Monte Carlo study of the pairing interaction
in the two-leg Hubbard ladder

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Abstract

Monte Carlo calculations of the irreducible particle-particle interaction on a two-leg Hubbard ladder doped near half-filling are reported. As the temperature is lowered, this interaction develops structure in momentum space similar to the magnetic susceptibility $\chi(q)$ and reflects the development of strong short-range antiferromagnetic correlations. Using this interaction, the eigenfunction of the leading singlet pair eigenvalue is found to have $d_{x^2-y^2}$ like symmetry. The single-particle spectral weight is also shown to peak near $(\pi, 0)$ and $(0, \pi)$ when the ratio of the inter- to intra-chain hopping $t_\perp/t \simeq 1.5$, leading to an increased tendency for pairing.
Numerical calculations, renormalization-group bosonization studies as well as strong-coupling treatments find that half-filled $t$-$J$ or Hubbard two-leg ladders have a spin gapped ground state with short range antiferromagnetic correlations \[1-3\]. Furthermore, these various techniques all find that when holes are doped into the ladder, $d_{x^2-y^2}$-like pairing correlations develop. This being the case, one would like to understand the nature of the effective interaction that gives rise to the $d_{x^2-y^2}$ pairing correlations for this system. Here, in order to address this question, we present Monte Carlo results for the irreducible particle-particle interaction $\Gamma_I$. In addition, we use $\Gamma_I$ and the single-particle Green’s function obtained from the Monte Carlo calculations to solve the Bethe-Salpeter equation in the singlet pairing channel. We find that the eigenfunction with the leading eigenvalue has $d_{x^2-y^2}$-like symmetry.

The Hubbard model Hamiltonian for a two-leg ladder has the form

$$H = -t \sum_{i,\lambda,s} \left( c_{i\lambda s}^\dagger c_{i+1\lambda s} + \text{h.c.} \right) - t_\perp \sum_{i,s} \left( c_{i1s}^\dagger c_{i2s} + \text{h.c.} \right) + U \sum_{i\lambda} n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here $t$ is the intra-chain one electron hopping, $t_\perp$ the inter-chain hopping and $U$ the on-site Coulomb interaction. The operators $c_{i\lambda s}^\dagger$ and $c_{i\lambda s}$ create and destroy electrons of spin $s$ on site $i$ of the $\lambda^{th}$ leg, respectively, and $n_{i\lambda s} = c_{i\lambda s}^\dagger c_{i\lambda s}$ is the occupation number for spin $s$ on site $i$ of the $\lambda^{th}$ leg.

Using Monte Carlo techniques, we have calculated the finite temperature two-particle Green’s function

$$G_2(x_4, x_3, x_2, x_1) = -\langle T c_\uparrow(x_4) c_\downarrow(x_3) c_\downarrow^\dagger(x_2) c_\uparrow^\dagger(x_1) \rangle. \quad (2)$$

Here $c_s^\dagger(x_i)$ with $x_i = (x_i, \tau_i)$ creates an electron of spin $s$ at site $x_i$ and imaginary time $\tau_i$ and $T$ is the usual $\tau$-ordering operator. Then, as previously discussed \[4\], one can take the Fourier transform of both the space and imaginary time variables and obtain $G_2(p', k', k, p)$ with $p' = (p', i\omega_n')$, etc. This two particle Green’s function can be expressed in terms of the exact single-particle propagator $G_s(p, i\omega_n)$ and the reducible particle-particle vertex $\Gamma(p', k', k, p)$.
\[ G_2(p', k', k, p) = -\delta_{p, p'} \delta_{k, k'} G_\downarrow(k) G_\uparrow(p) \]
\[ + \frac{T}{N} \delta_{p' + k', p + k} G^\uparrow(p') G_\downarrow(k') \Gamma(p', k', k, p) G_\downarrow(k) G_\uparrow(p). \]

Then from the Monte Carlo data for \( G \) and \( G^2 \), one can determine \( \Gamma(p', k', k, p) \). Finally, because the effective pairing interaction corresponds to the irreducible particle-particle interaction \( \Gamma_I \) in the zero energy and momentum center of mass channel, we have inverted the fully dressed \( t \)-matrix equation to find \( \Gamma_I \) in terms of \( \Gamma \) and \( G \). Setting \( k = -p \) and \( k' = -p' \), the fully dressed \( t \)-matrix equation becomes

\[ \Gamma(p'|p) = \Gamma_I(p'|p) - \frac{T}{N} \sum_k \Gamma(p'|k) G_\downarrow(-k) G_\uparrow(k) \Gamma_I(k|p), \]

which is solved to find \( \Gamma_I(p'|p) \). The effective pairing interaction in the singlet channel is

\[ V(p' - p) = \frac{1}{2} \left( \Gamma_I(p'|p) + \Gamma_I(-p'|p) \right). \]

We have carried out this calculation at different temperatures for various values of the hopping anisotropy \( t_\perp/t \), interaction strength \( U/t \) and filling \( \langle n \rangle = \langle n_{i\uparrow} + n_{i\downarrow} \rangle \). Here, we will show results for \( t_\perp/t = 1.5 \), \( U/t = 4 \), \( \langle n \rangle = 0.875 \) and a \( 2 \times 16 \) lattice. We have chosen this set of parameters, because the numerical density matrix renormalization group (DMRG) calculations find that for \( U/t = 4 \) and \( \langle n \rangle = 0.875 \), the \( d_{x^2-y^2} \) pairing correlations are strongest when \( t_\perp/t \approx 1.5 \) \[5\]. In addition, for these parameters we have good control of the maximum entropy analytic continuation of the Monte Carlo data, which is necessary to obtain the single-particle spectral weight \( A(p, \omega) \).

