Medium-range dielectric order in systems with collectivized electrons

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The problem of formation of a medium-range dielectric order (on a scale much larger than the interatomic one) due to electron–electron correlations and to scattering by an impurity in a system near a phase transition into a long-range order state is solved by a microscopic approach. It is shown that for a weak impurity potential the effect of medium-range order formation is stronger than the effect of long-range order suppression related to scattering by an impurity. The infuence of medium-range order on the one-particle excitation spectrum and on the density of states is considered. It is found that since the medium-range order in a system is due to correlations of electron and hole states "coupled" by a continuous set of inhomogeneity vectors (in contrast to the long-range order formed on a discrete set of such vectors), the density of states varies on an energy scale determined by the mean absolute value of these vectors. Therefore in a system undergoing phase transition into an inhomogeneous state with the modulus q_0 of inhomogeneity vectors the medium-range order forms in the density of states a pseudogap of scale length $v_F q_0$ (v_F is the Fermi velocity). This distinguishes such a system substantially from one, which tends to a phase transition into a homogeneous state ($q_0 \equiv 0$), where the medium-range order forms a pseudogap of scale length $v_F/\xi \ll v_F q_0$ (ξ is the correlation length). The possible role of medium dielectric order effects in high-T_c superconductors is discussed.

1. INTRODUCTION

Analysis of experimental data obtained during the years of study of high-T_c (HTSC) superconductivity reveals an important role of dielectric correlations in the mechanism of the latter. First, it is experimentally confirmed that there are strong spin correlations in the superconducting phase of LaSrCuO and YBaCuO.[1–3] Second, optical experiments[4–6] have reliably detected a pseudo-gap of electronic origin in the excitation spectrum of BaPbBiO and BaKBiO for superconducting compositions. Third, HTSC have very large static dielectric constants in the long wavelength limit,[7–9] which is interpreted as an indication of proximity of these substances to a point of instability in relation to the transition into ferroelectric phase. Fourth, anomalously high mobility of oxygen[10] and copper[11] ions has been observed in a number of experiments on YBaCuO, which can be related, from the microscopic point of view to electron instability to charge transfer from copper to oxygen.[12–14] Besides, temperature nonmonotonicity and changes in lattice parameters, and in the elastic and oscillation characteristics near the phase transition into superconducting phase can also be regarded as indirect evidence of strong dielectric correlations in HTSC.

All these data prompted to extensive theoretical studies of the nature of dielectric correlations in HTSC and their relation to superconductivity in these compounds.

It is reliably established that the electron-electron interaction in HTSC is not weak ($U/W \sim 1$, where U is the energy of one-center repulsion and W is the bandwidth). Owing to this, and in laminated HTSC also owing to their effective two-dimensionality, the point of electron instability with respect to the transition into the phase with long-range dielectric order is preceded by a wide interval of developed charge [in the case of a charge density wave (CDW)] or spin [in the case of a spin density wave (SDW)] fluctuations. In this interval electron-electron correlations form a medium-range order (falling off on a scale larger than the interatomic one), which means existence of local long-living charge or spin fluctuations.

Defects (impurities) inserted into HTSC by doping can also form, in their vicinity, regions of a medium CDW or SDW order. These regions of medium-range order in the vicinity of impurities constitute something like "frozen" fluctuations. Therefore the problem of fluctuations connected with electron–electron correlations can be treated in terms of the impurity problem. However, to go over from one problem to the other, it is necessary to replace in all final expressions the parameters $V_{12}N(0)$ and n_0, where V_{12} is the off-diagonal component of impurity scattering (see Sec. 2), $N(0)$ is the density of states at the Fermi level in the symmetric (initial) phase, and n_0 is the impurity concentration, by the parameters μ_{cr}/ε_F and n_ϕ, where μ_{cr} is the critical value of the incongruity parameter (see Sec. 2), ε_F is the Fermi energy, and n_ϕ is the concentration of local long-living regions of short-range order. Note also that n_ϕ should be determined, in a self-consistent way, by proximity of the system to the point of transition into the long-range order state.

It is known that scattering by a charged impurity suppresses the long-range order in systems with electron-hole coupling[15,16] (the $1/\tau$ effect). This is a second-order effect in the impurity potential related to different effect of a charged impurity on the electron and hole in the electron-hole pair. However, an impurity can produce in its vicinity the medium-range dielectric order even in such a range of system parameters for which the long-range order is not realized. This is a first-order effect in the impurity potential and predominates, when the latter is weak, over the effect of long-range order suppression. Two types of defect are possible: of the "local transition temperature" type, when the order in

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the vicinity of the defect arises at a temperature somewhat higher than the temperature of long-range ordering in the system, and of the "local field" type, when the medium-range order near the defect exists at any temperature.

Local structural transitions near the defects of the "local field" type been considered phenomenologically in Ref. 17. Defects of the "local transition temperature" type have been discussed in relation to band antiferromagnets (AF) above the Néel point.[18–20] The properties and structure of states localized at both types of defects in one-dimensional systems, undergoing transition into an inhomogeneous phase of the soliton lattice, have been considered in Ref. 21.

In the present study we treat microscopically, in terms of the "random field" impurity problem, the formation of medium-range dielectric order in systems above the point of transition into the long-range order state (the changeover to the problem of medium-range order formation by electron-electron correlations is carried out according to the rules mentioned above). The influence of the medium-range order on the one-particle excitation spectrum and density of states is considered, and the role that the medium-range dielectric order might play in HTSC is discussed.

We will solve the problem thus formulated in the limit of weak interaction ($U/W \ll 1$), in which it has an asymptotically exact solution. In this limit, the charge carriers are described in the framework of band approach, and the instability against electron-hole pairing is connected with the features of the excitation spectrum of collectivized electrons. As theoretical studies show, treating electron-electron correlations in the limits of weak ($U/W \ll 1$) and strong ($U/W \gg 1$) interactions lead to qualitatively equal results. Therefore one can hope that the results obtained in both limiting cases can be reasonably extrapolated to the region of intermediate interaction ($U/W \sim 1$) realized in HTSC.

2. MODEL HAMILTONIAN AND BASIC EQUATIONS

In the present study we use a model Hamiltonian for a semi-metal with congruent electron (1) and hole (2) bands whose extrema are the "nesting" vector $\mathbf{Q}$ apart:

$$\varepsilon_1(\mathbf{k}) = \varepsilon(\mathbf{k}) - \varepsilon_F,$$
$$\varepsilon_2(\mathbf{k}) = -\varepsilon(\mathbf{k}+\mathbf{Q}) + \varepsilon_F. \tag{1}$$

Note that the scheme of one-band metal with congruent parts of the Fermi surface separated by the "nesting" vector $\mathbf{Q}$ also reduces to model (1) by means of appropriate labeling of spectral regions separated by space at the vector $\mathbf{Q}$ near the Fermi surface.

We will make use of high density approximation, when all interactions can be assumed point-like.[22] It is well-known that a system described by model (1) is unstable against electron-hole pairing. In what follows we assume for definiteness that the system undergoes a phase transition into the state with charge ordering. The latter occurs, if the coupling constant g_s corresponding to the CDW is a maximum.[22] However, the results that follow hold also in the case of instability to a transition into the state with (AF) spin ordering, which occurs if the coupling constant g_t corresponding to the SDW is the greatest. It is necessary only to replace in all final expressions the coupling constant g_s of singlet pairing by the coupling constant g_t of triplet pairing, and replace the off-diagonal component of potential part of carrier scattering from impurity atoms by the off-diagonal component of the exchange part of scattering (see below).

