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Collective modes of spin, density, phase, and amplitude in exotic superconductors

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The equations of motion of pairlike excitations in the superconducting state are studied for various types of pairing using the random-phase approximation. The collective modes are computed of a layered electron gas described by a t-t' tight-binding band, where the electrons experience besides the long-range Coulomb repulsion an on-site Hubbard U repulsion and a nearest-neighbor attractive interaction. From numerical calculations we see that the collective-mode spectrum now becomes particularly rich. Several branches can occur below the continuum of quasiparticle excitations, corresponding to order-parameter fluctuations of various symmetries of pairing, and collective spin-density fluctuations. From the collective-mode softening near the nesting vectors it is concluded that in the d-wave paired state an instability occurs toward the formation of a spin-density wave.

I. INTRODUCTION

A well-known result of BCS theory is the variational wave function, describing the ground state of a superconductor. In the limit $\mathbf{Q} \to 0$ this function can be easily extended to describe a superconductor[1,2] moving at a small and uniform velocity $\mathbf{v} = (2m_e)^{-1}\hbar\mathbf{Q}$,

$$|\Psi\rangle = \left[\int d^3\mathbf{R} e^{i\mathbf{Q}\cdot\mathbf{R}} \int d^3\mathbf{r}\phi(\mathbf{r})\psi_\uparrow^\dagger(\mathbf{R}+\mathbf{r}/2) \times\psi_\downarrow^\dagger(\mathbf{R}-\mathbf{r}/2)\right]^{N/2} |0\rangle. \quad (1)$$

This function has the mathematical shape of a Bose condensate of pairs, where the wave function $\phi(\mathbf{r})$ describing the relative motion of electrons forming a pair is the Fourier transform of $v_k/u_k = \{[1+(\epsilon_k/\Delta_k)^2]^{1/2} - (\epsilon_k/\Delta_k)\}$, and $\exp(i\mathbf{Q}\cdot\mathbf{R})$ is the macroscopic wave function describing the center of mass motion of each pair. The similarity to a Bose condensate wave function is somewhat misleading, as also the wave function of a gas of uncorrelated fermions can be written in this form, in which case $\phi(\mathbf{r})$ is a nontrivial function with an r^{-2} tail. In the limit of a weak effective interaction $\phi(\mathbf{r})$ has an algebraic tail just as for the free electron gas. If the interaction is strong, $\phi(\mathbf{r})$ can be interpreted as a wave function describing the relative motion of two electrons forming a Bose-condensed pair.[3] If the effective interaction is an on-site attraction, the electrons pair up in a singlet-wave function with an enhanced probability to occupy the same site. Clearly if the electrons experience a strong on-site repulsion, the tendency towards pairing disappears. With a net attraction between electrons occupying neighboring sites in the lattice, it is still possible to form a paired state, but $\phi(r)$ has to be constructed such that the particles avoid the same site. This condition is, for example, fulfilled when $\phi(\mathbf{r})$ has a finite angular momentum.

One may wonder whether the analogy to Bose condensation can be drawn further, and consider the energy spectrum of pairlike excitations as a function of pair momentum. This problem was first treated by Bogoliubov *et al.*[4] and Anderson.[5] If the electrons experience an on-site repulsion, with a nearest-neighbor attraction, the collective-mode spectrum becomes particularly rich. It turns out that several branches occur below the continuum of quasiparticle excitations, corresponding to order-parameter fluctuations of various symmetries of pairing.[6] The existence of low-lying collective modes may be important when attempting to identify a superconducting gap in the infrared, Raman, or inelastic neutron scattering spectra of these materials.

Collective modes in superconductors have in the past attracted the attention for a variety of reasons: (1) Bogoliubov predicted the existence of a longitudinal collective mode with a soundlike dispersion.[4] Long-range Coulomb interactions make the spectrum identical to the plasmons of a normal Fermi gas, as was shown by Anderson.[5] (2) The collective mode spectrum naturally follows from a gauge-invariant formulation of BCS theory,[5] and a consistent explanation of the Meissner effect requires that the whole interaction Hamiltonian (as opposed to the reduced BCS Hamiltonian) be taken into account.[5,7] (3) As collective modes mediate electron-electron interactions, plasmons[8–10] and spin fluctuations[11–14] have been considered as possible candidates for a pairing mechanism. (4) Certain modes, in particular condensate phase fluctuations near or below the pair-breaking gap, are important for the thermal behavior, notably T_c, of the superconductor.[15] (5) An instability of the ground state and an incipient phase transition to a state with a lower energy follow from the softening of collective modes.[16–18] (6) Collective modes may show up in experimental spectra, such as in optical[19–21] or Raman spectroscopy.[22,23] (7) As there is no interplane hopping in a layered electron gas, the k-dependent plasmon spectrum becomes gapless,[24] which may give rise to an interesting behavior in the region for momentum and frequency values where the collective mode crosses 2Δ.[25,10]

(8) If there exists an electron-electron interaction in channels with a finite angular momentum L, excitons with the corresponding symmetries can exist.[6,16,19]

Usually modes of phase and density[25,10] are treated separately from amplitude modes[22,23] and spin fluctuations.[12,11,26] As we will see below, especially for a nonvanishing momentum, a coupling exists between the four collective-mode channels of spin density, charge, phase, and amplitude of the order parameter. The aim of this study is to derive general expressions for the collective modes in the superconducting state, using a unified approach including effects of finite momentum pairing. In the last section examples are given for the collective modes and the generalized susceptibility in the superconducting state. It is shown that a d-wave superconductor may become unstable with respect to the formation of a spin-density wave, or possibly a mixed spin-density wave (SDW) plus superconducting state, if an on-site repulsion is taken into account in addition to having an attractive interaction in the d-wave channel. More detailed calculations of various response functions and the comparison thereof to measurements on specific materials will follow in a future publication.

II. MODEL HAMILTONIAN

In the discussion of the collective modes we will make extensive use of two-particle creation operators. We will see below that the channels with $S_z = -1$, $S_z = 1$, and $S_z = 0$ are decoupled. In the $S_z = \pm 1$ channels there are triplet pair excitations and spin fluctuations. In the $S_z = 0$ channel there are spin fluctuations, density fluctuations, and fluctuations of phase and amplitude of the order parameter (singlet and triplet pair excitations). The corresponding operators are in the same order,

$$\begin{aligned}
\sigma_k(Q) &\equiv c^\dagger_{k+Q\uparrow} c_{k\uparrow} - c^\dagger_{-k\downarrow} c_{-k-Q\downarrow}, \\
\rho_k(Q) &\equiv c^\dagger_{k+Q\uparrow} c_{k\uparrow} + c^\dagger_{-k\downarrow} c_{-k-Q\downarrow}, \\
\phi_k(Q) &\equiv c_{-k-Q\downarrow} c_{k\uparrow} - c^\dagger_{k+Q\uparrow} c^\dagger_{-k\downarrow}, \\
\psi_k(Q) &\equiv c_{-k-Q\downarrow} c_{k\uparrow} + c^\dagger_{k+Q\uparrow} c^\dagger_{-k\downarrow}.
\end{aligned} \tag{2}$$

The remaining six combinations are $c^\dagger_{k+Q\sigma} c_{k\underline{\sigma}}$, (spin fluctuations with $S_z = \pm 1$) and $c_{-k-Q\sigma} c_{k\sigma}$ with the corresponding Hermitian conjugates (spin-triplet phase and amplitude fluctuations). When transformed to a Euclidean-space representation these operators acquire a more transparant physical meaning. For example the spin-density distribution function $n_\uparrow(r) - n_\downarrow(r)$ has as its Fourier transform $\sum_k \sigma_k(Q)$. Similar relations exist for the other operators, and the notation $\sigma(Q)$, $\rho(Q)$, $\phi(Q)$, and $\psi(Q)$ will be used to indicate the Fourier transforms of the spin-density, charge-density, phase, and gap-amplitude distributions in Euclidean space. We will consider a system of interacting electrons which can be described with the following Hamiltonian:

$$H = \sum_k \xi_k \rho_k(0) + \sum_Q \left\{ \frac{1}{2} V(Q) \rho(Q) \rho(-Q) + \frac{1}{8} U(Q) \left[\rho(Q)\rho(-Q) - \boldsymbol{\sigma}(Q) \cdot \boldsymbol{\sigma}(-Q) \right] \right\}, \tag{3}$$

where in $V(Q)$ I lumped together the Coulomb interaction with all other spin-independent interactions, which could be due to the coupling of the electrons to the other degrees of freedom of the solid. In principle, and in particular if the interaction kernel is derived from boson-exchange models such as the electron-phonon interaction, there can also be a separate dependence on the momentum of the interacting particles. For compactness of notation I will not explicitly include such a k and q dependence in the Hamiltonian.

With the spin-dependent interaction assumed here, the total spin of the system is still a good quantum number. Such terms can appear if the model Hamiltonian is derived from a more fundamental one by projecting out part of the Hilbert space. A well-known example is the occurrence of the Kondo exchange interaction in a magnetic impurity system after carrying out the Schrieffer-Wolff transformation. Other examples where such terms occur are the RKKY interaction in magnetic alloys and the superexchange in rare-earth-doped semiconductors. Also the on-site Hubbard U term is usually written in this form, although in this case the Pauli principle already automatically excludes occupation of the same site with parallel spins.

