Charge-density wave in a random potential

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Quasi-one-dimensional conductors have at low temperatures a gigantic dielectric susceptibility (superdielectrics) and produce on the x-ray patterns smeared-out spots at a momentum close to $2p_F$. This smearing attests to the absence of a long-range order in the charge-density wave. Both phenomena are attributed to the interaction of the charge-density wave with the impurities. A quantitative relation is established between the value of the dielectric susceptibility and the dimension of the spot on the x-ray pattern.

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1. INTRODUCTION

Quasi-one-dimensional semiconductors go over into a dielectric state at low temperatures. In this state, the electron density forms a three-dimensional lattice with a period equal to $1/2p_F$ along a preferred axis (charge-density wave, CDW). Two effects hinder the free motion of the CDW through a crystal: pinning by the crystal lattice and pinning by the impurity. The first effect is small if the period of the CDW and the period of the host lattice are almost noncommensurate.[1] In this case, which is realized in $K_2[Pt(CN)_4]Br_{0,3}\cdot 3H_2O$, (KCP), pinning by impurities is more significant. The pinning force depends on the impurity concentration and on the amplitude of the electron scattering by the impurities. This force determines the dielectric susceptibility and its frequency dependence. When the electron–impurity interaction is weak the static value of the dielectric susceptibility is large and dispersion sets in at relatively low frequencies. If the pinning by the impurity is stronger than by the crystal lattice, then the long-range order in the CDW vanishes. Consequently the δ-function singularity in the structure factor smears out near $2p_F$.[2–7] We shall establish below the relation between the width of the maximum of the structure function and the dielectric constant. Both quantities are determined by the amplitude of the electron scattering by the impurities and by the impurity concentration. The vanishing of long-range order in a periodic structure always occurs if the impurities are not coupled with this structure. This phenomenon was considered in[6] using as an example the destruction of the vortex lattice in type-II superconductors.

2. INTERACTION OF CHARGE DENSITY WAVE WITH IMPURITIES

In quasi-one-dimensional semiconductors the electrons move along individual filaments. The phonon spectrum can be three-dimensional in this case. The Hamiltonian that describes the interaction of the electrons with the phonons or impurities is of the form

$$H=H_0+H_1,$$

where

$$H_0=\sum_{\mathbf{p}}\omega(\mathbf{p})b_{\mathbf{p}}^{+}b_{\mathbf{p}}+\sum_{\mathbf{p}}\varepsilon(p)a_{\mathbf{p}}^{+}a_{\mathbf{p}}+\int\Delta(\mathbf{r})\psi^{+}(\mathbf{r})\psi(\mathbf{r})d^3\mathbf{r}, \tag{1}$$

$$H_1=\sum_i\int U(\mathbf{r}-\mathbf{r}_i)\psi^{+}(\mathbf{r})\psi(\mathbf{r})d^3\mathbf{r};\quad \Delta(\mathbf{r})=\sum_{\mathbf{p}}g\frac{1}{(2\omega(\mathbf{p}))^{1/2}}(b_{\mathbf{p}}^{+}+b_{\mathbf{p}})e^{i\mathbf{p}\mathbf{r}}. \tag{2}$$

Here

$$\psi(\mathbf{r})=\sum_{\mathbf{p}}a_{\mathbf{p}}e^{i\mathbf{p}\mathbf{r}},$$

$U(\mathbf{r})$ is the potential of the interaction of the electrons with the impurity, $\mathbf{r}_i$ are the impurity coordinates and are assumed to be randomly distributed, and the electron spectrum $\varepsilon(p)$ is assumed to be one-dimensional. Averaging over the states of the Hamiltonian (1) will be replaced by averaging over classical boson fields. As applied to quasi-one-dimensional systems, this method is described in[7,8]. Just as in these references, we make the substitution

$$\mathrm{Sp}\,e^{-H_0}\to\int e^{-F_0[\Delta]}D\Delta, \tag{3}$$

where the functional $F_0[\Delta]$ is equal to

$$F_0=-\ln\mathrm{Sp}\exp\Big\{\sum_{\mathbf{p}}\int_0^{1/T}d\tau\Big[\frac{\dot{\Delta}^2(\mathbf{p})}{2g^2}+\frac{\Delta^2(\mathbf{p})\omega^2(\mathbf{p})}{2g^2}\Big]+\int\Delta(\mathbf{r})\psi^{+}(\mathbf{r})\psi(\mathbf{r})d^3\mathbf{r}+\sum_{\mathbf{p}}\varepsilon(p)a_{\mathbf{p}}^{+}a_{\mathbf{p}}\Big\}. \tag{4}$$

The functional $F_0[\Delta]$ has a minimum at

$$\Delta(\mathbf{r})=\Delta_0\sin(\mathbf{Q}\mathbf{r}+\varphi), \tag{5}$$

where $Q_{\parallel}=2p_F$ and $Q_{\perp}$ is determined by the type of interaction between electrons of different filaments. In the self-consistent field approximation, $\Delta(r)$ is determined from the relation

$$\Delta(\mathbf{r})=[\langle\psi^{+}(\mathbf{r})\psi(\mathbf{r})\rangle_0-N]g^2/\omega^2(\mathbf{Q}), \tag{5a}$$

where $\langle\ \rangle_0$ is averaging with the Hamiltonian H_0, and N is the electron density. It follows from relation (5a) that

$$1=\frac{g^2}{\pi v\omega^2(\mathbf{Q})}\ln\frac{\varepsilon_F}{\Delta_0}, \tag{6}$$

v is the velocity on the Fermi surface.

