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Translated by W. F. Brown, Jr.

Density of electron levels in ferroelectric semiconductors

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(Submitted February 10, 1977)
Zh. Eksp. Teor. Fiz. **73**, 342–347 (July 1977)

We consider the effect of the electron-phonon interaction on the electron density of states $g(\epsilon)$ in polarized semiconductors with soft optical phonons. It is shown that for weakly doped semiconductors the value of g depends strongly on ϵ near the Fermi surface and has a minimum on this surface. $g(0)$ becomes anomalously small near the ferroelectric transition point.

PACS numbers: 71.20.+c, 71.38.+i

INTRODUCTION

The spectra of the lattice vibrations of certain polar degenerate semiconductors contain soft (temperature-dependent) phonons. In the long-wave region, the spectrum of such soft transverse optical phonons is determined by the relation $\omega_t^2(\mathbf{q})=\omega_0^2+s\mathbf{q}^2$, where ω_0 is an anomalously small gap ($\omega_0 \ll \omega_D$), and the dispersion s is of normal order of magnitude.

The electron-phonon-interaction singularities typical of this situation were discussed in detail by one of us.[1] The polarization part of the interaction is described, as usual, by a Fröhlich Hamiltonian. The transverse degrees of freedom make no contribution to the macroscopic polarization field. The corresponding deformation potential is usually small in comparison with the polarization potential. In the case of small ω_0 however, it is precisely the deformation contribution to the electron scattering by the lattice which is fundamental. In this paper we investigate the influence of this interaction on the electron level density $g(\varepsilon)$ of a degenerate weakly doped semiconductor for states near the Fermi surface.

2. CORRECTIONS TO THE VERTEX FUNCTION

The effective electron-electron interaction, which includes exchange of soft phonons at $T=0$, is given by[1]

$$D_0(\mathbf{q},\omega)=\frac{4\pi e^2}{K^2}|C|^2\frac{\varepsilon_0(\mathbf{q})\omega_t^2(\mathbf{q})}{\omega^2-\omega_t^2(\mathbf{q})+i\delta}, \tag{1}$$

where $\varepsilon_0(\mathbf{q})$ is the static part of the dielectric constant of the lattice, and $\mathbf{K}$ is the reciprocal-lattice vector. The constant $|C|<1$ is connected with the amplitude modulation of the Bloch functions. Using the Lyddane-Sachs-Teller relation for the long-wave region,[1] we represent the interaction (1) in the form

$$D_0(\mathbf{q},\omega)=4\pi^2\tilde{a}s^2/[\omega^2-\omega_t^2(\mathbf{q})+i\delta], \tag{2}$$

where we have introduced the dimensionless electron-phonon coupling constant

$$\tilde{a}=e^2|C|^2\varepsilon_\infty\omega_t^2/\pi s^3K^2, \tag{3}$$

ε_∞ is the dielectric constant due to the polarizability of the bound electrons, and ω_t is the frequency of the longitudinal optical phonons.

Let us examine the correction that must be introduced into the electron vertex function $\mathcal{T}$ as a result of the interaction (2) at $T=0$. The corresponding diagram is shown in Fig. 1. The electron line corresponds here to the zero-order Green's function

$$G_0(\varepsilon,\mathbf{p})=[\varepsilon-p^2/2m+i\delta\,\mathrm{sign}(|\mathbf{p}|-p_0)]^{-1}.$$

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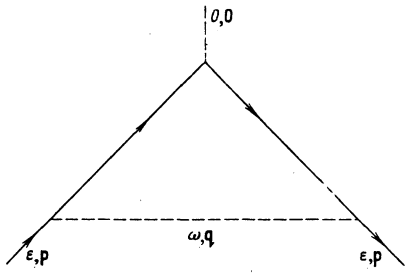


FIG. 1. First correction to the vertex function. The dashed and solid lines correspond respectively to the functions D_0 and G_0.