As we will discuss the equations of motion of the collective modes for a general form of the effective electron-electron interaction, it is worthwhile to summarize the expressions for the gap equation and the free energy. The thermodynamic potential at $T = 0$ of a BCS superconductor is the expectation value of the grand canonical Hamiltonian, and is easily obtained by taking the expectation value of Eq. (3) using the variational wave function of Eq. (1),

$$\Omega(\mu, V, v_{k_1}, ..., v_{k_N}) = 2 \sum_k |v_k|^2 (\xi_k - \mu) + \sum_{kq} \left[u_k v_k \lambda_{kq} u^*_q v^*_q + |u_k|^2 V(k-q) |v_q|^2 \right], \tag{4}$$

where λ_{kq} is the pairing potential. For the type of interaction introduced above one obtains $\lambda_{kq} = V(k-q) + \frac{1}{2}U(k-q) + \frac{1}{2}U(k+q)$ where the last term is the spin-flip scattering contribution contained in $\boldsymbol{\sigma}_k(Q) \cdot \boldsymbol{\sigma}_q(-Q)$. The last term in Eq. (4) corresponds to the exchange energy. From Ω one obtains the gap equation by calculating the minimum as a function of the set of variational parameters $v_{k_1}, ..., v_{k_N}$. The number of particles in the ground state is obtained by taking the first derivative with respect to μ. The resulting set of equations is

$$\begin{aligned}
-\sum_q u_q v_q \lambda_{kq} &= \frac{2 u_k v_k}{|u_k|^2 - |v_k|^2} \tilde{\epsilon}_k, \\
\sum_k |v_k|^2 &= N_e.
\end{aligned} \tag{5}$$

Apart from a shift in chemical potential the effect of the exchange energy term on the thermodynamic potential is to renormalize the single-particle dispersion $\epsilon_k = \xi_k - \mu$, which now has to be replaced with $\tilde{\epsilon}_k \equiv \epsilon_k - \sum_q |v_q|^2 V(k-q)$. After the ground state has been found from minimalization of the free energy, the quasiparticle spectrum is obtained, with the usual BCS-type energy dispersion $E_k = \left[\tilde{\epsilon}^2 + \Delta_k^2\right]^{1/2}$ and with Δ_k/E_k defined as $2u_k v_k$. In the following sections I will also use the (standard) notations $b_k \equiv u_k v_k$ and $z_k \equiv (|u_k|^2 - |v_k|^2)/2$.

If λ_{kq} has a nontrivial k dependence we can make a partial-wave decomposition

$$\lambda_{kq} = \sum_\alpha \psi_\alpha^*(k)\lambda_\alpha \psi_\alpha(q),$$

where $\{\psi_\alpha(k)\}$ is a complete set of orthogonal functions, chosen such as to diagonalize the pairing potential. We can make a similar expansion of the order parameter $\Delta_k = \sum_\alpha \Delta_\alpha \psi_\alpha(k)$ with the help of which one obtains the coupled gap equations

$$\Delta_\alpha = -\lambda_\alpha \sum_k \sum_\beta \frac{\psi_\alpha^*(k)\psi_\beta(k)\Delta_\beta}{2E_k}.$$

We notice that for $\Delta \to 0$ a decoupling of pairing channels occurs, depending on the presence of off-diagonal elements in the decomposition of $1/E_k \to 1/|\epsilon_k|$. As λ_{kq} is real $\{\psi_\alpha(k)\}$ can be chosen as real numbers. As a result, if also Δ_α is real, solutions with different symmetries may mix, leading to a breaking of spatial symmetry of the lattice.[27] If these channels are mixed "incoherently" (as in, e.g., $s + id$ pairing[28]), for $(T_c - T) \ll T_c$ the gap equations for s and d are decoupled.

III. EQUATIONS OF MOTION

The equations of motion are of the form $[H, \hat{O}] = \nu \hat{O}$, where $\hat{O}$ is a linear combination of pair operators representing an excitation of the system with energy ν. Although these equations have been treated extensively before, in the previous papers the coupling to the collective spin oscillation channel has not been considered. In particular a spin-dependent term was not included in earlier publications. As one of the aims of this paper is to discuss collective modes of spin density in the superconducting state, I rederive the equations of motion with this extended Hamiltonian.

In the superconducting state the equations of motion of spin density $[\sigma_k(Q)]$, charge density $[\rho_k(Q)]$, order-parameter phase $[\phi_k(Q)]$, and order-parameter amplitude $[\psi_k(Q)]$ are coupled in a nontrivial way. The commutator of each of these two-particle operators with the interaction part of the Hamiltonian generates products of four single-particle operators, which are approximated by taking the expectation value of all combinations of two of the operators appearing in this product. The resulting terms fall in two categories: those which have the same k value and those which are a weighted summation over k space. The latter give rise to the collective modes. In the first category one obtains (1) self-energy terms which can be absorbed in a shift of the chemical potential, (2) exchange self-energy terms, due to which ϵ_k is renormalized to $\tilde{\epsilon}_k \equiv \epsilon_k - \sum_q |v_q|^2 V(k-q)$, and (3) cross terms proportional to Δ_k, linking σ_k to ψ_k and ρ_k to ϕ_k operators.

Finally the category of weighted averages of two-particle operators over k space involves both direct and exchange terms, and is given by the expressions

$$\begin{aligned}
\mathbf{S}_k(Q) &\equiv \sum_q H_\sigma^i(k,q,Q)\sigma_q(Q),\\
\mathbf{R}_k(Q) &\equiv \sum_q H_\rho^i(k,q,Q)\rho_q(Q),\\
\mathbf{A}_k(Q) &\equiv \sum_q H_\phi^i(k,q,Q)\phi_q(Q),\\
\mathbf{B}_k(Q) &\equiv \sum_q H_\psi^i(k,q,Q)\psi_q(Q),
\end{aligned} \tag{6}$$

where I introduced

$$\begin{aligned}
H_\sigma^i(k,q,Q) &\equiv -\frac{1}{2}U(Q) - V(k-q) - \frac{1}{2}U(k-q),\\
H_\rho^i(k,q,Q) &\equiv 2V(Q) + \frac{1}{2}U(Q) - V(k-q) + \frac{1}{2}U(k-q),\\
H_\phi^i(k,q,Q) &\equiv V(k-q) + \frac{1}{2}U(k-q) + \frac{1}{2}U(k+q),\\
H_\psi^i(k,q,Q) &\equiv V(k-q) + \frac{1}{2}U(k-q) + \frac{1}{2}U(k+q).
\end{aligned} \tag{7}$$

With these definitions, and using the random-phase approximation (RPA) described above, the commutators of the pair operators can now be derived. The actual calculation is a straightforward, though rather laborious, exercise in commutator algebra. A detailed description of the various terms has been given by Anderson, and later discussed more extensively by Bardasis and Schrieffer, who retained a number of vertices in their final analysis which were neglected by Anderson. In the present paper all vertices discussed by Bardasis and Schrieffer are taken into account. The expressions are, however, modified due to the spin-dependent interaction term in Eq. (3). The set of commutators, including the exchange interactions, is

$$
\begin{aligned}
[H,\sigma_k(Q)] &= \tilde{\epsilon}^-_{kQ}\rho_k(Q) - \Delta^-_{kQ}\psi_k(Q) + z^-_{kQ}\mathbf{R}_k(Q) - b^-_{kQ}\mathbf{B}_k(Q),\\
[H,\rho_k(Q)] &= \tilde{\epsilon}^-_{kQ}\sigma_k(Q) - \Delta^+_{kQ}\phi_k(Q) + z^-_{kQ}\mathbf{S}_k(Q) - b^+_{kQ}\mathbf{A}_k(Q),\\
[H,\phi_k(Q)] &= -\tilde{\epsilon}^+_{kQ}\psi_k(Q) - \Delta^+_{kQ}\rho_k(Q) - b^+_{kQ}\mathbf{R}_k(Q) - z^+_{kQ}\mathbf{B}_k(Q),\\
[H,\psi_k(Q)] &= -\tilde{\epsilon}^+_{kQ}\phi_k(Q) - \Delta^-_{kQ}\sigma_k(Q) - b^-_{kQ}\mathbf{S}_k(Q) - z^+_{kQ}\mathbf{A}_k(Q).
\end{aligned}
\tag{8}
$$

Δ_k, $\tilde{\epsilon}_k$, b_k, and z_k were already defined in the previous section. For the sake of compactness of notation I introduced $b^\pm_{kQ} \equiv b_{k+Q} \pm b_k$, $z^\pm_{kQ} \equiv z_{k+Q} \pm z_k$, $\Delta^\pm_{kQ} \equiv \Delta_{k+Q} \pm \Delta_k$, and $\tilde{\epsilon}^\pm_{kQ} \equiv \tilde{\epsilon}_{k+Q} \pm \tilde{\epsilon}_k$.

The first two terms of all four commutators correspond to (1) the kinetic energy with exchange self-energy corrections [Fig. 1(a)] and (2) Boguliobov-Valatin particle-hole mixing [Fig. 1(a′)]. The remaining two terms in each of these expressions can be better described with reference to the definition of the collective coordinates in Eqs. (6) and (7.)

Let us first consider $\mathbf{R}_k(Q)$ and $\mathbf{S}_k(Q)$. The $V(Q)$, $U(Q)$, and $U(k-q)$ terms correspond to the polarization vertex in the commutators of σ_k and ρ_k [Fig. 1(b)]. In the commutators of ϕ_k and ψ_k the $V(Q)$, $U(Q)$, and $U(k-q)$ terms are polarization vertices combined with a particle-hole transformation on one of the legs [Fig. 1(b′)]. The $V(k-q)$ terms correspond to the exchange scattering vertex without [commutators of σ_k and ρ_k, Fig. 1(c)] and with a particle-hole transformation [commutators of ϕ_k and ψ_k, Fig. 1(c′)].

Finally $\mathbf{A}_k(Q)$ and $\mathbf{B}_k(Q)$ correspond to the direct particle-particle scattering vertex without [commutators of $\phi_k(Q)$ and $\psi_k(Q)$, Fig. 1(d)] and with particle-hole conversion [commutators of $\sigma_k(Q)$ and $\rho_k(Q)$, Fig. 1(d′)].

