Superconducting Gap for a Two-Leg *t*-*J* Ladder

Didier Poilblanc
Laboratoire de Physique Théorique CNRS-UMR5152, Université Paul Sabatier, F-31062 Toulouse, France

D. J. Scalapino
Physics Department, University of California, Santa Barbara, California 93106, USA

Sylvain Capponi
Department of Physics, Stanford University, Stanford, California 94305, USA,
and Laboratoire de Physique Théorique CNRS-UMR5152, Université Paul Sabatier, F-31062 Toulouse, France
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Single-particle diagonal and off-diagonal Green's functions of a two-leg *t*-*J* ladder at 1/8 doping are investigated by exact diagonalizations techniques. A numerically tractable expression for the superconducting gap is proposed and the frequency dependence of the real and imaginary parts of the gap are determined. The role of the low-energy gapped spin modes, whose energies are computed by a (one-step) contractor renormalization procedure, is discussed.

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In the BCS theory of superconductivity [1] the frequency and momentum dependence of the superconducting gap provide information about the frequency and momentum dependence of the pairing interaction [2]. In one spatial dimension quantum phase fluctuations destroy long-ranged superconducting (SC) order although the spectral gap is expected to survive [3]. In a doped two-leg spin ladder [4] the doped holes can form mobile singlet pairs [5] leading to dominant *algebraic* SC correlations [6] and a robust spin gap. In this Letter, motivated by previous work by two of the authors [7], we introduce a numerically tractable expression for the superconducting gap function which, as we argue, contains a nontrivial momentum and frequency dependence apart from an overall (vanishing in the thermodynamic limit) prefactor which accounts for 1D quantum phase fluctuations.

We shall consider here a generic two-leg *t*-*J* ladder,

$$\mathcal{H} = J_{\rm leg}\sum_{i,a}\vec{S}_{i,a}\cdot\vec{S}_{i+1,a} + J_{\rm rung}\sum_{i}\vec{S}_{i,1}\cdot\vec{S}_{i,2} + t_{\rm leg}\sum_{i,a}c^{\dagger}_{i,a}c_{i+1,a} + t_{\rm rung}\sum_{i}c^{\dagger}_{i,1}c_{i,2} + \text{H.c.}, \quad (1)$$

where $c_{i,a}$ are projected hole operators (spin indices are omitted) and $a(=1,2)$ labels the two legs of the ladder. Isotropic couplings, $t_{\rm leg} = t_{\rm rung} = t$ and $J_{\rm leg} = J_{\rm rung} = J$, will be of interest here. A value such as $J = 0.4$ (t is set to 1) and a doping of $\delta = 1/8$ are typical of superconducting ladder materials such as $Sr_{14-x}Ca_xCu_{24}O_{41}$ and these parameters will be assumed hereafter. Single-particle diagonal and off-diagonal spectral functions are computed by exact diagonalizations of $2\times L$ periodic ladders of size $L = 12$. The expression for the superconducting pairing function introduced previously in the context of the two-dimensional *t*-*J* model [7] is computed numerically from the knowledge of the diagonal and off-diagonal Green's functions of the doped two-leg ladder. The role of the low-energy collective triplet modes whose energies are obtained by a con trator renormalization [8,9] (CORE) calculation is investigated.

As established by numerical or bosonization techniques, in the parameter range considered here, the two-leg doped spin ladder exhibits dominant superconducting fluctuations [6] and its low-energy physics is governed by two (weakly gapped) collective spin modes (magnons), a gapped ($q_y = \pi$) charge mode, and a ($q_y = 0$) zero-energy collective charge mode [10–12] characteristic of a C1S0 phase of the Luther-Emery (LE) liquid universality class [13]. Prior to the investigation of spectral properties we have computed the lowest magnon excitations at hole density 1/8 on ladders with up to size 2×24 with $N_h = 6$ holes using an effective CORE Hamiltonian [9] as shown on Fig. 1(a). Our extrapolation gives a spin gap (for $q_y = \pi$) $\Delta^{\pi}_{\rm mag} \simeq 0.11$ significantly smaller than the spin gap $\sim J/2 = 0.2$ of the undoped spin ladder. On the other hand, the lowest $q_y = 0$ triplet (not shown) occurs at $\Delta^{0}_{\rm mag} \simeq 0.17$, close to the onset of the particle-hole continuum (discussed below).

