $\mathbf{p}(\mathbf{r}, t)$, $\psi(\mathbf{r}, t)$ is determined as a minimum of functional (1) with the additional condition

$$\int |\psi|^2 d\tau = 1; \quad (3)$$

hence,

$$\frac{\hbar^2}{2\mu} \delta \int |\nabla\psi|^2 d\tau - \int \mathbf{p}\delta\mathbf{D}[\psi] d\tau = 0. \quad (4)$$

In what follows, we assume that the ψ -function is already defined in this manner; then H is the Hamilton function describing the ion movement in the crystal.

We assume that the crystal is a system of ions performing small harmonic oscillations and express H via the corresponding normal coordinates and velocities of ions. The ion movement is determined with usual canonical Hamilton's equations (while differentiating H , expression (4) should be taken into account). Such equations are those for forced ion oscillations under the action of a force $\mathbf{D}(\mathbf{r}, t)$.

Let us consider a special case of motion when the polaron moves translationally as a whole with the velocity \mathbf{v} , i.e. when

$$\psi = \psi(\mathbf{r} - \mathbf{v}t), \quad \mathbf{D} = \mathbf{D}(\mathbf{r} - \mathbf{v}t), \quad \mathbf{p} = \mathbf{p}(\mathbf{r} - \mathbf{v}t). \quad (5)$$

Expanding \mathbf{D} and \mathbf{p} in the Fourier series, one obtains:

$$\mathbf{D} = \sum_{\mathbf{k}} \mathbf{D}_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r} - \mathbf{v}t)} = \sum_{\mathbf{k}} \mathbf{D}_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{r} - \omega_{\mathbf{k}}t)}, \quad \omega_{\mathbf{k}} = \mathbf{k}\mathbf{v}, \quad (6)$$

$$\mathbf{p} = \sum_{\mathbf{k}} \mathbf{p}_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{r} - \omega_{\mathbf{k}}t)}. \quad (7)$$

We note that the forced ion oscillations caused by the force \mathbf{D} can be obtained as a simple superposition of oscillations caused by separate harmonics of the form

$$\mathbf{D}_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{r} - \omega_{\mathbf{k}}t)}. \quad (8)$$

Certainly, these harmonics are not usual electromagnetic waves (their velocity $v \neq c$, they are characterized by a different dispersion law, and they are not transverse). However, since the polaron size exceeds the lattice constant, dominating in expansion (6) are the harmonics, whose wavelengths also exceed the lattice constant. In this case, the task can be reduced to the known limiting case of long waves. So that, when considering the forced oscillations of ions, harmonics (8) can be replaced by electromagnetic waves, the induction vector of which has the same amplitude and frequency. This change allows us to express the polarization of a dielectric via the dielectric constant $\varepsilon(\omega)$ defining the dispersion of electromagnetic waves in crystals as

$$\mathbf{p}_{\mathbf{k}} = c(\omega_{\mathbf{k}})/4\pi \mathbf{D}_{\mathbf{k}}, \quad c(\omega) = (1/n^2) - (1/\varepsilon(\omega)) \quad (9)$$

(when deducing the expression for $c(\omega)$, one should bear in mind that \mathbf{p} is only the inertial part of the specific polarization [2]). It is assumed that the crystal is polarized in an isotropic manner.

Relations (9) are the solution of the equation for forced oscillations. Equations (2), (4), and (9) define the functions ψ , \mathbf{D} , and \mathbf{p} , respectively. It is obvious that all three these equations are simultaneously satisfied with functions of form (5).

To determine the effective mass of a polaron, it is necessary to calculate energy (1) to within terms of the order of v^2 . In accordance with this and taking the parity of the function $\varepsilon(\omega)$ into account (we ignore the imaginary part of ε , i.e. the absorption), we represent $c(\omega)$ as the series

$$c(\omega_{\mathbf{k}}) = c_0 + c_2\omega_{\mathbf{k}}^2 + \dots \quad (10)$$

$$c_0 = (1/n^2) - (1/\varepsilon(0)), \quad c_2 = c_0/\omega_1^2, \quad (11)$$

where ω_1 is the limiting frequency of optical oscillations of ions (it and the “dispersion frequency” should not be confused). Since

$$\omega_{\mathbf{k}}^2 D_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{r} - \omega_{\mathbf{k}}t)} = -(\partial^2/\partial t^2) D_{\mathbf{k}} e^{i(\mathbf{k}\mathbf{r} - \omega_{\mathbf{k}}t)},$$

it is convenient to write the equations for forced oscillations (9) in the summed form:

$$\mathbf{p}(\mathbf{r}, t) = (1/4\pi)[c_0 \mathbf{D}(\mathbf{r}, t) - c_2 (\partial^2 \mathbf{D}/\partial t^2)]. \quad (12)$$

