Collective modes in the electronic polarization of double-layer systems in the superconducting state

F. Forsthofer, S. Kind, and J. Keller
Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany
(Received 5 October 1995)

Standard weak-coupling methods are used to study collective modes in the superconducting state of a double-layer system with intralayer and interlayer interaction, as well as a Josephson-type coupling and single-particle hopping between the layers by calculating the electronic polarization function perpendicular to the layers. Analytical results are derived for the mode frequencies corresponding to fluctuations of the relative phase and amplitude of the layer order parameters in the case of interlayer pairing and finite hopping t. An effect is found for finite k-dependent hopping: then the amplitude and phase fluctuations are coupled. Therefore two collective modes may appear in the dynamical c-axis conductivity below the threshold energy for breaking Cooper pairs. With help of numerical calculations we investigate the temperature dependence of the collective modes and show how a plasmon corresponding to charge fluctuations between the layers evolves in the normal state. [S0163-1829(96)04622-X]

I. INTRODUCTION

The problem of collective modes in superconductors is a very old one. Bogoliubov and Anderson[1,2] pointed out that charge oscillations can couple to oscillations of the phase of the superconducting order parameter via the pairing interaction. In a neutral system this would lead to a soundlike collective mode. In a charged system the frequency of this mode is pushed up to the plasma frequency due to the long-range Coulomb interaction,[3,4] and at these high frequencies this mode is of no importance for the superconducting properties.

The situation is different for modes which do not couple to long-range density fluctuations. Leggett[5] showed that in a two-band superconductor oscillations in the occupation difference between the two bands couple to phase fluctuations of the order parameters for the two bands giving rise to a collective mode with a frequency below 2Δ, the threshold energy for breaking Cooper pairs. Also oscillations of the amplitude of the order parameter are not perturbed by charge fluctuations. The frequency of this mode, however, is at the threshold for particle-hole excitations in normal isotropic superconductors. Only in special cases can overdamping of this mode be avoided.[6] Low-frequency collective modes may also exist in superconductors with a multicomponent order parameter.[7,8] Such order parameters are frequently discussed candidates for some heavy fermion superconductors.

Another possibility to avoid the influence of long-range Coulomb forces on the collective modes is realized in strongly anisotropic superconductors,[9] in particular in a periodic system of superconducting layers.[10,11] In the case of a finite value of the wave vector $q_\perp$ perpendicular to the layers, density fluctuations within the layers do not build up long-range Coulomb forces. In the limit $\vec{q} \to 0$ only the Coulomb interaction between the layers remains.

Recently the question of collective modes has been brought up again in connection with the multilayer structure of the high-T_c superconductors. In a double-layer system like Bi-Sr-Ca-Cu-O or Y-Ba-Cu-O one obtains two electronic bands for the motion of electrons parallel to the layers corresponding to states with symmetric or antisymmetric wave functions.[12] In the superconducting state both bands acquire gaps. In such systems one can discuss different collective modes[13–15] corresponding to fluctuations in the occupation number of the two bands and to charge oscillation between the two layers.

In a series of papers[16,17] we have investigated in detail the electronic polarization of double-layer systems in the normal and superconducting state and have studied the influence of charge fluctuations between the layers on the renormalization of transverse c-axis phonons. Here we have assumed a k-dependent tight-binding coupling between the layers and pairing interactions for electrons within the same and in different layers. In our numerical calculations[17] we included both the vertex corrections due to the BCS interaction and the Coulomb interaction between the layers, thus taking into account the effect of possible collective modes. We found a shift of phonon frequencies in the superconducting state which is in reasonable agreement with far-infrared experiments. As in this case we assumed a fairly large value for the tight-binding coupling the collective modes are strongly damped by quasiparticle excitations. In the present paper we analyze in more detail the conditions for undamped collective modes in the electronic polarization. The results depend crucially on the values of the different pairing interactions.

In principle one has to distinguish three different types of interactions: (1) an interaction between electronic densities within one layer, (2) an interaction between electronic densities in different layers, (3) an interaction between mixed densities from the two layers. All three interactions can be mediated by phonons (or other types of bosons): the first two by a change of local potentials induced by lattice displacements, the third one by a change of the hopping energy between the two layers. The first two interactions conserve the number of particles in the two layers, while the third interaction may interchange particles between the two layers. In particular, this interaction allows a transfer of two particles as in a Josephson coupling. This type of coupling, which can

also be derived from a second-order hopping process, has gained much interest recently. Anderson and co-workers have argued that in strongly correlated electron systems coherent single-particle hopping between the two layers is suppressed, while a coherent momentum conserving second-order hopping process is possible.[18] In such an interlayer-tunneling model without single-particle hopping two collective modes involving fluctuations of the phase and amplitude difference of the layer order parameters are found.[14]

The size of the effective hopping between the layers is currently under debate.[19,20] Therefore we investigate here collective modes for arbitrary hopping. If the suppression of single-particle hopping is due to strong correlation effects also deviations from Fermi-liquid behavior may be expected. In order to keep the discussion of collective modes as simple as possible we use here a Fermi-liquid description with a simple band structure and treat superconductivity within an extended BCS theory. The theory developed here is aimed at exploring the different possibilities for collective modes in double-layer systems. For a realistic description of high-T_c materials like Bi-Sr-Ca-Cu-O and Y-Ba-Cu-O one certainly has to include an angular-dependent hopping t_k and possibly d-wave pairing.

In a two-layer system one has to consider two order parameters corresponding to pairing of electrons in one layer and in different layers. This leads in general to different order parameters (and gaps) for the two bands which may even have different signs for s-wave pairing. Depending on the relative sign of the band order parameters one can distinguish between two different pairing types, which both have s-wave symmetry: In the case of dominant intralayer interaction the order parameters of the two bands have equal sign, while for dominant interlayer interaction they have opposite sign.[21–24] In Refs. 25 and 26 it is shown that antiferromagnetic interactions between the two layers favor a superconducting state with interlayer pairing and anisotropic s-wave symmetry.

In the following discussion we will consider all three types of pairing interactions mentioned above and will also take into account single-particle hopping between the layers. In this paper we consider only s-wave pairing by neglecting the k dependence of the pairing interaction. We discuss the collective modes for both pairing types and calculate the electronic polarization between the two layers, because this quantity enters directly the dynamical conductivity for electric-field vectors in the c direction. Our results extend earlier work on collective modes in two-layer systems mainly in the following respects: (1) we calculate collective modes in the case of interlayer pairing, (2) we find that a k-dependent tight-binding hopping between the layers couples amplitude and phase modes, making it possible that both modes appear below the threshold frequency in the optical conductivity.

Our paper is organized as follows: In the following section we specify our model and write down the interactions in a 4×4-Nambu matrix notation. Then we calculate the self-energies and discuss the self-consistency equations. In Sec. III we solve the vertex equations for the polarization function in the neutral and charged system. The collective modes for the k-independent hopping matrix element are studied in Sec. IV for intralayer pairing and interlayer pairing. In Sec. V

numerical results for the polarization function are presented. The results are summarized in Sec. VI.

II. NAMBU FORMALISM FOR TWO-BAND SYSTEMS

A. Model

We consider an electronic double-layer system described by the Hamiltonian

$$H_0 = \sum_{k\sigma} \epsilon_k (c_{1k\sigma}^\dagger c_{1k\sigma} + c_{2k\sigma}^\dagger c_{2k\sigma}) + t_k (c_{2k\sigma}^\dagger c_{1k\sigma} + c_{1k\sigma}^\dagger c_{2k\sigma}) \tag{1}$$

and the interaction

$$\begin{aligned} H_S = \frac{1}{2} \sum_{kk'q\sigma\sigma'} \sum_i \quad & + V_\parallel c_{ik+q\sigma}^\dagger c_{ik'-q\sigma'}^\dagger c_{ik'\sigma'} c_{ik\sigma} \\ & + V_\perp c_{ik+q\sigma}^\dagger c_{jk'-q\sigma'}^\dagger c_{jk'\sigma'} c_{ik\sigma} \\ & + J(c_{ik+q\sigma}^\dagger c_{ik'-q\sigma'}^\dagger c_{jk'\sigma'} c_{jk\sigma} \\ & + c_{ik+q\sigma}^\dagger c_{jk'-q\sigma'}^\dagger c_{ik'\sigma'} c_{jk\sigma}). \end{aligned} \tag{2}$$

Here t_k describes a tight-binding coupling between the two layers $i = (1,2), j = 3-i$. The couplings $V_\parallel$, $V_\perp$, J are effective pairing interactions. $V_\parallel$ describes the interaction between electronic densities within one layer, $V_\perp$ between different layers, and J is the coupling between mixed densities. The origin of these interactions is a combination of an attractive interaction due to the exchange of phonons (or other bosons) and a screened repulsive Coulomb interaction. This means that J is much smaller than $V_\perp$ and $V_\parallel$. Because J includes intrinsic tunneling of Cooper pairs from one layer to the other, J is called Josephson coupling. Here we neglect any momentum dependence of these interactions (except for a cutoff introduced later).

The Hamiltonian H_0 can be diagonalized by introducing fermionic operators $a_{\alpha k\sigma}$

$$a_{1k\sigma} = \frac{1}{\sqrt{2}}(c_{2k\sigma} - c_{1k\sigma}), \quad a_{2k\sigma} = \frac{1}{\sqrt{2}}(c_{2k\sigma} + c_{1k\sigma})$$

corresponding to states with antisymmetric and symmetric wave functions on the two layers (this symmetry is not broken by introducing the interactions). We then obtain two bands with quasiparticle energies

$$\epsilon_{1k} = \epsilon_k - t_k, \quad \epsilon_{2k} = \epsilon_k + t_k.$$

In order to treat superconductivity it is useful to combine the Fermi operators to a Nambu spinor[2,3]

$$\Psi_k = (a_{1k\uparrow}, a_{1-k\downarrow}^\dagger, a_{2k\uparrow}, a_{2-k\downarrow}^\dagger)^t.$$

With help of these spinors we can express the Hamiltonian of the two-layer system as follows (apart from constants):

$$H_0 = \sum_k \epsilon_k \Psi_k^\dagger D^{03} \Psi_k - t_k \Psi_k^\dagger D^{33} \Psi_k, \tag{3}$$

$$H_S = \frac{1}{2} \sum_{k,k',q} V(\Psi_{k+q}^\dagger D^{03}\Psi_k)(\Psi_{k'-q}^\dagger D^{03}\Psi_{k'})$$

$$+ \overline{V}(\Psi_{k+q}^\dagger D^{13}\Psi_k)(\Psi_{k'-q}^\dagger D^{13}\Psi_{k'})$$

$$+ J(\Psi_{k+q}^\dagger D^{33}\Psi_k)(\Psi_{k'-q}^\dagger D^{33}\Psi_{k'}). \tag{4}$$

Here $V = (V_\parallel + V_\perp)/2$, $\overline{V} = (V_\parallel - V_\perp)/2$. D^{jl} are 4×4 matrices in Nambu space which are constructed from two sets of Pauli matrices $D^{jl} = \tau_j \sigma_l$. Example:

$$D^{13} = \tau_1 \sigma_3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}.$$

The terms containing the matrices D^{03}, D^{33} describe the sum and difference of density operators of the two bands, while the term with D^{13} contains fermionic operators from different bands. Accordingly $\overline{V}$ leads to interband transitions, while V and J cause intraband transitions only. In principle, one can derive a further interaction mediated by phonons which couples operators characterized by the matrices D^{33} and D^{03}. Such an interaction is omitted here, because it has no influence on the interlayer polarization function.