We now turn to the investigation of the single-particle excitations. For a finite size system, it is convenient to define Green's functions so that the sets of electronlike (for $\omega < 0$) and holelike (for $\omega > 0$) poles coincide. The time-ordered diagonal Green's function is then defined as,

$$G(\mathbf{q},\omega) = \langle N|c^{\dagger}_{\mathbf{q},\sigma}\frac{1}{\omega - i\epsilon + H - \bar{E}_{N-1}}c_{\mathbf{q},\sigma}|N\rangle + \langle N-2|c_{\mathbf{q},\sigma}\frac{1}{\omega + i\epsilon - H + \bar{E}_{N-1}}c^{\dagger}_{\mathbf{q},\sigma}|N-2\rangle, \quad (2)$$

and the retarded one, $G_{\rm ret}(\mathbf{q},\omega)$, by the substitution $\omega + i\epsilon \to \omega - i\epsilon$ in the second term. ϵ is a small imaginary

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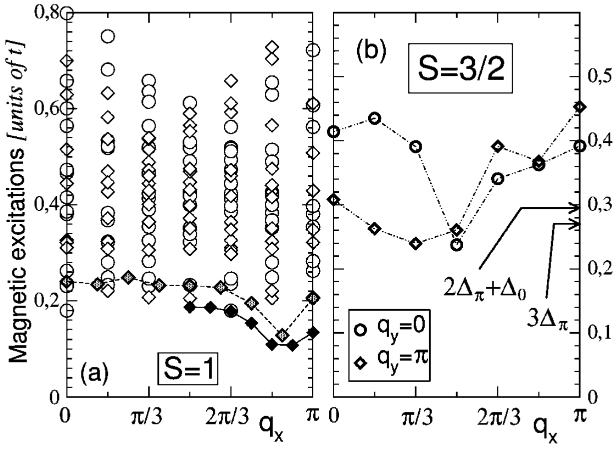

FIG. 1. Low-energy magnetic excitations at 1/8 doping and $J = 0.4$ for $q_y = 0$ (circles) and $q_y = \pi$ (diamonds) momenta. (a) Triplet collective mode obtained by CORE on 2×16 (shaded symbols) and 2×24 (solid symbols) ladders. The particle-hole continuum (open symbols) constructed from the data of Figs. 2 and 3 is also shown; (b) $S = 3/2$ excitations (measured from the chemical potential) calculated by ED of the 2×12 cluster. The onsets of the three quasiparticle continua are shown by arrows.

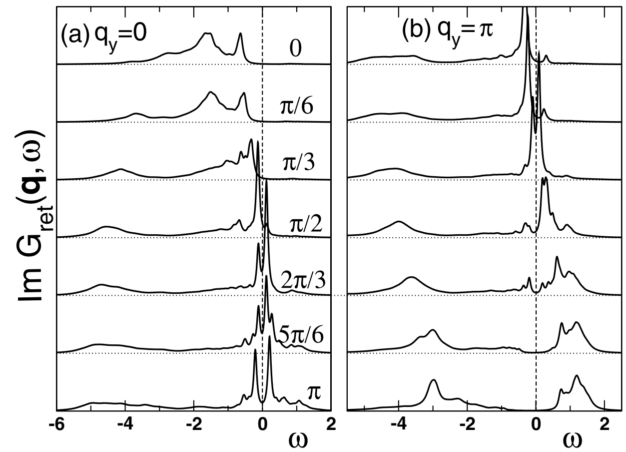

FIG. 2. Spectral function vs ω ($t = 1$) on a 2×12 ladder at 1/8 doping and $J = 0.4$ for two transverse momenta 0 and π in panels (a) and (b), respectively. Data for different chain momenta are shifted with respect to each other.

part set to 0.05 hereafter. Note that the "symmetrization" between ω and $-\omega$ implies using two ground states (GS) with particle numbers N and $N - 2$ surrounding the value $N - 1 = N_s - N_h$ corresponding to the actual hole density, i.e., here $N_h = 3$ holes on $N_s = 2L = 24$ sites. For convenience, the energy reference $\bar{E}_{N-1}$ is defined as the average between the GS energies of $|N\rangle$ and $|N-2\rangle$. $G(\mathbf{q}, \omega)$ and $G_{\rm ret}(\mathbf{q}, \omega)$ can be calculated using a standard continued-fraction method.

