Pair Structure and the Pairing Interaction in a Bilayer Hubbard model

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The bilayer Hubbard model provides a model system for which one can study the relationship between the structure of the Fermi surface, the spin-fluctuation spectrum and superconductivity. By varying the relative strength of the inter-layer one electron hopping \(t_{\perp}\) to the near-neighbor intra-layer hopping \(t\), one can alter the size and shape of the bonding and antibonding Fermi surfaces, change the momentum and frequency structure of the spin-fluctuation spectral weight, and move away from the Mott region. Previous Monte Carlo calculations \(^1\)-\(^6\) for a doped bilayer found evidence for an attractive pairing interaction in both the \(d_{x^2-y^2}\) (\(\cos k_x - \cos k_y\)) and \(k_z\) channels. The latter was called a \(d_z\) channel and corresponded to a pairfield function which had different signs on the bonding and antibonding Fermi surfaces. This is an \(A_{1g}\) gap and here we will refer to it as an \(s^\pm\) gap. The sign problem associated with the previous determinantal quantum Monte Carlo calculations prevented one from numerically exploring the low temperature properties of the doped bilayer. More recently, a functional renormalization group study \(^7\) found that as \(t_{\perp}/t\) increased, \(s^\pm\) pairing was favored over \(d_{x^2-y^2}\) pairing. Here using a dynamic cluster approximation\(^8\) (DCA) we will examine what the bilayer Hubbard model tells us about the pairing mechanism and the search for higher \(T_c\) materials.

The Hamiltonian for the bilayer Hubbard model shown in Fig. 1 can be written as

\[
H = -t \sum_{\langle ij \rangle} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) - t_{\perp} \sum_{i} (c^\dagger_{i\uparrow}\sigma c_{i\downarrow}\sigma + \text{h.c.}) - \mu \sum_{i} n_{i\sigma} + U \sum_{i} n_{i\uparrow}n_{i\downarrow}
\]

(1)

Here \(t\) and \(t_{\perp}\) are intra- and inter-layer near neighbor hopping parameters, \(\mu\) is the chemical potential and \(U\) is an onsite Coulomb interaction. The indices \(i\) and \(j\) run over the sites in both the \(m = 2\) (upper) and \(m = 1\) (lower) layers and \(\langle ij \rangle\) implies that only a single \(\langle ij \rangle\) near neighbor hopping is included in the sum. In the following we will measure energies in terms of \(t\) and set \(U = 6\). The bonding \(\langle k_z = 0 \rangle\) and anti-bonding \(\langle k_z = \pi \rangle\) bands are given by

\[
\varepsilon(k) = -2t(\cos k_x + \cos k_y) \pm t_{\perp} \cos k_z
\]

(2)

The \(k_z = 0\) bonding and \(k_z = \pi\) anti-bonding Fermi surfaces (FS) of the non-interacting system are shown in Fig. 1 for a filling \(\langle n \rangle = 0.95\) and two values of \(t_{\perp}/t\). There is an anti-bonding \(\langle k_z = \pi \rangle\) electron-like FS that forms around the \((k_x = 0, k_y = 0)\) \Gamma point of the 2D Brillouin zone and a bonding \(\langle k_z = 0 \rangle\) hole-like FS around the \((\pi, \pi)\) point. For \(\langle n \rangle = 0.95\), the topology of the non-interacting FS changes from two electron-like FS’s to one electron and one hole-like FS when \(t_{\perp}/t\) exceeds a critical value of order 0.1. Here we will focus on the behavior of the bilayer system for \(t_{\perp}/t\) greater than this value, although in some plots we will give the \(t_{\perp}/t = 0\) result. As \(t_{\perp}/t\) increases further, the FS’s shown in Fig. 1

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{a) The bilayer Hubbard lattice with near neighbor intra-layer \(t\) and inter-layer \(t_{\perp}\) hopping parameters and an onsite \(U\) Coulomb interaction. The bonding \(\langle k_z = 0 \rangle\) and antibonding \(\langle k_z = \pi \rangle\) Fermi surfaces for \(t_{\perp}/t = 0.5\) (b) and 2.0 (c) at a filling \(\langle n \rangle = 0.95\). A \(d_{x^2-y^2}\) gap structure is illustrated for the \(t_{\perp}/t = 0.5\) Fermi surface and an \(s^\pm\) gap structure is shown for \(t_{\perp}/t = 2.0\).}
\end{figure}
shrink and for $\langle n \rangle = 1$ the non-interacting system becomes a band insulator when $t_\perp > 4t$. Weak coupling fluctuation-exchange (FLEX) \[9\] as well as phenomenological spin-fluctuation calculations find superconductivity for the doped system with a $d_{x^2-y^2}$-like gap for $t_\perp/t = 0.5$ and an $s^\pm$-like gap for $t_\perp/t = 2.0$, as schematically illustrated in Fig. 1. This two-Fermi-surface model can be seen as an analog of the multi-Fermi-surface Fe-pnictide.

