Collective Excitations and Spectral Function in the Fermi-Liquid State of the *t*-*J* Model

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(Received 22 July 1991)

We analyze the nature of the single-particle excitations and the collective modes in the nonmagnetic phase of a generalized t-J model to next to leading order in $1/N$. We discuss the essential features of the spectral function of the t-J model and we evaluate it numerically for values of the parameters t, J, and of the doping level relevant to the copper-oxide planes.

PACS numbers: 71.28.+d, 74.65.+n, 79.60.−i

The characteristics of the one-particle Green's functions and the nature of the collective excitations in fermion systems where the local correlations are strong is a long-standing problem in condensed-matter physics. In the context of the simple, Hubbard-like models, two very important ideas, the existence of two broad incoherent peaks in the spectral function now known as Hubbard bands and the existence of a Luttinger Fermi surface, were advanced by Hubbard [1] and by Brinkman and Rice [2], respectively. Hubbard and followers used equation-of-motion schemes, which produce incoherent features in the spectral function as a result of the strong correlation. Unfortunately, these schemes do not produce quasiparticles and violate Luttinger's theorem [3]. Approaches based on the Brinkman-Rice-Gutzwiller [4] wave functions are consistent with a Fermi surface and strongly renormalized quasiparticle excitations; however, it is very difficult to construct in these schemes approximate variational excited states to calculate the spectral function and to recover the incoherent part of the spectrum.

In this Letter we calculate for the first time the one-particle spectral function in a generalized t-J model treated systematically to next to leading order in the $1/N$ expansion. This approach can be pursued very far analytically, and produces both Hubbard-like and Gutzwiller-like features in the spectral function. We find that the gross features of the Hubbard valence band have a simple interpretation in terms of a superposition of quasiparticles and a collective mode describing the coherent propagation of holes in a strongly correlated system. The collective mode reduces to the zero-sound mode in the long-wavelength limit. The exchange interactions between the spins do not affect the gross features of the spectral density but have a dramatic effect at low frequency. They produce very low-lying collective modes describing the propagation of staggered spin chirality and give rise to deviations from Fermi-liquid behavior at intermediate-energy scales. Our findings are in good agreement with recent numerical calculations [5,6].

We consider the SU(N) generalization of the t-J model [7] defined by

$$H=-\frac{t}{N}\sum_{\rm nn}(f_{i\sigma}^\dagger b_i f_{j\sigma}b_j^\dagger+\text{H.c.})+\frac{J}{N}\sum_{\rm nn}f_{i\sigma}^\dagger f_{i\sigma'}f_{j\sigma'}^\dagger f_{j\sigma}\,, \quad (1)$$

and the constraint $f_{i\sigma}^\dagger f_{i\sigma}+b_i^\dagger b_i=N/2$ with the sum over repeated $\sigma=1,\ldots,N$ implied. The spin-$\frac{1}{2}$ t-J model corresponds to the $N=2$ limit of Eq. (1) where b_i is a slave boson introduced to label an empty site and $f_{i\sigma}^\dagger$ is a fermion carrying the spin quantum number of the projected electron operator $c_{i\sigma}^\dagger=f_{i\sigma}^\dagger b_i$. The partition function of the model is a functional integral of the imaginary-time Lagrangian over the complex Bose field b, a Hubbard-Stratanovich field of expectation value $\Delta_{ij}=J\langle f_{i\sigma}^\dagger f_{j\sigma}\rangle/N$, Grassman variables f, and a Lagrange multiplier λ_i which enforces the constraint. In the large-N limit, the partition function is controlled in a large range of parameters by a saddle point uniform in the fields [7] $b^2=N\delta/2$, $\lambda_0=4t\Delta/J$, and $\Delta=J/N_s\times\sum_{\mathbf{k}}\cos k_x f(\varepsilon_{\mathbf{k}})$. It describes quasiparticles with dispersion $\varepsilon_{\mathbf{k}}=-2W(\cos k_x+\cos k_y)+\lambda_0-\mu$, $W=\Delta+tb^2/N$. The residual interactions are generated by the fluctuating part of the Bose fields: $b_i=(b+\sqrt{N}r_i)e^{i\theta_i}$, $i\lambda_i=\lambda_0+i\lambda_i$, and $\Delta_{i,\eta}=\Delta(1+R_{i,\eta})e^{iA_{i,\eta}}$. We work in the radial gauge [8] where the fermion excitations can be identified with the Fermi-liquid quasiparticles. The Lagrangian is given by