It is assumed that electrons and holes have different densities, owing to doping by impurities and existence of a reservoir (i.e., other bands overlapping with the ones under study but not participating in the pairing and providing total electroneutrality). For example, in the compound $La_{2-x}Sr_xCuO_4$ the role of doping, by impurities, of $2D$-bands formed by the CuO_2 plane is played by subsitution of Sr atoms for La atoms. In the $YBa_2Cu_3O_{6+\delta}$ compound the role of a reservoir is played by the $1D$-band formed by CuO chains and contributing to the Fermi surface, while the role of doping is played by changes in the oxygen content. Owing to the difference in electron and hole concentrations in the system, the model Hamiltonian should be supplemented by a term of the form

$$-\mu(\hat{n}_1+\hat{n}_2),$$

where $\hat{n}_{1,2}$ are electron density operators in the bands studied, and μ is the chemical potential. Because of this ($\mu \neq 0$), the Fermi surfaces of electron and hole bands turn out to be not exactly congruent, and therefore inhomogeneous solutions formed by a discrete set of wave vectors $\mathbf{q} \neq \mathbf{Q}$ (such that $|\mathbf{q}-\mathbf{Q}| \equiv q_0 \ll |\mathbf{Q}|$) may arise either for the CDW or for the SDW.[23,24]

The potential part of carrier scattering by impurity atoms can be written in the form of a matrix in the space of band and spin indices:

$$\hat{V}_{imp}(\mathbf{r}) = \sum_a \delta(\mathbf{r}-\mathbf{r}_a) \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \hat{I}, \tag{2}$$

where $\hat{I}$ is a unit matrix in spin space, and $V_{12} = V_{21}^*$. The impurity potential is considered point-like for simplicity. The off-diagonal, in band indices, component of potential scattering is the source of the long-range CDW order, while the off-diagonal component of the exchange part of scattering (proportional ot the scalar product of the impurity atom spin and the electron spin) is the source of the short-range SDW order.

The matrix elements V_{ij} ($i,j = 1,2$) in the space of band indices correspond to local renormalization of site energy levels ε_n and matrix elements t_{mn} of hopping between the neighbors in the basis of the Wannier functions:

$$\tilde{\varepsilon}_n = \varepsilon_n + V_{nn}, \quad \tilde{t}_{mn} = t_{mn} + V_{mn}$$

(The quantities with and without a tilde correspond to renormalized and bare matrix elements respectively). This renormalization leads to local changes in charge or spin density, producing either a local CDW or a local SDW, which fall off over scales of the order of the correlation length ξ.

All matrix elements V_{ij} ($i,j = 1,2$) have the same order of magnitude. In particular, the authors of Ref. 25, using the wave functions calculated in the tight-binding approximation for systems with bcc lattice,[26] have found that for a point-like impurity potential

$$V_{11} = V_{22} = V_{12}.$$

The effect of medium-range order formation in the impurity vicinity is "proportional" to V_{12}, while the "$1/\tau$ effect" of

long-range order suppression is "proportional" to the squares of matrix elements V_{ij} $(i,j=1,2)$. Therefore for a weak impurity potential the formation of a medium-range order near (below) the point of phase transition into the long-range-order state will predominate over the "$1/\tau$ effect."

The CDW amplitude is determined by the value of a singlet order parameter. $\Delta_s(\mathbf{r})$. The latter, in its turn, is related to the anomalous, in band indices, Green function by a self-consisting equation

$$\Delta_s(\mathbf{r})=\tilde{\Delta}_s(\mathbf{r})\exp(i\mathbf{Q}\mathbf{r}) = -\frac{1}{2}g_s\sum_{\omega_n,\alpha} G_{12}^{\alpha\alpha}(\mathbf{r},\mathbf{r},\omega_n)\exp(i\omega_n\tau), \quad \tau\to+0. \tag{3}$$

Here

$$G_{ij}^{\alpha\beta}(\mathbf{r},\mathbf{r}',\tau)=\langle T_\tau\Psi_{i\alpha}(\mathbf{r},\tau)\Psi_{j\beta}^{+}(\mathbf{r}',0)\rangle$$

are the temperature Green functions, $\Psi_{i\alpha}(\mathbf{r},\tau)$ is the field operator of annihilation for an electron of spin α in the ith band,

$$\omega_n=\pi(2n+1)T,$$

T is the temperature, and $\tilde{\Delta}_s(\mathbf{r})$ is a function slowly varying on the lattice-constant scale.

Since we have assumed for definiteness and without loss of generality that the system is unstable against the CDW formation, we have

$$G_{ij}^{\alpha\beta}(\mathbf{r},\mathbf{r}',\tau)=G_{ij}(\mathbf{r},\mathbf{r}',\tau)\delta_{\alpha\beta}. \tag{4}$$

In the high-density approximation the equations for the Green functions have a standard form $G_{ij}(\mathbf{r},\mathbf{r}',\omega_n)$

$$\begin{bmatrix} i\omega_n-\varepsilon_1(-i\nabla)-\mu-\varphi(\mathbf{r})-V_{11}(\mathbf{r}) & -(\Delta_s(\mathbf{r})+V_{12}(\mathbf{r})) \\ -(\Delta_s^*(\mathbf{r})+V_{12}^*(\mathbf{r})) & i\omega_n-\varepsilon_2(-i\nabla)-\mu-\varphi(\mathbf{r})-V_{22}(\mathbf{r}) \end{bmatrix} \times\begin{bmatrix} G_{11}(\mathbf{r},\mathbf{r}',\omega_n) & G_{12}(\mathbf{r},\mathbf{r}',\omega_n) \\ G_{21}(\mathbf{r},\mathbf{r}',\omega_n) & G_{22}(\mathbf{r},\mathbf{r}',\omega_n) \end{bmatrix}=\begin{bmatrix} \delta(\mathbf{r}-\mathbf{r}') & 0 \\ 0 & \delta(\mathbf{r}-\mathbf{r}') \end{bmatrix} \tag{5}$$

The potential $\varphi(\mathbf{r})$ in (5) is related to the long-range part of the Coulomb interaction resulting from screening of the impurity potential $V(\mathbf{r})$ and spatial redistribution of extra carriers, existing for $\mu\neq0$, due to inhomogeneous $\Delta_s(\mathbf{r})$. The potential $\varphi(\mathbf{r})$ obeys the Poisson equation, which has the following integral form

$$\varphi(\mathbf{r})=-\int\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}[n(\mathbf{r})-n]d\mathbf{r}', \tag{6}$$

where e is the electron charge, $n(\mathbf{r})$ is the difference in the electron and hole concentrations, and $n=\overline{n(\mathbf{r})}$ (the bar means averaging over the volume). Here we have already taken into account that the average value $\overline{\varphi(\mathbf{r})}=0$, since the system, as a whole, is electroneutral.

