Periodic structures in phase transitions of electron-phonon systems by a deformation interaction in a magnetic field

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We show that an instability is produced in an electron-phonon system in a quantizing magnetic field at $T \leq T_m$, where $T_m \sim b^4$ and where b is the electron-phonon interaction constant. At lower temperatures $T \sim \exp(-\text{const}/b^2)$, the instability becomes of the Peierls type. The new states are periodic-spatially charge and deformation distributions, and have a macroscopic period at $T \sim T_m$.

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1. It was predicted[1–5] that in electron-phonon systems with deformation interaction the velocity of sound would be renormalized to zero values, meaning loss of stability of the crystal and a phase transition to a new state. We have investigated the features of such phase transitions in a quantizing magnetic field **H** and will show that inhomogeneous states with periodic distributions of the electron and crystal density are realized in semiconductors with weakened Coulomb interaction. The free energy of an arbitrarily deformed semiconductor consists of the energy of the elastic deformation of the medium and the energy of the carriers in the field of the inhomogeneous deformation, and takes in the self-consistent-field approximation the form

$$F = \frac{\lambda}{2}\int d\mathbf{r}\,(\operatorname{div}\mathbf{u})^2 + \operatorname{Sp}\left\{\mu\hat{\rho} - T\ln\left(1 + e^{(\mu - \hat{\mathcal{H}})/T}\right) - \frac{\Phi}{2}(\hat{\rho} - \hat{\rho}_0)\right\}, \qquad (1)$$

λ is the elastic modulus, u is the displacement of the medium, μ is the chemical potential, $\hat{\rho}(\hat{\mathcal{H}},\mu)$ is the single-particle density matrix, $\hat{\rho}_0$ corresponds to a homogeneous state with electron density n_0, $\hat{\mathcal{H}} = \mathrm{W} + h(\mathbf{r})$, where W is the kinetic energy, $h = b\,\mathrm{div}u + \Phi$, b is the deformation-potential constant, Φ satisfies the Poisson equation, and T is the temperature.

2. The quasi-classical limit (1) for a homogeneous system $F(n_0, \mathrm{div}u)$ makes it possible to determine the regions of instability and the physical character of the resultant new states. If we eliminate from (1) the equilibrium value $\mathrm{div}u = -b/\lambda n_0$, then we find that the density dependence of the free energy $F(n_0)$ is

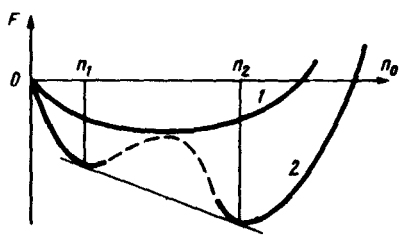

FIG. 1. Qualitative plots of $F(n_0)$. Curves 1 and 2 correspond to $T_2 < T_m < T_1$.

substantially different for different T (Fig. 1). The condition $F''_{n_0^2} > 0$ for the thermodynamic stability of the homogeneous states is violated at $A \equiv b^2/(\lambda d\mu/dn_0) \geq 1$. The oscillatory dependence of $d\mu(T, n_0)\, dn_0$ causes the last relation to be satisfied in a number of regions,[4] the boundaries of which are defined parametrically by

$$\sqrt{t} = \phi'(Z, \theta), \qquad t \equiv T(\lambda/Gb^2)^2; \tag{2a}$$

$$\kappa = \sqrt{t}\,\phi(Z, \theta) \qquad \kappa \equiv n_0 \lambda/G^2 b^2; \tag{2b}$$