We shall henceforth be interested in fluctuations of the phase φ, which vary slowly in space and in time. Expanding the functional near its minimum in terms of the slow changes of φ, we obtain

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$$F_0[\varphi]=\frac{1}{2}\int\Big[-\frac{Nm^*}{(2p_F)^2}\dot{\varphi}^2+C_\parallel\Big(\frac{\partial\varphi}{\partial z}\Big)^2+C_\perp\Big(\Big(\frac{\partial\varphi}{\partial x}\Big)^2+\Big(\frac{\partial\varphi}{\partial y}\Big)^2\Big)\Big]d^3\mathbf{r}\,dt. \quad (7)$$

The effective mass m^* in (7) is given by

$$m^*=m(1+\pi v\Delta_0^2/2g^2). \quad (8)$$

The elastic modulus $C_\parallel$ is equal to

$$C_\parallel=v/2\pi d^2, \quad (9)$$

d is the distance between the conducting filaments. The constant $C_\perp$ is expressed in terms of the phonon spectrum

$$C_\perp=\frac{\pi}{2g^2d^2}\Big(\frac{\partial^2\omega^2(\mathbf{k})}{\partial^2k_\perp}\Big)_{\mathbf{k}=\mathbf{Q}}\Delta_0^2. \quad (10)$$

In the low-temperature phase the thermal and quantum fluctuations do not influence the qualitative pictures and will not be taken into account here. To estimate them we calculate $\langle\varphi^2\rangle$ with the aid of the functional

$$\langle\varphi^2\rangle\sim\frac{g^2d^2}{v}\Big(\frac{\partial^2\omega^2(\mathbf{Q})}{\partial k_\perp^2}\Big)^{-1}_{k=Q}\sqrt{\frac{m}{m^*}}. \quad (11)$$

If the three-dimensionality effects are large enough, or if the adiabaticity condition $m^*\gg m$ is satisfied, then these fluctuations are quantitatively small.[8,9] What are substantial are the phase fluctuations due to the impurities. We consider below a case when the interaction with the impurities is weak enough, so that the mean free path is much larger than the particle–hole pair dimension. It is then possible to neglect their influence on the amplitude Δ_0. The influence on the phase is described by the Hamiltonian H_1. Near the extremum of F_0 the Hamiltonian H_1 must be replaced by the functional F_i:

$$F_i=\frac{\omega^2(\mathbf{Q})\Delta_0U(\mathbf{Q})}{g^2}\sum_i\sin(\mathbf{Qr}_i+\varphi(\mathbf{r}_i))=\int f(\mathbf{r})\sin(\mathbf{Qr}+\varphi(\mathbf{r}))\,d^3\mathbf{r}. \quad (12)$$

If the impurities have a random distribution and the interaction with them is weak, the random fields have a Gaussian distribution with a correlator

$$\langle f(\mathbf{r})f(\mathbf{r}')\rangle=\gamma\delta(\mathbf{r}-\mathbf{r}'), \quad (13)$$

$$\gamma=n(\omega^2(\mathbf{Q})\Delta_0U(\mathbf{Q})/g^2)^2. \quad (13a)$$

In formula (13a), n is the impurity concentration. The equation for the phase is determined by the condition that the functional F_0+F_1 be a minimum. In the absence of external field this equation takes the form

$$C_\perp\frac{\partial^2\varphi}{\partial r_x^2}+C_\perp\frac{\partial^2\varphi}{\partial r_y^2}+C_\parallel\frac{\partial^2\varphi}{\partial r_\parallel^2}=f(\mathbf{r})\cos(\mathbf{Qr}+\varphi(\mathbf{r})). \quad (14)$$

3. DESTRUCTION OF LONG RANGE ORDER

The existence of a long-range order is determined by the behavior of the phonon Green's function G at zero frequency

$$G=\langle b^+(0)b(\mathbf{R})\rangle. \quad (15)$$

At large distances, the main contribution to the form of the function G is made by the phase fluctuations:

$$G(\mathbf{R})=\frac{\omega(\mathbf{Q})\Delta_0^2}{g^2}\Pi(\mathbf{R})\cos\mathbf{QR}, \quad (16)$$

where

$$\Pi(\mathbf{R})=\langle e^{i(\varphi(\mathbf{R})-\varphi(0))}\rangle. \quad (17)$$

The thermal and quantum fluctuations in the low-temperature state lead to an insignificant decrease of $\Pi(\mathbf{R})$. If $\Pi(\mathbf{R})$ tends to a constant value at large $\mathbf{R}$, then long-range order exists in the system and the amplitude of the neutron or x-ray elastic scattering should have a δ-function singularity at a momentum equal to $\mathbf{Q}$. Let us verify that the impurities lead to an exponential or power-law decrease of $\Pi(\mathbf{R})$.

