Relevance of Interchain Hopping in Correlated Hubbard Chains

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Abstract

We demonstrate that the hopping of singlet electron pairs between Hubbard chains is relevant in the renormalization group sense if appropriate correlations exist between the chains.
Since the discovery of superconductivity in the copper oxide systems by Bednorz and Müller [1] various mechanisms have been proposed to account for the high superconducting transition temperatures in these materials. One candidate, the interlayer pair hopping mechanism [2], offers an explanation for the high transition temperatures in terms of a “blocked” single particle interlayer hopping and a relevant pair hopping between layers. An explanation of how such blocking of the single particle hopping can occur in a strongly correlated system, in spite of the relevance of the hopping operator, has been given elsewhere [3], as has an argument that this effect has already been experimentally observed [4]. Using the assumption of momentum space diagonality [5], pair hopping operators have been constructed which are relevant and lead to mean-field gap equation with a high superconducting transition temperature. In contrast, this paper will instead discuss the circumstances under which the real-space-local pair hopping operator $O_s(j) = (\psi_{1,\uparrow}^+(j) \psi_{1,\downarrow}^+(j+1) - \psi_{1,\downarrow}^+(j) \psi_{1,\uparrow}^+(j+1)) (\psi_{2,\uparrow}^+(j) \psi_{2,\downarrow}^+(j+1) - \psi_{2,\downarrow}^+(j) \psi_{2,\uparrow}^+(j+1)) + h.c.$, can become relevant for a model of coupled Hubbard chains, the prototypical model of an anisotropic, strongly correlated system. How a generalization to Hubbard planes might work will also be discussed.

The motivation for this work came from the recent discovery that the one dimensional Heisenberg model has a peculiar form of off-diagonal long range order [6,7] similar to that of the Fractional Quantum Hall Effect [8]. In particular, the overlap between the groundstate of the Heisenberg model with $N$ sites and the state obtained by adding a pair of sites in a singlet configuration to the groundstate of the $N-2$ site Heisenberg model is finite. This order has important implications for the renormalization group relevance of the operator, $O_s$, which hops singlet pairs of electrons between pairs of Hubbard chains as we now discuss.

The renormalization group relevance or irrelevance of the pair hopping operator, is determined by its scaling dimension. This can be obtained by examining the exponent with which its correlation functions decay for large separations. If $\langle O_s^+(j)O_s(0) \rangle$ decays at long distances like $j^{-2d}$, then $d$ is the scaling dimension of $O_s$. If the scaling dimension is less than 2, then $O_s$ is relevant in the infrared. In perturbing about the independent chains case,
the calculation can be simplified since the $O_s$ correlation function factorizes into the product of the singlet pair correlation functions in the isolated chains. The relevance or irrelevance of $O_s$ is then determined by the divergence or failure to diverge of the isolated-chain, pair susceptibility. For all positive $U$, the pair susceptibility is finite and $O_s$ is irrelevant for Hubbard chains coupled only by singlet pair hopping. We will see that this is not necessarily the case for Hubbard chains which are correlated.

To see how this comes about and what sort of correlations are required, we first discuss the large $U$ Hubbard model, where the exact wavefunction of Ogata and Shiba [9] can be used, together with the results of [7]. The Ogata-Shiba wavefunction is a product of spin and charge wavefunctions. The charge wavefunction is a spinless fermion determinant with the positions of the spinless fermions given by the real electron positions; the spin wavefunction is (for appropriate boundary conditions) the groundstate wavefunction of the Heisenberg model given by Bethe’s solution [10] with the positions of the electrons identified with the sites of the Heisenberg chain. The insertion of a singlet pair of electrons into a large $U$ Hubbard model acts on this wavefunction in a straightforward way, inserting a pair of spinless fermions into the charge wavefunction and a singlet pair of spins into the Heisenberg chain. The result of [7] is that the spin state obtained in this way has finite overlap with the true groundstate of the Heisenberg model with the appropriate number of sites. This allows us to write part of the action on the groundstate wavefunction of a singlet insertion purely in terms of the charge wavefunction: $\psi_{el,\uparrow}(j)\psi_{el,\downarrow}(j + 1) \rightarrow overlap \, \psi_{sf}^+(j)\psi_{sf}^+(j + 1)$

