Dynamics of one-dimensional electron-phonon systems at low temperatures

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The dynamical properties of the one-dimensional and quasi-one-dimensional Frölich model are investigated in the region $T_c < T \ll T_{c0}$, where T_c is the true temperature of the Peierls transition and T_{c0} is the transition temperature in the self-consistent field approximation. The dielectric permittivity, conductivity, density of electron states and dynamic structure factor are found.

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1. INTRODUCTION

1. It is well known that the interaction of electrons and phonons in quasi-one-dimensional (with respect to the electrons) conductors leads to a Peierls structural transition, i.e., to the appearance of a lattice deformation with period equal to or close to $2\pi/2p_F$ (cf. e.g., [1]). In the case when the important vibrational modes are also quasi-one-dimensional, the phase-transition temperature T_c lies substantially below the temperature T_{c0} determined by self-consistent field theory. Then in the region $T_c < T \ll T_{c0}$ one should observe the onset of short-range order, manifested in an increase in the range R_c of correlation of displacements of the lattice. In this case, according to a previous paper[2] by the authors, two situations are possible. The first of them occurs when the diameter $2p_F$ of the Fermi surface is close to half the length of the Brillouin reciprocal cell: $|2p_F - \pi/a| < T_{c0}/v_F$, where a is the period of the chain. In this case the correlation function has a maximum at wave vector $q_m = \pi/a$, and the correlation length increases exponentially with lowering of the temperature. The second situation occurs when the quantity $2p_F$ has a higher degree of commensurability with the period of the reciprocal lattice. In this case, in a broad temperature region the correlation length has a power-law increase: $R_c \sim v_F/T$, and the displacement correlation function is a maximum at $q_m = 2p_F$. However, on further lowering of the temperature umklapp processes begin to play a role. In this case R_c increases exponentially and q_m shifts to a point commensurable with $2\pi/a$. For example, at

$$|2p_F - \pi/2a| < (T_{c0}^2/v_F\varepsilon_F)\ln(\varepsilon_F/T_{c0})$$

commensurability begins to play a role when $T < (T_{c0}^2/\varepsilon_F)\ln(\varepsilon_F/T_{c0})$. In the cases when R_c is exponential the fluctuations of the lattice displacements can be assumed to be classical. For a power-law increase of R_c, however, there appears, as will be shown below, a new temperature scale $T_k \approx \omega_0[\ln(\varepsilon_F)T_{c0})]^{-1/2}$, where $\omega_0 \approx \omega_D$ is the unrenormalized frequency of phonons with momentum $q = 2p_F$. The calculation of the true transition temperature T_c can be carried out in analogy with the papers of Efetov and Larkin.[3]

2. In the present paper we shall investigate the dynamical properties of a one-dimensional system in the most interesting region, where R_c increases by a power law. We shall assume that the electron band is wide and the interaction with phonons at $T \gg T_{c0}$ is weak and $|\ln(\omega_D/T_{c0})| \lesssim 1$ (this condition implies the absence of instability with respect to a superconducting transition), and that the number of electrons per unit cell is not close to unity. The conditions listed are fulfilled in crystals of KCP compounds.[4]

We shall obtain expressions for the dynamic structure factor, permittivity, conductivity and density of electron states. These quantities have been investigated theoretically by different authors, both in the static[5,6] and in the dynamical[7,8] approximation with respect to the lattice displacements. In effect, however, these results were obtained in second order of perturbation theory in T_{c0}/ε and, consequently, are applicable only in the rather uninteresting region of electron energies $\varepsilon \gg T_{c0}$. Moreover,[7,8] a Rayleigh shape was postulated for the peak of the structure factor, and this is incorrect for quasi-one-dimensional systems for $T_c < T < T_{c0}$, as can be seen, e.g., from a comparison with the results of Efetov and Larkin.[3]

2. DESCRIPTION OF THE METHOD

1. The Hamiltonian of the system under consideration can be written in the form

$$\mathcal{H} = \int dx\, \bar\psi^+(x)\left[-iv\frac{\partial}{\partial x}\sigma_z - g\varphi(x)\sigma_+ - g\varphi^*(x)\sigma_-\right]\bar\psi(x) + \sum_q \omega(q)\, b_q^+ b_q; \qquad (1)$$

$$\bar\psi(x) = \begin{pmatrix}\psi_+(x)\\ \psi_-(x)\end{pmatrix}, \quad \psi_{\pm,k} = \psi_{\pm p_F + k},$$

where the ψ are the annihilation operators for electrons with momenta close to the Fermi boundaries $\pm p_F$, and σ_z, $\sigma_\pm = \sigma_x \pm i\sigma_y$ are the Pauli matrices; b_q^+ is the creation operator for a phonon with unrenormalized frequency $\omega(q)$;

$$\varphi(x) = \sum_{|q| \ll 2p_F}\left[\frac{\omega(2p_F+q)}{2}\right]^{1/2}(b_{2p_F+q} + b_{-2p_F+q}^+)\, e^{iqx}$$

is the complex field describing the lattice vibrations with momenta close to $\pm 2p_F$.

