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Dielectric transition in a quasi-one-dimensional system with repulsion

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It is shown that the interaction between electrons located on different chains may lead to a three-dimensional dielectric transition even if the electrons on a single chain repel one another. The relevant interaction constant of electrons on a single chain is obtained. If the converse inequality holds, the ground state of the system is metallic.

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1. INTRODUCTION

Materials possessing a chain structure have been intensively investigated in recent years. We have in mind experiments on complexes on a TCNQ base and complexes of variable valence on a Pt or Ir base and so on. Such quasi-one-dimensional systems should in principle possess a number of interesting properties. Nevertheless, in spite of the large variety of states theoretically possible, almost all the known quasi-one-dimensional systems are dielectrics at low temperatures.

In the present research, we consider one of the possible mechanisms of dielectric transition. As a model, we consider a system of parallel metallic chains arranged in a lattice. The interaction between electrons located on each chain is assumed to be large in comparison with the interaction between electrons on different chains. This interaction can be a direct Coulomb interaction or indirect, through phonons. The interaction through phonons becomes significant at temperatures below the Debye temperature; therefore, in the initial junctions we consider only the Coulomb interaction.

The case of repulsion brought about by the Coulomb interaction is usually considered to be "uninteresting." The fact is that the simplest calculation by the molecular-field method,[1] with neglect of the interaction between neighboring chains, leads to the conclusion that any sort of transition is absent. An exception is the case of just one electron per unit cell. We shall not consider this case. We shall show that allowance for an arbitrarily weak interaction between electrons on different chains leads to a renormalization of the interaction of the electrons on a single chain and, in final analysis, to a dielectric transition. The characteristic feature of this transition is that the renormalized interaction between electrons on different chains becomes of the order of the renormalized interaction on a single chain. This leads to the suppression of purely one-dimensional fluctuations and makes possible the description of the transition by means of the molecular-field method. We shall use the very well known method of summation of principal terms—the "parquet" method.

In the one-dimensional case, there exist two particular scattering channels, those of Cooper and Peierls. The first corresponds to coupling of two electrons on opposite ends of the Fermi surface,1) while the second corresponds to coupling of an electron and hole at opposite ends of the Fermi surface, with total momentum $2p_F$.

Both channels give logarithmic integrals of the order of $\ln(\tilde{\omega}/T)$, where $\tilde{\omega} \sim \varepsilon_F$. Summation of terms of the form $(g\ln(\tilde{\omega}/T))^n$ leads to a system of parquet equations. Following Gor'kov and Dzyaloshinskiĭ,[2] we write down the complete vertex part, explicitly separating the dependence on the spins $(\alpha\beta\gamma\delta)$ and the numbers of chains2) $(iklm)$:

$$\Gamma_{\alpha\beta\gamma\delta}^{iklm}(++--) = \gamma_1{}^{ik}\delta_{\alpha\gamma}\delta_{\beta\delta}\delta_{il}\delta_{km} - \gamma_2{}^{ik}\delta_{\alpha\delta}\delta_{\beta\gamma}\delta_{im}\delta_{kl}.$$

Here the signs ± correspond to an electron located at one "Fermi point" $\pm p_F$ or another; γ_1 corresponds to scattering with momentum transfer $2p_F$; γ_2 corresponds to scattering with zero momentum transfer.

We shall not derive the parquet equations, but use the equations obtained in Ref. 2. In contrast to Ref. 2, we shall consider the case in which electrons are repelled on one chain, i.e., the nonrenormalized constants g_1, $g_2 > 0$. We shall show that, upon satisfaction of the inequality $2g_2 - g_1 > 0$, the interaction between electrons located on different chains increases like $1/T^{g_2 - g_1/2}$ with decrease in temperature. When this interaction becomes of the order of the interaction on a single chain, the equations become nonlinear. Therefore, it is possible to prove rigorously that a three-dimensional dielectric transition takes place only in the case of certain limitations on the initial conditions. This is either a limitation on the signs of the interaction constants between chains or the requirement of rapid decrease of the interaction on different chains.

We shall not take into account effects connected with hops of electrons between chains. This means that the temperature at which the logarithmic integrals are cut off is always assumed to be higher than the energy of the transverse motion of the electrons $(T > \omega_\perp)$.[2]

2. INSTABILITY IN THE QUASI-ONE-DIMENSIONAL SYSTEM WITH REPULSION ON A SINGLE CHAIN. MOVING POLE

We make use of the equations for the complete vertices γ_1, γ_2 as functions of the logarithmic variable

$$\xi = \ln\frac{\tilde{\omega}}{\max(T, \omega, v_F p)}$$

obtained in the parquet approximation[2]:

$$\gamma_1{}^{ik} = g_1{}^{ik} - \int_0^\xi d\xi' \left[\gamma_1{}^{ik}\gamma_2{}^{ik} - \gamma_1{}^{ik}\gamma_2 + \sum_l \gamma_1{}^{il}\gamma_1{}^{lk}\right],$$
$$\gamma_2{}^{ik} = g_2{}^{ik} - \frac{1}{2}\int_0^\xi d\xi' (\gamma_1{}^{ik})^2. \qquad (1)$$

