Reports of the Academy of Sciences of the USSR

Yu. I. Gorkun and K. B. Tolpygo

1958

SovietRxiv

Abstract

Full Text

Reports of the Academy of Sciences of the USSR

1958, Volume 120, No. 3

PHYSICS

Yu. I. Gorkun and K. B. Tolpygo

FEATURES OF THE MOTION OF FAST CURRENT CARRIERS IN POLAR CRYSTALS

(Presented by Academician A. F. Ioffe on 25 XII 1957)

1. In the study of a number of phenomena one has to deal with the motion of fast electrons in solids. These include, in particular, electrical breakdown and secondary, photo-, and autoelectronic emission in semiconductors and dielectrics.

The very important question of how polarons—the principal current carriers in ionic crystals ([1],[2])—behave with increasing energy has hardly been investigated. Here we shall give the results of such an investigation in the limiting case of very strong coupling, when the energy of the polaron is given with high accuracy by the semiclassical theory ([1]). The treatment will be carried out for not very fast electrons, whose energy, however, may considerably exceed the thermal energy.

2. S. I. Pekar ([1]), in considering a moving polaron, restricted himself to the case of absence of resonance between the polarization waves and the natural frequencies of the crystal, $\omega_K \, \mathbf{K} \cdot \mathbf{v} \ll \omega_K$ ($\mathbf{K}$ is the wave vector of one of the main harmonics in the expansion of the polaron field $D(\mathbf{r})$, $\mathbf{v}$ is the velocity of the polaron). The method of N. N. Bogolyubov ([3]), which in the zeroth approximation gives results coinciding with those of the semiclassical theory, does not require this restriction; however, it contains improper integrals, whose evaluation can be justified by taking anharmonicity into account. This is most simply done in the classical treatment of lattice vibrations, which will be used below in the form ([4]).

The fluctuation motion of a polaron, whose center of gravity moves with velocity $\mathbf{v}$, in the absence of an external field is described by the equation

$$\left(-\frac{\hbar^2}{2m^*} + U(\mathbf{r}) - E\right)\psi = 0, \tag{1}$$

where

Figure 1

Figure 1: Figure 1

$$U(\mathbf{r}) = -\frac{4\pi e^2 c}{V} \sum_K \frac{\omega_K^2}{K^2} \frac{\int e^{-i\mathbf{K}\mathbf{r}'} |\psi(\mathbf{r}')|^2 \, d\tau'}{\omega_K^2 - (\mathbf{K}\cdot\mathbf{v})^2 - i\Gamma'(\mathbf{K}\mathbf{v})} e^{i\mathbf{K}\mathbf{r}}; \tag{2}$$

$$c = \frac{1}{n^2} - \frac{1}{\varepsilon};$$

V is the volume of the fundamental region of the crystal; Γ is the anharmonicity constant. For a polaron of sufficiently large radius one may restrict oneself to taking into account interaction only with the longitudinal optical branch and neglect the dependence of ω_K on $\mathbf{K}$. Equation (1) was solved by the variational method for two approximating functions ([5]):

$$\psi_1(\mathbf{r}) = \sqrt{\frac{\alpha^3}{\pi}} e^{-\alpha r}, \qquad \psi_2(\mathbf{r}) = \sqrt{\frac{\alpha^3}{\pi(1 + 9\beta^2/2\alpha^4)}} \left[1 + \beta r^2 P_2(\cos\vartheta)\right] e^{-\alpha r}; \tag{3}$$

P_2 is the Legendre polynomial; ϑ is the angle between $\mathbf{v}$ and $\mathbf{r}$. The results are given in Fig. 1 as a function of the dimensionless velocity $u = v/\omega r_0$, where $r_0 = \hbar^2/m^* e^4 c^2$. The negative value of the parameter β shows that a fast polaron is somewhat compressed in the direction of motion.

3. The total energy of the polaron-crystal system, with anharmonicity taken into account, is found to be

$$\overline{H} = E + \frac{e^2\omega^4 c}{2\pi} \int \frac{\left|\int e^{-i\mathbf{K}\mathbf{r}} |\psi(\mathbf{r})|^2 d\tau\right|^2 d\mathbf{K}}{\left[(\omega^2 - (\mathbf{K}\mathbf{v})^2)^2 + \Gamma^2(\mathbf{K}\mathbf{v})^2\right] K^2} - \frac{e^2\omega^2 c}{4\pi^2} \int \frac{\left|\int e^{-i\mathbf{K}\mathbf{r}} |\psi(\mathbf{r})|^2 d\tau\right|^2 d\mathbf{K}}{\left[\omega^2 - (\mathbf{K}\mathbf{v})^2 - i\Gamma(\mathbf{K}\mathbf{v})\right] K^2}; \tag{4}$$

for $u > 1$ it depends substantially on the magnitude Γ/ω. In Fig. 2 the dependence of $\overline{H}$ on u (energy in units of $m^* e^4 c^2/\hbar^2$) is given for NaCl (Γ—according to (6)). For comparison, the curves $m^* v^2/2$ and $Mv^2/2$ are shown, where M is the effective mass of the polaron according to the data of (1).

