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Pairing and excitation spectrum in doped t-J ladders

Hirokazu Tsunetsugu
Theoretische Physik, Eidgenössische Technische Hochschule, 8093 Zürich, Switzerland
and Interdisziplinäres Projektzentrum für Supercomputing, ETH-Zentrum, 8092 Zürich, Switzerland

Matthias Troyer
Theoretische Physik, Eidgenössische Technische Hochschule, 8093 Zürich, Switzerland;
Interdisziplinäres Projektzentrum für Supercomputing, ETH-Zentrum, 8092 Zürich, Switzerland;
and Centro Svizzero di Calcolo Scientifico, 6924 Manno, Switzerland

T. M. Rice
Theoretische Physik, Eidgenössische Technische Hochschule, 8093 Zürich, Switzerland
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Exact-diagonalization studies for a doped t-J ladder (or double chain) show hole pairing in the ground state. The excitation spectrum separates into a limited number of quasiparticles which carry charge $+|e|$ and spin $\frac{1}{2}$ and a triplet mode. At half-filling the former vanish but the latter evolves continuously into the triplet band of the spin liquid. At low doping the quasiparticles form a dilute Fermi gas with a strong attraction but simultaneously the Fermi wave vector, as would be measured in photoemission, is large.

The properties of strongly correlated electrons confined to a ladder (or double chain) and described by t-J or Hubbard models have been the subject of intensive investigation recently.[1–6] The reason lies in the unusual spin-liquid nature of the undoped parent system.[1,7,8] The key question is the evolution of the finite gap in the spin excitation spectrum upon doping. The spin gap remains in other spin liquids systems and is a sign of strong superconducting fluctuations.[9,10] A recent analysis of the t-J ladder using a mean-field (MF) theory with Gutzwiller renormalization of the matrix elements to account for the strong correlations, gave a continuous evolution of the spin gap with doping.[3] The short-range resonance-valence-bond (RVB) state evolves into a superconductor with modified d-wave symmetry within this MF theory for the t-J ladder. A tendency towards modified d-wave superconductivity was also found in a renormalization group calculation[6] and in a very recent numerical study of the Hubbard ladder although no actual enhancement of the superconducting correlations was reported.[4] In this paper we report on the properties of finite t-J ladders up to a size of 10×2 sites using a Lanczos diagonalization method. We find results which give clear evidence of hole pairing and a modified d-wave RVB state in lightly doped systems in agreement with the MF theory. An interesting difference however is the discontinuous evolution of the excitation spectrum upon doping. Upon doping new quasiparticle (QP) excitations appear carrying both charge and spin. These excitations are in addition to a band of spin triplets which evolve continuously away from the undoped spin liquid. This separation of the excitation spectrum into bound holon-spinon QP's and collective triplet excitation contrasts with the full spin-charge separation found in a Luttinger liquid.

Another reason for special interest is the possibility of realizing a lattice of weakly coupled ladders in the compounds $SrCu_2O_3$ (Ref. 11) and also $(V\,O)_2P_2O_7$.[12] In the first case the ladders are isotropic with equal hopping matrix elements and exchange couplings along rungs and legs and we concentrate on this case.

The t-J ladder we will study reads

$$\begin{aligned}\mathcal{H} = -t\sum_{j,\sigma}\Bigg[\Bigg(\sum_{a=1}^{2} c^{\dagger}_{a\sigma}(j)c_{a\sigma}(j{+}1) \\ +c^{\dagger}_{1\sigma}(j)c_{2\sigma}(j)\Bigg) + \text{H.c.}\Bigg] \\ +J\sum_{j,a}[\mathbf{S}_a(j)\cdot\mathbf{S}_a(j{+}1) - \tfrac{1}{4}n_a(j)n_a(j{+}1)] \\ +J'\sum_{j}[\mathbf{S}_1(j)\cdot\mathbf{S}_2(j) - \tfrac{1}{4}n_1(j)n_2(j)],\end{aligned} \tag{1}$$

