Evolution of the Spin Gap Upon Doping a 2-Leg Ladder

D. Poilblanc\textsuperscript{a}\textsuperscript{*}, O. Chiappa\textsuperscript{a} and J. Riera\textsuperscript{b}\textsuperscript{†},
\textsuperscript{a}Laboratoire de Physique Quantique & UMR–CNRS 5626, Université Paul Sabatier, F-31062 Toulouse, France
\textsuperscript{b}Instituto de Física Rosario, Consejo Nacional de Investigaciones Científicas y Técnicas, y Departamento de Física, Universidad Nacional de Rosario, Avenida Pellegrini 250, 2000-Rosario, Argentina

S.R. White\textsuperscript{c}\textsuperscript{‡} and D.J. Scalapino\textsuperscript{d}\textsuperscript{§}
\textsuperscript{c}Department of Physics and Astronomy, University of California, Irvine, CA 92697
\textsuperscript{d}Department of Physics, University of California, Santa Barbara CA 93106
(November 17, 2021)

The evolution of the spin gap of a 2-leg ladder upon doping depends upon the nature of the lowest triplet excitations in a ladder with two holes. Here we study this evolution using various numerical techniques for a \(t-t’\)-\(J\) ladder as the next-near-neighbor hopping \(t’\) is varied. We find that depending on the value of \(t’\), the spin gap can evolve continuously or discontinuously and the lowest triplet state can correspond to a magnon, a bound magnon-hole-pair, or two separate quasi-particles. Previous experimental results on the superconducting two-leg ladder \(\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_2\text{O}_4\) are discussed.

PACS: 71.27.+a, 75.50.Ee, 71.10.-w, 75.40.Mg

Studies of strongly-correlated electrons confined to two-leg ladders and described by \(t-J\) and Hubbard models have provided important insights into the high \(T_c\) cuprate puzzle. These models are known to exhibit a gapped spin liquid state at half-filling and upon doping to evolve into a Luther-Emery state characterized by \(d_{x^2-y^2}\)-like pairing and \(4k_F\) CDW correlations. A key feature of the Luther-Emery state is the existence of a gap \(\Delta_S\) in the excitation energy of the spin degrees of freedom. If there is such a bound magnon-pair with energy \(\Delta_{MP}\), then it will set the spin gap in the doped ladder provided \(\Delta_{MP} < \Delta_M\). Such a scenario occurs e.g. in ladders with anisotropic Heisenberg ladder and near neighbor exchange interaction \(J\). However, as discussed by Tsunetsugu \textit{et. al}. \cite{5}, there can be a discontinuous evolution of the spin gap upon doping. In particular, they note that a pair can be dissociated into two charge \(|e|\) and spin \(S = 1/2\) quasi-particles, and the low-energy continuum for such scattering is set by the pair-binding energy \(\Delta_P\). Then, if the pair-binding energy is less than the half-filled spin gap (\(\Delta_P < \Delta_M\)), there will be a discontinuous decrease in the spin gap upon doping to a value equal to the pair-binding energy \(\Delta_P\). Thus, while there is still an \(S = 1\), \(K = (\pi, \pi)\) magnon excitation with energy \(\Delta_M\) in the infinitesimally doped ladder, if \(\Delta_M > \Delta_P\) a lower energy \(S = 1\) state exists in which a pair is dissociated into two quasi-particles.

There is a low energy continuum of excited states corresponding to two quasi-particles, each in an even parity \(k_y = 0\) state, which have a total momentum \((k_x, k_y) = (0, 0)\). Here \(k_y = 0\) for a bonding and \(\pi\) for an anti-bonding quasi-particle respectively. The singlet and triplet continua start at the same energy \(\Delta_P\). In addition to these scattering states, there can also be a bound \(S = 1\) state in which a bonding and an anti-bonding quasi-particle with momentum \(k_y = \pi\) hybridize with a magnon excitation of the spin background \[\text{[6]}.\]

