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Dynamics of Spin and Charge Fluctuations in a $t-J$ Model

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Abstract. We review the phase diagram of a $t-J$ model that we have recently determined in the context of an $1/N$ expansion, and calculate the spin-spin dynamical structure factor and the real part of the finite-frequency conductivity in the canted antiferromagnetic (CAF) phase.

1. Introduction

The dynamics of mobile holes in a doped Heisenberg antiferromagnet is of considerable current interest because such a system, usually described by the $t-J$ model, is believed to capture the low-energy physics of the high-T_c cuprate superconductors. Expressed in terms of Hubbard operators, $\chi^{ab} = |a><b|$, the $t-J$ Hamiltonian reads,

$$H = -t \sum_{<i,j>} \chi_i^{0\mu}\chi_j^{\mu 0} + \frac{1}{2}J \sum_{<i,j>} (\chi_i^{\mu\nu}\chi_j^{\nu\mu} - \chi_i^{\mu\mu}\chi_j^{\nu\nu}) + \frac{1}{2}J \sum_{\substack{<i,l,j>\\ i\neq j}} (\chi_i^{0\mu}\chi_l^{\mu\nu}\chi_j^{\nu 0} - \chi_i^{0\mu}\chi_l^{\nu\nu}\chi_j^{\mu 0}), \quad (1)$$

where index 0 corresponds to a hole, and the Greek indices $\mu, \nu, \ldots$, can take two distinct values, for a spin-up and a spin-down electron. The form of (1) is identical to that emerging in the large-U limit of the Hubbard Hamiltonian on a square lattice with nearest-neighbor hopping t, in which case the exchange constant is $J = 4t^2/U$. In Ref.[1] we generalized the local constraint associated with (1) to $\chi_i^{00} + \chi_i^{\mu\mu} = N$, and took the commutation properties of the χ^{ab}'s to be those of the generators of the $U(3)$ algebra. A generalized Holstein-Primakoff realization can then be employed to develop an $1/N$ expansion, setting $N = 1$ at the end of the calculation.

2. Phase Diagram

At half-filling ($n_e = 1$) the ground state of (1) in the large-N limit reduces to the conventional Néel antiferromagnetic state while for large enough hole doping $(1 - n_e)$ and t/J a Nagaoka ferromagnetic (FM) state is stabilized. Close to half-filling ($n_e \lesssim 1$), however, the competition between antiferromagnetic and ferromagnetic tendencies leads to a phase-separated (PS) ground state consisting of a 'no-hole' insulating antiferromagnetic region and a 'hole-rich' ferromagnetic region. We have verified the existence of phase separation in the large-N limit both by direct minimization of (1) as well as by the standard Maxwell construction. Finally, close to half-filling and for $t/J \leq 1.118$ a uniform-density two-sublattice canted antiferromagnetic (CAF) configuration is stabilized. In this metallic CAF state the spins on each sublattice are parallel to each other but form an angle θ_c with the spins of the opposite sublattice. The complete phase diagram is shown in Fig.1 where we note also the possibility of phase separation into an antiferromagnetic and a CAF region. Some experimental support to this general picture comes from neutron-scattering and other measurements indicating phase separation or spin canting in oxygen-doped high-T_c materials.

3. Spin and Charge Fluctuations

To assess the dependence of the magnetic dynamics on doping we have calculated the spin-spin dynamical structure factor $S^{\alpha\alpha}(q,\omega)$ for the CAF phase in the harmonic approximation, [2]. With the help of $S^{\alpha\alpha}(q,\omega)$ we may define 'average frequencies' $\tilde{\omega}_{zz}(q)$ of maximal spectral weight in the

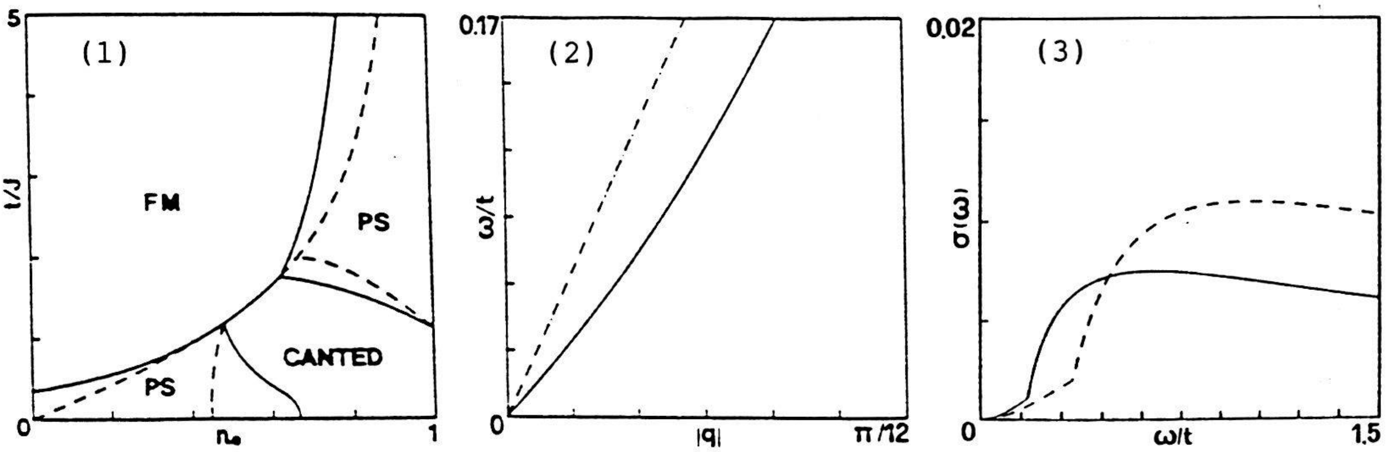

FIG. 1. Phase diagram in two dimensions. The dashed lines represent limits of metastability. The solid lines are the true critical lines obtained with the Maxwell construction.

FIG. 2. Average magnon frequencies *vs* crystal momentum along the diagonal of the Brillouin zone for $t/J = 1$ and $1 - n_e = 0.01$. Small-q region illustrating the reduction of $\bar{\omega}_{zz}$ (solid line) relative to its undoped $n_e = 1$ value (dashed-dotted line).

FIG. 3. Optical absorption (in units of $e^2/\hbar$) *vs* frequency for $t/J = 1$ and $1 - n_e = 0.01$ (solid line) or $1 - n_e = 0.02$ (dashed line). The crossover frequency above which $\sigma(\omega)$ rises sharply coincides with the corresponding energy gap $\Delta/t = 0.175$ (solid line) or $\Delta/t = 0.342$ (dashed line).

transverse direction (i.e., perpendicular to the antiferromagnetic ordering) which correspond to conventional magnons. Fig.2 shows typical results indicating the reduction of the average magnon velocity almost by a factor of 2 upon doping with 1% of holes, in qualitative agreement with the long-wavelength spin-wave softening observed by neutron-scattering [3] in $YBa_2Cu_3O_{6.37}$.

We have also studied effects of charge fluctuations by calculating the Kubo formula for the real part of the finite-frequency conductivity $\sigma(\omega)$, i.e., the optical absorption, for the CAF phase, [4]. Fig.3 shows typical results. We note that below a characteristic crossover frequency Δ the absorption is very small, while above Δ it rises sharply to a broad maximum, in qualitative agreement with measurements of the normal-state mid-infrared absorption band in $YBa_2Cu_3O_{7-\delta}$ films [5]. As shown in detail in [4], Δ identifies with an energy gap developing upon hole doping in one of the two branches of elementary excitations, at the corner of the square Brillouin zone.

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