Moments of the ARPES spectral function of an undoped Mott insulator.

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We derive analytic expressions for the first three frequency moments of the single particle spectral function for one hole in a Mott insulator in terms of equilibrium spin correlation functions of the insulating state. We show that the “remnant Fermi surface” detected in ARPES experiments is, in fact, a reflection of the strong antiferromagnetic correlations of the system, not a reflection of the original band-structure Fermi surface. We suggest that ARPES data could be used to measure the magnetic specific heat.

I. THE CALCULATION

A. Half-filled Hubbard model at large U

The large U Hubbard model at half filling is the simplest model that produces the large charge gap and the antiferromagnetic tendencies observed experimentally in CuO planes. The Hamiltonian,

\[ \hat{H} = -\sum_{\sigma,i,j} t_{ij} C_{i,\sigma}^\dagger C_{j,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow} \]

contains a strong onsite repulsion term \( U \sum_j n_{j,\uparrow} n_{j,\downarrow} \) that freezes (together with the lattice potential) charge motion at half-filling provided that the kinetic energy term is small enough to be treated as a perturbation, \( |t_{ij}| \ll U \).

When \( t_{ij}/U = 0 \) the ground state consists of singly occupied sites, has energy zero, is \( 2^N \)-fold degenerate where \( N \) is the size of the system, and is completely characterized by the spin configuration, \( \{S_i\} \).

The perturbative effects of the kinetic energy modify all of the above statements except the last one: each of the perturbed states, though it contains an admixture of doubly occupied sites, can still be labeled by the spin configuration of the unperturbed state from which it has evolved. Thus the expectation value of any operator in the ground state manifold can always be expressed in terms of spin variables. Formally this is accomplished by computing perturbatively in powers of \( t_{ij}/U \) the unitary transformation \( \exp[i\hat{X}] \) that expresses the evolution of the low energy unperturbed states \( \{|S_i\} \rangle \) as a function of increasing kinetic energy

\[ \langle \{S_i\} \rangle = e^{-i\hat{X}} \langle \{S_i\} \rangle > \]

\[ < \hat{O} > = < \{S_i\} | e^{i\hat{X}} \hat{O} e^{-i\hat{X}} | \{S_i\} >, \]

where \( \hat{O} \) is any observable.

In the familiar fashion, this transformation maps the low energy physics of the Hubbard Hamiltonian into an effective Heisenberg antiferromagnet whose leading term is:

\[ \hat{H}_{\text{eff}} = e^{i\hat{X}} \hat{H} e^{-i\hat{X}} \]

\[ = -\frac{1}{2} \sum_{i,j} 4t_{ij}^2 \left( 1 - \hat{S}_i \cdot \hat{S}_j \right) + \mathcal{O}(t_{ij}^4/U^3). \]
B. The spectral function

The emission spectral function is

\[ A(\tilde{k}, w) = \frac{1}{2} \sum_{\sigma, m, n} e^{-\beta E_n} \langle m | C_{\tilde{k}, \sigma}^\dagger n > | 2 \delta(\omega + E_m - E_n) \]

\[ = \frac{1}{2} \sum_{\sigma} \int dt e^{iwt} < C_{\tilde{k}, \sigma}^\dagger(t) C_{\tilde{k}, \sigma}(0) >. \tag{5} \]

Frequency moments of \( A(\tilde{k}, w) \) correspond to ground state (or thermodynamic) averages of the following operators:

\[ n_\tilde{k} = \int \frac{d\omega}{2\pi} A(\tilde{k}, \omega) = \frac{1}{2} \sum_{\sigma} < C_{\tilde{k}, \sigma}^\dagger C_{\tilde{k}, \sigma} > \tag{6} \]

\[ A_1(\tilde{k}) = \int \frac{d\omega}{2\pi} \omega A(\tilde{k}, \omega) \]

\[ = -\frac{1}{2} \sum_{\sigma} < C_{\tilde{k}, \sigma}^\dagger [\hat{H}, C_{\tilde{k}, \sigma}] > \tag{7} \]

\[ A_2(\tilde{k}) = \int \frac{d\omega}{2\pi} \omega^2 A(\tilde{k}, \omega) \]

\[ = \frac{1}{2} \sum_{\sigma} < C_{\tilde{k}, \sigma}^\dagger [\hat{H}, [\hat{H}, C_{\tilde{k}, \sigma}] ] >. \tag{8} \]

A systematic evaluation of these averages, using the perturbative expression for \( X \) in powers of \( t_{ij} / U \), can be found in the Appendix.