It is easy to find the local variation of the electron density, if we know the Green functions and density of states at the Fermi level, N_p, in the bands forming the reservoir. Since the variation of the electron density in the reservoir bands equals

$$N_p(\mu-\mu_0+\varphi(\mathbf{r})),$$

where μ_0 is the chemical potential in the absence of the impurity potential in the symmetric phase, i.e. for

$$\Delta_s(\mathbf{r})=\varphi(\mathbf{r})=\hat{V}_{imp}(\mathbf{r})=0,$$

we have

$$n(\mathbf{r})=2T\sum_{\omega_n}\{G_{11}(\mathbf{r},\mathbf{r},\omega_n)\exp(i\omega_n\tau)+G_{22}(\mathbf{r},\mathbf{r},\omega_n) \times\exp(-i\omega_n\tau)\}+N_p(\mu-\mu_0+\varphi(\mathbf{r})), \quad \tau\to+0 \tag{7}$$

The chemical potential μ_0 is found from Eqs. (5) and (7), if we set $\mu=\mu_0$, $\Delta_s(\mathbf{r})=\varphi(\mathbf{r})=\hat{V}_{imp}(\mathbf{r})=0$, and $n(\mathbf{r})=n$:

$$\mu_0=\frac{n}{4N(0)}, \tag{8}$$

where

$$N(0)=m^2v_F/2\pi^2$$

is the density of states in bands 1 and 2 at the Fermi level [we have assumed, for simplicity, that the spectrum $\varepsilon(k)$ is isotropic, i.e., $\varepsilon(\mathbf{k})=\mathbf{k}^2/2m$], and v_F is the Fermi velocity.

Thus, Eqs. (3), and (5)–(7) form a closed system allowing to find the order parameter $\Delta_s(\mathbf{r})$, the long-range Coulomb potential $\varphi(\mathbf{r})$, and the chemical potential μ in terms of system parameters, as well as carrier excitation spectra $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$, the difference n in electron and hole concentrations, and the coupling constant g_s.

3. LOCAL CDW

It is well known (see Refs. 23 and 24) that when the scattering by impurities is absent [$\hat{V}_{imp}(\mathbf{r})=0$] at $T=0$, the system under study experiences a phase transition into an inhomogeneous state with long-range dielectric order, if

$$|\mu|<\mu_{cr},$$

where

$$\mu_{cr}=0{,}755\Delta_0, \quad \Delta_0=2\varepsilon_F\exp(-1/g_s),$$

and ε_F is the Fermi energy. The formation of a spatially inhomogeneous solution for the order parameter occurs for a discrete set of wave vectors $\mathbf{q}$, lying close to the "nesting" vector $\mathbf{Q}$, such that

$|\mathbf{q}-\mathbf{Q}| \equiv q_0 \approx 2{,}4|\mu|/v_F$.

In the presence of the impurity potential the right-hand side of the self-consistency equation (3) contains a source whose magnitude is proportional to V_{12}. As a result, a solution for $\Delta_s(\mathbf{r})$ localized near the impurity exists even above the transition into the state with long-range order. We will find this solution at $T=0$ for the values of the incongruity parameter close to (larger than) μ_{cr}.

For this purpose we go over in the system (3), (5)–(7) to the momentum representation, introducing, as usual, the Fourier components $\Delta_s(\mathbf{q})$, $\varphi(\mathbf{q})$, $n(\mathbf{q})$ and $G_{ij}(\mathbf{k},\mathbf{k}+\mathbf{q},\omega_n)$. Then we expand $G_{12}(\mathbf{k},\mathbf{k}+\mathbf{q},\omega_n)$ in a series in $\Delta_s(\mathbf{q})$ and $V_{ij}(\mathbf{q})$ and retain in the right-hand side of the self-consistency equation (3) the terms linear in $\Delta_s(\mathbf{q})$ and $V_{12}(\mathbf{q})$, which is valid in the Born approximation

$$|V_{ij}|N(0) \ll 1, \quad i,j=1,2. \tag{9}$$

Then Eq. (3) is rewritten in the form

$$\frac{1}{g_s}\Delta_s(\mathbf{q}) = \Pi(\mathbf{q},\mu)\left\{\Delta_s(\mathbf{q}) + V_{12}\sum_a \exp(-i\mathbf{q}\mathbf{r}_a)\right\}, \tag{10}$$

where the polarization operator $\Pi(\mathbf{q},\mu)$ is

$$\Pi(\mathbf{q},\mu) = -\frac{T}{N(0)}\sum_{\omega_n}\int G_{11}^{0}(\mathbf{k},\omega_n)\,G_{22}^{0}(\mathbf{k}-\mathbf{q},\omega_n) \times \exp(i\omega_n\tau)\,\frac{d\mathbf{k}}{(2\pi)^3}, \quad \tau\to+0, \tag{11}$$

and

$$G_{ii}^{0}(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - \varepsilon_i(\mathbf{k}) - \mu}$$

is the Green function of a free particle in the ith band.

Assuming that

$$\frac{|\mu|-\mu_{cr}}{\mu_{cr}} \ll 1, \qquad \frac{|\mathbf{q}-\mathbf{Q}|-q_0}{q_0} \ll 1$$

[the latter assumption is justified by the final result for $\Delta_s(\mathbf{r})$], we expand the polarization operator $\Pi(\mathbf{q},\mu)$, having a maximum for $|\mathbf{q}-\mathbf{Q}| = q_0$, in a series in these parameters:

$$\Pi(\mathbf{q},\mu) = \frac{1}{g_s} - \frac{|\mu|-\mu_{cr}}{\mu_{cr}} - 0{,}284\left(\frac{v_F}{\mu_{cr}}\right)^2 (|\mathbf{q}-\mathbf{Q}|-q_0)^2. \tag{12}$$

From (10)–(12) we find

$$\Delta_s(\mathbf{q}) = \frac{V_{12}}{g_s}\,\frac{\sum_a \exp(-i\mathbf{q}\mathbf{r}_a}{(|\mu|-\mu_{cr})/\mu_{cr} + 0{,}284(v_F/\mu_{cr})^2(|\mathbf{q}-\mathbf{Q}|-q_0)^2}. \tag{13}$$

In the configuration space we have correspondingly

$$\Delta_s(\mathbf{r}) = \frac{V_{12}}{g_s}\,\frac{2q_0\xi\mu_{cr}^2}{1{,}136\pi v_F^2} \times \sum_a \frac{\exp\{iQ(\mathbf{r}-\mathbf{r}_a) - |\mathbf{r}-\mathbf{r}_a|/\xi\}\sin(q_0|\mathbf{r}-\mathbf{r}_a|)}{|\mathbf{r}-\mathbf{r}_a|}, \tag{14}$$

where the correlation length

$$\xi = \left(\frac{0.568 v_F^2}{2\mu_{cr}(|\mu|-\mu_{cr})}\right)^{1/2}$$

determines the effective size of the medium-range order region near the impurity.