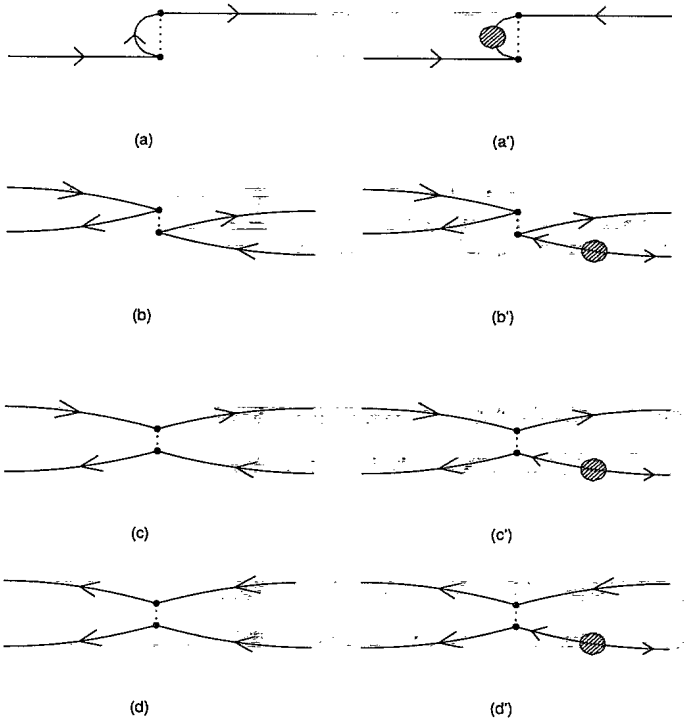

FIG. 1. Diagrams taken into account in the RPA. Exchange self-energy (a), particle-hole mixing [(a′)], polarization vertex [(b) and (b′)], exchange scattering [(c) and (c′)], and direct particle-particle scattering [(d) and (d′)]. Diagrams (b′), (c′) and (d′) exist only in the superconducting state.

If we apply the equations of motion to a general operator of the form

$$
\hat{O} = \sum_k \Big[v_{1,k}(Q)\sigma_k(Q) + v_{2,k}(Q)\rho_k(Q) + v_{3,k}(Q)\phi_k(Q) + v_{4,k}(Q)\psi_k(Q) \Big],
$$

we find that they can be written in matrix form as

$$
H^0(k,Q)\mathbf{v}_k(Q) + \sum_q H^i(k,q,Q)\Gamma(q,Q)\mathbf{v}_q(Q) = \nu\mathbf{v}_k(Q).
\tag{9}
$$

The interaction Hamiltonian H^i contains the matrix elements of Eq. (7) on the diagonal, and is zero elsewhere. We furthermore use the zeroth-order Hamiltonian describing noninteracting quasiparticles,

$$
H^0(k,Q) \equiv \begin{pmatrix} 0 & \tilde{\epsilon}^-_{kQ} & 0 & -\Delta^-_{kQ} \\ \tilde{\epsilon}^-_{kQ} & 0 & -\Delta^+_{kQ} & 0 \\ 0 & -\Delta^+_{kQ} & 0 & -\tilde{\epsilon}^+_{kQ} \\ -\Delta^-_{kQ} & 0 & -\tilde{\epsilon}^+_{kQ} & 0 \end{pmatrix},
\tag{10}
$$

and the dimensionless matrix containing coherence factors,

$$
\Gamma(k,Q) \equiv \begin{pmatrix} 0 & z^-_{kQ} & 0 & -b^-_{kQ} \\ z^-_{kQ} & 0 & -b^+_{kQ} & 0 \\ 0 & -b^+_{kQ} & 0 & -z^+_{kQ} \\ -b^-_{kQ} & 0 & -z^+_{kQ} & 0 \end{pmatrix}.
\tag{11}
$$

The collective modes can be found by looking for poles in the correlation functions, in particular the density-density and the spin-spin correlation functions $\langle\langle T\rho(\mathbf{r},\tau)\rho(\mathbf{r}',0)\rangle\rangle_\nu$ and $\langle\langle T\sigma(\mathbf{r},\tau)\sigma(\mathbf{r}',0)\rangle\rangle_\nu$, where $\rho(\mathbf{r},\tau)$, etc., are the Heisenberg representation of the operators $\sum_{\mathbf{Q}} \exp(i\mathbf{Q}\cdot\mathbf{r})\rho(\mathbf{r})$ which were defined in the previous section. In the superconducting state also $\langle\langle T\phi(\mathbf{r},\tau)\phi(\mathbf{r}',0)\rangle\rangle_\nu$ and $\langle\langle T\psi(\mathbf{r},\tau)\psi(\mathbf{r}',0)\rangle\rangle_\nu$ become relevant. Together with the six off-diagonal correlation functions, the four diagonal functions define a 4×4 two-particle Green's function matrix. The matrix $K^0_{kq}(Q,\nu) = [\nu - H^0(k,Q) - i0^+]^{-1}\delta_{k,q}$ corresponds to the Lehmann representation of this Green's function in the absence of residual interactions (i.e., with $H^i = 0$). As this describes the response of a gas of noninteracting quasiparticles there are no poles corresponding to collective modes. The generalized susceptibility $\chi^0(Q,\nu) = -\sum_{k,q}\Gamma(k,Q)K^0_{k,q}(Q,\nu)$. If we now include H^i, we can calculate the Green's functions in the RPA by applying the Dyson equation

$$K_{kq}(Q,\nu) = K^0_{kq}(Q,\nu)\delta_{k,q} + K^0_{kk}(Q,\nu)\sum_{k'} H^i(k,k',Q)\Gamma(k',Q)K_{k'q}(Q,\nu). \tag{12}$$

We can use the same partial-wave decomposition as introduced in the previous section where we discussed the gap equation. It is straightforward to show that the above Dyson equation has the solution

$$\chi_{\alpha,\beta}(Q,\nu) = \sum_{\gamma}\chi^0_{\alpha,\gamma}(Q,\nu)\left(1+H^i\chi^0\right)^{-1}_{\gamma,\beta}, \tag{13}$$

where I used the partial-wave decomposition

$$\chi_{\alpha,\beta}(Q,\nu) = -\sum_{kq}\psi_\alpha(k)\Gamma(k,Q)K_{kq}(Q,\nu)\psi_\beta(q),$$

with similar expressions for χ^0 and H^i. The collective modes correspond to the zeros of the determinant of

$$\delta_{\alpha,\beta}\delta_{i,j} + \sum_{\mu,l} H^i_{\alpha,\mu;i,l}\chi^0_{\mu,\beta;l,j}, \tag{14}$$

which can be determined numerically, and in some limiting cases also analytically. The expression of the response function Eq. (13) corresponds to calculating the series of diagrams depicted in Fig. 1. It is possible to improve further by taking into account the screening of the vertex in all of these diagrams, except in the polarization vertices of Figs. 1(b) and 1(b′), as this would lead to double counting. (N.B. Although in this paper the pairing interaction is introduced as an independent model parameter, one should keep in mind that for an electronic mechanism of superconductivity such as a spin fluctuation or plasmon-intermediated interaction, the pairing arises precisely from such diagrams.) This procedure was proposed by Anderson, Rickayzen, and also by Bardasis and Schrieffer. Moreover, in the next section we will see that in the normal state the σ and ρ channels are completely decoupled for all values of Q. This implies that the sum over diagrams for the charge fluctuations does not contain any vertex correction due to the spin fluctuations and vice versa. Hence, it is necessary in this case to screen all vertices in the charge-fluctuation channel with the spin fluctuations, and vice versa. As has been shown by Rickayzen, in the superconducting state the screening properties are basically the same as in the normal state.[7]

One has to be cautious with this procedure of screening the vertices, as, by making the RPA *before* calculating the sum over diagrams, certain classes of vertex corrections are omitted. As a result inconsistencies may arise, as can be seen from the following example: If we consider the Hubbard U model, the on-site interaction can be introduced either using an on-site spin-independent (V) or a singlet-only (U) term as defined in Eq. (3). The expressions for the equation of motion should be independent of this choice, as the Pauli exclusion principle automatically projects out the double occupancy of the same site with equal spins. Indeed, we can check from Eq. (7) that this requirement is satisfied as long as we do not introduce screening. If we follow the recipe that in the first two lines of Eq. (7) the polarization diagrams $U(Q)$, $V(Q)$, and $U(k-q)$, but not the exchange diagram $V(k-q)$, should be replaced with the bare interaction, we arrive at a different result depending on whether we introduce the on-site interaction through a singlet-only or a spin-independent interaction.

This inconsistency is removed if we replace the direct *and* exchange terms in H^i_σ with the charge screened value. In the same way screening with spin fluctuations should be introduced "by hand" in the direct *and* exchange terms in H^i_ρ. Finally all three terms in H^i_ϕ and H^i_ψ should be replaced with the charge- *and* spin-fluctuation-screened vertices.