$$\mathcal{L}=\sum_{\mathbf{k},n}f_{\mathbf{k},\sigma}^\dagger(i\nu_n-\varepsilon_{\mathbf{k}})f_{\mathbf{k},\sigma}+N\sum_q\left[\varepsilon_q^b r_q^2+i\frac{2b}{\sqrt{N}}\lambda_q r_{-q}+\frac{\Delta^2}{J}(A_q^2+R_q^2)\right]$$
$$+\frac{\Delta}{W}\sum_q\left[\mathcal{J}_q\cdot\mathbf{A}_{-q}+\mathcal{T}_q\cdot\mathbf{R}_{-q}+i\frac{W}{\Delta}\rho_q\lambda_{-q}+\frac{tb/\sqrt{N}}{\Delta}\mathcal{E}_q r_{-q}\right], \quad (2)$$

where $q=(\mathbf{q},i\omega_n)$. The fields λ and r are the usual slave-boson fields which couple to the quasiparticle density and energy density operators $(\rho,\mathcal{E})$. The phase and amplitude (A_μ,R_μ) of the bond variables couple to the current and stress operators $(\mathcal{J}^\mu,\mathcal{T}^\mu)$,

$$(\rho_q,\mathcal{E}_q,\mathcal{J}_q^\mu,\mathcal{T}_q^\mu)=\sum_{\mathbf{k}}\left(1,(\varepsilon_{\mathbf{k}_+}+\varepsilon_{\mathbf{k}_-}),\frac{\partial\varepsilon_{\mathbf{k}}}{\partial k_\mu},\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_\mu^2}\right)f_{\mathbf{k}_+,\sigma}^\dagger f_{\mathbf{k}_-,\sigma}\,, \quad (3)$$

with $\mathbf{k}_\pm = \mathbf{k} \pm q/2$. The potential terms in Eq. (2) contain the vacuum tadpole diagrams. Notice that the value of the r-r vertex is the dispersion of a boson $\varepsilon^b_\mathbf{q} = 2t(\Delta/J)(2-\cos q_x - \cos q_y)$ with a weakly renormalized bandwidth $8t\Delta/J$, while the λ-r vertex is a consequence of the Bose condensation. The Bose field propagators $D_{\alpha\beta} = \langle \phi^\alpha_q \phi^\beta_{-q} \rangle$, with $\phi^\alpha = (r, \lambda, R_\mu, A_\mu)$, are given by $D^{-1}(q) = D_0^{-1}(q) + \chi^0(q)$, where D_0^{-1} are the bare boson propagators in Eq. (2) and the χ^0 are fermion polarization bubbles calculated with the vertices in Eq. (3).

First we turn to the collective modes of the model. The density-density correlation χ_ρ to leading order in $1/N$ is given by $-4b^2 D_{rr}$. Figure 1 shows that χ''_ρ has a particle-hole continuum with a well-defined cutoff $\approx q v_F$, with v_F the renormalized Fermi velocity which defines a mass renormalization $m^*/m = t/(\Delta + tb^2/N)$. In the region $|\omega| \gg q v_F$, the density-density correlation function is dominated by a collective mode $\chi_\rho(\mathbf{q},\omega) \simeq N[(1+F^s_1/2)/m^*](\Delta/J)q^2/(\omega^2 - \omega^2_\mathbf{q})$. The dispersion of this mode, $\omega_\mathbf{q} \simeq (\varepsilon^b_\mathbf{q} + c^2 q^2)^{1/2}$, is analogous to that of the phase mode of a Bose superfluid. In the long-wavelength limit this mode reduces to the zero-sound mode of a Fermi liquid, i.e., $\omega_\mathbf{q} \simeq c|q|$, which is undamped for $(J/t)^2 \ll \delta$. The sound velocity in this case is

$$c^2 = \frac{1}{m^{*2}} \left[\frac{\Delta}{J\rho_0} F^s_0 \left(1 + \frac{1}{2} F^s_1 \right) + A_1 F^s_1 + A_2 F^s_2 + A_3 F^s_1 F^s_2 \right]. \tag{4}$$

