Effect of the $W$-term for a $t-U-W$ Hubbard ladder

S. Daul 1, D. J. Scalapino 2 and Steven R. White 3

1 Institute for Theoretical Physics, University of California, Santa-Barbara CA 93106.
2 Physics Department, University of California, Santa-Barbara CA 93106.
3 Department of Physics and Astronomy, University of California, Irvine CA 92697.

Antiferromagnetic and $d_{x^2-y^2}$-pairing correlations appear delicately balanced in the 2D Hubbard model. Whether doping can tip the balance to pairing is unclear and models with additional interaction terms have been studied. In one of these, the square of a local hopping kinetic energy $H_W$ was found to favor pairing. However, such a term can be separated into a number of simpler processes and one would like to know which of these terms are responsible for enhancing the pairing. Here we analyze these processes for a 2-leg Hubbard ladder.

The interplay of antiferromagnetism and $d_{x^2-y^2}$ superconductivity in the 2D Hubbard model remains an open question. [1] Weak coupling calculations originally suggested that doping could drive the ground state from an antiferromagnet to a $d_{x^2-y^2}$ superconductor. [2] However, numerical Monte Carlo calculations have found only short range $d_{x^2-y^2}$ pairing correlations. [3] This may be due to the finite lattice sizes that have been studied, the difficulty in attaining low temperature results or possibly that the $t-U$ Hubbard model lies just outside the superconducting parameter regime.

One approach to this problem is then to add various terms to the basic Hubbard model and see what it takes to drive it into a superconducting state. In this spirit, a recent Monte Carlo study [4] added a term $H_W$, involving the square of the local hopping kinetic energy around a site,

$$H_W = -W \sum_i K_i^2$$  \hspace{1cm} (1)

with $K_i$ equal to the local kinetic energy involving site $i$ and its near neighbors at $i + \delta$,

$$K_i = \sum_{\sigma=\uparrow,\downarrow} \left( c_{i,\sigma}^\dagger c_{i+\delta,\sigma} + c_{i+\delta,\sigma}^\dagger c_{i,\sigma} \right).$$  \hspace{1cm} (2)

With $H_W$ added to the 2D $t-U$ Hubbard model, the half-filled system exhibited a transition from an antiferromagnetic phase to a $d_{x^2-y^2}$-pairing phase at a critical value of $W$. Separating $H_W$ into various pieces, it was found that it contained one-electron hopping terms, exchange interactions and triplet and singlet four particle scattering terms. One would like to understand which of these terms or what combination of the terms are responsible for enhancing superconductivity. Unfortunately because of the fermion sign problem it has not been possible to carry out a Monte Carlo calculations for the individual terms. However, density matrix renormalization group (DMRG) techniques [6] can be used to study the individual pieces of the $H_W$ interaction. Here we describe the results of such a study for a 2-leg ladder. For such a system, we can determine the effect of the individual terms for both the half-filled and the doped system. As we will discuss in the conclusion, it is important to note that the half-filled 2-leg ladder has a spin gap which distinguishes it from the 2D half-filled Hubbard model. Nevertheless, it is instructive to see what effect the various parts of $W$ have on the pairing correlations for a ladder.

We begin with the usual Hubbard Hamiltonian

$$H_U = -t \sum_{\langle ij \rangle, \sigma=\uparrow,\downarrow} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$  \hspace{1cm} (3)

with a one electron hopping kinetic energy and an onsite Coulomb interaction $U$. The sum $\langle ij \rangle$ is over all pairs of nearest neighbors. We will measure all energies in units of $t$. We then add the interaction (1) with $W$ positive. Monte Carlo calculations for a 2D half-filled system with the Hamiltonian

$$H = H_U + H_W$$  \hspace{1cm} (4)

find a quantum phase transition between an antiferromagnetic Mott insulator and a $d_{x^2-y^2}$-wave superconducting phase when $W$ is increased to a value of order 0.35. [5] However, the 2D Hubbard model at half-filling has an antiferromagnetic ground state while a 2-leg ladder is characterized by a spin gap. [5] Thus, as we will see, the behavior of a two-leg ladder as $W$ is turned on, can be different.

