Superconducting gap for a two-leg tJ ladder

Didier Poilblanc
Laboratoire de Physique Théorique CNRS-FRE2603, Université Paul Sabatier, F-31062 Toulouse, France

D. J. Scalapino
Physics department, University of California, Santa Barbara, CA 93106

Sylvain Capponi
Department of Physics, Stanford University, Stanford, CA 94305 & Laboratoire de Physique Théorique CNRS-FRE2603, Université Paul Sabatier, F-31062 Toulouse, France

(Dated: May 8, 2019)

Single-particle diagonal and off-diagonal Green’s functions of a 2-leg t-J ladder at 1/8-doping are investigated by Exact Diagonalisations 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 are discussed.

PACS numbers: PACS numbers: 75.10.-b, 75.10.Jm, 75.40.Mg

In the BCS theory of superconductivity the frequency and momentum dependence of the superconducting gap provide information about the frequency and momentum dependence of the pairing interaction. In one spatial dimension quantum phase fluctuations destroy long-ranged SC order although the spectral gap is expected to survive. In a doped two-leg spin ladder the doped holes can form mobile singlet pairs leading to dominant algebraic SC correlations and a robust spin gap. In this Letter, motivated by previous work by two of the authors, we introduce a numerically tractable expression for the superconducting gap function which, as we argue, contains a non-trivial momentum dependence of the pairing interaction. In the BCS theory of superconductivity the frequency and momentum dependence of the superconducting gap are determined. The role of the low-energy gapped spin modes whose energies are computed by Exact Diagonalisations techniques, in the parameter range considered here, the 2-leg doped spin ladder exhibits dominant superconducting fluctuations and its low-energy physics is governed by

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 $2 \times 16$ (shaded symbols) and $2 \times 24$ (closed symbols) ladders. The particle-hole continuum (open symbols) constructed from the data of Figs. 2 & 3 is also shown; (b) $S = 3/2$ excitations (measured from the chemical potential) calculated by ED of the $2 \times 12$ cluster. The onsets of the 3-quasi-particle continua are shown by arrows.

where $c_{i,a}$ are projected hole operators and $a (\pm 1, 2)$ labels the two legs of the ladder. Isotropic couplings, $t_{leg} = t_{rung} = t$ and $J_{leg} = J_{rung} = J$, will be of interest here. A value like $J = 0.4$ ($t$ is set to 1) and a doping of $\delta = 1/8$ are typical of superconducting ladder materials such as Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ and these parameters will be assumed hereafter. Single-particle diagonal and off-diagonal spectral functions are computed by Exact Diagonalisations 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 tJ model is computed numerically from the knowledge of the diagonal and off-diagonal Green’s functions of the 2-leg ladder. The role of the low-energy collective triplet modes whose energies are obtained by a Contractor-Renormalisation (CORE) calculation is investigated.

As established by numerical or Bosonisation techniques, in the parameter range considered here, the 2-leg doped spin ladder exhibits dominant superconducting fluctuations 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 characteristic of a C150 phase of the Luther-Emery (LE) liquid universality class. 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 \times 24 with \(N_h = 6\) holes using an effective CORE hamiltonian as shown on Fig. 4(a). Our extrapolation gives a spin gap \((\Delta \approx 0.11)\) significantly smaller than the spin gap \(J / 2 = 0.2\) of the undoped spin ladder. On the other hand, the lowest \(q_y = 0\) triplet (not shown) occurs at \(\Delta^0 \approx 0.17\), 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 electron-like and hole-like quasi-particle bands with the chemical potential reference energy \(\omega = 0\) and \(\omega = \pi(\text{antibonding})\) quasi-particle bands with the chemical potential reference energy \(\omega = 0\) and \(\omega = \pi(\text{antibonding})\) quasi-particle bands. The data for the single-particle spectral function \(A(q, \omega) = -\frac{1}{\pi} \text{Im} G_{\text{ret}}(q, \omega)\) shown in Fig. 2 can be fairly well described by (i) BCS-like \(q_y = 0\) (bonding) and \(q_y = \pi\) (antibonding) quasi-particle 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 \(2 \times 8\) cluster at the same hole density. Note 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 which gives \(k_{F1} + k_{F2} = 7\pi/8\). The low-energy peaks of \(A(q, \omega)\) plotted vs momentum in Fig. 3 exhibit BCS-like dispersions \(\pm \sqrt{\epsilon^2(q) + \Delta^2(q)}\) 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 be obtained by considering all combinations of any two of the lowest single-particle excitations. Figs. 4(a) and 4(b) give further evidence that bound triplet-hole pair excitations sits below this continuum.

The superconducting Gorkov’s off-diagonal one-electron time-ordered Green’s function \(F(q, t)\) defined by

\[
F(q, t) = i \langle T c_{-q, \sigma}(t/2) c_{q, \sigma}(-t/2) \rangle ,
\]