The overlap is just a constant, except for the following consideration: since the momenta of the groundstates of the $N$ and $N + 2$ site Heisenberg models differ by $\pi$, the finite overlap changes sign every time the inserted singlet is displaced one site in the Heisenberg model or past one electron in the large $U$ Hubbard model. This means that $\psi_{el,\uparrow}(j)\psi_{el,\downarrow}(j + 1) \rightarrow const \, e^{i\pi \sum_{j<i} n_j} \psi_{sf}^+(j)\psi_{sf}^+(j + 1)$ where the constant is a number of order unity (see [7]). The correlation function of $\psi_{sf}^+(j)\psi_{sf}^+(j + 1)$ with its Hermitean conjugate is just a free fermion correlation function and so decays like $j^{-2}$. This would make pair hopping marginally relevant even at infinite $U$, except for the presence of the alternating sign induced
by $e^{i\pi \sum_{i<j} n_j}$. To make the pair susceptibility of an isolated Hubbard chain diverge we could modify its correlations so that there was an expectation value for $-1$ raised to a power given by the number of particles to the left of site $j$. This would involve radically changing the correlation structure of the chain, in effect requiring electrons to come in pairs. The only obvious way to do this is to change the sign of $U$, in which case finding a diverging pair susceptibility is not surprising. Negative $U$ models are unlikely to be relevant to the cuprates. Fortunately we are interested in the pair susceptibility only for what it can tell us about the relevance of the interchain pair hopping operator. In that case, the operator that needs to acquire and expectation value is $-1$ raised to the power given by the total number of particles in both chains to the left of site $j$. States with this property can be constructed for positive $U$ and a reasonable choice for the interchain coupling as explained below.

In order to discuss which types of correlations between the chains satisfy this requirement it is convenient to introduce the Abelian bosonization formalism or Luttinger liquid approach to the one dimensional Hubbard model $[\text{11,12}]$. In that language the effective low energy Hamiltonian of the Hubbard model becomes:

$$H = \frac{1}{4\pi} \int dx \left( v_\rho K_\rho (\partial \Theta_\rho)^2 + v_\rho K_\rho^{-1} (\partial \Phi_\rho)^2 + v_\sigma K_\sigma (\partial \Theta_\sigma)^2 + v_\sigma K_\sigma (\partial \Phi_\sigma)^2 \right)$$

(1)

where $K_\rho$ is $U$ dependent ranging from 1 at $U = 0$ to $\frac{1}{2}$ as $U \to \infty$, $K_\sigma$ is fixed at unity by $SU(2)$ invariance and bosonic representations of all operators can be constructed from those of the electron operator $[\text{11}]:$

$$\Psi^\dagger_\uparrow(x) \sim \sqrt{\frac{\partial \Phi_\uparrow(x)}{\pi}} \sum_{m \text{ odd}} \exp \left( i [m \Phi_\uparrow(x) + \Theta_\uparrow(x)] \right)$$

(2)

In particular, the bosonized form of the pair insertion operator is given by:

$$\Psi^\dagger_\uparrow(x) \Psi^\dagger_\downarrow(x) \sim \frac{1}{\pi} \sqrt{\partial \Phi_\uparrow(x) \partial \Phi_\downarrow(x)} \sum_{m,n \text{ odd}} \exp \left( i [m \Phi_\downarrow(x) + \Theta_\downarrow(x) + n \Phi_\uparrow(x) + \Theta_\uparrow(x)] \right)$$

$$\sim \rho_0 \exp \left( i \Theta_\rho(x) \right) \cos \Phi_\sigma(x) + \ldots$$

(3)

where $\rho$ and $\sigma$ subscripts label the symmetric and antisymmetric combinations of the up and down spin phase fields. The bosonized form of the pair hopping operator is given by:
where \( S \) and \( A \) subscripts label symmetric and antisymmetric combinations of the phase fields of the two chains. The leading contribution to the bosonized form of 
\[
O_s(x) \sim \rho_0^2 \cos \Theta_{p,A}(x) \left[ \cos \Phi_{\sigma,A} + \cos \Phi_{\sigma,A} \right] + \ldots
\]
(4)

acquire expectation values (provided things are not contrived so that several of the above acquire expectation values which sum to zero). The first of the cosines can not acquire a non-zero expectation value for a generic filling fraction while, following equation 4, the second would introduce a gap into the antisymmetric, charge sector of the model so that the correlation functions of \( O_s \) would decay exponentially. However, an expectation value for either of the other two cosine operators will dramatically enhance the correlations of \( O_s \), as can clearly be seen from equation 4 as well as from the more physically intuitive argument we have given for large \( U \).