4. EXCITATION SPECTRUM AND DENSITY OF STATES IN A SYSTEM WITH MEDIUM CDW OR SDW ORDER

When considering the influence of inhomogeneities on physical parameters indicative of a system as a whole (such as thermodynamic properties, energy spectrum, density of states, etc.), it is necessary to average these parameters over spatial position of inhomogeneities. As a result, the momentum $\mathbf{k}$ turns out to be a natural quantum number in the problem. Let us consider the effect of medium-range dielectric order on the spectrum of one-particle excitations $E_i(\mathbf{k})$ and density of states $N_i(\omega)$ in the bands $i=1,2$. These quantities are expressed through the self-energy part $\Sigma_i(\omega,\mathbf{k})$ of the corresponding band:

$$E_i - \mu - \varepsilon_i(\mathbf{k}) - \mathrm{Re}\,\Sigma_i(E_i,\mathbf{k}) = 0, \tag{15}$$

$$N_i(\omega) = \frac{1}{\pi}\int \frac{|\mathrm{Im}\,\Sigma_i(\omega,\mathbf{k})|}{[\omega-\mu-\varepsilon_i(\mathbf{k})-\mathrm{Re}\,\Sigma_i(\omega,\mathbf{k})]^2 + [\mathrm{Im}\,\Sigma_i(\omega,\mathbf{k})]^2} \times \frac{d\mathbf{k}}{(2\pi)^3}, \tag{16}$$

In the "cross" technique[27] self-energy parts are given by the following expressions:

$$\Sigma_i(\omega,\mathbf{k}) = n_0\int \frac{|\Delta_1(\mathbf{q})|^2}{\omega-\mu+\varepsilon_i(\mathbf{k}-\mathbf{q})+i\cdot 0\,\mathrm{sgn}\,\omega}\,\frac{d\mathbf{q}}{(2\pi)^3}. \tag{17}$$

where n_0 is the impurity concentration, and $\Delta_1(\mathbf{q})$ is the order parameter (13) for one impurity atom.

Two requirements must be fulfilled, if we want to use the "cross" technique. The first is related to the contribution of neglected "localization" diagrams:

$$\frac{|\mathrm{Im}\,\Sigma_i(E_i(\mathbf{k}),\mathbf{k})|}{\varepsilon_F} \ll 1. \tag{18}$$

The second one, making use of the Born approximation in the potential $\Delta_1(\mathbf{q})$, reduces, in our case, to the inequality

$$\left[\frac{V_{12}N(0)}{g_s}\,\frac{\pi}{2}\left(\frac{\mu_{cr}}{\varepsilon_F}\right)^2 \xi q_0\right]^2 \ll 1. \tag{19}$$

Using (13), we get from (17) the following expressions for $\Sigma_i(\omega,\mathbf{k})$ for $\mathbf{k}$ near the Fermi surface of the corresponding band i:

$$\begin{cases} \operatorname{Im}\Sigma_i(\tilde{\omega},\mathbf{k}) = -u\varepsilon_F \operatorname{sgn}(\tilde{\omega}+\mu) \\ \times\left\{\frac{\pi}{2} - \operatorname{arctg}\left[\xi q_0\left(\frac{|\tilde{\omega}+\varepsilon_i(\mathbf{k})|}{v_F q_0} - 1\right)\right]\right. \\ \left. - \frac{(|\tilde{\omega}+\varepsilon_i(\mathbf{k})|/v_F q_0 - 1) - (\xi q_0)^{-2}}{\xi q_0(|\tilde{\omega}+\varepsilon_i(\mathbf{k})|/v_F q_0 - 1)^2 + (\xi q_0)^{-1}}\right\}, \\ \operatorname{Re}\Sigma_i(\omega,\mathbf{k}) = u\varepsilon_F \frac{2}{\pi}\xi q_0 \int_0^\infty \frac{x}{[1+(\xi q_0)^2(x-1)^2]^2} \\ \times \ln\left|\frac{x+(\tilde{\omega}+\varepsilon_i(\mathbf{k}))/v_F q_0}{x-(\tilde{\omega}+\varepsilon_i(\mathbf{k}))/v_F q_0}\right| dx. \end{cases} \tag{20}$$

We have introduced the notations $\tilde{\omega} = \omega - \mu$, and

$$u = 28.8\left[\frac{V_{12}N(0)}{g_s}\right]^2\left(\frac{\mu_{\text{кр}}}{\varepsilon_F}\right)^5 n_0\xi^3. \tag{21}$$

It follows from (20) that for $|\tilde{\omega} + \varepsilon_i(\mathbf{k}) \pm v_F q_0| \gtrsim v_F/\xi$ and at $\tilde{\omega} = -\varepsilon_i(\mathbf{k}) \pm v_F q_0$

$$\begin{cases} \operatorname{Re}\Sigma_i(\tilde{\omega},\mathbf{k}) \approx u\varepsilon_F \ln\left|\frac{1+(\tilde{\omega}+\varepsilon_i(\mathbf{k}))/v_F q_0}{1-(\tilde{\omega}+\varepsilon_i(\mathbf{k}))/v_F q_0}\right|, \\ \qquad\qquad |\tilde{\omega}+\varepsilon_i(\mathbf{k}) \pm v_F q_0| \gtrsim \frac{v_F}{\xi}, \\ \operatorname{Re}\Sigma_i(\tilde{\omega}=-\varepsilon_i(\mathbf{k})\pm v_F q_0, \mathbf{k}) \approx 0{,}64 u\varepsilon_F \xi q_0. \end{cases} \tag{22}$$

Using (20), (21) and (18), we find

$$\frac{\varepsilon_F}{v_F q_0} u \ll 1. \tag{23}$$

Figure 1 shows $\operatorname{Re}\Sigma_i(\tilde{\omega},\mathbf{k})$ and $\operatorname{Im}\Sigma_i(\tilde{\omega},\mathbf{k})$ as functions of $x = \tilde{\omega} + \varepsilon_i(\mathbf{k})$ (solid lines). According to (16), the intersection points of the plots of $\operatorname{Re}\Sigma_i(\tilde{\omega},\mathbf{k})$ and $[x - 2\varepsilon_i(\mathbf{k})]$ give the spectrum of elementary excitations $E_i(\mathbf{k})$, and $\operatorname{Im}\Sigma_i[E_i(\mathbf{k}),\mathbf{k}]$ give their damping. The general form of the spectrum E_i as a function of $\varepsilon_i(\mathbf{k})$ for different values of the parameter $2u\varepsilon_F/v_F q_0$ is shown in Fig. 2. As is well-known, quasiparticles are well defined if the condition

$$\operatorname{Im}\Sigma_i(E_i(\mathbf{k}),\mathbf{k}) \ll 1,$$

is fulfilled. This is realized in the system under study in spectral regions

$$|E_i(\mathbf{k}) + \varepsilon_i(\mathbf{k})| \gtrsim v_F q_0. \tag{24}$$

Substituting (20) into (16), we find the following expression for the density of states near the Fermi surface:

$$N_i(E) = N(0)\int_{-\infty}^{\infty} \times \frac{1}{\pi}\frac{\operatorname{Im}\Sigma_i(y)/v_F q_0}{[E - y - \operatorname{Re}\Sigma_i(y)/v_F q_0]^2 + [\operatorname{Im}\Sigma_i(y)/v_F q_0]^2} dy, \tag{25}$$

where

$$y = (\tilde{\omega}+\varepsilon_i(\mathbf{k}))/v_F q_0, \quad E = 2\tilde{\omega}/v_F q_0.$$

Expressions (20) and (25) show that

$$v_F q_0 \approx 1{,}8\Delta_0,$$

where Δ_0 is the mean-field gap for

$$T = \mu = V_{imp}(\mathbf{r}) = 0$$

(see Sec. 3), is the characteristic energy scale of the density of states.