We write down the equations for γ_1^{ik} and γ_2^{ik} in differential form:

$$\frac{d\gamma_1{}^{ik}}{d\xi} = -\gamma_1{}^{ik}\gamma_2{}^{ik} + \gamma_1{}^{ik}\gamma_2{}^{ii} - \sum_l \gamma_1{}^{il}\gamma_1{}^{lk},$$
$$\frac{d\gamma_2{}^{ik}}{d\xi} = -\frac{1}{2}(\gamma_1{}^{ik})^2. \qquad (2)$$

If only the constants of interaction on a single chain are different from zero, then Eqs. (2) have a simple solution:[1]

$$\gamma_1 = \frac{g_1}{1+g_1\xi}, \quad \gamma_2 = g_2 - \frac{1}{2}g_1 + \frac{{}^1\!/_2 g_1}{1+g_1\xi}. \qquad (3)$$

In the case of repulsion of electrons on a single chain, $g_1 > 0$, the solution does not contain singularities as $T \to 0$, $\xi \to \infty$. Let the interaction between electrons on nearest chains be small in comparison with the interaction on a single chain and much greater than the interaction with more remote chains. Then we have, in first order in $\gamma^{i\,i+1}$,

$$\frac{d\gamma_1^{i\,i+1}}{d\xi} = \gamma_1^{i\,i+1}(\gamma_2 - 2\gamma_1), \quad \frac{d\gamma_2^{i\,i+1}}{d\xi} = 0. \qquad (4)$$

Substituting (3) in (4) and integrating, we obtain

$$\gamma_1^{i\,i+1} = g_1^{i\,i+1}\exp\int_0^\xi d\xi'(\gamma_2 - 2\gamma_1) = \frac{g_1^{i\,i+1}}{(1+g_1\xi)^{3/2}}\exp\left(g_2 - \frac{1}{2}g_1\right)\xi. \qquad (5)$$

In the case of repulsion on a single chain, $g_1 > 0$, the limiting behavior of $\gamma_1^{i\,i+1}$ as $T \to 0$ is determined by the sign of the expression $g_2 - \frac{1}{2}g_1$:

$$\gamma_1^{i\,i+1} \sim \frac{1}{T^{g_2 - g_1/2}}.$$

If $g_2 - \frac{1}{2}g_1 > 0$, then $\gamma_1^{i\,i+1}$ increases with decrease in temperature and becomes of the order of γ_1, γ_2 at

$$\xi_0 \sim \frac{1}{g_2 - {}^1\!/_2 g_1}\ln\frac{g}{g_1^{i\,i+1}}$$

or

$$T_0 \sim \tilde{\omega}\exp\{-\ln(g/g_1^{i\,i+1})/(g_2 - {}^1\!/_2 g_1)\}.$$

Substituting (3) and (5) in Eq. (2) for the next nearest chain $\gamma_{1,2}^{i\,i+2}$, we see that $\gamma_1^{i\,i+2}$ becomes of the order of γ_1, γ_2 simultaneously with $\gamma_1^{i\,i+1}$ and so on. Thus, at $\xi \sim \xi_0$ it is necessary to solve the problem of the interaction of electrons on a large number of chains.

A similar situation arises in the case of the attraction of electrons on a single chain, $g_1 < 0$. Then a pole singularity appears in the solution (3) at $\xi_0 = -(g_1)^{-1}$. As is seen from (4), the interaction of the electrons on different chains increases more rapidly than on a single chain, as $(1 + g_1\xi)^{-3/2}$, and in this case also, it is necessary to solve the problem of the interaction of many chains.

In the Fourier representation in terms of difference of the coordinates of the chains ρ^{ik}:

$$\gamma(\mathbf{q}) = \sum_k \gamma^{ik}\exp(i\mathbf{q}\rho^{ik}), \quad \gamma^{ik} = \int_S \gamma(\mathbf{q})\exp(i\mathbf{q}\rho^{ik})\frac{d^2q}{S},$$

