The magnetic susceptibility of the \( t-J \) model at low hole doping

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We compute the dynamical magnetic susceptibility of the \( t-J \) model in its commensurate flux phase at low hole doping. We compare the calculations with experiments and exact diagonalization studies.

It has long been recognized that an essential ingredient in any theory of high \( T_c \) superconductivity is a description of the accompanying magnetic behavior \([1]\). Therefore, a great deal of effort has been invested in studying the magnetic behavior of the \( t-J \) model, one of the simplest models thought to capture the physics of the high temperature superconductors \([2]\). Because the \( t-J \) model is very strongly correlated, it is not easily solvable. Nonetheless, two of the present authors applied a novel calculational technique to this model and the resulting optical response function agreed very well with exact diagonalization studies \([3,4]\). In this paper, we extend this calculational formalism in order to calculate zero temperature magnetic properties of the \( t-J \) model. We find quantitative agreement with exact diagonalization studies at low dopings and show that our results are consistent with several experimental properties of the high \( T_c \) materials.

We will study the \( t-J \) Hamiltonian

\[
\mathcal{H}_{t-J} = -t \sum_{<ij>} c_{i\sigma}^\dagger c_{j\sigma} + \frac{J}{2} \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}
\]

where \(<i,j>\) denotes the Hermitian sum over nearest neighbor pairs, and no lattice site may be doubly occupied. In the gauge theory of the \( t-J \) model, the spin and charge degrees of freedom are treated as separate while the Gutzwiller constraint of having no doubly occupied sites is enforced by a gauge field degree of freedom. The corresponding Lagrangian is

\[
\mathcal{L} = \sum_j \left\{ \sum_\sigma f_{j\sigma}^\dagger \left( i \hbar \frac{\partial}{\partial t} + \phi_j \right) f_{j\sigma} + b_j^\dagger \left( i \hbar \frac{\partial}{\partial t} + \phi_j \right) b_j - \phi_j \right\} \\
- \sum_{<j,k>} \left\{ -\frac{t_J}{2} |\chi_{jk}|^2 + \chi_{jk} \left[ \frac{J}{2} \sum_\sigma f_{j\sigma}^\dagger f_{k\sigma} + tb_j^\dagger b_k \right] \\
+ \left[ \frac{t_J}{2} - \frac{J}{2} \right] b_j^\dagger b_k^\dagger b_k b_j \right\}, \tag{2}
\]

where \( c_{i\sigma}^\dagger = f_{i\sigma}^\dagger b_i \) and \( b_i^\dagger \) is a bosonic operator that creates a charge one spinless excitation at site \( i \), and \( f_{i\sigma}^\dagger \) is a neutral operator that creates a spin \( \sigma \) excitation at site \( i \). The time component of the \( U(1) \) gauge field at site \( j \) is given by the Lagrange multiplier \( \phi_j \) while the phase of the Hubbard-Stratonivich variable \( \chi_{jk} \) is the integral of the spatial component of this gauge field along the link joining sites \( j \) and \( k \).

Our calculational procedure requires us to define a saddle point of this gauge theory \([5]\). We first define the mean-field Hamiltonians for the Fermi and Bose sectors

\[
\mathcal{H}_b = -t \chi_o \sum_{<j,k>} e^{i\phi_{jk}} b_j^\dagger b_k \tag{3}
\]

\[
\mathcal{H}_f = -\frac{J \chi_o}{2} \sum_{<j,k>} e^{ia_{jk}} f_j^\dagger f_k \tag{4}
\]

where we have assumed that \( \chi_{jk} = \chi_{kj}^\dagger \) has a link-independent magnitude \( \chi_o \) given by

\[
\chi_o^2 = -\frac{1}{JN} \langle 0 | \mathcal{H}_f + \mathcal{H}_b | 0 \rangle. \tag{5}
\]

It is important to note that the value of \( \chi_o \) is twice that predicted by the saddle point procedure. This bandwidth enhancement is a known effect of Gutzwiller projection \([6]\). The commensurate flux saddle point is defined by choosing mean-field values for \( a_{jk} \), the value of the gauge field along the link joining sites \( j \) and \( k \), such that each plaquette of the lattice encloses \((1 - \delta)/2\) flux quanta, where \( \delta \) is the percentage of empty sites. We are able to investigate small fluctuations about these mean-field values for the flux per plaquette by employing perturbation theory. One of the reasons we choose the commensurate flux saddle point is that it minimizes the total energy of these mean field Hamiltonians in the relevant doping range \([6]\). For the fermions, \( \mathcal{H}_f \) is a Hofstadter Hamiltonian \([7]\) with \( M/N = (1 - \delta)/2 \) flux quanta per plaquette \((M, N: \text{relatively prime integers})\). In order to perform
calculations in the bose sector, a statistical transmutation is employed that allows us to treat the bosons in their fermionic representation \( \tilde{F} \). This assumption stabilizes the theory at zero temperature because the bosons are no longer degenerate and have a corresponding mean-field Hamiltonian with an energy gap. In addition, this approximation is consistent with known variational results \( \tilde{F} \).