To calculate the correlator $\Pi(\mathbf{R})$ (17) it is necessary to solve Eq. (14) at an arbitrary $f(\mathbf{R})$, substitute the solution in (17), and then average by using (13). We choose as the zeroth approximation the solution of (14) in an approximation linear in $f(r)$

$$\varphi^{(0)}(\mathbf{r})=\int G(\mathbf{r}-\mathbf{r}_1)f(\mathbf{r}_1)\cos\mathbf{Qr}_1\,d^3\mathbf{r}_1, \quad (18)$$

where the function $G(\mathbf{r})$ satisfies the equation

$$C_\parallel\frac{\partial^2G}{\partial r_\parallel^2}+C_\perp\Big(\frac{\partial^2G}{\partial r_x^2}+\frac{\partial^2G}{\partial r_y^2}\Big)=\delta(\mathbf{r}). \quad (19)$$

The Fourier component $G(\mathbf{k})$ of this function is

$$G(\mathbf{k})=1/(C_\parallel k_\parallel^2+C_\perp k_\perp^2). \quad (20)$$

Substituting (18) in (17), we obtain $\Pi(\mathbf{R})$ at large distances:

$$\Pi(\mathbf{R})=\exp\Big\{-\frac{\langle(\varphi(\mathbf{R})-\varphi(0))^2\rangle}{2}\Big\}=\exp\Big\{-\frac{\gamma}{8\pi C_\parallel^{1/2}C_\perp}\Big(\frac{R_\parallel^2}{C_\parallel}+\frac{R_\perp^2}{C_\perp}\Big)^{1/2}\Big\}. \quad (21)$$

In the derivation of (21) and everywhere else below it was assumed that the impurities are weak enough

$$8\pi C_\parallel^{1/2}C_\perp\gamma^{-1}\gg\max\{v\Delta_0^{-1}C_\parallel^{-1/2},dC_\perp^{-1/2}\}.$$

Formula (21) shows that arbitrarily weak impurities destroy the long-range order. In exactly the same manner it is possible to calculate the average order parameter $\langle\Delta\cos\mathbf{Q}\cdot\mathbf{R}\rangle$:

$$2\langle\Delta\cos\mathbf{QR}\rangle=\Delta_0\langle e^{i\varphi}\rangle=\Delta_0\exp(-\langle\varphi^2\rangle/2)=0. \quad (22)$$

It follows from all the foregoing that even weak inhomogeneities disrupt the phase transition.

Formulas analogous to (21) and (22) were obtained in [6] in the course of the solution of the problem of a vortex lattice in a random potential in a superconductor. For the CDW they have been written out in[3,4], where account was taken of only the zeroth approximation for φ [Eq. (18)]. It could be verified, however, that each of the succeeding terms of the expansion obtained by solving Eq. (14) by iteration, is not small and generally speaking the zeroth approximation is insufficient. None the less, in the calculation of mean values such as (21) and (22), the contribution of the sum of all the expansion terms higher than the zeroth is exactly equal to zero, and formulas (21) and (22) remain valid.

To prove this statement and to calculate eventually the dynamic characteristics, it is convenient to use the diagram technique developed in[10]. To this end, we expand the right hand of (14) in powers of φ and solve the resultant equation by iteration. The simplest diagram corresponding to $\varphi^{(0)}(\mathbf{r})$ is shown in Fig. 1a. The solid

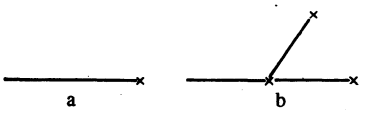

FIG. 1.

line corresponds to the Green's functions $G(\mathbf{r}-\mathbf{r}_1)$ and the cross to the random field $f(\mathbf{r}_1)\cos\mathbf{Q}\cdot\mathbf{r}$. The integration is with respect to the coordinate of the cross. A more complicated diagram is shown in Fig. 1b. A diagram of arbitrary order constitutes a "tree." Each line is set in correspondence to a Green's function $G(\mathbf{r}_i-\mathbf{r}_j)$, and the vertices correspond to

$$f(\mathbf{r}_i)\frac{1}{m_i!}\frac{d^{m_i}}{d\mathbf{r}_i^{m_i}}\cos\mathbf{Q}\mathbf{r}_i.$$

Any number of lines can converge in each vertix. The only line that leads from some cross in the point i to the "base of the tree," is defined as incoming into point i, and the remaining lines are outgoing. Then m_i is equal to the number of lines that go out of the point i (to the order of the i-th vertex). Integration is carried out over the coordinates of all the points with crosses.