(S is the area of the reciprocal cell), Eq. (2) is written down in the following form:

$$\frac{d\gamma_1(\mathbf{q})}{d\xi} = -\gamma_1^2(\mathbf{q}) + \gamma_1(\mathbf{q}) \int\limits_S \gamma_2(\mathbf{q}_1) \frac{d^2q_1}{S} - \int\limits_S \gamma_1(\mathbf{q}-\mathbf{q}_1)\gamma_2(\mathbf{q}_1) \frac{d^2q_1}{S},$$
$$\frac{d\gamma_2(\mathbf{q})}{d\xi} = -\frac{1}{2}\int\limits_S \gamma_1(\mathbf{q}-\mathbf{q}_1)\gamma_1(\mathbf{q}_1)\frac{d^2q_1}{S}. \qquad (6)$$

It has been shown[2] that the Eqs. (2) and (6) can have a singularity of the "standing pole" type:

$$\gamma_1^{ik} = \frac{A_{ik}}{\xi-\xi_0}, \quad \gamma_2^{ik} = \frac{B_{ik}}{\xi-\xi_0} \qquad (7)$$

or a singularity of the "moving pole" type:

$$\gamma_1(\mathbf{q}) \sim \frac{1}{\xi-\xi_0(\mathbf{q})}, \quad \gamma_2(\mathbf{q}) \sim \ln|\xi-\xi_0(\mathbf{q})|, \qquad (8)$$

where $\xi_0(\mathbf{q})$ is a significant function of the transverse quasimomentum. The solutions (7) and (8) correspond to different physical states of the quasi-one-dimensional system. Because of the nonlinearity of the equations, it is impossible to indicate which initial conditions correspond to one solution or the other. Consequently, all the states considered in Ref. 2 are possible in principle in our case. Nonetheless, for the physically important case of an initial interaction between chains that falls off rapidly with distance, we can show that the singularity is of the form of a moving pole. The existence of a solution of the moving pole type can be demonstrated also without the condition of rapid decrease in the interaction of the electrons on different chains, but with a limitation on the sign of this interaction. This is either the requirement of attraction of all electrons on different chains or the requirement of alternation of repulsion and attraction as the distance between chains increases (see the Appendix). In all probability, the solution of the standing pole type (7) is a special case of the solution of the moving pole type (8) with a degenerate dependence $\xi_0(\mathbf{q}) = \xi_0$ and is realized only under specific initial conditions.

The fact that the pole part $\gamma_1(\mathbf{q})$ contains a dependence on the transverse quasimomentum q means that near the transition the basic contribution to Eq. (6) for $\gamma_1(\mathbf{q})$ is made by the term which does not contain the integration over q. This term has the form $\sum_l \gamma_1^{il}\gamma_1^{lk}$ in the coordinate representation and describes the contribution of the Peierls channel to γ_1^{ik}.

Actually, in the absence of hops of electrons between chains, transitions with participation of electrons on intermediate chains are possible only in the Peierls channel. The fact that the pole singularity arises only in the Peierls channel means that a dielectric transition is taking place.

The transition is accompanied by the appearance of a charge-density wave with longitudinal component $2p_F$ and transverse component $\mathbf{q}_0$ ($\mathbf{q}_0$ is that value of $\mathbf{q}$ at which $\xi_0(\mathbf{q})$ has a minimum). The charge-density waves on different chains are in phase, $\mathbf{q}_0 = [0, 0]$ if the unrenormalized interaction between the chains is one of attraction, and in counterphase, $\mathbf{q}_0 = [\pi, \pi]$ if it is one of repulsion. These cases are considered in the Appendix. In the general case, the vector $\mathbf{q}_0$ is generally incommensurate with the transverse vectors of the reciprocal lattice and is temperature dependent.

If the electrons on one chain attract one another, $g_1 < 0$, then in all the cases considered in the Appendix, a moving pole is also formed. But, as is seen from (5), this takes place when all $|\gamma_1^{ik}| > 1$, i.e., the parquet approximation is inapplicable. Therefore, it is entirely possible that arguments favoring a dielectric transition at $g_1 < 0$ can turn out to be incorrect.

The conclusion that a moving pole exists is valid also in the case of complicated systems consisting of sublattices of conducting chains imbedded in one another, as, for example, TTF-TCNQ. It can be shown that the formation of a moving pole in the subsystems TTF and TCNQ takes place simulataneously. Denoting the chains of TTF and TCNQ by the indices a and b, we write down equations$^{3)}$ similar to the first of Eqs. (6), in the form

$$\frac{d\gamma_1^{aa}(\mathbf{q})}{d\xi} = -\gamma_1^{aa}(\mathbf{q})\gamma_1^{aa}(\mathbf{q}) - \gamma_1^{ab}(\mathbf{q})\gamma_1^{ba}(\mathbf{q}) + \dots,$$
$$\frac{d\gamma_1^{ab}(\mathbf{q})}{d\xi} = -\gamma_1^{ab}(\mathbf{q})\gamma_1^{bb}(\mathbf{q}) - \gamma_1^{aa}(\mathbf{q})\gamma_1^{ab}(\mathbf{q}) + \dots, \qquad (9)$$
$$\frac{d\gamma_1^{bb}(\mathbf{q})}{d\xi} = -\gamma_1^{ba}(\mathbf{q})\gamma_1^{ab}(\mathbf{q}) - \gamma_1^{bb}(\mathbf{q})\gamma_1^{bb}(\mathbf{q}) + \dots$$