For the interactions $V, \overline{V}, J$ a cutoff has to be introduced either in momentum space or frequency space. We introduce the cutoff in momentum space:

$$V, \overline{V}, J \begin{cases} \neq 0 & \text{if } |\epsilon_k - \mu|, |\epsilon_{k'} - \mu| < \omega_c \\ = 0, & \text{otherwise}, \end{cases} \tag{5}$$

ω_c is the cutoff energy, μ the chemical potential. Note that the cutoff has been introduced for the energy ϵ_k and not for the band energies $\epsilon_{\alpha k}$. Otherwise we obtain inconsistencies in solving the vertex equations.

In the following we are primarily interested in the calculation of the interlayer polarization function which is the correlation function of the electronic polarization perpendicular to the layers. The latter is described (up to a factor $ed/2$, where d is the layer separation and e is the electronic charge) by the operator

$$P = \sum_{k\sigma} c_{2k\sigma}^\dagger c_{2k\sigma} - c_{1k\sigma}^\dagger c_{1k\sigma}. \tag{6}$$

There are three other operators which couple to the interlayer polarization in the vertex equations. These are

$$\Phi = -i\sum_k c_{2k\uparrow}^\dagger c_{2-k\downarrow}^\dagger - c_{1k\uparrow}^\dagger c_{1-k\downarrow}^\dagger - c_{2-k\downarrow}c_{2k\uparrow} + c_{1-k\downarrow}c_{1k\uparrow},$$

$$A = \sum_k c_{2k\uparrow}^\dagger c_{2-k\downarrow}^\dagger - c_{1k\uparrow}^\dagger c_{1-k\downarrow}^\dagger + c_{2-k\downarrow}c_{2k\uparrow} - c_{1-k\downarrow}c_{1k\uparrow}, \tag{7}$$

$$j = -i\sum_{k\sigma} c_{2k\sigma}^\dagger c_{1k\sigma} - c_{1k\sigma}^\dagger c_{2k\sigma}.$$

In Nambu space a 4×4 matrix corresponds to each operator:

$$P^{jl} = \sum_k \Psi_k^\dagger D^{jl} \Psi_k, \tag{8}$$

where $P = P^{13}$, $\Phi = P^{12}$, $A = P^{11}$, $j = P^{20}$.

Φ and A are called phase and amplitude operator in the literature,[14] because in the case that the phases of the layer order parameters are zero, Φ and A measure the difference of the phases and amplitudes of the layer order parameters. j is related to the interlayer current density. This is strictly so only in the case of constant interlayer hopping $t_k = t$ and vanishing Josephson coupling J; then the equation of motion $2tj = \dot{P}$ is fulfilled. In the case $J \neq 0$ the current-density operator becomes more complicated; it contains also two-particle operators. Nevertheless j will be called the current operator in the following.

B. Self-consistency equations

The Green's functions can be combined to a 4×4-Nambu matrix. We assume the Green's-function matrix to be diagonal in the band indices:

$$G(k,z) = \begin{pmatrix} G_1(k,z) & 0 \\ 0 & G_2(k,z) \end{pmatrix}, \tag{9}$$

where $G_\alpha(k,z)$ are 2×2 matrices for each band. This assumption which neglects pairing in different bands is reasonable since the two bands (in the presence of a finite tight-binding coupling) have different symmetries,[24] and this symmetry is preserved by the interaction H_S. One consequence of this assumption is that the phases of the order parameters $\langle c_{ik\uparrow} c_{i-k\downarrow} \rangle$ for pairing in one layer are equal for the two layers (equal amplitude and phase). Intraband pairing seems to be the ground state for all negative values of J, while it may become unstable for large positive $J \gg |t_k|$. This is supported by the calculation of the ground state of a model with two electrons on two sites with all the interactions contained in the Hamiltonian $H_0 + H_S$. Defining operators $a_{\alpha\sigma} = (1/\sqrt{2})(c_{2\sigma} \pm c_{1\sigma})$ for the single-particle eigenstates of H_0 one finds that the ground state contains only diagonal terms $a_{\alpha\uparrow}^\dagger a_{\alpha\downarrow}^\dagger |0\rangle$ as long as the Josephson coupling is attractive $J \leq 0$ but contains nondiagonal terms for large positive values $J \gg |t_k|$. In our numerical calculations of the polarization function we will show that an instability occurs for large positive Josephson coupling J.

The bare Green's function is given by

$$G_{0\alpha}^{-1}(k,z) = z\sigma_0 - (\epsilon_{\alpha,k} - \mu)\sigma_3. \tag{10}$$

In the presence of the pairing interaction we have self-energy corrections:

$$G^{-1}(k,z) = G_0^{-1}(k,z) - \Sigma(z), \tag{11}$$

where the self-energy $\Sigma(z)$ contains contributions from intraband and interband interactions:

$$\Sigma = -\frac{1}{\beta}\sum_{k\omega_m} VD^{03}G(k,i\omega_m)D^{03} + \overline{V}D^{13}G(k,i\omega_m)D^{13}$$

$$+ JD^{33}G(k,i\omega_m)D^{33}. \tag{12}$$

The self-energy is diagonal in the band indices

$$\Sigma = \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \tag{13}$$

and the 2×2 components Σ_α are given by

$$\Sigma_1=-\frac{1}{\beta}\sum_{k\omega_m} W\sigma_3 G_1(k,i\omega_m)\sigma_3+\overline{V}\sigma_3 G_2(k,i\omega_m)\sigma_3,$$

$$\Sigma_2=-\frac{1}{\beta}\sum_{k\omega_m} W\sigma_3 G_2(k,i\omega_m)\sigma_3+\overline{V}\sigma_3 G_1(k,i\omega_m)\sigma_3$$

(14)

with the intraband interaction $W=V+J$. While the interactions V, J enter in the same way into the self-energy, this is not so in the vertex equations. Therefore J cannot simply be incorporated into the interaction V by a proper redefinition.

Writing $\Sigma_\alpha=-\Delta_\alpha\sigma_1-x_\alpha\sigma_3$ we have

$$G_\alpha^{-1}(k,z)=z\sigma_0-\xi_{\alpha k}\sigma_3+\Delta_\alpha\sigma_1$$

(15)

with $\xi_{\alpha k}=\epsilon_{\alpha k}+x_\alpha-\mu$.

Δ_α is the energy gap of band α. x_α is an energy shift due to the pairing interaction which is also present in the normal state. In a one-layer system x_α can be incorporated into the chemical potential μ, but this is not possible in the two-layer system with interlayer hopping.

Performing the frequency summation we get the following self-consistency equations for the gaps and energy shifts:

$$\Delta_1=-W\Delta_1 I_1-\overline{V}\Delta_2 I_2,$$

$$\Delta_2=-W\Delta_2 I_2-\overline{V}\Delta_1 I_1,$$

(16)

$$x_1=-WK_1-\overline{V}K_2,$$

$$x_2=-WK_2-\overline{V}K_1$$

(17)

with the integrals

$$I_\alpha=\sum_k\frac{1}{2E_{\alpha k}}\tanh\frac{\beta E_{\alpha k}}{2},\quad K_i=\sum_k\frac{\xi_{\alpha k}}{2E_{\alpha k}}\tanh\frac{\beta E_{\alpha k}}{2}$$

and $E_{\alpha k}=\sqrt{\xi_{\alpha k}^2+\Delta_\alpha^2}$.

Without a cutoff the integrals I_i would diverge. Approximately the integrals have the values

$$I_\alpha\simeq N_\alpha\ln(2\omega_c/\mathrm{Max}(\Delta_\alpha,T)),$$

(18)

where N_α is the density of states of band α per spin at the Fermi surface, and ω_c is the cutoff.

The self-consistency equations (17) describing the energy shifts $x_{1,2}$ of the two bands can be solved approximately by observing that the integrands are nearly step functions. Assuming constant density of states N_1, N_2 (this is given by a quadratic two-dimensional dispersion) and k-independent interlayer hopping t one finds

$$x_1=WN_1(t+x_1)-\overline{V}N_2(t-x_2),$$

$$x_2=-WN_2(t-x_2)+\overline{V}N_1(t+x_1).$$

(19)

In the limit of $W,\overline{V}\rightarrow0$ and cutoff $\omega_c\rightarrow\infty$ these shifts vanish, but the ratio $(x_2-x_1)/(W-\overline{V})$ stays finite $[N_0=(N_1+N_2)/2]$:

$$\frac{x_2-x_1}{W-\overline{V}}\rightarrow-2N_0t.$$

(20)

The solution of the gap equations for a two-band system is discussed already by Leggett;[5] the qualitative results can be summarized as follows: There exists no solution, if $W>0$ and $W^2>\overline{V}^2>0$; then the intralayer $W_\parallel=V_\parallel+J$ and the interlayer coupling $W_\perp=V_\perp+J$ are repulsive. There are two nontrivial solutions, if $W<0$ and $W^2>\overline{V}^2>0$; in this case $W_\parallel$ and $W_\perp$ are attractive. The solution corresponding to the ground state depends on the sign of the interband interaction $\overline{V}$. If $\overline{V}<0$, the state where the gaps have the same sign ($\Delta_1\Delta_2>0$) is stable; if $\overline{V}>0$, then the gaps have opposite signs ($\Delta_1\Delta_2<0$). The reason is a term in the free-energy proportional to $\overline{V}\cos(\phi_1-\phi_2)$, where ϕ_1,ϕ_2 are the phases of the order parameters Δ_1,Δ_2.

If the density of states for the two bands are equal (this happens for a constant density of states and for k-independent interlayer hopping t) the two integrals I_i are equal for equal values of the gaps ($I_1=I_2$ for $\Delta_1^2=\Delta_2^2$) then for all solutions of the gap equations one always finds $|\Delta_1|=|\Delta_2|$ and $x_1=-x_2$ irrespective of the values of the coupling constants, i.e., one either has pure intralayer pairing for $W_\parallel<0$ with $(\Delta_1+\Delta_2)/2=\Delta_\parallel\neq0$, $(\Delta_2-\Delta_1)/2=\Delta_\perp=0$ or pure interlayer pairing for $W_\perp<0$ with $\Delta_\perp\neq0$ and $\Delta_\parallel=0$. In the more general case the density of states of the two bands is different at the Fermi surface, and the two integrals have different values also in the case of equal or vanishing gaps, and the two order parameters are coupled.

For the numerical solutions of the self-consistency equations and vertex equations with k-dependent hopping we use the following simple model by choosing two bands with quadratic dispersion but different effective masses (and different density of states):

$$\epsilon_{1k}=\epsilon_k-t_k=k^2/(2m_1)-t_0,$$

$$\epsilon_{2k}=\epsilon_k+t_k=k^2/(2m_2)+t_0.$$

(21)

In the numerical calculations we use the following dispersion parameters to get k-dependent hopping:

$$2m_1/\hbar^2=1\ \mathrm{eV}^{-1}\ \text{Å}^{-2},\quad 2m_2/\hbar^2=1.2\ \mathrm{eV}^{-1}\ \text{Å}^{-2},$$

$$t_0=0,\quad \mu=0.3\ \mathrm{eV},\quad \omega_c=0.25\ \mathrm{eV}.$$

(22)

For the intraband and interband coupling constants $W=V+J$ and $\overline{V}$, entering the self-consistency equations we choose

$$N_0W=-0.139,\quad N_0\overline{V}=\pm0.185.$$

(23)

We have chosen these values for the coupling constants in order to get T_c values which are appropriate for high-T_c superconductors and ensure also the appearance of the collective modes we want to study.