where j runs over L rungs, and σ $(=\uparrow,\downarrow)$ and a $(=1,2)$ are spin and leg indices. We take $t = 1$ as the energy units. The first term is the kinetic energy and the J (J') are exchange couplings along the ladder (rungs). The local constraint excludes double occupancy at every site $[n_{a\uparrow}(j)n_{a\downarrow}(j) = 0]$. Although the isotropic case $J' = J$ is of most interest, we study also the limit of $J' \gg J, 1$, which can be easily understood and is a good starting point to trace back to the isotropic case. Periodic or antiperiodic boundary conditions (PBC, APBC) are used along the ladder and then the wave vector $\mathbf{k} = (k_x, k_y)$ is well defined, k_x (k_y) are along the ladder (rungs).

To begin we summarize the properties of spin excitations at half-filling. In this case (1) reduces to the Heisenberg spin ladder (aside from a constant). Several different approaches have shown it has a spin-liquid ground state with a finite excitation gap.[1,7,8] In the limit of $J' \to \infty$, the ground state is an ensemble of singlet rungs and the total spin is trivially $S = 0$. Low-lying excitations are Bloch states of one triplet with energy $J' + J\cos k_x$, and have a minimum at $k_x = \pi$. With decreasing J'/J, the

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dispersion becomes more linear with a smaller gap, but at $J' = J$ the gap remains finite ($\Delta_{\rm spin} = 0.5J$).

The first evidence of enhanced superconducting fluctuations in the t-J ladder is the formation of a bound pair of two holes doped into half-filling. The ground state wave function is calculated by the Lanczos method up to $L = 10$ and found to have $S = 0$ and $\mathbf{k} = (0,0)$. The two holes have a positive binding energy defined by $E_B \equiv 2E_{\rm g.s.}(2L-1) - E_{\rm g.s.}(2L) - E_{\rm g.s.}(2L-2)$, where $E_{\rm g.s.}(N)$ denotes the ground-state energy for N electrons. In Fig. 1, we show E_B for $L = 8$ and $J = 0.3$ as a function of the rung exchange, J'. The binding energy is positive down to the isotropic value, $J' = J = 0.3$ appropriate for a cuprate. The same calculation for four holes indicates no phase separation up to the largest value $J' = 3.0$.

In the limit of strong rung coupling $J' \gg J, 1$, this binding can be easily understood. At half-filling every rung forms a spin singlet. A single hole breaks a singlet so the second hole is attracted to the same rung to avoid breaking another singlet bond. The binding energy is therefore $E_B \sim J' - 2$ asymptotically.

The hole binding in the ground state is also seen directly in the hole-hole correlation function, $\langle n_{ah}(j) n_{a'h}(j')\rangle$ [$n_{ah}(j) \equiv 1 - n_a(j)$: hole density]. We calculated the size of the bound hole pair ξ by fitting $\langle n_{1h}(i) n_{2h}(j)\rangle \sim$ const. $\times$ $(e^{-|i-j|/\xi} + e^{-(L-|i-j|)/\xi})$ for $|i-j| = \frac{L}{2}$ and $\frac{L}{2} - 1$. The results are shown in the inset of Fig. 1 for $L = 6, 8$, and 10. In the strong coupling limit $J' \gg J, 1$, the two holes are confined to the same rung and $\xi \to 0$. The size of the bound hole pair increases with decreasing J', but is still quite short, $\xi \approx 2$, even for isotropic coupling $J' = 0.3$. Note at this value, the hole-hole correlation is maximum for holes on neighboring rungs, i.e., $\langle n_{1h}(j) n_{2h}(j+1)\rangle$.

One of the most interesting properties of the t-J ladder is that there are two distinct types of spin excitations upon doping. Let us start from the large J' limit, where they are easily distinguished. The first is the triplet excitation similar to that at half-filling and arises when a singlet rung away from the hole pair is excited to a triplet. The triplet propagates along the ladder with the matrix element $\frac{J}{2}$, and can also pass through the hole pair. For the second type of spin excitation, the presence of the holes is essential. The bound hole pair in the ground state dissociates into two separate holons, each of which is now bound to a spinon on the same rung to form a QP with charge $+|e|$ and spin $\frac{1}{2}$.[13] In this sense, these holon-spinon bound pairs are similar to QP's in conventional Fermi liquids.