$G = \sqrt{2m/\hbar^2}\, 2\pi^2 r_H^2$, $r_H^2 = \hbar/m\omega$, $\theta = \hbar\omega/T$, $Z = \mu/T, \omega$ is the cyclotron frequency, m is the effective mass, $\phi = \Sigma_{n=0} \Phi_{-1/2}(Z - n\theta)$, and Φ_s is the Fermi integral. The first region (the quantum limit) is adjacent to the point $T = 0$, $n_0 = 0$ (Fig. 2), while the other regions are similar to the first and the characteristic concentrations in them correspond to $\mu(n_0)$ values which are multiples of $\hbar\omega$. Each region has its own maximum point $T = T_m \propto b^4$, which depends in power-law fashion on the interaction constant. We note that in a magnetic field instability can occur at all values of n_0 if the temperature is low enough (at $H = 0$ the threshold values of n_0 are high even as $T \to 0$). At $T < T_m$ there is an interval of values of n_0 where the homogeneous state is absolutely unstable. Without allowance for the Coulomb repulsion, the minimum of F corresponds to heterogeneous states with stratification into phases of decreased and increased concentrations $n_1 < n_0$ and $n_2 > n_0$, respectively. Allowance for the electrostatic interaction leads to a mixing of the phases with different densities. An unlimited breakup of the phases is not profitable, since it is accompanied, for example, by an increase of the kinetic energy of the electrons. As a result, an inhomogeneous structure should be produced, with a spatially periodic distribution of the electron density and a compatible deformation, the period of which is determined by the competition between the electrostatic energy and the energy connected with the homogeneity. The latter is determined by the change of the free energy of the electron in the inhomogeneous field $h(\mathbf{r})$, with allowance for the quantum properties, compared with its quasi-classical value.

3. Assuming that h in (1) is small, let us calculate the change of the specific free energy of the system on going to the inhomogeneous state

$$\Delta F = \frac{b^2}{2\lambda} \sum_{\mathbf{q}} \frac{1 + \nu\Pi}{\nu^2} |h_{\mathbf{q}}|^2 + \ldots, \qquad \nu = \frac{4\pi e^2}{\epsilon_0 q^2} - \frac{b^2}{\lambda}, \tag{3}$$

$\Pi(Z, \mathbf{q})$ is the static polarization operator,[6] h_q is the Fourier component of $h(\mathbf{r})$, and ϵ_0 is the dielectric constant. From (3) follows the absolute-instability condition $1 + \nu\Pi \leq 0$, which can be represented in the form

FIG. 2.

$$A(t, Z) \geqslant {}^1/l^2 q^2 + \Pi_0 \Pi^{-1} \equiv \tau(q_\perp, q_\parallel, t, Z), \qquad l^2 \equiv \epsilon_0/4\pi e^2 \Pi_0 . \tag{4}$$

where $q_\perp$ and $q_\parallel$ are the transverse and longitudinal components of $\mathbf{q}$ relative to H. $\Pi_0 = \Pi(q=0)$ (4) generalizes the quasiclassical criterion $A \geq 1$, and takes into account the Coulomb interaction and the dispersion of F over the quantum and de Broglie lengths r_H and k_F^{-1}, respectively. The stability limit $\kappa = \kappa(t)$ is determined by those $q = q_0$ for which τ is minimal: $\tau'_{q_\perp}(q_{\perp 0}, q_{\parallel 0}) = 0$ and $\tau'_{q_\parallel}(q_{\perp 0}, q_{\parallel 0}) = 0$. An investigation of these equations together with (4) and (2b) shows that the $\kappa(t)$ curve has sections on which there develops either a longitudinal instability with $\mathbf{q} \| \mathbf{H}$ (L instability) or a transverse instability with $\mathbf{q} \perp \mathbf{H}$ (T instability).

The character of the L instability is determined essentially by the evolution of the known singularity[6,7] of the one-dimensional polarization operator $\Pi(q_\parallel)$ when t and κ are varied. Let us follow the behavior of the L boundary when $q_{\parallel 0}$ varies along this boundary. At $T \ll \mu$ we obtain $\Pi/\Pi_0 \approx \ln(\mu/T) \gg 1$ in a narrow interval near $2k_F$. It follows then from (4) that the instability sets in for wave vectors $q_{\parallel 0} \approx 2k_F$ at a temperature

$$T \lesssim 4\gamma_C \mu \exp[-1/A(1 - q_*^2/4k_F^2)], \qquad q_*^2 \equiv 1/Al^2 , \tag{5}$$

