The 2-Leg Hubbard Ladder:
Computational Studies of New Materials

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Abstract

Computational studies of basic models of strongly-correlated electron systems can provide guidance in the search for new materials as well as insight into the physical mechanisms responsible for their properties. Here, we illustrate this by examining what numerical computations have shown us about the 2-leg Hubbard ladder.
This workshop in honor of Zachary Fisk’s 60th birthday is to explore the future of materials physics, an area to which he has contributed so much. It addresses the challenges and opportunities posed by complex materials. Here, in this session on computation, I want to focus on the problems of strongly interacting electronic systems, specifically the problem of the 2-leg Hubbard ladder. While this is a special case, I believe it illustrates the way in which numerical studies of simple models can help in the search for new materials, such as the cuprate ladder materials \[1,2\], as well as how such calculations can provide insight into more general problems such as that posed by the high \(T_c\)-layered cuprates. It also represents an example of a case in which the interest in these materials arose from numerical calculations, which suggested that an undoped ladder would have a spin gap and a doped system would have power law pairing correlations \[3\].

The Hamiltonian for the 2-leg Hubbard ladder is

\[
H = -t \sum_{i,\lambda,s} \left( c_{i+1,\lambda s}^{\dagger} c_{i,\lambda s} + c_{i,\lambda s}^{\dagger} c_{i+1,\lambda s} \right) - t_\perp \sum_{i,s} \left( c_{i,1s}^{\dagger} c_{i,2s} + c_{i,2s}^{\dagger} c_{i,1s} \right) + U \sum_{i,\lambda} n_{i,\lambda\uparrow} n_{i,\lambda\downarrow} \quad (1)
\]

Here \(c_{i,\lambda s}^{\dagger}\) creates an electron of spin \(s\) at rung \(i\) on leg \(\lambda = 1\) or 2. The hopping along a leg is \(t\) and across a rung is \(t_\perp\). There is an onsite Coulomb interaction \(U\) and the filling is set by a chemical potential in the Monte Carlo simulations and by a fixed electron number in the density matrix renormalization group (DMRG) calculations.

The general properties of the 2-leg ladder \[4\], which have been found from both numerical \[5,6\] and analytic studies \[7–9\], can be summarized as follows. At half-filling, the ground state has both a charge gap \(\Delta_c\) and a spin gap \(\Delta_s\). It is an insulator with short-range antiferromagnetic correlations and spin gapped \(S = 1\) magnon excitations. As \(t_\perp/t\) increases the ground state of the half-filled ladder adiabatically crosses over from a spin-gapped Mott insulator to a band insulator \[5\] and \(\Delta_s/\Delta_c\) goes to 1. For small values of \(U\), this crossover to the band insulator occurs when \(t_\perp/t\) approaches 2. This corresponds to the value at which the bottom of the antibonding band rises above the top of the bonding band and the non-interacting, half-filled system becomes a Bloch insulator. When the spin gapped Mott insulator is doped so that the site occupation \(n = 1 - x\), the system goes into a Luther-Emery phase \[10\] with power law pair field and \(4k_F\)-CDW correlations. The sign of the rung-rung pair field correlations are positive while the rung-leg correlations are negative, implying “\(d\)-wave-like” pairing. In the Luther-Emery phase, the power law decay of the pair field \(\ell^{-1/2\kappa}\) is conjugate to the \(\ell^{-2\kappa}\) decay of the \(4k_F\)-CDW correlations. As one goes towards the insulating state, Umklapp processes play an important role \[11\] and Schulz \[9\] has shown that \(\kappa \rightarrow 1\) and the pairing correlations are dominant. Finally, we note that the superfluid density vanishes as the doping \(x\) goes to 0.

These properties make the 2-leg Hubbard ladder an interesting laboratory for studying the effect of various parameters on the pairing. In Figure 1, a DMRG calculation \[5\] of the rung-rung pair field correlation function

\[
D(\ell) = \langle \Delta_{i+\ell}^{\dagger} \Delta_i \rangle \quad (2)
\]

is shown for a \(2 \times 32\) ladder with a hole doping of \(x = 0.125\), \(U/t = 8\), and different values of \(t_\perp/t\). Here

\[
\Delta_i^{\dagger} = \left( c_{i,1\uparrow}^{\dagger} c_{i,2\downarrow} + c_{i,1\uparrow}^{\dagger} c_{i,2\downarrow} \right) \quad (3)
\]
creates a singlet pair on the \( i \)th rung. As \( t_\perp/t \) increases, the pairing correlations initially increase. However, as shown for \( t_\perp/t = 2 \), when \( t_\perp/t \) becomes too large, we find that the pairing correlations are suppressed. A closer look at this behavior is shown in Fig. 2a. Here an average strength of the rung-rung pairing correlations