Figure 3 shows the results of computer calculations for the following sets of parameters

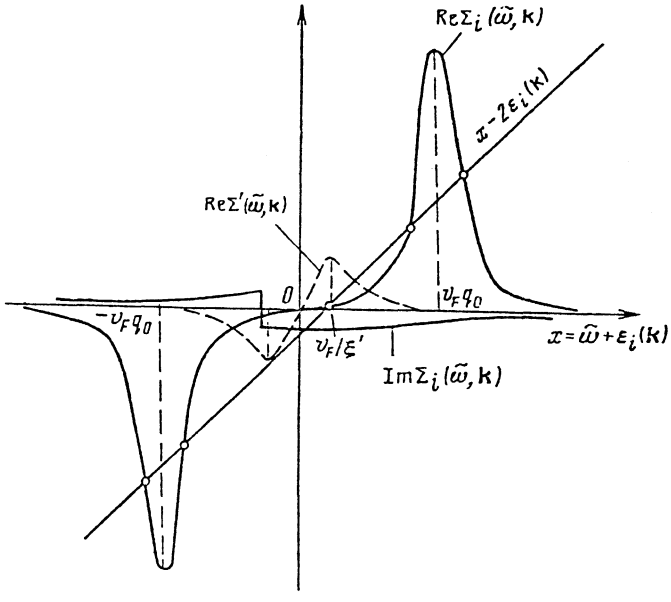

FIG. 1. Self-energy part in a system with medium-range dielectric order unstable against the transition into an inhomogeneous state (solid lines) and into a homogeneous one (dashed lines).

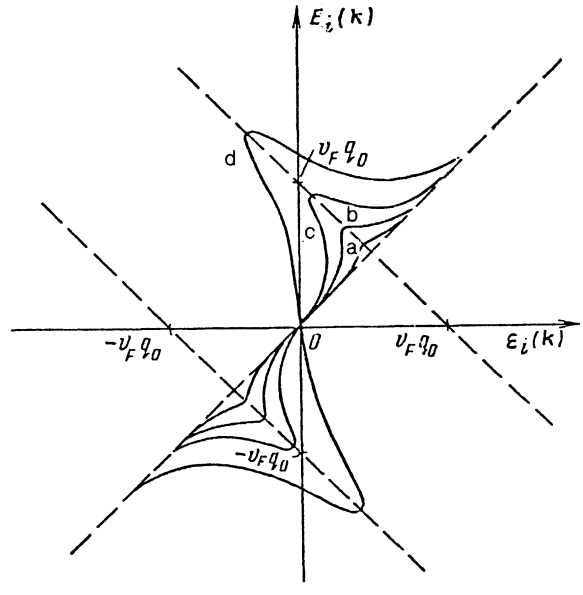

FIG. 2. One-particle excitation spectrum $E_i(\mathbf{k})$ of a system with medium-range dielectric order unstable against the transition into an inhomogeneous state (plots *a*, *b*, and *c* correspond to $2u\varepsilon_F/v_F q_0 < 1$, and plot *d* to $2u\varepsilon_F/v_F q_0 > 1$).

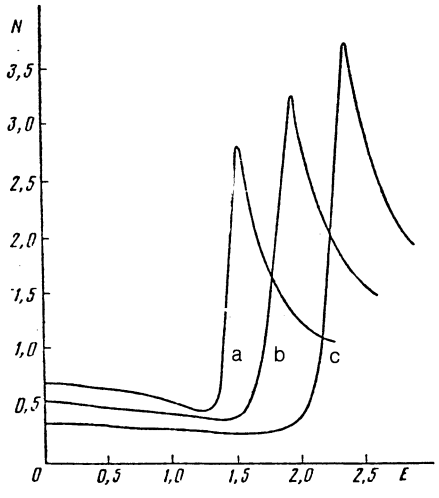

FIG. 3. Density of states in a system with medium-range dielectric order unstable against the transition into an inhomogeneous state.

a) $2u\varepsilon_F/v_Fq_0=0{,}2$ $\xi q_0=8$,
b) $2u\varepsilon_F/v_Fq_0=0{,}4$ $\xi q_0=10$,
c) $2u\varepsilon_F/v_Fq_0=0{,}8$, $\xi q_0=12$.

Evidently, we get a pseudogap structure of the density of states with a characteristic energy scale of the pseudogap $\sim v_F q_0$ and well pronounced peaks of the density of states at its boundary. The coordinates of these peaks are found from the condition that the absolute value of

$$\left.\frac{dE_i(\mathbf{k})}{d\varepsilon_i(\mathbf{k})}\right|_{E_i(\mathbf{k})=\tilde{\omega}_{max}},$$

is minimal, which, together with (20) and (22), gives

$$\tilde{\omega}_{max}=\pm\frac{1}{2}v_Fq_0\left\{1+\frac{2u\varepsilon_F/v_Fq_0}{1+(1+2u\varepsilon_F/v_Fq_0)^{1/2}}+\frac{u\varepsilon_F}{v_Fq_0}\ln\frac{(1+(1+2u\varepsilon_F/v_Fq_0)^{1/2})^2}{2u\varepsilon_F/v_Fq_0}\right\}. \tag{26}$$

Thus, the pseudogap width equals $2|\tilde{\omega}_{\max}|$. The amplitude of the density of states at the maixmum, $N(\tilde{\omega}_{\max})$, is proportional to $\tilde{\omega}_{\max}$. Outside the pseudogap energy scale, for

$$|\tilde{\omega}|\geqslant|\omega_{max}|+v_F/\xi$$

the density of states is

$$N(\tilde{\omega})\approx N(0)\frac{\tilde{\omega}}{(\tilde{\omega}^2-\tilde{\omega}_{max}^2)^{1/2}},$$

as in the case of commensurate CDW with long-range order in the system.

When the system moves away from the point of instability against the transition into the state with long-range CDW or SDW order [this corresponds to the increase in the parameter u [see (21)] and correlation length ξ], the density of states grows on the energy scale of the pseudogap, while the peak amplitude falls off (see Fig. 3). The peaks themselves draw together in such a way that the pseudogap width is always larger than $v_F q_0$ [see (26)]. Such an evolution of the CDW-pseudogap has been found in optical experiments[4-6] on $BaPb_{1-x}Bi_xO_3$ in the Pb concentration range, where the long-range CDW order is suppressed.

As has already been noted, well defined quasiparticles exist in the spectral regions given by (24). It is just these sepctral regions that lie outside the energy interval of the pseudigap and turn into quasiparticles when the long-range order sets in. The states inside the pseudogap have a very strong damping and therefore contribute mainly to the incoherent part of the spectral function $A(\mathbf{k},\omega)$, which is the integrand in (16).

Before discussing the physical cause of formation, by the medium-range order, of a pseudogap on a characteristic energy scale

$$v_Fq_0\gg v_F/\xi,$$

in a system, which tends to a phase transition into an inhomogeneous state, we consider the same problem for a system near (above) the point of phase transition into a homogeneous (i.e., with $q_0\equiv 0$) state. For this purpose, instead of (12), we must use

$$\Pi(\mathbf{q},\mu)=\frac{1}{g_s}-\frac{|\mu|-\mu'_{cr}}{\mu'_{cr}}-\alpha\left(\frac{v_F}{\mu'_{cr}}\right)^2\mathbf{q}^2, \tag{12'}$$

where

$$\mu'_{cr}={}^1/_2\Delta_0=\varepsilon_F\exp(-1/g_s)$$

(see Ref. 28),

$$\alpha=\frac{7\zeta(3)}{48\pi^2},$$

and $\zeta(3)\approx 1.2$ is the Riemann zeta-function for the argument equal to 3.

