A toy model of interlayer pair hopping

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We extend the correlated electron model of Baskaran [Mod. Phys. Lett. B5, 643(1991)] to the case of coupled layers. We show that the nature of the non-Fermi liquid ground state leads to the absence of electron-like quasiparticles at the Fermi surface, thereby suppressing coherent transport of electrons between the coupled layers ("confinement"). On the other hand, motion of singlet pairs between the layers is not blocked. We also discuss how pair tunneling can be used to construct a superconducting ground state.
The study of correlated electronic systems has attracted considerable attention in recent times. In particular, the arguments advanced by Anderson and collaborators in favor of (a) failure of Fermi liquid theory in two dimensions [1], (b) spin-charge separation [2], (c) irrelevance of single particle hopping between coupled Hubbard chains and/or planes [3] and (d) interlayer pair hopping [4] have evinced a lot of debate [5]. Though most of these features are present in the one dimensional Hubbard model, the two dimensional model is yet to be solved. Therefore, it would be instructive to examine an interacting system of electrons which would exhibit these features in two and/or higher dimensions. Such a study would further our understanding of strongly correlated electronic systems.

A step in this direction was taken by one of us [6] who proposed and solved a model of strongly interacting fermions in d-dimensions. The advantage of this model is that it can be solved exactly to show the breakdown of Fermi liquid theory and the emergence of spin-charge decoupling, thus illustrating two of the four features we listed above. In this letter, we extend this work to the case of coupled layers and examine the remaining two features, viz., single particle hopping between the coupled layers and interlayer pair hopping. We show that while the non-Fermi liquid ground state leads to a suppression of coherent one-electron motion between the coupled layers, motion of singlet pairs is not blocked. Both these results are obtained exactly. Finally, we discuss how long range superconducting order can be obtained in the presence of a residual intralayer pairing mechanism acting in conjunction with pair tunneling and how the scale of the superconducting transition temperature $T_c$ is governed by the interlayer hopping matrix element $t_\perp$.

We begin by writing the model hamiltonian of ref. [6],

$$H_o = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \ c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + J \sum_{\vec{k}\vec{k}'} \vec{S}_{\vec{k}} \cdot \vec{S}_{\vec{k}'} ,$$  \hspace{1cm} (1)

where $\vec{S}_{\vec{k}} = c^\dagger_{\vec{k}\alpha} \sigma_{\alpha\beta} c_{\vec{k}\beta}$ is the spin operator ($S = \frac{1}{2}$) in momentum space and $\epsilon_{\vec{k}}$ is assumed to be of the form $\hbar^2 \vec{k}^2 / 2m$ for simplicity [7]. The primed sum indicates the absence of the $k = k'$ term in the summand. Thus $H_o$ is a $t - J$ model in momentum space. As shown in [6], $H_o$ can be solved exactly in d-dimensions and the ground state $|G\rangle_o$ is given by
\[ |G\rangle_o = P_S \prod_{k_1<|k|<k_2} c_{k\sigma_k}^\dagger \prod_{|k|<k_1} c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle, \] 

(2)

where \( P_S \) is a singlet projection operator and \( \{\sigma_k\} \) is any \( k \)-dependent spin configuration in momentum space in the singly occupied annulus of radii \( k_1 \) and \( k_2 \) such that the condition \( \sum_{k_1<|k|<k_2} S_k^z = 0 \) is satisfied. The radii \( k_1 \) and \( k_2 \) are determined by the equations

\[
\epsilon_{k_2} - \epsilon_{k_1} = J \\
\sum_{k_1<|k|<k_F} = \sum_{k_2>|k|>k_F},
\]

where \( k_F \) is the Fermi wave vector of the noninteracting Fermi sea. The ground state is therefore a filled doubly occupied Fermi sea up to radius \( k_1 \); between radii \( k_1 \) and \( k_2 \), it is singly occupied and the electrons inside this annulus form a total singlet in momentum space. Therefore, the momentum distribution function \( n_k \) (at zero temperature) is given by

\[
n_k = \begin{cases} 
1 & \text{if } |k| < k_1 \\
\frac{1}{2} & \text{if } k_1 < |k| < k_2 
\end{cases}
\]

