Dynamical charge susceptibility in layered cuprates: Beyond the conventional random-phase-approximation scheme

M. Eremin,[1] I. Eremin,[1,2] and S. Varlamov[1,3]
[1]*Physics Department, Kazan State University, Kremlyovskaya 18, 42008 Kazan, Russia*
[2]*Institut für Theoretische Physik, Freie Universität Berlin, D-14195 Berlin, Germany*
[3]*Brandenburgische Technische Universität Cottbus, D-03013 Cottbus, Germany*
(Received 11 January 2001; published 13 November 2001)

The analytical expression for a dynamical charge susceptibility in layered cuprates has been derived in the framework of a singlet-correlated band model beyond the random-phase-approximation (RPA) scheme. Our calculations performed near optimal doping regime show that there is a peak in the real part of the charge susceptibility $\chi_{\mathrm{ch}}(\mathbf{q},\omega)$ at $\mathbf{Q}=(\pi,\pi)$ at strong enough intersite Coulomb repulsion. Together with strong maximum in the Im $\chi_{\mathrm{ch}}(\mathbf{Q},\omega)$ at low frequencies, it confirms the formation of low-energy collective excitations or charge fluctuations. This justifies that these excitations are important and together with spin fluctuations can contribute to the Cooper pairing in layered cuprates. Analyzing the charge susceptibility with respect to the instability we obtain a new plasmon branch, $\omega_{\mathbf{q}}$, along the Brillouin zone (BZ). In particular, we have found that it goes to zero around $\mathbf{Q}\approx(\pi,\pi)$.

DOI: 10.1103/PhysRevB.64.214512 PACS number(s): 74.72.−h, 75.40.Gb, 74.20.Mn, 71.45.Lr

I. INTRODUCTION

The phenomenon of high-temperature superconductivity cannot be completely understood without clarification of a "pseudogap" feature observed by many experimental techniques in the normal state of underdoped cuprates. There are few informative reviews and papers devoted to this problem (see, for example, Refs. 1–4). One of the most reasonable points of view is that a pseudogap in the density of states appears due to an instability in two-dimensional copper-oxygen planes. The important question to answer is, what is the physical origin of this possible instability in layered cuprates? In a recent paper the pseudogap phenomenon has been considered in a context of a new hidden order parameter with orbital antiferromagnetism (a special case of d-wave order parameter[5]). Constructing the integral equation for the extended charge density wave (CDW) instability in a frame of the t-J Hamiltonian proposed by Anderson *et al.*[6] it is easy to prove that for $q=(\pi,\pi)$ the order parameter for the charge instability indeed has a d-wave symmetry. However, the order parameter is imaginary,[7] and therefore it is not a usual charge density wave. This reminds us of an old problem of the itinerant currents studied many years ago in semiconductors.[8,9]

Perhaps the most convincing evidence about the instability in layered cuprates can be obtained directly within the analysis of a dynamical charge and a spin susceptibilities. In contrast to the spin susceptibility, the role played by the instabilities in the charge channel with respect to a pairing and a pseudogap formation is not clear. Moreover, the form of the charge susceptibility beyond the random-phase approximation (RPA) scheme was much less investigated. In particular, there is no agreement concerning its analytical form if the effect of strong electron correlations is taken into account (for example, compare the results in Refs. 10–12). Therefore, the theoretical investigation in this direction becomes very actual.

Here, using the singlet-correlated band model (Refs. 13 and 14 and references therein), which under a simplified assumption about the energy dispersion and the screened Coulomb repulsion is equivalent to t-J model,[15] using the projecting Hubbard-like operators,[16] we derive the expression for the dynamical charge susceptibility beyond the RPA scheme. We analyze the obtained expression numerically and find that the charge susceptibility shows a peak at $\mathbf{Q}=(\pi,\pi)$ similarly to the spin susceptibility only if one takes into account a strong enough intersite Coulomb repulsion. Investigating the denominator of the charge susceptibility we have found a possible dispersion curve of CDW-like excitations ω_q, for slightly underdoped cuprates.

II. MODEL HAMILTONIAN AND BACKGROUND

The Hamiltonian of the singlet-correlated band model in terms of Hubbard-type projecting operators, $\Psi_i^{\alpha,\beta}=|i,\alpha\rangle\langle i,\beta|$ reads as

$$H=\sum t_{ij}\Psi_i^{pd,\sigma}\Psi_j^{\sigma,pd}+\sum_{i>j}J_{ij}\left((S_iS_j)-\frac{n_in_j}{4}\right)+\sum_{i>j}G_{ij}\delta_i\delta_j, \tag{1}$$

where t_{ij} is a hopping integral and J_{ij} is a superexchange constant of copper spins, $\sigma=\pm1/2$. The symbol pd corresponds to a Zhang-Rice singlet with one hole placed on copper and the second hole distributed on neighboring oxygen sites[15] and carrying spin states. G_{ij} is a screened intersite Coulomb repulsion of doped holes. Since we are working in a one-band approximation, the hole doping is determined as $\delta_i=\Psi_i^{pd,dp}$. $1+\delta=\langle\Sigma\Psi_i^{\sigma\sigma}+2\Psi_i^{pd,dp}\rangle$ defines a chemical potential and $1_i=\Sigma_\sigma\Psi_i^{\sigma\sigma}+\Psi_i^{pd,dp}$ expresses the completeness relation. The Ψ operators obey the specific commutation relation and on-site multiplication rules of Hubbard-like operators which can be found elsewhere.[17,18] The spin and density operators are expressed by projecting operators as follows:

$$S_i^+=\Psi_i^{\uparrow,\downarrow},\quad S_i^-=\Psi_i^{\downarrow,\uparrow},\quad S_i^z=\frac{1}{2}(\Psi_i^{\uparrow,\uparrow}-\Psi_i^{\downarrow,\downarrow}). \tag{2}$$