It is clear that to produce an expectation value for a cosine operator whose argument is a combination of the spin phase fields in the different chains, we need to correlate the spin structure between the two chains. Phenomenologically, many of the cuprate compounds exhibit “spin gap” behavior [13] and the fact that this behavior is clearest for the two-layer per unit cell compounds [14,15] suggests that the spins in different layers are indeed correlating at low temperature in the cuprates. Further, density matrix renormalization group studies of Hubbard chains coupled by an interlayer hopping find a spin gap phase for a broad range of hopping strengths [16]. It is therefore natural to seek two-chain spin sector
states which posses a spin gap and an expectation value for either $\cos \Phi_{\sigma,S}$ or $\cos \Phi_{\sigma,A}$. One candidate state is the analogue of the disordered state found for coupled Heisenberg chains \[\text{[17]}\] where $\cos \Theta_{\sigma,A}$ and $\cos \Phi_{\sigma,S}$ take on expectation values. This state should result if the dominant coupling between the two chains is an antiferromagnetic coupling of the small momentum pieces of the spin density operators. The spin coupling operator then takes the form $\cos \Phi_{\sigma,S} \cos \Theta_{\sigma,A}$ and is marginally relevant for an antiferromagnetic coupling. Since the symmetric and antisymmetric sectors are decoupled this should lead to expectation values for $\cos \Phi_{\sigma,S}$ and $\cos \Theta_{\sigma,A}$, separately. The dual state where $\cos \Phi_{\sigma,A}$ and $\cos \Theta_{\sigma,S}$ acquire expectation values also has the correct properties, but we are unaware of any operator which would naturally give rise to this state.

In the former state, as a consequence of the expectation value for $\cos \Phi_{\sigma,S}$, the singlet pair hopping, $O_s$, contains a piece given by $\text{const.} \cos \Theta_{\rho,A}$. This operator is relevant with scaling dimension $K_{\rho}^{-1}$, ranging between 1 and 2 for the positive $U$ Hubbard model \[\text{[18]}\], and can be expected to dominate the low energy physics. In the infinite $U$ limit, the charge sector of the model can be re-fermionized, with the operator, $\cos \Phi_{\sigma,S}$ becoming nothing more than pair hopping of the otherwise free, spinless fermions. The equivalent, refermionized model is two chains of free spinless fermions coupled only by a hopping between the chains of pairs of fermions at opposite Fermi points. In effect, hopping a singlet pair of electrons is equivalent to hopping a pair of free holons. (Note that the charge part of the electron operator in one dimension is a semion, not a spinless fermion, and that it is only the hopping of a pair of electrons which can be written in terms of the hopping of a pair of spinless fermions, and then only in the large $U$ limit for correlated chains; the “holon” we are discussing is a true spinless fermion and not equivalent to some of the other uses of the term.) Although the one-dimensional, two chain version can not acquire long range pairing order of its holons, a higher dimensional analogue of this state is ideal for realizing the interlayer pair hopping mechanism for high $T_c$ and one would expect the hopping to act as an effective attractive interaction, leading to holon pairing.

It is interesting to see how the invariance of the pair insertion to a spatial interchange of
the electrons in a Cooper pair would occur in the above framework. The electron insertion is equivalent to a singlet insertion plus a holon pair insertion, and the holon pair insertion is odd under a spatial interchange so that the eveness of the electrons under spatial interchange occurs only because the singlet insertion is also odd under spatial interchange. The holon and spinons are effectively \( p \)-wave paired so that electrons are either \( s \) or \( d \)-wave paired, which are the same in one dimension. If the correct two dimensional generalization of the solution of the one dimensional Hubbard model has an analogous version of spin-charge separation to the one dimensional solution then one expects to find the pairing of spinless fermion holons at large \( U \) in a \( p \)-wave channel, and, since the singlet insertion is odd under a 180\(^\circ\) rotation of the singlet pair, the natural symmetry for the electron pairing would actually be \( d \)-wave. Since the singlet is tied to the real space lattice, \( d_{x^2-y^2} \) is the natural choice.