The energies and allowed numbers of the two types of spin excitations are different. The triplet can be excited only at the rungs without holes, whereas the second type needs a hole. Therefore the number of possible excitations is proportional to $(1-\delta)$ and δ, respectively, where δ is the hole doping.

The second type of spin excitations have lower energies in the large J' region as follows. For both types at least two singlets have to be broken with energy cost J', but their kinetic energies differ. In the first type, rungs are occupied by a hole pair and by a triplet. The hole pair and the triplet move independently along the ladder with the matrix elements $(J' - \frac{4}{J'})^{-1}$ and $\frac{J}{2}$, respectively. In the second type, two rungs are occupied by only one electron in a bonding orbital with kinetic energy gain (-2). These singly occupied rungs move with the matrix element $\frac{1}{2}$. Therefore the total gain of kinetic energy is much larger for the second type when $J' \gg 1, J$. Accordingly the lowest spin triplet excitation is of the second type as shown in Fig. 1, and $\Delta_{\rm spin} \sim E_B$. With decreasing J', the two excitations become closer to each other in energy.

The different characters of the two types of excitations are clearly distinguished by the hole-hole and spin-hole correlation functions. Figure 2 shows the correlation functions calculated by the Lanczos method for the two excitations with $S^z = 1$ for $J = 0.3$ and $J' = 0.3$, and 3.0. In the QP excitation (dotted line), the hole-hole correlation is maximum for the longest separation, but for

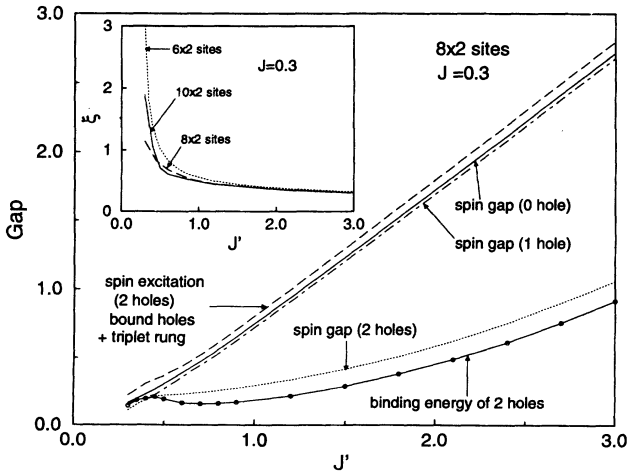

FIG. 1. Binding energy of two holes, spin gap, and energy of the triplet excitation away from the bound hole pair. Inset shows the size of the bound hole pair for the ground state.

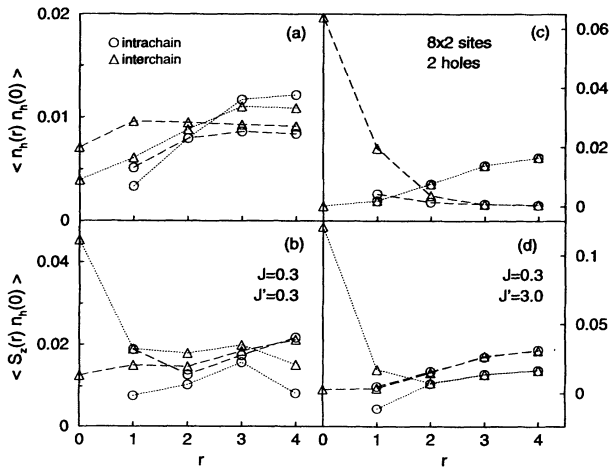

FIG. 2. Hole-hole [(a),(c)] and spin-hole [(b),(d)] correlation functions for the two triplet states. Dotted lines are for the lowest triplet state (QP excitation) and dashed lines are for the triplet state with a bound pair.

the spin-hole correlations on the same rung. This tendency is obvious for the large rung coupling $J' = 3.0$, but still holds down to the isotropic value $J' = 0.3$. For the other excitations (dashed line), at $J' = 3.0$ the two holes are strongly bound on the same rung and repel the triplet. With decreasing J', the hole pair becomes more extended as in the singlet ground state. The most dominant configuration at $J' = 0.3$ is that the two holes are in the neighboring rungs and different legs.