(we omit the integral terms). It is then seen that if there is a singularity in $\gamma^{aa}(\mathbf{q})$ at $\mathbf{q} = \mathbf{q}_0$, then this singularity exists also in $\gamma^{ab}(\mathbf{q}_0)$ and in $\gamma^{bb}(\mathbf{q}_0)$. (If $g_1^{ab}(\mathbf{q}_0) = 0$ for any reason, then the transitions take place independently in the different subsystems.)

3. EQUATION FOR THE DIELECTRIC GAP

The fact that a singularity arises only in one of two scattering channels allows us to apply the ladder approximation, analogous to BCS, near the transition. The effective vertex of the interaction of an electron and a hole will be the sum S^{ik} of all diagrams that are irreducible to a Peierls channel (Fig. 1). True, in contrast to BCS, S^{ik} in the parquet approximation is a function of the maximum momentum or frequency to the right or left of the S^{ik} cross section (see Fig. 1) or the corresponding logarithmic variables ξ and ξ':

$$S^{ik}(\xi, \xi') = \begin{cases} S^{ik}(\xi) & (\xi < \xi') \\ S^{ik}(\xi') & (\xi > \xi') \end{cases}$$

where

$$S^{ik}(\xi) = g_1^{ik} + C_1^{ik}(\xi) - {}^1/_2 (g_2^{ii} + C_2^{ii}(\xi))\delta_{ik},$$

here C_1^{ik} and C_2^{ii} are the contributions made to γ_1^{ik} and γ_2^{ii} by diagrams that are reducible in the Cooper channel.

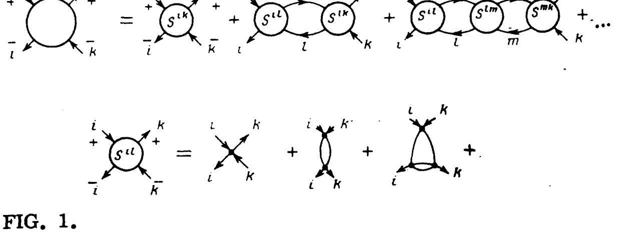
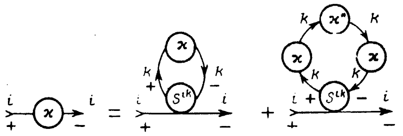


FIG. 1.

$$C_1^{ik}=-\int_0^{\xi} d\xi'\gamma_1^{ik}\gamma_2^{ik},\quad C_2^{ii}=-\frac{1}{2}\int_0^{\xi} d\xi'[(\gamma_1^{ii})^2+(\gamma_2^{ii})^2].$$

At $\xi\sim\xi_0$ the function $S^{ik}(\xi)$ does not have singularities.

We write down the equation for the dielectric gap $\varkappa$ with accuracy to within components of third order in $\varkappa$:



(10)

On the right side of (10) summation over all chains k is understood.

We shall not take into account the diagram with $\varkappa$ inserted in S^{ik}. Actually, if we insert a $G\varkappa G$ or $G\varkappa G\varkappa^*G$ line in place of any G line in S^{ik}, then the integration in the corresponding cross section will not be logarithmic and the resultant diagram will have an additional smallness $\sim g$ besides the smallness $(\varkappa/T)^n$ corresponding to an expansion in $\varkappa$. We write down (10) in the coordinate representation:

$$\varkappa^{ii}(r_1r_2)=T\sum_{\omega_n}\sum_{k}\iiiint \tilde{S}^{ik}(r_1r_2r_3r_4)G_{\omega_n}(r_3r_4)\varkappa^{kk}(r_5r_6)G_{\omega_n}(r_6r_4)\,dr_3dr_4dr_5dr_5$$
$$-T\sum_{\omega_n}\sum_{k}\iint\dots\int \tilde{S}^{ik}(r_1r_2r_3r_4)G_{\omega_n}(r_3r_5)\varkappa^{kk}(r_5r_6)\cdot$$
$$\cdot G_{\omega_n}(r_6r_7)\varkappa^{kk}(r_7r_8)\cdot G_{\omega_n}(r_8r_9)\varkappa^{kk}(r_9r_{10})G_{\omega_n}(r_{10}r_4)\,dr_3\dots dr_{10},\tag{11}$$

where $\tilde{S}^{ik}$ differs from the dimensionless quantity S^{ik} by the factor $2\pi v_F$.