If there is such a bound magnon-pair with energy \(\Delta_{MP}\), then it will set the spin gap in the doped ladder provided \(\Delta_{MP} < \Delta_M\). Such a scenario occurs e.g. in ladders with anisotropic Heisenberg ladder and near neighbor exchange interaction \(J\). The Hamiltonian for the \(t-t’-J\) ladder is

\begin{equation}
H = J \sum_{i,\lambda} \langle \tilde{S}_{i,\lambda} \cdot \tilde{S}_{i+1,\lambda} - \frac{1}{4} n_{i,\lambda} n_{i+1,\lambda} \rangle + \frac{1}{4} n_{i,1} n_{i,2}
+ t \sum_{i,\lambda,s} (c_{i,\lambda,s}^\dagger c_{i+1,\lambda,s} + h.c.) + t' \sum_{i,s} (c_{i,1,s}^\dagger c_{i+1,2,s} + h.c.)
+ \frac{1}{2} \sum_{i,s} (\Sigma_{s} c_{i,\lambda,s}^\dagger c_{i,\lambda,s} + h.c.),
\end{equation}

Here \(c_{i,\lambda,s}^\dagger\) creates an electron of spin \(s\) on site \(i\) of leg \(\lambda = 1\) or 2, \(\tilde{S}_{i,\lambda} = (c_{i,\lambda,s}^\dagger \tilde{\sigma}_{s,s'} c_{i,\lambda,s'})/2\) and \(n_{i,\lambda} = \Sigma_{s} c_{i,\lambda,s}^\dagger c_{i,\lambda,s}\). We have taken both the near-neighbor leg and rung one-electron hopping matrix elements equal to \(t\) and the diagonal next-near-neighbor term equal to \(t'\). The exchange interaction \(J\) is taken as isotropic between near-neighbor leg and rung sites and throughout this \(J/t = 0.5\).

We begin with our conclusions shown in Fig. 1(a)…
where we have plotted the excitation energies $\Delta E$ of various triplet states versus $t'$. The spin gap $\Delta_S$ of the two leg $t$-$t'$-$J$ ladder doped with two holes is defined as the difference between the ground state energies of the system with two holes and $S = 1$ and $S = 0$ respectively.

$$\Delta_S = E_0 (n_h = 2, S = 1) - E_0 (n_h = 0, S = 0). \quad (2)$$

The stars in Fig. 1(a) show $\Delta_S$ versus $t'/t$ obtained from DMRG results on $2 \times L$ ladders with $L = 32$. The dashed line is the DMRG result for the magnon excitation of the undoped ladder obtained from

$$\Delta_M = E_0 (n_h = 0, S = 1) - E_0 (n_h = 0, S = 0). \quad (3)$$

That this difference in ground state energies corresponds to the $(\pi, \pi)$ magnon is known from ED calculations in which the momentum of the excitation is specified. The open diamonds show the triplet excitation energy in the $K = (\pi, \pi)$ sector, obtained from a finite size scaling analysis using ED. Finally, the solid curve in Fig. 1 corresponds to the pair-binding energy calculated with DMRG from

$$\Delta_P = E_0 (n_h = 2, S = 0) + E_0 (n_h = 0, S = 0)$$

$$- 2E_0 \left( n_h = 1, S = \frac{1}{2} \right) \quad (4)$$

with $n_h$ the number of holes relative to the half-filled ladder (in agreement with the ED results for $t' = 0$ in Ref. [7]). As shown in Fig. 1(b), $\Delta_P$ sets the two quasi-particle continuum. Here infinite size extrapolated ED results for the lowest energy excited singlet and triplet states in the $K = (0, 0)$ sector are plotted as open symbols and the solid circles are DMRG data for the pair-binding energy $\Delta_P$, Eq. (4). These energies are in good agreement, consistent with a picture in which a pair dissociates into two quasi-particles.