After integrating with respect to the frequency ω and with respect to the angles we obtain

$$\mathcal{T}_1(\varepsilon, \mathbf{p}) = \frac{\tilde{\alpha} s^{1/2}}{2} \left\{ \int_{p-p_0}^{p+p_0} \frac{q^2\,dq}{\omega_t(q)} \times \left[\frac{1+(p^2-p_0^2+q^2)/2pq}{[\eta-\omega_t(q)+(p^2-p_0^2)/2m][\eta-\omega_t(q)-(q^2+2pq)/2m]} + \frac{1-(p^2-p_0^2+q^2)/2pq}{[\eta+\omega_t(q)+(p^2-p_0^2)/2m][\eta+\omega_t(q)-(q^2-2pq)/2m]} \right] + 2\left(\int_0^{p-p_0} + \int_{p+p_0}^{\infty} \right) \frac{q^2\,dq}{\omega_t(q)\,[(\eta-\omega_t(q)-q^2/2m)^2-(pq/m)^2]} \right\}. \quad (4)$$

Here $\eta = \varepsilon - p^2/2m$. The external ends of the diagram on Fig. 1 correspond to an almost-real electron, since η is assumed to be small.

Near the Fermi surface $p - p_0 \ll p_0$ the first integral in the right-hand side of (4) diverges logarithmically in the region $\Omega \ll q \ll p_0$, where

$$\Omega = \max\left\{ \frac{\omega_0}{s^{1/2}}, \frac{|\eta|}{s^{1/2}}, \frac{v_F|p-p_0|}{s^{1/2}} \right\}. \quad (5)$$

In the other regions of the values of q all the integrals converge and yield negligibly small corrections of order $\tilde{\alpha} s/v_F^2$. Ultimately we have

$$\mathcal{T}_1 = \alpha \ln(p_0/\Omega), \quad \alpha = \tilde{\alpha} s^{1/2}/v_F. \quad (6)$$

An analogous expression is obtained also for the hole scattering $p < p_0$.

In the case of simultaneous proximity to the ferroelectric transition point (small ω_0), to the mass shell (small $|\eta|$), and to the Fermi surface (small $|\xi_p| = v_F|p-p_0|$) the effective coupling $\alpha \ln(p_0/\Omega)$ is no longer weak. The problem is now to find the renormalized vertices and Green's functions in the principal logarithmic approximation.

3. RENORMALIZED FUNCTIONS

It is necessary first to consider the question of the screening of the phonon interaction by the free carriers in the case of a Fermi filling. In the "empty" lattice of an ionic crystal, the nonrenormalized interaction can be regarded as a sum of two terms

$$D_0(q, \omega) = D_0^t(q, \omega) + D_0^l(q, \omega). \quad (7)$$

The first term takes into account the direct Coulomb interaction of the electrons and their interaction via exchange of a longitudinal optical phonon. According to Gurevich *et al.*[2] we have for a cubic crystal

$$D_0^l(q, \omega) = \frac{4\pi e^2}{q^2}\left[\varepsilon_\infty^{-1} - (\varepsilon_\infty^{-1} - \varepsilon_0^{-1}) \frac{\omega_t^2}{\omega_t^2 - \omega^2} \right]. \quad (8)$$

In the frequency region $\omega \ll \omega_t$ which will henceforth be of importance to us we have

$$D_0^l(q, \omega) = 4\pi e^2/\varepsilon_0 q^2. \quad (9)$$

Using for D_0^t the expression (2), we obtain

$$D_0(q, \omega) = \frac{4\pi e^2}{\varepsilon_0 q^2} \frac{\omega^2 - \omega_t^2(q) + (q/K)^2 \varepsilon_0 \varepsilon_\infty |C|^2 \omega_t^2}{\omega^2 - \omega_t^2(q)}. \quad (10)$$