Figure 1 shows the dispersion for the two bands in the normal state and the quasiparticle dispersions in the superconducting state at zero temperature in the k region $|\epsilon_k-\mu|<\omega_c$. Figures 2(a), 2(b) show the temperature dependence of the gaps for negative $\overline{V}$ (a) and positive $\overline{V}$ (b). Because the effective masses m_1 and m_2 are nearly the same
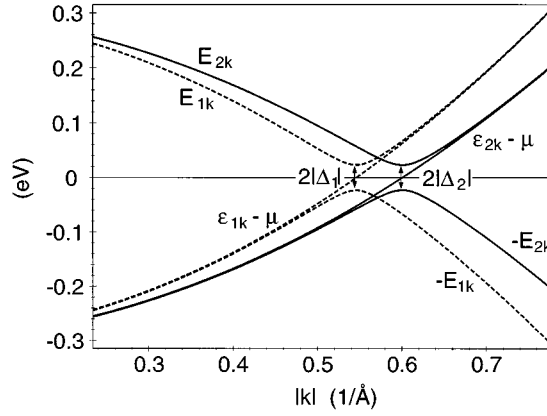
FIG. 1. Dispersions in the normal state ϵ_{1k}, ϵ_{2k} and quasiparticle dispersions in the superconducting state ($T=0$) in the k region $|\epsilon_k| < \omega_c$. The parameters (22,23) are used.

(22) the values of the two gaps Δ_1 and Δ_2 are nearly the same. For repulsive interband coupling $\overline{V}$ the stable gaps have different signs. In both cases intralayer and interlayer pairing are mixed. But for negative $\overline{V}$ intralayer pairing dominates, for positive $\overline{V}$ interlayer pairing dominates. T_c is 155 K. We have also calculated the level shifts x_i. They are practically temperature independent.

III. VERTEX EQUATIONS

Now we will set up the integral equations for the vertex functions corresponding to the interlayer polarization and related operators defined in (8) for the neutral and charged system. We are interested in optical response functions for electric-field vectors perpendicular to the layers. Here we can assume that the external wave vector is zero.
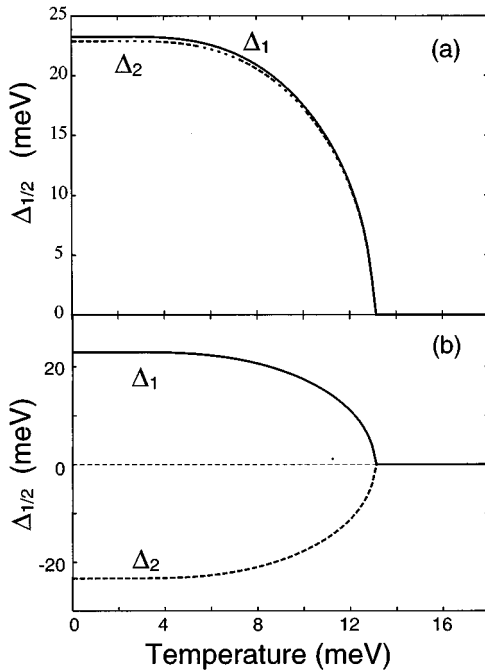

FIG. 2. Gaps as function of temperature for negative (a) and positive interband coupling $\overline{V}$ (b). The parameters (22,23) are used.

A. Neutral system

We consider response functions where the bare vertex is one of the matrices D^{jl}, corresponding to the operators (8). In the standard ladder approximation the vertex equation for the renormalization of a vertex with matrix D^{jl} reads

$$\Gamma^{jl}(i\omega_s) = D^{jl} - \frac{1}{\beta}\sum_{k\omega_n} V D^{03} G(k,i\omega_n)$$
$$+ i\omega_s \Gamma^{jl}(i\omega_s) G(k,i\omega_n) D^{03}$$
$$+ \overline{V} D^{13} G(k,i\omega_n+i\omega_s)\Gamma^{jl}(i\omega_s)G(k,i\omega_n)D^{13}$$
$$+ J D^{33} G(k,i\omega_n+i\omega_s)\Gamma^{jl}(i\omega_s)G(k,i\omega_n)D^{33}.$$
(24)

The vertex function depends only on the external frequency ω_s, not on the momentum k (apart from the cutoff) and the internal frequency of the Green's function, because the interactions are assumed to be constant. The label jl indicates to which bare vertex the vertex function belongs. In the case of the polarization we have to consider the matrix D^{13}. Of course, due to the interactions the renormalized vertex Γ^{jl} contains also contributions from other matrices.

The interactions V, J induce only intraband transitions, the interaction $\overline{V}$ only interband transitions. These interactions do not change the off-diagonal character of the bare vertices, therefore we can make the following ansatz for the renormalized vertex of the neutral system:

$$\Gamma^{jl} = \begin{pmatrix} 0 & \gamma \\ \hat{\gamma} & 0 \end{pmatrix} \tag{25}$$

with 2×2 matrices $\gamma(i\omega_s)$, $\hat{\gamma}(i\omega_s)$. Then the system of vertex equations can be written as two coupled equations for 2×2 matrices:

$$\gamma + W' B + \overline{V}\hat{B} = I,$$
$$\hat{\gamma} + W'\hat{B} + \overline{V}B = \hat{I}, \tag{26}$$

where $W' = V - J = (V_\parallel + V_\perp)/2 - J$. The 2×2 matrices I and $\hat{I}$ are the upper right and lower left part of the matrix D^{jl}. In the case of the polarization D^{13} we have $I = \sigma_3$, $\hat{I} = -\sigma_3$. The quantities B are defined as

$$B(i\omega_s) = \frac{1}{\beta}\sum_{\omega_n}\sum_k \sigma_3 G_1(k,i\omega_n+i\omega_s)\gamma(i\omega_s)G_2(k,i\omega_n)\sigma_3,$$

$$\hat{B}(i\omega_s) = \frac{1}{\beta}\sum_{\omega_n}\sum_k \sigma_3 G_2(k,i\omega_n+i\omega_s)\hat{\gamma}(i\omega_s)G_1(k,i\omega_n)\sigma_3,$$
(27)

depending linearly on $\gamma(i\omega_s)$. Note, that in contrast to the self-consistency equations (16, 17) ($W = V + J$), the interaction J enters here with another sign ($W' = V - J$).

For the solution of this system of equations it is convenient to decompose $\gamma, \hat{\gamma}$ and also $B, \hat{B}$ into Pauli matrices:

$$\gamma = \gamma_0\sigma_0 + \gamma_1\sigma_1 + \gamma_2 i\sigma_2 + \gamma_3\sigma_3,$$

$$B = B_0\sigma_0 + B_1\sigma_1 + B_2 i\sigma_2 + B_3\sigma_3. \tag{28}$$

If we write the coefficient functions γ_i as vector $\underline{\gamma} = (\gamma_0, \gamma_1, \gamma_2, \gamma_3)$ we can express the linear dependence of $\underline{B}$ on these coefficients in matrix form:

$$\underline{B} = K\underline{\gamma}, \quad \hat{\underline{B}} = \hat{K}\hat{\underline{\gamma}}. \tag{29}$$

The 4×4 matrices $K, \hat{K}$ are integrals over products of Green's functions. For notational convenience it is useful to introduce an extra factor i for the σ_2 component in (28). The structure of K is given in (A3) and the functions are listed in (A5). With help of these matrices K, $\hat{K}$ the vertex equations can be written as

$$(1 + W'K)\underline{\gamma} + \overline{V}\hat{K}\hat{\underline{\gamma}} = \underline{I},$$

$$(1 + W'\hat{K})\hat{\underline{\gamma}} + \overline{V}K\underline{\gamma} = \hat{\underline{I}}. \tag{30}$$

The matrix $\hat{K}$ differs from the matrix K only by the sign of some elements in the first row and column. More precisely: $\hat{K} = gKg$ with g being the diagonal matrix $g = \text{diag}(-1,1,1,1)$. $\underline{I}$ is a vector given by $(0,0,0,1)$, $(0,0,-i,0)$, $(0,1,0,0)$, $(-i,0,0,0)$ for P^{13}, P^{12}, P^{11}, P^{20}, respectively. $\hat{\underline{I}}$ fulfills: $\hat{\underline{I}} = g\underline{I}$. The second equation in (30) can be reduced to the first equation by setting

$$\hat{\underline{\gamma}} = g\underline{\gamma}, \tag{31}$$

and it is sufficient to solve the first equation

$$\sum_j (\delta_{ij} + (W' + \overline{V}g_{ii})K_{ij})\gamma_j = I_i, \tag{32}$$

which is a set of four linear equations.

A closer inspection of the integral contained in the matrix K shows that two of the integrals K_{11} and K_{22} are badly convergent. They depend logarithmically on the cutoff in momentum space in a similar way as the integrals in the self-consistency equations (18). These badly convergent integrals can be eliminated by using relations (B19,B20) which can be derived from Ward identities. Then the cutoff is only needed in the calculation of the gaps Δ_i.

In general the correlation functions of the neutral system are given by

$$\langle\langle P^{ij}; P^{lm} \rangle\rangle_{i\omega_s} = \frac{1}{\beta}\sum_{\omega_n} \sum_k \text{Tr}\{D^{ij}G(k, i\omega_n + i\omega_s)\Gamma^{lm}(i\omega_s)G(k, i\omega_n)\}. \tag{33}$$

Especially the polarization function is determined by

$$\langle\langle P; P \rangle\rangle_{i\omega_s} = \frac{1}{\beta}\sum_{\omega_n} \sum_k \text{Tr}\{D^{13}G(k, i\omega_n + i\omega_s)\Gamma^{13}(i\omega_s)G(k, i\omega_n)\}. \tag{34}$$

The polarization function can be expressed by the matrix B (27) or by the matrix K using the commutation relations for the Pauli matrices and the development into Pauli matrices (28):

$$\langle\langle P, P \rangle\rangle = \langle\langle P^{13}, P^{13} \rangle\rangle = 4K_{3j}\gamma_j^{13}. \tag{35}$$
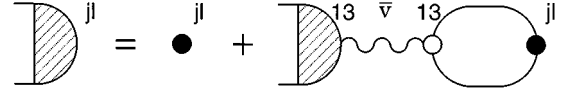

FIG. 3. Diagrammatic representation of the vertex Y^{jl} of the charged system with help of the vertex Γ^{jl} (full circle) of the neutral system. The interband Coulomb interaction $\overline{v}$ couples to the correlation function $\langle\langle P^{13}, P^{jl} \rangle\rangle$ of the neutral system.

Later we want to discuss the influence of the polarization $\langle P \rangle$ on the order parameter. Therefore we need the correlation functions

$$\langle\langle A, P \rangle\rangle = \langle\langle P^{11}, P^{13} \rangle\rangle = -4K_{1j}\gamma_j^{13}, \tag{36}$$

$$\langle\langle \Phi, P \rangle\rangle = \langle\langle P^{12}, P^{13} \rangle\rangle = -4iK_{2j}\gamma_j^{13}. \tag{37}$$

B. Charged system

Up to now we have only considered neutral superconductors. The long-range Coulomb interaction is known to have important consequences for the collective modes.[1-4] Here we are interested in the optical properties for field vectors perpendicular to the layers in the long-wavelength limit $q \rightarrow 0$. Then we have to consider only the Coulomb interaction arising from charge fluctuations between the layers. These Coulomb forces stay finite in the long-wavelength limit but nevertheless are sizable. They can be incorporated in the vertex equations in a random-phase-approximation-type manner.