We transform from the variables r_1 and r_2 to their arithmetic mean $\mathbf{R}$ and difference r. We shall assume $\mathbf{R}$ to be a three-dimensional vector. It is then not necessary to write the numbers of the chains i and k.

We change $\mathbf{R}$ and r to the Fourier components $\mathbf{P}$ and p. The vector $\mathbf{P}$ corresponds to the total quasimomentum of the paired particles and contains the longitudinal and transverse components $\mathbf{P}=\{P,\mathbf{q}\}$. The quantity $|p|-p_F$ is the distance of the paired particles from the Fermi surface. Near $P=2p_F$ and $\mathbf{q}=\mathbf{q}_0$, we carry out an expansion, limiting ourselves to terms of second order in $P-2p_F$ and $\mathbf{q}-\mathbf{q}_0$. After simple calculations we obtain

$$\varkappa(P,\mathbf{q},p)=T\sum_{\omega_n}\int S(\mathbf{q}_0,p,p')G_{\omega_n}(p')\varkappa(P,\mathbf{q},p')$$
$$\times G_{\omega_n}(p'+2p_F)\frac{dp'}{2\pi}+\frac{1}{4}(P-2p_F)^2T\sum_{\omega_n}\int\varkappa(P,\mathbf{q},p')$$
$$\times\frac{\partial^2}{\partial p'^2}G_{\omega_n}(p')G_{\omega_n}(p'+2p_F)\tilde{S}(\mathbf{q}_0,p,p')\frac{dp'}{2\pi}$$
$$+\frac{1}{4}(\mathbf{q}-\mathbf{q}_0)^2T\sum_{\omega_n}\int\varkappa(P,\mathbf{q},p')\frac{\partial^2}{\partial q^2}\tilde{S}(\mathbf{q},p,p')|_{\mathbf{q}=\mathbf{q}_0}G_{\omega_n}(p')$$
$$\times G_{\omega_n}(p'+2p_F)\frac{dp'}{2\pi}-T\sum_{\omega_n}\int\varkappa(P,\mathbf{q},p')|\varkappa(P,\mathbf{q},p')|^2\cdot$$
$$\times G^2_{\omega_n}(p')G^2_{\omega_n}(p'+2p_F)\tilde{S}(\mathbf{q}_0,p,p')\frac{dp'}{2\pi}.\tag{12}$$

In the BCS theory, one always separates the variables by writing $\varkappa(P,\mathbf{q},p)$ in the form $\varkappa(P,\mathbf{q})f(p)$, and obtains an equation for $\varkappa(P,\mathbf{q})$. In our case, because of the one-dimensionality of the G functions of the electrons, this cannot be done; therefore, we write $\varkappa(P,\mathbf{q},p)$ in the form

$$\varkappa(P,\mathbf{q},p)=\varkappa(P,\mathbf{q})f(p)+f_1(P,\mathbf{q},p),\tag{13}$$

where the function $f(p)$ satisfies the equation

$$f(p)=T_0\sum_{\omega_n}\int\frac{dp'}{2\pi}f(p')G_{\omega_n}(p')G_{\omega_n}(p'+2p_F)\tilde{S}(\mathbf{q}_0,p_1,p')\tag{14}$$

with the normalization $f(p_F)=1$ and $f_1(P,\mathbf{q},p)$ is a small correction. In what follows, we shall show that the corrections to the equation for $\varkappa(P,\mathbf{q})$ due to $f_1(P,\mathbf{q},p)$ are small.

We substitute (13) and (14) in (12). We have left in f_1 only terms of first order. We write down the remaining integrals in terms of logarithmic variables:

$$S(\mathbf{q}_0,\xi_0,\xi)\left\{\frac{T-T_0}{T_0}\varkappa(P,\mathbf{q})+\frac{v_F^2}{2}\eta(P-2p_F)^2\varkappa(P,\mathbf{q})\right.$$
$$\left.+\eta\varkappa(P,\mathbf{q})|\varkappa(P,\mathbf{q})|^2+3\eta|\varkappa(P,\mathbf{q})|^2f_1(P,\mathbf{q},\xi_0)\right\}+f_1(P,\mathbf{q},\xi)$$
$$-\int_0^{\xi_0}S(\mathbf{q}_0,\xi,\xi')f_1(P,\mathbf{q},\xi')\,d\xi'\cdot$$
$$+\frac{1}{4}(\mathbf{q}-\mathbf{q}_0)^2\varkappa(P,\mathbf{q})\int_0^{\xi_0}f(\xi')\frac{\partial^2}{\partial\mathbf{q}^2}S(\mathbf{q},\xi,\xi')|_{\mathbf{q}=\mathbf{q}_0}d\xi',\tag{15}$$

