POSSIBILITY OF "SUPERTHERMAL CONDUCTIVITY" IN SEMICONDUCTORS

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The possible existence of undamped energy flow in a two-band system with pairing is demonstrated. A proof is given of the Landau criterion for superfluidity in the case of crystalline periodicity. The superfluid motion is stable with respect to Umklapp processes and scattering by impurities.

In semiconductors with a narrow gap and in semimetals with a small current carrier concentration, as Keldysh and Kopaev[1] and the authors[2] showed, the Coulomb interaction between electrons and holes may, at low temperatures, lead to substantial rearrangement of the spectrum. This rearrangement is accompanied by the formation of bound electron-hole pairs, precipitating into the Bose condensate at temperatures less than a certain critical temperature T_c. Previously,[2] on the basis of an analogy with the case of superconductivity, it was conjectured that the Bose condensate behaves like a superfluid. However, the possible existence of superfluidity in the model under consideration requires special proof, since it is essential to introduce the crystal lattice (band structure) into the problem, and the direct application of a Galilean transformation would imply trivial motion of the crystal as a whole.

The Hamiltonian of the system under consideration has the form

$$H = H_0 + H_1 + H_2,$$
$$H_0 = \sum_{\mathbf{p}} (E_{c\mathbf{p}} a_{c\mathbf{p}}^+ a_{c\mathbf{p}} + E_{v\mathbf{p}} a_{v\mathbf{p}}^+ a_{v\mathbf{p}}),$$
$$H_1 = \sum_{\mathbf{p}+\mathbf{q}=\mathbf{p}'+\mathbf{q}'} V(\mathbf{p}, \mathbf{p}') a_{c\mathbf{p}}^+ a_{v\mathbf{q}}^+ a_{v\mathbf{q}'} a_{c\mathbf{p}'}, \tag{1}$$

where for small values of p

$$E_{c\mathbf{p}} = E_{c0} + p^2/2m_c, \quad E_{v\mathbf{p}} = E_{v0} - p^2/2m_v. \tag{2}$$

Here c and v denote, respectively, the conduction and valence bands; $V(\mathbf{p}, \mathbf{p}')$ is the matrix element of the Coulomb interaction. The quasimomentum is measured in each band from its extremum (see [2]); the dependence on spin indices is inessential. Umklapp processes and scattering by impurities are attributed to H_2. This part of the interaction does not lead to singularities in the scattering amplitude and may be discarded in connection with an examination of the problem of rearrangement of the spectrum. H_2 can be taken into account as a perturbation acting on the rearranged state, which we shall do below.

We shall likewise not take the electron-phonon interaction into account since its role in comparison with the Coulomb interaction, as V. V. Tolmachev[3] showed, is determined by the ratio of the Debye frequency to the energy corresponding to the radius of the Coulomb interaction, but in the case of interest to us, close to the band edge, the Coulomb interaction is weakly screened so that the indicated ratio is large.

In order to obtain a state of thermodynamic equilibrium with a nonvanishing energy current, it is necessary to introduce an additional integral of the motion into the Gibbs distribution. The operator

$$\mathbf{P} = \sum_{\mathbf{p}} \mathbf{p} (a_{c\mathbf{p}}^+ a_{c\mathbf{p}} + a_{v\mathbf{p}}^+ a_{v\mathbf{p}}), \tag{3}$$

commutes with the Hamiltonian; therefore, in order to clarify the question of superfluidity it is necessary to start from the distribution

$$\exp\{-(H_0 + H_1 - \mu N - \mathbf{u}\mathbf{P})/kT\}, \tag{4}$$

where $\mathbf{u}$ is a Lagrange multiplier having the dimension of a velocity.

If we change to the operators $b_{c\mathbf{p}} = a_{c,\mathbf{p}+m_c\mathbf{u}}$, $b_{v\mathbf{p}} = a_{v,\mathbf{p}-m_v\mathbf{u}}$, then (4) takes the form of the usual Gibbs distribution without the term $\mathbf{u}\cdot\mathbf{P}$. A transformation to new quasiparticles corresponding to a rearranged ground state is accomplished with the aid of the canonical transformation

$$b_{c\mathbf{p}} = U_{\mathbf{p}}\alpha_{2\mathbf{p}} - V_{\mathbf{p}}\alpha_{1\mathbf{p}}, \quad b_{v\mathbf{p}} = V_{\mathbf{p}}\alpha_{2\mathbf{p}} + U_{\mathbf{p}}\alpha_{1\mathbf{p}}, \tag{5}$$

