Bi- and Tri-layer splittings in a new formulation for the $t-J$ model of cuprates

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Abstract

The $t-J$ model of the cuprates is formulated in a novel fashion in terms of a single spin and charge particle along with flux tubes. The theory has been developed[1,2] to simulate ARPES spectra and this earlier formulation is here applied to compare the $\mathbf{k} = \{\pi, 0\}$ spectra for mono, bi- and tri-layer Bi cuprates.

Key words: High T_c cuprates; theory $t-J$ model; ARPES; multi-layer cuprates

The theory described here[1,2] is based upon the standard $t-J$ model,

$$H = -t \sum_{<ij>\sigma} \tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma} + J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $< ij >$ indicates a sum on near-neighbours and where the tilde on $\tilde{c}^\dagger_{i\sigma}$ implies no double occupation. The formulation [1,2] is based upon the Jordan-Wigner (J-W) transformation. There is a single particle for each of the spin and charge sectors. The fermion $f^\dagger_n$ creates an up spin and $b^\dagger_n$ a hole at site n, these relative a vacuum which has a down spin at every site. The J-W transformation is realised using *unitary* operators, $u^\dagger_n = \exp[-i\int_0^{n-1}\mathbf{a}\cdot d\mathbf{r}]$ where $\mathbf{a}$ is the vector potential due to flux tubes attached to each particle and where 0 is an arbitrary origin. A physical electron creation operator is $c^\dagger_{n\uparrow} = f^\dagger_n b_n$ or $c^\dagger_{n\downarrow} = u^\dagger_n b_n$ while, e.g., the spin raising operator is conveniently written as $S^+_n f^\dagger_n u_n$ while $S_{zn} = f^\dagger_n f_n - 1/2$. The representation of H is similar to that for slave bosons *except* that the down spin fermion has been replaced by the flux tube operator[1,2].

In analogy with the quantum Hall effect, the flux tubes are non-trivial. The vacuum $|-N/2\rangle$, the fully aligned, ferromagnetic state, is highly degenerate. The state $|-N/2+1\rangle \propto S^+|-N/2\rangle$ is equivalent due to the rotation invariance of H. Special for the non-polarised state is the vacuum $|0\rangle$ which has the *total* $S_z = 0$. *Any* state with $S_z = 0$ can be projected out from this. The $u^\dagger_n$ can be commuted past such a projection to act directly on $|0\rangle$. Consider an operator such as $S^+_n = f^\dagger_n u_n$. Since there is a $f^\dagger_n$ to the left $u_n|0\rangle = f_n u_n f^\dagger_n|0\rangle = f_n S^+_n|0\rangle$. The expansion of $S^+_n = (S^+/N) + \ldots$ so that $u_n|0\rangle$ contains a vacuum off-diagonal term $(1/N)f_n[S(S+1)]^{1/2}|1\rangle = (1/2)f_n|1\rangle$, where in the matrix element, $S = N/2$ and is large. The net effect is $u_n|0\rangle \to (1/2)f_n|1\rangle$, i.e., the action of u_n is the same as the effect of f_n *plus* a change in the vacuum state. The vacuum *diagonal* matrix element of u_n is simply a phase factor determined by the particle positions.

This dual role of the flux tubes reflected by u_n allows the formalism to contain both spinwave and spinon excitations in a natural way. The vacuum diagonal part of $S^+ = f^\dagger_n u_n$ creates a single $S = 1$ spinwave. The vacuum off-diagonal part $S^+ \to f^\dagger_n f_n$, i.e., leads to particle-hole *spinon* excitations. The vacuum diagonal part of $c^\dagger_{n\downarrow} = u^\dagger_n b_n$ corresponds to a boson plus unit flux tube and is a composite fermion, while off-diagonal part $c^\dagger_{n\downarrow} \to f^\dagger_n b_n$ and is a boson-holon-fermion-spinon-particel-hole pair.