The renormalized interaction is

$$D^{-1}(q, \omega) = D_0^{-1}(q, \omega) - \Pi(q, \omega).$$

The polarization operator in the Thomas-Fermi approximation ($\omega \ll v_F q$) is equal to

$$\Pi = -\varepsilon_\infty \varkappa^2/4\pi e^2, \quad (11)$$

where the reciprocal screening lengths is $\varkappa = (4e^2 m p_0/\pi\varepsilon_\infty)^{1/2}$. As a result we have

$$D(q, \omega) = \frac{\omega^2 - \omega_t^2(q) + (q/K)^2 \varepsilon_0 \varepsilon_\infty |C|^2 \omega_t^2}{\varepsilon_0 q^2 [\omega^2 - \omega_t^2(q)] + \varepsilon_\infty \varkappa^2 [\omega^2 - \omega_t^2(q) + (q/K)^2 \varepsilon_0 \varepsilon_\infty |C|^2 \omega_t^2]}. \quad (12)$$

The long-wave spectrum of the soft phonons is now determined by the poles of the function (12):

$$\tilde{\omega}_t^2(q) = \omega_t^2(q) - \frac{\varkappa^2 |C|^2 \varepsilon_0 \varepsilon_\infty^2 \omega_t^2}{K^2} \frac{q^2}{\varepsilon_0 q^2 + \varepsilon_\infty \varkappa^2}. \quad (13)$$

The qualitative form of the spectrum (13) is shown in Fig. 2. In the region $q^2 \ll \varepsilon_\infty \varkappa^2/\varepsilon_0$, the dispersion s changes:

$$\tilde{\omega}_t^2(q) = \omega_0^2 + \tilde{s} q^2. \quad \tilde{s} = s - \varepsilon_0 \varepsilon_\infty |C|^2 \omega_t^2/K^2. \quad (14)$$

An apparent renormalization of the gap takes place in the region $q^2 \gg \varepsilon_\infty \varkappa^2/\varepsilon_0$:

$$\tilde{\omega}_t^2(q) = \tilde{\omega}_0^2 + s q^2. \quad \tilde{\omega}_0^2 = \omega_0^2 - \varkappa^2 |C|^2 \varepsilon_\infty^2 \omega_t^2/K^2. \quad (15)$$

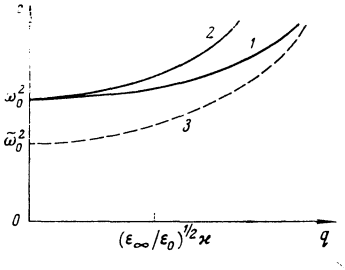


FIG. 2. Long-wave spectrum of soft phonons. Curve 1 corresponds to the renormalized spectrum (13) and curve 2 to the nonrenormalized spectrum. The auxilliary curve 3 corresponds to the relation $\omega^2 = \tilde{\omega}_0^2 + sq^2$.

It is convenient to represent the D function (12) in the form

$$D(q,\omega)=\frac{4\pi e^2}{\varepsilon_0 q^2+\varepsilon_\infty\varkappa^2}+\frac{4\pi^2\bar{a}s^{1/2}}{\omega^2-\tilde{\omega}_t^2(q)}\frac{\varepsilon_0^2 q^4}{(\varepsilon_0 q^2+\varepsilon_\infty\varkappa^2)^2}. \tag{16}$$

The logarithmic corrections to the vertex function are connected with second term in formula (16) and correspond to the region $q^2\gg\varepsilon_\infty\varkappa^2/\varepsilon_0$. As to the first term of (16), it does not lead to divergences and will no longer be written out. Thus,

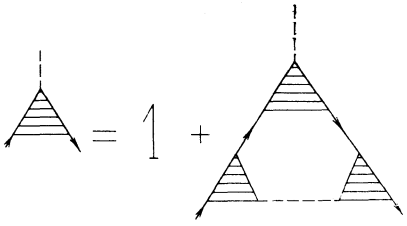
$$D(q,\omega)=\frac{4\pi^2\bar{a}s^{1/2}}{\omega^2-\tilde{\omega}_0^2-sq^2+i\delta},\qquad q^2\gg\frac{\varepsilon_\infty\varkappa^2}{\varepsilon_0}. \tag{17}$$

It is easy to verify that the screening does not enter among the cutoff parameters of (5). Indeed,

$$\omega_0\varepsilon_0^{1/2}/(\varepsilon_\infty s)^{1/2}\varkappa\sim(\varepsilon_\infty K/p_0)^{1/2}\gg 1,$$

and the cutoff parameter $\omega_0/s^{1/2}\sim\tilde{\omega}_0/s^{1/2}$ certainly exceeds $(\varepsilon_\infty\varkappa^2/\varepsilon_0)^{1/2}$.