As there is no discontinuity in the occupancy at \( k_F \), viz., \( Z_{k_F} = 0 \), the result implies a complete breakdown of Fermi liquid theory. (We note here that it is possible to restrict the range of the \( k \)-space superexchange interaction to a shell of desired width about the Fermi surface, leading to an asymptotic failure of Fermi liquid theory as opposed to a complete breakdown as above.) Since the ground state is known exactly, this feature can also be seen by writing down the explicit form of the one-electron Green’s function \( G(k, \omega) \). \( G(k, \omega) \) is defined in the usual manner as

\[
G(k, \omega) = -i \int_{-\infty}^{+\infty} e^{-i\omega t} \langle T c_{k\uparrow}(t) c_{k\uparrow}^\dagger(0) \rangle \, dt.
\]

We use the equation of motion method to evaluate \( G(k, \omega) \) exactly. The time dependence of \( c_{k\uparrow} \) will be governed by commutators that occur in the equation of motion for \( G(k, \omega) \) such as,

\[
[ H, c_{k\uparrow} ] = -\left( \epsilon_k - \frac{3J}{4} \right) c_{k\uparrow} - J c_{k\downarrow} \sum_p S_p^- - J c_{k\uparrow} \sum_p S_p^z.
\]
The expectation values of such commutators are evaluated with respect to one of the infinitely many ground states. Since the ground state is a total singlet it follows that

\[
\langle c_{k\uparrow}^\dagger \left[ H, c_{k\uparrow} \right] \rangle = -(\epsilon_k - \frac{3J}{4}) \langle c_{k\uparrow}^\dagger c_{k\uparrow} \rangle
\]

(Here, we note that it is not necessary for us to know the exact form of the ground state wave function. We only need to know that the ground state is a total singlet.) A similar line of reasoning will hold good for the higher order terms in the expression for \( c_{k\uparrow}(t) \). This simplifies our calculation of \( G(k, \omega) \) and we find that \( G(k, \omega) \) is given by

\[
G(k, \omega) = \frac{1}{i\omega - (\epsilon_k - \frac{3J}{4})}.
\]

The pole that is present at \( \omega = \epsilon_k \) in the case of the non-interacting system is absent and instead we now obtain a pole at \( \omega = \epsilon_k - \frac{3J}{4} \). The new pole has its residue contributed by one of the many (\( \sim N \)) degenerate states. All these states are characterized by a double occupancy at point \( k \) and one unpaired spin elsewhere in the singly occupied \( k \)-space annulus of radii \( k_1 \) and \( k_2 \). It is this which gives a potentially incoherent character to the spectral weight. For example, by choosing \( J \) in (1) to be dependent on momentum, it is possible to lift the degeneracy of these states and this would spread the pole to a truly incoherent background. This behaviour should be contrasted with the shifted pole structure in say, a mean field CDW or BCS state where the new poles essentially correspond to one or two new eigen states that are not incoherent. Thus it is clear that the shifting of the pole at \( k_F \) is not a simple energy denominator effect or an energy shift effect. We can also see this by considering the motion of singlets, viz., the Green’s function of a singlet pair \( S(k, k'; \omega) \). We define

\[
S(k, k'; \omega) = -i \int_{-\infty}^{+\infty} \langle T \, b_{kk'}(t) \, b_{kk'}^\dagger(0) \rangle \, e^{-i\omega t} \, dt,
\]

where

\[
b_{kk'}^\dagger = \frac{1}{\sqrt{2}} \left( c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\uparrow}^\dagger \right),
\]

is the creation operator of a singlet bond between \( k \) and \( k' \). As in the case of \( G(k, \omega) \), we
can evaluate $S(k, k'; \omega)$ exactly. We find that

$$S(k, k'; \omega) = \frac{1}{i\omega - (\epsilon_k + \epsilon_{k'})},$$

i.e., the pole gets shifted back and the two particle (singlet) Green’s function has the same form as that of the non interacting system! This is essentially due to the singlet correlations induced by the $k$-space superexchange term in $H_o$. Thus we see that while the pole at $k_F$ disappears in the case of the one-electron Green’s function it persists in the two electron (singlet) Green’s function. Obviously, this cannot happen if the vanishing of the pole were a simple energy denominator or an energy shift effect.