The data for the single-particle spectral function $A(\mathbf{q}, \omega) = -\frac{1}{\pi}{\rm Im}G_{\rm ret}(\mathbf{q},\omega)$ shown in Fig. 2 can be fairly well described by (i) BCS-like $q_y = 0$ (bonding) and $q_y = \pi$ (antibonding) quasiparticle bands with the chemical potential reference energy $\omega = 0$ and (ii) a broad incoherent background extending further away towards negative energies in agreement with a calculation on a smaller 2×8 cluster at the same hole density [14]. Note that the peaks of the low-energy bandlike features narrow near the chemical potential. Note also that the approximate Fermi momenta $(k_{F,1}, 0)$ which lies between $(5\pi/6, 0)$ and $(2\pi/3, 0)$ and $(k_{F,2}, \pi) \sim (\pi/3, \pi)$ are in rough agreement with Luttinger's theorem [15](which gives $k_{F1} + k_{F2} = 7\pi/8$). The low-energy peaks of $A(\mathbf{q}, \omega)$ plotted vs momentum in Fig. 3 exhibit BCS-like dispersions $\pm\sqrt{\tilde{\epsilon}^2_{(\mathbf{q})} + \Delta^2(\mathbf{q})}$ with the magnitudes of the gaps $\Delta(k_{F1}, 0) \equiv \Delta_0 \simeq 0.115$ and $\Delta(k_{F2}, \pi) \equiv \Delta_\pi \simeq 0.090$. Here, the solid points denote the maximum spectral weight and the open circles the BCS-like shadow band. Note that the particle-hole continuum can been obtained by considering all combinations of any two of the lowest single-particle excitations. Figures 1(a) and 1(b) give further evidence that bound triplet-hole pair excitations sits below this continuum [10].

The superconducting Gorkov's off-diagonal one-electron time-ordered Green's function [1] defined by

$$F(\mathbf{q}, t) = i\langle Tc_{-\mathbf{q},-\sigma}(t/2)c_{\mathbf{q},\sigma}(-t/2)\rangle, \qquad (3)$$

can be computed in a finite system by taking the expectation value between the two GS $|N\rangle$ and $|N-2\rangle$ differing by two particles, hence reflecting superconducting fluctuations. Note that these states are both spin singlets so that the (Fourier transformed in time) Green-function, $F(\mathbf{q}, \omega)$, is *even* in frequency and can be expressed as,

$$F(\mathbf{q}, \omega) = \tilde{F}_{\mathbf{q}}(\omega + i\epsilon) + \tilde{F}_{\mathbf{q}}(-\omega + i\epsilon), \qquad (4)$$

where

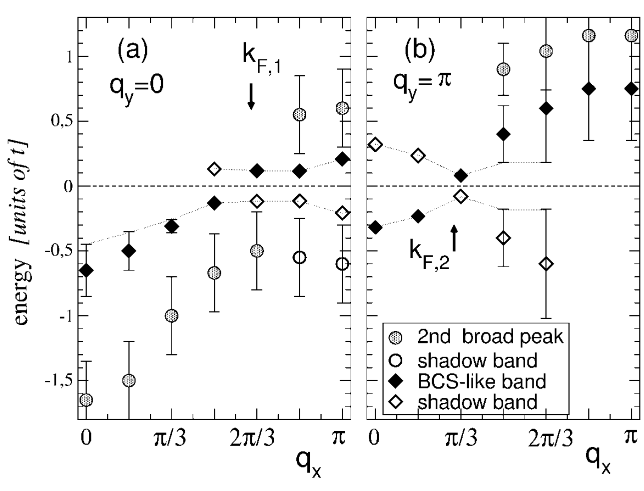

FIG. 3. Momentum dispersion of the low-energy peaks seen in Fig. 2. Error bars give the widths of the peaks (if any) and the dotted lines correspond to the lowest excitation energies.

$$\tilde{F}_{\mathbf{q}}(z) = \langle N-2|c_{-\mathbf{q},-\sigma}\frac{1}{z-H+\bar{E}_{N-1}}c_{\mathbf{q},\sigma}|N\rangle, \quad (5)$$

is defined for all complex z (with $\mathrm{Im}\, z \neq 0$). Following Ohta *et al.* [16] who extended the continued-fraction method to deal with off-diagonal Green's functions, we have computed $F(\mathbf{q}, \omega)$ on a 2×12 ladder at a hole density of 1/8 and for all momenta. Sharp low energies features are found near momenta $(k_{F,1}, 0)$ and $(k_{F,2}, \pi)$ as shown in Fig. 4. As the diagonal Green's function, the off-diagonal one is also gapped. The equal-time pair amplitude $\langle c_{-\mathbf{q},-\sigma}c_{\mathbf{q},\sigma}\rangle$ corresponding to the integrated weight $(1/2i\pi)\int_{-\infty}^{\infty} F(\mathbf{q}, \omega)\, d\omega$ is plotted in Fig. 5 showing maxima in the vicinity of the (estimated) Fermi momenta. Note also in Figs. 4 and 5 that the pair amplitudes have opposite signs for the two transverse momenta 0 and π, reminiscent of a two-dimensional (2D) d-wave orbital symmetry.