We shall make use of the functional formulation (developed in quantum electrodynamics[9] and in statistical physics[10]) of the problem of averaging expressions con-

FIG. 1.

structed from electron and phonon operators $\bar{\psi}$ and φ. The method of functional integration was first applied, albeit in implicit form, in a paper by Ferrell in 1964,[6] in which he proved that long-range superconducting order is absent in the one-dimensional case. The operations performed below, and the corresponding calculations of Efetov and Larkin[3] for another model, are, in essence, a repeat of Ferrell's calculations for the correlation functions.

The statistical phonon and electron Green functions on the imaginary axis of times τ are determined by the following functional integrals:

$$D(x,\tau;x',\tau')=\int\varphi(x,\tau)\varphi^*(x',\tau')Z^{-1}Z\{\varphi\}D\varphi, \tag{2}$$

$$G(x,\tau;x',\tau')=\int G(x,\tau;x',\tau'|\varphi)Z^{-1}Z\{\varphi\}D\varphi; \tag{3}$$

where

$$Z\{\varphi\}=\exp\left\{-\int dx\int_0^\beta d\tau\left[\varphi^*D_0^{-1}\varphi+\int_0^{g}\langle\mathscr{H}_{int}(g'\varphi)\rangle_\varphi\frac{dg'}{g'}\right]\right\}, \tag{4}$$

$$Z=\int Z\{\varphi\}D\varphi,\quad D_0^{-1}=1-\omega_0^{-2}\frac{\partial^2}{\partial\tau^2},\quad \omega_0=\omega(2p_F), \tag{5}$$

and $G(x,\tau;x',\tau'|\varphi)$ is the one-electron Green function calculated for a fixed classical field $\varphi(x,\tau)$. The functional integration is performed with Bose boundary conditions: $\varphi(x,0)\equiv\varphi(x,\beta)$.

By writing $Z\{\varphi\}=\exp[-\mathscr{F}\{\varphi\}]$, we obtain that, for $\varphi=\text{const}$, the free energy $\mathscr{F}\{\varphi\}$ coincides with the free energy of a Peierls insulator, calculated without allowance for fluctuations of the order parameter. For $T\ll T_{c0}$ this energy has a sharp absolute minimum at $g|\varphi|=\Delta(T)$, where $\Delta(T)\approx T_{c0}$ is the magnitude of the gap in the electron spectrum of the Peierls insulator. Consequently, only small and slowly varying deviations from this extremal state are important in the integrals in formulas (2), (3) and (5). To distinguish these deviations we write

$$g\varphi(x,\tau)=(\Delta+\delta(x,\tau))\exp[i\chi(x,\tau)],\quad \mathscr{F}\{\varphi\}\equiv\mathscr{F}\{\delta,\chi\}.$$

2. In the calculation of the electron Green function $G(x,\tau;x',\tau'|\varphi)$ the fluctuations $\delta(x,\tau)$ of the modulus are, generally speaking, a small perturbation, while the perturbation from fluctuations of the phase is slowly varying but not small. We shall find it more convenient to perform a transformation such that, as a result, it will also be possible to treat the phase fluctuations as a small perturbation. For this we introduce

$$\tilde{G}(x,\tau;x',\tau'|\varphi)=\exp[-\tfrac{1}{2}i\chi(x,\tau)\sigma_z]G(x,\tau;x',\tau'|\varphi)\exp[\tfrac{1}{2}i\chi(x',\tau')\sigma_z] \tag{6}$$

and define $\tilde{G}\equiv\tilde{G}(x-x',\tau-\tau')$ in terms of $\tilde{G}(x,\tau;x',\tau'|\varphi)$ by analogy with formula (3). The most important linear response functions of the system, e.g., the permittivity, conductivity and paramagnetic susceptibility, are expressed in terms of integrals, of the type (2), of products $\tilde{G}(x,\tau;x',\tau'|\varphi)\otimes\tilde{G}(x',\tau';x,\tau|\varphi)$ contracted with the matrix $\hat{I}$ or $\hat{\sigma}_z$. It is obvious that these functions are invariant under the transformation (6). The density of electron states, which is determined by the analytic continuation of the function $G(x,\tau;x',\tau')$, is approximately invariant under the transformation (6) in the case when we can neglect the time dependence of the phase: $\chi(x,\tau)\to\chi(x)$. It will be shown below that this approximation covers all the important regions of the spectrum. The interaction energy is also easily expressed in terms of the function $\tilde{G}$:

$$\langle\mathscr{H}_{int}\rangle_\varphi=(\Delta+\delta)\,\mathrm{Sp}\,\tilde{G}(x,\tau;x,\tau|\varphi)\hat{\sigma}_x \tag{7}$$

($\langle\cdots\rangle_\varphi$ in formulas (4) and (7) denotes the trace over the electron states for given phonon states).