the coefficients of which are found from the condition for minimization of the energy for given average values of the operators N and $\mathbf{P}$ and for given entropy,[3] i.e., $U_{\mathbf{p}}$ and $V_{\mathbf{p}}$ satisfy the equations

$$\left(\frac{\partial}{\partial U_{\mathbf{p}}}\langle H_0+H_1-\mu N-\mathbf{uP}\rangle\right)_{N_{2,1}(\mathbf{p})}=0,$$

$$U_{\mathbf{p}}^2+V_{\mathbf{p}}^2=1, \qquad (6)$$

where $N_{2,1}(\mathbf{p}) = \langle \alpha_{2,1\mathbf{p}}\alpha_{2,1\mathbf{p}}\rangle$ is the occupation number for quasiparticles.

Substituting (5) into (6), we find:

$$U_{\mathbf{p}}={}^1/_2(1+E_{\mathbf{p}}/\varepsilon_{\mathbf{p}}), \qquad V_{\mathbf{p}}={}^1/_2(1-E_{\mathbf{p}}/\varepsilon_{\mathbf{p}}), \qquad (7)$$

where

$$E_{\mathbf{p}}={}^1/_2(E_{c\mathbf{p}}-E_{v\mathbf{p}}), \qquad \varepsilon_{\mathbf{p}}=(E_{\mathbf{p}}^2+\Delta_{\mathbf{p}}^2)^{1/2}$$

and $\Delta_{\mathbf{p}}$ is determined by the equation

$$\Delta_{\mathbf{p}}=\sum_{\mathbf{p}'}V(\mathbf{p},\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{2\varepsilon_{\mathbf{p}'}}(N_{1\mathbf{p}'}-N_{2\mathbf{p}'}). \qquad (8)$$

The spectrum of elementary Fermi excitations is defined as the variational derivative of the total energy with respect to the number of quasiparticles:

$$\omega_{n\mathbf{p}}=\left(\frac{\delta\langle H_0+H_1\rangle}{\delta N_{n\mathbf{p}}}\right)_{U_{\mathbf{p}}}+\sum_{\mathbf{p}'}\left(\frac{\delta\langle H_0+H_1\rangle}{\delta U_{\mathbf{p}'}}\right)_{N_{n\mathbf{p}}}\frac{\delta U_{\mathbf{p}'}}{\delta N_{n\mathbf{p}}}.$$

The second term, as one can easily see, is of order of magnitude $(1/2)(m_c + m_v)u^2$, and in the linear approximation in $\mathbf{u}$ we find:

$$\omega_{n\mathbf{p}}=\frac{m_v-m_c}{m_v+m_c}E_{\mathbf{p}}+(-1)^n\varepsilon_{\mathbf{p}}+\mathbf{up}, \quad n=1,2. \qquad (9)$$

The rearranged state is stable if min ω_2 > max ω_1. This inequality is satisfied for $u < u_{cr}$. As the calculations show, in the most interesting case of contact of the bands of the unrearranged spectrum ($E_{c0} = E_{v0}$; in this case the rearrangement of the spectrum is maximum[2]) we have in order of magnitude

$$^1/_2(m_c+m_v)u_{cr}^2=\Delta. \qquad (10)$$

Formula (10) has an obvious physical meaning: The state of motion disappears when the kinetic energy of a pair is comparable with the value of the binding energy.

In the ground state $N_{2\mathbf{p}} = 0$, $N_{1\mathbf{p}} = 1$, and the quasiparticle current is determined by the formula

$$\mathbf{J}=2\sum_{\mathbf{p}-m_v\mathbf{u}}\frac{\partial\omega_{1\mathbf{p}}}{\partial\mathbf{p}}. \qquad (11)$$

The index under the summation sign indicates that $\mathbf{p} - m_v\mathbf{u}$ runs over an elementary cell in reciprocal space (this follows from formula (5), according to which $\alpha_{1\mathbf{p}} = a_{v,\mathbf{p}-m_v\mathbf{u}}$ far away from band extrema). It is easy to find that the current (11), like the current

$$2\sum_{\mathbf{p}}\left(\frac{\partial E_{c\mathbf{p}}}{\partial\mathbf{p}}\langle a_{c\mathbf{p}}^+a_{c\mathbf{p}}\rangle+\frac{\partial E_{v\mathbf{p}}}{\partial\mathbf{p}}\langle a_{v\mathbf{p}}^+a_{v\mathbf{p}}\rangle\right),$$

determined in terms of the "hole" operators is equal to zero, i.e., just as it should be, the distribution (4) is not associated with transport of charge and mass.