A long-ranged superconducting GS is characterized by a frequency-dependent gap function $\Delta_{\mathrm{SC}}(\mathbf{q}, \omega)$ directly proportional to $F(\mathbf{q}, \omega)$. A definition such as

$$\Delta_{\mathrm{SC}}(\mathbf{q}, \omega) = \frac{2\omega F(\mathbf{q}, \omega)}{G(\mathbf{q}, \omega) - G(\mathbf{q}, -\omega)}, \quad (6)$$

is consistent with Nambu-Eliashberg theory [1] as shown by two of the authors [7]. From a numerical calculation of $G(\mathbf{q}, \omega)$ and $F(\mathbf{q}, \omega)$, $\Delta_{\mathrm{SC}}(\mathbf{q}, \omega)$ has been obtained in a 2D t-J model [7], extending previous work by Ohta *et al.* [16] who fit the spectral weight $\mathrm{Im}F(\mathbf{q}, \omega)/\pi$ to a $d_{x^2-y^2}$ BCS-Bogoliubov quasiparticle form [1]. In contrast to a true SC state, a doped two-leg ladder (for parameters used here) exhibits long distance power law pair field correlations which decay as x^{-1/K_ρ}. Here K_ρ is the Luttinger liquid parameter associated with the massless charge mode. This implies [17] that for a ladder of length L, the off-diagonal Green's function $F(\mathbf{q}, \omega)$ decays as $(\xi/L)^{1/2K_\rho}$. Here the coherence length ξ is proportional to the inverse of the spin gap. Thus, we expect that $\Delta(\mathbf{q}, \omega)$ given by Eq. (6) will vary as $(\xi/L)^{1/2K_\rho}$. Using a CORE calculation supplemented by conformal invariance identities [9], we obtain, for $\delta = 1/8$ and $J = 0.4$, $\tilde{K}_\rho \simeq 0.65$ ($K_\rho = 2\tilde{K}_\rho$) in agreement with previous exact diagonalization (ED) evaluations [13] and density matrix renormalization group data [18]. We then expect the SC gap function $\Delta_{\mathrm{SC}}(\mathbf{q}, \omega)$ to vanish in the thermodynamic limit due to Cooper pair phase fluctuations. Indeed, using, e.g., a standard low-energy long-wavelength LE field theory, it can be shown that the SC Green's function decays with system size such as $(1/L)^{1/2K_\rho}$ due to SC phase fluctuations [17]. However, apart from this prefactor, $\Delta_{\mathrm{SC}}(\mathbf{q}, \omega)$ *calculated on a finite system* can provide information on the dynamics of pairing at intermediate distances.

In our case L/ξ is only of order 2 to 3 so that the scaling factor $(\xi/L)^{1/2K_\rho}$ is of order 1 and we will simply normalize [19] $\Delta_{\mathrm{SC}}(\mathbf{q}, \omega)$ so that $\Delta_{\mathrm{SC}}(k_{F1}, 0, \omega = 0) = 0.12t$ and $\Delta_{\mathrm{SC}}(k_{F2}, \pi, \omega = 0) = -0.09t$. Using this normalization, we have plotted the real and imaginary parts of $\Delta_{\mathrm{SC}}(\mathbf{q}, \omega)$ for the bonding $\mathbf{q} = (2\pi/3, 0)$ and antibonding $\mathbf{q} = (\pi/3, \pi)$ Fermi momenta in Fig. 6. As expected for a d-wave-like gap, the sign of the gap changes when one goes from $(k_{F1}, 0)$ to (k_{F2}, π). Otherwise, the frequency dependence of both the real and imaginary parts of the gap is quite similar. The imaginary part of the gap appears to onset at values of $\omega \sim \Delta_0 + \Delta_{\mathrm{mag}}^{\pi}$ where $\Delta_0 \sim 0.12$ is the superconducting gap and $\Delta_{\mathrm{mag}}^{\pi} \sim 0.11$ is the magnon gap. The imaginary part of the gap then increases until one passes through the particle-hole spectrum [10] and then decreases at yet higher energies. The real part of the gap increases slightly and then when ω increases