3. Performing the transformation (6) in the equation of motion for the Green function $G(x,\tau;x',\tau'|\varphi)$, we obtain that the function $\tilde{G}(x,\tau;x',\tau'|\varphi)$ can be regarded as the Green function of the effective electron system in a field χ, δ, defined by the Hamiltonian:

$$\tilde{\mathscr{H}}=\int\tilde{\psi}^+(x)\left[-iv\frac{\partial}{\partial x}\sigma_z-\Delta\sigma_x-\delta\sigma_x+\frac{1}{2}v\frac{\partial\chi}{\partial x}I+\frac{i}{2}\frac{\partial\chi}{\partial\tau}\sigma_z\right]\tilde{\psi}(x)\,dx. \tag{8}$$

The first two terms in the expression (8) describe the unperturbed electron states in the Peierls insulator.

Treating the last three terms in (8) as a perturbation and taking formulas (4) and (7) into account, we find that

$$Z\{\varphi\}=\exp\left[-\int dx\int_0^\beta d\tau\mathscr{L}_{ph}\{\varphi\}\right], \tag{9}$$

where, in accordance with the expressions (4) and (7), the effective phonon Lagrangian $\mathscr{L}_{ph}$ is determined in the quadratic approximation by the diagrams of Fig. 1a. In this figure the shaded circle denotes the potential $\Delta\sigma_x$ and the unshaded circles signify either $\frac{1}{2}i\sigma_z\partial\chi/\partial\tau$ or $\frac{1}{2}vI\partial\chi/\partial x$. The solid lines denote the Green functions of (9).

Carrying out the calculations to within small terms $\sim e^{-\Delta/T}$, we obtain the effective free-phonon Lagrangian,

$$\mathscr{L}_{ph}=\int dx\left\{\frac{v}{8\pi}\left[\left(\frac{\partial\chi}{\partial x}\right)^2+\frac{1}{u^2}\left(\frac{\partial\chi}{\partial\tau}\right)^2\right]+\frac{1}{\pi v}\left[\delta^2+\frac{\pi}{36}\left(\frac{v}{\Delta}\right)^2\left(\frac{\partial\delta}{\partial x}\right)^2+\frac{1}{8}\left(\frac{v}{u\Delta}\right)^2\left(\frac{\partial\delta}{\partial\tau}\right)^2\right]\right\}, \tag{10}$$

where $u=v(\omega_0/\Delta)(g^2/8\pi v)^{1/2}$ is the effective velocity of the sound associated with the oscillations of the phase. By virtue of the conditions postulated in the Introduction, $s\ll u\ll v$ always, where s is the velocity of the acoustic phonons. The terms with time derivatives in (10) are determined by the bare Green function in the expression (4)—the corrections from $\langle\mathscr{H}_{\text{int}}\rangle_\varphi$ are of relative order u^2/v^2. On the other hand, the terms containing gradients are determined by the interaction.

In combination with the Bose boundary conditions[1)] the expressions (8) and (11) specify the resulting effective

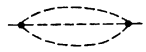

FIG. 2.

system as an insulator with an acoustic (χ) and an optical (δ) branch of the vibration spectrum. The difference from real systems is that the decay of a phonon into an electron–hole pair is forbidden. The green functions of the operators χ and δ are equal to

$$D_\chi = \frac{-4\pi u^2}{v^2(\omega_n^2+u^2q^2)}, \quad D_\delta = \frac{-4\pi\Delta^2u^2}{v(\omega_n^2+8\Delta^2u^2/v^2)}. \tag{11}$$

(For the optical phonons we have neglected the dispersion, since the theory as a whole is applicable for $q \ll \Delta/v$.)

Owing to the smallness of u/v and T/Δ, scattering of electrons is important only in the vicinity of the boundaries of the forbidden band, i.e., when $||\varepsilon| - \Delta/2| \ll \Delta$ and $|\xi| \ll \Delta$. In this region it is convenient to perform a canonical transformation of the electron operators, thereby diagonalizing the one-electron part of the Hamiltonian (8). In the new basis, in the leading approximation in ξ/Δ, we obtain the following expression for the phonon-mediated electron–electron interaction:

$$U_{\text{eff}} = {}^1/_4 D_\chi(k, \omega_n) I\otimes I + D_\delta(k, \omega_n)\ \sigma_z\otimes\sigma_z. \tag{12}$$

A qualitative description of the electron states lying in the neighborhood of the chemical potential $\varepsilon = 0$, i.e., in the middle of the forbidden band, can be obtained by interpolating data on the tails of the density of electron states, obtained in the neighborhoods of the boundaries $\varepsilon = \pm\Delta/2$.