We now ask if coherent hopping of electrons between coupled layers is possible in the presence of an interlayer hopping term

$$\sum_{k\sigma} t_\perp(k) \left( c^\dagger_{k\sigma} d_{k\sigma} + h.c. \right),$$

Here, $t_\perp(k)$ is the dispersion along the c-axis and $c$ and $d$ represent the coupled layers. (Though our results are valid for d-dimensions, we shall continue to use the term “layer” throughout.) The hamiltonian $H$ is now given by

$$H = \sum_{k\sigma} \epsilon_k \left( c^\dagger_{k\sigma} c_{k\sigma} + d^\dagger_{k\sigma} d_{k\sigma} \right) + J \sum'_{kk'} \bar{S}_c^{k} \cdot \bar{S}_c^{k'} + \bar{S}_d^{k} \cdot \bar{S}_d^{k'} + \sum_{k\sigma} t_\perp(k) \left( c^\dagger_{k\sigma} d_{k\sigma} + h.c. \right).$$

We check for c-axis current by evaluating the Green’s function

$$G^\perp(k, \omega) = -i \int_{-\infty}^{+\infty} \langle T c^\dagger_{k\sigma}(t) d_{k\sigma}(0) \rangle e^{-i\omega t} dt.$$

If this has a pole structure, it would mean that electrons can be transported along the c-direction. In such a case, the interlayer coupling would be termed a “relevant operator”. We evaluate $G^\perp(k, \omega)$ by defining the operators $\alpha_{k\sigma}$ and $\beta_{k\sigma}$,

$$\alpha_{k\sigma} = \frac{1}{\sqrt{2}} \left( c_{k\sigma} + d_{k\sigma} \right)$$

$$\beta_{k\sigma} = \frac{1}{\sqrt{2}} \left( c_{k\sigma} - d_{k\sigma} \right),$$
and reexpressing the hamiltonian in terms of these operators. It is easily verified that $H$
can be rewritten as

$$H = \sum_{k\sigma} \left[ (\epsilon_k - t_\perp(k)) \beta_{k\sigma}^\dagger \beta_{k\sigma} + (\epsilon_k + t_\perp(k)) \alpha_{k\sigma}^\dagger \alpha_{k\sigma} \right]$$

$$+ \frac{J}{2} \sum_{kk'} S_{k}^\alpha \cdot \bar{S}_{k}^\alpha + S_{k}^\beta \cdot \bar{S}_{k}^\beta + 2 S_{k}^\alpha \cdot \bar{S}_{k}^\beta$$

$$+ \frac{J}{2} \sum_{kk'}' (S_{k}^{\alpha\beta} + S_{k}^{\beta\alpha} \cdot (S_{k'}^{\alpha\beta} + S_{k'}^{\beta\alpha}),$$

where we have defined

$$\bar{S}_{k}^\alpha = \frac{1}{2} \alpha_{k\mu}^\dagger \bar{\sigma}_{\mu\nu} \alpha_{k\nu},$$

$$\bar{S}_{k}^{\alpha\beta} = \frac{1}{2} \alpha_{k\mu}^\dagger \bar{\sigma}_{\mu\nu} \beta_{k\nu},$$ etc.