$F^s_0 = (4t\rho_0|\epsilon_0| - J\rho_0\epsilon_0^2)/2W$, $F^s_1 = -2\Delta/(\Delta + tb^2/N)$, and $F^s_2 = (J\rho_0\epsilon_0^2 - 4J\rho_0 + 4\Delta)/2W$ are the Landau parameters that describe the residual quasiparticle interactions. The A's in Eq. (4) are dimensionless constants given in terms of $I_n = \sum_\mathbf{k} \cos^n(k_x)\delta(\varepsilon_\mathbf{k}/2W)$, with $\rho_0 = I_0$ and $\epsilon_0 = \mu/2W$. At shorter wavelengths $\omega_\mathbf{q} \simeq \varepsilon^b_\mathbf{q}$, we recover the dispersion

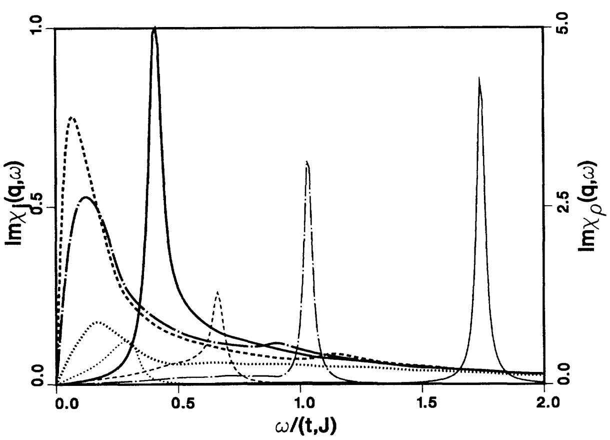

FIG. 1. The spectrum of density and transverse-current correlation functions in frequency units of t and J, respectively, at $J/t = 0.3$ and $\delta = 0.2$. The thick curves are the χ''_j at $\mathbf{q} = (\pi,\pi)$ (solid), $(1.0, 0.77)\pi$ (dashed), $(1.0, 0.83)\pi$ (dot-dashed), and $(2/3, 2/3)\pi$ (dotted). The light curves are the χ''_ρ at $\mathbf{q} = (\pi,\pi)$ (solid), $(2/3, 2/3)\pi$ (dot-dashed), $(1/2, 1/2)\pi$ (dashed), and $(1/6, 1/6)\pi$ (dotted).

of the slave bosons. The boson r_q represents this collective mode in the density channel. It describes the coherent propagation of charge excitations (holons [9]) in an infinite-U system.

The other important low-energy collective excitation is related to the phase fluctuation of the valence bond. The physical quantity in this case is the dynamical plaquette flux variable $\Phi_q = 2(\sin q_x/2)A_y(q) - 2(\sin q_y/2)A_x(q)$. It has been shown [10,11] that Φ is proportional to the local spin chirality $\mathscr{C}_i = \mathrm{Tr}[n_i(\mathbf{S}_{i+x} \cdot \mathbf{S}_{i+x+y} \times \mathbf{S}_{i+y})]$, where the trace means a cyclic permutation within a plaquette. The transverse current-current correlation function $\chi_j(\mathbf{q},\omega) = \langle \mathcal{J}_q \mathcal{J}_{-q} \rangle_{\mathrm{trans}}$ can be expressed as $\chi_j = (NW\Delta/J)^2 \langle \Phi_q \Phi_{-q} \rangle / \sin^2(q_\mu/2)$. The spectral function χ''_j is plotted in Fig. 1. We find that the interactions between the spins produce a particle-hole bound state at $Q = (\pi,\pi)$ just below the onset of continuum with a binding energy $E_b \simeq (16W/\pi)e^{-32W/\pi J + \mathrm{const}}$. This collective mode is an excited state with staggered spin chirality. As the wave vector q is reduced to the incommensurate values $(\pi, \pi - q_0)$, where q_0 is proportional to the hole concentration, the peak in χ''_j moves to lower energies and the gap in the spectrum vanishes. When the mode enters the particle-hole continuum at smaller wave vectors it gives rise to a large incoherent background which extends to very low energies (Fig. 1). The existence of low-energy excitations carrying staggered spin chirality is consistent with the findings of small-cluster simulations [6]. This feature should be observable in the current-current correlation function at *large* wave vectors. Unfortunately this regime is not easily accessible experimentally.