3. DYNAMICS OF THE PHONONS

1. The relations obtained above enable us to determine the characteristics of the system as a function of the imaginary time τ. Assuming that the analytic continuation to real frequencies of the final expressions is equivalent to that of individual terms of the perturbation-theory series, we shall use the well-known analytic-continuation methods of the diagram technique.

We shall consider the damping of the acoustic phonons, which is essential in the following. It is determined by the anharmonicities that arise from the further expansion of $\mathcal{F}\{\delta, \chi\}$. (The interaction of the phase with the real acoustic phonons is small in the ratio $(\Delta/\varepsilon_F)^2$.) The fourth-order terms are determined by diagrams of the type of Fig. 1b. In order of magnitude,

$$\mathcal{L}_{ph}^{(4)} \approx \frac{1}{v\Delta^2}[(v\chi')^4 + (\dot\chi)^2(v\chi')^2 + \Delta\delta(v\chi')^2 + \Delta\delta\dot\chi^2 + \ldots]. \tag{13}$$

Here we have omitted combinations which give either a small or an unimportant effect. The contributions of the higher anharmonicities to the damping of the oscillations of the phase fall off like powers of T/Δ and u/v.

The damping is determined by the imaginary part of the diagram of Fig. 2. The analytic continuation of diagrams of this type is most simply determined by the technique developed in a paper by one of the authors[11]. We obtain

$$D_\chi(k, \omega) = 4\pi u^2 v^{-1}[\omega^2 - u^2k^2 + 2i\omega\Gamma(uk, \omega)],$$

where the relaxation frequency $\Gamma(uk, \omega)$ is determined by the expression

$$\Gamma(uk,\omega) = \frac{1}{2}\frac{1}{6}\left(\frac{4\pi}{v}\right)^4\Lambda^2\frac{\omega}{n(\omega)}\sum_{\alpha_i=\pm1}\int\frac{dk_1dk_2dk_3}{(2\pi)^2}\delta(k-k_1-k_2-k_3)$$
$$\times\delta(\omega-\alpha_1\omega(k_1)-\alpha_2\omega(k_2)-\alpha_3\omega(k_3))\,\alpha_1\omega(k_1)\,\alpha_2\omega(k_2)\,\alpha_3\omega(k_3)\,n(\alpha_1\omega(k_1))$$
$$\times n(\alpha_2\omega(k_2))\,n(\alpha_3\omega(k_3)), \tag{14}$$

here, the scattering amplitude Λ is, according to (13), of order $\Lambda \sim v^3/\Delta^2$.

The integrals in formula (14) converge at frequencies $\omega(k_i) \lesssim T$, and, consequently, we have the right to consider only the quantum region $T \ll \Delta u/v$. In this case the largest contribution is given by that region of integration over the momenta in which sign $k_i = \alpha_i$. In this region the energy conservation law is satisfied identically when the momentum conservation law is fulfilled, i.e., the argument of the second δ-function is identically equal to zero. This circumstance is a consequence of the one-dimensionality of the system and of the linearity of the dispersion law. A finite result for the damping on the mass shell can be obtained by taking into account the non-one-dimensionality of the system and corrections to the phonon dispersion law, and also by carrying out a self-consistent calculation of the damping. The calculations show that the last effect is the least important. Therefore, we shall consider only the first two.

With allowance for the nonlinearity, the acoustic-phonon spectrum has the following form:

$$\omega(k) = uk(1 - C\xi_0^2k^2),$$

where the coefficient $C \approx 1$ will be omitted in the following. Bearing in mind that values $\omega(k_i) \ll T$ will be important, we obtain from (14), for $\omega \to uk$,

$$\Gamma(\omega,\omega) \sim \omega^2\frac{v^2}{u^2}\frac{T^2}{\Delta^4}\iint d\omega_1 d\omega_2\,\delta\left(\frac{v^2}{u^2}\frac{1}{\Delta^2}[\omega^3 - 3(\omega_1+\omega_2)(\omega-\omega_1)(\omega-\omega_2)]\right),$$

whence

$$\Gamma(\omega,\omega) \sim \frac{\omega^2T^2}{\Delta^2}\left[\max\left\{\omega, \left(w\frac{u^2}{v^2}\Delta^2\right)^{1/3}, \left(\Gamma(\omega,\omega)\frac{u^2}{v^2}\Delta^2\right)^{1/3}\right\}\right]^{-1}, \tag{15}$$

where w is the characteristic width of the spectrum. Determining $\Gamma(\omega, \omega)$ self-consistently, we obtain from (15):

$$\begin{aligned}
&\frac{\Gamma(\omega,\omega)}{\omega} \sim \frac{T^2}{\Delta^2}, && T\frac{u}{v} \ll \omega \ll T,\\
&\frac{\Gamma(\omega,\omega)}{\omega} \sim \left(\frac{v\omega}{uT}\right)^{1/2}\frac{T^2}{\Delta^2}, && \left(w\frac{u^2}{v^2}\Delta^2\right)^{1/3} \ll \omega \ll T\frac{u}{v},\\
&\frac{\Gamma(\omega,\omega)}{\omega} \sim \frac{\omega}{(wu^2\Delta^2/v^2)^{1/4}}, && \omega \ll \left(w\frac{u^2}{v^2}\Delta^2\right)^{1/3}.
\end{aligned} \tag{16}$$