q^* does not depend on κ, and $\ln\gamma_C$ is the Euler constant. It is seen that the Coulomb interaction "shuts off" the instability for concentrations at which $2k_F \leq q^*$. At large concentrations, the L boundary is determined by the relation $T = \gamma_C \mu e^{-1/A}$, which is typical of a transition of the Peierls type.[7] It follows from (5) that the phase-transition temperature increases with increasing A. The highest temperatures $T \sim \mu$ are reached in the region $A \sim 1$, if the inequality $k_F l \gg 1$ is satisfied in this region. The L boundary is then close to the quasiclassical curve $A(\kappa, t) = 1$, and the maximum temperature is $T \approx T_m \sim b^4$. The singularity of Π then becomes smoothed out and the Coulomb term becomes essential for the determination of $q_{\parallel 0}$ from (4). As a result we obtain for $\kappa \approx \kappa_m \equiv \kappa(t_m)$ the relation $q_{\parallel 0} \approx \sqrt[3]{k_F^2 l^{-1}}$, and on the left wing of the L boundary we have $(\kappa < \kappa_m) - q_{\parallel 0} \approx \sqrt{k_F l^{-1}}$.

At low concentrations (in the region $A \gtrsim 1$), where the L instability is hindered by the Coulomb repulsion, the transition into the inhomogeneous state is determined by the T instability. Its boundary is always similar to the $A = 1$ curve, and is close to this curve at $r_H^{-1} l \gg 1$ in which case $q_{\perp 0} \approx \sqrt{r_H^{-1} l^{-1}}$. Thus, the left-hand wing of the phase diagram is of the T type and the right-hand wing of the L type (Fig. 2).

4. The produced inhomogeneous states can be described by a free energy of the type (1), i.e., in the same model that predicts the instability of the initial phase. Let us consider by way of example a periodic L structure $h(x) = \Sigma_{n \neq 0} h_{nq} e^{inqx}$ in the actual vicinity of the temperatures $T \approx T_m$. The equations for h_{nq} are obtained by variation of (3) with allowance for the terms of higher order in h. The amplitudes of the higher harmonics are excluded from them with the aid of the fundamental ($|h_{nq}| \sim |h_q|^n$) and the connection between h_q and the period q^{-1} is determined and makes it possible to compare the relative convenience of the structures with different periods:

$$A - A_0 - (q - q_0)^2/q_x^2 = \beta \Pi_0^{-1} |h_q|^2, \quad \Delta F \cong -\beta |h_q|^4, \quad A - A_0 << A_0 \equiv r(q_0), \tag{6}$$

where $q_x/q_0 \sim (k_F l)^{2/3} \gg 1$ and $\beta \approx |d^2\Pi_0/d\mu^2| \sim \Pi_0/T_m^2$. At the instability boundary ($A = A_0$) there is a unique solution (6) corresponding to $h_{q0} = 0$, $q = q_0$. At $A > A_0$

we obtain a set of finite values h_q for the interval $|q-q_0| \sim q_x\sqrt{A-A_0}$. The largest amplitude and accordingly the greatest decrease of F is reached in accordance with (6) for the solution with $q=q_0$. Thus, in the vicinity of T_m there should be realized weakly-inhomogeneous states with a spatial period $q^{-1} \sim \sqrt[3]{k_F^2 l}$ and with an amplitude $h \sim T_m\sqrt{A-A_0}$. These states arise via second-order phase transitions.

We present an order-of-magnitude estimate of the critical values of T_m and $n(T_m)$:

$$T_m \approx (\hbar\omega)^2/E_a\,\xi\,, \quad na_0^3 \approx (\hbar\omega)^2/E_a^2\,\xi\,, \qquad \xi = 9\pi^4(m_0 a^2/ma_0^2)^3\,,$$

where m_0 is the mass of the free electron, a_0 is the lattice constant, a is the Bohr radius, and E_a is an energy on the order of the atomic energy (it is assumed that $b \sim E_a$, $\lambda \sim E_a/a_0^3$). The condition that the electron gas be ideal $e^2n^{1/3}/\epsilon_0 \ll T$ leads to the inequality $H \gg H_0 = (a/a_0\epsilon_0)^{3/4}(mc/e\hbar)\sqrt{\xi}\,E_a$ for the magnetic field. For example, at $m=m_0$, $\epsilon_0=400$, $E_a=10$ eV, and $a_0/a=10$ we obtain $H_0=5\times10^4$ Oe. Putting $H=3\times10^5$ Oe we get $T_m=17$ K, $n=10^{18}$ cm^{-3}.

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