For example, the diagram of Fig. 1b corresponds to the expression

$$-\frac{1}{2!}\int G(\mathbf{r}-\mathbf{r}_2)G(\mathbf{r}_2-\mathbf{r}_3)G(\mathbf{r}_2-\mathbf{r}_1)f(\mathbf{r}_1)$$
$$\times\cos\mathbf{Q}\mathbf{r}_1 f(\mathbf{r}_2)\cos\mathbf{Q}\mathbf{r}_2 f(\mathbf{r}_3)\cos\mathbf{Q}\mathbf{r}_3\, d^3\mathbf{r}_1\, d^3\mathbf{r}_2\, d^3\mathbf{r}_3. \qquad (23)$$

To calculate the correlator Π (17) we expand the exponential in powers of φ. The general term of this series $\langle\varphi(\mathbf{R}_1)\ldots\varphi(\mathbf{R}_N)\rangle$ comprises N trees. We denote the correlator $\langle f(\mathbf{r})f(\mathbf{r}')\rangle=\gamma\delta(\mathbf{r}-\mathbf{r}')$ by a dashed line. Then, after averaging all the vertices, crosses turn out to be connected with the vertices by dashed lines. Diagrams in which connections of even-order vertices with odd-order vertices are encountered contain in the integrand rapidly oscillating factors $e^{i\mathbf{Q}\cdot\mathbf{r}}$, and are therefore small.

We consider now any two vertices of like parity joined by a dashed line. The junctions can be of two types: 1) Connection between two vertices such that it is possible to go from each vertex along solid lines to the base of the tree without crossing another vertex. 2) The connection between two vertices is such that it is impossible to go from either vertex to the base without crossing at the same time the other vertex. We note that if the joined vertices pertain to different trees, then the connection must be of the first type. Examples of connections of the first and second type are shown in Figs. 2a, b, c, and 2d, e, respectively.

Let the connection between the j-th and i-th vertices be of the first type and let the sum of the orders of the connected vertices be $2N\geq 2$. Cutting off a line outgoing, say, from the i-th vertices and attaching it to the j-th one, we obtain a diagram that corresponds to exactly the same integral, but with a different coefficient. It is easy to see that there are $2N+1$ such diagrams. The sum of the coefficients S_{ij} is then

$$S_{ij}=\left\langle\int\sum_{m=0}^{2N}\frac{d^m\cos\mathbf{Q}\mathbf{r}_i}{d\mathbf{r}_i^m}\frac{d^{2N-m}\cos\mathbf{Q}\mathbf{r}_j}{d\mathbf{r}_j^{2N-m}}\frac{1}{m!}\frac{1}{(2N-m)!}f(\mathbf{r}_i)f(\mathbf{r}_j)\,d^3\mathbf{r}_i\,d^3\mathbf{r}_j\right\rangle. \qquad (24)$$

Averaging and using the Leibnitz formula, we verify that the quantity under the integral sign is the derivative of a periodic function, and S_{ij} is equal to zero at $N\geq 1$.

In Fig. 2, the diagrams a, b, and c are cancelled out (connection of the first kind). It is easy to verify that if the connection is of the second type, then the sum of diagrams obtained by cutting off the outgoing lines of one vertex and attaching them to the other is equal to zero. The difference from the first case lies only in the fact that it is impossible to cut off the branch on which the second vertex is situated. The diagrams cancelled out in Fig. 2 are now d and e (connection of the second type).

Thus, the only diagrams left are those corresponding to the use of the zeroth approximation (18) for φ, and this confirms the validity of formulas (21) and (22).

The cancellations described above take place if the correlation of the potential at different points is a δ function. Allowance for a small smearing leads to a small renormalization of the coefficients C and γ in formulas (21) and (22).

It was assumed above that the period of the CDW is not commensurate with the period of the host lattice. If they are commensurate, then an additional term appears in Eq. (14)[11]

$$-\beta\sin M\varphi, \qquad (25)$$

where $\beta\sim(\Delta_0/\varepsilon_F)^M$ and M is the order of the commensurability. To destroy the long-range order in this case it is necessary that the concentration of the impurities be higher than critical. In order of magnitude, the critical value in formulas (13) and (13a) is equal to

$$\gamma_c\sim\sqrt{C_\parallel C_\perp}\sqrt{\beta M}. \qquad (26)$$

To verify this, we calculate the correlator $\langle\varphi_k\varphi_{-k}\rangle$ in two limiting cases. If $\gamma\ll\gamma_c$, only small φ are significant in (25), and the sine function can be replaced by a linear term. Then

$$\langle\varphi^2\rangle=\gamma\int\frac{d^3\mathbf{k}}{[C_\parallel k_\parallel^2+C_\perp k_\perp^2+\beta M]^2}=\frac{\gamma}{8\pi C_\perp(\beta M C_\parallel)^{1/2}}\ll 1. \qquad (27)$$