It is convenient to decompose the interaction $H_W$ as follows [6]

$$H_W = \sum_i H_{W_i},$$  \hspace{1cm} (5)

with

$$H_{W_i} = -4W_i \sum_i (n_{i\uparrow} + n_{i\downarrow})$$  \hspace{1cm} (6a)
\[ H_{W_2} = -W_2 \sum_{i,\delta,\delta'} \sum_{\sigma} c_{i,\delta,\sigma}^\dagger c_{i+\delta',\sigma} \]  
(6b)

\[ H_{W_3} = -W_3 \sum_{i,\delta,\delta'} \sum_{\sigma} (c_{i,\delta,\sigma}^\dagger \sigma - c_{i+\delta',\sigma}^\dagger - c_{i,\delta,\sigma} + \text{h.c.}) \]  
(6c)

\[ H_{W_4} = +W_4 \sum_{i,\delta,\delta'} \left( T_{i,\delta,1}^\dagger T_{i,\delta,1} + T_{i,\delta,-1}^\dagger T_{i,\delta,-1} + T_{i,\delta',0}^\dagger T_{i,\delta,0} \right) \]  
(6d)

\[ H_{W_5} = -W_5 \sum_{i,\delta} \Delta_{i\delta}^x \Delta_{i\delta}^y \]  
(6e)

\[ H_{W_6} = -W_6 \sum_{i,\delta \neq \delta'} \Delta_{i\delta}^x \Delta_{i\delta'}^y. \]  

Here \( T_{i,\delta,1}^\dagger = c_{i,\delta,\uparrow}^\dagger c_{i+\delta,\downarrow} \), \( T_{i,\delta,-1}^\dagger = c_{i,\delta,\downarrow}^\dagger c_{i+\delta,\uparrow} \), \( T_{i,\delta,0}^\dagger \) \( = (c_{i,\delta,\uparrow}^\dagger c_{i+\delta,\downarrow} + c_{i,\delta,\downarrow}^\dagger c_{i+\delta,\uparrow}) / \sqrt{2} \) are triplet pair creation operators, and \( \Delta_{i\delta}^x = (c_{i,\delta,\uparrow}^\dagger c_{i,\delta,\downarrow} - c_{i,\delta,\downarrow}^\dagger c_{i,\delta,\uparrow}) / \sqrt{2} \) is a singlet pair creation operator. If one sets all the \( W_i \) equal to \( W \), the original \( H_W \) interaction (6) is recovered. Here we will examine the effect of the individual terms. \( H_{W_1} \) renormalizes the chemical potential and \( H_{W_2} \) contains nearest-neighbor and next-nearest-neighbor on-site one-electron hopping terms. \( H_{W_3} \) scatters an onsite singlet to neighbors sites while \( H_{W_4} \), which comes with a positive sign, is a triplet scattering term. Finally \( H_{W_5} \) and \( H_{W_6} \) involve singlet pairs. It had been thought for the 2D system that the relevant terms for the quantum transition were \( H_{W_5} \) and \( H_{W_6} \). [8]

Here, in order to determine the effects of the individual terms, we have studied the model on a two-leg ladder using DMRG techniques. All the runs were done on \( 2 \times 32 \) ladders keeping up to 800 states leading to a maximum discarded weight of \( 10^{-6} \). We calculated the singlet pairing correlation function \( D_{\alpha\beta}(\ell) \) defined as

\[
D_{xx}(\ell) = \langle \Delta_x(i + \ell) \Delta_x^\dagger(i) \rangle \\
D_{xy}(\ell) = \langle \Delta_x(i + \ell) \Delta_y^\dagger(i) \rangle \\
D_{yy}(\ell) = \langle \Delta_y(i + \ell) \Delta_y^\dagger(i) \rangle
\]  
(7-9)

where \( \Delta_x(i) = c_{i,\delta,\uparrow}^\dagger c_{i,\delta,\downarrow} - c_{i,\delta,\downarrow}^\dagger c_{i,\delta,\uparrow} \), \( \delta_x = (1,0) \) and \( \delta_y = (0,1) \). For clarity, in the following we show the rung-rung correlation function \( D_{yy}(\ell) \). \( D_{xx}(\ell) \) and \( D_{yy}(\ell) \) were always positive while \( D_{xy}(\ell) \) was negative corresponding to a \( d_{x^2-y^2} \)-like structure.