The resulting phenomenology is in excellent agreement with that observed in the bilayer cuprates, including the lack of correlation of \( T_c \) with \( \rho_{ab}(T)/T \) emphasized by Anderson [19], the strong correlation of \( T_c \) with the number of layers [2], the gap symmetry and the presence of a spin gap phase. For materials with one or three layers per unit cell a theory of two coupled chains is clearly a bad starting point. The evidence for the absence of a spin gap in these materials [13,14] is therefore not inconsistent with the idea of interlayer spin correlations, which we require here to change the relevance of the pair hopping. The spins in odd layer per unit cell compounds may still correlate with each other, but, with an odd number of layers per unit cell, there is no natural way to put everything into singlets and gap the entire spin spectrum.

Coupled Hubbard chains have been studied previously in references [20], [21] and [22], none of which considered the scenario envisioned here for reasons which we now discuss briefly. The first set of works focused on the relevance of single particle hopping between Hubbard chains. A single particle hopping operator with an appreciable coefficient should be present in the cuprates; we have chosen to ignore the effects of single particle hopping for several reasons. First, the theoretical work of [3] suggests that for strongly correlated,
anisotropic systems the coherent effects of single particle hopping may vanish, despite the relevance of the hopping operator, while [4] argued that this effect has already been observed experimentally. Second, photoemission data of [23], which have an energy resolution of 8 meV, show no evidence of the Fermi surface splitting for the coupled planes in BISCO 2212, despite that fact that a coherent single particle hopping should produce such a splitting for the Fermi surfaces of the symmetric and antisymmetric fermions and the scale of the splitting predicted by band theory calculations is of order tenths of an electron volt [24]. Lastly, the highly anisotropic resistive properties of the cuprates essentially rule out coherent three dimensional transport [25] suggesting that single particle interlayer hopping is not dominating the low energy physics as would naively be expected. We therefore believe it is appropriate to consider a model where the single particle hopping is neglected.

References [21] and [22] focused on Hubbard chains with an antiferromagnetic coupling of the $2k_F$ pieces of the spin operators in the two chains. These works were primarily concerned with how an isolated two dimensional Hubbard model might be better understood through the study of coupled Hubbard chains. In this context those works noted that the resulting expectation values for $\cos \Phi_{\rho,A}$, $\cos \Theta_{\sigma,A}$ and $\cos \Phi_{\sigma,S}$ lead to an enhanced tendency towards interchain pairing and the formation of a spin-gap. If one believes that high temperature superconductivity and spin gap behavior are present for isolated copper oxide planes then these are significant results. On the other hand, considered as a one-dimensional version of coupled planes, their state would be unfavorable to interlayer pair hopping because the antisymmetric charge sector has a gap, leading to the exponential decay of the correlations of $O_s$ and so is not a candidate for the effects we are interested in.