Let $Y^{il}(i\omega_s)$ be the vertex for the charged system. The vertex equation for Y^{il} is obtained from the vertex of the neutral system (24), if Γ^{jl} is replaced by $Y^{il}(i\omega_s)$, and on the right-hand side (rhs) of the vertex equation (24) the following term is included:

$$D^{13}\overline{v}\frac{1}{\beta}\sum_{\omega_n k} \text{Tr}\{D^{13}G(k, i\omega_n + i\omega_s)Y^{jl}(i\omega_s)G(k, i\omega_n)\} \tag{38}$$

with $\overline{v} = \lim_{|q| \rightarrow 0} e^2 \pi (1 - e^{-d|q|})/(|q|\epsilon_0) = e^2\pi d/\epsilon_0$ the Coulomb interaction between the layers. For a periodic double-layer system $\overline{v}$ has to be replaced by $\pi e^2 d(c-d)/c\epsilon_0$, where d is the distance between the two layers in one unit cell and c is the distance between the unit cells. The vertex equation for Y^{jl} can also be expressed by correlation functions and the vertex of the neutral system Γ^{jl}, as shown in Fig. 3. This equation reads

$$Y^{jl} = \Gamma^{jl} + Y^{13}\overline{v}\langle\langle P^{13}, P^{jl} \rangle\rangle, \tag{39}$$

where the correlation function $\langle\langle P^{13}, P^{jl} \rangle\rangle$ of the neutral system to which the interband Coulomb-interaction couples is given by

$$\langle\langle P^{13}, P^{jl} \rangle\rangle = \frac{1}{\beta}\sum_{\omega_n} \sum_k$$

$$\text{Tr}\{D^{13}G(k, i\omega_n + i\omega_s)\Gamma^{jl}(i\omega_s)G(k, i\omega_n)\}. \tag{40}$$

From this the vertex function Y^{13} for the electronic polarization is easily calculated

$$Y^{13} = \Gamma^{13}/(1 - \overline{v}\langle\langle P^{13}, P^{13} \rangle\rangle), \tag{41}$$

and we get for the polarization function for the charged system

$$\langle\langle P,P\rangle\rangle^C_{i\omega_s}=\langle\langle P,P\rangle\rangle_{i\omega_s}/(1-\bar{v}\langle\langle P,P\rangle\rangle_{i\omega_s}), \quad (42)$$

and the correlation functions (36), (37)

$$\langle\langle A,P\rangle\rangle^C_{i\omega_s}=\langle\langle A,P\rangle\rangle_{i\omega_s}/(1-\bar{v}\langle\langle P,P\rangle\rangle_{i\omega_s}),$$

$$\langle\langle\Phi,P\rangle\rangle^C_{i\omega_s}=\langle\langle\Phi,P\rangle\rangle_{i\omega_s}/(1-\bar{v}\langle\langle P,P\rangle\rangle_{i\omega_s}). \quad (43)$$

IV. ANALYTICAL DISCUSSION OF THE COLLECTIVE MODES

In general the four vertex equations (32)

$$\sum_j [\delta_{ij}+(W'+\bar{V}g_{ii})K_{ij}]\gamma_j=I_i \quad (44)$$

have to be solved numerically. But in some limits the equations can be simplified so that analytical results for the collective modes can be derived: (1) in the normal state and (2) in the limit of momentum-independent tight-binding coupling t_k between the layers.

In the following we need the special form of the matrix K given in Appendix A:

$$K=\begin{pmatrix} H^{++} & -\widetilde{Y} & -\widetilde{Z} & \widetilde{X} \\ \widetilde{Y} & -H^{-+} & X & Z \\ \widetilde{Z} & X & -H^{--} & Y \\ \widetilde{X} & -Z & -Y & H^{+-} \end{pmatrix}. \quad (45)$$

Furthermore we need the following combinations of coupling constants, which are listed here for completeness:

$$W=V+J, \quad W_\parallel=V_\parallel+J, \quad W_\perp=V_\perp+J,$$

$$W'=V-J, \quad W'_\parallel=V_\parallel-J, \quad W'_\perp=V_\perp-J \quad (46)$$

with $V=(V_\parallel+V_\perp)/2$, $\bar{V}=(V_\parallel+V_\perp)/2$. Of special importance is the limit, where all pairing interactions are small

$$VN_0, \quad \bar{V}N_0, \quad JN_0\ll 1. \quad (47)$$

This will be called the weak-coupling limit in the following.

A. Normal state

In the normal state the functions $Z,\widetilde{Z},Y,\widetilde{Y}$ vanish, because they are proportional to the gaps (A5). Therefore the set of equations (44) decouples. With $\underline{I}=(0,0,0,1)$ we obtain for the polarization vertex $\gamma=\gamma^{13}=\gamma^P$:

$$\gamma_0=-W'_\perp\widetilde{X}/N, \quad \gamma_1=\gamma_2=0,$$

$$\gamma_3=(1+W'_\perp H^{++})/N \quad (48)$$

with $N=(1+W'_\perp H^{++})(1+W'_\parallel H^{+-})-W'_\parallel W'_\perp\widetilde{X}^2$. The polarization function (35) is then given by

$$\langle\langle P,P\rangle\rangle_{i\omega_s}=4[(1+W'_\perp H^{++})H^{+-}-W'_\perp(\widetilde{X})^2]/N. \quad (49)$$

In the case of momentum-independent hopping ($t_k=t$) this expression can be simplified considerably by using the relations between the different matrix elements derived from the Ward identities (B18) and the approximation $(x_2-x_1)/W_\perp=-2tN_0$. We obtain

$$\langle\langle P;P\rangle\rangle_{i\omega_s}=16N_0t^2(1+2N_0J)/M \quad (50)$$

with

$$M=(i\omega_s)^2-4t^2[1-2(\bar{V}-2J)N_0-4J(\bar{V}-J)N_0^2].$$

The polarization function has a simple pole which is shifted with respect to the simple particle-hole excitation energy $2t$ due to the pairing interactions. In the weak-coupling limit (47) we recover as result the bare polarization function, which is given by H^{+-}. In the charged system there exists then a plasmon describing interlayer charge fluctuations at $\omega^2=(2t)^2(1+\bar{v}4N_0)$.

B. k-independent hopping matrix element t

In the case of momentum-independent tight-binding coupling ($t_k=t$) the solution for the self-consistency equations (17, 16) has the form

$$\Delta_1=\pm\Delta_2 \quad \text{and} \quad x_1=-x_2, \quad (51)$$

independent of the details of the band dispersion ϵ_k. Then there exists a symmetry relation between the band dispersions $\xi_{1k}=\xi_k-t-x_1$ and $\xi_{2k}=\xi_k+t-x_2$ ($\xi_k=\varepsilon_k-\mu$) and the quasiparticle dispersions:

$$\xi_2(\xi_k)=-\xi_1(-\xi_k),$$

$$E_1(-\xi_k)=E_2(\xi_k). \quad (52)$$

Due to this symmetry some matrix functions K_{ij} vanish and therefore (44) is reduced to a system of three coupled equations. We have to distinguish the two cases $\Delta_1=\pm\Delta_2$.

1. Intralayer pairing $\Delta_1=\Delta_2$

In the case of dominant intralayer interaction $W_\parallel$ the band gaps are equal ($\Delta_1=\Delta_2=\Delta_\parallel$) and interlayer pairing vanishes [$\Delta_\perp=(\Delta_2-\Delta_1)/2=0$]. Three functions are zero because of the relation (52)

$$Z(i\omega_s)=X(i\omega_s)=\widetilde{Y}(i\omega_s)=0. \quad (53)$$

Therefore the second equation of the vertex equations (44) can be solved easily

$$\gamma_1^j,\gamma_1^\Phi,\gamma_1^P=0, \quad \gamma_1^A(i\omega_s)=1/[1-W_\parallel H^{-+}(i\omega_s)],$$

$$\gamma_l^A=0, \quad l=0,2,3. \quad (54)$$

This means that oscillations of the amplitude A do not couple to oscillations of the current j, polarization P, and phase Φ. But the density, phase, and current oscillations couple to each other. The Coulomb interaction does not affect the amplitude fluctuations. This is in agreement with the results found in Refs. 14,15, where a double-layer system with $t=0$ is investigated. In the case of k-dependent hopping all these quantities couple, which will be demonstrated below by our numerical results.

The frequencies of the collective modes are determined by the zeros of the denominator of the vertex functions γ^{jl}. For the current, phase, and polarization oscillations the frequency of the collective mode is given by the determinant of the corresponding 3×3 matrix of the vertex-equation system (44); the collective mode of the amplitude oscillations is determined by (54).

The functions $K(\omega + i\delta)$ obtain imaginary parts at temperature $T = 0$, when the frequency of the external field is large enough to break Cooper pairs $[\omega > \min(E_{1k} + E_{2k}) = \sqrt{(2\hat{t})^2 + (2\Delta_\parallel)^2}$ with $\hat{t} = t + (x_1 - x_2)/2]$. We are interested in undamped collective modes below the particle-hole threshold. In order to derive a simple approximation for the collective mode frequencies, we shall assume small frequencies $\omega \ll \sqrt{(2\hat{t})^2 + (2\Delta_\parallel)^2}$, a small hopping matrix element $(\hat{t}/\Delta_\parallel)^2 \ll 1$, and zero temperature.

The functions K (A5) can be evaluated with help of an expansion in $\hat{t}/\Delta_\parallel$ and $\omega/2\Delta_\parallel$:

$$H^{+-}(\omega) \approx -N_0 + \omega^2 C, \quad H^{++} \approx (2\hat{t})^2 C,$$

$$Y(\omega) \approx \omega\{N_0 + [(2\hat{t})^2 - \omega^2]C\}/(2\Delta_\parallel),$$

$$\widetilde{Z}(\omega) \approx -2\hat{t}N_0/(2\Delta_\parallel), \quad \widetilde{X} \approx -\omega 2\hat{t}C, \tag{55}$$

where $C = -N_0/(8\Delta_\parallel^2)$. Here $-(x_2 - x_1)/(W_\perp 2\hat{t})$ has been approximated by the density of states at the Fermi level N_0 [see (19)].

With these expressions we expand the determinant up to second order in $\hat{t}/\Delta_\parallel$ or $\omega/(2\Delta_\parallel)$

$$\mathrm{Det} = \frac{N_0 W_\parallel'}{(2\Delta_\parallel)^2}(1 - \omega_0^2 W_\parallel' C)(\omega^2 - \omega_P^2). \tag{56}$$

Here ω_P is the frequency of the collective phase mode in the neutral system

$$\omega_P^2 = \{\omega_0^2 + (2\hat{t})^2[1 - W_\perp'(N_0 - \omega_0^2 C)]\}\frac{1 - W_\parallel' N_0}{1 - \omega_0^2 W_\parallel' C} \tag{57}$$

with

$$\omega_0^2 = \frac{(2\Delta_\parallel)^2}{N_0}\frac{-2J}{V_\parallel^2 - J^2}.$$

This reduces to a simple result in the weak-coupling limit (47):

$$\omega_P^2 = (2t)^2 + \omega_0^2. \tag{58}$$

Because we have assumed small frequencies the formula is only valid for small ω_0, i.e., $|J/V_\parallel|$ has to be small. The expression for the frequency ω_0 has been derived already by Leggett.[5] Here we see how the mode frequency is modified by the interlayer hopping t. It is justified to call this mode phase mode, because it appears as a resonance in the polarization function due to its coupling to the phase fluctuation.