Let us now calculate K^0 by inverting $[\nu - H^{qp}]$. The determinant is

$$\begin{aligned}|\nu - H^{qp}| &= \nu^4 - 2\nu^2(E^2_{k+Q}+E^2_k) + (E^2_{k+Q}-E^2_k)^2 \\ &= [\nu^2-(E_{k+Q}+E_k)^2][\nu^2-(E_{k+Q}-E_k)^2].\end{aligned} \tag{15}$$

The zeroth-order two-particle Green's function is then

$$K^0 = |\nu - H^{qp}|^{-1}\begin{pmatrix} \nu(\nu^2-\tilde\epsilon^{+2}-\Delta^{+2}) & \tilde\epsilon^-(\nu^2-\tilde\epsilon^{+2}) & -\nu\tilde\epsilon^-\Delta^+ & \tilde\epsilon^+\tilde\epsilon^-\Delta^+ \\ & -\tilde\epsilon^+\Delta^+\Delta^- & +\nu\tilde\epsilon^+\Delta^- & +(\Delta^{+2}-\nu^2)\Delta^- \\ \tilde\epsilon^-(\nu^2-\tilde\epsilon^{+2}) & \nu(\nu^2-\tilde\epsilon^{+2}) & -\nu^2\Delta^+ & \nu\tilde\epsilon^+\Delta^+ \\ -\tilde\epsilon^+\Delta^+\Delta^- & -\nu\Delta^{-2} & +(\tilde\epsilon^+\tilde\epsilon^- + \Delta^+\Delta^-)\Delta^- & -\nu\tilde\epsilon^-\Delta^- \\ -\nu\tilde\epsilon^-\Delta^+ & -\nu^2\Delta^+ & \nu(\nu^2-\tilde\epsilon^{-2}) & \tilde\epsilon^+(\tilde\epsilon^{-2}-\nu^2) \\ +\nu\tilde\epsilon^+\Delta^- & +(\tilde\epsilon^+\tilde\epsilon^- + \Delta^+\Delta^-)\Delta^- & -\nu\Delta^{-2} & +\tilde\epsilon^-\Delta^+\Delta^- \\ \tilde\epsilon^+\tilde\epsilon^-\Delta^+ & \nu\tilde\epsilon^+\Delta^+ & \tilde\epsilon^+(\tilde\epsilon^{-2}-\nu^2) & \nu(\nu^2-\tilde\epsilon^{-2}-\Delta^{+2}) \\ +(\Delta^{+2}-\nu^2)\Delta^- & -\nu\tilde\epsilon^-\Delta^- & +\tilde\epsilon^-\Delta^+\Delta^- & \end{pmatrix}. \tag{16}$$

The 4×4 matrix $K^0\Gamma$ becomes

$$K^0\Gamma = |\nu - H^{qp}|^{-1} \begin{pmatrix} -\nu^2(z^-\tilde{\epsilon}^- + b^-\Delta^-) + (b^-\Delta^+ + z^-\tilde{\epsilon}^+) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) & z^-\nu^3 + \nu z^-(\tilde{\epsilon}^{+^2} + \Delta^{+^2}) + \nu b^+(\tilde{\epsilon}^+\Delta^- - \tilde{\epsilon}^-\Delta^+) & \nu^2(b^+\tilde{\epsilon}^- - z^+\Delta^-) + (z^+\Delta^+ - b^+\tilde{\epsilon}^+) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) & b^-\nu^3 + \nu z^+(\tilde{\epsilon}^+\Delta^- - \tilde{\epsilon}^-\Delta^+) - \nu b^-(\tilde{\epsilon}^{+^2} + \Delta^{+^2}) \\ z^-\nu^3 + \nu z^-(\tilde{\epsilon}^{+^2} + \Delta^{-^2}) + \nu b^-(\tilde{\epsilon}^+\Delta^+ - \tilde{\epsilon}^-\Delta^-) & -\nu^2(z^-\tilde{\epsilon}^- + b^+\Delta^+) + (b^+\Delta^- + z^-\tilde{\epsilon}^+) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) & b^+\nu^3 + \nu z^+(\tilde{\epsilon}^+\Delta^+ - \tilde{\epsilon}^-\Delta^-) - \nu b^+(\tilde{\epsilon}^{+^2} + \Delta^{-^2}) & \nu^2(b^-\tilde{\epsilon}^- - z^+\Delta^+) + (z^+\Delta^- - b^-\tilde{\epsilon}^+) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) \\ \nu^2(-b^-\tilde{\epsilon}^+ + z^-\Delta^+) + (z^-\Delta^- + b^-\tilde{\epsilon}^-) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) & \nu^3 b^+ - \nu z^-(\tilde{\epsilon}^+\Delta^- - \tilde{\epsilon}^-\Delta^+) - \nu b^+(\tilde{\epsilon}^{-^2} + \Delta^{-^2}) & -\nu^2(z^+\tilde{\epsilon}^+ + b^+\Delta^+) + (b^+\Delta^- + z^+\tilde{\epsilon}^-) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) & \nu^3 z^+ - \nu z^+(\tilde{\epsilon}^{-^2} + \Delta^{-^2}) - \nu b^-(\tilde{\epsilon}^-\Delta^+ - \tilde{\epsilon}^+\Delta^-) \\ b^-\nu^3 - \nu z^-(\tilde{\epsilon}^+\Delta^+ - \tilde{\epsilon}^-\Delta^-) - \nu b^-(\tilde{\epsilon}^{-^2} + \Delta^{+^2}) & -\nu^2(b^+\tilde{\epsilon}^+ - z^-\Delta^-) - (z^-\Delta^+ - b^+\tilde{\epsilon}^-) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) & z^+\nu^3 - \nu z^+(\tilde{\epsilon}^{-^2} + \Delta^{+^2}) + \nu b^+(\tilde{\epsilon}^+\Delta^+ - \tilde{\epsilon}^-\Delta^-) & -\nu^2(z^+\tilde{\epsilon}^+ + b^-\Delta^-) + (z^+\tilde{\epsilon}^- + b^-\Delta^+) \times(\tilde{\epsilon}^+\tilde{\epsilon}^- + \Delta^+\Delta^-) \end{pmatrix}. \tag{17}$$

From inspection of the matrix elements it turns out that they all contain the factor $(\nu^2 - (E_{k+Q} - E_k)^2)$ in the numerator. As the same term appears in the denominator, these factors cancel. $K^0\Gamma$ turns out to be symmetric, and the exact result is

$$\Gamma K^0 = K^0\Gamma = \frac{E_{k+Q} + E_k}{2E_kE_{k+Q}((E_{k+Q} + E_k)^2 - \nu^2)} \times \begin{pmatrix} -E_{k+Q}E_k + \Delta_k\Delta_{k+Q} + \tilde{\epsilon}_k\tilde{\epsilon}_{k+Q} & \nu\frac{E_{k+Q}\tilde{\epsilon}_k - E_k\tilde{\epsilon}_{k+Q}}{E_{k+Q}+E_k} & \tilde{\epsilon}_{k+Q}\Delta_k - \tilde{\epsilon}_k\Delta_{k+Q} & -\nu\frac{E_{k+Q}\Delta_k - E_k\Delta_{k+Q}}{E_{k+Q}+E_k} \\ \nu\frac{E_{k+Q}\tilde{\epsilon}_k - E_k\tilde{\epsilon}_{k+Q}}{E_{k+Q}+E_k} & -E_{k+Q}E_k - \Delta_k\Delta_{k+Q} + \tilde{\epsilon}_k\tilde{\epsilon}_{k+Q} & \nu\frac{E_{k+Q}\Delta_k + E_k\Delta_{k+Q}}{E_{k+Q}+E_k} & -\tilde{\epsilon}_{k+Q}\Delta_k - \tilde{\epsilon}_k\Delta_{k+Q} \\ \tilde{\epsilon}_{k+Q}\Delta_k - \tilde{\epsilon}_k\Delta_{k+Q} & \nu\frac{E_{k+Q}\Delta_k + E_k\Delta_{k+Q}}{E_{k+Q}+E_k} & -E_{k+Q}E_k - \Delta_{k+Q}\Delta_k - \tilde{\epsilon}_{k+Q}\tilde{\epsilon}_k & \nu\frac{E_{k+Q}\tilde{\epsilon}_k + E_k\tilde{\epsilon}_{k+Q}}{E_{k+Q}+E_k} \\ -\nu\frac{E_{k+Q}\Delta_k - E_k\Delta_{k+Q}}{E_{k+Q}+E_k} & -\tilde{\epsilon}_{k+Q}\Delta_k - \tilde{\epsilon}_k\Delta_{k+Q} & \nu\frac{E_{k+Q}\tilde{\epsilon}_k + E_k\tilde{\epsilon}_{k+Q}}{E_{k+Q}+E_k} & -E_{k+Q}E_k + \Delta_k\Delta_{k+Q} - \tilde{\epsilon}_k\tilde{\epsilon}_{k+Q} \end{pmatrix}. \tag{18}$$

IV. EXAMPLES

In this section I will apply the formalism outlined above to a number of examples with an increasing degree of complexity in relation to the type of electron-electron interaction that is assumed. The energy dispersion is assumed to be of the form

$$\epsilon_k = -2t\,[\cos(k_xa) + \cos(k_ya)] - 2t'\cos(k_xa)\cdot\cos(k_ya) - \mu, \tag{19}$$

where a, b, and c are the lattice parameters. The t and t' terms are due to nearest-neighbor and next-nearest-neighbor hopping in a square lattice. If $t' = 0$ at half filling of the band, such a dispersion relation has the remarkable property that the Fermi surface forms a perfect square, with a diverging effective mass over the entire Fermi surface. In practice this situation will never occur, as there will always be some finite coupling between next-nearest neighbors. This causes a bulging of the Fermi surface, which eventually transforms into a rotated Fermi surface if $|t'| \gg |t|$.

In all examples I will restrict the discussion to systems where electrons have an on-site attraction or repulsion, a nearest-neighbor interaction, or both, as well as the long-range e^2/r repulsive interaction. Moreover, the discussion is limited to the situation where a single band crosses the Fermi surface, and tight-banding language will be used for the description of this band. In particular I will consider a tight-binding band on a three-dimensional (3D) square lattice, with a strong anisotropy leading to quasi-two-dimensional behavior. A convenient set of functions to be used for the partial-wave decomposition of H^i is then the set of harmonic functions

$$\begin{aligned} &s: && \psi_0(k) = 1, \\ &s^*: && \psi_1(k) = \cos(k_xa) + \cos(k_yb), \\ &d_{x^2-y^2}: && \psi_2(k) = \cos(k_xa) - \cos(k_yb), \\ &p_x: && \psi_3(k) = \sqrt{2}\sin(k_xa), \\ &p_y: && \psi_4(k) = \sqrt{2}\sin(k_yb), \\ &d_{xy}: && \psi_5(k) = 2\sin(k_xa)\sin(k_yb), \\ &\text{etc.} \end{aligned} \tag{20}$$

The k-space representation of the on-site Hubbard U

interaction $\sum_i U_0 n_{i\uparrow} n_{i\downarrow}$ is the k-independent function $U(k-q) = U_0 \psi_0(k)\psi_0(q)$. If we consider the nearest-neighbor interaction $\frac{1}{2}V_1 \sum_{\langle i,j\rangle} n_i n_j$ we find, by means of a direct Fourier transformation of the operators $n_i = c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow}$, that this can be cast in the form $\frac{1}{2}\sum_Q V(Q)\rho(Q)\rho(-Q)$ with $V(Q) = 2V_1\psi_1(Q)$, so that we obtain the partial-wave decomposition

$$V(k-q) = V_1 \Big[\psi_1(k)\psi_1(q) + \psi_2(k)\psi_2(q) - \psi_3(k)\psi_3(q) - \psi_4(k)\psi_4(q) \Big]. \tag{21}$$

A singlet-only nearest-neighbor interaction $\frac{1}{4}U_1 \sum_{\langle i,j\rangle}(c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger)(c_{j\downarrow}c_{i\uparrow} - c_{j\uparrow}c_{i\downarrow})$ can be cast in the form $\frac{1}{8}\sum_Q U(Q)\,[\rho(Q)\rho(-Q) - \boldsymbol{\sigma}(Q)\cdot\boldsymbol{\sigma}(-Q)]$ with $U(Q) = 2U_1\psi_1(Q)$; hence it has the same partial-wave expansion as $2V_1\psi_1(Q)$. However, from Eq. (7) we see that the singlet-only interaction has other prefactors, and is summed over $U(k-q)$ and $U(k+q)$ in the pairing channel.