As seen from (22), in this limit the impurity have little effect on the long-range order. If $\gamma\gg\gamma_c$, then the term (25) can be taken into account as a perturbation. Calculating $\langle\varphi_k\varphi_{-k}\rangle$ accurate to terms of second order in β, we get

$$\langle\varphi_k\varphi_{-k}\rangle=\frac{\gamma}{(C_\parallel k_\parallel^2+C_\perp k_\perp^2)^2}\left(1+\left(\frac{8\pi C_\perp(C_\parallel\beta M)^{1/2}}{\gamma}\right)^4\right). \qquad (28)$$

Thus, at $\gamma\gg\gamma_c$ the commensurability effects lead only to an inessential change of the correlation radius in formula (21).

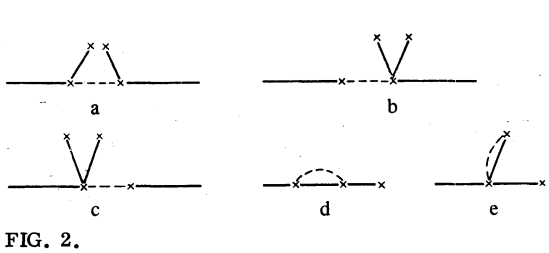

FIG. 2.

The results obtained above pertained to compounds in which no large Coulomb forces arise in the case of slow phase fluctuations. For example, in TTF-TCNQ there exists an electron and hole CDW. Therefore no space charge is produced in the case of slow fluctuations. The short-range part of the Coulomb interaction leads only to a change of the coefficients $C_{\parallel}$ and $C_{\perp}$. In compounds of the KCP type only one chain of the platinum atoms is conducting. In this case the spatial variations of the phase φ denote a change in the charge density ρ.[11]

$$e\partial\varphi/\partial r_{\parallel}=\pi\rho(r)\,d^2. \tag{29}$$

The Coulomb interaction leads to the appearance in the functional of an additional term F_c:

$$F_c[\varphi]=\frac{1}{2}\sum_{k}\frac{4e^2k_{\parallel}^2|\varphi_k|^2}{(\varepsilon_{\parallel}k_{\parallel}^2+\varepsilon_{\perp}k_{\perp}^2)\pi d^4}. \tag{30}$$

In formula (30) $\varepsilon_{\parallel}$ and $\varepsilon_{\perp}$ are the dielectric constants along and across the filaments at high frequencies. The Green's function $G(\mathbf{k})$ then takes the form

$$G_0^{-1}(\mathbf{k})=C_{\parallel}k_{\parallel}^2+C_{\perp}k_{\perp}^2+\frac{4e^2}{\pi d^4}\frac{k_{\parallel}^2}{\varepsilon_{\parallel}k_{\parallel}^2+\varepsilon_{\perp}k_{\perp}^2}. \tag{31}$$

The last term, which describes the Coulomb interaction, has a singularity if the angle between the vector $\mathbf{k}$ and the z axis is small. Just as in the theory of phase transitions,[12] the problem becomes formally four-dimensional and $\langle\varphi^2\rangle$ diverges logarithmically at small k. Therefore $\Pi(R)$ decreases in power-law fashion in the case of large R. The corresponding calculations and a comparison with experiment are presented for KCP in[5] and yield

$$\Pi(R_{\parallel})=(R_{\parallel}^2C_{\perp}^2/C_{\parallel}^2\varepsilon_{\perp}e^2)^{-\alpha/2}, \tag{32}$$

where

$$\alpha=\frac{\gamma\varepsilon_{\perp}^{1/2}d^2}{32C_{\perp}^{1/2}(4\pi e^2)^{1/2}}; \tag{32a}$$

with $\alpha\approx 0.055$ in KCP.

4. DIELECTRIC CONSTANT

Most quasi-one-dimensional compounds have at low temperatures a large dielectric constant. There are several explanations for this phenomenon. In compounds of the KCP type, an electron CDW is produced with a period that is not commensurate with the period of the host lattice. The motion of this wave makes the main contribution to the dielectric constant. Without allowance for the interaction with the impurities, the static dielectric constant would be infinite. The weak interaction with the impurities makes the dielectric constant finite but large.