Evaluating the polarization function (35) of the neutral system for small frequencies and small hopping matrix element we obtain

$$\langle\langle P, P\rangle\rangle_\omega = 4N_0 \frac{\omega_P^2(1 - \omega_0^2 W_\parallel' C) - \omega^2 \omega_0^2 C(1 - W_\parallel' N_0)}{(\omega^2 - \omega_P^2)(1 - \omega_0^2 W_\parallel' C)(1 - W_\parallel' N_0)}. \tag{59}$$

Inserting (59) into the polarization function with Coulomb interaction (42) we get the phase-mode frequency in the charged system:

$$\omega_C^2 = \{\omega_0^2 + (2\hat{t})^2[1 - W_\perp'(N_0 - \omega_0^2 C)]\}\frac{1 + N_0(4\bar{v} - W_\parallel')}{1 + \omega_0^2 C(4\bar{v} - W_\parallel')}. \tag{60}$$

In the weak-coupling limit (47) and for small $|\omega_0^2 C|$ we have

$$\omega_C^2 = (\omega_0^2 + (2t)^2)(1 + 4N_0\bar{v}). \tag{61}$$

The interband Coulomb interaction $\bar{v}$ shifts the mode up to higher frequencies. $\bar{v}$ is proportional to the distance d between the layers. In order to get a phase mode below the particle-hole threshold, it is necessary that the distance of the layers and the Josephson coupling constant J be small. If the Josephson coupling J is zero, the resonance appears at $2t$ as in the normal state but still below the particle-hole threshold.

In order to understand how the superconducting order parameter couples to the polarization, we calculate the correlation functions (43) in the weak-coupling limit. Applying the same approximations as before $[(t/\Delta_\parallel)^2 \ll 1, \omega^2 \sim O(t^2), \omega_0^2 \sim O(t^2)]$ we find

$$\langle\langle A, P\rangle\rangle^C = 0, \tag{62}$$

$$\langle\langle \Phi, P\rangle\rangle^C \approx -4iN_0 \frac{1}{N_0 W_\parallel}\frac{\omega 2\Delta_\parallel}{\omega^2 - \omega_C^2}. \tag{63}$$

The imaginary factor i indicates that $\langle\Phi\rangle(t)$ is oscillating with a phase shift of $\pi/2$ in comparison to $\langle P\rangle(t)$. A finite value of $\langle\Phi\rangle(t) = -i\mathrm{Im}(\langle c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger\rangle - \langle c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger\rangle)$ means that the phases of the intralayer order parameters are oscillating. The mode corresponds to the collective tunneling of Cooper pairs between the layers without pair breaking.

The denominator of γ_1^A (54) determines the amplitude mode. With the relations (B21) and using Ward identities (B18) we get

$$\frac{1}{\gamma_1^A(\omega)} = 1 - \frac{W_\parallel'}{W_\parallel} - \left(\frac{(2\hat{t})^2 - \omega^2}{(2\Delta_\parallel)^2} + 1\right)W_\parallel'\frac{2\Delta_\parallel Y(\omega)}{\omega}. \tag{64}$$

For vanishing Josephson coupling ($W_\parallel'/W_\parallel = 1$) the amplitude mode lies just at the particle-hole threshold:

$$\omega_A^2 = (2\hat{t})^2 + (2\Delta_\parallel)^2.$$

For finite Josephson coupling an approximate analytical result can be obtained with (55):

$$\omega_A^2 = (2\hat{t})^2 + 2[\omega_0^2 + (2\Delta_\parallel)^2]. \tag{65}$$

Because we assumed small frequencies, this result is only valid if ω_0^2 is negative, which is obtained for positive J. For the general solution we refer to the numerical calculation.

The formula for the phase (58) and amplitude modes (65) shows how the mode frequencies are shifted by the hopping

t and the results of Refs. 5 and 14 are modified. Note, however, that the particle-hole threshold is shifted too.

2. Interlayer pairing $\Delta_1 = -\Delta_2$

In the case of dominant interlayer interaction, when $\Delta_\perp = (\Delta_2 - \Delta_1)/2 \neq 0$, $\Delta_\parallel = (\Delta_2 + \Delta_1)/2 = 0$, the following three functions are zero because of (52):

$$\widetilde{Z}(i\omega_s) = X(i\omega_s) = Y(i\omega_s) = 0. \qquad (66)$$

The third column and line of the vertex equation matrix (44) are zero with the exception of the diagonal element. Now the oscillations of Φ are decoupled from the the oscillations of the other quantities, while j, A, and P couple to each other.

Again we study the limit of small frequencies $\omega \ll \sqrt{(2\hat{t})^2 + \Delta_\perp^2}$ and small hopping $|\hat{t}/\Delta_\perp|^2 \ll 1$. The functions can be approximated as

$$H^{++} \approx -N_0 + \omega^2 C, \quad H^{+-} \approx (2\hat{t})^2 C,$$

$$\widetilde{Y} \approx \omega\{N_0 + [(2\hat{t})^2 - \omega^2]C\}/(2\Delta_\perp),$$

$$Z \approx -2\hat{t}N_0/(2\Delta_\perp), \quad \widetilde{X} \approx -\omega 2\hat{t}C,$$

$$H^{-+} \approx 1/W_\perp - [\omega^2 - (2\hat{t})^2]N_0/(2\Delta_\perp)^2, \qquad (67)$$

where $C = -N_0/8\Delta_\perp^2$ and $\hat{t} = t + (x_1 - x_2)/2$ as before. From the vanishing of the determinant of the three coupled equations we now obtain for the frequency of the collective mode determining polarization and amplitude oscillations:

$$\omega_P^2 = \{\omega_0^2 + (2\hat{t})^2[1 - W_\parallel'(N_0 - \omega_0^2 C)]\}\frac{1 - W_\perp' N_0}{1 - \omega_0^2 W_\perp' C} \qquad (68)$$

with

$$\omega_0^2 = \frac{(2\Delta_\perp)^2}{N_0}\frac{2(\overline{V} - J)}{V^2 - (\overline{V} - J)^2}.$$

In the weak-coupling limit (47) the mode in the neutral system becomes

$$\omega_P^2 = (2t)^2 + \omega_0^2. \qquad (69)$$

Expanding the nominator and denominator of the polarization function (35) up to second order in $\hat{t}/\Delta_\perp$ and $\omega/2\Delta_\perp$ we obtain

$$\langle\langle P,P\rangle\rangle_\omega = 4(N_0 - \omega_0^2 C)\frac{(2\hat{t})^2(1 - W_\perp' N_0)}{(\omega^2 - \omega_P^2)(1 - \omega_0^2 W_\perp' C)}, \qquad (70)$$

which in the weak-coupling limit and for $\omega_0^2 \sim O(t^2)$ becomes

$$\langle\langle P,P\rangle\rangle \approx 4N_0\frac{(2t)^2}{\omega^2 - \omega_P^2}. \qquad (71)$$

For the correlation functions (36, 37) we find

$$\langle\langle A,P\rangle\rangle \approx 4N_0\frac{1}{N_0 W_\perp}\frac{2t\Delta_\perp}{\omega^2 - \omega_P^2},$$

$$\langle\langle \Phi,P\rangle\rangle = 0. \qquad (72)$$

The polarization function (71) is zero, if the single-particle hopping t vanishes. This is in contrast to the case of intralayer pairing, where the pair tunneling due to J produces density fluctuations between the layers and therefore spectral weight in the polarization function even in the absence of single-particle hopping.

The correlation function (72) shows that a finite polarization $\langle P\rangle(t)$ is connected with a finite amplitude $\langle A\rangle(t) = \text{Re}(\langle c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger\rangle - \langle c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger\rangle)$. This means that the polarization is associated with the building of intralayer pairs $\langle c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger\rangle$, $\langle c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger\rangle$.

In the frequency ω_0^2 the coupling $\overline{V}$ now appears in the nominator apart from the Josephson coupling J. $\overline{V}$ is proportional to the difference of the intralayer $V_\parallel$ and interlayer coupling $V_\perp$ and is related to the energy difference between intralayer and interlayer pairing. The mode can only exist if the energy $\overline{V}$ for formation of intralayer pairs is small or the Josephson coupling J compensates this energy ($J \approx \overline{V}$). The second possibility is a quite unrealistic one, because J is normally much smaller than $\overline{V}$.

The collective mode in the charged system is given by

$$\omega_C^2 = \{\omega_0^2 + (2\hat{t})^2[1 + (4\overline{v} - W_\parallel')(N_0 - \omega_0^2 C)]\}\frac{1 - W_\perp' N_0}{1 - \omega_0^2 W_\perp' C}. \qquad (73)$$

Only the term containing the single-particle hopping is influenced by the Coulomb interaction. This is consistent with the picture of interlayer pairing. The hopping of interlayer pairs produces no charge fluctuation between the layers. When an interlayer pair is tunneling, one electron jumps to the upper layer, the other to the lower layer and the charge density on the layers does not change.

In a similar way as above we obtain for the frequency of the phase mode, which is now decoupled from the polarization:

$$\omega_\Phi^2 = (2\hat{t})^2 + 2[\omega_0^2 + (2\Delta_\perp)^2]. \qquad (74)$$

Because we assumed small frequencies, this result is only valid, if ω_0^2 is negative, which is obtained for negative $\overline{V} - J$. For the general solution we refer to the numerical calculation.

In comparison to the case of intralayer pairing the modes have changed their role. The amplitude mode is now the low-lying excitation and is coupled to the electronic polarization. As in the ground state of interlayer pairing the layer order parameters $\langle c_{1\uparrow} c_{1\downarrow}\rangle$ and $\langle c_{2\uparrow} c_{2\downarrow}\rangle$ are zero and it is no longer justified to call oscillations of Φ phase oscillations. We kept this name for convenience only.

V. NUMERICAL RESULTS

In the general case of k-dependent hopping when intralayer and interlayer pairing are mixed it is not possible to derive simple expressions for the dispersions of the collec-
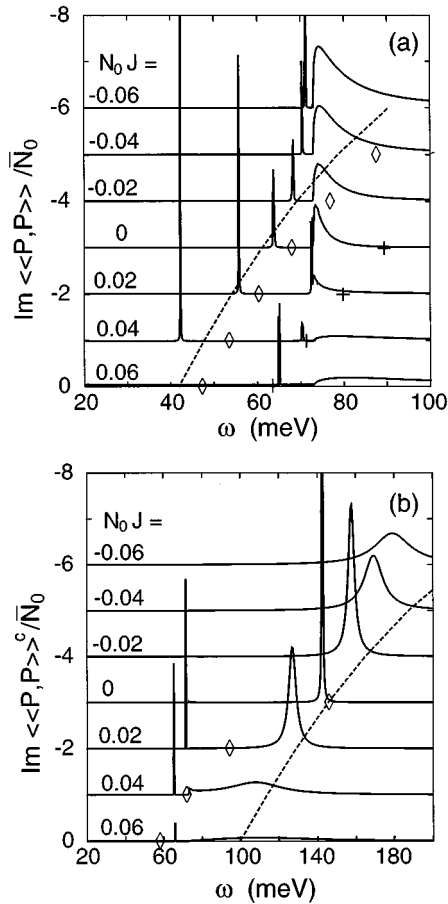
FIG. 4. Imaginary parts of the polarization function in the neutral (a) and charged (b) system at $T=0$ in the case of dominant intralayer pairing for different Josephson couplings J. The parameter sets (22,23) are used. The results are normalized by $\bar{N}_0 = 13 N_0$. The different lines are shifted by equal units. The rhombs, crosses, and dashed lines in the figures correspond to various approximation formulas for the collective mode frequencies discussed in the text.

tive modes. We made numerical calculations for the polarization functions with the dispersion parameters (22) and coupling constants

$$N_0 W = -0.139, \quad N_0 \bar{V} = \pm 0.185, \quad N_0 \bar{v} = 1.3 \quad (75)$$

for constant $W = V + J$ and variable Josephson coupling J for dominating intralayer ($\bar{V} < 0$) and interlayer pairing ($\bar{V} > 0$), in order to study the influence of the Josephson coupling J and the temperature dependence of the collective modes. We present results both for the neutral system and taking into account the Coulomb interaction $\bar{v}$ between the layers. To resolve the δ peaks of the collective modes at $T=0$ below the particle-hole threshold we have introduced a small imaginary part (10^{-3} meV) to the frequency.