In the following, we will use the DCA to study the Hubbard bilayer with $U = 6$ and $\langle n \rangle = 0.95$. The DCA maps the bulk lattice problem onto an effective periodic cluster embedded in a self-consistent dynamic mean-field that is designed to represent the remaining degrees of freedom. The DCA calculations were carried out on an $N = 2 \times (L \times L)$ cluster with $L = 4$ and the effective cluster problem was solved using a Hirsch-Fye quantum Monte Carlo algorithm \[10\].

The magnetic susceptibility is given by
\[
\chi(q) = \int_0^\beta d\tau \langle m_q^- (\tau) m_q^+ (0) \rangle
\]
(3)

Here
\[
m_q^+ = \frac{1}{\sqrt{N}} \sum_k c_{k+q}^+ c_{k}\n
\]
(4)

and
\[
c_{k} = \frac{1}{\sqrt{N}} \sum_{(\ell,m)} e^{i(k \cdot \ell + k_z m)} c_{\ell m}\n
\]
(5)

Fig. 2 shows plots of $\chi(\pi, \pi, 0)$ and $\chi^{-1}(0)$ versus $t_\perp$ at a temperature $T = 0.4$. For the undoped system at $T = 0$,

the AF order vanishes for $t_\perp \gtrsim 2.0$ and the ground state is a disordered valence bond (VB) phase with a spin gap \[6\]. Here, for the doped system, one sees that for $t_\perp \sim 2$ the near neighbor in plane $(\pi, \pi, 0)$ response is suppressed and as $t_\perp$ increases further, the low energy interlayer spin-fluctuations become gapped as the interlayer valence bond singlets form. This crossover is also clearly seen in the behavior of the inverse spin susceptibility $\chi^{-1}(q = 0)$.

As noted, weak coupling calculations have found both $d_{x^2-y^2}$ ($B_{1g}$) and $s^\pm$ ($A_{1g}$) pairing correlations for the Hubbard bilayer model. Here, in order to probe the superconducting response we have used the DCA to calculate the pairfield susceptibilities.

\[
P_\alpha(T) = \int_0^\beta d\tau \langle \Delta_\alpha (\tau) \Delta_\alpha^\dagger (0) \rangle
\]
(6)

associated with each of these symmetries. For the $d_{x^2-y^2}$-wave we have taken
\[
\Delta_{x^2-y^2}^\downarrow = \frac{1}{\sqrt{N}} \sum_k (\cos k_x - \cos k_y) c_{k^\dagger}^+ c_{-k^\dagger}
\]
(7)

and for the $s^\pm$ case \[11\]
\[
\Delta_{s^\pm}^\dagger = \frac{1}{\sqrt{N}} \sum_k \cos k_z c_{k^\dagger}^+ c_{-k^\dagger}
\]
(8)

Here, $k = (k_x, k_y, k_z)$ with $k_z = 0$ and $\pi$. In Fig. 3 results for these pairfield susceptibilities are shown for different values of $t_\perp$ versus temperature. For $t_\perp = 0.5$,

one sees in Fig. 3a, that the $d_{x^2-y^2}$-wave susceptibility is rising the most rapidly at low temperatures followed by the $s^\pm$-wave response. In Fig. 3b, for $t_\perp = 1.0$ the
The pairing interaction is given by the irreducible particle-particle scattering vertex $\Gamma(K, K')$ which describes the scattering of a singlet pair from the state $(K, -K)$ to $(K', -K')$ with $K = (K, i\omega_n)$. Given this vertex and the dressed single-particle Green’s functions, one can solve the Bethe-Salpeter equation to find the pairing eigenvalues $\lambda_\alpha$ and eigenfunctions $\varphi_\alpha(K)$ [12]. For the bilayer Hubbard model, the leading pairing eigenvalue at small values of $t_\perp$ corresponds to the $B_{1g}$ ($d_{x^2-y^2}$) state and, as $t_\perp$ exceeds 1, switches to the $A_{1g}$ ($s^\pm$) state. A measure of the pairing strength $V_\alpha$ for a given pairing state is

$$V_\alpha = \frac{1/N \sum_{\mathbf{K}, \mathbf{K'} } \varphi_\alpha(\mathbf{K}, \pi T) \Gamma(\mathbf{K}, \pi T, \mathbf{K'}, \pi T) \varphi_\alpha(\mathbf{K'}, \pi T) }{ \sum_{\mathbf{K}} \varphi_\alpha^2(\mathbf{K}, \pi T) }$$