Below we shall need the value of the damping at $k = 0$. In analogy with (15), (16), we obtain

$$\frac{\Gamma(0,\omega)}{\omega} \sim \frac{u^2}{v^4}\frac{T^2\omega}{\Delta^2}\Big/\left(\frac{u^2}{v^2}\Delta^2\max\{\omega, w\}\right)^{1/4}, \quad T\frac{u}{v} \ll \omega, w \ll T, \tag{17}$$

$$\frac{\Gamma(0,\omega)}{\omega}\sim\frac{u^4}{v^4}\frac{T^2}{\Delta^2}\left(\frac{v\omega}{uT}\right)^{1/2},\quad \omega, w\ll T\frac{u}{v}.$$

(The extra factor u^4/v^4 appears in (17) on account of the fact that the terms $\chi^2(v\chi')^2$ in the expression (13) are small in the ratio u^2/v^2 compared with the terms $(v\chi')^4$ that played the principal role for $k\neq 0$.)

2. The fact, established above, that the damping of the oscillations of the phase is small enables us to calculate the dynamic structure factor $S(k,\omega)$ determining the neutron scattering:

$$\frac{d\sigma}{d\omega\,d\Omega}\sim S(k,\omega)=\int dt\,dx e^{i(\omega t-kx)}\langle\exp\{-iQd(0,0)\}\exp\{iQd(x,t)\}\rangle,$$

where $d=(1+\delta/\Delta)d_0\cos(2p_F x+\chi)$ is the lattice displacement ($d_0=\Delta/\omega_0 g\rho^{1/2}$, where ρ is the linear density, is the equilibrium displacement of the lattice in the self-consistent field theory). Since $d_0 p_F\sim(\Delta/\varepsilon_F)(v/g^2)^{1/2}\ll 1$, we have, for $Q=2p_F+k$,

$$S(k,\omega)\approx(d_0p_F)^2\int dt\,dx e^{i(\omega t-kx)}[K(x,t)+K_\delta(x,t)],\tag{18}$$

where the correlation functions

$$K(x,t)=\langle\exp\{i[\chi(0,0)-\chi(x,t)]\}\rangle,\quad K_\delta(x,t)=\Delta^{-2}\langle\delta(0,0)\delta(x,t)\rangle\tag{18a}$$

are expressed in terms of the retarded Green functions[11]:

$$K(k,\omega)=\operatorname{Im}K^R(k,\omega)(1+n(\omega)).$$

(In formula (18) it has been taken into account that the correlation length $R_\delta\sim v/\Delta$ of deviations of the modulus is much smaller than the correlation length $R_\chi\sim v/T$ of the phase.)

In accordance with (11),

$$K_\delta=4\pi\frac{u^2}{v}\delta\left(\omega^2-8\left(\frac{u}{v}\Delta\right)^2-\frac{2\pi}{9}u^2k^2\right)(1+n(\omega)).$$

We shall find the function $K^R(k,\omega)$ by analytic continuation of the temperature Green function $\mathcal{K}(k,\omega_n)$. In the coordinate representation we obtain

$$\mathcal{K}(x,\tau)=Z^{-1}\int D\chi\exp\{i[\chi(0,0)-\chi(x,\tau)]\}=\exp\{D_\chi(x,\tau)-D_\chi(0,0)\}.\tag{19}$$

We expand the exponential in formula (19) in a power series and, by the method developed earlier,[11] perform the analytic continuation in each of its terms. Writing, for $0<\tau<\beta$,

$$D_\chi(x,\tau)=2\frac{u}{v}\int\frac{d\eta}{\eta}\cos\left(\eta\frac{x}{u}\right)e^{-\eta\tau}(1+n(\eta)),$$

we obtain

$$\mathcal{K}(x,\tau)=\sum_n\frac{(2u/v)^n}{n!}\prod_{i=1}^n\int\frac{d\eta_i}{\eta_i}\left[\cos\left(\eta_i\frac{x}{u}\right)e^{-\eta_i\tau}-1\right](1+n(\eta_i)).\tag{20}$$