\[
\bar{D} = \frac{1}{5} \sum_{\ell=8}^{12} D(\ell)
\]  

is shown versus \( t_\perp/t \) for \( U/t = 8 \) at several dopings. In Fig. 2b, \( \bar{D} \) versus \( t_\perp/t \) is shown for various values of \( U/t \) at a doping \( x = 0.0625 \). Separate calculations of the pair gap show that it has the same behavior as \( \bar{D} \) as a function of \( t_\perp/t \) and \( x \). The strength of the pair binding increases as \( x \) decreases and the Mott insulating state is approached while, as noted previously, the superfluid density decreases as \( x \) goes to zero. The pairing also depends upon \( U \), and as shown in Fig. 2b, peaks for \( U \) of order the bandwidth. For values \( U \) large compared with the bandwidth, the effective exchange interaction varies as \( U^{-1} \) and both the insulating spin gap and the pairing strength decrease as \( U \) increases.

The peak in \( \bar{D} \) as a function of \( t_\perp/t \) can be understood in terms of the behavior of the single-particle spectral weight \( A(p, \omega) \). Results for \( A(p, \omega) \) obtained from a maximum entropy analytic continuation of Monte Carlo data [12] for a 2-leg ladder at \( T = 0.25t \) with \( U/t = 4, t_\perp/t = 1.5 \), and \( \langle n \rangle = 0.875 \) are shown in Fig. 3. Here, the solid curves are for the bonding band (\( p_y = 0 \)) and the dotted curves are for the antibonding band (\( p_y = \pi \)). One sees that for this value of \( t_\perp/t \), the bonding band has spectral weight near the fermi level for \( p \approx (\pi, 0) \) while the antibonding band has its spectral weight near the fermi level for \( p \approx (0, \pi) \). These Fermi points can be connected by scatterings involving a large momentum transfer where, as we will see, the effective pairing interaction \( V \) is strong. Furthermore, the peak in both the bonding and antibonding spectral weight is seen to disperse very slowly near the bonding and antibonding fermi points leading to a large density of states at the fermi energy. For a value of \( t_\perp/t \sim 1.6 \) which is slightly larger, the dispersion becomes even flatter and \( \bar{D} \) peaks. At still larger values of \( t_\perp/t \), the antibonding band pulls away from the Fermi energy leaving only the bonding band with spectral weight near the Fermi level. In this case, the doped system behaves like a one-band Luttinger liquid and the pairing correlations vanish.

These computations suggest that an array of weakly coupled ladders should exhibit superconductivity and that \( T_c \) can be enhanced by adjusting the ratio of the effective rung-to-leg hopping as well as optimally doping the system. Additional calculations [13] have shown that the pairing can be further enhanced if an exchange interaction \( J_\perp \vec{S}_{i1} \cdot \vec{S}_{i2} \) is added. In a \( CuO_2 \) model, such an additional exchange term can be seen to arise from intermediate states in which the two exchanged electrons virtually occupy the oxygen site rather than one of the \( Cu \) sites. Chemically, one might try to enhance the rung hopping and the rung exchange by substitutions off the ladder plane that change the Madelung energy of the rung O. A more radical approach would be to replace the rung O by another element such as \( S \). Clearly, the 2-leg ladder materials represent an important area of new materials that merit further study.

Beyond this, however, computational studies of the 2-leg ladder have provided insight into the more general problem of the high \( T_c \) cuprates. Using Monte Carlo simulations [12], one can extract the effective pairing interaction \( V(q, \omega_m) \). While these calculations for a doped
ladder were restricted to temperature $T \geq 0.25t$ because of the “fermion sign” problem, they showed that the momentum, Matsubara frequency and temperature dependence of $V(q, \omega_m)$ was remarkably similar to that of the spin susceptibility

$$\chi(q, \omega_m) = \frac{T}{N} \int_0^\beta d\tau e^{-i\omega_m \tau} \sum_q e^{i\mathbf{q} \cdot \mathbf{r}_t} \left\langle M^z_{i+\mathbf{r}_t}(\tau)M^z_i(0) \right\rangle \tag{5}$$

Here $M^z_i = (n_{i\uparrow} - n_{i\downarrow})/2$. A comparison of $V(q, \omega_m = 0)$ versus $q$ with $\chi(q, \omega_m = 0)$ for various temperatures is shown in Figures 4a and b. As the temperature decreases and the short-range antiferromagnetic correlations evolve in $\chi(q)$, the effective interaction grows in strength and a broad peak appears at large momentum transfers. It is this interaction which leads to the strong scattering of pairs from regions near the bonding fermi points $(p_{Fb}, 0)$ and $(-p_{Fb}, 0)$ to regions near the antibonding fermi points $(p_{Fa}, \pi)$ and $(-p_{Fa}, -\pi)$ and hence to the pair binding.