Now, it is easy to obtain the expression for the crystal energy U_p . Taking into account that the work performed in a unit volume of the crystal per unit time is

$$\mathbf{D}\dot{\mathbf{p}} = (\mathbf{D}/4\pi) [c_0 \dot{\mathbf{D}} - c_2 \ddot{\mathbf{D}}], \quad (13)$$

and setting the energy of a unit volume without field (a polaron is far away) to be equal to zero, we obtain

$$U_p = (c_0/8\pi) \int \mathbf{D}^2 d\tau + (3c_2/8\pi) \int \dot{\mathbf{D}}^2 d\tau. \quad (14)$$

Substituting (12) and (14) in formula (1) for the energy of the system, we get

$$H = \frac{\hbar^2}{2\mu} \int |\nabla\psi|^2 d\tau - \frac{c_0}{8\pi} \int \mathbf{D}^2 [\psi] d\tau + \frac{c_2}{8\pi} \int \dot{\mathbf{D}}^2 [\psi] d\tau. \quad (15)$$

The case of immovable polaron ($v = 0$, $\dot{\mathbf{D}} = 0$) was considered in detail by one of the authors in previous works [2, 3], where the ground-state wave function $\psi = \psi_0(\mathbf{r})$ of a polaron and the respective energy

$$H_0 = -0.0547 (\mu e^4/\hbar^2) c_0^2 \quad (16)$$

were obtained. Taking this solution as a zero approximation and passing to the case of a uniformly moving polaron, it can be shown that the ψ -function and the energy acquire small corrections, if the velocity

$$v \ll r_m \omega_1, \quad (17)$$

where r_m is the polaron radius [2].

To within terms of the order of v^2 , the energy can be written in the form

$$H = H_0 + \frac{1}{2} M v^2,$$

$$M = \frac{c_2}{3} \left[\int_0^\infty \left(\frac{\partial \mathbf{D}[\psi_0]}{\partial r} \right)^2 r^2 dr + 2 \int_0^\infty \mathbf{D}^2 [\psi_0] dr \right]. \quad (18)$$

By substituting $D[\psi_0]$ from (3), we get that the effective mass of a polaron

$$\begin{aligned} M &= 5.8 \times 10^{-3} (\mu e^2/\hbar^2)^3 e^2 c_0^3 c_2 = \\ &= 9.08 \times 10^3 (\mu/m)^3 c_0^3 c_2 \text{ g}, \end{aligned} \quad (19)$$

where m is the free electron mass, μ is the effective electron mass in the ordinary conduction band. As usual, M turns out to be considerably higher than the electron mass (in the case of NaCl, it is 432 times higher).

By considering the motion of a polaron in an external electric field \mathbf{E} and equating the power developed by this field to the energy increment (18) per second, we obtain an ordinary equation of motion for the polaron:

$$M\dot{\mathbf{v}} = e\mathbf{E}. \quad (20)$$

It has been assumed above that the uniform motion of a polaron is conservative, i.e. harmonics (8) keep stationary forced oscillations of ions but do not generate natural oscillations of ions. However, in reality, the forced ion oscillations generate natural oscillations due to some anharmonism (heat is released). In this case, some deceleration of a polaron is observed. The energy given to the lattice by a polaron can be formally calculated as the absorption of above-mentioned electromagnetic waves equivalent to harmonics (8) in the crystal. The calculation has shown [4] that the braking force is proportional to the velocity, and the mobility of the polaron in an external field is

$$u = 0.262 \times 10^{-13} \frac{\varepsilon(0)^{3/2}}{b(\mu/m)^3 c_0^3} \text{ abs. un.} \quad (21)$$