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,
field correlations which decay as $x^{-1/Kρ}$. Here $K_ρ$ is the Luttinger liquid parameter associated with the massless charge mode. This implies \[16\] that for a ladder of length $L$, the off-diagonal Green’s function $F(q, ω)$ decays as $(ξ/L)^{1/2 Kρ}$. Here the coherence length $ξ$ is proportional to the inverse of the spin gap. Thus, we expect that $Δ(q, ω)$ given by Eq. \[6\] will vary as $(ξ/L)^{1/2 Kρ}$. Using a CORE calculation supplemented by conformal invariance identities \[8\], we obtain, for $δ = 1/8$ and $J = 0.4$, $K_ρ ≈ 0.65$ in agreement with previous ED evaluations \[12\] and DMRG data \[17\]. We then expect the SC gap function $Δ_{SC}(q, ω)$ 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 like $(1/L)^{3π8}$ due to SC phase fluctuations \[16\]. However, apart from this prefactor, $Δ_{SC}(q, ω)$ calculated on a finite system can provide informations 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 $(ξ/L)^{1/2 Kρ}$ is of order one and we will simply normalize $Δ_{SC}(q, ω)$ so that $Δ_{SC}(k_F1, 0, ω = 0) = 0.12t$ and $Δ_{SC}(k_F2, π, ω = 0) = −0.09t$. Using this normalization, we have plotted the real and imaginary parts of $Δ_{SC}(q, ω)$ for the bonding $q = (2π/3, 0)$ and antibonding $q = (π/3, π)$ Fermi momenta in Fig. \[4\]. 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 $ω ≈ Δ_0 + Δ_{mag}^π$ where $Δ_0 ≈ 0.12$ is the superconducting gap and $Δ_{mag}^π ≈ 0.11$ is the magnon gap. The imaginary part of the gap then increases until one passes through the particle-hole spectrum \[4\] and then decreases at yet higher energies. The real part of the gap increases slightly and then when $ω$ increases beyond the electron-hole spectrum, the real part of the gap drops.

Thus, we believe that this approach to calculating $Δ_{SC}(q, ω)$ allows one to probe the internal structure of a pair. Clearly, additional calculations, particularly for the 2-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.

**Acknowledgments**

D.J. Scalapino would like to acknowledge support from the US Department of Energy under Grant No DE-FG03-85ER45197. D. Poilblanc thanks M. Sigrist (ETH-Zürich) for discussions and aknowledges hospitality of the Physics Department (UC Santa Barbara) where part of this work was carried out. Numerical computations were done on the vector NEC-SX5 supercomputer at IDRIS (Paris, France). We thank E. Orignac for useful com-
Superconducting amplitudes

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.

0 0,2 0,4 0,6 0,8 1
-0,2
0 0,2 0,4 0,6 0,8 1
-0,2

\( -0,1 \)
0
0,1
0,2

FIG. 6: Real (a) and imaginary (b) parts of the superconducting gap vs \( \omega \), normalization as discussed in the text, obtained by ED results for a \( 2 \times 12 \) 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.

[1] J.R. Schrieffer, *Theory of Superconductivity* (Benjamin, NY 1964).
[2] J. Voit, *Eur. Phys. J. B* **5**, 505 (1998); F.H.L. Essler and A.M. Tsvelik, [cond-mat/0205294](https://arxiv.org/abs/cond-mat/0205294) (2002).
[3] E. Dagotto and T.M. Rice, *Science* **271**, 618 (1996).
[4] E. Dagotto, J. Riera, and D.J. Scalapino, *Phys. Rev. B* **45**, 5744 (1992).
[5] C. A. Hayward et al., *Phys. Rev. Lett.* **75**, 926 (1995).
[6] D. Poilblanc and D.J. Scalapino, *Phys. Rev. B* **66**, 052513 (2002).
[7] C. J. Morningstar and M. Weinstein, *Phys. Rev. D* **54**, 4131 (1996). For Hubbard models see E. Altman and A. Auerbach, *Phys. Rev. B* **65**, 104508 (2002).
[8] On the \( 2 \times 24 \) ladder, \( 2 \times 2 \) plaquette bosonic triplet and hole pair states are retained to construct a range 2 effective hamiltonian. On the \( 2 \times 16 \) ladder, additional one-hole fermionic plaquette states are also kept; S. Capponi and D. Poilblanc, *Phys. Rev. B* **66**, 180503 (2002).
[9] D. Poilblanc, D.J. Scalapino, and W. Hanke, *Phys. Rev. B* **52**, 6796 (1995); D. Poilblanc et al., *Phys. Rev. B* **62**, R14633 (2000).
[10] L. Balents and M.P.A. Fisher, *Phys. Rev. B* **53**, 12133 (1996) and references therein.
[11] The second charge mode is gapped.
[12] M. Troyer, H. Tsunetsugu, and T.M. Rice, *Phys. Rev. B* **53**, 251 (1996); C.A. Hayward and D. Poilblanc, *Phys. Rev. B* **53**, 11721 (1996).
[13] D. Poilblanc, J. Riera and E. Dagotto, *Eur. Phys. J. B* **7**, 53 (1999).
[14] P. Gagliardini, S. Haas, and T. M. Rice, *Phys. Rev. B* **58**, 9603 (1998).
[15] Y. Ohta, T. Shimozato, R. Eder, and S. Maekawa, *Phys. Rev. Lett.* **73**, 324 (1994).
[16] A bozonization calculation shows that \( \Delta(q,\omega) \) given by Eq. 6 factors into an \( L^{-1/2} e^{\rho} \) factor times a function of \( \omega \) and \( q \) which is independent of \( L \). E. Orignac and D. Poilblanc, [cond-mat/0303053](https://arxiv.org/abs/cond-mat/0303053).
[17] T. Siller, M. Troyer, T.M. Rice and S.R. White, *Phys. Rev. B* **63**, 195106 (2001).
[18] Strickly speaking, the gap should be defined at the gap edge so that, for example \( \Delta_{SC}(k_{F1},0,\omega = \Delta_0(k_{F1},0)) = \Delta_0(k_{F1},0) \). However, since \( \Delta_{SC}(q,\omega) \) is relatively flat out to energies of order \( \Delta_0 \), we have set \( \omega = 0 \).