As discussed below, we have used ED, in which the momentum of the state can be specified, as well as DMRG calculations of the hole and spin correlations in order to interpret the results shown in Fig. 1(a). Here we summarize what these show. Basically, there are three different regimes set by $t'/t$. For $-0.5 < t'/t < -0.2$, the discontinuous drop in the spin gap with doping reflects the fact that the pair binding energy $\Delta_P$ is less than the $(\pi, \pi)$ magnon energy $\Delta_M$ of the undoped ladder. Thus, when the system is doped, a singlet pair can dissociate into two separate quasi-particles with total spin $S = 1$, reducing the spin gap $\Delta_S$ from $\Delta_M$ to $\Delta_P$. In this region, there is a bound magnon-hole pair with a minimum energy at $(\pi, \pi)$ but its energy $\Delta_{MP}$ is larger than $\Delta_P$ so that the spin gap is set by $\Delta_P$. In the region $-0.2 \leq t'/t \leq 0.35$, the situation changes. The pair binding energy $\Delta_P$ becomes greater than the energy to create a bound magnon-hole pair $\Delta_{MP}$, but $\Delta_{MP}$ is less than the energy to create a separate magnon $\Delta_M$. Thus, in this parameter region the lowest energy triplet state of the 2-hole doped ladder has momentum $(\pi, \pi)$ and corresponds to a bound magnon-hole pair so that $\Delta_S = \Delta_{MP}$. Finally, for $0.35 < t'/t < 0.5$, the energy of the triplet $K = (\pi, \pi)$ excitation becomes equal to the $S = 1$ magnon energy of the undoped ladder. Here DMRG calculations of the spin and charge correlations show that the excitation corresponds to a magnon which is uncorrelated with the bound singlet pair. Thus, in this region, there is no discontinuity in the spin gap upon doping.

ED calculations were carried out on $2 \times L$ ladders with $L$ an odd number of sites. Both periodic and anti-periodic boundary conditions for $L$ up to 13 were used [10]. In Fig. 2 we show results for the triplet excitation energies in the $K = (\pi, \pi)$ sector for a sequence of $2 \times L$ ladders with 2 holes for various values of $t'$. Here the excitation energy is measured relative to the 2-hole $K = (0, 0)$ ground state. The lowest triplet $K = (\pi, \pi)$ state is found to be separated from a quasi-continuum of higher energy states. In Fig. 2, the error bars mark the difference between the results obtained using periodic and anti-periodic boundary conditions with the open symbols marking the mean value. Since the actual longitudinal momentum for a finite ladder is $\pi (1 - 1/L)$, we have extrapolated these results using a scaling form $A + B/L + c/L^2$. The solid symbols denote the DMRG calculation of the spin gap $\Delta_S$, Eq. (2), for an open $2 \times 32$ ladder with 2 holes (larger lattices are also included for $t' = 0$). For $-0.2 \leq t'/t \leq 0.5$, the extrapo-
lated ED results for the \( K = (\pi, \pi) \) triplet pass through the DMRG spin gap \( \Delta_S \). However, for \( t' = -0.5 \), the DMRG determined spin gap lays well below the extrapolated \( K = (\pi, \pi) \) triplet. As discussed in the introduction, for \(-0.2 \leq t'\), the spin gap is set by the excitation in the triplet \( K = (\pi, \pi) \) sector. However, for \( t' \lesssim -0.2 \), the spin gap is set by the onset of the two quasi-particle continuum \( \Delta_P \) which goes to zero as \( t' \) approaches \(-0.5\). Note that, even when \( \Delta_S < \Delta_{MP} \), the magnon-hole pair state could still be locally stable if the decay process into 2 quasi-particles with the same momentum \((\pi, \pi)\) is impossible. Although the ED results approach the \( K = (\pi, \pi) \) magnon energy of the undoped ladder for \( t' > 0.35 \), DMRG results show that the character of the triplet excitation changes from a bound magnon-hole-pair to a separate magnon and hole-pair state. Thus, in this regime, the spin gap is set by the excitation energy of the magnon \( \Delta_M \) and is therefore continuous upon doping.