Finally we have to take into account the long-range Coulomb interaction. Here we will use the lattice Fourier transform of e^2/r. The screening of the Coulomb interaction for part of the vertices has been discussed above, and is essential, as a bare Q^{-2} interaction is known to create a singularity at the Fermi level within the random-phase approximation. I will use the convention in the remainder of this paper that $V(Q)$ is the bare Coulomb repulsion at large distances, whereas for shorter distances U_0 and V_1 are the projections of $V(Q)$ on the on-site interaction and the spin-independent nearest-neighbor interaction, respectively. Taking all these terms together we obtain for a model with a "singlet-only" nearest-neighbor interaction,

$$\begin{aligned}
&H_\sigma^i(0,0) = -U_0^\rho - U_1^\rho\psi_1(Q),\\
&H_\sigma^i(\alpha,\alpha) = -U_1^\rho/2 \quad (\alpha = 1,2),\\
&H_\rho^i(0,0) = 2V^\sigma(Q) - U_0^\sigma + U_1^\sigma\psi_1(Q),\\
&H_\rho^i(\alpha,\alpha) = U_1^\sigma/2 \quad (\alpha = 1,2),\\
&H_\phi^i(0,0) = U_0^{\rho\sigma},\\
&H_\phi^i(\alpha,\alpha) = U_1^{\rho\sigma} \quad (\alpha = 1,2).
\end{aligned} \tag{22}$$

For all symmetries we have $H_\psi^i(\alpha,\beta) = H_\phi^i(\alpha,\beta)$. The upper indices ρ and σ indicate whether screening with charge or spin fluctuations is implied. The minus sign in front of the U_0 term in $H_\rho^i(0,0)$ is not a misprint. As $2V(Q)$ "contains" the on-site Hubbard term, the sum of these two contributions is $+U_0$. In principle one should also include higher harmonics, as the expansion of $V(Q)$ does not end at ψ_4. However, as the expansion only appears as a *screened* interaction in expression (22), it is reasonable to work with a model where such interaction terms are neglected. If the nearest-neighbor interaction is spin independent, we must also include p_x and p_y symmetries of pairing, and we obtain

$$\begin{aligned}
&H_\sigma^i(0,0) = -U_0^\rho,\\
&H_\sigma^i(\alpha,\alpha) = -V_1^\rho \quad (\alpha = 1,\ldots,4),\\
&H_\rho^i(0,0) = 2V^\sigma(Q) - U_0^\sigma,\\
&H_\rho^i(\alpha,\alpha) = -V_1^\sigma \quad (\alpha = 1,\ldots,4),\\
&H_\phi^i(0,0) = U_0^{\rho\sigma},\\
&H_\phi^i(\alpha,\alpha) = V_1^{\rho\sigma} \quad (\alpha = 1,\ldots,4).
\end{aligned} \tag{23}$$

In the previous section we have seen that in addition to the partial-wave expansion of H^i, we also have to make a similar expansion of ΓK^0. The expression for this product is given in Eq. (18). The partial-wave expansion of this expression is in general complicated, and has to be done with the help of a computer. Some limiting cases exist, however, where the integrals can be solved, especially when an expansion for small Q can be made. Some of these limiting cases will be treated in the subsequent sections. In addition numerical calculations will be given at general values of the collective mode momentum Q.

A. Normal-state limit

In the nonsuperconducting limit Eq. (18) has only nonvanishing matrix elements on the diagonal. Furthermore, only the charge and spin channels are relevant in the absence of off-diagonal order. Let us make the further assumption that the electrons interact with each other via an on-site Hubbard U repulsion, which is therefore independent of k. After the summation over k we obtain for the top-left corner of Eqs. (18),

$$H^i(Q)\chi^0 = -\sum_k \frac{(\epsilon_{k+Q} - \epsilon_k)(f_k - f_{k+Q})}{\nu^2 - (\epsilon_{k+Q} - \epsilon_k)^2} \times \begin{pmatrix} -U_0^\rho & 0 \\ 0 & 2V^\sigma(Q) - U_0^\sigma \end{pmatrix}, \tag{24}$$

where the f_k are Fermi occupation factors. Let us assume for this part of the discussion that the momentum of the electrons in the plane is unbounded. In that case the Fourier transform of e^2/r is discrete in the direction perpendicular to the planes, and continuous along the planes, so that[24] $V(Q) = 2\pi e^2 d^2 \sinh(Q_\parallel d)[Q_\parallel d]^{-1}[\cosh(Q_\parallel d) - \cos(Q_\perp d)]^{-1}$, where d is the interlayer distance. Let us define $\tilde{Q} = \sqrt{4\pi e^2/V(Q)}$, which has the property $\lim_{Q\to 0}\tilde{Q} = Q$. If we assume that we have a cylindrical Fermi surface, with an isotropic Fermi velocity v_F, and a Fermi wave vector k_F, we obtain with $\epsilon - 1 = 2V(Q)\chi^0(2,2)$, and $\nu_p^2 \equiv 2e^2 d^{-1}\hbar k_F v_F$,

$$\epsilon = 1 - 2V(Q)\frac{2\pi k_F}{d}\frac{(2\pi)^{-3}}{\hbar v_F}\int_0^{2\pi} d\phi \frac{\hbar^2 Q_\parallel^2 v_F^2 \cos^2\phi}{\nu^2 - \hbar^2 Q_\parallel^2 v_F^2\cos^2\phi}$$

$$= 1 - \frac{2\nu_p^2}{\hbar^2\tilde{Q}^2 v_F^2}\left\{\left(1 - \frac{\hbar^2 Q_\parallel^2 v_F^2}{\nu^2}\right)^{-1/2} - 1\right\}. \tag{25}$$

The plasma dispersion relation becomes

$$\nu = \nu_p \frac{Q_\parallel}{\tilde{Q}} \frac{1+\hbar^2\tilde{Q}^2 v_F^2/(2\nu_p^2)}{\left\{1+\hbar^2\tilde{Q}^2 v_F^2/(4\nu_p^2)\right\}^{1/2}} = \nu_p \frac{Q_\parallel}{\tilde{Q}} \left\{1+\frac{3}{8}\frac{\hbar^2\tilde{Q}^2 v_F^2}{\nu_p^2}+\cdots\right\}. \quad (26)$$

The spin susceptibility per unit cell (Ω_u is the area in the 2D plane) is

$$\chi(1,1) = \frac{1-(1-\hbar^2 Q_\parallel^2 v_F^2/\nu^2)^{-1/2}}{W + U_0[(1-\hbar^2 Q_\parallel^2 v_F^2/\nu^2)^{-1/2}-1]}, \quad (27)$$

where $W \equiv \frac{\hbar^2\pi}{m\Omega_u}$ is the effective bandwidth. We see that in the high-frequency limit ($\nu \gg \hbar Q_\parallel v_F$) $\chi^{\mathrm{HF}}(1,1) = -E_F Q_\parallel^2 \Omega_u [\nu^2 + U_0 E_F Q_\parallel^2 \Omega_u]^{-1}$, and in the low-frequency limit $\chi^{\mathrm{LF}}(1,1) = (W-U_0)^{-1}$. Hence the ac susceptibility is suppressed, whereas the static susceptibility is enhanced. A magnetic instability occurs for $U_0 \approx W$. The above expressions are derived assuming a free electron dispersion. If the Fermi surface has nesting vectors,[12] instabilities for specific values of Q are often found.

B. *s*-wave superconductivity

For s symmetry, and neglecting the radial k dependence of the pairing potential, the partial-wave decomposition of χ^0 and H^i is trivially achieved by summing over all k. As a model for the pairing interaction we adopt $U(k-q) = -g$. As is usually done in the gap equation, one can limit the energy range of the interactions in these expressions by putting $\Delta = 0$ for energies larger than a scaling value (the Debye frequency for phonon-mediated pairing). For the long-range Coulomb interaction we take again $V(Q) = 4\pi e^2 Q^{-2}$. Due to the fact that $\epsilon_{k+Q} = \epsilon_{-k-Q}$ we obtain after summation that $\chi^0(1,2) = \chi^0(1,3) = \chi^0(1,4) = 0$. Hence the spin fluctuations are fully decoupled from the other three and can be considered separately. The remaining diagonal and off-diagonal susceptibilities are finite, and the following expressions are required:

$$\begin{aligned}
\chi^0(1,1) &= -\sum_k \frac{(E_k+E_{k+Q})(E_kE_{k+Q}-\Delta_k\Delta_{k+Q}-\epsilon_k\epsilon_{k+Q})}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},\\
\chi^0(2,2) &= -\sum_k \frac{(E_k+E_{k+Q})(E_kE_{k+Q}+\Delta_k\Delta_{k+Q}-\epsilon_k\epsilon_{k+Q})}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},\\
\chi^0(3,3) &= -\sum_k \frac{(E_k+E_{k+Q})(E_kE_{k+Q}+\Delta_k\Delta_{k+Q}+\epsilon_k\epsilon_{k+Q})}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},\\
\chi^0(4,4) &= -\sum_k \frac{(E_k+E_{k+Q})(E_kE_{k+Q}-\Delta_k\Delta_{k+Q}+\epsilon_k\epsilon_{k+Q})}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},
\end{aligned} \quad (28)$$

$$\begin{aligned}
S &= \sum_k \frac{(E_k+E_{k+Q})}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},\\
T &= \sum_k \frac{(E_k+E_{k+Q})(\epsilon_k+\epsilon_{k+Q})}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},\\
M &= \sum_k \frac{(E_k+E_{k+Q})(\epsilon_k-\epsilon_{k+Q})^2}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)},\\
N &= \sum_k \frac{(E_k-E_{k+Q})(\epsilon_{k+Q}-\epsilon_k)}{2E_kE_{k+Q}\left(\nu^2-[E_k+E_{k+Q}]^2\right)}.
\end{aligned}$$

Let us first consider the spin susceptibility. As now $\chi(1,1) = \frac{\chi^0(1,1)}{1+g\chi^0(1,1)}$ with $g>0$ for a BCS interaction, the spin fluctuations are pushed to a slightly higher energy.