Let us now preliminarily discuss the nature of the density wave formation in a frame of our model. We are going to study the objects that can be described by the following operators:

$$\eta_q=\frac{1}{2}\sum A(\mathbf{k},\mathbf{q},\omega)[\Psi_{k+q}^{pd,\uparrow}\Psi_k^{\uparrow,pd}+\Psi_{k+q}^{pd,\downarrow}\Psi_k^{\downarrow,pd}], \tag{3}$$

$$\xi_q=\frac{1}{2}\sum B(\mathbf{k},\mathbf{q},\omega)[\Psi_k^{\uparrow,pd}\Psi_{k+q}^{pd,\uparrow}-\Psi_k^{\downarrow,pd}\Psi_{k+q}^{pd,\downarrow}], \tag{4}$$

where $A(\mathbf{k},\mathbf{q},\omega)$ and $B(\mathbf{k},\mathbf{q},\omega)$ are charge- and spin-excitation amplitudes, respectively. The frequencies of harmonic motion of these objects can be found in a conventional manner:

$$i\frac{\partial\eta_q}{\partial t}=[\eta_q,H]=\omega_q^c\eta_q,\quad i\frac{\partial\xi_q}{\partial t}=[\xi_q,H]=\omega_q^s\xi_q. \tag{5}$$

The real part of η_q corresponds to a conventional CDW order parameter, whereas its imaginary part is responsible for a charge current formation.[9,19] The latter also looks very similar to the proposed earlier flux phase[20] and orbital antiferromagnetism.[5] The real part of ξ_q represents the well-known spin density wave (SDW) and its imaginary quantity is closely related to the so-called spin current formation.[9,19] Symmetry aspects of this interesting problem have been discussed very recently by Nayak[21] and therefore we do not study this problem here. One can immediately see from Eqs. (3) and (4) that the equations for the frequency determination of the real and imaginary parts look very similar and seem to be a good starting point to study both the collective charge and the spin excitations in layered cuprates.

Calculating the commutators using the simplest Hubbard decoupling scheme[16] (for details see the next section) one can find that $A(\mathbf{k},\mathbf{q},\omega)$ and $B(\mathbf{k},\mathbf{q},\omega)$ can be taken in the usual form:

$$A(\mathbf{k},\mathbf{q},\omega)=\frac{1}{\omega_q^c-\epsilon_{k+q}+\epsilon_k},\qquad B(\mathbf{k},\mathbf{q},\omega)=\frac{1}{\omega_q^s-\epsilon_{k+q}+\epsilon_k}, \tag{6}$$

and frequencies are determined by the relations

$$1=\frac{1}{2}\sum\frac{t_{k+q}n_{k+q}-t_kn_k}{\omega_q^c-\epsilon_{k+q}+\epsilon_k}-\left(\frac{J_q}{4}-G_q\right)\sum\frac{n_k-n_{k+q}}{\omega_q^c-\epsilon_{k+q}+\epsilon_k}, \tag{7}$$

$$1=\sum\frac{t_{k+q}\tilde{n}_{k+q}-t_k\tilde{n}_k}{\omega_q^s-\epsilon_{k+q}+\epsilon_k}-\frac{1}{2}J_q\sum\frac{\tilde{n}_{k+q}-\tilde{n}_k}{\omega_q^s-\epsilon_{k+q}+\epsilon_k}, \tag{8}$$

where $n_k=\frac{1}{2}(n_k^{\uparrow}+n_k^{\downarrow})$ and $n_k^{\sigma}=\langle\Psi_k^{pd,\sigma}\Psi_k^{\sigma,pd}\rangle$ is a quasiparticle number, $\epsilon_k=P_{pd}t_k$ is the energy dispersion of the itinerant carriers, $P_{pd}=(1+\delta)/2$ is the Hubbard-type bandwidth narrowing factor. In Eq. (8) $\tilde{n}_k=\frac{1}{2}(\tilde{n}_k^{\uparrow}+\tilde{n}_k^{\downarrow})$ and $\tilde{n}_k^{\sigma}=\langle\Psi_k^{\sigma,pd}\Psi_k^{pd,\sigma}\rangle$ are quasiparticle numbers in the electron representation. The Fourier transforms of the integrals t_k, J_q, and G_q are determined by the conventional expressions

$$t_k=2t_1(\cos k_x+\cos k_y)+4t_2\cos k_x\cos k_y+\cdots, \tag{9}$$

$$J_q=2J_1(\cos q_x+\cos q_y)+4J_2\cos q_x\cos q_y+\cdots, \tag{10}$$

$$G_q=2G_1(\cos q_x+\cos q_y)+4G_2\cos q_x\cos q_y+\cdots, \tag{11}$$

where $t_1(J_1,G_1)$, $t_2(J_2,G_2)$, and t_3 refer to the first, second, and third neighbors, respectively. For simplicity we put a lattice constant equal to unity. The choice of parameters for the hopping integrals is determined by the correct Fermi surface topology and the presence of a van Hove singularity in the vicinity of the Fermi level as observed in the experiment.[22] This holds at $t_1=72$ meV, $t_2=0$, and $t_3=12$ meV. The screened Coulomb repulsion of the doped holes and the superexchange integral between nearest copper spins were taken as G_1 in the range 70–170 meV and $J_1=135$ meV in accordance with first-principles estimations[23] and inelastic neutron scattering experiments,[24] respectively. The range for variation of G_1 was taken in agreement with the calculation of the pseudogap formation temperature in underdoped cuprates on the basis of a CDW type of scenario.[14]