It is also useful to consider a strong-coupling local picture of the pairing. Figure 5 shows the results of a DMRG calculation of the amplitude for removing 2 electrons

$$\langle N - 2 | (c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}) | N \rangle \tag{6}$$

from a half-filled 2-leg ladder. The phase of this amplitude has been chosen so that the rung amplitude is positive. Here one sees a clear “$d_x^2-y^2$-like” structure and from the size of the amplitude, one can judge that the pair is extended over about 10 sites. This amplitude is probing a property of the half-filled ground state and although the superfluid density for the undoped ladder vanishes, this spin-gapped Mott state contains latent $d_x^2-y^2$-like pairs. To illustrate this, consider a 2 × 2 segment of a ladder in which the 4-sites are numbered in a clockwise manner. In a ladder with short-range antiferromagnetic correlations, the half-filled, 4-site cluster has a ground state

$$|\psi\rangle = N_0 \left( \Delta^\dagger_{14}\Delta^\dagger_{23} - \Delta^\dagger_{12}\Delta^\dagger_{34} \right) |0\rangle \tag{7}$$

with $\Delta^\dagger_{ij} = c^\dagger_{i\uparrow}c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow}c^\dagger_{j\uparrow}$. This superposition of valence bonds has $d_x^2-y^2$-like symmetry. The power law quasi-long-range-order superconducting pairing phase arises when these latent pairs are “freed” by the doping.

In summary, the dependence of the pairing correlations on the ratio of the rung-to-leg hopping parameters $t_\perp/t$, the strength of the Coulomb interaction $U/t$ and the doping $x$ provide insight into the search for new ladder materials that could exhibit enhanced superconductivity. The effective pairing interaction $V(q, \omega_m)$ shown in Fig. 4a and the resonating valence bond structure shown in Fig. 5, illustrate the momentum space and real space nature of the pairing process for the 2-leg Hubbard ladder. The short coherence length and the relatively high energy scale set by the gap magnitude of the 2D layered high $T_c$ cuprates suggest that the basis pairing mechanism in these materials involves short-range physics. Thus we expect that what has been learned about the pairing process in the 2-leg ladder will also be relevant to the layered cuprates.

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[16] It would be natural to call this a short-range RVB state [P.W. Anderson, *Science* **235** (1987) 1169; S.A. Kivelson, D.S. Rokhsar, and J.P. Sethna, *Phys. Rev. B* **35** (1987) 8865.] except that the term RVB carries a variety of special connotations with it such as spinons. As noted, a half-filled ladder has only \(S = 1\) spin-gapped magnon excitations and is adiabatically connected to a band insulator.
FIG. 1. The equal-time pair-field correlation function $\langle \Delta_i \Delta_j^\dagger \rangle$ versus $|i-j|$ for $\langle n \rangle = 0.875$, $U/t = 8$ and various values of $t_\perp/t$. 
FIG. 2. a) $\bar{D}$ versus $t_\perp/t$ for $U/t = 8$ at fillings $\langle n \rangle = 0.75$, 0.875, and 0.9375. b) $\bar{D}$ versus $t_\perp/t$ for various values of $U/t$ at filling $\langle n \rangle = 0.9375$.

FIG. 3. Single-particle spectral weight $A(p, \omega)$ versus $\omega$ for $t_\perp/t = 1.5$, $T = 0.25t$, $U/t = 4$, and $\langle n \rangle = 0.875$. The solid curves denote the results for the bonding band ($p_y = 0$) and the dotted curves denote the results for the antibonding band ($p_y = \pi$).
FIG. 4. a) Momentum-dependence of the effective interaction $V(q)$ for $U = 4t$, $\langle n \rangle = 0.875$, and $t_\perp = 1.5t$. Here $V(q)$ is measured in units of $t$, $q_y = \pi$ and $V(q)$ is plotted as a function of $q_x$. b) Momentum-dependence of the magnetic susceptibility $\chi(q)$ for $U = 4t$, $\langle n \rangle = 0.875$, and $t_\perp = 1.5t$. Here, $q_y = \pi$ and $\chi(q)$ is plotted as a function of $q_x$. 
FIG. 5. Schematic drawing of the pair-wave function showing the values of the off-diagonal matrix element $\left\langle N - 2 | (c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}) | N \right\rangle$ for removing a singlet pair between near-neighbor sites.