The two types of excitations have different contributions to the spin susceptibility and structure factor,

$$\mathcal{S}(\mathbf{k},\omega) \equiv \sum_{\alpha} \left|\langle \alpha | S^{+}_{\mathbf{k}} | \text{g.s.}\rangle\right|^2 \delta(\omega - E_\alpha + E_{\text{g.s.}}). \quad (2)$$

Here $|\alpha\rangle$ and $|\text{g.s.}\rangle$ denote an $S = 1$ eigenstate and the ground state with energies E_α and $E_{\text{g.s.}}$. As was discussed before the spin excitations with separate holes have lower energies. However at $\delta \ll 1$, their number is smaller ($\propto \delta$) than the excitations with the bound hole pairs and triplet rungs ($\propto 1 - \delta$). Therefore with decreasing temperature the susceptibility will show a large exponential drop at $T \sim J'$ and a smaller drop further at $T \sim \Delta_{\text{spin}}$, corresponding to the different excitation energies. Figure 3 shows the structure factor, $\mathcal{S}(\mathbf{k},\omega)$, for two holes in 8×2 sites. Large peaks are seen around $\mathbf{k} = (\pi,\pi)$ and the energy of the order of J'. These are due to the excitations away from bound hole pairs. On the other hand, the QP excitations do not have large weights in spite of their lower excitation energies, because of the change in the charge configuration from the ground state. This point would be important when comparing to neutron scattering experiments.

Finally we discuss the one-particle Green's function where we can see QP excitations directly. By using the Lanczos method combined with a continued fraction method, we calculate the spectral function for two holes. The electron and hole parts of the spectral function are defined as

$$\begin{aligned} A_e(\mathbf{k},\omega) \equiv & \sum_{\alpha} |\langle \alpha, 2L-1 | c^{\dagger}_{\mathbf{k}\sigma} | \text{g.s.}, 2L-2\rangle|^2 \\ & \times \delta(\omega - E_\alpha(2L-1) + E_{\text{g.s.}}(2L-2) + \mu), \\ A_h(\mathbf{k},\omega) \equiv & \sum_{\alpha} |\langle \alpha, 2L-3 | c_{\mathbf{k}\sigma} | \text{g.s.}, 2L-2\rangle|^2 \\ & \times \delta(\omega + E_\alpha(2L-3) - E_{\text{g.s.}}(2L-2) + \mu), \end{aligned} \quad (3)$$

where $|\alpha, N\rangle$ is an eigenstate for N electrons with the energy $E_\alpha(N)$ and g.s. denotes the ground state. Positive (negative) energies correspond to the electron (hole) part. The chemical potential is defined by $\mu \equiv \frac{1}{2}[E_{\text{g.s.}}(2L-1) - E_{\text{g.s.}}(2L-3)]$. The results are shown in Fig. 4 for $L = 8$ and $J = J' = 0.3$. The wave vector along the ladder $k_x = \frac{2\pi}{L} n$ (n: integer) are for PBC and $k_x = \frac{2\pi}{L}(n + \frac{1}{2})$ for APBC. The ground-state energy $E_{\text{g.s.}}(2L-2)$ and the chemical potential μ in Eq. (3) are the average over both boundary conditions.