Regarding Eqs. (7) and (8) we would like to note two important features. Both equations determine the condition of the instability of the system with respect to the mentioned types of charge and spin instabilities. In other words, Eqs. (7) and (8) determine the divergences of charge and spin susceptibilities in the normal state. In contrast to the usual RPA-type expression the first terms in Eqs. (7) and (8) are proportional to the hopping integral and result from the strong electron correlation effects due to a no-double-on-site occupancy constraint.[18] It reflects the existence of the very large on-site Coulomb repulsion leading to a renormalization and an enhancement of the susceptibilities (or in other words the presence of strong electron correlation). This non-Fermi-liquid correction was firstly deduced by Hubbard and Jain[25] for the spin susceptibility. The second remark is that as one can see from Eqs. (7) and (8), the screened intersite Coulomb repulsion does not play any role in determining the spin dispersion in contrast to the charge one. Therefore it becomes clear that the equations for charge and spin collective excitations are quite different in the presence of the intersite Coulomb interaction in contrast to what was widely implied. However, our present approach is quite preliminary and in order to see the difference between charge and spin collective excitations in more detail we will calculate the dynamical charge susceptibility and compare its form with the spin counterpart obtained earlier.[26]

III. DYNAMICAL CHARGE SUSCEPTIBILITY: IMPROVED DECOUPLING SCHEME FOR THE EQUATION OF MOTION

We start from the definition of the Fourier transform of the amplitude of the density operator

$$\delta\times\delta_{q,0}+e_q=\Psi_q^{pd,pd}=\frac{1}{N}\sum_k e_{kq}=\frac{1}{2N}\sum_k(\Psi_k^{pd,\uparrow}\Psi_{k+q}^{\uparrow,pd}+\Psi_{k+q}^{pd,\downarrow}\Psi_k^{\downarrow,pd}), \tag{12}$$

where $\delta_{q,0}$ is a delta function and the Fourier transform is defined as

$$\Psi_k^{pd,\uparrow}=\frac{1}{\sqrt{N}}\sum_j \Psi_j^{pd,\uparrow}e^{i\mathbf{k}\cdot\mathbf{R}_j}. \tag{13}$$

In the next step we derive the equation of motion for the two retarded Green's functions

$$\omega_q^c\langle\langle e_q|e_{-q}\rangle\rangle_\omega=\frac{i}{2\pi}\langle[\Psi_q^{pd,pd},\Psi_{-q}^{pd,pd}]\rangle+\langle\langle[\Psi_q^{pd,pd},H]|e_{-q}\rangle\rangle_\omega \tag{14}$$

and

$$\omega_q^c\langle\langle e_{kq}|e_{-q}\rangle\rangle_\omega=\frac{i}{2\pi}\langle[e_{kq},e_{-q}]\rangle+\langle\langle[e_{kq},H]|e_{-q}\rangle\rangle_\omega . \tag{15}$$

We calculate the commutators using the on-site representation of the operators. For example, for the kinetic part of the Hamiltonian H_t, it has a form

$$[\Psi_i^{pd,\uparrow}\Psi_j^{\uparrow,pd},H_t]=\Psi_i^{pd,\uparrow}\sum_l t_{jl}\{\Psi_j^{\uparrow,\downarrow}\Psi_l^{\downarrow,pd}+(\Psi_j^{\uparrow,\uparrow}+\Psi_j^{pd,pd})\Psi_l^{\uparrow,pd}]-\sum_l t_{li}\{\Psi_l^{pd,\downarrow}\Psi_i^{\downarrow,\uparrow}+\Psi_l^{pd,\uparrow}(\Psi_i^{\uparrow,\uparrow}+\Psi_i^{pd,pd})\}\Psi_j^{\uparrow,pd}. \tag{16}$$

This exact result leads, however, to the appearance of a Green's function of higher order. Therefore we made a decoupling in several steps. First, using the equation for the determination of the chemical potential and the definition of the density and spin operators determined in previous section, one can find

$$\Psi_j^{\uparrow,\uparrow}+\Psi_j^{pd,pd}=\frac{1+\delta}{2}+\frac{e_j}{2}+s_j^z, \tag{17}$$

$$\Psi_j^{\downarrow,\downarrow}+\Psi_j^{pd,pd}=\frac{1+\delta}{2}+\frac{e_j}{2}-s_j^z, \tag{18}$$

where δ is an average number of the doped holes per one unit cell as already mentioned and e_i its modulation. The next step is to distinguish the cases $i=j$ and $i\neq j$. In the latter case the right-hand side of Eq. (16) can be approximated within the usual approximation technique:

$$\sum_l t_{jl}\left\{\Psi_j^{\uparrow,\downarrow}\langle\Psi_i^{pd,\uparrow}\Psi_l^{\downarrow,pd}\rangle+\frac{1+\delta}{2}\Psi_i^{pd,\uparrow}\Psi_l^{\uparrow,pd}+\left(\frac{e_j}{2}+s_j^z\right)\times\langle\Psi_i^{pd,\uparrow}\Psi_l^{\uparrow,pd}\rangle\right\}-\sum_l t_{li}\left\{\langle\Psi_l^{pd,\downarrow}\Psi_j^{\uparrow,pd}\rangle\Psi_i^{\downarrow,\uparrow}+\frac{1+\delta}{2}\Psi_l^{pd,\uparrow}\Psi_j^{\uparrow,pd}+\left(\frac{e_i}{2}+s_i^z\right)\langle\Psi_l^{pd,\uparrow}\Psi_j^{\uparrow,pd}\rangle\right\}, \tag{19}$$

where s_i^z is zero in the paramagnetic phase.

As for the case $i=j$, it can be calculated exactly as

$$[\Psi_i^{pd,pd},H_t]=\sum_l t_{il}(\Psi_i^{pd,\uparrow}\Psi_l^{\uparrow,pd}+\Psi_i^{pd,\downarrow}\Psi_l^{\downarrow,pd})-\sum_l t_{li}(\Psi_l^{pd,\uparrow}\Psi_i^{\uparrow,pd}+\Psi_l^{pd,\downarrow}\Psi_i^{\downarrow,pd}). \tag{20}$$

Using the Fourier transformation (13) we can write the commutator (16) in the equation of motion as follows:

$$[e_{kq},H_t]=P_{pd}(t_k-t_{k+q})e_{kq}+\frac{1}{4N}\sum_{k'}[t_{k'+q}(n_{k'+q}^{\uparrow}+n_{k'+q}^{\downarrow})-t_{k'}(n_{k'}^{\uparrow}+n_{k'}^{\downarrow})]e_q+\frac{2-P_{pd}}{2N}\sum_{k'}(t_{k'}-t_{k'+q})e_{k'q}. \tag{21}$$

The last term in Eq. (21) still leads to a high-order Green's function but fortunately it can be reduced to the previous one with the help of Eq. (20), which yields

$$\frac{\omega_q}{2}\langle\langle e_q|e_{-q}\rangle\rangle=\sum_k (t_k-t_{k+q})\langle\langle e_{kq}|e_{-q}\rangle\rangle. \tag{22}$$

Considering the superexchange and Coulomb screening parts of the Hamiltonian, H_J and H_c, we notice that the operator $\Psi_i^{pd,pd}$ commutes with these terms of the Hamiltonian and therefore the case $i=j$ does not contribute to the equation of motion. This is in contrast to the spin susceptibility where the additional noncommutation of the spin operator S_q^+ led to a fact that the ordinary Hubbard 1 decoupling scheme is not sufficient and additional consideration is required.[26] Strictly speaking, it means that although spin and charge degrees of freedom are still coupled as in the case of the usual Fermi liquid, the simple relations of the RPA approximation of the usual Fermi-liquid approach do not hold. Thus, for the case of $i\neq j$ in the site representation we have

$$[\Psi_i^{pd,\uparrow}\Psi_j^{\uparrow,pd},H_J]=\frac{1}{2}\sum_l J_{il}\{\Psi_i^{pd,\downarrow}\Psi_l^{\downarrow,\uparrow}\Psi_j^{\uparrow,pd}-\Psi_i^{pd,\uparrow}\Psi_l^{\downarrow,\downarrow}\Psi_j^{\uparrow,pd}\}-\frac{1}{2}\sum_l J_{jl}\{\Psi_i^{pd,\uparrow}\Psi_j^{\downarrow,pd}\Psi_l^{\uparrow,\downarrow}-\Psi_i^{pd,\uparrow}\Psi_j^{\uparrow,pd}\Psi_l^{\downarrow,\downarrow}\}, \tag{23}$$

whereas for case of $i=j$

$$[\Psi_i^{pd,pd},H_J]=0. \tag{24}$$

Restricting ourselves to an absence of the long-range spin order we can write

$$[e_{kq},H_J]=\frac{1}{4N}J_q\{[n_k^{\uparrow}+n_k^{\downarrow}]-[n_{k+q}^{\uparrow}+n_{k+q}^{\downarrow}]\}e_q. \tag{25}$$

For the Coulomb screening part of the Hamiltonian the result reads

$$[e_{kq},H_c]=-\frac{1}{2N}G_q\{[n_k^{\uparrow}+n_k^{\downarrow}]-[n_{k+q}^{\uparrow}+n_{k+q}^{\downarrow}]\}e_q. \tag{26}$$

Substituting Eq. (21) and Eqs. (25) and (26) into the equation of motion (27) and taking into account the absence of the external magnetic field, we get finally

$$\omega_q\langle\langle e_{kq}|e_{-q}\rangle\rangle=\frac{1}{2\pi}(n_{k+q}-n_k)+P_{pd}(t_k-t_{k+q})\langle\langle e_{kq}|e_{-q}\rangle\rangle+\left[\frac{1}{4}(t_{k+q}n_{k+q}-t_kn_k)+\left(G_q-\frac{J_q}{4}\right)\times(n_{k+q}-n_k)+\frac{(2-P_{pd})}{2}\omega_q\right]\langle\langle e_q|e_{-q}\rangle\rangle. \tag{27}$$