Instead of (13), we find

$$\Delta_s'(\mathbf{r})=\frac{V_{12}}{g_s}\frac{(\mu'_{cr})^2}{4\pi\alpha v_F^2}\sum_a\frac{\exp\{i\mathbf{Q}(\mathbf{r}-\mathbf{r}_a)-|\mathbf{r}-\mathbf{r}_a|/\xi'\}}{|\mathbf{r}-\mathbf{r}_a|}, \tag{14'}$$

where the correlation length is

$$\xi'=\left(\frac{\alpha v_F^2}{\mu'_{cr}(|\mu|-\mu'_{cr})}\right)^{1/2}.$$

For the self-energy parts, instead of (20), we get

$$\begin{cases}\operatorname{Im}\Sigma_i'(\tilde{\omega},\mathbf{k})=-\dfrac{u'\varepsilon_F\operatorname{sgn}(\tilde{\omega}+\mu)}{1+(\xi'/v_F)^2(\tilde{\omega}+\varepsilon_i(\mathbf{k}))^2}\\ \operatorname{Re}\Sigma_i'(\tilde{\omega},\mathbf{k})=u'\varepsilon_F\dfrac{(\xi'/v_F)(\tilde{\omega}+\varepsilon_i(\mathbf{k}))}{1+(\xi'/v_F)^2(\tilde{\omega}+\varepsilon_i(\mathbf{k}))^2},\end{cases} \tag{20'}$$

where

$$\tilde{\omega}=\omega-\mu$$

and

$$u'=\frac{\pi^3}{8\alpha^2}\left[\frac{V_{12}N(0)}{g_s}\right]^2\left(\frac{\mu'_{cr}}{\varepsilon_F}\right)^4 n_0(\xi')^2\frac{v_F}{\varepsilon_F}. \tag{21'}$$

Inequality (18), together with (20), gives

$$\frac{\varepsilon_F}{\mu'_{cr}}u'\ll 1. \tag{23'}$$

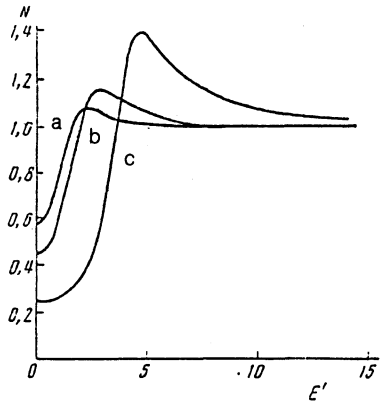

FIG. 4. Density of states in a system with medium-range dielectric order unstable against the transition into a homogeneous state.

It is necessary to replace (19) by

$$\left[\frac{1}{4\alpha}\frac{V_{12}N(0)}{g_s}\left(\frac{\mu'_{cr}}{\varepsilon_F}\right)^2\right]^2 \ll 1. \qquad (19')$$

The plot of $\mathrm{Re}\,\Sigma_i'(\tilde{\omega},\mathbf{k})$ is shown in Fig. 1 (dashed line).

Substituting (20') into (16), we get

$$N(E') = N(0)\int_{-\infty}^{\infty}\frac{1}{\pi} \times \frac{|\mathrm{Im}\,\Sigma_i'(y')|/(v_F/\xi')}{[E'-y'-\mathrm{Re}\,\Sigma_i'(y')/(v_F/\xi')]^2+[\mathrm{Im}\,\Sigma_i'(y')/(v_F/\xi')]^2}dy', \qquad (25')$$

where

$$y' = \frac{\tilde{\omega}+\varepsilon(\mathbf{k})}{v_F/\xi'}, \quad E' = \frac{2\tilde{\omega}}{v_F/\xi'}.$$

Expressions (20') and (25') show that the medium-range order in a system undergoing a phase transition into a homogegeneous state gives rise to a characteristic scale length v_F/ξ' of the density of states. Figure 4 shows the results of computer calculations of $N_i(E')$ for the following parameters

a) $2u'\varepsilon_F\xi'/v_F=1$,
b) $2u'\varepsilon_F\xi'/v_F=2$,
c) $2u'\varepsilon_F\xi'/v_F=8$.

The phase transition into a homogeneous state with long-range order is due to the correlation of an electron with momentum $\mathbf{k}$ from band 1 and a hole with momentum $\mathbf{k}-\mathbf{Q}$ from band 2. In contrast to this, the medium-range order in such a system is formed due to correlations of an electron with momentum $\mathbf{k}$ from band 1 with an ensemble of holes from band 2 whose momenta lie inside a sphere of effective radius $(\xi')^{-1}$ with the center at the point $\mathbf{k}-\mathbf{Q}$ (Fig. 5). The phase volume of these states is $4/3\pi(\xi')^{-3}$. As a result, the characteristic energy scale length for the density of states is v_F/ξ'.

The phase transition into an inhomogeneous state with long-range order is due to the correlation of an electron of momentum $\mathbf{k}$ from band 1 and a discrete (finite) set of hole states from band 2 with momenta $\mathbf{k}-\mathbf{q}$. The vectors $\mathbf{q}$ are given by the absolute value of the inhomogeneity vector $\mathbf{q}-\mathbf{Q}$:

$$|\mathbf{q}-\mathbf{Q}| = q_0 \approx 2{,}4|\mu|/v_F.$$

The medium-range order in such a system is formed by the correlated motion of an electron with momentum $\mathbf{k}$ from band 1 and an ensemble of holes from band 2, both inside a spherical layer of effective thickness ξ^{-1}. The radius of the sphere equals q_0 and its center is at the point $\mathbf{k}-\mathbf{Q}$ (Fig. 5). The phase volume occupied by this ensemble (the volume of spherical layer) is large and equal to

$$4\pi q_0^2\xi^{-1} \gg {}^4/_3\xi^{-3}.$$

This is why the medium-range order in a system undergoing phase transition into an inhomogeneous state forms a pseudogap on a characteristic energy scale

$$\sim v_F q_0 \gg v_F/\xi.$$

Such a system with medium-range order is much closer in its properties [the excitation spectrum, density of states (and, as a result, thermodynamic properties), optical and tunnel characteristics, etc.] to a system with long-range dielectric order than a system with medium-range order unstable against the phase transition into a homogeneous state. This is also reflected in the fact that the ratio of correlation lengths in these two cases, under the condition of equal proximity to the transition point, is

$$\frac{\xi}{\xi'} = \left(\frac{0{,}568\,\mu'_{cr}}{\alpha\mu_{cr}}\right)^{1/4} \approx 5.$$

The effect of anitferromagnetic spin fluctuations on the excitation spectrum and density of states of a two-dimensional metal given by the Hubbard model for $T=0$ and occupation deviating from half occupation ($\mu \neq 0$) has recently been discussed.[29] However, attention has mainly been paid to the case of system instability against the transition

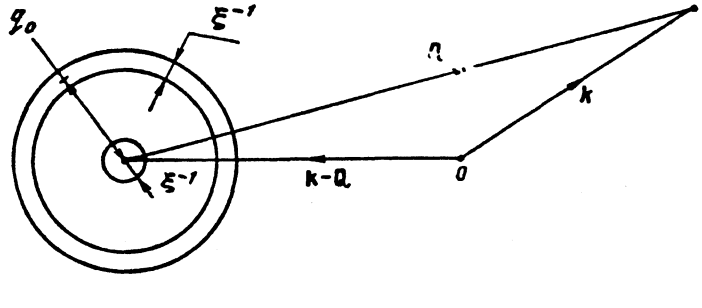

FIG. 5. To the question of correlation between an electron of momentum $\mathbf{k}$ from band 1 and holes of momenta $\mathbf{k}-\mathbf{q}$ from band 2 in systems with medium-range order.

into a homogeneous state with the SDW. The random phase approximation has been used and the solution has been extrapolated to the region of intermediate and strong interaction ($U/W \geqslant 1$), where the size of the ordering region is determined by the ineratomic distance.[30] The pseudogap energy scale is therefore determined by the quantity

$$\frac{v_F}{a} \sim W \gg v_F q_0$$

(here a is the interatomic distance), as found by the authors of Ref. 29.