There are large weights for the bonding $(B)(k_y = 0)$ and antibonding $(A)(k_y = \pi)$ orbitals only near the Fermi energy $\omega = 0$, and they seem to constitute QP bands. Away from the Fermi energy, the individual QP peaks

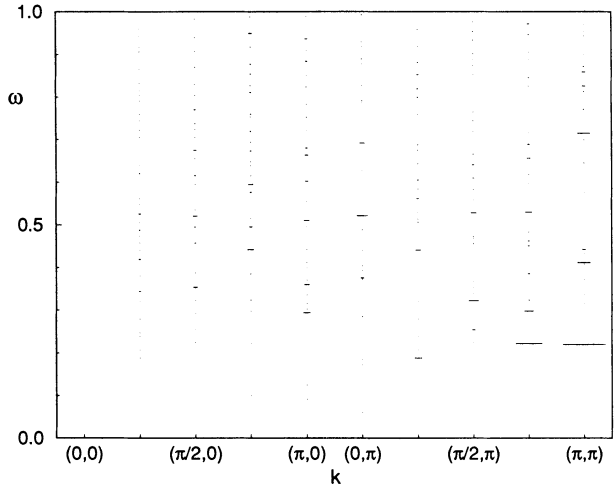

FIG. 3. Spin structure factor, $\mathcal{S}(\mathbf{k},\omega)$, for the t-J ladder with two holes and APBC. $L = 8$ and $J = J' = 0.3$. The width of each line represents the strength of the excitation.

are much less prominent and there is an incoherent part with the energy of the order of 1.

The QP spectrum is consistent with the MF theory based on the d-wave RVB state. Without holes the B and A bands are degenerate because the kinetic energy is zero. Upon hole doping, $\langle c^{\dagger}_{1\sigma}(j) c_{2\sigma}(j)\rangle$ on a rung becomes finite and the two bands are split. The B band is pushed down and occupied by more electrons, while the A band is pushed up and occupied by less electrons. The QP with energy closest to $\omega = 0$ has a wave vector nearest to the original Fermi k_F: ($k_x = \frac{5\pi}{8}$ for B and $k_x = \frac{3\pi}{8}$ for A). Because of the band splitting, $k_F^B > k_F^A$, but the Luttinger sum rule is satisfied, $k_F^B + k_F^A = (1 - \delta)\pi$. This means the Fermi surface is large, consistent with photoemission experiments on cuprates.

It is important to notice the QP peaks near the Fermi energy have their counterparts on the opposite side of the Fermi energy. An electronic QP peak at energy $\omega > 0$ has a shadow hole peak at energy around $-\omega < 0$, and *vice*

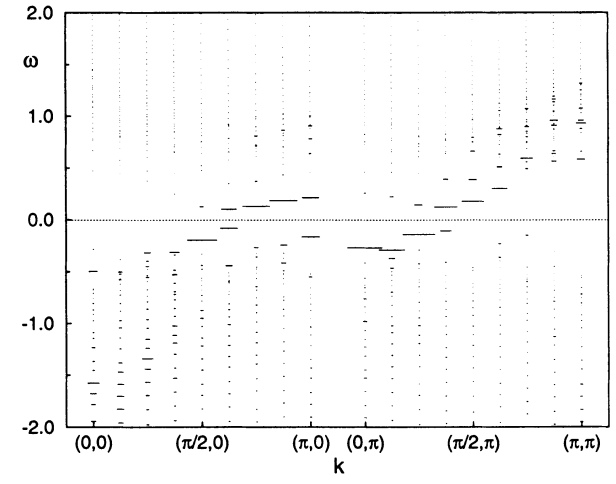

FIG. 4. Spectral function of the one-particle Green's function, $A(\mathbf{k},\omega)$, for two holes. $L = 8$ and $J = J' = 0.3$. The width of each line represents the strength of the excitation.