Performing a sum over **k** we obtain the expression for the dynamical charge susceptibility in a form

$$\chi_{\rm ch}(\mathbf{q},\omega)=\frac{\chi_0(\mathbf{q},\omega)}{1+(G_q-J_q/4)\chi_0(\mathbf{q},\omega)+\chi_1(\mathbf{q},\omega)-z_1(\mathbf{q},\omega)}, \tag{28}$$

where $\chi_0(\mathbf{q},\omega)$ is an ordinary Pauli-Lindhard response function

$$\chi_0(\mathbf{q},\omega)=\frac{1}{N}\sum_k\frac{n_k-n_{k+q}}{\omega+i0^+-\epsilon_k+\epsilon_{k+q}}. \tag{29}$$

The most interesting $\chi_1(\mathbf{q},\omega)$ and $z_1(\mathbf{q},\omega)$ terms describe the contributions due to no-double occupancy constraint and projecting nature of Hubbard operators:

$$\chi_1(\mathbf{q},\omega)=\frac{1}{2N}\sum_k\frac{t_kn_k-t_{k+q}n_{k+q}}{\omega+i0^+-\epsilon_k+\epsilon_{k+q}}, \tag{30}$$

$$z_1(\mathbf{q},\omega)=\frac{2-P_{pd}}{2N}\sum_k\frac{\omega+i0^+}{\omega+i0^+-\epsilon_k+\epsilon_{k+q}}. \tag{31}$$

The comparison of the obtained equation with our preliminary consideration resulting in Eq. (7) shows that the important term $z_1(\mathbf{q},\omega)$ appears in the right-hand side of Eq. (28). To our knowledge this term was not pointed out for the charge susceptibility so far. It acts as a frequency-dependent "molecular field" caused by the transfer hopping term of the Hamiltonian (1) and, as we shall see below, play some role in the formation of collective modes around (π,π).

For comparison we also show the part of a spin susceptibility related to a formation of the current carriers. Excluding the possible contribution to the spin susceptibility from a spin wave of localized moments,[26] the same kind of procedure, as explained above, yields the following expression for the spin susceptibility:

$$\chi_{sp}^{+-}(\mathbf{q},\omega)=\frac{\chi_0^{+-}(\mathbf{q},\omega)}{1+(J_q/2)\chi_0^{+-}(\mathbf{q},\omega)+\chi_1^{+-}(\mathbf{q},\omega)-z_2^{+-}(\mathbf{q},\omega)}, \tag{32}$$

where

$$\chi_0^{+-}(\mathbf{q},\omega)=\frac{1}{N}\sum_k\frac{\tilde{n}_k^{\uparrow}-\tilde{n}_{k+q}^{\downarrow}}{\omega+i0^+-\epsilon_k^{\uparrow}+\epsilon_{k+q}^{\downarrow}}, \tag{33}$$

$$\chi_1^{+-}(\mathbf{q},\omega)=\frac{1}{N}\sum_k\frac{t_k\tilde{n}_k^{\uparrow}-t_{k+q}\tilde{n}_{k+q}^{\downarrow}}{\omega+i0^+-\epsilon_k^{\uparrow}+\epsilon_{k+q}^{\downarrow}}, \tag{34}$$

$$z_2^{+-}(\mathbf{q},\omega)=(1-P_{pd})\frac{1}{N}\sum_k\frac{\omega+i0^+}{\omega+i0^+-\epsilon_k^{\uparrow}+\epsilon_{k+q}^{\downarrow}}. \tag{35}$$

Using the anticommutator relation we can substitute in Eqs. (33)–(35) $\tilde{n}_k^{\sigma}=-n_k^{\sigma}+P_{pd}$, which holds at zero external magnetic field. In this case the right-hand side of expression (32) is reduced to a form

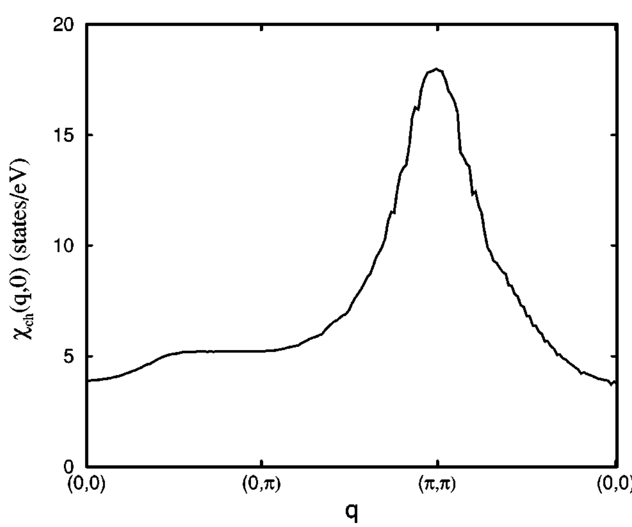

FIG. 1. Momentum dependence of the Re $\chi_{\rm ch}(\mathbf{q},0)$ through the route of the Brillouin zone (0,0)-$(\pi,0)$-(π,π)-(0,0) at $T=100$ K.

$$\chi_{sp}^{+-}(\mathbf{q},\omega)=\frac{\sum_k \frac{f(\epsilon_{k+q})-f(\epsilon_k)}{\omega+i0^+-\epsilon_k+\epsilon_{k+q}}}{\sum \frac{\left(t_{k+q}-\frac{1}{2}J_q\right)f(\varepsilon_{k+q})-\left(t_k-\frac{1}{2}J_q\right)f(\varepsilon_k)+\omega+i0^+}{(\omega+i0^+-\epsilon_k+\epsilon_{k+q})}}, \tag{36}$$

which is quite different from the conventional RPA one. Here, $f(\varepsilon_k)=\{1+\exp[(\varepsilon_k-\mu)/k_BT]\}$ is a Fermi function. The mutual relation of charge and spin susceptibility functions as well as their differences are especially clear from the comparison of Eqs. (28) and (32).