As already noted in the Introduction, the large values of the static dielectric constant in the long wavelength limit[7-9] and anomalously high mobility of oxygen[10] and copper[11] ions in HTSC are, evidently, related to the proximity of these systems to instability against charge transfer from copper (in cuprate superconductors) or bismuth [in Ba(K,Pb)BiO] to oxygen (charge instability). In Refs. 12–14 the charge instability has been regarded as a cause of radical increase in the superconducting transition temperature due to peculiar momentum and frequency dependences of electron–electron interaction in the Cooper channel.

The theory developed in the present paper for medium-range CDW or SDW order in systems close to the instability against the transition into an inhomogeneous state suggests the following scenario of evolution of HTSC under doping. Undoped systems (La_2CuO_4, $YBa_2Cu_3O_6$, $BaBiO_3$, etc.) are unstable against the formation of long-range CDW or SDW order due to the "nesting" of the Fermi surface in the initial antibonding band (mainly copper for cuprate HTSC and bismuth for $BaBiO_3$). This band splits into two subbands and the upper part of the bonding (mainly, oxygen) band falls into the energy interval of the formed CDW or SDW gap. With doping the long-range charge or spin order is suppressed, the subbands draw together, but the medium-range order (with $q_0 \neq 0$) prevents the CDW or SDW pseudogap from "collapsing." For certain doping (probably, corresponding to the superconductivity optimum) the distance between the Fermi level in the oxygen band and the maximum of the density of states, which corresponds to the upper CDW or SDW subband, turns out to be smallest. This doping corresponds precisely to the greatest proximity of the system to charge instability connected with the carrier interaction in the oxygen and upper CDW or SDW subband. In the next section we consider the exitation spectrum and density of states of a system close to charge instability.

5. BEHAVIOR OF A SYSTEM CLOSE TO CHARGE INSTABILITY

As the model of a bare excitation spectrum of a system tending to charge instability we use the two-band spectrum (1), where it is necessary, however, to replace ε_F by $-E_g/2$ (E_g is the band gap width). Furthermore, we assume that the semiconductor is a direct-band one, i.e., we set $Q = 0$.

In the isotropic case [$\varepsilon(k) = \mathbf{k}^2/2m$] at $T = 0$ the polarization operator (11) [it is necessary to replace $N(0)$ by the quantity $N(E_g) = m(mE_g)^{1/2}/2\pi$ having the dimensions of the density of states] is

$$\Pi(q,\mu) = \frac{1}{2}\left\{\frac{\tilde{p}^2+1}{\tilde{q}}\ln\frac{(\tilde{p}+\tilde{q}/2)^2+1}{(\tilde{p}-\tilde{q}/2)^2+1} - \frac{\alpha^2+1}{\tilde{q}}\ln\frac{(\alpha+\tilde{q}/2)^2+1}{(\alpha-\tilde{q}/2)^2+1} + 2\tilde{p} - 2\alpha - 2(\tilde{q}^2/4+1)^{1/2}\left(\operatorname{arctg}\frac{\tilde{p}+\tilde{q}/2}{(\tilde{q}^2/4+1)^{1/2}} + \operatorname{arctg}\frac{\tilde{p}-\tilde{q}/2}{(\tilde{q}^2/4+1)^{1/2}} - \operatorname{arctg}\frac{\alpha+\tilde{q}/2}{(\tilde{q}^2/4+1)^{1/2}} - \operatorname{arctg}\frac{\alpha-\tilde{q}/2}{(\tilde{q}^2/4+1)^{1/2}}\right)\right\}, \tag{27}$$

where

$$\tilde{p} = \frac{(2m\omega_0)^{1/2}}{(mE_g)^{1/2}}, \quad \tilde{q} = \frac{|\mathbf{q}|}{(mE_g)^{1/2}}, \quad \alpha = \left(\frac{2|\mu|}{E_g} - 1\right)^{1/2}$$

and ω_0 is the cutoff energy of the order of the allowed band width.

In the limit of interest,

$$\tilde{p} \gg 1, \quad \tilde{p} \gg \tilde{q}, \quad \tilde{p} \gg \alpha$$

Eq. (27) reduces to

$$\Pi(q,\mu) = \frac{1}{2}\left\{4\tilde{p} - 2\alpha - 2\pi(\tilde{q}^2/4+1)^{1/2} - \frac{\alpha^2+1}{\tilde{q}}\ln\frac{(\alpha+\tilde{q}/2)^2+1}{(\alpha-\tilde{q}/2)^2+1} + 2(\tilde{q}^2/4+1)^{1/2} + 1\left(\operatorname{arctg}\frac{\alpha+\tilde{q}/2}{(\tilde{q}^2/4+1)^{1/2}} + \operatorname{arctg}\frac{\alpha-\tilde{q}/2}{(\tilde{q}^2/4+1)^{1/2}}\right)\right\}. \tag{28}$$

If we study (28) as a function of $\mathbf{q}$, we find that $\Pi(\mathbf{q},\mu)$ has a single maximum at the point $\mathbf{q} = 0$. Expanding (28) in a series in $\tilde{q} \ll 1$ and $\alpha \ll 1$, we get

$$\Pi(q,\mu) = 2\tilde{p} - \pi - {}^1/_3\alpha^3 - {}^1/_8\pi\tilde{q}^2. \tag{29}$$

The critical value of doping at which the long-range dielectric order can arise in the limit of weak interaction [$g = \lambda N(E_g) \ll 1$, where λ is a dimensional interaction constant for band-1 electrons and band-2 holes] is given by the equation

$$\frac{1}{g} = \Pi(\mathbf{q}=0,\mu). \tag{30}$$

As noted in the previous section, in HTSC doping leads to relative motion of the oxygen and upper CDW or SDW bands. With increasing μ (we assume for definiteness that $\mu > 0$, which corresponds to hole HTSC E_g decreases. Therefore in the framework of the model considered we must assume that E_g is a function of μ, and for a certain composition range (in which, as shown by experiment, conditions optimal for superconductivity are realized in HTSC) the system is close to but above the point of formation of long-range dielectric order. Equation (30) may not have any solution for any value of the parameter μ. In what follows we will consider precisely this situation, which is evidently realized in HTSC.