The method of finding the renormalized vertex $\mathcal{T}$ in the principal logarithmic approximation, for the case of weak coupling, is well known.[3] The significant diagrams contain interaction lines that enclose not more than one of all the elementary vertices of the diagram of Fig. 1. The momenta transferred along these lines are $q_i\ll p$, so that in any section of the diagram the electron momentum remains close to its initial value. Taking the foregoing into account, the equation for the complete three-point diagram takes the form



(18)

To establish the connection between the renormalized electron propagator G in the complete vertex $\mathcal{T}$ we use the scalar and vector Ward identities

$$\frac{\partial G^{-1}}{\partial\varepsilon}=\mathcal{T},\qquad\frac{\partial G^{-1}}{\partial\mathbf{p}}=-\mathbf{v}\mathcal{T}. \tag{19}$$

Relations (19) are formally of the same form as for the case of a single electron without a Fermi background.[4] It is easy to verify that differentiation of the Fermi step actually makes no contribution to the logarithmic vertex. Therefore

$$G^{-1}(\eta,x)=\eta\mathcal{T}(x),\quad x=\alpha\ln(p_0/\Omega). \tag{20}$$

Taking (20) into account, the equation for the vertex (18) is rewritten in the form

$$\partial\mathcal{T}/\partial x=\mathcal{T}(x),\quad\mathcal{T}(0)=1. \tag{21}$$

Consequently,

$$\mathcal{T}(\Omega)=(p/\Omega)^\alpha, \tag{22}$$

$$G(\eta,\Omega)=(\Omega/p)^\alpha\eta^{-1}. \tag{23}$$

Let us compare the results (23) with the piezopolaron Green's function obtained by Édel'shtein.[4] There is no infrared divergence in this case. The vertex $\mathcal{T}$ ceases to depend on η already at $|\eta|<\max\{\omega_0,|\xi_p|\}$. A branch point can occur only at the critical point for states along the Fermi surface. However, the carrier scattering by impurities, which is discussed in the next section, is such that in this case the pole character of the G functions is preserved, and its residue becomes renormalized.

4. STATE DENSITY

We proceed to calculate the density of states near the Fermi surface. As usual

$$g(\varepsilon)=\frac{2}{\pi}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\operatorname{sign}(p_0-|\mathbf{p}|)\operatorname{Im}G(\varepsilon,\mathbf{p}). \tag{24}$$

The energy ε will be reckoned from the level of the chemical potential (the Fermi energy). In the absence of the interaction (2), the state density is constant in a wide energy range $|\varepsilon|\ll\varepsilon_F$ and is equal to $g_0=mp_0/\pi^2$. Now, however, we have for $|\varepsilon|\lesssim\omega_0$

$$g(\varepsilon)=(\omega_0/s^{1/2}p_0)^\alpha g_0, \tag{25}$$

and in the interval $\omega_0\lesssim|\varepsilon|\ll s^{1/2}p_0\ll\varepsilon_F$

$$g(\varepsilon)=(\varepsilon/s^{1/2}p_0)^\alpha g_0. \tag{26}$$

An approximate form of the state-density curve is shown in Fig. 3. Since $g(0)\ll g_0$, the state density is anomalously small in the region of the Fermi energies. Therefore, for example, the paramagnetic susceptibility $\chi\sim g(0)$ of these substances should be anomalously small.