IV. NUMERICAL RESULTS AND DISCUSSION

Let us first analyze the behavior of the obtained expression for the dynamical charge susceptibility (28). In Fig. 1 we present the calculated Re $\chi_{\rm ch}(\mathbf{q},0)$ for the set of parameters described above. The peak around (π,π) reflects the nesting properties of the Fermi surface enhanced by the RPA type of the denominator. The structure of the real part of the charge susceptibility at zero frequency looks very similar to the spin counterpart. Originally it comes from the nesting properties of the Fermi surface resembled by χ_0. However, the additional enhancement due to the denominator is quite different in origin in both cases. In the spin susceptibility it results due to the superexchange interaction having a maximum at (π,π). In the charge susceptibility the contribution from J_q has a different sign and therefore should suppress the peak. On the other hand, an inclusion of the intersite Coulomb screening repairs the situation and again leads to the strong commensurate peak around (π,π). As we will see later, this peak is strongly dependent only on the value of the intersite Coulomb repulsion. This is a quite remarkable fact if one remembers that the calculations of the charge and spin susceptibility in the frame of the one-band Hubbard Hamiltonian with on-site U or ordinary t-J model show that the charge susceptibility is rather small at $\mathbf{Q}=(\pi,\pi)$ in contrast to the spin susceptibility.[27] This often led to the exclusion of the charge degrees of freedom from the pairing interaction. However, as it is seen here, the significant contribution to the charge susceptibility comes from the intersite screened Coulomb repulsion between doped holes. Since this interaction plays the most important role in the underdoped case one would expect the significant contribution to the pairing interaction from the charge susceptibility too.

This fact is also seen from Fig. 2 where we present the imaginary part of the charge susceptibility at $\mathbf{Q}=(\pi,\pi)$ with and without the screened Coulomb repulsion G_1. Without the intersite Coulomb repulsion one sees that the charge susceptibility shows no features at low energies. This indicates that the superexchange mechanism itself cannot lead to any charge instabilities in the system. The situation changes drastically if one switches on the screened Coulomb repulsion between doped holes. In particular, at $G_1=70$ meV the charge susceptibility shows a strong peak at $\omega_{\rm cf}\approx 15$ meV. This is quite comparable with the typical spin fluctuation frequency, $\omega_{\rm sf}$ that results from the approximate position of the peak in Im χ_s.[28] On the basis of Figs. 1 and 2, we can conclude that the charge susceptibility may play an important role in the scattering mechanism and in the Cooper pairing instability. However, such a large value of the intersite Coulomb interaction could only be expected at a low doping level. Therefore, we think that the spin-fluctuation scenario of superconductivity is much more robust than the charge-fluctuation one in high-T_c cuprates. One would expect, however, a strong CDW-like instability in underdoped cuprates since the intersite Coulomb repulsion is most important at a low doping concentration.

In order to analyze these possible instabilities in the charge subsystem we also investigate the charge susceptibility with respect to a CDW formation. The CDW frequency range can be obtained analyzing the denominator of the dynamical charge susceptibility expression (28). Therefore, we solve the equation

$$1+\left(G_q-\frac{J_q}{4}\right)\chi_0(\mathbf{q},\omega)+\chi_1(\mathbf{q},\omega)-z_1(\mathbf{q},\omega)=0 \tag{37}$$

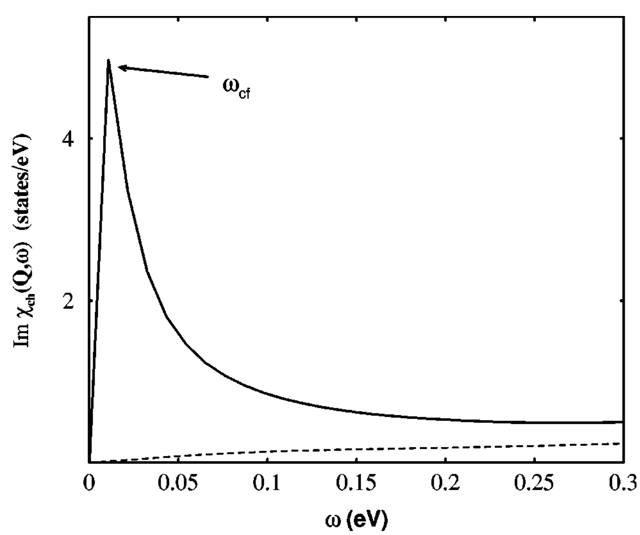

FIG. 2. Frequency dependence of the Im $\chi_{\rm ch}(\mathbf{Q},\omega)$ at $Q=(\pi,\pi)$ for $G_1=0$ (long-dashed curve) and $G_1=70$ meV (solid curve) at $T=100$ K. The arrow indicates the approximate position of the maximum at $\omega_{cf}\approx 15$ meV.