Fig. 1. Dependence of the parameters of the wave functions on the dimensionless velocity of the polaron. a, b—for ψ_2; c—for ψ_1; a_0, b_0—for $\psi_0(r')$ (9). The scale αr_0 refers to the curves a, a_0, c; β_0—to the curve b_0, βr_0^2—to the curve b.

4. Since, in the motion of a fast polaron, there is resonance between the natural frequencies and the frequency of the driving force, it is not, strictly speaking, stationary. A continuous transfer of energy from the polaron to

Figure 2

Figure 2: Figure 2

the crystal occurs, i.e., braking of the polaron. The amount of energy lost, $\mathcal{E}(v)$, was calculated in (7) for a Gaussian polaron function under the assumption that the shape of the polaron is independent of velocity. As the calculations of V. Yasinskii and A. I. Nosar' and one of us (5) have shown, under this assumption $\mathcal{E}(v)$ is little sensitive to the choice of the approximating function. The situation is different when the deformation of a moving polaron is taken into account. In Fig. 3 the curves of the dependence of $\lg \mathcal{E}(u)/(m^*e^4c^2\omega/16\hbar^2)$ on $\lg u$ are given for the functions ψ_1 and ψ_2 (3) and, for comparison, for the best function of a rigid polaron (1),

$$\psi_3 \sim (1 + \alpha r + \beta r^2)e^{-\alpha r}. \tag{5}$$

As was to be expected, in the actual range of velocities the deformable polaron experiences noticeably smaller energy losses.

Fig. 2. 1—dependence of the total energy of the system on the velocity of the polaron; 2—$Mv^2/2$; 3—$m^*v^2/2$ (at the points $\overline{H}/(m^*e^4c^2/\hbar^2) = 0.05$ on the ordinate axis and $u = 2$ on the abscissa axis, the scales have been changed).

5. The properties of fast current carriers considered in the preceding sections may manifest themselves in photoemission and secondary electron emission when the excited electron moves toward the surface, when the electric field E_0 is small. On the contrary, in pre-breakdown (and possibly also breakdown) states, in field electron emission from polar crystals, and also in the motion of current carriers in blocking layers, one must reckon with the direct influence of the field on the form of the polarization well and of the polaron ψ-function. We shall restrict ourselves to consideration of "self-consistent" quasistationary motion of a polaron along the field, when its velocity is constant in time and the resonant energy loss $\mathcal{E}(u)$ is exactly compen-

is compensated by the work of the field evE_0. The corresponding time-dependent Schrödinger equation has the form

$$\frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m^*}\Delta + U(\mathbf{r}, t) - e\mathbf{E}_0 \cdot \mathbf{r} - \mathcal{E}(v)\right]\psi(\mathbf{r}, t). \tag{6}$$

Its special feature is the presence in the Hamiltonian of the phenomenological rate of energy loss to "friction," $\mathcal{E}(v)$, which in what follows will itself be determined through $\psi(\mathbf{r}, t)$. This is precisely what constitutes our self-consistency.

We seek a particular solution of (6) in the form

$$\psi(\mathbf{r},t)=\psi_0(\mathbf{r}-\mathbf{v}t)e^{\frac{i}{\hbar}[m^*\mathbf{v}\cdot\mathbf{r}-\varphi(t)]}; \tag{7}$$

ψ_0 and $\varphi(t)$ are real functions. After substituting (7) and (6), and separating the imaginary part from the real part, we obtain

$$\varphi(t)=-\left(W_0+\frac{m^*v^2}{2}\right)t+evE_0t^2,$$

$$\left[-\frac{\hbar^2}{2m^*}\Delta+U(\mathbf{r}')-e\mathbf{E}_0\cdot\mathbf{r}'\right]\psi_0(\mathbf{r}')=W_0\psi_0(\mathbf{r}'),\qquad \mathbf{r}'=\mathbf{r}-\mathbf{v}t. \tag{8}$$

The approximating function ψ_0 was taken in the form

$$\psi_0(\mathbf{r}')=\sqrt{\frac{\alpha^3}{\pi(7+\beta^2)}}\left[1+\alpha r'(1+\beta\cos\vartheta)\right]e^{-\alpha r'}; \tag{9}$$

ϑ is the angle of $\mathbf{r}'$ with the direction of $\mathbf{v}$ (and $\mathbf{E}_0$). The form of ψ_0, as well as the polaron velocity v, are determined by the field E_0 from equation (8), expression $U(r)$ (2), and the stationarity condition

$$evE_0=\mathcal{E}(v). \tag{10}$$

The results of calculations for α and β are given in Fig. 1 (the curves are furnished with the subscript 0).

Fig. 3. Dependence of the radiation power on the polaron velocity.
1 –for ψ_3 (5); 2 –for ψ_1; 3 –for ψ_2; 4 –for $\psi_0(\mathbf{r}')$ (9)

Fig. 4. Potential energy of the electron in the polarization well in the presence of an external field $E_{0\,\max}$ in the direction of the field

The radiation power of the oscillations is shown in Fig. 3. For convenience, the velocity u has been taken as the argument instead of the field E_0. The dependence of the polaron velocity on the field, as well as the polaron mobility μ, is given in Table 1. The large values of μ at small velocities were obtained because the principal mechanism determining μ as $v\to 0$–anharmonism–was not taken into account.