We now turn to the gauge-invariant one-particle Green's function of the electrons $G_{\mathrm{el}}(x,\tau) = -\langle T_\tau f_\sigma(x,\tau) b^\dagger(x,\tau) f^\dagger_\sigma(0,0) b(0,0) \rangle$. In the unitary gauge,

$$\begin{aligned} G_{\mathrm{el}}(x,\tau) &= b^2 G_{11}(x,\tau) + b\sqrt{N} G_{21}(x,\tau) \\ &\quad + b\sqrt{N} G_{12}(x,\tau) + N G_{22}(x,\tau), \\ G_{11} &= -\langle T_\tau f_\sigma(x,\tau) f^\dagger_\sigma(0,0) \rangle, \\ G_{21} &= G_{12} = -\langle T_\tau f_\sigma(x,\tau) r(x,\tau) f^\dagger_\sigma(0,0) \rangle, \\ G_{22} &= -\langle T_\tau f_\sigma(x,\tau) f^\dagger_\sigma(0,0) r(x,\tau) r(0,0) \rangle. \end{aligned} \tag{5}$$

G_{11} describes the propagation of quasiparticles. From a Fermi-liquid point of view, G_{21} and G_{12} describe residual hybridization of the quasiparticles and the incoherent part of the one-particle excitation spectrum. A charge excitation can propagate either as a quasiparticle or as a quasiparticle plus holon, which at large energies is a natural form of propagation in an infinite-U system. Since the quasiparticles carry relatively small energies but can take arbitrarily large momenta, the incoherent part of G_{el} depends rather weakly on momentum but extends over a large energy interval. The spectral function $A(\mathbf{k},\omega) = -2\,\mathrm{Im}G_{\mathrm{el}}(\mathbf{k},\omega)$ obeys the sum rule $\int d\omega A(\mathbf{k},\omega)/2\pi = [1 + (N-1)\delta]/2$, i.e., the total spectral weight is

$(1+\delta)/2$ in the physical limit $N=2$. This quantity is less than 1 since an amount of $(1-\delta)/2$ of the doubly occupied Hilbert space is pushed to infinity as $U\to\infty$. Our spectral function therefore describes the structure of the lower Hubbard band.

To calculate Eq. (5) it is important to isolate the diagrams of the perturbation theory that are irreducible with respect to the quasiparticle Green's function G_{11}. Because of the existence of G_{12} and G_{22} there are three irreducible self-energies Σ_n, Σ_a, and $\Sigma_{\rm inc}$ shown in Fig. 2. The electron Green's function is then expressed in terms of the self-energies as

$$G_{\rm el}(\mathbf{k},\omega)=\frac{N[b/\sqrt{N}+\Sigma_a(\mathbf{k},\omega)]^2}{\omega-\varepsilon_{\mathbf{k}}-\Sigma_n(\mathbf{k},\omega)}+\Sigma_{\rm inc}(\mathbf{k},\omega)\,. \quad (6)$$