The generalized susceptibility for density, phase, and amplitude can be expressed using the above definitions as

$$\begin{pmatrix} -\chi^0(1,1)+2\Delta^2 S & -\nu\Delta S & \Delta T \\ -\nu\Delta S & -\chi^0(3,3) & -\nu(T+N)/2 \\ \Delta T & -\nu(T+N)/2 & -\chi^0(4,4) \end{pmatrix}.$$

Using the gap equation, $\left(1 = \sum_k \frac{g}{2E_k}\right)$ it is easy to prove that $\chi^0(3,3) = 1/g - \nu^2 S/2 + M/2$ and $\chi^0(4,4) =$

$\chi^0(3,3) + 2\Delta^2 S$. Using these properties, we see that the matrix $1 + H^i\chi^0$ becomes

$$\begin{pmatrix} 1+2V_Q\chi^0(1,1) - 4V\Delta^2 S & 2V_Q\nu\Delta S & -2V_Q\Delta T \\ -g\nu\Delta S & g(\nu^2 S - M)/2 & -g\nu(T+N)/2 \\ g\Delta T & -g\nu(T+N)/2 & g([\nu^2 - 4\Delta^2]S - M)/2 \end{pmatrix}$$

and the collective modes can be calculated from the determinant

$$0 = [1 - 2V_Q\chi^0(1,1)]\left\{(\nu^2 S - M)\left([\nu^2 - 4\Delta^2]S - M\right) - \nu^2(T-N)^2\right\} + 4V\Delta^2\left\{(N^2 + 2TN)S\nu^2 + M(S^2[\nu^2 - 4\Delta^2] - T^2\right\}. \tag{29}$$

To further analyze this expression we need to make a series expansion for small Q. In what follows we will neglect N ($\propto Q^2$, but with a vanishing prefactor if the gap has electron-hole symmetry). Furthermore we notice that we can write $2V_Q\chi^0(1,1) \approx -\nu_p(Q)^2(\nu^2 - W^2 - 4\Delta^2)^{-1}$, $M \approx S\langle(\mathbf{v}_F \cdot \mathbf{Q})^2\rangle$, $V_Q M \approx -(1 + W^2/4\Delta^2)V_Q\chi^0(1,1)$, and $T \approx -2\mu_F S$, where $\mu_F = E_F - W/2$, and W is the effective bandwidth. Retaining only leading orders in $\langle(\mathbf{v}_F \cdot \mathbf{Q})^2\rangle$ we see that the collective modes can now be solved from

$$2[\nu^2 - W^2 - 4\Delta^2 - \nu_p(Q)^2](\nu^2 + 2\Delta^2)\langle(\mathbf{v}_F \cdot \mathbf{Q})^2\rangle = (\nu^2 - 4\Delta^2 - 4\mu_F^2)(\nu^2 - W^2 - 4\Delta^2)[\nu^2 - \nu_p(Q)^2]. \tag{30}$$

Hence we see that the negative U Hubbard model permits in principle four collective modes: a spin-density oscillation discussed above, a plasma mode, and two additional modes, which are, however, situated in the two-quasiparticle continuum, and therefore are strongly damped. Interestingly the plasmalike mode can exist at frequencies above and below the gap, depending on the initial value of $\nu_p(Q)$ in the normal state. As has been discussed by Fertig and Das Sarma[25] a layer dispersion relation as discussed above permits the existence of low-lying plasmons *below* the gap. Another mechanism for reducing the plasma frequency in the superconducting state is strong damping of the motion perpendicular to the planes, as we recently discussed.[29]

C. *s*-wave superconductivity in a layered electron gas

If the superconductor is strongly anisotropic, the plasma energy for $Q \to 0$ depends on the direction of propagation. An extreme example of this arises when the mass in one of the three directions is infinite, resulting in a system which behaves two dimensional from the point of view of the single-particle band structure, whereas the Coulomb forces are three dimensional. A simple model exhibiting such behavior is an infinite stack of two-dimensional layers. The electrodynamics of this system was already discussed by several authors[24,9,8] using hydrodynamic calculations, as well as with the random-phase approximation. The resulting plasmon spectrum of such a metal is, in the limit of a large wavelength, $\nu(\mathbf{Q}) = \nu_p Q_\parallel |\mathbf{Q}|^{-1}$, which for $Q_\perp = 0$ saturates at the value ν_p, while for finite values of $Q_\perp$ it has an acoustic-like dependence on $Q_\parallel$.

This implies that here we have a system which on the one hand has a density of charge carriers characteristic of a metal and, provided that there is a pairing mechanism, therefore has the potential of becoming a BCS-like superconductor. On the other hand the dynamical response of the electrons in one of the directions is more characteristic of a semiconductor or an insulator. This combination provides us with an example where the Anderson-Higgs mechanism does *not* shift the Goldstone mode to a high energy, in spite of the fact that the particles interact through a long-range Coulomb force. Here we will use the dispersion introduced in Eq. (19) with $t' = 0$. In this example $W = 4t$ is the bandwidth. For the long-range Coulomb forces we take the lattice Fourier transform of e^2/r, which has $\Omega_u^{-1} 4\pi e Q^{-2}$ as its long-wavelength limiting behavior, and possesses

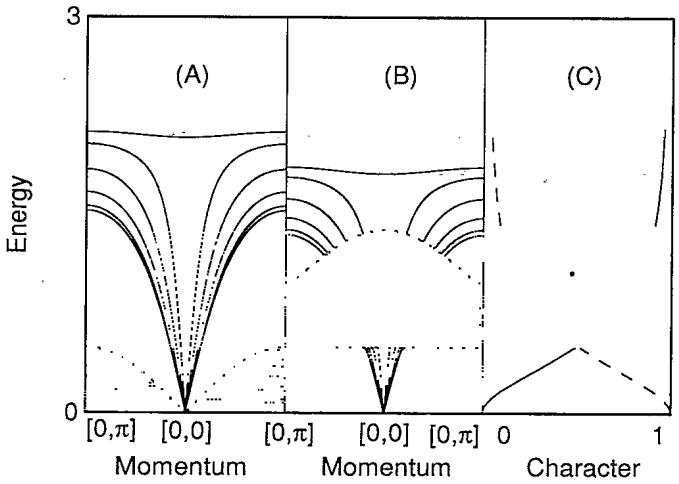

FIG. 2. Collective-mode spectrum of a superconducting layered electron gas, assuming *s*-wave pairing. The parameters are $E_F/(4t) = 0.35$, $\mathrm{Ry}/(4t) = 4.0$. $Q_\perp c$ is varied with 0 to π with increments of 0.2π (top to bottom solid curves). The dashed curves are the boundaries of the region of Landau damping. (a) Normal metal, U=0 and (b) superconducting state, $U/(4t) = -0.67$. (c) The amount of ρ (solid line) and ϕ (dashed line) character of the collective modes as a function of collective-mode energy. The interruption occurs where the modes become Landau damped.

the same periodicity in k space as the tight-binding band. $\mathrm{Ry}^* = e^2 d^{-1}$ is the effective Rydberg which, together with the Fermi energy, sets the scale of the plasma frequency in the planar direction ($\nu_p = 2\sqrt{E_F \mathrm{Ry}^*}$ for $E_F << W$). For the pairing interaction we adopt the same model as in the previous section, with the following set of parameters: $E_F/W = 0.35$, $g/W = 0.6729$ (resulting in $\Delta/W = 0.25$), and $\mathrm{Ry}^*/W = 4.0$. In Fig. 2(a) the result is displayed with $Q_\perp$ as a parameter in the range from 0 to $d^{-1}\pi$, and agrees well with the calculations of Fertig and Das Sarma, and those by Côté and Griffin.[25,10] Due to the model assumption of an energy-independent attraction, the electron-hole continuum becomes a broadband already for zero momentum in the two-particle channel. In Fig. 2(b) the same set of calculations is displayed for the normal state. The plasma frequencies become somewhat smaller in the superconducting state, which is due to the fact that the gap in this example is relatively large. It reflects a well-known property of the negative U Hubbard model that the mass of a pair is enhanced due to the fact that two particles have to hop simultaneously.[30] Also a strong qualitative difference arises, which is not directly evident from these curves. This is the change in character of the modes. In Fig. 2(c) the distribution of weight of the mode over the density, gap-phase, and gap-amplitude branches is displayed. First of all we notice that the contribution of the latter is negligible. The second interesting feature is that the nature of the collective mode changes gradually from a pure phase fluctuation at low energy to a 50/50 % phase-density mixture at the edge of the particle-hole continuum. Inside the electron-hole continuum the collective modes are damped. (Although they may still persist as a resonance, they cannot be identified from the zeros of a determinant.) However, for energies larger than the particle-hole continuum of our band we see that the density-fluctuation character dominates.