where

$$\eta=\frac{7}{8}\frac{\zeta(3)}{(\pi T_0)^2}.$$

We can apply to f_1 the condition of orthogonality to f in the logarithmic integration:

$$\int_0^{\xi_0}f_1(\xi)f(\xi)\,d\xi=0.$$

We multiply (15) by $f(\xi)$ and integrate over ξ:

$$\frac{(\mathbf{q}-\mathbf{q}_0)^2}{2}\int_0^{\xi_0}d\xi\,f(\xi)\int_0^{\xi}d\xi'\,f(\xi')\frac{\partial^2}{\partial\mathbf{q}^2}S(\mathbf{q},\xi_0,\xi')|_{\mathbf{q}=\mathbf{q}_0}\varkappa(P,\mathbf{q})$$
$$+\int_0^{\xi_0}d\xi\,S(\mathbf{q}_0,\xi_0,\xi)f(\xi)\left\{\frac{T-T_0}{T}\varkappa(P,\mathbf{q})+\frac{v_F^2\eta}{2}(P-2p_F)^2\varkappa(P,\mathbf{q})\right.$$
$$\left.+\eta\varkappa(P,\mathbf{q})|\varkappa(P,\mathbf{q})|^2+3\eta|\varkappa(P,\mathbf{q})|^2f_1(P,\mathbf{q},\xi_0)\right\}.\tag{16}$$

We note that the integral in front of the curly brackets is equal to unity. (see (14)). Comparing (16) with (15), we can establish the fact that $f_1(P,\mathbf{q},p)\sim(\mathbf{q}-\mathbf{q}_0)^2\ \ (P,\mathbf{q})$; therefore, we can neglect the last term in (16). We obtain the Ginzburg–Landau equation for the order parameter:

$$\left\{\frac{T-T_0}{T_0}+\frac{v_F^2\eta}{2}(P-2p_F)^2+\frac{1}{2}(\mathbf{q}-\mathbf{q}_0)^2\int_0^{\xi_0}d\xi f(\xi)\int_0^{\xi}d\xi' f(\xi')\right.$$
$$\left.\times\frac{\partial^2}{\partial\mathbf{q}^2}S(\mathbf{q},\xi_0,\xi')|_{\mathbf{q}=\mathbf{q}_0}+\eta|\varkappa(P,\mathbf{q})|^2\right\}\varkappa(P,\mathbf{q})=0.\tag{17}$$

The function $S(\xi)$ can be calculated with logarithmic accuracy by solving Eq. (6) numerically. Knowing $S(\xi)$, we can determine $f(\xi)$. We write down (14) in the logarithmic variables:

$$f(\xi)=\int_0^{\xi_0}d\xi' f(\xi')S(\mathbf{q}_0,\xi,\xi').\tag{18}$$

Differentiating with respect to ξ, we get

$$f'(\xi)=S'(\mathbf{q}_0,\xi)\int_{\xi}^{\xi_0} f(\xi')\,d\xi'.$$

We introduce the function

$$F(\xi)=\int_{\xi}^{\xi_0} f(\xi')\,d\xi',$$

then $f(\xi)$ is determined from the solution of the equation

$$F''(\xi)=S'(\mathbf{q}_0,\,\xi)F(\xi) \tag{19}$$

with initial conditions $F(\xi_0)=0$ and $F'(\xi_0)=1$.

With the help of (17), we can determine (see, for example, Ref. 4) the region of applicability of the theory of the molecular field:

$$\left|\frac{T_0-T}{T_0}\right| \gg \left[\int_0^{\xi_0} d\xi f(\xi)\int_0^{\xi} d\xi' f(\xi')\frac{\partial^2}{\partial q^2}S(\mathbf{q},\xi_0,\xi)\,|_{\mathbf{q}=\mathbf{q}_0}\right]^{-2}\sim g^2. \tag{20}$$

From (17) and (12), we can establish the expression for the free energy. Substituting the equilibrium value of $\varkappa$ in it and differentiating twice with respect to the temperature, we obtain (exactly as in BCS theory) the expression for the temperature jump at the transition point:

$$C_d-C_n=\frac{4mp_F}{7\zeta(3)}T_0. \tag{21}$$

It is not difficult to establish the fact that the logarithmic corrections that are typical of one-dimensional systems are lacking in the heat capacity and the permittivity. Actually, the complete vertex in the corresponding diagram (Fig. 2) does not contain any singularity at the transition point. The value of the gap at zero temperature is connected with the transition temperature in the usual way: $\varkappa=\pi T_0/\gamma$, where $\ln\gamma=C=0.577$.