The coefficient b is experimentally determined by measuring the absorption of electromagnetic waves in a crystal: namely, $b\omega$ is the imaginary part of the refraction index of a crystal for waves with frequency $\omega \ll \omega_1$. The braking force \mathbf{R} can be expressed in terms of the mobility and the velocity of a polaron as

$$\mathbf{R} = -e\mathbf{v}/u. \quad (22)$$

Neglecting a weak braking and quantizing the motion of a polaron as a whole (without field), we can ascertain that the motion can be described by plane waves (like the motion of the mass center of any complex particle with internal degrees of freedom). Therefore, the dependence of the density of energy levels for the translational motion of a polaron on its kinetic energy has the same form as that in the case of a free particle with mass M and spin $1/2$.

The thermodynamically equilibrium concentration of polarons is expressed by the usual formula

$$n = (2/h^3)(2\pi M kT)^{3/2} e^{(\zeta - H_0)/kT},$$

where ζ is the chemical potential of electrons in a crystal. However, the coefficient of the exponential factor is usually by many orders higher than that in the case of electrons. Due to the interaction of polarons with thermal oscillations of ions, the Maxwell distribution for polaron velocities is established.

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Received January 20, 1948

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Lev Davidovich Landau was the outstanding physicist-theorist of the XX century, Full Member of the Academy of Sciences of the USSR, the Nobel Prize winner in physics (1962) "For pioneer investigations in the theory of condensed matter and especially of liquid helium".

During 1932–1937, he was Head of the Department of Theoretical Physics at the Ukrainian Physical-Technical Institute in Kharkov (now NSC "Kharkov Institute of Physics and Technology" of NAS of Ukraine), L.D. Landau headed a chair at Kharkov State University also. Since 1937, he was Head of the Theoretical Department of the Institute for Physical Problems of the Academy of Sciences of the USSR in Moscow. He is a founder of the Kharkov's scientific school of theoretical physics.

L.D. Landau's investigations cover practically all branches of theoretical physics, ranging from fluid mechanics to quantum field theory [1]. L.D. Landau predicted the existence of neutron stars (W. Baade, F. Zwicky, L.D. Landau), he constructed a general theory of phase transitions of the second order (1936–1937). The Ginzburg-Landau equation is of great importance in the theory of superconductivity. The Landau levels, Landau diamagnetism, and Landau-Lifshits equation are well known

in physics. L.D. Landau constructed the theory of superfluid liquid helium-II [2] and the theory of the Fermi liquid [3–5]. L.D. Landau's investigations in plasma physics and in the theory of magnetism are of great importance. L.D. Landau formulated the theory of a two-component neutrino (independently of A. Salam, T. Lee, and C. Yang, 1957) and proposed the principle of conservation of the combined parity in the weak interactions of elementary particles [6].

A significant part in the L.D. Landau's heritage belongs to the world-famous "Course of Theoretical Physics" written jointly with E.M. Lifshits in many volumes.

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PEKAR SOLOMON ISAKOVYCH (16.03.1917–08.06.1985)

S.I. Pekar was born in Kyiv. He was graduated from Kyiv State University in 1938. At the age of 24, he was conferred the Doctor degree for his candidate thesis "Studies on the Theory of Semiconductors". From 1941 up to his death, S.I. Pekar was working at the Academy of Sciences of UkrSSR as the Head of the Department of Theoretical Physics (1941-1960 – Institute of Physics, 1960–1985 – Institute of Semiconductors). Since 1946, he was Professor. S.I. Pekar headed the Chair of Theoretical Physics at Kyiv State University in 1944–1949 and in 1953–1962. There, he founded the specialization "physicist-theorist" for students and postgraduates. In 1961, S.I. Pekar was elected Academician of the Academy of Sciences of UkrSSR without intermediate grade "Corresponding member". He is the author of several important discoveries in solid-state physics. Two of them are commonly recognized peaks of the world science: the theory of autolocalized states of electrons named polarons by him (1946) and the discovery of additional light waves in crystals (1957) plus a new theory of crystallooptics (the phenomenon was officially registered as a discovery).