Since $\langle T c_{k\sigma}^\dagger(t) d_{k\sigma}(0) \rangle = \langle T d_{k\sigma}^\dagger(t) c_{k\sigma}(0) \rangle$ by symmetry, we can write

$$G^\perp(k, \omega) = -i \int_{-\infty}^{+\infty} e^{-i\omega t} \left[ \langle T c_{k\sigma}^\dagger(t) \alpha_{k\sigma}(0) \rangle - \langle T \beta_{k\sigma}^\dagger(t) \beta_{k\sigma}(0) \rangle \right].$$

Though we could not write down the exact ground state wave function we have nevertheless
been able to obtain the exact form of $G^\perp(k, \omega)$ by exploiting the symmetry between the two
layers $c$ and $d$ and by using the fact that the ground state wave function $|GS\rangle$ must be a
total singlet, viz.,

$$\sum_k (S_{k}^{c-} + S_{k}^{d-}) |GS\rangle \equiv 0,$$

(where $S^{c-}$ and $S^{d-}$ are the usual spin lowering operators) as well as the symmetry between
the coupled layers by virtue of which

$$\sum_k S_{k}^{cz} - S_{k}^{dz} |GS\rangle \equiv 0 \text{ etc.},$$

In terms of the $\alpha$ and the $\beta$ operators, we then have the following conditions satisfied by
the ground state $|GS\rangle$.

$$\sum_k (S_{k}^{\alpha-} + S_{k}^{\beta-}) |GS\rangle = 0,$$

$$\sum_k (S_{k}^{\alpha z} + S_{k}^{\beta z}) |GS\rangle = 0.$$
and
\[ \sum_k (S_{k}^{\alpha\beta} - S_{k}^{\beta\alpha}) |GS\rangle = 0 , \]
\[ \sum_k (S_{k}^{\alpha\beta z} + S_{k}^{\beta\alpha z}) |GS\rangle = 0 . \]

Using these conditions, we arrive at the form of the Green’s function for interlayer motion,
\[ G^\perp (k, \omega) \propto \left[ \frac{\langle \alpha^{\dagger} \alpha^{\dagger} k \sigma \rangle}{i\omega - (\epsilon_k - t_\perp (k) - \frac{3J}{4})} + \frac{\langle \beta^{\dagger} \beta^{\dagger} k \sigma \rangle}{i\omega - (\epsilon_k + t_\perp (k) - \frac{3J}{4})} \right] . \]

Since in general, \( \langle \alpha^{\dagger} k \sigma \alpha k \sigma \rangle \) and \( \langle \beta^{\dagger} k \sigma \beta k \sigma \rangle \leq 1 \), we see again that there will be no pole structure in the Green’s function for energies less than \( \frac{3J}{4} \) as in the single layer case. As discussed before, these two poles are also potentially incoherent and modifying the form of \( J \) would spread the pole to an incoherent background. Thus the non Fermi liquid nature of the ground state persists in the presence of interlayer hopping and this causes the bare hopping matrix element to get renormalized to zero. This is the phenomenon of “confinement” which is being studied extensively in coupled Hubbard chains/planes.

We now turn our attention to the Green’s function for singlet transport between the layers \( S^{cd}(k, k'; \omega) \). It is not difficult to see that \( S^{cd}(k, k'; \omega) \) is given by
\[ S^{cd}(k, k'; \omega) \propto \left[ \frac{\langle \alpha^{\dagger} k \uparrow \alpha^{\dagger} k' \downarrow \rangle}{i\omega - (\epsilon_k - t_\perp (k) + \epsilon_{k'} - t_\perp (k'))} + \frac{\langle \beta^{\dagger} k \uparrow \beta^{\dagger} k' \downarrow \rangle}{i\omega - (\epsilon_k + t_\perp (k) + \epsilon_{k'} + t_\perp (k'))} \right] . \]