The condition that $\Pi(\mathbf{q} = 0,\mu)$ has a maximum, as a function of μ, gives an equation for μ_{cr}:

$$-\left(\frac{2m\omega_0}{mE_g(\mu_{cr})}\right)^{1/2}\frac{dE_g(\mu)}{d\mu}\Big|_{\mu=\mu_{cr}}=\left(\frac{2\mu_{cr}}{E_g(\mu_{cr})}-1\right)^{1/2}$$

$$\times\left(1-\frac{\mu_{cr}}{E_g(\mu_{cr})}\frac{dE_g(\mu)}{d\mu}\Big|_{\mu=\mu_{cr}}\right). \quad (31)$$

Using (10) and (29), we find the solution for the order parameter $\Delta(\mathbf{q})$ in the case of charge instability:

$$\Delta(\mathbf{q})=\frac{V_{12}\Pi(0,\mu)}{\frac{1}{g}-\Pi(0,\mu)}\frac{\sum_a \exp(i\mathbf{q}\mathbf{r}_a)}{1+\xi^2\mathbf{q}^2}, \quad (32)$$

where the correlation length is

$$\xi=\left(\frac{\pi}{8mE_g(1/g-\Pi(0,\mu))}\right)^{1/2}.$$

In configuration space we have correspondingly

$$\Delta(\mathbf{r})=\frac{V_{12}\Pi(0,\mu)}{4\pi(1/g-\Pi(0,\mu))\xi^2}\sum_a\frac{\exp(-|\mathbf{r}-\mathbf{r}_a|/\xi)}{|\mathbf{r}-\mathbf{r}_a|}. \quad (33)$$

Using (32), we find from (17) the following expressions for self-energy parts $\Sigma_i(\omega,\mathbf{k})$, $i=1,2$ (the upper sign corresponds to $i=1$, the lower to $i=2$):

$$\begin{cases} \operatorname{Im}\Sigma_i(\tilde\omega,\mathbf{k})=-\dfrac{\pi uE_g}{\xi k}\left\{\dfrac{1}{1+\xi^2[k-(2m(\mp\tilde\omega-E_g/2))^{1/2}]^2}\right. \\ \left.-\dfrac{1}{1+\xi^2[k-(2m(\mp\tilde\omega-E_g/2))^{1/2}]}\right\} \\ \times\theta\left(\mp\tilde\omega-\dfrac{E_g}{2}\right)\operatorname{sgn}(\tilde\omega+\mu), \\ \operatorname{Re}\Sigma_i(\tilde\omega,\mathbf{k}) \\ =\pm\dfrac{2uE_g}{\xi k}\displaystyle\int_0^\infty\frac{q}{(1+q^2)^2} \\ \times\ln\left|\dfrac{\pm\tilde\omega+E_g/2+(k+q\xi^{-1})^2/2m}{\pm\tilde\omega+E_g/2+(k-q\xi^{-1})^2/2m}\right|dq, \end{cases} \quad (34)$$

where $\tilde\omega=\omega-\mu$, $k=|\mathbf{k}|$ and a dimensionless parameter u is introduced:

$$u=\left(\frac{V_{12}\Pi(0,\mu)m(mE_g)^{1/2}}{\pi^2}\right)^2 n_0\xi^3. \quad (35)$$

Using Eq. (16) for the density of states $N_i(\omega)$ together with (34), we find (as before, the upper sign corresponds to $i=1$, while the lower one to $i=2$):

$$\begin{cases} N_i(\tilde\omega)=N_i^+(\tilde\omega)+N_i^-(\tilde\omega), \\ N_i^+(\tilde\omega)=(1/4\pi^2)[1+(\tilde\omega^2-\pi uE_g\xi^{-2}/m)^{1/2}/|\tilde\omega|]^{1/2} \\ \times m[2m(\tilde\omega^2-\pi uE_g\xi^{-2}/m)^{1/2}-E_g/2]^{1/2} \\ \times\theta[\pm\tilde\omega-(E_g^2/4+\pi uE_g\xi^{-2}/m)], \\ N_i^-(\tilde\omega)=(uE_g/8\pi\tilde\omega^2\xi^2) \\ \times[2m(\mp\tilde\omega-E_g/2)]^{1/2}\theta(\mp\tilde\omega-E_g/2), \\ u\ll 1. \end{cases} \quad (36)$$

The contribution of $N_i^+(\tilde\omega)$ to the density of states is related to well defined quasiparticles (with infinite lifetime) having the dispersion law

$$E_i(\mathbf{k})=\pm[\varepsilon_i^2(\mathbf{k})+\pi uE_g\xi^{-2}/m]^{1/2}.$$

The renormalization constant (residue) of these quasiparticles is

$$z_i(\mathbf{k})=\frac{1}{2}\left(1+\frac{\varepsilon_i(\mathbf{k})}{E_i(\mathbf{k})}\right).$$

The contribution $N_i^-(\tilde\omega)$ to the density of states is related to the splitting of a part of the density of states from band i (owing to which the residue $z_i(\mathbf{k})$ corresponding to the quasiparticles $E_i(\mathbf{k})$, which form $N_i^+(\tilde\omega)$, is strictly less than unity) and transfer of this part to the extremum of the opposite band.

The relations $N_i^+(\tilde\omega)$ and $N_i^-(\tilde\omega)$, $i=1,2$ (thin lines) and $N(\tilde\omega)=N_1(\tilde\omega)+N_2(\tilde\omega)$ (thick line) are shown in Fig. 6. The density of states corresponding to the seed spectrum $\varepsilon_i(\mathbf{k})$ is shown by dashed lines.

6. CONCLUSION

In the present study we have used a microscopic approach to examine the formation of regions having medium-range charge or spin order and the influence of these regions on the excitation spectrum and density of states of a system above the point of phase transition into the state with long-range CDW or SDW order. As a source of medium-range

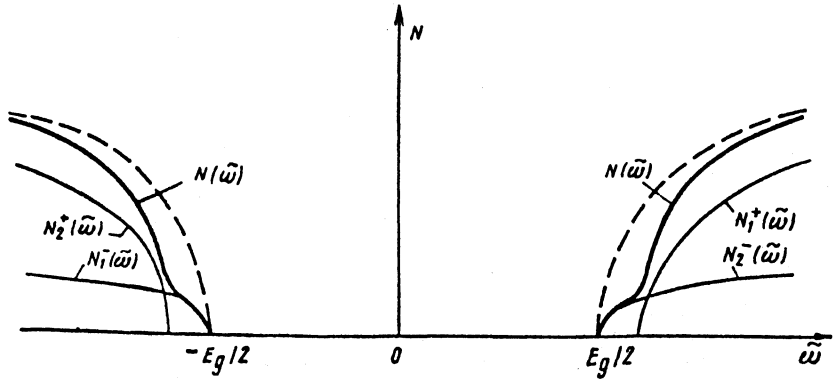

FIG. 6. Density of states for a system near charge instability.

order we have used an impurity potential of the "random field" type. However, as already noted in Introduction, all the results, with appropriate notations, can be transferred to the case of dynamic fluctuations resulting from charge or spin electron-electron correlations in the system.

We have assumed that $T = 0$, but the results will be qualitatively valid if we consider the system near the whole line of phase transition into the state with long-range order in the "temperature-doping" coordinates.

We have considered the system above the point of transition into the state with long-range dielectric order. However, the effects of medium-range order will also play an important role below (but near) the point of this transition. In particular, as shown in Sec. 2, the effect of medium-range order formation is stronger than the "$1/\tau$ effect" of long-range order suppression. Therefore, below (but near) the point of transition into the state with long-range ordering the quantity $|\langle\Delta\rangle|$ determined by the long-range order is smaller than the quantity $\langle|\Delta|\rangle$ determined mainly by the medium-range order (as usual, the brackets mean averaging over the impurities in the system). Therefore the pseudogap structure of the density of states will be observed also below the phase transition point.

The long-range order will manifest itself in suppression of the density of states in the middle of the pseudogap on small (of order $|\langle\Delta\rangle|$ energy scales.

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