FIG. 2. A finite-size scaling analysis of the lowest triplet eigenenergies of a \( 2 \times L \) ladder with 2 holes in the \( K = (\pi, \pi) \) sector measured with respect to the \( K = (0,0) \) ground state singlet for various values of \( t' \). The open symbols are ED data obtained on closed ladders up to \( 2 \times 13 \) in size. The mean value between periodic and antiperiodic boundary conditions is denoted by the open symbols. The error bars are given by the energy difference between the two boundary conditions. The full symbols are DMRG results for the spin gap \( \Delta_S \) defined by Eq. (2).

In order to get a clearer picture of the nature of the triplet excitations which determine the spin gap, we have used DMRG results to study the spin and hole correlations in these states. In Fig. 3 a center section of a \( 2 \times 32 \) ladder with \( t' = 0 \) is shown. The upper and middle diagrams show the probability of finding the second hole when the first hole is projected out at the center of the upper leg for the singlet and triplet state respectively. In both of these states, the two holes are bound and the most probable configuration for \( J/t = 0.5 \) corresponds to having the holes on diagonal sites. Note that the triplet-bound state is more extended than the singlet bound state. The lowest diagram shows the spin distribution for the \( S_z = 1 \) triplet state when the two holes are projected out at their most probable sites. It is clear that this state is a bound magnon-hole pair.

FIG. 3. Structure of the ground state and the lowest energy triplet state of a 2-leg ladder with 2 holes and \( t' = 0 \). In the top and middle diagrams, the diameter of the black circles is proportional to the probability of finding the second hole when one hole is projected out at the center of the upper leg for the ground singlet and lowest energy triplet states respectively. Note that the triplet state is more extended than the singlet bound state. The bottom diagram provides the spin distribution in the triplet state.

Similar calculations for \( t' = -0.5 \) show that in the triplet state the two holes are unbound while for \( t' = 0.5 \) the two holes are bound into a singlet and uncorrelated with the spin 1 excitation. This behavior is shown in Fig. 4, where we have plotted

\[
\langle S_z(\ell_x) \rangle \equiv \langle S_z(\ell_x,1)P_h(i)P_h(j) \rangle / \langle P_h(i)P_h(j) \rangle \tag{5}
\]

versus \( \ell_x \) for \( t' = 0, -0.5, \) and 0.5. Here \( P_h(i) \) is the projection operator for a hole at the \( i \)th site. For \( t' = 0 \), we have set \( i = (16,2) \) and \( j = (17,1) \), corresponding to the most probable hole location. Here, as previously illustrated in Fig. 3, we see that the spin is bound to the hole-pair. For \( t' = 0.5 \) we again have a situation where the holes are most likely to sit close to each other, and here we have projected them onto \( i = (16,1) \) and \( j = (16,2) \). However, in this case, the spin 1 is spread out corresponding to a magnon which is not bound to the hole-pair. Finally, for \( t' = -0.5 \), one finds that the lowest energy triplet excitation corresponds to two separate quasi-particles.
We finish with a brief discussion of some experimental results for the superconducting two-leg doped ladder Sr$_2$Ca$_2$Cu$_{24}$O$_{41}$ [12]. Nuclear magnetic resonance measurements of the copper-63 Knight shift and relaxation time $T_1$ suggest a collapse of the spin gap with pressure. We believe this signals the appearance of new low lying triplet excitations upon doping the ladder planes and points towards a negative value of $t'$ [3]. In this regime, due to the presence of a low-energy quasi-particle continuum located predominantly around the zone center, momentum-resolved experiments like inelastic neutron scattering would be essential to search for sharp finite energy triplet excitations.

![Graph](attachment:image.png)

FIG. 4. Here, for three different values of $t'$ we show $\langle S_z(\ell_x) \rangle$ (as defined by Eq. (3)) versus $\ell_x$. For $t' = 0$, we take $i = (16, 2)$, and $j = (17, 1)$, one of the most probable locations for the two holes, and one sees that a magnon is tightly bound to the hole pair. For $t' = 0.5$, we have $i = (16, 1)$ and $j = (16, 2)$, also one of the most probable locations for the holes. Here we see a magnon which is not bound to the hole pair. For $t' = -0.5$, in order to illustrate how separate $S = 1/2$ spins are bound to each hole, we plot $\langle S_z(\ell_x) \rangle$ with $i = (8, 1)$ and $j = (25, 1)$.