It follows from (29) that the interaction with the external electric field E leads to an additional term F_E in the free-energy functional

$$F_E[\varphi]=-\int\frac{e\varphi(t)E(t)}{\pi d^2}d^3\mathbf{r}\,dt. \tag{33}$$

It is assumed in (33) that the field $\mathbf{E}(t)$ is directed along the filaments. Minimizing the functional $F=F_0+F_c+F_i+F_E$ (formulas (7), (12), (30), and (33)), we obtain an equation for:

$$G_0^{-1}\varphi_k(t)+\int f(\mathbf{r})\cos(\mathbf{Qr}+\varphi)e^{i\mathbf{kr}}d^3\mathbf{r}=\frac{e}{\pi d^2}E_k(t), \tag{34}$$

where

$$G_0^{-1}=\frac{Nm^*}{(2p_F)^2}\frac{\partial^2}{\partial t^2}+C_{\parallel}k_{\parallel}^2+C_{\perp}k_{\perp}^2+\frac{4e^2k_{\parallel}^2}{(\varepsilon_{\parallel}k_{\parallel}^2+\varepsilon_{\perp}k_{\perp}^2)\pi d^4}. \tag{35}$$

Expanding the sine in (34) and solving this equation by iterations, we can obtain φ in the form of a series in f and E. In the approximation linear in the electric field we obtain for φ an expression in the form of a series in f, each term of which is represented graphically by a tree (see Fig. 1b). The difference from the static case lies in the fact that in one of the zeroth-order vertices $f(\mathbf{r})\cos\mathbf{Q}\cdot\mathbf{r}$ is replaced by $Ee/\pi d^2$. In addition, the frequency ω of the external field passes along the trunk joining this vertex with the base of the tree. All the segments of this trunk represent the Green's function $G(\omega)$, while the segments of the branches, just as in the static case, represent the Green's function $G(0)$. Averaging over the impurities means, as before, the interconnection of all the crosses in all possible manners. Unlike the static case, however, there is no complete cancellation of the diagrams, since different parts of the diagrams contain different Green's functions $G(\omega)$ and $G(0)$. For example, the self-energy part Σ is represented in first orders by the diagrams 3a and 3b, and is equal to

$$\Sigma_1=\gamma\int\frac{d^3\mathbf{k}}{(2\pi)^3}[G(\omega)-G(0)]. \tag{36}$$

We consider first the case of a weak Coulomb interaction, when the parameter α is large and the last term in (35) can be disregarded. We shall substitute henceforth in the skeleton diagrams the exact Green's functions, $G^{-1}=\tilde{G}_0^{-1}-\Sigma$. The Green's functions represented by the "stubs," as in Fig. 3a, are not renormalized, just as in the static case. In second order in γ, the self-energy part Σ_2 is represented by the diagrams 3c and 3d, and is equal to

$$\Sigma_2(\mathbf{k})=\gamma^2\int G(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k})[G(\mathbf{k}_1)G(\mathbf{k}_2)-G_0(\mathbf{k}_1)G_0(\mathbf{k}_2)]\frac{d^3\mathbf{k}_1\,d^3\mathbf{k}_2}{(2\pi)^6}, \tag{37}$$

where G_0 is the static Green's function (20). In third order in γ, the self-energy part of Σ_3 is equal to

$$\begin{aligned}\Sigma_3(\mathbf{k})=2\gamma^3\int G(\mathbf{k}_1+\mathbf{k}_2)[&2G(\mathbf{k}_1+\mathbf{k})G(\mathbf{k}_2)G(\mathbf{k}_3)G(\mathbf{k}_1+\mathbf{k}_3)\\&-G(\mathbf{k}_1+\mathbf{k})G(\mathbf{k}_2)G_0(\mathbf{k}_3)G_0(\mathbf{k}_1+\mathbf{k}_3)\\&-G_0(\mathbf{k}_1+\mathbf{k})G_0(\mathbf{k}_2)G_0(\mathbf{k}_3)G(\mathbf{k}_1+\mathbf{k}_3)]\frac{d^3\mathbf{k}_1\,d^3\mathbf{k}_2\,d^3\mathbf{k}_3}{(2\pi)^9}.\end{aligned} \tag{38}$$

Putting

$$-\frac{Nm^*}{(2p_F)^2}\omega^2-\Sigma(0)=\varkappa,$$

we obtain for $\varkappa$ the algebraic equation

$$\varkappa+\frac{\omega^2Nm_*}{(2p_F)^2}=\tilde{\gamma}\sqrt{\varkappa}+1.1\tilde{\gamma}^2+\frac{2.3\tilde{\gamma}^3}{\sqrt{\varkappa}}+\ldots, \tag{39}$$

where $\tilde{\gamma}=\gamma/4\pi C_{\perp}\sqrt{C_{\parallel}}$.

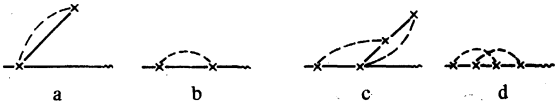

FIG. 3.