The pole structure is got back when singlet transport is considered. So we see that while one electron motion between the coupled layers is blocked (the corresponding Green’s function being completely incoherent), singlets can be transported freely. Another way of interpreting this result is to say that while the state describing an electron-hole excitation between the layers, \( c_{k\sigma} d_{k\sigma} |N^c; N^d\rangle \) suffers an orthogonality catastrophe
\[ \langle (N + 1)^c; (N - 1)^d | c_{k\sigma} d_{k\sigma} |N^c; N^d\rangle = 0 , \]
there is a finite overlap between states that are connected by pair hopping, viz.,
\[ \langle (N - 2)^c; (N + 2)^d | b_{kk'}^{d\dagger} b_{kk'}^c |N^c; N^d\rangle \neq 0 . \]
Now that we have shown that it is possible to transport pairs of electrons between the two coupled layers, the next obvious question would be to ask if such a process leads to superconductivity. Since we have calculated the interlayer two particle Green’s function, we can, in principle calculate the Josephson current between the coupled layers and discuss the nature of the superconducting state. But we adopt the following perturbative approach which not only illustrates the pair hopping mechanism but also enables us to compare our results with those obtained earlier in the context of high temperature superconductivity from interlayer tunneling [4], [9], [10]. As we have shown that the interlayer single electron Green’s function does not have a pole at $\epsilon_k$ whereas the two electron (singlet) Green’s function does, it is enough to consider only pair hopping processes that are generated perturbatively. Let us consider the interlayer hopping as perturbing the initial ground state $|G\rangle_o$ by breaking, for instance, a singlet bond between momentum states $k$ and $-k$ with the rest of the wave function being undisturbed. This results in the creation of a particle hole excitation between the layers which we treat as an intermediate state in perturbation theory. It is easy to see that second order perturbation theory leads to an effective interaction of the form

$$-\frac{1}{3} \sum_k t_\perp^2(k) c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger d_{-k\downarrow} d_{k\uparrow}. \quad (3)$$

This hamiltonian resembles the holon pair hopping hamiltonian that was first introduced by Wheatley, Hsu and Anderson [4]. However there is an important difference since the pair hopping interaction above is extremely local in $k$-space. This is because the interlayer hopping matrix element $t_\perp(k)$ (which generates the pair hopping process) conserves the momentum parallel to the layers. The significance of this fact and its implications were first discussed by Anderson [8]. Such a pair hopping hamiltonian has been studied recently by several people [9], [10]. In particular, one can for instance do a mean field calculation with the pairing interaction as given by (3) and obtain the superconducting transition temperature

$$k_B T_c \sim \frac{t_\perp^2(k)_{\text{max}}}{J}.$$

Note that $T_c$ depends on the pairing interaction in a simple manner unlike the BCS case.
But the extreme \((k\text{-space})\) locality of the pairing interaction will suppress any finite temperature phase transition since the phases of various pairing amplitudes \(\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle\) do not get correlated. However, it is clear that any residual pairing interaction such as an intralayer BCS interaction which is non local in \(k\text{-space}\) will correlate the phases of various pairing amplitudes and will result in long range superconducting order. It should be emphasized that the scale of \(T_c\) will still be set by the strength of the pair tunneling interaction rather than that of the intralayer interaction as long as \(\frac{t^2}{J} > V_{BCS}\) [10].

Before we conclude we would like to point out that the model under consideration was introduced to mimic the single occupancy constraint in a realistic model such as the large \(U\) Hubbard model, where it is speculated that forward scattering of a pair of electrons becomes singular asymptotically close to the Fermi surface. The model discussed in this letter does not show this asymptotic behaviour but leads to a complete breakdown of Fermi liquid theory. We believe this model can be made more realistic by introducing a suitable momentum dependent \(J\) in (1). This is a topic of future study.

To summarize, we have been able to illustrate several features of interlayer pair hopping that have been proposed in connection with high temperature superconductivity such as “confinement”, \(k\text{-space}\) locality of the pair hopping interaction and the analytic dependence of \(T_c\) on the strength of the pair hopping interaction. Our results assume added significance owing to the fact we have derived these features from a microscopic hamiltonian, albeit a toy one.

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