Effective pairing interaction in a system with an incipient band

T. A. Maier, V. Mishra, and D. J. Scalapino

1Computational Sciences and Engineering Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6164, USA
2Department of Physics, University of California, Santa Barbara, CA 93106-9530, USA

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The nature and mechanism of superconductivity in the extremely electron-doped FeSe based superconductors continues to be a matter of debate. In these systems, the hole-like band has moved below the Fermi level, and various spin-fluctuation theories involving pairing between states near the electron Fermi surface and states of this incipient band have been proposed. Here, using a dynamic cluster quantum Monte Carlo calculation for a bilayer Hubbard model we show that the pairing in these systems can be understood in terms of an effective retarded attractive interaction between electrons near the electron Fermi surface.

The proposal that spin-fluctuation scattering of pairs between the electron and hole Fermi surfaces of the Fe-based superconductors provides the pairing mechanism in these materials is challenged by the occurrence of superconductivity in FeSe monolayers on STO, and K and Li FeSe intercalates. In these materials the hole band near Γ is submerged below the Fermi level leaving only an electron-like Fermi surface (FS) around the M point. Various authors have suggested that an s± pairing state can be formed in which a gap appears on the incipient band with the opposite sign to the gap on the electron Fermi surface.

Here using a dynamic cluster approximation (DCA) quantum Monte Carlo (QMC) calculation for a bilayer Hubbard model we show that this physics can be described in terms of an effective pairing interaction for the fermions near the electron Fermi surface. Unlike the usual momentum dependent spin-fluctuation pairing interaction, this effective interaction is essentially independent of momentum transfer, but depends upon the Matsubara frequency transfer. It is local in space but retarded in time. While the resulting superconducting state is similar to that of the incipient band pairing proposals, the introduction of an effective interaction provides a different perspective on the pairing interaction. In this case, just as in the traditional electron-phonon superconductors, it is the frequency dependence of the pairing interaction rather than its momentum dependence that is important. As a consequence, it is the sign change of the gap with frequency that characterizes the pairing.

The system we will study is a bilayer Hubbard model with

\[
H = t \sum_{\langle i,j \rangle m\sigma} (c^\dagger_{jm}c_{im} + \text{h.c.}) + t_\perp \sum_{i\sigma} (c^\dagger_{i1\sigma}c_{i2\sigma} + \text{h.c.}) -\mu \sum_{im\sigma} n_{im\sigma} + U \sum_{im} n_{im\uparrow}n_{im\downarrow}. \tag{1}
\]

The operator \(c^\dagger_{im\sigma}\) creates an electron on the \(i\)th site of the \(m=1\) or 2 layer with spin \(\sigma\) and \(n_{im\sigma} = c^\dagger_{im\sigma}c_{im\sigma}\). Here \(t\) is the intra-layer near neighbor hopping, \(t_\perp\) the inter-layer hopping and \(U\) the on site interband Coulomb interaction.

The bandstructure for periodic boundary conditions is

\[
\varepsilon_k = 2t(\cos k_x + \cos k_y) + t_\perp \cos k_z - \mu. \tag{2}
\]

The results which will be shown are obtained from a DCA calculation on a \((4 \times 4) \times 2\) cluster with 16 sites in each layer. In the DCA, the momentum space is coarse-grained and thereby the lattice problem is reduced to a finite size cluster embedded in a mean-field that is self-consistently determined to represent the remaining lattice degrees of freedom. This 32-site cluster problem is then solved with a continuous-time auxiliary-field QMC algorithm. While the \(k\) dependence of irreducible quantities, i.e. the single-particle self-energy and the irreducible two-particle vertex functions, is reduced to the 32 cluster momenta, the full lattice \(k\)-dependence is retained in the Green’s function through the dispersion Eq. (2). In this approximation, correlations within a length-scale set by the cluster size are treated accurately by QMC, while longer-ranged correlations beyond the cluster are treated at a mean-field level.