In (20) we Fourier-transform to discrete frequencies $\omega_n=2\pi Tn$, replace $i\omega_n$ by $\omega+i\delta$ and perform the inverse Fourier transformation to real times $t>0$. We obtain

$$K^R(x,t)=\sum\frac{1}{n!}[(A(x,t))^n-(A^*(x,t))^n];$$

$$A(x,t)=2\frac{u}{v}\int\frac{d\eta}{\eta}\left[\cos\left(\eta\frac{x}{u}\right)e^{-i\eta t}-1\right](1+n(\eta))$$

$$=\frac{u}{v}\ln\left[\left(\frac{T_0}{T}\right)^2\operatorname{sh}(\pi Tt_+)\operatorname{sh}(\pi Tt_-)\right]-i\pi\frac{u}{v}\theta\left(t-\frac{|x|}{u}\right);$$

$$t_\pm=t\pm|x|/u,\quad T_0=\Delta u/v.$$

As a result we obtain

$$K^R(t,x)=2\sin\left(\pi\frac{u}{v}\right)\left[\left(\frac{T_0}{T}\right)^2\operatorname{sh}(\pi Tt_+)\operatorname{sh}(\pi Tt_-)\right].\tag{21}$$

Taking the Fourier transform of the expression (21) and taking (18) and (18a) into account, we obtain an expression for the structure factor:

$$S(k,\omega)=\frac{u(p_Fd_0)^2}{8\pi^2\Gamma^2(u/v)T^2}\left(\frac{T}{T_0}\right)^{2u/v}e^{\omega/2T}$$

$$\times\left|\Gamma\left(\frac{u}{2v}+i\frac{\omega+ku}{4\pi T}\right)\Gamma\left(\frac{u}{2v}+i\frac{\omega-ku}{4\pi T}\right)\right|^2.\tag{22}$$

Taking into account the smallness of u/v, it follows from (22) that

1) $|\omega|\ll T$, $|ku|\ll T$,

$$S(k,\omega)=\frac{32\pi^2u^3v^{-2}p_F^2d_0^2T^2(T/T_0)^{2u/v}}{[(\omega+ku)^2+(2\pi Tu/v)^2][(\omega-ku)^2+(2\pi Tu/v)^2]}.$$

2) $|\omega-ku|\ll T$; $|\omega+ku|\gg T$,

$$S(k,\omega)=\frac{8\pi^2u^3v^{-2}p_F^2d_0^2(T/T_0)^{u/v}}{(\omega-ku)^2+(2\pi Tu/v)^2}\left(\frac{T_0}{|\omega|}\right)^{1-u/v}\exp\left\{\frac{\omega}{T}0(-\omega)\right\};$$

3) $|\omega-ku|\gg T$, $|\omega+ku|\gg T$,

$$S(k,\omega)=2\pi^2\frac{u^3p_F^2d_0^2}{v^2T_0^2}\left(\frac{T_0^2}{\omega^2-k^2u^2}\right)^{1-u/v}\exp\left\{\frac{2\omega-|\omega-ku|-|\omega+ku|}{4T}\right\}.$$

The integral structure factor $S(k)$ is equal to

$$S(k)=\left(2\frac{T}{T_0}\right)^{2u/v}\left(\frac{p_Fd_0}{\pi}\right)^2\Gamma\left(1-2\frac{u}{v}\right)u\sin\left(\frac{\pi u}{v}\right)$$

$$\times\frac{1}{T}\operatorname{ch}\left(\frac{ku}{2T}\right)\left|\Gamma\left(\frac{u}{v}+i\frac{uk}{2\pi T}\right)\right|^2.\tag{23}$$

From (23) we obtain

1) $|ku|\ll T$:

$$S(k)=\left(\frac{2T}{T_0}\right)^{2u/v}\frac{4\pi T(p_Fd_0)^2}{v[k^2+(2\pi T/v)^2]},$$

2) $|ku|\gg T$:

$$S(k)=(p_Fd_0)^2\frac{u^2}{v}\frac{2\pi}{T_0}\left(\frac{T_0}{u|k|}\right)^{1-2u/v}.$$

4. THE ELECTRON SPECTRUM

The character of the electron–photon interaction can be elucidated using the example of the first-order correction to the electron self-energy (Fig. 3.). For the retarded Green function this quantity is equal to

$$\Sigma_R(\varepsilon,p)=\sum_\lambda c_\lambda\int\frac{vdq}{2\pi}\frac{\omega_\lambda(q)}{[\varepsilon-\varepsilon(p+q)]^2-[\omega_\lambda(q)]^2}$$

$$\times\left\{\omega_\lambda(q)\operatorname{th}\frac{\varepsilon(p+q)}{2T}+[\varepsilon-\varepsilon(p+q)]\operatorname{cth}\frac{\omega_\lambda(q)}{2T}\right\},\tag{24}$$

FIG. 3.