6. Using the $\psi_0(\mathbf{r}')$ found, one can solve the problem of the destruction of the polaron by the field more consistently than was done in [8], and check whether a polaron level still lies inside the polarization well. In Fig. 4 the course of $U(r)-eE_0r$ is given for the maximum (breakdown) field corresponding to $u\approx 2$. The horizontal straight line represents the energy level W_0. Thus, the direct action of the external field on the polaron cannot lead to its destruction. The transition of the polaron to a band state can-

can occur only as a result of "breakaway," i.e., a violation of the stationarity equation (10). The breakaway moment corresponds to the maximum of the field E_0 as a function of the polaron velocity.

Table 1

u	$\frac{E_0}{ec/r_0^2}$	$\frac{\mu}{\omega_0^3/ec}$
0.2979	$1.166 \cdot 10^{-8}$	$2.55 \cdot 10^{9}$
0.5809	$1.264 \cdot 10^{-5}$	$4.59 \cdot 10^{8}$
4.9516	$1.749 \cdot 10^{-3}$	$5.44 \cdot 10^{4}$
2.009	$7.174 \cdot 10^{-3}$	$2.80 \cdot 10^{4}$
0.419	$4.379 \cdot 10^{-3}$	$1.01 \cdot 10^{3}$

Taking into account the dependence of the polaron shape on the field (the function $\psi_0^{(9)}$), this gives $u \approx 2$, whence

$$E_{0\,\max} \approx 7.2 \cdot 10^{-3} \frac{ec}{r_0^2} = \frac{c}{r_0^2}\, 10^{-9}\ \frac{\mathrm{V}}{\mathrm{cm}}.$$

If the direct influence of the field on the form $\psi(r)$ is not taken into account, the stationarity condition (10) gives $E_0 = \mathcal{E}(v)/ev$, and $E_{0\,\max}$ is determined by the equation

$$\frac{1}{v}\frac{d\mathcal{E}}{dv} - \frac{1}{v^2}\mathcal{E}(v) = 0.$$

Table 2 gives the values of the constant

$$B = \frac{r_0^2}{c}\, 10^9 E_{0\,\max}$$

and $u_{\max}$ for various forms of the approximating function.

Table 2

	$e^{-\alpha^2 r^2}$	ψ_s	ψ_1	ψ_2	$[1+\alpha r(1+\beta\cos\vartheta)]e^{-\alpha r}$
B	2.8	3.12	2.1	1.26	1
$u_{\max}$	3.98	3.71	2.4	1.88	2

If this quantity is calculated from the experimental values of the breakdown fields[9], taking m^* from [1], then for potassium and rubidium halides one obtains $B \sim 0.4$–0.5, for KF and sodium halides $B \sim 0.2$–0.3, and for LiF $B \sim 0.055$. It

is natural to expect that the breakdown field is greater than, or at least equal to, the polaron breakaway field $E_{0\,\max}$. The comparison presented with experiment gives the opposite picture. It is possible that, because of the spread of velocities, a small fraction of polarons "break away" earlier and cause breakdown. Real crystals, which have imperfections, are apparently electrically less strong than ideal ones. It is possible that the true effective masses m^*, and consequently also c/r_0^2, for the crystals considered are smaller than those calculated in [1]. This idea is suggested by the circumstance that the agreement of the theory with experiment is the better, the larger the radius of the polaron state, i.e., the more accurate the approximation of the theory [1].

In conclusion, let us note that the limiting approximation of strong coupling is not suitable for most crystals. In the case of intermediate coupling, as the polaron velocity increases, a further weakening of the coupling occurs [10]. This circumstance should be taken into account in the further development of the theory of fast polarons.

Received
25 XII 1957

REFERENCES

[1] S. I. Pekar, *Research on the Electronic Theory of Crystals*, Moscow–Leningrad, 1951.
[2] 7th All-Union Conference on the Properties of Semiconductors, ZhTF, **21**, No. 2, 231 (1951).
[3] N. N. Bogolyubov, Ukr. Mat. Zh., **2**, 3 (1950).
[4] K. B. Tolpygo, Tr. Kievsk. Gos. Univ., Matem. Sborn., No. 5, 99 (1951).
[5] Yu. I. Gorkun, ZhTF, **27**, 1764 (1957).
[6] M. Czerny, Zs. Phys., **65**, 600 (1930).
[7] K. B. Tolpygo, Z. I. Uritskii, ZhETF, **30**, 929 (1956).
[8] M. I. Klinger, ZhETF, **26**, 166 (1954).
[9] V. A. Tsinchenko, Usp. Fiz. Nauk, **54**, 185 (1954).
[10] V. M. Buimistrov, S. I. Pekar, ZhETF, **33**, 1271 (1957).

Note: Figure translations are in progress. See original paper for figures.