In the following we will set \(t_\perp/t = 2.5, U/t = 8\) and take a filling \(n = 1.15\). For these parameters, the single-particle spectral weight \(A(k, \omega)\), obtained from a Maximum Entropy estimation, plotted in Fig. 1(a), shows evidence of a \(k_z = 0\) electron Fermi surface around the \(M\) point and an incipient \(k_z = \pi\) hole band that has dropped just below the Fermi energy at the \(\Gamma\) point. Consistent with this, the momentum distribution \(\langle n(k) \rangle\) for \(k_z = 0\) shown in Fig. 1(b) sharpens at \(k_F\) as the temperature is reduced, while for \(k_z = \pi\), \(\langle n(k) \rangle\) fades away as \(T\) decreases indicating that the \(k_z = \pi\) band lays below the Fermi energy. Further evidence of an incipient \(k_z = \pi\) band is seen in the behavior of the intrinsic pairfield susceptibility

\[
P_{k_z}^0(T) = \frac{T}{N} \sum_{k_z,\omega_n} \phi^2(\omega_n)G_{k_z}(k, \omega_n)G_{k_z}(-k_z, -\omega_n). \tag{3}
\]

Here we have used a smooth frequency cut-off \(\phi(\omega_n) = (\pi^2T^2 + \omega_n^2)/(\omega_n^2 + \omega_c^2)\) with \(\omega_c = t\). \(G_{k_z}(k, \omega_n)\) is the
dressed single particle propagator associated with the $k_z = 0$ or $\pi$ bands, $k = (k_x, k_y)$ and $\omega_n = (2n + 1)\pi T$ is a Matsubara frequency. The intrinsic pairfield susceptibility is expected to exhibit a Cooper $\log(t/T)$ behavior when there is a Fermi surface. As shown in Fig. 2 one

sees this type of behavior for the $k_z = 0$ electrons, but $P_\pi^0(T)$ for the $k_z = \pi$ hole band remains flat as $T$ decreases.

With this in mind, we consider the pairing interaction $\Gamma(K, K')$ with $K = (k_x, k_y, i\omega_n)$ and $K' = (k'_x, k'_y, i\omega_{n'})$ between fermion pairs near the $k_z = 0$ electron FS. This interaction can be separated into two particle-particle scattering vertices

$$\Gamma(K, K') = \Gamma_1(K, K') + \Gamma_2(K, K'). \quad \text{(4)}$$

The first of these, $\Gamma_1$, involves intermediate pair scattering processes near the electron Fermi surface ($k_z = 0$) while $\Gamma_2(K, K')$ involves the incipient ($k_z = \pi$) hole band. A schematic illustration of $\Gamma_2(K, K')$ is shown in Fig. 3.

$\Gamma_1$ is irreducible in both the $k_z = 0$ and $k_z = \pi$ particle-particle channels while $\Gamma_2$ is irreducible in only the $k_z = 0$ channel. As shown in the Feynman diagram in Fig. 3, $\Gamma_2$ can be written as

$$\Gamma_2(K, K') = -\frac{T}{N} \sum_{K''} \Gamma^0_{0\pi}(K, K'')G_\pi(K'')G_\pi(-K'') \times \Gamma_{\pi0}(K'', K'). \quad \text{(5)}$$

Here the $\Gamma^0_{0\pi}$ vertex involves pairs with $k_z = 0$ near the electron FS which scatters to states in the incipient $k_z = \pi$ band. It is irreducible in both the $k_z = 0$ and $\pi$ two particle channels. The single particle Green’s function $G_\pi(K'')$ is the dressed electron propagator on the incipient band and the vertex $\Gamma_{\pi0}$ is only irreducible in the $k_z = 0$ channel, so that $\Gamma_2$ contains multiple scattering processes involving pairs on the incipient $k_z = \pi$ band.

The important momentum dependence of the pairing interaction which involves the inter-band $k_x - k'_x = \pi$ scattering has been separated out and the $\Gamma$ vertices in Eq. (5) are slowly varying functions of $k_x - k'_x$ and $k_y - k'_y$. 

FIG. 1: (a) The single particle spectral weight $A(k, \omega)$ at $T = 0.2$ for $t_\perp = 2.5$, $n = 1.15$ and $U = 8$ shows an electron pocket around the $(k_x = \pi, k_y = \pi)$ $M$ point for $k_z = 0$ and an incipient hole band laying below the Fermi energy and centered at the $(k_x = 0, k_y = 0)$ $\Gamma$ point for $k_z = \pi$. (b) The momentum occupation $\langle n(k) \rangle$ plotted for $k$ running from $\Gamma$ to $M$ sharpens at the electron FS as the temperature is decreased, and is suppressed at $\Gamma$ as the $k_z = \pi$ band drops below the Fermi energy.