The resummation (6) is exact irrespective of the value of N [12]. To evaluate the one-particle Green's function we insert in Eq. (6) the self-energies (shown in Fig. 2) calculated to order $1/N$ using the triangle microzone method with a 60×60-point discretization of the first Brillouin zone. The one-particle spectral function $A(\mathbf{k},\omega)$ is plotted in Fig. 3 for $\delta=0.2$, $J/t=0.3$, and $N=2$. The spectrum contains a quasiparticle peak of weight $\sim\delta$ with a dispersion characterized by its bandwidth $8(\Delta+t\delta/2)$ and a broad background extending over a scale of $2t$ which carries the bulk of the spectral weight of the valence band. The spectral function is very asymmetric for particlelike and holelike excitations. At positive frequencies the weight is rather small, $O(\delta)$, while at negative frequencies it is of order unity. Physically, this is due to the large on-site Coulomb repulsion U which makes it easier to add a hole than an electron to the system close to half filling. The incoherent background arises from $\Sigma_{\rm inc}$, Σ_a, and Σ_n. Their contributions can be estimated in the small-doping limit. The anomalous self-energy Σ_a ensures a cancellation of the order-unity spectral weight at positive frequencies while it adds up to the contributions from $\Sigma_{\rm inc}$ and Σ_n at negative frequencies to provide a background of area $(1-\delta)/2$. The total spectral weight is $(1+\delta)/2$ in agreement with the sum rule.

The hole part of the spectrum has a sharp edge $\omega_{\rm edge}$. As the quasiparticle peak disperses through the Fermi surface, the edge of the continuum moves to lower energies away from the Fermi level (see Fig. 3). This feature has been seen in exact diagonalization of small clusters of the t-J model by Stephan and Horsch [5]. In our model the position of the edge is given as $\omega_{\mathbf{k}}^{\rm edge}\simeq-\varepsilon_Q^b+\varepsilon_{\mathbf{k}+Q}$ with $q=Q=(\pi,\pi)$.

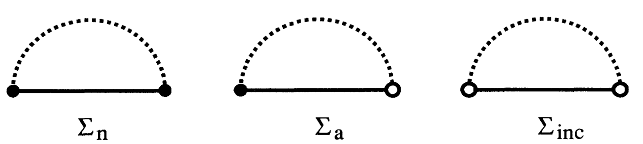

FIG. 2. The leading-order $1/N$ self-energies in Eq. (6). Solid lines: quasiparticle Green's function $G_0=(i\nu_n-\varepsilon_{\mathbf{k}})^{-1}$. Dashed lines: Bose propagators $D_{\alpha\beta}$. The solid circles represent the fermion-boson vertices and the open circles indicate that only the Bose field r enters with unity vertex.

It is useful to compare our findings with the description of the spectral function in the *weak* coupling of the Hubbard model [13]. In this case the spectral function has *dispersive* features which are shadows of the quasiparticles which would have existed if the spins had condensed in spin-density waves. In this case the quasiparticles are close to the center of an approximately symmetric band. We find that in the infinite-U limit the only dispersive features are in the edges of a band, which is extremely asymmetric for positive and negative energies. The quasiparticles sit very near the top of the position of the lower Hubbard band in the insulating limit.

The calculated integrated spectral function qualitatively agrees with the simple phenomenological model recently proposed by Matho [14]. However, his model does not incorporate the particle-hole asymmetry of the incoherent part of the spectrum. In addition, the edges of the quasiparticle band and the incoherent part of the spectrum do not coincide.

The role of the slave bosons in the Fermi-liquid phase is very different from that in the high-temperature regime where the bosons are not condensed, as originally envisioned by Anderson and Zou [15]. We have shown here that the bosons are responsible for the incoherent features in the spectrum and have a characteristic energy of order t. Nagaosa and Lee [10] have shown that in the high-temperature phase the bosons are coherent excitations with an energy scale J. They find that the integrated spectral function is given by $\Gamma(\omega)=\delta+\theta(-\omega)|\omega|/J$. The particle-hole asymmetry originates from the fact that when the bosons are not condensed the Bose spectral function is nonzero only at positive frequencies. In the Fermi-liquid phase we find that $\Gamma(\omega)=\delta+\theta(-\omega)|\omega|/t$. The asymmetry stems from the subtle cancellation be-