A plot of $V_\alpha$ versus $t_\perp$ is shown on the left hand side of Fig.4. On the right hand side of this figure we have plotted the integrated spin-fluctuation spectral weights for the intra- and inter-layer near-neighbor spin fluctuations

$$I_\nu = \frac{1}{N} \sum_{\mathbf{K}} \int \frac{d\omega}{\pi} \frac{\chi_\nu'(\mathbf{K}, \omega)}{\omega} \cos K_\nu$$

$$= \frac{1}{N} \sum_{\mathbf{K}} \chi_\nu(\mathbf{K}, 0) \cos K_\nu$$

(10)

Here $K_\nu = K_\perp$ for the intra-layer fluctuations and $K_\nu$ for the inter-layer fluctuations, and $\chi_\nu(\mathbf{K}, \omega)$ is the spin-susceptibility calculated on the $2 \times (4 \times 4)$ cluster. As $t_\perp$ increases, the dominant spin-fluctuations change from intra-layer to inter-layer. The inter-layer spin fluctuations give rise to the scattering of pairs between the bonding and anti-bonding Fermi surfaces and lead to $s^\pm$ pairing. We believe that the similarity of the $t_\perp$ dependence of $I_\nu$ and the pairing strengths $V_\alpha$ provides evidence linking the structure of the spin fluctuation spectral weight to the pairing mechanism and the resulting gap structure in this model. This spin-fluctuation picture differs from an alternate strong coupling scenario in which $U$ is assumed larger than the bandwidth and superconductivity is viewed as arising from the melting of a valence bond phase with doping [12]. We believe that the spin-fluctuation picture provides a more appropriate framework for $U$ of order the bandwidth, which corresponds to the parameter region in which the pairing is strongest.

Although we cannot carry out the finite size scaling analysis one would need to determine $T_c$, we have estimated $T_c$ values from the temperature at which the DCA results for $P_\nu(T)$ diverge. We find that the maximum $T_c$ for the $s^\pm$ phase is significantly larger than that for the $d$-wave phase even though, as seen in Fig. 4, the maximum value of $V_d$ exceeds that of $V_{s^\pm}$. This is because, at $\langle n \rangle = 0.95$, the $t_\perp \to 0$ system is near the Mott state and the quasi-particle weight is strongly suppressed. At larger values of $t_\perp$, where $V_{s^\pm}$ peaks, the bilayer system with an intermediate $U = 6$ has moved into a semi-metallic phase which has only a moderate renormalization of the quasi-particles. It is interesting to note that the maximum $T_c$ for the $s^\pm$ phase with $\langle n \rangle = 0.95$ is more than a factor of two larger than the $T_c$ obtained from a corresponding DCA estimate of the single-layer case at optimal doping. In this case, the $T_c$ of the single-layer system has been increased by doping away from half-filling so as to suppress the quasi-particle Mott renormalization. However, this reduces the strength of the pairing interaction. In the bilayer case, one can move away from the Mott region by increasing $t_\perp$ and at the same time still achieve a large interaction strength as shown in Fig.4. Thus we conclude that multi Fermi surface materials can offer a possible pathway to higher $T_c$ superconductivity.

To conclude, in this paper we have reported DCA results for the pair structure and pairing interaction for a bilayer Hubbard model. By increasing the relative size of the inter-layer hopping $t_\perp$ to the intra-layer hopping $t$ at a fixed doping, we have shown that one can tune the system from a $d_{x^2-y^2}$ ($B_{1g}$) superconductor to an $s^\pm$ ($A_{1g}$) superconductor. We then examined the strength of the pairing interactions in these channels as $t_\perp/t$ was varied and showed that they were correlated with the relative strengths of the near-neighbor intra-layer to inter-layer spin fluctuations respectively. When the inter-layer spin fluctuations become dominant, an $s^\pm$ superconducting phase is favored. The ability to change the nature of the superconducting state by varying a one-electron param-
eter in the Hamiltonian represents a useful approach for studying the relationship between the pair structure and the underlying pairing interaction as well as identifying the basic correlations which are responsible for pairing.

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[11] Here we have taken the simplest form factors for a given symmetry. For example, one could take \( \cos k_x - a(\cos k_x + \cos k_y) \) for the \( s^\pm \) case and obtain a better overlap with the leading \( s^\pm \) eigenfunction of the particle-particle Bethe-Salpeter equation. However, as long as one has some overlap, the susceptibility will diverge at the leading pairing instability having \( s^\pm \) symmetry.
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