In Fig. 1 we plot the effective pairing interaction \( V \) versus \( q_x = p'_x - p_x \) for \( q_y = p'_y - p_y = \pi \). Here we have set \( \omega_n = \omega_{n'} = \pi T \) corresponding to \( \omega_m = 0 \) energy transfer. The three curves correspond to temperatures \( T = 1.0t \), \( 0.5t \) and \( 0.25t \). One can see that as the temperature decreases, the effective pairing interaction becomes increasingly positive at large momentum transfer \( q \to (\pi, \pi) \). As shown in Figure 2, the magnetic susceptibility

\[ \chi(q) = \frac{1}{N} \int_0^\beta d\tau \sum_\ell e^{i\mathbf{q}\cdot\ell} \langle m_{\ell+\ell}(\tau) m^+_{\ell}(0) \rangle \]

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also develops structure at large momentum transfers over this same temperature region. Thus it is clear that the effective pairing interaction is associated with the development of short-range antiferromagnetic correlations.

It is also of interest to study the Bethe-Salpeter equation for the singlet particle-particle channel

$$\lambda_\alpha \phi_\alpha(p, i\omega_n) = -\frac{T}{N} \sum_{p', i\omega_{n'}} \Gamma_1(p, i\omega_n | p', i\omega_{n'}) |G(p', i\omega_{n'})|^2 \phi_\alpha(p', i\omega_{n'}).$$  \hspace{1cm} (7)

Fig. 3 shows the eigenfunction $\phi(p, i\omega_n)$ of the leading eigenvalue versus $p$ for $\omega_n = \pi T$. We observe that $\phi(p, i\pi T)$ has $d_{x^2-y^2}$-like momentum structure in the sense that it has opposite signs and is largest near $(\pi, 0)$ on the bonding band and near $(0, \pi)$ on the antibonding band. This is associated with the structure of the irreducible interaction $\Gamma_1$ and the single-particle spectral weight $A(p, \omega)$ which we will study below [6].

The temperature dependence of the leading eigenvalue $\lambda_1$ is plotted in Fig. 4(a). As previously discussed, when the temperature is lowered, short-range antiferromagnetic correlations develop and the effective pairing interaction increases at large momentum transfer. This leads to an increase in $\lambda_1$ as shown in Fig. 4(a). We believe that $\lambda_1$ will approach unity at low temperatures where power-law $d_{x^2-y^2}$-like pairing correlations have been shown to exist using density matrix renormalization group techniques [2]. In Fig. 4(b), we show the dependence of the leading eigenvalue $\lambda_1$ on the hopping anisotropy $t_\perp/t$. According to the DMRG calculations [3], for $U/t = 4$ and $\langle n \rangle = 0.875$ the pairing correlations in the ground state are strongest when $t_\perp/t \simeq 1.5$. In Fig. 4(b), we do not observe a strong dependence of $\lambda_1$ on $t_\perp/t$ because of the thermal smearing effects at $T = 0.25t$.

In addition to the irreducible interaction vertex $\Gamma_1$, the single-particle Green’s function $G(p, i\omega_n)$ is also important in determining the structure of the leading eigenfunction of the Bethe-Salpeter equation. Using a numerical maximum entropy procedure [7], we have calculated the single-particle spectral weight

$$A(p, \omega) = -\frac{1}{\pi} \text{Im} \, G(p, \omega).$$  \hspace{1cm} (8)
This is plotted in Fig. 5 for $t_{\perp}/t = 1.5$ as a function of $\omega$ for different $p$. Here, the solid curves are for the bonding band ($p_y = 0$) and the dotted curves are for the antibonding band ($p_y = \pi$). We see that for this value of $t_{\perp}/t$, the bonding band has spectral weight near the Fermi level for $p \sim (\pi, 0)$, and the antibonding band has spectral weight near the Fermi level for $p \sim (0, \pi)$. Hence, these Fermi points can be connected by scatterings involving $q = (\pi, \pi)$ momentum transfer. Since $\Gamma_{IS}$ is large and repulsive for $q \sim (\pi, \pi)$, the leading eigenfunction $\phi$ of the Bethe-Salpeter equation has opposite signs for $p$ near $p = (\pi, 0)$ and $(0, \pi)$, as seen in Fig. 2.

These calculations provide further insight into the structure of the effective pairing interaction and the single-particle spectral weight which lead to the pairing correlations in the two-leg Hubbard ladder. Specifically, the momentum structure of the effective interaction $V(q)$ clearly reflects the existence of short-range antiferromagnetic correlations as the cause of the increasing positive strength of $V(q)$ at large momentum transfer. Secondly, the enhanced spectral weight in the bonding band near $(\pi, 0)$ and the antibonding band near $(0, \pi)$ are reminiscent of a similar effect observed in the two-dimensional Hubbard model near half-filling [8,9] and in the ARPES of the cuprates [10]. This enhanced low lying spectral weight associated with the renormalized quasiparticles is such that pair scattering processes with momentum transfers near $(\pi, \pi)$ have increased phase space. These two features appear to play an important role in the development of pairing on the two-leg ladder, just as they do for the two-dimensional Hubbard model.

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FIG. 1. 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 $q_x$.

FIG. 2. 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. 3. Momentum dependence of the $d_{x^2-y^2}$ eigenfunction $\phi(p, i\pi T)$. These results are for $T = 0.25t$, $U = 4t$, $\langle n \rangle = 0.875$ and $t_\perp = 1.5t$.

FIG. 4. (a) Temperature dependence of the leading eigenvalue $\lambda_1$ for $t_\perp = 1.5t$. (b) $\lambda_1$ vs $t_\perp/t$ for $T = 0.25t$. These results are for $\langle n \rangle = 0.875$ and $U = 4t$. 
FIG. 5. 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 ($p_y = \pi$).