Equation (39) yields $\varkappa$ and consequently also the dielectric constant ε as a function of the frequency

$$\varepsilon-1=\frac{4e^2}{\pi\varkappa d^4}=\frac{4e^2f(x)}{\pi d^4\bar\gamma^2},\quad x=\frac{(Nm^*)^{1/3}}{2p_F}\frac{\omega}{\bar\gamma^2}. \tag{40}$$

Equation (39) enables us to find ε at high frequencies. For $x\gg1$ we have

$$f(x)=-\frac{1}{x^2}-\frac{i}{x^3}+\frac{1.1}{x^4}. \tag{41}$$

At small x we can hope to attain numerical accuracy by including a sufficiently large number of the terms of the series in the right-hand side of (39). If we retain one, two, or three terms of the series, we obtain the following sequence of values of $f_i(0)$:

$$f_1=1;\quad f_2=0.36;\quad f_3=0.23. \tag{42}$$

Thus, in the case of weak interaction of the electrons with the impurities, the static dielectric constant is large but finite. The statement that ε is finite follows from the fact that Eq. (39) has at $\omega=0$ a solution at finite $\varkappa$. The solution is valid, in any case, not only if the first three calculated terms of the series are positive, but also all the remaining terms. If the series is of alternating sign, then one cannot exclude the possibility, as in the theory of phase transition, that ε can increase in power-law fashion at low frequencies. We regard as more reasonable the first possibility, which is analogous to that existing in the theory of the Kondo effect, when ε is finite at low frequencies and can be expanded in powers of ω^2. If we use Eq. (39), then we obtain for $f(x)$ at small x

$$f(x)=0.23+0.15x^2. \tag{43}$$

In the considered case of weak Coulomb interaction, the frequency dependence of $\varepsilon(\omega)$ has two regions, $x\gg1$ and $x\ll1$.

If the Coulomb interaction is strong enough, so that the parameter α (32a) is small, then there exists an intermediate frequency region where the effective number of conducting electrons depends logarithmically on the frequency. In the region of high frequencies $\omega\gg\tilde\omega$, the expansion (41) is valid. The value of $\tilde\omega$ is determined from the condition that the first and fourth terms of (35) be equal

$$\tilde\omega^2\sim\frac{p_F^2C_\perp e^2}{Nm^*C_\parallel\varepsilon_\perp d^4}. \tag{44}$$

We assume for simplicity that the equality $C_\parallel/C_\perp\gg\varepsilon_\parallel/\varepsilon_\perp$ is satisfied. As shown in[3], this case conforms to the experimental situation. In the region $\omega\ll\tilde\omega$, the expansion in γ leads to logarithmic integrals. To sum the higher-order logarithms, we use the renormalization group method or the "parquet" equations. The second-order diagrams for the effective vertex Γ are shown in Fig. 4. The corresponding "parquet" equation is

$$\Gamma=\gamma+\int GG\Gamma^2\frac{d^3k}{(2\pi)^3}. \tag{45}$$

Solving this equation with logarithmic accuracy, we obtain for the dimensionless effective interaction $\tilde\Gamma=\alpha\Gamma/\gamma$:

$$\Gamma=\frac{\alpha}{1-3\alpha\ln(-\tilde\omega^2/\omega^2)}=\frac{1}{3\ln(-\omega^2/\omega_T^2)},\quad \omega_T^2=\tilde\omega^2e^{-1/3\alpha}. \tag{46}$$

Expression (46) is valid at high frequencies $\omega\gg\omega_T$, where $\tilde\Gamma\ll1$. In this region $G(\omega)$ can be obtained from the formula

$$\frac{\partial G^{-1}(\omega)}{\partial\omega^2}=\mathcal{T}(\omega). \tag{47}$$

$\mathcal{T}(\omega)$ in (47) satisfies the equation

$$\mathcal{T}=\frac{Nm^*}{(2p_F)^2}+\int\mathcal{T}\Gamma GG\frac{d^3k}{(2\pi)^3}. \tag{48}$$

Solving (48) and substituting $\mathcal{T}(\omega)$ in (47), we obtain an expression for $\varepsilon(\omega)$:

$$\varepsilon(\omega)-1=\frac{4\pi e^2N}{m^*\omega^2}\left(3\alpha\ln\frac{\omega^2}{\omega_T^2}-3i\alpha\pi\right). \tag{49}$$

Formula (49) is valid at sufficiently high frequencies $\omega\gg\omega_T$, when $\tilde\Gamma\ll1$. We assume, just as in the theory of the Kondo effect, that $\varepsilon(\omega)$ assumes a constant value at low frequencies. The value of $\varepsilon(0)$ can be obtained with exponential accuracy by substituting in (49) the value of ω at which $\tilde\Gamma$ is of the order of unity

$$\varepsilon(0)\sim\frac{4\pi e^2N}{m^*\tilde\omega^2}e^{1/\alpha}. \tag{50}$$

To find in (50) the dependence of the pre-exponential factor on α, it is necessary to write down the equation of the renormalization group accurate to the next term:

$$\frac{d\Gamma}{d\xi}=3\Gamma^2+12\Gamma^3,\quad \xi=\ln\frac{em^*\tilde\omega^2}{4\pi e^2N}. \tag{51}$$