II. THE SPECTRAL WEIGHT, \( n_\tilde{k} \)

We begin with a discussion of the spectral weight because it has an immediate physical interpretation as the occupation probability. As shown in the Appendix,

\[ n_\tilde{k} = \frac{1}{2} [1 - \frac{4\epsilon_\tilde{k}}{U} + O(t^3/U^3)] \tag{9} \]

where

\[ \epsilon_\tilde{k} = -\sum_j S_{0j} t_{0j} e^{i\tilde{k} \cdot \tilde{R}_j} \tag{10} \]

and

\[ S_{ij} = < \frac{1}{4} - \tilde{S}_i \cdot \tilde{S}_j >. \tag{11} \]

is the equilibrium spin correlation between spins i and j. \( \epsilon_\tilde{k} \) is a sort of renormalized band energy in which each hopping matrix element \( t_{ij} \) is renormalized by a factor of \( S_{ij} \). However, this renormalized energy does not correspond in any simple way to the energy of any elementary excitation of the system. Note that the non-interacting free electron band is given by \( \epsilon_\tilde{k} = -\sum_j t_{0j} e^{i\tilde{k} \cdot \tilde{R}_j} \).

This expression for \( n_\tilde{k} \) can be derived in a different, simpler manner, which is readily generalizable to more complicated situations, such as the three band Cu-O or Emery model. From the Hellman-Feynman theorem, it follows that

\[ \sum_{\sigma} < [c_{\tilde{k}\sigma}^\dagger c_{\sigma} + H.C.] >= -\partial E / \partial t_{ij} = [\partial J_{ij} / \partial t_{ij}] S_{ij} \]

where \( E \) is the internal energy, which can be computed using the effective Hamiltonian \( \hat{H}_{eff} \). From the expression for \( J_{ij} \) in terms of \( t_{ij} \), the result in Eq. 4 follows immediately.

A. The remnant fermi surface

At low temperatures, the short-range spin correlation functions are essentially temperature independent, and equal to their value in the ground state. To be concrete, let us consider the Hubbard model with nearest, second, and third neighbor hopping, \( t, t', \) and \( t'' \), respectively; this sort of model was used in the numerical studies to fit the dispersions seen in ARPES. The zero temperature spin correlations of the corresponding spin 1/2 Heisenberg model have been computed fairly accurately in numerical studies. For the Heisenberg model with only nearest-neighbor exchange coupling, the spin correlation functions are \( S_{01} \approx 7/12 \) and \( S_{03} \approx S_{02} \approx \frac{1}{20} \) between nearest, next-nearest, and third nearest neighbor sites, respectively. These correlations are, moreover, found to be relatively insensitive to the inclusion of a modest amount of further neighbor exchange couplings, which anyway are expected to be quite small since \( J'/J = [t'/t]^2 \).

In computing \( \epsilon_\tilde{k} \) the antiferromagnetic correlations between neighboring spins imply a factor of 1/2 renormalization of \( t \), compared to a factor of 1/20 renormalization of \( t' \) and \( t'' \). Since in most cases of physical interest, \( |t'|, |t''| \ll 10|t| \), even when \( t' \) and \( t'' \) are large enough to make significant shifts in the original Fermi surface defined by \( \epsilon_\tilde{k} \), the occupation probability is well approximated (Figure 1) as

\[ n_\tilde{k} \approx \frac{1}{2} [1 - \frac{7(t \cos(k_x) + \cos(k_y))}{3U}] \tag{13} \]

It is both \( \frac{1}{2} \) and has the steepest slope along the Fermi surface of the non-interacting electrons with only the nearest neighbor hopping. In fact, ARPES experiments that observe such momentum dependence of \( n_\tilde{k} \) have been interpreted as an indication that there is a “remnant Fermi surface” in the undoped Mott insulator. By contrast, our result suggests that the observed \( n_\tilde{k} \) is reflective of the the spin physics of the strongly correlated Neel state rather than a vestige of the original Fermi surface.
corresponding to a summation over sites a given near-neighbor distance away on the square lattice.