FIG. 4.

where the index $\lambda(=0, a)$ labels the phonon branches, $c_a = \pi/2$, $c_0 = \pi/4$, $\omega_0(q) = \sqrt{8}u\Delta/v$, $\omega_a(q) = uq$, and $\varepsilon(p) = \Delta/2 + v^2p^2/2$. When $\lambda = a$, in the denominator of formula (24) we can neglect the term $\omega_\lambda^2(q)$ if $|\xi| \gg \Delta u/v$ or if $||\varepsilon| - \Delta/2| \gg \Delta(u/2v)^2$. When $\lambda = 0$ we have the single condition $||\varepsilon| - \Delta/2| \gg \Delta u/v$. In the numerator of formula (24) we can always assume that $\tanh(\varepsilon/2T) = 1$. If $T \gg \Delta u/v$, the frequencies $\omega_\lambda(q) \ll T$ for all q. When all the conditions enumerated are fulfilled,

$$\Sigma_R(\varepsilon, p) = \frac{3}{2}\pi \int \frac{v\,dq}{2\pi} \frac{T}{\varepsilon - \varepsilon(q)} = \frac{3}{2} T \left(\frac{\Delta}{2\varepsilon - \Delta}\right)^{1/2}.$$

Consequently, for $T \gg \Delta u/v$ the phonons play the role of a random Gaussian external field $V(x)$ with correlation function

$$\langle V(x)V(0)\rangle = {}^3/_2 \pi T \delta(x).$$

The integral density of states in this case was found in the paper[12] by Halperin:

$$\frac{1}{N(\varepsilon)} = \int_0^\infty \left(\frac{\pi}{t}\right)^{1/2} \exp\left\{-\frac{t^3}{12} - 2t\frac{\varepsilon - \Delta/2}{\varepsilon_0}\right\} dt,$$

$$N(\varepsilon) \sim \frac{(2E)^{1/2}}{\pi} \exp\left\{-\frac{4}{3}\left(\frac{2E}{\varepsilon_0}\right)^{3/2}\right\}, \quad \varepsilon_0 = \left[\left(\frac{3\pi}{2}\right)^2 T^2 \Delta\right]^{1/3} \quad (25)$$

for

$$E = \Delta/2 - \varepsilon \gg \varepsilon_0.$$

Since, in estimates, we must always bear in mind that $||\varepsilon| - \Delta/2| \gtrsim \varepsilon$ we have

$$\frac{||\varepsilon| - \Delta/2|}{\Delta} > \left(\frac{T}{\Delta}\right)^{2/3} > \left(\frac{u}{v}\right)^{2/3} \gg \frac{u}{v}.$$

Consequently, the use of the static approximation is self-consistent. It can also be seen from the latter inequalities that, for $T \approx \Delta u/v$,

$$\varepsilon_0/\Delta \sim (u/v)^{2/3} \gg u/v.$$

Consequently, the static approximation also remains valid for $T \ll \Delta u/v$. In this region, $\coth(\omega_\lambda(q)/2T) \to 1$ and, as can be seen from (17), the optical vibrations give the largest contribution. We again obtain formulas (25), with ε_0 replaced by $\bar{\varepsilon}_0 = (\pi u^2/2v^2)^{1/3}\Delta$. Since $\bar{\varepsilon}_0 v/\Delta u \approx (v/u)^{1/3} \gg 1$, the static approximation is fulfilled as before, as we should expect.

We note that the width over which the band edge is smeared out is always large compared with the temperature. The one-electron excitations in the dielectric are distributed near the extrema of the function $n_F(\varepsilon)dN/d\varepsilon$. From formula (25) and the form of ε_0 and $\bar{\varepsilon}_0$ we can obtain the result that, for $T \ll \Delta u/v$, this extremum lies at the center of the forbidden band, i.e., the results obtained are applicable only in order of magnitude. In the region $T \gg \Delta u/v$ the extremum of the electron distribution function is also found to be located at $\varepsilon = 0$. This result, however, depends in an essential way on the numerical coefficients and can change when the model is made more complicated (the extremum shifts to the boundaries $\varepsilon = \pm\Delta/2$ of the forbidden band).

5. ELECTROMAGNETIC PROPERTIES

The electromagnetic response function $Q(k, \omega) = -J(k, \omega)/A(k, \omega)$ is determined by the diagrams of Fig. 4. In combination with the diamagnetic term $Q_d = -Ne^2/m$, the first, normal diagram (Fig. 4a) gives

$$Q_0 = \frac{e^2v}{3\pi}\frac{\omega^2}{\Delta^2},$$

which corresponds to the normal dielectric permittivity $4e^2v/3\Delta^2$ of a one-dimensional narrow-band dielectric. The second, anomalous part (Fig. 4b) arises from the term

$$\frac{i}{2}\frac{\partial\chi}{\partial\tau}\tilde{\psi}^+\sigma_z\tilde{\psi}$$

in the Hamiltonian (8). It reflects the fact that the quantity $\chi/2p_F$ is the average coordinate of the electron-phonon system and, consequently, is proportional to the dipole moment. Its contribution can be regarded as the precursor of the Fröhlich conduction via the Goldstone mode[13] in the ordered phase. We obtain

$$Q_a(k, \omega) = -e^2\pi^{-2}\omega^2 D_\chi(\omega, k),$$

whence, for $k = 0$, the complex dielectric permittivity is equal to

$$\varepsilon(\omega) = \frac{4e^2v}{3\Delta^2} - \frac{16e^2u^2/v}{\omega^2(1 + 2i\Gamma(0, \omega)/\omega)}.$$