Having defined the underlying formalism, let us now calculate the mean field spinon polarization bubble,

\[
\chi_0(q, \omega) = \frac{1}{N} \sum_n \left[ \frac{|\langle 0 | S^+_n | n \rangle|^2}{\omega - E_{n0} + i\eta} - \frac{|\langle 0 | S^-_n | n \rangle|^2}{\omega + E_{n0} + i\eta} \right],
\]

where \( S^+_n = \sum_k f_{k+q}^\dagger f_k, \ S^-_n = \sum_k f_{k+q} f_k \), \( E_{n0} = E_n - E_0 \), and the sum is carried out over all excited states \( |n\rangle \) of \( \mathcal{H}_f \).

Next we perform a vertex correction in order to account for the gauge field fluctuations that impose the Gutzwiller constraint. We approximate the gauge field interaction as an instantaneous onsite repulsive potential of strength \( U \). We require that \( U = 1.78 J \chi_0 \), the value found in variational studies of the Heisenberg antiferromagnet \( \tilde{F} \). This value of \( U \), without Gutzwiller projection, generates the exact amount of antiferromagnetic order which minimizes the energy of the projected flux ground state. We assume that the repulsive core of the gauge field interaction between spinons is relatively unaffected at low doping. The reason is that the core is short-ranged and therefore immune to “screening” effects. Therefore, \( U \) is not an adjustable parameter in this calculation. The vertex correction is easily performed, and the resulting expression for the corrected susceptibility is

\[
\chi_q(\omega) = (1 - \delta)^2 \frac{\chi_0^0(\omega)}{1 + U \chi_0^0(\omega)},
\]

where the doping-dependent prefactor is implicit in the relation

\[
S_j = \frac{1}{2} f_{j\alpha}^\dagger [\sigma^\alpha \beta f_{j\beta} (b_j^\dagger)] \simeq (1 - \delta) \frac{1}{2} f_{j\alpha}^\dagger [\sigma^\alpha \beta f_{j\beta}].
\]

FIG. 1. Comparison of \( S(q, \omega) \) calculated from Eq. (8) (solid lines) with the exact diagonalization results of ref. [12] (dashed lines) at two different momenta for two, three and four holes on a 16-site cluster for \( J/t = 0.4 \). Both calculations use \( \eta = J/2 \).

Let us now compare our calculation of \( S(q, \omega) = -\text{Im} \chi_q(\omega) \) with the exact diagonalization results of ref. [12] (\( \odot \), \( J/t = 0.4 \)) and ref. [13] (\( \Box \), \( J/t = 0.25; +, J/t = 0.5 \)). Inset: Brillouin zone, with special points labeled. Bottom: \( S(q) \) for \( \delta = 5/41 \) (solid line) compared with the two-hole results of ref. [12] (\( \odot \), \( J/t = 0.4 \)) and ref. [13] (+, \( J/t = 0.4 \)). Inset: \( S(q) \) calculated for (top to bottom) \( \delta \approx 1/16, 1/8, 3/16, \) and 1/4. Note that our \( S(q) \) is independent of \( t/J \).
middle and bottom respectively). The exact diagonalization values are shown as dotted lines. The solid lines were obtained from Eq. (8). We wish to point out the following basic similarities:

- There is a single coherent peak with a characteristic energy scale of $J$ at $q = 0$. The energy of this pole increases substantially with doping.
- Elsewhere in the zone, (e.g. $q = \frac{3}{2}Q$) the spectral weight is not especially doping-dependent, nor is it very coherently distributed.

The unphysical sharp structure in both calculations has been smoothed out considerably through the use of a large value of $\eta (= J/2)$. With the value of $U$ held fixed, there are no adjustable parameters in our equation for $S(q, \omega)$. Furthermore, we have not scaled the $y$ axes.

We shall now calculate $S(q) = \int_0^\infty d\omega S(q, \omega)$ to see how the integrated spectral weight is distributed over the Brillouin zone. This gives an idea of the extent of magnetic correlation at momentum $q$. Fig. 2 compares $S(q)$ with the exact diagonalization results of refs. [13–15]. As expected, the correlation is greatest near $Q$ and is suppressed elsewhere in the zone. While the exact diagonalization results are weakly dependent on $J/t$ at $Q$, our calculation is independent of $J/t$. The doping dependence and absolute magnitude of $S(q)$ are both reproduced quite well. Again, we emphasize that there are no adjustable parameters.