A. Dominant intralayer pairing

First we discuss the results for the case of dominant intralayer pairing ($\bar{V} < 0, \Delta_1 \Delta_2 > 0$). In Fig. 4 the spectrum of the collective modes (sharp spikes) and the form of the particle-hole spectrum at $T=0$ are shown. The imaginary

parts of the polarization function in the neutral 4(a) and the charged system 4(b) are calculated for different Josephson couplings J and constant intraband $W = V + J$ and interband coupling $\bar{V}$. For comparison results of the approximation formulas are plotted, too. The rhombs and crosses in (a) refer to the formulas for the phase (57) and amplitude mode (65), respectively, calculated with a constant averaged hopping $t = -30.5$ meV. The dashed line represents the phase mode frequency (58) in the weak-coupling limit.

For negative Josephson couplings J a collective mode, the phase mode, lies just below the particle-hole threshold. With increasing positive J the phase-mode peak moves to lower frequencies.

For positive J another mode, the amplitude mode, becomes visible near the particle-hole threshold. For increasing J the peak moves to smaller frequencies. Thus, two superconducting collective modes can occur in the polarization function perpendicular to the layers. This effect is caused by the coupling of the phase and amplitude fluctuations.

The two approximation formulas for the phase mode, represented by the rhombs and the dashed line, give qualitatively the right position of the collective-mode frequencies, as long as the peaks are below the particle-hole threshold. The same holds for the approximated values for the amplitude mode (crosses).

For $N_0 J \gtrsim 0.06$ the peak of the phase mode has passed zero, and its frequency has become imaginary. This behavior is also obtained by using the approximation formula (58). We believe that this instability indicates a phase transition from intraband to interband pairing. This is supported by a study of a two-site model with two electrons (see the self-consistency equation), where a strong positive coupling J leads to a ground state consisting of interband Cooper pairs ($a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger$).

In Fig. 4(b) the influence of the Coulomb interaction between the layers is shown. A plasmon exists within the particle-hole continuum. This mode is caused by charge fluctuations between the layers. The damping of this mode increases with increasing $|J|$. The particle-hole threshold peak is strongly suppressed if there exists a collective mode with large spectral weight above the threshold. Again the approximation formula for the phase mode in the weak-coupling limit, represented by the dashed line in Fig. 4(b), gives the right position of the plasmon peak for small $|J|$. The plasmon mode and phase mode coincide for small $|J|$.

But for positive J a peak below the particle-hole threshold appears ($N_0 J = 0.02, 0.04$). This peak can be attributed to phase fluctuations by comparing the peak positions with the analytical results obtained for constant t (rhombs). The amplitude peak lies just at the particle-hole threshold at $N_0 J = 0.04$ and can be seen at $N_0 J = 0.06$. Those peaks which we have attributed to the phase and amplitude modes have large spectral weight in the correlations functions $\langle\langle \Phi, \Phi \rangle\rangle$ and $\langle\langle A, A \rangle\rangle$, respectively.

Now we discuss the temperature dependence of the polarization functions for large positive (0.05) and negative (-0.06) Josephson coupling. Figure 5 shows the imaginary part of the bare polarization function (a), the polarization function in the neutral system (b), and the real part of the optical conductivity in the charged system (c). The latter is related to the polarization function by $\sigma(\omega + i\delta)$
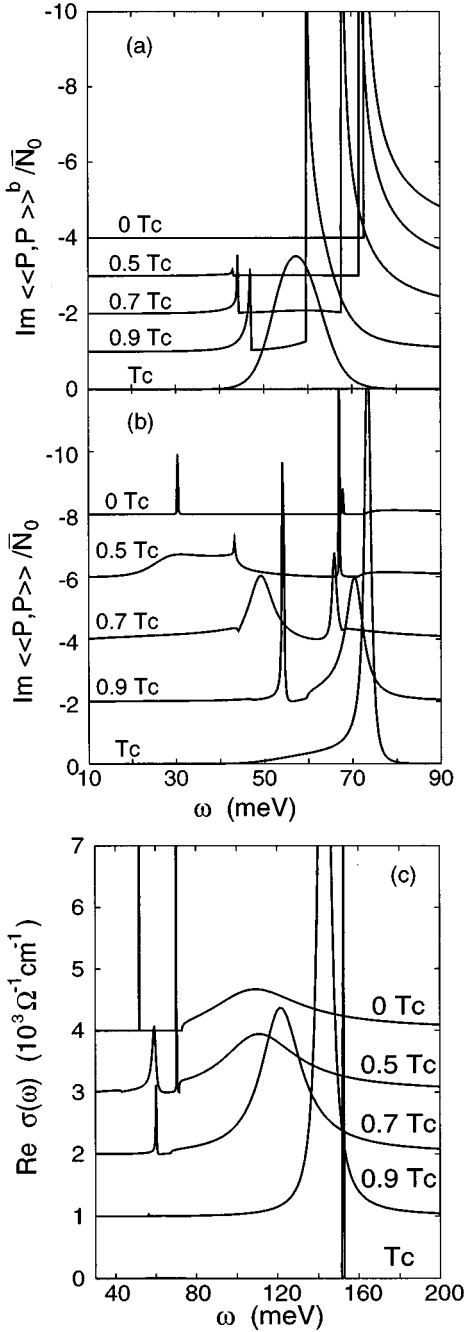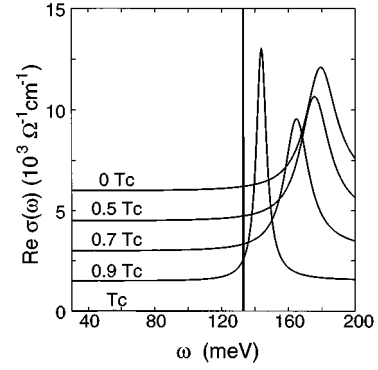
FIG. 6. Real part of the optical conductivity $\sigma(\omega)$ in the case of dominant intralayer pairing for different temperatures T and negative Josephson coupling $N_0 J = -0.06$. The parameters (22,23) are used, $d = 3$ Å . The different lines are shifted by equal units.

Coulomb interaction between the layers shifts the collective modes associated with density fluctuations to higher frequencies [Fig. 5(c)], whereas the amplitude mode near the particle-hole threshold is only slightly shifted.

In the case of negative J, which is the more realistic one, if this coupling is produced by the exchange of a boson, the Coulomb interaction shifts the collective modes into the region of particle-hole excitations. Figure 6 shows the temperature dependence of the remaining density-fluctuation spectrum.

B. Dominant interlayer pairing

In the case of dominant interlayer pairing ($\bar{V} > 0, \Delta_1 \Delta_2 < 0$) it is possible to produce the same peak structures in the polarization function as in the case of dominant intralayer pairing. Figure 7 shows the imaginary parts of the polarization function in the neutral (a) and charged (b) system for selected J values. The structures are nearly the same as in Fig. 4. For J greater equal $\bar{V}$ collective modes below the particle-hole threshold can occur in the polarization function of the neutral system and for relatively large positive J also in the polarization function for the charged system. The damping behavior of the plasmon is quite similar as in the case of dominant intralayer pairing. For negative and small positive J the plasmon peak is strongly damped.

An example for the temperature dependence of the imaginary part of the polarization function in the neutral (full lines) and charged (dashed lines) system is shown in Fig. 8. The plasmon (dashed line) has the same behavior as in Fig. 6.

VI. CONCLUSIONS

In this paper we have studied collective modes in superconducting double-layer systems which are connected with charge fluctuations between the layers. In our model we assumed a single-particle tight-binding hopping t_k between the layers and considered three different types of pairing interactions: an intralayer interaction $V_\parallel$, an interlayer interaction $V_\perp$, and a Josephson-type coupling J which allows a transfer of two particles between the layers. With these interactions we set up a system of vertex equations within a conserving approximation. The collective modes then appear as reso-

FIG. 5. Imaginary parts of the bare polarization function (a), the polarization function in the neutral system (b), and the real part of the optical conductivity in the charged system (c) in the case of dominant intralayer pairing for different temperatures T and positive Josephson coupling $N_0 J = 0.05$. The parameters (22,23) are used. The different lines are shifted by equal units. In (c) we choose as distance between the layers $d = 3$ Å .

$= i\omega (ed/2)^2 \langle\langle P, P \rangle\rangle^C_{\omega + i\delta}$. In Fig. 5(a) only particle-hole excitations with energy $|E_{1k} + E_{2k}|$ are visible at $T = 0$. For finite temperatures also excitations with $|E_{1k} - E_{2k}|$ from excited levels are possible at lower frequencies. The broad peak at T_c is due to interband transitions with different t_k values. Figure 5(b) shows the complicated transition from two distinct collective modes at $T = 0$ (phase and amplitude mode) to a collective density fluctuation in the normal state. The
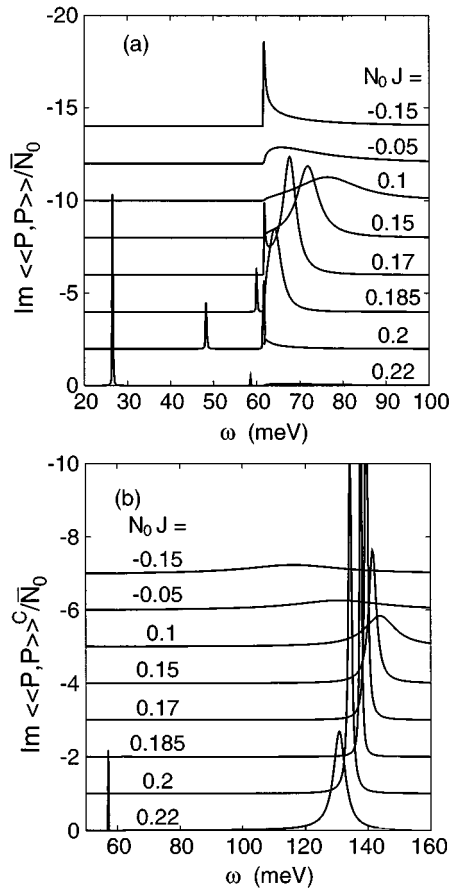
FIG. 7. Imaginary part of the polarization function in the neutral (a) and charged (b) system in the case of dominant interlayer pairing for different Josephson couplings and temperature $T=0$. The parameters (22,23) are used.

nances in the vertex functions. So we were able to study the interplay of the three types of interlayer interactions t_k, $V_\perp$, and J, which has not been investigated so far together.