4. PHONONS

The expression for the temperature of the dielectric transition $T_0\sim\tilde{\omega}\exp\{-(1/g)\ln(g/g^{i\,i+1})\}$ contains an additional smallness: therefore, the transition takes place at a temperature known to be below the Debye temperature. Account of the phonon mechanisms at $T<\omega_D$ leads to a renormalization of the constants of interaction and of the limits of integration[2]:

$$\tilde{\xi}=\ln\frac{\tilde{\omega}}{T}\to\xi=\ln\frac{\omega_D}{T},$$

$$\gamma_1^{ik}(\xi_D)-g_{ep}^2\delta_{ik}\to g_1^{ik},\quad \gamma_2^{ik}(\xi_D)\to g_2^{ik},$$

where g_{ep} is the constant of electron-phonon interaction. We shall assume that the inequalities for the interaction constants, which we have used, do not change here. At $T\sim\omega_D$, the effective interaction constant of electrons and holes S^{ik} experiences a jump. The delta-shaped singularity in $S'(\mathbf{q}_0,\xi)$ leads to a break in the function $F(\xi)$, i.e., a jump in the value of the dielectric gap. Thus, below the transition point, a singularity of the order of $(T_0/\omega_D)^2$ occurs in the density of states at $\omega\sim\omega_D$.

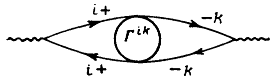


FIG. 2.

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APPENDIX

We write down the first of Eqs. (2) in the form

$$\frac{d\gamma_1^{ik}}{d\xi}=\gamma_1^{ik}(\gamma_2-2\gamma_1)-\gamma_1^{ik}\gamma_2^{ik}-\sum_{l\neq i,k}\gamma_1^{il}\gamma_1^{lk}. \tag{A.1}$$

At some ξ let all $\gamma_{1,2}^{ik}<0$ ($i\neq k$, and also $\gamma_2-2\gamma_1>0$). Then all the terms in (9) are negative. We write down the following equations for γ_1, γ_2:

$$\frac{d\gamma_1}{d\xi}=-\sum_k(\gamma_1^{ik})^2,\quad \frac{d\gamma_2}{d\xi}=-\frac{1}{2}(\gamma_1)^2. \tag{A.2}$$

The increments γ_1 are at least twice the increment in γ_2 and these increments are negative. Therefore, the inequality $\gamma_2-2\gamma_1>0$ is preserved. The signs of the second and third terms of (A.1) are also preserved. Therefore, all the γ^{ik} ($i\neq k$) will be negative for all succeeding ξ.

The first of the Eqs. (6) is equal to the sum of Eqs. (A.1) with the factors $\exp(i\mathbf{q}\rho^{ik})$. Since all the terms of this sum are negative, the derivative of $\gamma_1(\mathbf{q})$ is maximum in absolute value at $\mathbf{q}=0$ and increases. Therefore, $\gamma_1(0)$ becomes less than zero at some ξ. We write down for $d\gamma_1(0)/d\xi$ the inequality

$$-\frac{3}{2}\gamma_1^2(0)\leqslant\frac{d\gamma_1(0)}{d\xi}\leqslant-\gamma_1^2(0)+\gamma_1(0)\gamma_2\leqslant-\frac{\gamma_1^2(0)}{2}. \tag{A.3}$$

Thus, $\gamma_1(0)$ has a pole singularity. In order to make clear the character of the singularity in the vicinity of $\mathbf{q}=0$, we differentiate (6) twice with respect to $\mathbf{q}$. At $\mathbf{q}=0$, we obtain

$$\frac{dA(0)}{d\xi}=-2A(0)\gamma_1(0)+A(0)\int_S\gamma_2(\mathbf{q})\frac{d^2q}{S}-\\-\int_S A(\mathbf{q})\gamma_2(\mathbf{q})\frac{d^2q}{S}, \tag{A.4}$$

where

$$A(\mathbf{q})=\frac{\partial^2\gamma_1(\mathbf{q})}{\partial\mathbf{q}^2}=-\sum_{i\neq k}(\rho_{ik})^2\gamma_1^{ik}e^{i\mathbf{q}\rho^{ik}},$$

Near the pole, we write the integral terms in (6) at $\mathbf{q}=0$ in the form $\gamma_1(0)\,(\Lambda_1-\Lambda_2)$. We denote the residues in Λ_1 and Λ_2 by δ_1 and δ_2. Here, $-\frac{1}{2}\leqslant(\delta_{1,2})\leqslant 0$. Then

$$\operatorname{Res}\gamma_1(0)=\frac{1}{1-\delta_1+\delta_2}$$

We write down for $A(0)$ an inequality similar to (A.3):

$$-2\gamma_1(0)+\delta_1\gamma_1(0)\leqslant\frac{1}{A(0)}\frac{dA(0)}{d\xi}\leqslant-\frac{5}{2}\gamma_1(0). \tag{A.5}$$

The residue on the left side of (A.4) is equal to

$$-\frac{2-\delta_1}{1-\delta_1+\delta_2}=-1-\frac{1-\delta_2}{1-\delta_1+\delta_2}<-1.$$

Therefore, the degree of the pole singularity in A(0) $=\partial^2\gamma_1(\mathbf{q})/\partial\mathbf{q}^2|_{\mathbf{q}=0}$ is higher than first, i.e., $\gamma_2(\mathbf{q})$ has the form $1/(\xi-\xi_0(\mathbf{q}))$ near the pole.