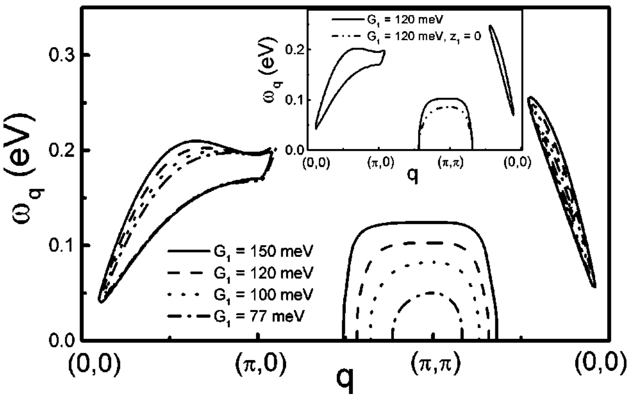

FIG. 3. Momentum dependence of the CDW frequencies at different values of the Coulomb repulsion G_1. In the inset two curves are shown for $G_1 = 120$ meV with and without taking into account the term $z_1(\mathbf{q},\omega)$.

through the route of the Brillouin zone (0,0)-(π,0)-(π,π)-(0,0).

In Fig. 3 we present the resulting energy dispersion of the CDW-type frequency, ω_q, in a slightly underdoped regime ($\langle\tilde{n}\rangle = 0.86$) and at temperature $T = 100$ K for different values of G_1. As one can see, there are three disconnected branches of the frequency curves. We focus our attention on those that go to zero because $\omega_Q = 0$ means the instability of the charge subsystem with respect to a long-range order phase transition at wave vector $\mathbf{Q}$. It is natural to interpret this mode as a frequency of the phase motion mode (phason), whereas others refer to the amplitude modes. Most importantly, at $G_1 = 70$ meV (not shown) there is only one point of $\omega_q = 0$ where the instability wave vector corresponds exactly to $\mathbf{Q} = (\pi,\pi)$. With increasing G_1 we obtain a set of the instability wave vectors around (π,π) along the instability contour. Therefore, the system becomes degenerate. In order to show that these wave vectors are equivalent with respect to the enhancement of Im $\chi_{\mathrm{ch}}(\mathbf{q},\omega)$ we also show in Fig. 4 the mesh of the Im $\chi_{\mathrm{ch}}(\mathbf{q},\omega)$ versus frequency and momentum along the routes of the Brillouin zone $(0,0)\rightarrow(\pi,\pi)$ and $(\pi,0)\rightarrow(\pi,\pi)$ close to the instability points. One sees that in both cases the enhancement of the charge susceptibility is almost the same. Finally we remark on the importance of $z_1(\mathbf{q},\omega)$ term. In the inset of Fig. 3 we show the momentum dependence of CDW frequencies at $G_1 = 120$ meV with and without taking into account $z_1(\mathbf{q},\omega)$. In the latter case one sees a slight decrease of $\omega_{\mathbf{q}}$ in the vicinity of (π,π), while the intersections with the $\omega = 0$ axis do not move at all. This relates to the fact that $z_1(\mathbf{q},\omega)$ describes the effect of the strong electron correlations, namely, no double-occupancy constraint, which is important in underdoped cuprates.

In the case of the degeneracy the behavior of the system becomes more complicated. In order to answer the question at which actual wave vector the instability will occur here one has to take into account the interaction of the current carriers with a lattice potential or a pinning effect. This is out of the scope of the present investigation. Note, the presence of the phason mode will also lead to the difference of the photoemission spectra between α and β points of the Fermi surface as observed recently.[29] One sees also from Fig. 3 that this mode exists at large enough value of G_1 which is possible only in the underdoped regime.

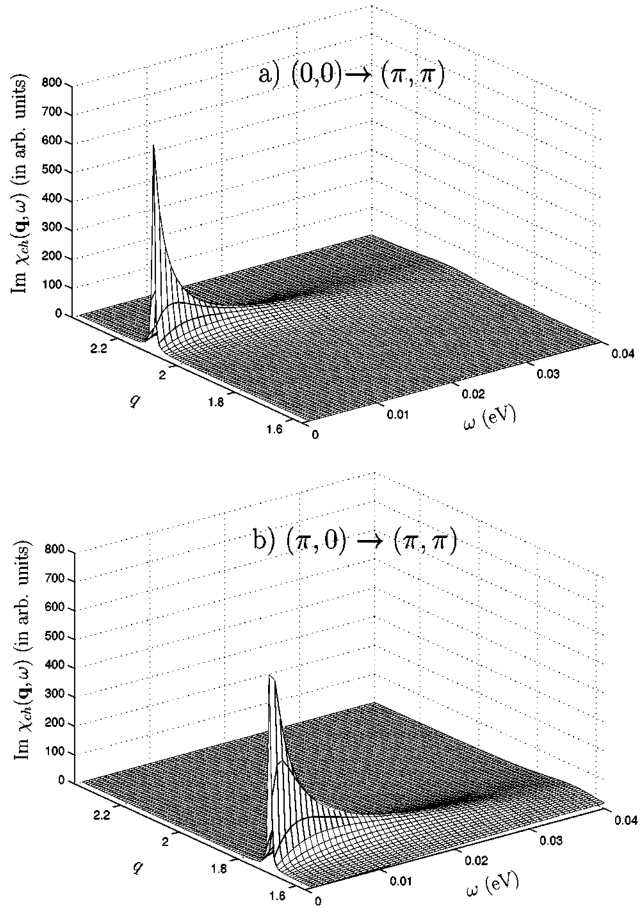

FIG. 4. Calculated imaginary part of the charge susceptibility versus frequency and momentum at $G_1 = 120$ meV. (a) Along $(\pi,\pi)\rightarrow(0,0)$ route of the BZ. (b) Along $(\pi,\pi)\rightarrow(\pi,0)$ route of the BZ.