The energy current is calculated from the formula

$$\mathbf{Q}=2\sum_{\mathbf{p}-m_v\mathbf{u}}\omega_{1\mathbf{p}}\frac{\partial\omega_{1\mathbf{p}}}{\partial\mathbf{p}} \qquad (12)$$

and turns out to be equal to

$$\mathbf{Q}=-2\gamma_1\Delta N_{\text{pair}}\mathbf{u}, \qquad (13)$$

where

$$N_{\text{pair}}=2\sum_{\mathbf{p}}\langle a_{c\mathbf{p}}^+a_{c\mathbf{p}}\rangle=\frac{\gamma_2}{4\pi^2}\Delta^{3/2}m^{3/2}\hbar^{-3} \qquad (14)$$

is the number of electrons in the conduction band, which is equal to the number of pairs in the case of nonoverlapping (for $T > T_c$) bands; γ_1 and γ_2 are numerical coefficients close to unity.

Thus $\mathbf{Q}$ has the meaning of a transport of binding energy (-2Δ) by pairs moving with velocity $\mathbf{u}$, and one can say that the state under consideration represents superfluid motion of the Bose condensate of bound pairs with velocity $\mathbf{u}$. One can say that the current $\mathbf{Q}$ brings about a thermodynamically reversible heat transport that takes place at a zero temperature gradient. One can represent the mechanism of thermal conductivity as the creation of pairs at the heat outlet, their propagation without resistance to the point of heat supply, and subsequent annihilation with release of negative energy (-2Δ). One can estimate the critical heat current corresponding to the critical velocity u_{cr} with the aid of Eqs. (10), (13), and (14), keeping in mind that Δ is of the order of T_c:

$$Q_{cr}\cong\frac{m}{m_0}\left(\frac{m}{m_c+m_v}\right)^{1/2}T_c^3\cdot10^{-2}\,[\text{J}\cdot\text{cm}^{-2}\,\text{sec}^{-1}], \qquad (15)$$

where T_c is expressed in degrees, $m = 2m_cm_v/(m_c + m_v)$, m_0 is the mass of a free electron. For example, for $m_c = m_v = 10^{-1}\,m_0$ and $T_c = 10\,°K$ the current $Q \approx 1\ \text{J-cm}^{-2}\,\text{sec}^{-1}$. This magnitude is quite accessible to measurement.

As mentioned above, Umklapp processes and scattering by impurities do not lead to singularities in the scattering amplitude and may be considered in perturbation theory. The effect of these interactions is characterized by the transition probability

$$W_{fi}=(2\pi/\hbar)\,|M_{fi}|^2\delta(E_f-E_i).$$

The ground state with a given value of u may change only as a result of the appearance of elementary excitations. Such a process is accompanied by an increase of energy and therefore its probability is equal to zero. In principle, a transition without change of energy is possible to an excited state characterized by a smaller value of u. However, the probability for such a transition is macroscopically small since it leads to a change in the motion of the system as a whole.

The role of the perturbation may manifest itself only in renormalization of the gap. For Umklapp processes, the order of magnitude of this renormalization is

$$\delta E = \sum_{\mathbf{p},\,\mathbf{p}'} \frac{4\pi e^2}{K^2} \langle a_{c\mathbf{p}}{}^+ a_{v\mathbf{p}} \rangle \langle a_{v\mathbf{p}'}{}^+ a_{c\mathbf{p}'} \rangle = \frac{4\pi e^2}{K^2} \frac{\Delta^2}{V_{av}{}^2},$$

where K is the period of the reciprocal lattice, and V_{av} is a certain average interaction determined by the equation $V_{av} \Sigma(\Delta/2\epsilon) = \Delta$. It is clear that δE is always $\ll \Delta$.

In conclusion, let us consider the simplest possible experiments with regard to the observation of superthermal conductivity for semiconductors having a narrow gap. Certain semiconductors, which change into the metallic state under an increase of temperature or under pressure, may turn out to be suspicious in this respect. This happens, for example, for certain oxides of titanium and vanadium,[4] and for InSb.[5] One can observe "superthermal conductivity" in the absence of a temperature gradient for small heat currents. In addition, as we saw above, the rearranged state disappears for thermal currents larger than the critical current. Therefore, by passing a large heat current through the material for $T < T_c$, one can expect the appearance of metallic conductivity and the vanishing of weak antiferromagnetism (if such existed[2]).

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