Thus, the sufficient conditions for the formation of a moving pole for $\gamma_1^{i\,i+1} < 0$ are the following (at $\xi = 0$): a) all $g_{1,2}^{ik} < 0$ $(i \neq k)$ or b) all $g^{i\,i+k} \ll (g/n!)(g_1^{i\,i+1}/g)^n$. This means that on the right sides of Eq. (9) we have left only terms with $\gamma_1^{i\,i+1}$ from (5) and at some ξ, all the γ_k^{ik} become less than zero.

If $\gamma_1^{i\,i+1} > 0$, then the moving pole is formed under the conditions: c) $g_1^{i\,i+2} < 0$, $g_1^{i\,i+3} > 0$, ... all $g_2^{ik} < 0$ or b). Here all the γ_1^{ik} will have alternating signs. Therefore the singularity appears at $q \neq 0$. For example, for a square lattice of chains, $\mathbf{q} = [\pi, \pi]$.

[1)] We shall also make use of the mixed representation. The momentum along the corresponding chain and its number are indicated here. On each chain, the electrons occupy in the one-dimensional reciprocal cell the region between $-p_F$ and $+p_F$. We then make use of the term "Fermi point."

[2)] In place of g^{ik}, γ^{ik}, we shall also use the notation $g^{i\,i+n}$, $\gamma^{i\,i+n}$, where n is the minimum number of transitions between nearest chains, which must be undergone in order to proceed from chain i to chain k. For the quantities g^{ii}, γ^{ii}, we shall use the notation g, γ.

[3)] The Fermi momenta are the same in both subsystems. The difference in the Fermi energies can be removed by renormalization of the constants. But the variables $\xi^{a,b} = \ln(\tilde{\omega}/\max\{T, \omega, v_F^{a,b}p\})$ are nevertheless all differently defined because of the difference between the Fermi velocities. Therefore, Eqs. (9) can be written down only at $\omega = 0$, $p = 0$ in the investigation of the temperature dependence of $\gamma(\xi)$.

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Energy spectrum of the donors in GaAs and Ge and its reaction to a magnetic field

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The spectrum of the submillimeter photoconductivity of *n*-GaAs and *n*-Ge in a magnetic field up to 60 kOe at helium temperatures was investigated. A large number of lines due to transitions between excited states of the donors have been investigated, and the measurement results were used to determine a number of levels of the energy spectrum in a wide range of magnetic fields. For GaAs, these data are compared with calculations of the energy spectrum of the hydrogen atom in magnetic fields up to $\sim 2 \times 10^9$ Oe. For the donors in Ge, the energy spectrum is investigated at different orientations of the magnetic field relative to the crystallographic axes (**H** ∥ [100], [111], [110]), and these results are also compared with the corresponding calculations.

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INTRODUCTION

The photoexcitation spectrum of shallow impurities in many superconductors lies in the submillimeter band and makes it possible to obtain information not only on the properties of the impurities, and particularly on its energy spectrum, but also on the semiconducting crystal itself. The results of submillimeter spectroscopy of semiconductors are of interest for atomic spectroscopy. By using as a model a shallow impurity in a semiconductor, it is possible to obtain in a number of cases experimental data which cannot be obtained by studying the atoms in free space. A sufficiently well-known example is the problem of the properties of atoms in very strong magnetic fields. Indeed, from the point of view of the influence on the impurity-atom spectrum, the effective magnetic field is equivalent to one that is larger by 4–6 orders of magnitude than in the case of atoms in free space. This is caused by the small characteristic energies and by the strong interaction of the shallow-impurity atoms with the external magnetic field, a fact explained by the low effective mass m^* of the electron (hole) and the large dielectric constant $\varkappa$ of the medium—the semiconducting crystal. The impurity-atom spectrum therefore turns out to be strongly shifted towards longer wavelengths.

We have investigated the energy spectrum of shallow impurities in Ge and GaAs and the effect exerted on it by a magnetic field H, using for this purpose a highly sensitive backward-wave-tube (BWT) submillimeter spectrometer of high resolution.[1] It is customary to use for such measurements long-wave infrared gratings and interference spectrometers. In particular, three groups have recently published papers[2,3] on the spectroscopy of residual shallow impurities in ultrapure Ge

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