V. CONCLUSION

We have obtained in a frame of the singlet-correlated band model beyond the RPA approximation a new analytical expression for the dynamical charge susceptibility. We have shown that it produces a strong peak at $\mathbf{Q} = (\pi,\pi)$ at large enough screened Coulomb repulsion between doped holes. This may result in a significant contribution to the pairing interaction from the charge susceptibility at low doping level where the Coulomb repulsion plays an important role. The analysis of the instability of the system with respect to a CDW formation shows that the charge subsystem is most unstable along the contour of the Brillouin zone around (π,π). Our finding strongly supports the relevance of a CDW type of instability as an origin for the pseudogap formation in optimally and underdoped cuprates.

ACKNOWLEDGMENTS

It is our pleasure to thank V. Yushankhai, D. Manske, and G. Seibold for stimulating discussions. This work was supported by the Russian Scientific Council on Superconductivity (Grant No. 98014) and partially by the Swiss National Foundation (Grant No. 7SUPJ062258). I.E. was supported by the Alexander von Humboldt Foundation.

[1] T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999).
[2] J. L. Tallon, G. V. M. Williams, and J. W. Loram, Physica C **338**, 9 (2000).
[3] R. S. Markiewicz, C. Kusko, and V. Kidambi, Phys. Rev. B **60**, 627 (1999).
[4] V. J. Emery, S. A. Kivelson, and O. Zachar, Phys. Rev. B **56**, 6120 (1997).
[5] S. Chakravarty, R. B. Laughlin, D. Morr, and Ch. Nayak, Phys. Rev. B **63**, 094503 (2001).
[6] P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).
[7] I. Eremin and M. Eremin, J. Supercond. **10**, 459 (1997); S. Varlamov, M. Eremin, and I. Eremin, Pis'ma Zh. Éksp. Teor. Fiz. **66**, 533 (1997) [JETP Lett. **66**, 569 (1997)].
[8] Yu. V. Kopaev, Fiz. Tverd. Tela **8**, 223 (1966) [Sov. Phys. Solid State **8**, 175 (1966)].
[9] B. I. Halperin and T. M. Rice, Solid State Phys. **21**, 116 (1968).
[10] G. Jackeli and N. M. Plakida, Phys. Rev. B **60**, 5266 (1999).
[11] R. Zeyher and M. L. Kulic, Phys. Rev. B **54**, 8985 (1996).
[12] G. Santoro, S. Scandolo, and E. Tosatti, Phys. Rev. B **59**, 1891 (1999).
[13] I. Eremin, M. Eremin, S. Varlamov, D. Brinkmann, M. Mali, and J. Roos, Phys. Rev. B **56**, 11 305 (1997).
[14] M. Eremin, S. Varlamov, and I. Eremin, Appl. Magn. Reson. **19**, 355 (2000).
[15] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[16] J. Hubbard, Proc. R. Soc. London, Ser. A **281**, 401 (1964).
[17] N. M. Plakida, R. Hayn, and J. L. Richard, Phys. Rev. B **51**, 16 599 (1995).
[18] M. V. Eremin, S. G. Solovjanov, S. V. Varlamov, D. Brinkmann, M. Mali, R. Markendorf, and J. Roos, Pis'ma Zh. Éksp. Teor. Fiz. **60**, 118 (1994) [JETP Lett. **60**, 125 (1994)].
[19] H. J. Schulz, Phys. Rev. B **39**, 2940 (1989).
[20] I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988).
[21] Ch. Nayak, Phys. Rev. B **62**, 6135 (2000).
[22] Z.-X. Shen and D.-S. Dessau, Phys. Rep. **253**, 1 (1995).
[23] L. F. Feiner, J. H. Jefferson, and R. Raimondi, Phys. Rev. B **53**, 8751 (1996).
[24] G. Aeppli, S. M. Hayden, H. A. Mook, Z. Fisk, S.-W. Cheong, D. Rytz, J. P. Remeika, G. P. Espinosa, and A. S. Cooper, Phys. Rev. Lett. **62**, 2052 (1989).
[25] J. Hubbard and K. P. Jain, J. Phys. C **1**, 1650 (1968).
[26] A. Yu. Zavidonov and D. Brinkmann, Phys. Rev. B **58**, 12 486 (1998).
[27] See, for example, D. J. Scalapino, Phys. Rep. **250**, 329 (1995).
[28] Y. Zha, V. Barzykin, and D. Pines, Phys. Rev. B **54**, 7561 (1996).
[29] Z.-X. Shen and J. R. Schrieffer, Phys. Rev. Lett. **78**, 1771 (1997).