In general the *low energy* excitations are spinons and

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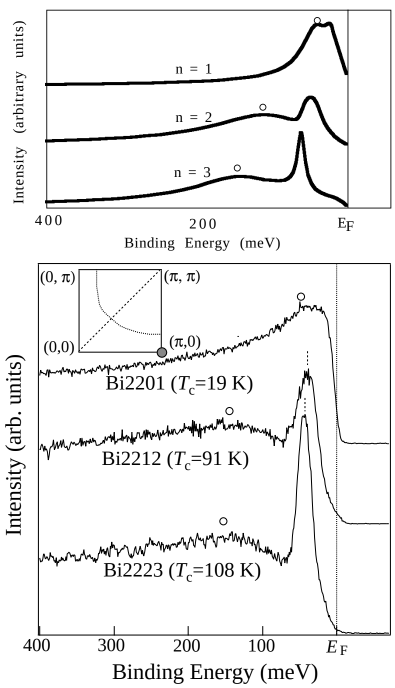

Fig. 1. The top panel is a theoretical simulation of ARPES spectra for a n-layer system, using the theory[1,2]. Details of parameters will be given elsewhere. The botom panel shows experiment of [3] for Bi materials.

holons since on the long time scale the spinwave and composite fermions are destroyed by averaging of the $u_n^\dagger$ phases. As in many theories, the fermion spinons form a d-wave BCS type ground state[2]. The *high energy hole excitations* see an approximately frozen spin configuration and *are* composite fermions which leads to a band width $\sim 8t$. The low energy boson holons condense at low temperatures. The low energy decomposition of a physical electron into spinon and holons thereby also has two parts, e.g., $c_{n\downarrow}^\dagger \to f_n^\dagger b_n \to f_n^\dagger \langle b_n \rangle + f_n^\dagger b_n'$ where b_n' is the operator for the non-condensed part of the holon field. Again, as in other approaches, the part $f_n^\dagger \langle b_n \rangle$ of $c_{n\downarrow}^\dagger$ implies that the spinon density of states is reproduced at the Fermi level in the physical electron density of states. Here, since the filled states correspond to up spin, and the empty states down spins, this band *must* have particle-hole symmetry reflecting the equivalence of the two spin directions, i.e., the spinon band at the Fermi surface is half-filled independent of doping[1,2]. A physical electron can also propagate as a spinon-holon-particle-hole pair. With a condensate, the holon energy is pinned to the chemical potential, i.e., to the physical electron Fermi level, which in turn coincides with the spinon Fermi level. It follows the that the spinon-holon-particle-hole propagator also forms a band centered at the Fermi level.

The present authors have distilled this approach into an approximate expression[2] which can be used to simulate the density of states near the Fermi surface and hence be compared with ARPES data. In these simulations the superconducting peaks appear with holon condensation at T_c and reflect the $f_n^\dagger \langle b_n \rangle$ part of $c_{n\sigma}^\dagger$. The spinon-holon-particle-hole part $f_n^\dagger b_n$ is reflected as a "quasi-particle" band. These two contributions to $c_{n\sigma}^\dagger$ mix and interact.

Some of the above is illustrated by the differences between single bi- and tri-layer Bi high T_c cuprates with $\mathbf{k} = \{\pi, 0\}$. Both the simulations based upon the present theory and experiment[3,4] are shown in Fig. 1. The parameters used in the simluations are similar to those detailed in earlier work[2] but adapted to different hole concentrations x, gaps and condensed fractions. Details of the simulations will be given elsewhere. The mono-layer compound shows no coherence peak mainly because both the condensed fraction 0.45 along with the gap are small and the coherence peak is absorbed into the quasi-particle resonance for this angle. For the bi-layer system the gap is almost twice as large and condensed fraction in the theory has been increased to 0.55. The bonding band lies about 150 meV below the Fermi surface, reflecting the maximum bi-layer splitting, and the coherence peak seen below the Fermi surfaces actually belongs to the anti-bonding band which is above. In the tri-layer system the condensed faction 0.6 is again larger as is the gap. The simulations indicate that for $\mathbf{k} = \{\pi, 0\}$ the coherence peak arises mainly from the non-bonding band despite the fact that the larger gap and T_c is most probably due to a larger pair amplitude in the middle layer.

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