Due to the interaction $V_\perp$ Cooper pairs with electrons in different layers are formed. Depending on the relative size of the different interactions one finds dominating interlayer or intralayer pairing. In the case of constant hopping t we calculated analytically the frequency of the collective modes. It
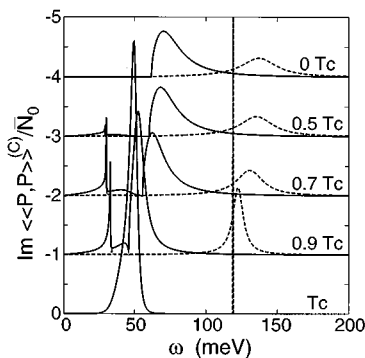

FIG. 8. Imaginary part of the polarization function in the neutral (full lines) and charged (dashed lines) system in the case of dominant interlayer pairing for different temperatures and Josephson coupling $J=0$. The parameters (22,23) are used.

is of the form $\omega = \sqrt{(2t)^2 + \omega_0^2}$ in the neutral system. In the case of intralayer pairing ω_0^2 is proportional to the ratio $-J/|V_\parallel|$, while for interlayer pairing it is proportional to $(V_\parallel - V_\perp - 2J)/|V_\parallel + V_\perp|$ (in the limit that theses ratios are small). The former result is in agreement with the result for the collective mode obtained by Wu and Griffin[14] for $t=0$. The difference $V_\parallel - V_\perp$ is related to the energy difference for intralayer and interlayer pairing. If the ground state is built by interlayer pairs the polarization is connected with the formation of intralayer pairs.

In order to find an undamped collective mode it is important that its frequency is below the particle-hole threshold $\sqrt{(2t)^2 + (2\Delta)^2}$. As for realistic systems $\omega_0^2 > 0$ the best chances to observe a collective mode is for the case of intralayer pairing and small Josephson coupling J. However, one has to keep in mind that the Coulomb interaction between the layers leads to a further shift to higher frequencies. This Coulomb interaction is proportional to the distance between the layers but can be reduced by a large phononic polarizability of the intermediate layers. We would like to add that a similar set of collective modes exists for spin fluctuations between the layers.[28] Here the influence of the Coulomb interaction on the mode frequency is absent.

In principle one has to distinguish two different modes which in the literature sometimes are called the phase and amplitude mode. For $\omega_0^2 < 0$ the two collective modes can both have frequencies below the particle-hole threshold for the same coupling parameters in the neutral system. However, in the case of constant t and equal values of the two gaps (pure intralayer or interlayer pairing), only one of these modes couples to the electronic polarization and will show up in the optical spectra. This is different for mixed intralayer and interlayer pairing and finite hopping (this occurs in our model for k-dependent hopping t_k). Then both phase and amplitude oscillations couple to the charge oscillation between the layers. Therefore in the c-axis optical conductivity two collective mode peaks can appear below the particle-hole threshold for low enough Coulomb interaction.

For a more realistic parameter region (negative J and strong Coulomb interaction) only one collective mode, the plasmon corresponding to charge fluctuations between the layers, exists. In this case most of the weight of the polarization spectrum is concentrated in the plasmon peak; the particle-hole excitations and, in particular, the peak at the threshold of particle-hole excitations are strongly suppressed. Therefore it is difficult to determine the threshold energy for breaking up Cooper pairs or the superconducting gap with optical c-axis experiments. It is remarkable that the plasmon peak is much narrower in the normal state than in the superconducting state. That is due to the stronger quasiparticle dispersion in the superconducting state, allowing a much wider range of interband transition energies.

Up to now the c-axis plasmon is not detected in the layered high-T_c superconductors Y-Ba-Cu-O or Bi-Sr-Ca-Cu-O. One explanation could be that in these compounds the single-particle hopping t is suppressed by correlation effects, as suggested by Anderson. In that case one has to assume also a strong quasiparticle damping. On the other hand, the interlayer polarization (the real part of the susceptibility) is certainly present and has a big influence on the renormaliza-

tion of c-axis phonons.[17] Therefore the most natural explanation for the absence of the c-axis plasmon and related collective modes is probably that the interlayer hopping t_k extends over a large energy range with a strong angular dependence[12] like $t_k = t_\perp [\cos(k_x a) - \cos(k_y a)]^2$, and in addition that the superconducting order parameter vanishes on some parts of the Fermi surface like in d-wave pairing. In that case the collective mode lies in the frequency range of particle-hole excitations and is strongly damped.

ACKNOWLEDGMENTS

APPENDIX A: MATRIX ELEMENTS

For the matrix K_{ij} we have to calculate the following integrals:

$$K_{ij} = \frac{1}{\beta} \sum_{\omega_n k} \frac{1}{2} \text{Tr}\{\bar{\sigma}_i^T \sigma_3 G_1(k, i\omega_n + i\omega_s) \bar{\sigma}_j G_2(k, i\omega_n) \sigma_3\},$$
(A1)

where σ_i are Pauli matrices and the matrices $\bar{\sigma}_j$ are defined by

$$\bar{\sigma}_j = \sigma_j \quad \text{for } j = 0,1,3, \quad \bar{\sigma}_2 = i\sigma_2, \quad \bar{\sigma}_2^T = -i\sigma_2.$$

Defining the integrals

$$H^{\pm\pm}(i\omega_s) = \frac{1}{\beta} \sum_{\omega_n} \sum_k [(i\omega_n + i\omega_s) i\omega_n \pm \xi_{1k}\xi_{2k}$$
$$\pm \Delta_1\Delta_2]/N,$$

$$(X/\widetilde{X})(i\omega_s) = \frac{1}{\beta} \sum_{\omega_n} \sum_k [(i\omega_n + i\omega_s)\xi_{2k} \mp i\omega_n \xi_{1k}]/N,$$

$$(Y/\widetilde{Y})(i\omega_s) = \frac{1}{\beta} \sum_{\omega_n} \sum_k [(i\omega_n + i\omega_s)\Delta_2 \mp i\omega_n \Delta_1]/N,$$

$$(Z/\widetilde{Z})(i\omega_s) = \frac{1}{\beta} \sum_{\omega_n} \sum_k [\xi_{1k}\Delta_2 \pm \xi_{2k}\Delta_1]/N$$
(A2)

with

$$N = [(i\omega_n + i\omega_s)^2 - E_{1k}^2][(i\omega_n)^2 - E_{2k}^2],$$

the matrix K can be written as

$$K = \begin{pmatrix} H^{++} & -\widetilde{Y} & -\widetilde{Z} & \widetilde{X} \\ \widetilde{Y} & -H^{-+} & X & Z \\ \widetilde{Z} & X & -H^{--} & Y \\ \widetilde{X} & -Z & -Y & H^{+-} \end{pmatrix}.$$
(A3)

The different signs come from the commutation relations for the Pauli matrices. Integrals of this type are common in vertex equations for superconductors[11] and for antiferromagnetic systems.[27]

The frequency summations are all of the general form

$$J(k, i\omega_s) = \frac{1}{\beta} \sum_{\omega_n} \frac{F(i\omega_n + i\omega_s, i\omega_n)}{[(i\omega_n + i\omega_s)^2 - E_{1k}^2][(i\omega_n)^2 - E_{2k}^2]},$$
(A4)

where the functions $F(z_1, z_2)$ are given by

$$H^{\pm\pm}: F(z_1, z_2) = z_1 z_2 \pm \xi_{1k}\xi_{2k} \pm \Delta_1\Delta_2,$$

$$(X/\widetilde{X}): F(z_1, z_2) = z_1 \xi_{2k} \mp z_2 \xi_{1k},$$

$$(Y/\widetilde{Y}): F(z_1, z_2) = z_1 \Delta_2 \mp z_2 \Delta_1,$$

$$(Z/\widetilde{Z}): F(z_1, z_2) = \xi_{1k}\Delta_2 \pm \xi_{2k}\Delta_1.$$
(A5)

After performing the frequency summations with help of Poisson's summation formula we obtain

$$J(k, i\omega_s) = \frac{1}{8E_{1k}E_{2k}} \left(\tanh\frac{\beta E_{1k}}{2} + \tanh\frac{\beta E_{2k}}{2} \right)$$
$$\times \left(\frac{F(-E_{1k}, E_{2k})}{i\omega_s + E_{1k} + E_{2k}} - \frac{F(E_{1k}, -E_{2k})}{i\omega_s - E_{1k} - E_{2k}} \right)$$
$$+ \frac{1}{8E_{1k}E_{2k}} \left(\tanh\frac{\beta E_{1k}}{2} - \tanh\frac{\beta E_{2k}}{2} \right)$$
$$\times \left(\frac{F(E_{1k}, E_{2k})}{i\omega_s - E_{1k} + E_{2k}} - \frac{F(-E_{1k}, -E_{2k})}{i\omega_s + E_{1k} - E_{2k}} \right).$$
(A6)

One notices that the first term containing contributions from the creation or destruction of two quasiparticles in different bands remains finite also for $T \to 0$. The second term with transfer of quasiparticles from one band to the other vanishes in that limit. Using the expressions for the function $F(z', z)$ the different matrix elements are easily calculated. One observes that the integrals $H^{\pm\pm}, Z, \widetilde{Z}$ are even functions of ω_s, while the integrals $X, \widetilde{X}, Y, \widetilde{Y}$ are odd functions.

APPENDIX B: VERTEX FUNCTIONS AND WARD IDENTITIES

We derive some useful relations between different integrals of the matrix K, which are based on the conserving approximation used for the calculation of self-energies and vertex functions. Similar relations for a one-band system are calculated, e.g., in Ref. 6.

The vertex equation in the neutral system in the ladder approximation has the general form (24):

$$\Gamma^{jl}(i\omega_s)=D^{jl}-L\{\Gamma^{ij}\} \qquad (B1)$$

with

$$L\{\Gamma\}=\frac{1}{\beta}\sum_{\omega_n k} VD^{03}G(k,i\omega_n+i\omega_s)\Gamma(i\omega_s)G(k,i\omega_n)D^{03}$$
$$+\overline{V}D^{13}G(k,i\omega_n+i\omega_s)\Gamma(i\omega_s)G(k,i\omega_n)D^{13}$$
$$+JD^{33}G(k,i\omega_n+i\omega_s)\Gamma(i\omega_s)G(k,i\omega_n)D^{33}. \qquad (B2)$$

We consider only vertex functions Γ, which are off-diagonal in the band indices:

$$\Gamma=\begin{pmatrix} 0 & \gamma \\ \hat{\gamma} & 0 \end{pmatrix}. \qquad (B3)$$

Then L is also off-diagonal in the band indices and can be written as

$$L=\begin{pmatrix} 0 & \lambda \\ \hat{\lambda} & 0 \end{pmatrix}. \qquad (B4)$$

Now let us define a k-dependent vertex function:

$$\Gamma_k^a(i\omega_s)=G^{-1}(k,i\omega_n+i\omega_s)D^{13}-D^{13}G^{-1}(k,i\omega_n), \qquad (B5)$$

then the right upper corner is

$$\gamma_k^a=i\omega_s\sigma_3+2\hat{t}_k\sigma_0-i(\Delta_1+\Delta_2)\sigma_2, \qquad (B6)$$

where $\hat{t}_k=(\xi_{2k}-\xi_{1k})/2$.