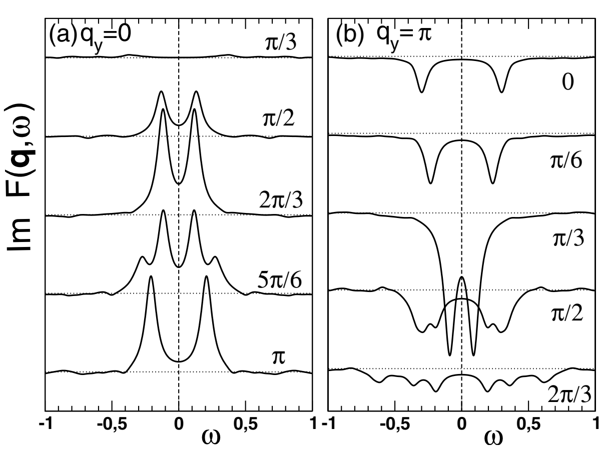

FIG. 4. Spectral weight of the superconducting Green's function. Same conventions as in Fig. 2. Note the change of sign between transverse momenta 0 and π.

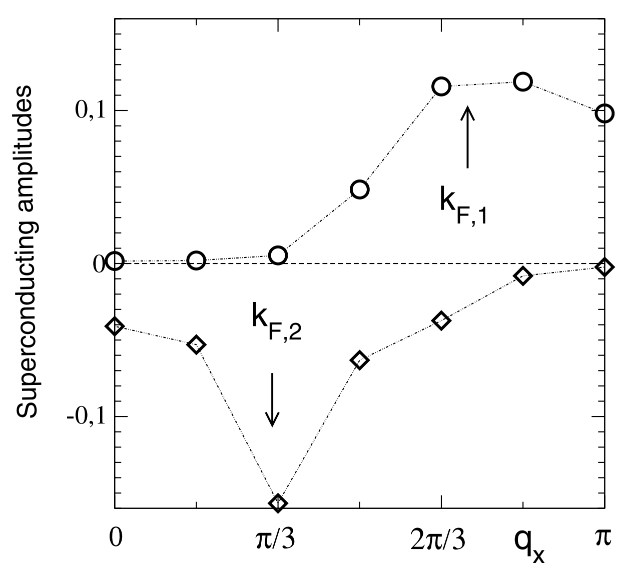

FIG. 5. Superconducting amplitude as a function of the chain momentum q_x for the bonding $q_y = 0$ (solid circles) and antibonding $q_y = \pi$ (open circles) transfer momenta.

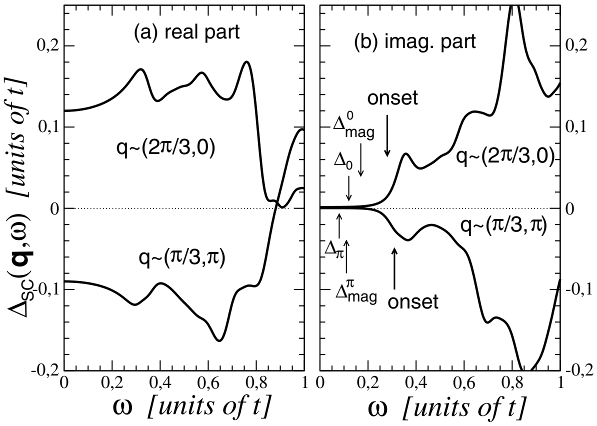

FIG. 6. Real (a) and imaginary (b) parts of the superconducting gap vs ω, normalization as discussed in the text, obtained by ED results for a 2×12 t-J ladder at the two bonding and antibonding Fermi momenta $(2\pi/3, 0)$ and $(\pi/3, \pi)$. An imaginary damping $\epsilon = 0.05$ is used and the irrelevant offset $F(0, 0) \propto i\epsilon$ has been subtracted.

beyond the electron-hole spectrum, the real part of the gap drops.

Thus, we believe that this approach to calculating $\Delta_{SC}(\mathbf{q}, \omega)$ allows one to probe the internal structure of a pair. Clearly, additional calculations, particularly for the two-leg Hubbard ladder will be of interest in providing further insight into the relationship between frequency dependence of the gap and the dynamics of the pairing interaction.

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