The results for the half-filled case with \( U = 4 \) and \( W_i = 0 \) or 0.25 are shown in Fig. 1. In the plot of \( D_{yy}(\ell) \) we have kept \( \ell \leq 12 \), with the measurements made in the central portion of the ladder. In this region the effects of the open ends are negligible. We clearly see in part (a) that when all \( W_i \) are turned on there is an enhancement of the pairing (as found in the 2D Monte-Carlo simulations). However, if we only turn on \( W_5 \), there is a suppression of pairing. For the 2-leg ladder, this can be understood by noting that \( H_{W_5} \) can be written as an antiferromagnetic exchange interaction

\[
H_{W_5} = 2W_5 \sum_{\langle ij \rangle} \left( S_i S_j - \frac{1}{4} n_i n_j \right). \tag{10}
\]

Now as one knows, [8] a 2-leg Heisenberg ladder has a spin gap \( \Delta_s \approx 0.51J \). Thus the effect of \( H_{W_5} \) at half-filling is to increase the spin gap by a factor of order \( W_5 \) and this leads to an exponentially more rapid decay of the pairing correlations.

Fig. 1 (b) shows the effect of the other terms. \( H_{W_3} \) has no effect as expected since it just renormalizes the chemical potential and we have fixed \( \langle \hat{n} \rangle = 1 \). The additional one electron hopping term \( H_{W_4} \) leads to only a small change in the pairing. However \( H_{W_5} \) which scatters an onsite singlet to neighbors sites enhances the pairing despite the presence of \( U \) which lowers the double occupancy.
We now investigate the nature of the magnetic ordering by examining the spin–spin correlation function
\[ S(r) = \langle S_\ell^+ S_{\ell+r}^- \rangle \] (11)
where \( S_\ell^+ \) (\( S_\ell^- \)) are the spin raising (lowering) operators corresponding to \( S_\ell = c_\ell^\dagger \sigma_{s_\ell} c_{\ell s} \). We then perform a Fourier transform to obtain the static structure factor
\[ S(q) = \sum_r e^{iqr} S(r). \] (12)

The resulting structure factor is plotted in Fig. 4 for various \( W_i \) interactions. As previously noted, the effect of \( W_3 \) is to increase the spin gap which leads to a broadening of the Lorentzian and a decrease of its peak at \((\pi, \pi)\). When all of the \( W_i \) terms are present, \( S(q) \) appears to simply be reduced in magnitude at all \( q \) values indicating a reduction of the local moment \( \sqrt{\langle S_\ell^2 \rangle} \) due to the delocalization effects of \( H_W \).

We now turn to the doped case and consider the same lattice with \( U = 4 \) and 8 holes corresponding to a filling \( \langle n \rangle = 0.875 \). Fig. 5 show results for \( D_{yy}(\ell) \). We clearly see in part (a) that in this case the inclusion of \( H_{W_5} \) enhances the pairing while in part (b) we see that all of the remaining terms are essentially irrelevant. Thus the \( W_5 \) term, which corresponds to adding a near neighbor exchange \( J = 2W_5 \) enhances the pairing correlation in the doped system.
Thus we conclude, that while $H_W$ with $U = 4t$ can slightly enhance the pairing correlations of a half-filled ladder, this is in fact a small effect. Furthermore, for large values of $U/t$, $H_W$ leads to a suppression of the half-filled pairing correlations. This can be understood in terms of the dominance of $H_{W_5}$, which represents an effective antiferromagnetic exchange increasing the spin gap and suppressing the pairing correlations. However, for the doped ladder, $W_5$ acts to enhance the pairing correlation since it increases the effective exchange interaction and the pair binding energy. Clearly, in light of the 2D results, where it was found that $H_W$ could lead at half-filling to a $d_{x^2-y^2}$ pairing state, one would like to extend the DMRG calculations to a 3-leg ladder which has a vanishing spin gap at half-filling.

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