FIG. 2: The intrinsic pairfield susceptibilities $P_0^0(T)$ and $P_\pi^0(T)$ versus $T$. $P_0^0(T)$ exhibits a $\log(t/T)$ Cooper instability associated with the $k_z = 0$ Fermi surface while $P_\pi^0(T)$ for the incipient band remains flat as $T$ decreases.
The important variables are the Matsubara energies $\omega_n$ and $\omega_{n'}$. The gap is an even function of $\omega_n$ so that it is useful for plotting to introduce symmetrized vertices \[ \tilde{\Gamma}(\omega_n, \omega_{n'}) = \Gamma(\omega_n, \omega_{n'}) + \Gamma(\omega_n, -\omega_{n'}) \] (6)

with $\omega_n$ and $\omega_{n'}$ varying over positive Matsubara frequencies. Results for $\tilde{\Gamma}_1(\omega_n, \omega_{n'})$ and $\tilde{\Gamma}_2(\omega_n, \omega_{n'})$ are plotted in Fig. 4 (a-b) for $k$ and $k'$ set to $(\pi, \pi)$. The contribution to the pairing interaction from pair scatterings on the FS, $\tilde{\Gamma}_1(\omega_n, \omega_{n'})$, is positive while the contribution from the virtual pair scattering involving the $k_z = \pi$ band, $\tilde{\Gamma}_2(\omega_n, \omega_{n'})$, is negative. The strength of the attractive $\tilde{\Gamma}_2$ is associated with the spin-fluctuation $k'_z - k_z = \pi$ scattering processes that scatter pairs between the electron Fermi surface and the incipient band. It is this transfer rather than the scattering interactions on the incipient band that is important. The $\omega_{n'} = \omega_n$ cleft in $\tilde{\Gamma}_2(\omega_n, \omega_{n'})$ shown in Fig. 4 (b) corresponds to having zero center of mass energy in this transfer process.

Combining $\Gamma_1$ and $\Gamma_2$, the resulting effective pairing interaction $\Gamma$ is attractive at low Matsubara frequencies and repulsive at higher frequencies. Using $\Gamma$ in the Bethe-
FIG. 5: (a) The leading eigenvalue $\lambda_s(T)$ of the Bethe-Salpeter equation as $T$ decreases. (b) The momentum dependence of the gap function $\phi(k, \omega_n)$ of the leading eigenvalue for $\omega_n = \pi T$ for $k$ values near the FS as shown in the inset and (c) its frequency dependence for $k = (\pi/2, \pi/2)$ for $T = 0.125t$. $\phi(k, \omega_n)$ changes sign leading to a reduction of the effect of the repulsive $\Gamma_1$ interaction on $\lambda_s(T)$.

Salpeter equation \cite{16}

$$\frac{T}{N} \sum_{K'} \Gamma(K, K') G_\pi(K') G_\pi(-K') \phi(K') = \lambda \phi(K)$$ \hspace{1cm} (7)

with $K = (k_x, k_y, \omega_n)$, we find the leading eigenvalue shown in Fig. 5, and the $k$ and $\omega_n$ dependence of the eigenfunction $\phi(k, \omega_n)$ shown in 5b and 5c. As noted, the irreducible vertex $\Gamma(K, K')$, and therefore the eigenfunction $\phi(K)$ only depend on the 32 DCA cluster momenta, while the Green’s function $G(K)$ retains the full momentum dependence of the lattice \cite{17}. The eigenfunction $\phi(k, \omega_n)$ is essentially independent of $k$ as shown in Fig. 5, but changes sign as $\omega_n$ increases. This sign change is such that the gap function is positive over the frequency regime characteristic of the spin-fluctuations.

This is similar to the frequency dependence of the gap in the traditional electron-phonon-Coulomb problem. The eigenfunction $\phi(k, \omega_n)$ is positive when $|\omega_n - \omega_{n'}| < \omega_0$ and then changes sign at higher frequencies leading to a suppression of the repulsive part of the potential. Putting this another way, if the interaction were cut-off when $|\omega_n - \omega_{n'}|$ exceeded several times the exchange energy, the remaining part of $\Gamma_1$ would be replaced by a smaller pseudopotential.

To summarize, in this picture (1) antiferromagnetic order is suppressed as the hole (or electron) band becomes incipient, leaving strong $k' - k = \pi$ spin-fluctuations and (2) the pairing interaction arises from these spin fluctuation scattering processes which involve intermediate states on the incipient band and give rise to an attractive retarded pairing interaction for the fermions on the remaining electron Fermi surface.

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