Their state is clearly relevant to Hubbard chains with a weak antiferromagnetic coupling, since the coupling of the $2k_F$ pieces of the spin operator is more relevant that the coupling of the small momentum pieces. On the other hand there are a number of reasons to prefer an analogue of the state without a charge gap for the cuprates. One reasons is that, at half-filling, the two dimensional analog of the $2k_F$ piece of the spin operator in one dimension is the Neel order parameter. Coupling the Neel order in two planes will produce optical and
acoustic magnons rather than a spin gap, so if one attributes spin gap behavior to interlayer
coupling (rather than intralayer physics as intended in [21,22]) the coupling focused on in
those works does not lead to a spin gap in two dimensions. Away from half-filling, there
in no clear analogue of the $2k_F$ piece of the spin operator and the the spin operator should
involve low energy pieces with (if there is Fermi surface) all momenta which span the Fermi
surface. This should disfavor a state based on a particular wavevector, which would be the
analogue of $2k_F$. Another factor favoring the operator we consider is that the spin energy
scale is much smaller than the charge energy scale for the large $U$ Hubbard model, so an
operator which seeks to modify only spin degrees of freedom should be correspondingly more
effective at a given strength than one that require the modification of both spin and charge
degrees of freedom. Further, coupled plane states analogous to that of [21,22] would have
an interlayer pairing similar to that discussed in [26]. The drawback of such a state is that
an interlayer pair should transform trivially under rotations in the $ab$ plane [20] whereas
current experimental evidence strongly supports a gap transforming with $d$-wave symmetry
[27]. Finally, there is the issue of the exact effects of the relevant single particle hopping
operator which should be present in any model meant to be relevant to the cuprates. Both
the interchain correlations discussed here and those discussed in [21] and [22] require that
it be possible to effectively eliminate $t_\perp$, the interchain hopping. This can be done as in
[22] for a more general model where the spin-spin coupling between the chains in introduced
independent of the interchain hopping so that it can dominate over $t_\perp$ simply because of its
coefficient. However, if one takes the perspective that any spin coupling between the chains
should arise as a superexchange coupling obtained from integrating out the single particle
hopping, then the problem arises that $t_\perp$ is more relevant than the spin-spin coupling and
should dominate the physics. It is possible [28] that this operator is removed by incoherence
effects resulting from strong interactions so that it one can effectively integrate out $t_\perp$ and
consider the operators generated at higher order, however, no rigorous prescription exists
for doing so since it would require a full understanding of the strong-coupling, incoherent
fixed point proposed in [3] which is not presently available. In the absence of such an
understanding, it is not clear that the operator which is more relevant at the $t_\perp = 0$ fixed point need dominate the flow away from the strong-coupling, incoherent fixed point. We have therefore chosen to consider a state dominated by the coupling of the non-alternating pieces of the spin operator.

In summary, we have considered a model of coupled Hubbard chains different than those considered previously and have found that appropriate correlations between the chains can lead to the renormalization group relevance of the interchain pair hopping operator. The relevance can be considered to result from the hidden ODLRO of the one dimensional Heisenberg chain \[7\] together with interchain correlations. The most reasonable candidate for such correlation is a state resulting from coupling the small momentum pieces of the spin operators in the two chains, leading to a spin gap. The resulting state would realize an interchain version of the interlayer tunneling theory of superconductivity \[2\], provided that the divergent, one-dimensional fluctuations of a single pair of chains were stabilized by some coupling to the other pairs in a three dimensional array of such chains. The natural generalization to coupled planes should exhibit $d_{x^2-y^2}$ symmetry, a spin gap and a high transition temperature dependent on the interlayer coupling, but not on the in-layer resistivity, in precise agreement with the phenomenology of the high $T_c$ cuprates.

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$$\Delta E = -\sum_m \frac{|\langle 0 | H' | M \rangle|^2}{E_m}$$  \hspace{1cm} (9)

or if $H' = \lambda O$ then

$$\Delta E = -\lambda^2 \int \frac{d\omega}{\omega} \rho_O(\omega)$$  \hspace{1cm} (10)

where $\rho_O(\omega)$ is the spectral function for the operator $O$ defined to be $\sum_m |\langle 0 | O | M \rangle|^2 \delta(E_M - \omega)$. For spectral functions which do not vanish as $\omega \to 0$ the shift is logarithmically divergent, signalling that the perturbation, $H'$, must be treated in nearly degenerate perturbation theory, not in ordinary perturbation theory and the
usual approach to integrating it will generate nonsensical answers. Our definition for coherence is essentially that the spectral function does not vanish sufficiently quickly. For $t_\perp$ this situation is complicated by the effects of the Fermi statistics of the electrons on the spectral function. For free particles, the spectral function of $t_\perp$ vanishes identically since Fermi statistics prevent any hops in the ground state, however, $t_\perp$ clearly needs to be treated in degenerate perturbation theory and is coherent. We believe that the essential point still holds that the coefficients of operators generated at second order will diverge unless the response to the perturbation is incoherent. More detailed arguments will be given elsewhere [29].

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