\[ A_n(\vec{k}) = \sum_j A_j^2 \gamma_j(\vec{k}), \]
\[ \gamma_j(\vec{k}) = \sum_{\vec{R}=j^n \mu n.n.} e^{-i\vec{k} \cdot \vec{R}^i}, \]  

One notices that all computed moments are finite. Although the existence of the moment expansion is a general requirement of any physical system, it is more rule than exception that approximations lead to divergencies past some finite order. Though we haven’t constructed an explicit proof, there are indications that the expansion is well behaved for the Hubbard model.

In principle, the moment expansion can be used to study the QP dispersion \( E_\vec{k}^n \) directly: a coherent oscillation results in \( E_\vec{k}^n \) contribution to \( A_n(\vec{k}) \). The crudest (single mode) approximation of this sort identifies \( E_\vec{k} = A_1(\vec{k})/n_\vec{k} \). We found it to be in a surprising agreement with previously obtained results for the momentum dependence of the QP energy in t-t'-t''-J as well as t-J models (one needs to assume that term proportional to t does not contribute to QP dispersion). Since \( E_\vec{k} \) rather seriously overestimates the overall bandwidth, it isn’t clear if one is justified claiming to have obtained even an approximate QP energy yet. Another likely use of our results (or rather their extension to higher moments and orders in perturbation theory) can be in comparing with spectral functions obtained by other means (either numerics, self-consistent Born approximation or other).

In conclusion, we have outlined a well controlled method for analysing the spectral moments of a hole in a Mott insulator. We find the occupation probability, \( n_\vec{k} \),

\[ n_\vec{k} \approx \frac{1}{2} \left[ 1 + \frac{8t(cos(k_x) + cos(k_y))}{U} \right] S_1, \]

by measuring the temperature dependence of \( S_1 \) (as extracted from \( n_\vec{k} \)) and differentiating it one gets the magnetic contribution to the specific heat. The specific heat extracted in this manner contains only the contribution from the spin fluctuations.

III. HIGHER MOMENTS

Higher spectral moments correspond to the derivatives \( <C_{\vec{k}}^i(t)C_{\vec{k}}^j(0)> \) at \( t=0 \) and thus provide further insight into the problem of a hole in a Mott insulator. Our results for first and second moments, \( A_1(\vec{k}) \) and \( A_2(\vec{k}) \), are presented in a table below. The moments are written as sums over momentum space Fourier harmonics, each

\[
\begin{array}{ccc}
\hline
i & A_1^i & A_2^i \\
\hline
1 & t\left(\frac{3}{4} - S_1\right) & -t\left(\frac{3}{4} - S_1\right) - \frac{3}{4}tS_1 \\
2 & \frac{1}{4}t^2(S_2 + 2S_1) & \frac{1}{4}t^2(S_2 + 2S_1) \\
3 & \frac{1}{4}t^2(S_3 + 2S_2) & \frac{1}{4}t^2(S_3 + 2S_2) \\
4 & \frac{1}{4}t^2(S_4 + 2S_3) & \frac{1}{4}t^2(S_4 + 2S_3) \\
5 & \frac{1}{4}t^2(S_5 + 2S_4) & \frac{1}{4}t^2(S_5 + 2S_4) \\
6 & \frac{1}{4}t^2(S_6 + 2S_5) & \frac{1}{4}t^2(S_6 + 2S_5) \\
7 & \frac{1}{4}t^2(S_7 + 2S_6) & \frac{1}{4}t^2(S_7 + 2S_6) \\
8 & \frac{1}{4}t^2(S_8 + 2S_7) & \frac{1}{4}t^2(S_8 + 2S_7) \\
9 & \frac{1}{4}t^2(S_9 + 2S_8) & \frac{1}{4}t^2(S_9 + 2S_8) \\
10 & \frac{1}{4}t^2(S_{10} + 2S_9) & \frac{1}{4}t^2(S_{10} + 2S_9) \\
\hline
\end{array}
\]
is in agreement with the well established experimental result, which as our calculation suggests is strongly constrained by the presence of AF order. We further propose that the temperature dependence of $n_\gamma$ can be used to study the specific heat of the Neel transition. The implications of our results for higher moments are yet to be understood properly.