Let us now address the issue of discommensuration in $S(q, \omega)$. The plateau in $S(q)$ near $Q$ widens upon doping, an effect clearly visible in the inset in the lower half of Fig. 2. The widening plateau is an indication of discommensuration of the antiferromagnetic correlations away from the ordering vector $Q$. The extent of this is usually characterized by a scalar quantity $q_d$, where

$$q_d = \frac{1}{\pi} |q_d - Q|,$$

and $q_d$ is a momentum at which the greatest magnetic scattering occurs. Neutron scattering experiments performed on $La_{2-x}Sr_xCuO_4$ have given values of $q_d$ at $\delta = 0.075$ and $0.14$ (c.f. Fig. 3, bottom right panel) along with our calculation of $q_d(\delta)$. The upper right panel shows how we estimate $q_d$ from $S(q, \omega)$. This particular example shows a doping of $15/107 \approx 0.14$. The lowest energy poles in $S(q, \omega)$ occur at an energy $\omega_0 = 1.14 J$, and are distributed around $Q$ in a ring-like manner (dark shading). At higher dopings, the ring becomes increasingly diamond-shaped, with more spectral weight along the faces than at the corners. To be consistent with the experiments, we take $q_d$ in the $(\pi, 0)$ direction and calculate $q_d$ as shown.

While the magnitude of the discommensuration does agree with the experimentally obtained values from $La_{2-x}Sr_xCuO_4$, the distribution does not. The experiments clearly show that discommensurate momenta appear at four points in the $(0, \pm\pi)$ and $(\pm\pi, 0)$ directions, not in a ring around $Q$. This disagreement between our calculation and the experimental data does not necessarily call into question the validity of our calculation. Exact diagonalization studies of the $t-J$ Hamiltonian are as yet unable to determine which type of discommensuration it exhibits. Resolution of this issue will have to wait until clusters of large enough size can be studied. For now, we note that the discommensuration effect that
we calculated is due to the existence of a finite concentration of empty lattice sites. Because this distribution is uncorrelated (i.e. there is no charge order), all directions look equivalent to spin excitations of momentum $\mathbf{q}$. Therefore, a ring of discommensurate momenta forms around the ordering vector $(\pi, \pi)$. We expect this to change if the ground state is modified to include axis-aligned charge ordering, a modification which would require the addition of another Hartree-Fock parameter. The formation of such “stripes” is thought by some to be an essential ingredient of high $T_c$ superconductivity \cite{17}, and it has indeed been observed in experiments \cite{20} and other calculations \cite{19}. However, the instability is indicated by a vanishing gap to spin excitations as $\delta \to \delta_c^-$, where $\delta_c \simeq 0.02$. Above $\delta_c$, the lowest lying spin excitation requires a finite energy $\omega_0$. Fig. \ref{fig:4} illustrates the boundary between the stable regime ($\delta > \delta_c$, $\omega_0 > 0$) and the unstable regime ($\delta < \delta_c$, $\omega_0 = 0$). We have included the values of the Néel temperature measured in ref. \cite{20} for La$_{2-\delta}$Sr$_\delta$CuO$_4$ at dopings $\delta \leq 0.02$.

While our calculation of the minimum doping of the spin disordered phase $\delta_c$ agrees with experimental studies of La$_{2-\delta}$Sr$_\delta$CuO$_4$, our calculation of the gap to spin excitations $\omega_0$ in this phase does not. Neutron scattering investigations of the high $T_c$ materials indicate a gap to spin excitations with an energy scale closer to the superconducting gap than to $J$ \cite{21}. Both our calculation and the exact diagonalization work thus far greatly overestimate the value of $\omega_0$. While this may be a finite size effect in the exact diagonalizations, we attribute it to a overly large mean-field energy gap that is expected to be reduced by broadening and damping effects such as those considered in ref. \cite{22} with respect to the fractional statistics gas.

To summarize, we have calculated the zero temperature magnetic properties of the $t$-$J$ Hamiltonian in its commensurate flux phase. We find quantitative agreement with exact diagonalization calculations of the spin correlation function \cite{12} and the spin structure factor \cite{3, 13}. We also find discommensuration of magnetic order away from $(\pi, \pi)$ comparable in magnitude to that observed in La$_{2-\delta}$Sr$_\delta$CuO$_4$ \cite{16}, but the details remain to be clarified. The instability to an antiferromagnetic phase occurs at a value of $\delta$ close to that found in experiments \cite{21} and other calculations \cite{19}. However, the gap to spin excitations in the commensurate flux phase is approximately five times larger than indicated by experiment \cite{21}. Nevertheless, the $t$-$J$ model seems to be well described by a gauge theory of new particles identified with the spin and charge coordinates of the original electrons. We therefore present these calculations as a further test of the gauge theory of spinons and holons and as a justification for continued efforts to remedy its shortcomings.

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