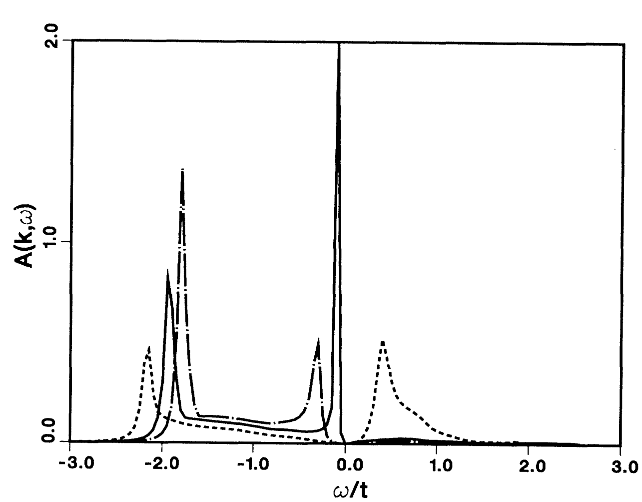

FIG. 3. The spectral functions for $J/t=0.3$ and $\delta=0.2$ at $\mathbf{k}=0.86(\pi/2,\pi/2)$ (solid curve), $\mathbf{k}=0.67(\pi/2,\pi/2)$ (dot-dashed curve), and $\mathbf{k}=1.2(\pi/2,\pi/2)$ (dashed curve).

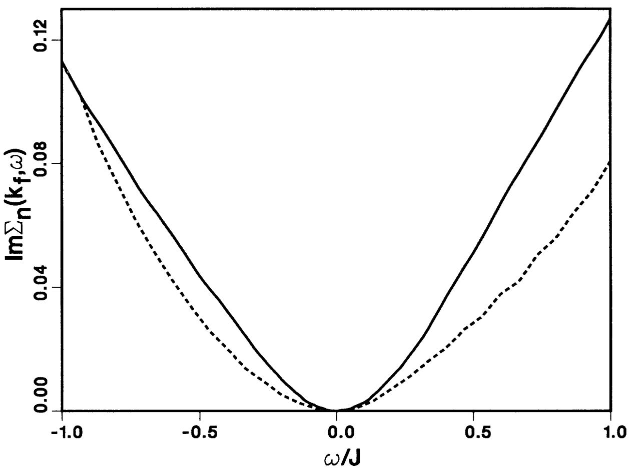

FIG. 4. The imaginary part of self-energy $\Sigma_n''(k,\omega)$ close to the Fermi energy for the t model (dashed line) and the t-J model (solid line) with $J/t=0.3$ at $\delta=0.2$.

tween the normal and anomalous diagrams. Therefore for energy scales smaller than the full bandwidth t, the linear part of the normal-state tunneling density of states is very small.

We conclude with a discussion of the low-energy behavior of the self-energy of the model. While J does not change the gross features of the lower Hubbard band it gives rise to low-lying spin chirality excitations found earlier. We find that the interaction of the quasiparticles with these excitations produces a low-energy scale ω_c in the t-J model above which $\mathrm{Im}\Sigma_n(\mathbf{k},\omega)\propto|\omega|$. The imaginary part of the quasiparticle self-energy Σ_n is plotted in Fig. 4 for $J=0$ and $J/t=0.3$ at 20% doping. In the large-U limit, the collective modes can be thought of as evolving continuously from the incoherent spectrum of the parent insulating state rather than as bound states of quasiparticle and quasihole pairs. The spin-liquid state which evolves smoothly into the Fermi-liquid state has low-lying chirality excitations with large wave vectors. Their characteristic energy scale ω_c is much smaller than J. A large-N estimation gives $\omega_c\approx J/\pi^2$. Upon doping, these modes interact with the single-particle excitations, which further reduces the scale of particle-hole excitations. As a result, the quasiparticles are strongly scattered causing anomalous damping above a scale on the order of ω_c. Notice that in this parameter range the system is close to an instability against spontaneous formation of incommensurate flux. This is a very subtle instability because it does not show any precursor effect in the spin-spin or density-density correlation function. Beyond this instability point there are many metastable states with very low energy. The uniform state minima, in this regime, are rather shallow and we expect non-Gaussian fluctuations to become more important in this region and to reduce even further the scale above which the departure from Fermi-liquid behavior emerges.

We would like to thank A. Ruckenstein, E. Abrahams, T. K. Lee, C. de Melo, S. Sachdev, and X. F. Wang for useful discussions. The support of NSF Grant No. DMR-8915895 is gratefully acknowledged.

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