To summarize, using ED and DMRG calculations, we have found that the spin gap can evolve in different ways when two holes are doped into a 2-leg ladder. When the 2 holes are added, it is possible that the lowest energy triplet state simply remains the $K = (\pi, \pi)$ magnon so that there is no change in $\Delta_S$. In this case the 2 added holes remain in a bound $d_{x^2-y^2}$-like singlet state and a triplet magnon similar to that of an undoped ladder is created. As the length of the ladder increases, the interaction between these two entities becomes negligible. We see this happening for $t' \gtrsim 0.35$. It is also possible that the lowest energy triplet state has $K = (0, 0)$ and is set by the two-quasi-particle continuum corresponding to the pair-binding energy $\Delta_P$. In this case, there is a discontinuous change in the spin gap upon doping and the lowest energy triplet state arises from the dissociation of a pair into two quasi-particles. We see this for the present model when $t' \lesssim -0.2$. Finally, for the intermediate region $-0.2 \lesssim t' \lesssim 0.35$ we find that the lowest energy triplet state has $K = (\pi, \pi)$ and corresponds to a bound magnon-hole pair with energy $\Delta_{MP} < \Delta_M$. In this case, there is again a discontinuous evolution in the spin gap from $\Delta_M$ to $\Delta_{MP}$ upon doping.

We would like to acknowledge useful discussions with Ian Affleck. S.R. White and D.J. Scalapino acknowledge support from the NSF under grant # DMR98-70930 and grant # DMR98-17242 respectively. D. Poilblanc thanks IDRIS (Paris) for allocation of CPU time on the NEC SX5 supercomputers.

[1] E. Dagotto and T.M. Rice, Science, 271, 618 (1996); E. Dagotto, J. Riera, and D.J. Scalapino, Phys. Rev. B, 45, 5744 (1992); T. Barnes, E. Dagotto, J. Riera and E. S. Swanson, Phys. Rev. B, 47, 3196 (1993); T.M. Rice, S. Gepalan, and M. Sigrist, Europhys. Lett., 23, 445 (1993).
[2] C. A. Hayward et al., Phys. Rev. Lett. 75, 926 (1995).
[3] H. Tsumetsugu, M. Troyer, and T.M. Rice, Phys. Rev. B, 49, 16078 (1994).
[4] M. Troyer, H. Tsumetsugu, and T.M. Rice, Phys. Rev. B, 53, 251 (1996).
[5] H.H. Lin, L. Balents, and M.P.A. Fisher, Phys. Rev. B, 58, 1794 (1998).
[6] In fact the global stability of the magnon-hole pair can be inferred from the positiveness of its binding energy defined by $\Delta_{bind} = \min \{\Delta_P, \Delta_M\} - \Delta_{MP}$.
[7] J. Riera, D. Poilblanc and E. Dagotto, Eur. Phys. J. B 7, 53 (1999).
[8] C.A. Hayward and D. Poilblanc, Phys. Rev. B, 53, 11721 (1996); D. Poilblanc, D.J. Scalapino, and W. Hanke, Phys. Rev. B, 52, 6796 (1995).
[9] S.R. White, Phys. Rev. B, 48, 10345 (1993).
[10] For details on the role of the parity of the ladder length see Ref. [1].
[11] S.R. White and D.J. Scalapino, Phys. Rev. B, 55, 6504 (1997).
[12] H. Mayaffre et al., Science 279, 345 (1998) and references therein.
[13] $t'/t \simeq -0.35$ has been suggested for the 2D high-$T_C$ cuprates. See e.g. C. Kim et al., Phys. Rev. Lett. 80, 425 (1998).