The plasmon-dispersion, which is coupled to the s-phase fluctuating channels for small q, is acoustic for finite $Q_\perp/Q_\parallel$, and so the Landau criterion[31] remains satisfied in spite of having a gapless plasmon spectrum.

D. Phase versus spin-fluctuating modes in a layered electron gas

Let us now consider the singlet-only nearest-neighbor pairing interaction U_1. In the discussion of the resonating valence bond state[32,33,28] the t-J model has been used, where $J = -U_1$, and a reduction of the double occupancy of the same site is included, either by replacing the bare hopping parameter t with an effective one, or by using more elaborate schemes. It is not the aim of the present discussion to address the t-J model. Instead we consider a Fermi liquid, with an on-site repulsion (U_0) which is not too strong, and an attractive interaction between electrons on a neighboring site (U_1). As the actual band structure in these systems is experimentally known to be better described by the three-band model of Zaanen, Sawatzky, and Allen[34] (which is again a simplified version of the real valence band structure involving six oxygen $2p$ bands and five copper $3d$ bands for the occupied states, as well as unoccupied $3s$ and $3p$ states) a transformation to a single-band Hamiltonian will in principle generate both an effective Hubbard U_0 and an intersite U_1.[35–37] Examples of such transformations can be found in the work by Emery[38] and by Jansen.[39] However, also other, more complicated types of interactions are generated when making such transformations, notably the correlated hopping term (with six operators) which, as has been shown by Hirsch, promotes superconductivity of hole carriers.[40] The interaction considered by Jansen, as well as the correlated hopping term treated by Hirsch, effectively provides an *on-site* attraction, which, when considered on its own, promotes pairing in the (nonextended) s-wave channel. Also the U_1 term contains contributions from the virtual exchange of spin fluctuations.[11,41] As has been discussed by Scalapino *et al.*,[12] such processes give rise to an attraction on nearest-neighbor sites, and increase the on-site repulsion between electrons. As the exchange spin fluctuations are really vertex corrections due to the H^i_σ channel, one could schematically regard U_1 in Eq. (22) as the vertex correction of U_0. As such corrections are necessarily retarded, and therefore rather ill represented by the nonretarded interaction assumed here, the present analysis can at best provide a qualitative picture.

(BZA) Baskaran, Zhou, and Anderson[33] considered pairing of the s^* type near half filling, Emery considered $d_{x^2-y^2}$ pairing, and Kotliar studied both s^*- and d-type pairing. As we will see, the s^*-type pairing is not a stable solution near half filling, and is dominated by pairing of the d type. As the latter again tends to be unstable with respect to the antiferromagnetic Mott-Hubbard insulating state at half filling, superconductivity can only exist sufficiently far away from this region. As the optimal T_c would have been reached at half filling for a symmetrical band, this would lead to the conclusion that superconductivity is only a marginal effect in such a system. However, the high-T_c cuprates do not have an electron-hole symmetrical band, and the Fermi surface is known to be strongly distorted from the perfect square that arises from considering only nearest-neighbor hopping. This actually comes to the rescue: As a function of band filling it pulls apart the regions where antiferromagnetism and high T_c have their highest stablility. The three coupled gap equations are (with $x \equiv k_x a$ and $y \equiv k_y a$)

$$\left(1 + \sum_k \frac{\tanh E_k/(2k_BT)}{2E_k} \begin{bmatrix} U_0 & U_0[\cos x + \cos y] & U_0[\cos x - \cos y] \\ U_1[\cos x + \cos y] & U_1[\cos x + \cos y]^2 & U_1[\cos^2 x - \cos^2 y] \\ U_1[\cos x - \cos y] & U_1[\cos^2 x - \cos^2 y] & U_1[\cos x - \cos y]^2 \end{bmatrix}\right) \begin{pmatrix} \Delta_s \\ \Delta_{s^*} \\ \Delta_d \end{pmatrix} = 0, \tag{31}$$

together with a fourth expression, which determines the chemical potential by constraining the electron occupation number $\sum_k (1-\epsilon_k/E_k) = N_e$. For a sufficiently small value of U_1 or for T near T_c, where Δ becomes small, the denominator has the fourfold symmetry of the crystal, and the cross terms linking s^* to d are zero for symmetry reasons. Hence only s and s^* are coupled provided that $U_0 \neq 0$. If Δ becomes large compared to the bandwidth, *a priori* there is no reason why mixing between s and d is forbidden, and indeed we will see that such a mixing takes place for a large value of U_1.

I still need to specify the electron dispersion relation before we can solve the gap equations. For the dispersion relation we now use Eq. (19) with $t' = -0.7t$. The shape of the Fermi surface obtained with this choice of parameters is very close to what has been calculated with the local density approximation for, e.g., La_2CuO_4 and $YBa_2Cu_3O_7$.[42,43] Due to the finite value of t' a significant change occurs in the density of states (DOS) at the Fermi energy as a function of the number of electrons per unit cell. The DOS is now asymmetric, and the maximum is shifted to the "hole-doped" side of the point where the band is half filled. Of course the direction in which this occurs is dictated by the sign of t'. With $t' < 0$ we mimic the situation encountered in the CuO_2 planes of the high-T_c cuprates.

The phase diagram, displayed in Fig. 3, was calculated by searching numerically for the minimum of the Helmholtz free energy [Eq. (4) + μN_e, using μ as a Lagrange parameter to keep the number of electrons fixed] as a function of Δ_s, Δ_{s^*}, and $\Delta_{d(x^2-y^2)}$. The boundaries, which are indicated in this diagram, are calculated for $T = 0.01W$, where $W = 4t$ is the bandwidth. For $T = 0$ no sharp phase boundaries exist. Somewhat surprisingly, for $|U_1|$ larger than a critical value (which depends on n_e), the ground state is of mixed s and d symmetry. It is worthwhile to mention in this context that the region of sd mixing almost coincides with the region of p-wave symmetry, if we use a spin-independent interaction (V_1) instead.

The phase diagram with $t'/t = -0.7$ and $U_1/(4t) = -0.5$, and $U_0/(4t) = 0$ is displayed in Fig. 4. Due to

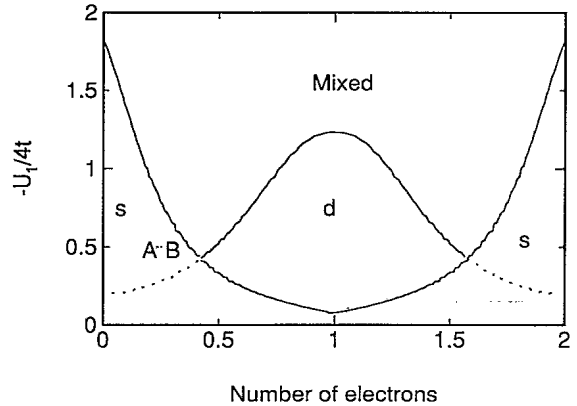

FIG. 3. Phase diagram in the U_1-n plane, where n is the number of electrons per unit cell, with $t' = -0.7$ and $U_0/(4t) = 0$.

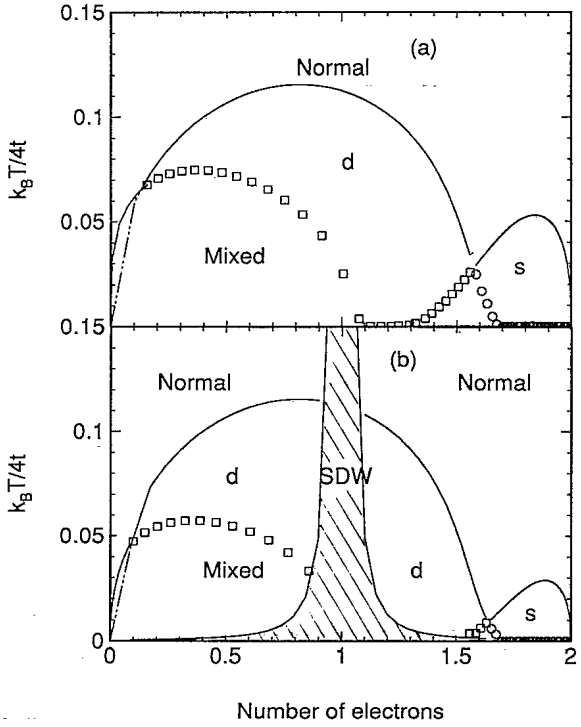

FIG. 4. (a) Phase diagram in the T-n plane, where n is the number of electrons per unit cell, with $t' = -0.7t$ and $U_0/(4t) = 0$, and $U_1/(4t) = -0.5$. (b) The same with $U_0/(4t) = 1$.

breaking of electron-hole symmetry, the diagram is now asymmetric around half occupation of the band. Roughly speaking s^* pairing is favored far away from half filling of the band, whereas d-wave pairing becomes the most stable solution near half filling. We also notice from this plot that the asymmetry implies that the highest T_c's and d-pairing superconductor are to be expected on the left-hand ("hole-doped") side of half filling. Lower T_c's and s pairing occur on the right-hand side, in agreement with the result of Micnas *et al.*[44]

Let us now consider the Δ/T_c ratio following from the gap equation. Within the context of BCS theory we have $\Delta_0(T) = 0$ at T_c, so that T_c follows from

$$\frac{-2}{U_1} = \sum_q \epsilon_q^{-1} \tanh\left(\frac{\epsilon_q}{2k_B T_c}\right)[\cos q_x a \pm \cos q_y a]^2, \qquad (32)$$

where the $\pm$ sign refers again to the two symmetries of pairing. This equation can be easily solved numerically. The result is that for extended s-wave pairing the ratio $2\Delta_0/k_B T_c$ is 6.5, whereas for d-wave pairing it rises gradually from 4 if $|U_1| \ll W$, up to 6.5 in the limit where $|U_1| \gg W$. This is not sensitive to the value of the parameter t'. We should keep in mind here that Δ_0 is the maximum value reached by $\Delta(k)$ [respectively, at the $(\pi, 0)$ and (π, π) points for d and s^* pairing].