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APPENDIX A: EVALUATION OF MOMENTS

To compute the moments we first express them in terms of real space electronic correlations

$$n_k = \frac{1}{2} \sum_\sigma < C^\dagger_{k,\sigma} C^{}_{k,\sigma} >$$

$$= \frac{1}{2} \{ 1 + \sum_{i,\sigma} < C^\dagger_{i,\sigma} C^{}_{0,\sigma} > \gamma_i(k) \} \quad (A1)$$

$$A_1(\vec{k}) = - \frac{1}{2} \sum_\sigma < C^\dagger_{k,\sigma} [\hat{H}, C^{}_{k,\sigma}] >$$

$$= \epsilon_k n_k + \frac{U}{2} \sum_{i,\sigma} \gamma_i(k) < C^\dagger_{i,\sigma} C^{}_{0,\sigma} n_{0,-\sigma} > \quad (A2)$$

$$A_2(\vec{k}) = \frac{1}{2} \sum_\sigma < C^\dagger_{k,\sigma} [\hat{H}, [\hat{H}, C^{}_{k,\sigma}] >$$

$$= \epsilon_k n_k \vec{E}_k + \frac{U^2}{2} \sum_{i,\sigma} \gamma_i(k) < C^\dagger_{i,\sigma} C^{}_{0,\sigma} n_{0,-\sigma} >$$

$$+ \frac{U}{2} \sum_{i,\sigma} \gamma_i(k) t_{j,0} < C^\dagger_{i,\sigma} (-C^\dagger_{j,\sigma} n_{0,-\sigma})$$

$$+ C^\dagger_{j,-\sigma} C^{}_{0,-\sigma} C^{}_{0,\sigma} + C^\dagger_{j,-\sigma} C^{}_{0,-\sigma} C^{}_{0,\sigma} > \quad (A3)$$

As before $\gamma_i(k) = \sum_{R_i} e^{-i\vec{k} \cdot \vec{R}_i}$, where the sum is over i’th nearest neighbors.

Next, these electronic correlations are evaluated perturbatively $(S_{ij} = < \frac{1}{2} - \vec{S}_i \cdot \vec{S}_j >)$:

$$\sum_\sigma < C^\dagger_{i,\sigma} C^{}_{0,\sigma} > = \frac{4t_{i0}}{U} S_{i0} + O(t^3/U^3) \quad (A4)$$

$$\sum_\sigma < C^\dagger_{i,\sigma} C^{}_{0,\sigma} n_{0,-\sigma} > = \frac{2t_{i0}}{U} S_{i0}$$

$$+ \sum_{j, R_j} \frac{t_{iR_j} t_{R_j0}}{U^2} (3S_{iR_j} - S_{R_j0} - S_{i0} + 3i < \vec{S}_i (\vec{S}_{R_j} \times \vec{S}_0) >) \quad (A5)$$

On a square lattice and in a state that doesn’t break time reflection invariance $\gamma_i(\vec{k}) < \vec{S}_i \cdot (\vec{S}_{R_j} \times \vec{S}_0) >= 0$ the second sum is (for different $i$):

$$\begin{array}{c|c}
1 & 4tt' S_{20} + 2tt' S_{10} \\
2 & 2(2S_1 - S_2)t^2 + 4S_3 t' t'' \\
3 & (2S_1 - S_2)t^2 + 2(2S_2 - S_3)t' t'' \\
4 & 2(S_1 + S_2)t' t'' + 2(S_1 + S_3 - S_4)t'^2 \\
5 & (2S_2 - S_3)t'^2 + 2(S_3 - S_5)t'^2 \\
6 & 2(S_1 + S_3 - S_6)t' t'' \\
7 & 2(S_2 + S_3 - S_7)t'^2 \\
10 & (2S_3 - S_10)t'^2 \\
\end{array}$$

Substituting these terms into $A_1, A_2, A_3$ yields results of Section III.

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8. When this is no longer the case $< \vec{S}_i \cdot (\vec{S}_{R_j} \times \vec{S}_0) >$ gives rise to sink$_x$ (sink$_y$) contributions to spectral moments resulting in $A_n(\vec{k}) \neq A_n( -\vec{k})$. 