The static value of the dielectric constant $\varepsilon(0)$ corresponds, apart from a numerical factor, to a value of the parameter ξ such that $\tilde\Gamma$ becomes of the order of unity. Solving (51), we get

$$\frac{1}{3\Gamma}-\frac{4}{3}\ln\left(4+\frac{1}{\Gamma}\right)=-\xi+\frac{1}{3\alpha}-\frac{4}{3}\ln\left(4+\frac{1}{\alpha}\right), \tag{52}$$

from which we obtain the value of $\varepsilon(0)$:

$$\varepsilon(0)=B\frac{\varepsilon_\perp C_\parallel}{C_\perp}\alpha^{4/3}e^{1/\alpha}, \tag{53}$$

where B is a number on the order of unity.

It was assumed that $\varepsilon_\perp C_\parallel\gg C_\perp\varepsilon_\parallel(\infty)$. In the opposite limiting case formula (53) contains $\varepsilon_\parallel(\infty)$ in place of $\varepsilon_\perp C_\parallel/C_\perp$.

5. CONCLUSION

Bergman, Price, and Lee[5] estimated the parameter α from the dimension of the spot on the x-ray diffraction pattern ($\alpha\approx0.055$). They also obtained the estimates $C_\parallel\approx1.5\times10^{-2}$ eV/Å, $C_\perp\approx10^{-5}$ eV/Å, $\varepsilon_\perp\approx3$, and $\varepsilon_\parallel(\infty)\approx340$. Substituting these quantities in (53), we get

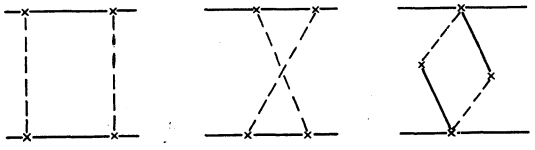

FIG. 4.

$\varepsilon \simeq 10^4$. The experimental value is $\varepsilon = 1200$.[13] Recognizing that formula (53) was obtained accurate to a numerical factor and that the parameters that enter in it are not very accurately known, the agreement between theory and experiment can be regarded as satisfactory.

Lee, Rice, and Anderson[1] have discussed other effects to lead to a large dielectric constant. One of these effects is connected with the relatively small gap in the electronic spectrum and yields for ε of KCP a value 340, which is less than the observed $\varepsilon = 1200$. The second effect is connected with the CDW motion. It was assumed in[1] that the finite ε is due to the pinning of the wave by the host lattice as a result of commensurability effects. It is difficult to estimate the magnitude of these effects. It appears that in KCP the pinning by the host lattice is weaker than the pinning by impurities, which was considered above, for otherwise the long-range order would not vanish.

It is possible to distinguish between the two pinning mechanism by means of the frequency dependence of ε. The qualitative behavior is the same in both cases: a resonant maximum should appear in the far infrared at frequencies $\omega^2 = 4\pi Ne^2/m^*\varepsilon(0)$, and at higher frequencies $\varepsilon(\omega)$ is negative and decreases quadratically with frequency. At low temperatures, however, in the case of pinning by the lattice, the imaginary part is small at all frequencies, and the resonance is narrow. In the case of pinning by impurities, the resonant maximum is broad. The behavior of the function $\varepsilon(\omega)$ is qualitatively the same in the case of weak and strong Coulomb interaction, and is described by Eq. (39) at sufficiently low frequencies, when the activation conduction can be neglected. It follows from this equation that at low frequencies $\omega \ll \omega_T$ the quantity $\varepsilon(\omega)$ is real and increases with frequency like $\varepsilon(\omega) = \varepsilon(0)(1 + c\omega^2/\omega_T^2)$, and an imaginary part of ε appears at $\omega \sim \omega_T$; in the resonance region, the imaginary and real components of ε are of the same order. At $\omega \gg \omega_T$ the imaginary part of $\varepsilon(\omega)$ is smaller than the real part, and their ratio decreases with increasing frequency in power-law fashion in the case of a weak Coulomb interaction (formulas (40) and (41)) or logarithmically in the case of a strong Coulomb interaction (formula (49)).

A maximum of the dielectric constant $\varepsilon(\omega)$ at frequencies $\omega \sim 0.002$–0.003 eV was observed in experiment.[14] The real and imaginary parts were of the same order, thus also indicating that the pinning by the impurities is stronger.

In compounds of the TTF–TCNQ type below the transition point there are two charge-density waves, electron hole. These waves are coupled with each other and do not transport any charge. The Coulomb effects are also inessential here. It is possible to apply to these substances the results of Sec. 3 for static correlators in the case of a weak Coulomb interaction: the correlation function should decrease exponentially at large distances. The greater part of the dielectric constant of these compounds is evidently due not to pinning by impurities, but to the weak interaction of the CDW of opposite signs.

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