In Fig. 5, $T_c^{\rm MF}/W$ is displayed as a function of $|U_1|/W$ for the d-wave channel. First of all we notice that for $|U_1| > W/4$ the value of $T_c^{\rm MF}$ is about $|U_1|/4$. For $|U_1|/W \ll 1$ this crosses over to a quadratic dependency $T_c^{\rm MF} = 4|U_1|^2/W$. For comparison a similar curve is dis-

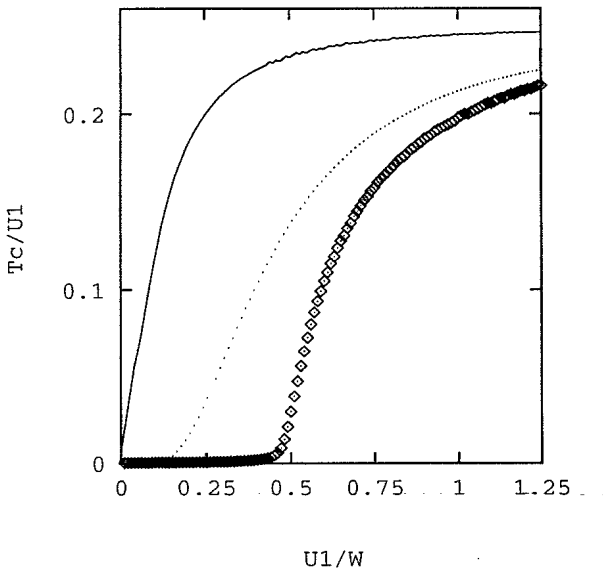

FIG. 5. Solid curve: $T_c/|U_1|$ calculated for the d-wave channel of the exchange-only model with $t' = 0$ and 1 electron per site. The same curve is obtained for $t' = -0.7t$ with 0.7 electron per site. Open lozenges: T_c of the s^*-wave channel with the latter parameters. Dotted curve: $T_c/|U|$ versus $|U|/W$ for the negative U Hubbard model taking a square DOS.

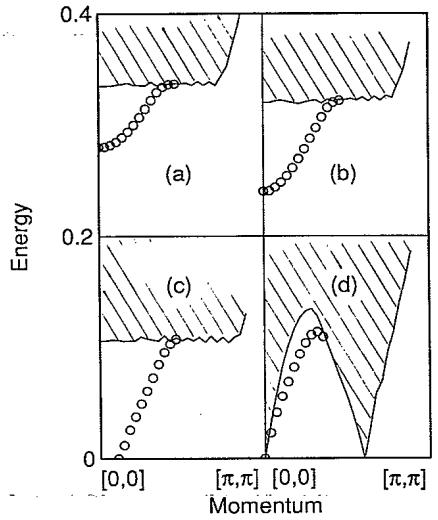

FIG. 6. Phase-fluctuating collective mode versus momentum for a layered electron gas with long-range Coulomb interactions (Ry* = 20), an on-site repulsive interaction ($U_0/W = 0.5$), and a nearest-neighbor attractive interaction $U_1/W = -0.5$. The number of electrons is $n_e = 0.2$ (a), $n_e = 0.25$ (b), $n_e = 0.3$ (c), and $n_e = 0.4$ (d).

played for conventional s-wave pairing, using the negative U Hubbard model in a band with a square DOS. We notice that the mean-field transition temperature with the latter model becomes $T_c^{\mathrm{MF}} = |U_0|/4$ for large $|U_0|$ (which is actually outside the range of validity of the BCS weak coupling approach[30,45]) and has the familiar BCS-like $\exp(-W/|U_0|)$ behavior for small U_0. The T_c for the extended s-wave pairing lies again below the negative U_0 curve, and is only finite above a threshold value of $|U_1|$ as discussed above.

Let us now consider the collective modes for the examples along the line AB indicated in the phase diagram of Fig. 3. The result is displayed in Fig. 6. We see that a soft mode develops if we approach the phase boundary between s- and d-wave superconductivity. The transition takes place exactly when the mode has developed into a Bogoliubov sound mode. If we keep imposing the s symmetry for the ground state, while actually being in the d-wave part of the phase diagram, we always find a soft mode of phase-fluctuating character, indicating that the solution is unstable. If we allow the ground-state wave function to become d-wave paired, the gap disappears, and a sound-wave phase-fluctuation mode occurs directly below the particle-hole continuum. Both the Bogoliubov mode and the lower bound of the particle-hole continuum are soundlike, so that according to the argument of Landau *et al.*[31] a supercurrent flow is still possible in spite of the fact that there is no gap.

If $t'/t = -0.7$ and $U_1/(4t) = -0.5$, and $U_0/(4t) = 0$, the phase diagram for which is displayed in Fig. 4, we can anticipate that again d-wave phase fluctuations exist below the particle-hole continuum. In addition, because there is an on-site repulsive U_0, a branch of spin fluctu-

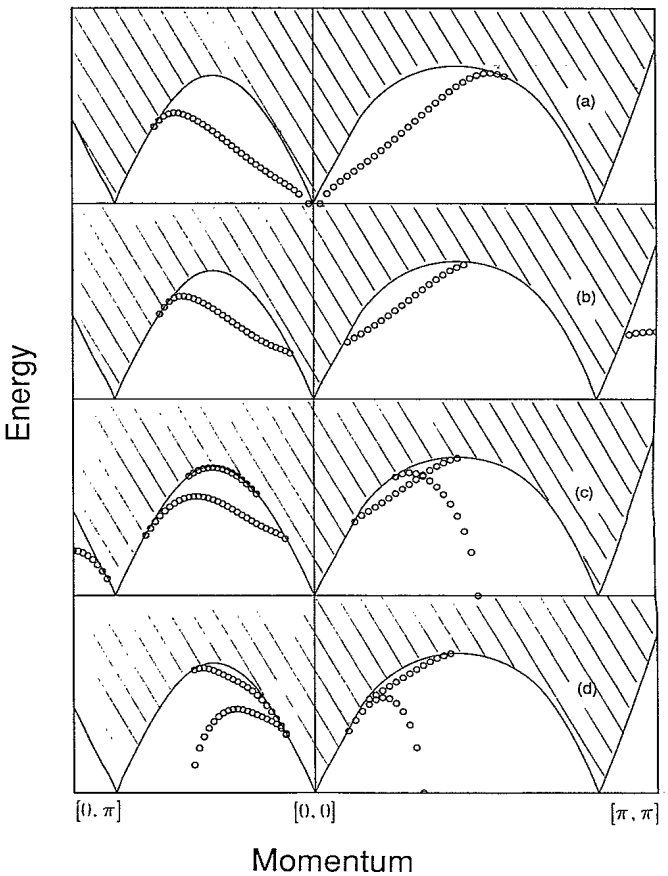

FIG. 7. The collective modes in the d-wave paired state, using $U_1/(4t) = -0.5$, and $n_e = 0.85$, and with $U_0/(4t) = 0$ (a), 0.5 (b), 1 (c), and 1.5 (d).

ations can be pulled below the particle-hole continuum. In Fig. 7 the collective-mode spectrum is displayed, using $U_1/(4t) = -0.5$, and $n_e = 0.85$, and with $U_0/(4t)$ ranging from 0 to 1.5. In the plot for $U_0 = 0$ we already notice that the particle-hole continuum has eight points in k space where it touches the horizontal axis: The Fermi surface crosses the node lines $k_x = \pm k_y$ at the coordinates $(\pm(\pi-\delta)/2, \pm(\pi-\delta)/2)$, hence the particle-hole spectrum is gapless for the Q vectors $(0, \pm(\pi-\delta))$, $(\pm(\pi-\delta), 0)$, and $(\pm(\pi-\delta), \pm(\pi-\delta))$. Precisely for these Q values the spin (and charge) susceptibility acquires the largest value, also in the superconducting state; hence if we switch on a finite value of the repulsive on-site U_0, a spin-density wave starts to develop around the $(\pm\pi, \pm\pi)$ points on the Fermi surface. Clearly the ground state is no longer of the form of Eq. (1), and the corrections may become strong enough to completely destroy superconductivity. As, on the other hand, the spin-density wave exists around a portion of the Fermi surface where the gap is zero (and therefore contributes the least to the ground-state energy), whereas the maximum gap value is at the $[\pm\pi, 0]$ and $[0, \pm\pi]$ points, there may actually be a coexistence of superconductivity and a spin-density wave in different portions of the Fermi surface.

From Fig. 7 we can see that the region taking part in the formation of the spin-density wave quickly spreads around the $(\pm(\pi-\delta)/2, \pm(\pi-\delta)/2)$ points if $U_0/(4t)$ increases, leaving a small region around $[\pm\pi, 0]$ and $[0, \pm\pi]$ for the formation of a superconducting condensate if $U_0/(4t) = 1$. The phase diagram for $U_0/(4t) = 1$, and $U_1/(4t) = -0.5$ is indicated in Fig. 4(b). The shaded area roughly indicates the region with an instability towards a SDW. In principle a mixed SDW-superconducting state may exist for all concentrations. It is not possible to decide from the numerical results presented above whether or not there is a sharp phase boundary separating regions with a magnetic instability from superconducting regions.

V. CONCLUSIONS

A unified approach is presented to the calculation of the collective modes of spin, charge, phase, and amplitude in superconductors with a nontrivial pairing interaction. The expressions for the dynamical spin and charge susceptibilities are generalized to take into account superconductivity at general values of momentum and frequency. Several examples are treated. Notably the response functions of a layered charged electron gas, with a pairing interaction in the d-wave channel, are considered in the absence and presence of an on-site Hubbard repulsive interaction. An incipient instability toward a spin-density wave follows from the softening of the collective-mode spectrum near $\mathbf{Q} = (\pi, \pi)$ in the d-wave paired state.

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