versa. These peaks indicate that the QP excitations are those of the Bogoliubov QP's as in BCS theory, i.e., mixture of an electron and a hole ($\alpha^\dagger_{\mathbf{k}} = u_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}$). The weights in the electron and hole parts are proportional to $|u_{\mathbf{k}}|^2$ and $|v_{\mathbf{k}}|^2$. They are holelike around $k_x = 0$ and electronlike around $k_x = \pi$ for both B and A bands. There exists a finite energy gap in the QP spectra. The electron and hole branches both come close to the Fermi energy at $k_x \sim \frac{\pi}{2}$, but instead of passing through they move away from it. The energy gap is $0.18t$ at $\mathbf{k} = (\frac{5\pi}{8}, 0)$ and $0.23t$ at $\mathbf{k} = (\frac{3\pi}{8}, \pi)$, corresponding to a QP gap $2\Delta_{\mathrm{QP}} \simeq 0.2 (\simeq \frac{2J}{3})$. It is interesting to note that the Stephan-Horsch results for $A(\mathbf{k}, \omega)$ in two-dimensional clusters[14] show similar behavior for $\mathbf{k}$ points not along $(1,1)$ but no shadow peaks for $\mathbf{k} \parallel (1,1)$, indicating $d_{x^2-y^2}$ pairing also.

The results of our exact diagonalization studies show that the doped t-J ladder belongs to a different universality class than the single chain. Here the separation is into a limited number of quasiparticle excitations carrying charge $+|e|$ and spin $\frac{1}{2}$ which vanish as $\delta \to 0$, and a triplet collective mode which remains as $\delta \to 0$. So the triplet mode is *not* a collective mode of the quasiparticles. This separation resembles in certain ways the proposal of Sokol and Pines for a doped quantum critical regime[15] and also Chubukov and Sachdev for collective and Fermion contributions to the susceptibility.[16] Note the quasiparticles do not behave as a usual Fermi liquid. Although their number is strictly limited when $\delta \ll 1$, yet their pairing energy is finite as $\delta \to 0$. In this sense they resemble a dilute Fermi gas with a strong attraction giving pair binding.[17] However if we look at the dispersion energy of an added hole that would be seen in photoemission, then from Fig. 4 it is characterized by the large Fermi surface. The quasiparticles do not form a usual Fermi liquid but display a new and interesting mixture of dilute Fermi gas and large Fermi surface behavior.

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[1] E. Dagotto, J. Riera, and D. J. Scalapino, Phys. Rev. B **45**, 5744 (1992); T. Barnes *et al.*, *ibid.* **47**, 3196 (1993).
[2] T. M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. **23**, 445 (1993).
[3] M. Sigrist, T. M. Rice, and F. C. Zhang, Phys. Rev. B **49**, 12 058 (1994).
[4] R. M. Noack, S. R. White, and D. J. Scalapino (unpublished).
[5] S. Gopalan, T. M. Rice, and M. Sigrist, Phys. Rev. B **49**, 8901 (1994).
[6] D. V. Khveshchenko and T. M. Rice (unpublished); D. V. Khveshchenko (unpublished).
[7] R. Hirsch, Diplomarbeit, University of Köln, 1988.
[8] S. P. Strong and A. J. Millis, Phys. Rev. Lett. **69**, 2419 (1992).
[9] M. Ogata, M. U. Luchini, and T. M. Rice, Phys. Rev. B **44**, 12 083 (1991).
[10] M. Imada, Phys. Rev. B **48**, 550 (1993), and references therein.
[11] M. Takano *et al.*, JJAP Series 7, 3 (1992).
[12] D. C. Johnston *et al.*, Phys. Rev. B **35**, 219 (1987).
[13] Similar excitations are also found for a t-J chain with frustrated couplings in K. Takano and K. Sano, Phys. Rev. B **48**, 9831 (1993); I. Bose and S. Gayen, *ibid.* **48**, 10 653 (1993).
[14] W. Stephan and P. Horsch, Phys. Rev. Lett. **66**, 2258 (1991).
[15] A. Sokol and D. Pines, Phys. Rev. Lett. **71**, 2813 (1993).
[16] A. V. Chubukov and S. Sachdev, Phys. Rev. Lett. **71**, 169 (1993).
[17] C. A. R. Sá de Melo, M. Randeria, and J. R. Engelbrecht, Phys. Rev. Lett. **71**, 3202 (1993).