Inserting Γ^a into the rhs of (B2) some of the Green's function cancel, and the integrals are reduced to those which also occur in the self-energies (14). In particular we obtain for the 2×2 matrix in the right upper corner

$$\lambda^a=\sum_k\sum_{\omega_n} W'[G_2(k,i\omega_n)\sigma_3-\sigma_3 G_1(k,i\omega_n+i\omega_s)]+\overline{V}[G_1(k,i\omega_n)\sigma_3-\sigma_3 G_2(k,i\omega_n+i\omega_s)]$$
$$=\frac{1}{W^2-\overline{V}^2}\{W'[\sigma_3(-W\Sigma_2+\overline{V}\Sigma_1)+(W\Sigma_1-\overline{V}\Sigma_2)\sigma_3]+\overline{V}[\sigma_3(-W\Sigma_1+\overline{V}\Sigma_2)+(W\Sigma_2-\overline{V}\Sigma_1)\sigma_3]\}$$
$$=\frac{W'+\overline{V}}{W+\overline{V}}(\Delta_2+\Delta_1)i\sigma_2+\frac{W'-\overline{V}}{W-\overline{V}}(x_2-x_1)\sigma_0. \qquad (B7)$$

On the other hand we can calculate $L\{\Gamma\}$ in another way. With the quantities B and $\hat{B}$ defined in (27), λ is given by

$$\lambda^a=W'B+\overline{V}\hat{B}. \qquad (B8)$$

Because of the k dependence of the vertex function γ_k^a we introduce the k dependent 4×4 matrix functions K_k and $\hat{K}_k$, which are related to K and $\hat{K}$ by

$$K=\sum_k K_k, \qquad \hat{K}=\sum_k \hat{K}_k.$$

The same relations we needed for deriving the vertex equation (44) hold for the k-dependent quantities K_k, $\hat{K}_k$, γ_k^a, and $\hat{\gamma}_k^a$. Therefore we find

$$\underline{\lambda}^a=(W'+g\overline{V})\sum_k K_k\underline{\gamma}_k^a, \qquad (B9)$$

where g is the diagonal matrix $g=\text{diag}(-1,1,1,1)$. Thus we arrive at the first identity

$$(W+g\overline{V})\sum_k K_k\underline{\gamma}_k^a=(x_2-x_1,0,\Delta_2+\Delta_1,0)^t. \qquad (B10)$$

Note on the lhs stands W not W', because the factor $W'+g\overline{V}$ cancels.

In a similar way we find a second relation starting from

$$\Gamma_k^b(i\omega_s)=G^{-1}(k,i\omega_n+i\omega_s)D^{10}-D^{10}G^{-1}(k,i\omega_n). \qquad (B11)$$

Inserting this into the integral L we obtain

$$\lambda^b=\sum_k\sum_{\omega_n} W'\sigma_3 G_2(k,i\omega_n)\sigma_3-\overline{V}\sigma_3 G_1(k,i\omega_n)\sigma_3$$
$$-W'\sigma_3 G_1(k,i\omega_n+i\omega_s)\sigma_3+\overline{V}\sigma_3 G_2(k,i\omega_n+i\omega_s)\sigma_3$$
$$=\frac{W'+\overline{V}}{W-\overline{V}}(\Sigma_1-\Sigma_2) \qquad (B12)$$

or

$$\sum_k K_k\underline{\gamma}_k^b=\frac{1}{W-\overline{V}}[0,(\Delta_2-\Delta_1),0,-(x_2-x_1)]^t. \qquad (B13)$$

In the case of vanishing Josephson coupling and k-independent hopping t the first relation is identical with the Ward identity

$$i\omega_s\Gamma^P+2it\Gamma^j=\Gamma^a, \qquad (B14)$$

which follows from the continuity equation $2tj=\dot{P}$ [compare the discussion to (8)]. Γ^P is here the polarization vertex

and Γ^j the current vertex. The second relation follows from the conservation of the spin density. Between the relative spin polarization

$$P^{10} = \sum_k c^\dagger_{2k\uparrow} c_{2k\uparrow} - c^\dagger_{2k\downarrow} c_{2k\downarrow} - c^\dagger_{1k\uparrow} c_{1k\uparrow} + c^\dagger_{1k\downarrow} c_{1k\downarrow}$$

(B15)

and the spin current in the z direction

$$P^{23} = -i \sum_k c^\dagger_{2k\uparrow} c_{1k\uparrow} - c^\dagger_{1k\uparrow} c_{2k\uparrow} - c^\dagger_{2k\downarrow} c_{1k\downarrow} + c^\dagger_{1k\downarrow} c_{2k\downarrow},$$

(B16)

the continuity equation $\dot{P}^{10} = 2t P^{23}$ holds in the case $J \to 0$ and $t = $ const. From this equation one finds the Ward identity

$$i\omega_s \Gamma^{10} + 2it\Gamma^{23} = \Gamma^b.$$

(B17)

More relations are obtained by replacing the matrix D^{13} by D^{11} or D^{12}. These relations, however, are not of practical use.

From the above relations we obtain the following identities between the different integrals:

$$2H^{t++} + \widetilde{Z}2\Delta_\parallel + \widetilde{X}i\omega_s = (x_2 - x_1)/W_\perp,$$

(B18)

$$2\widetilde{Y}^t - X2\Delta_\parallel + Zi\omega_s = 0,$$

$$2\widetilde{Z}^t + H^{--}2\Delta_\parallel + Yi\omega_s = 2\Delta_\parallel/W_\parallel,$$

$$2\widetilde{X}^t + Y2\Delta_\parallel + H^{+-}i\omega_s = 0,$$

$$H^{++}i\omega_s + \widetilde{Y}2\Delta_\perp + 2\widetilde{X}^t = 0,$$

$$\widetilde{Y}i\omega_s + H^{-+}2\Delta_\perp + 2Z^t = 2\Delta_\perp/W_\perp,$$

$$\widetilde{Z}i\omega_s - X2\Delta_\perp + 2Y^t = 0,$$

$$\widetilde{X}i\omega_s + Z2\Delta_\perp + 2H^{t+-} = (x_2 - x_1)/W_\perp,$$

where $W_\parallel = V_\parallel + J = W + \overline{V}$, $W_\perp = V_\perp + J = W - \overline{V}$ and $\Delta_\parallel = (\Delta_2 + \Delta_1)/2, \Delta_\perp = (\Delta_2 - \Delta_1)/2$. Here the quantities K^t_{ij} are integrals similar to K_{ij} with the integrand multiplied by $\bar{\tau}_k = t_k + (x_1 - x_2)/2$ before the momentum integration. In the case of momentum-independent hopping matrix element t_k we have $K^t_{ij} = \hat{t} K_{ij}$.

The identities can be used to eliminate the badly converging integrals H^{-+} and H^{--}:

$$H^{-+} = \frac{1}{W_\perp} - \frac{1}{\Delta_2 - \Delta_1}(i\omega_s \widetilde{Y} + 2Z^t),$$

(B19)

$$H^{--} = \frac{1}{W_\parallel} - \frac{1}{\Delta_1 + \Delta_2}(i\omega_s Y + 2\widetilde{Z}^t).$$

(B20)

Here the integrals on the rhs do not need a cutoff.

In the two special cases of pure intralayer and interlayer pairing one can derive from the definitions of the functions (A5) two further relations:

$$H^{-+} = H^{--} + (\Delta_1 + \Delta_2)Y/i\omega_s \quad \text{if} \quad \Delta_1 = \Delta_2, \quad \text{(B21)}$$

$$H^{--} = H^{-+} + (\Delta_2 - \Delta_1)\widetilde{Y}/i\omega_s \quad \text{if} \quad \Delta_1 = -\Delta_2.$$

(B22)

[1] P. W. Anderson, Phys. Rev. **110**, 827 (1958); **110**, 1900 (1958); N. N. Bogoliubov, Nuovo Cimento **7**, 794 (1958).

[2] J. R. Schrieffer, *Superconductivity* (Benjamin, New York, 1964).

[3] Y. Nambu, Phys. Rev. **117**, 648 (1960).

[4] P. Martin, in *Superconductivity*, edited by R. D. Parks (Dekker, New York, 1969), pp. 371–379.

[5] A. J. Leggett, Prog. Theor. Phys. (Jpn.) **36**, 901 (1966).

[6] P. B. Littlewood and C. M. Varma, Phys. Rev. B **26**, 4883 (1982).

[7] P. J. Hirschfeld, W. O. Puttika, and P. Wölfle, Phys. Rev. Lett. **69**, 1447 (1992).

[8] H. Monien, L. Tewordt, and K. Scharnberg, Solid State Commun. **63**, 1027 (1987).

[9] P. Wölfle, J. Low Temp. Phys. **95**, 191 (1994).

[10] H. A. Fertig and S. Das Sarma, Phys. Rev. B **44**, 4480 (1991); R. Côtè and A. Griffin, *ibid.* **48**, 10 404 (1993).

[11] D. van der Marel, Phys. Rev. B **5**, 1147 (1995).

[12] O. K. Andersen, O. Jepsen, A. I. Liechtenstein, and I. I. Mazin, Phys. Rev. B **49**, 4145 (1994); O. K. Andersen, A. I. Liechtenstein, O. Jepsen, and F. Paulsen, J. Phys. Chem. Solids **56**, 1573 (1995).

[13] M. E. Palistrant, Physica C **235-240**, 2135 (1994).

[14] Wen-Chin Wu and A. Griffin, Phys. Rev. Lett. **74**, 158 (1995); Phys. Rev. B **51**, 15 317 (1995).

[15] K. Kuboki and P. A. Lee, J. Phys. Soc. Jpn. **64**, 3179 (1995).

[16] G. Hastreiter, U. Hofmann, J. Keller, and K. F. Renk, Solid State Commun. **76**, 1015 (1990); G. Hastreiter, D. Strauch, J. Keller, B. Schmid, and U. Schröder, Z. Phys. B **89**, 129 (1992).

[17] G. Hastreiter and J. Keller, Solid State Commun. **85**, 967 (1993); G. Hastreiter, F. Forsthofer, and J. Keller, *ibid.* **88**, 769 (1993).

[18] P. W. Anderson, Science **256**, 1526 (1992); S. Chakravarty, A. Sudbo, P. W. Anderson, and S. Strong, *ibid.* **261**, 337 (1993).

[19] H. Ding *et al.*, Phys. Rev. Lett. **74**, 2784 (1995).

[20] R. Liu *et al.*, Phys. Rev. B **46**, 11 056 (1992).

[21] R. Combescot and X. Leyronas, Phys. Rev. Lett. **75**, 3732 (1995).

[22] A. A. Golubov and I. I. Mazin, Physica C **243**, 153 (1995).

[23] I. I. Mazin and V. M. Yakovenko, Phys. Rev. Lett. **75**, 4134 (1995).

[24] D. Z. Liu, K. Levin, and J. Maly, Phys. Rev. B **51**, 8680 (1995).

[25] A. I. Liechtenstein, I. I. Mazin, and O. K. Andersen, Phys. Rev. Lett. **74**, 2303 (1995).

[26] B. Normand, H. Kohno, and H. Fukuyama, J. Phys. Soc. Jpn. **64**, 3903 (1995).

[27] W. Brenig, J. Low Temp. Phys. **99**, 319 (1995).

[28] F. Forsthofer, J. Keller, and C. Helm (unpublished).