Bearing in mind that, according to (17), $\Gamma(0, \omega)/\omega \ll 1$, we obtain expressions for the permittivity and conductivity:

$$\varepsilon(\omega) = \frac{4}{3}\frac{e^2v}{\Delta^2}\left(1 - 12\frac{u^2}{v^2}\frac{\Delta^2}{\omega^2}\right),$$

$$\sigma(\omega) = \frac{4}{\pi}\frac{e^2u^2}{v^2}\frac{\Gamma(0, \omega)}{\omega^2}.$$

According to (17), in a strictly one-dimensional system,

$$\sigma(\omega) \sim e^2v\left(\frac{u}{v}\right)^6 \begin{cases} ((u\Delta/v)^2\omega)^{-1/3}, & uT/v \ll \omega \ll T, \\ (u\Delta\omega/v)^{-1/3}, & \omega \ll uT/v, \end{cases} \quad (26)$$

The expression (26) obtained above for the conductivity takes into account the damping of the phase oscillations as a result of the intrinsic anharmonicity. It should be borne in mind that there also exists the possibility of decay of these oscillations into an electron-hole pair. The change in the function $D_\chi(\omega, k)$ as a result of such processes can be taken into account by noting that, according to (8), the quantities $\dot{\chi}/2e$ and $v\chi'/2e$ are equivalent to the vector and scalar potential, respectively. The Fermi velocity v plays the role of the velocity of light. We obtain immediately that

$$D_x(\omega, k)=\frac{4\pi}{v}\left[\frac{\omega^2}{u^2}-k^2+\pi\frac{\omega^2}{e^2v^3}\tilde{Q}(\omega, k)\right]^{-1},$$
$$\tilde{Q}(\omega, k)=2e^2v/\pi+i\omega\sigma^{(n)}$$

is the electromagnetic response function, calculated without allowance for the diamagnetic term. The real part $\mathrm{Re}\tilde{Q}$ gives an unimportant renormalization of the sound velocity: $u^{-2}\to u^{-2}+2v^{-2}$. The imaginary part

$$\mathrm{Im}\,\tilde{Q}\sim\omega e^{-\Delta/T},$$

inasmuch as the normal conductivity $\sigma^{(n)}$ should have a finite value under conditions of strong electron–phonon interaction. Consequently, we have obtained the result that the contribution of polarization processes to the damping of the phase oscillations is negligibly small compared with the contribution of the decay processes due to the anharmonicities.

The results obtained for the conductivity also remain valid in the ordered phase of the quasi-one-dimensional system, i.e., for $T<T_c$.

In conclusion we shall discuss the sensitivity of the results obtained to the inclusion of coupling between the phase oscillations and the electric field in a quasi-one-dimensional system. This coupling leads to a renormalization of the sound velocity:

$$u^2\to\tilde{u}^2\left(1+16\pi\frac{e^2}{\hbar v}\ln\frac{S_\perp}{S_0}\right)^2,$$

where $S_\perp=a_\perp^2$ is the transverse cross-sectional area of the unit cell, S_0 is the area of the transverse localization of the electron states, and $\xi_0=v/\Delta$, and to the appearance of a gap in the sound spectrum[13,14]:

$$\omega^2(k)\to\tilde{\omega}^2(k)=\tilde{u}^2k_\parallel^2+16\pi\frac{e^2}{\hbar v}\frac{\tilde{u}^2}{S_\perp}\frac{k_\parallel^2}{k_\parallel^2+k_\perp^2}. \qquad (27)$$

The gap in the spectrum (27) effectively exists for $k_\parallel \gg k_\perp$, while for $k_\parallel \ll k_\perp$ the renormalization becomes unimportant. Inasmuch as all the quantities investigated above were defined initially on one filament, i.e., were integral quantities over the transverse quasi-momenta, the expressions obtained remain unchanged over longitudinal distance $|x| \gg a_\perp$.

For the conductivity this means that we should consider the region $\omega \gg u/a_\perp$. At lower frequencies the damping of the phase oscillations will be determined by polarization effects. It is possible that this effect explains the appearance of the low-frequency peak in the infrared spectra of KCP.[15]

The expressions (22) and (23) for the structure factor are applicable for $k_\parallel \ll a_\perp^{-1}$. For larger $k_\parallel$ the phase oscillations will give qualitatively the same contribution to $S(k, \omega)$ as the oscillations of the modulus of the gap. The electron-spectrum parameters ε_0 and $\bar{\varepsilon}_0$ found above acquire an additional numerical factor of order unity if $\max\{\varepsilon_0, \bar{\varepsilon}_0\} > \Delta(a_\perp/\xi_0)^2$.

[1)]This elementary quantization of the phase is possible only in a one-dimensional system, in which vortices cannot arise.

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