In connection with the impurity character of the conductivity, the following should be noted. The electron mean free path time τ into the scattering by impurities is of the usual order of magnitude and is not connected with the critical behavior of the lattice. In the region of the concentrations and temperatures considered above we have $\tau\sim10^{-13}$ sec. The momenta of importance in the logarithmic integration should satisfy the relation $q\ll1/v_F\tau$. The damping does not enter among the cutoff parameters if $\omega_0\gtrsim s^{1/2}/v_F\tau\sim1$K. The last inequality always holds for ferroelectric transitions of first order close to second order.

The results of this study can be applicable to narrow-

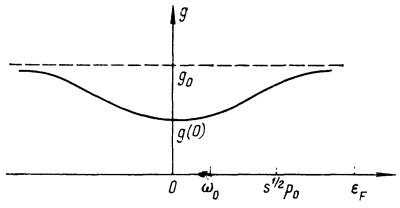


FIG. 3. Electron level density near the Fermi surface.

band IV–VI compounds whose static dielectric constant is anomalously large at low temperatures. Thus, for example, soft TO modes were observed in PbTe,[5] SnTe,[6] $Pb_{1-x}Sn_xTe$[7] and others. It should be noted that the explanation offered by Kawamura *et al.*[8] for the existence of soft modes in the semiconductors, as consequences of the interaction of the electrons with the soft photons, seems unsatisfactory from our point of view. As follows from formulas (14) and (15) of the present paper, allowance for the polarization interaction in addition to the deformation interaction, makes the gap-renormalization effect illusory.

In conclusion, the authors thank D. I. Khmel'nitskiĭ for constant interest in the work and for valuable remarks, and A. M. Finkel'shteĭn and V. M. Édel'shteĭn for a useful discussion of the results.

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Translated by J. G. Adashko

Dynamics of Onsager-Feynman vortices in a rotating superfluid system of the pulsar type

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(Submitted February 9, 1977)
Zh. Eksp. Teor. Fiz. 73, 348–354 (July 1977)

Equations are derived for the description of the dynamics of a vortex lattice in a rotating superfluid system of the pulsar type. The observed time dependence of the angular velocity of the normal part of the system is attributed to interaction of the system with Onsager-Feynman vortices.

PACS numbers: 67.90.+z

1. The nonstationary rotation of He II has been under intensive experimental investigation in recent years (see, e.g., the review)[1] in connection with a check on the premise that a pulsar is a superconducting system in which the interaction of the superfluid (neutron) component with the normal (proton) component is effected via Onsager-Feynman vortices.

It is known (detailed references to the original sources are contained, e.g., in the review)[1] that the time dependence of the angular velocity of pulsars has not yet found a satisfactory explanation. It was shown in experiments[2-3] that an analogous behavior of the angular velocity with time is observed also for rotating He II. These experiments have shown convincingly that the nature of the time dependence of the angular velocity should be the same for He II as for pulsars. We shall not present here the arguments (advanced already in[1]) that lead to this conclusion.

It is shown in the present paper that allowance for the motion of the vortex lattice and its interaction with the normal component in a rotating superfluid liquid, under conditions when there is no equilibrium between the actual angular velocity of the normal component and the number of vortices in the system, explains fully the experimentally observed time dependence of the angular velocity.

The application of our approach to the observed dependence of the angular velocity of a pulsar can explain the mechanisms of the radiative losses of the star, its structure (it permits measurements of the angular momenta of the superfluid and normal components and of the core) and yields quantitative information on the coefficients of viscous-friction of the vortices against the normal component.

We assume throughout that the normal component moves like a rigid body (i.e., it duplicates fully the rotation of the vessel or of the core). For pulsars it is legitimate to disregard the drag waves in the normal component, inasmuch as in pulsars the normal (charged) component is frozen into the core (if the latter exists) by the ultrastrong magnetic field of the stars. The analysis is carried out in the laboratory frame.

We note also the following important feature of the employed terminology. The symbol v_0 denotes throughout the proper velocity of the superfluid-component velocity. By this we mean the velocity due to extraneous forces (usually connected with external sources of pres-

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