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Phase lamination in a t–J bilayer at finite temperature

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ABSTRACT

A bilayered t–J model is investigated with a slave boson mean field theory. A spontaneous phase lamination (PL) into a layer dominated by antiferromagnetism (AFM) and a layer dominated by superconductivity (SC) is found at a low doping density and low temperature regime. Raising the temperature removes the PL and SC, turns the system into a homogeneously antiferromagnetic (AF) bilayer, and eventually a homogeneously paramagnetic bilayer at high temperature. The PL circumvents the competition between AFM and SC, and may result in a higher superconducting transition temperature. The density of states of low energy single particle excitation in the homogeneously AF state at intermediate temperature is reduced by the AF scattering. The relation between this study and the bilayered superconducting cuprates is discussed.

1. Introduction

The underdoped (UD) superconducting cuprates are susceptible to instability of spatial inhomogeneity with various charge, spin, and orbital orders [1–4]. There can be competition between the orders, and inhomogeneity in the cuprates has always been an issue since the discovery of the compounds. The inhomogeneity can be directly visualized by a scanning tunneling microscopy (STM) probe [5]. When an UD cuprate is cooled down from a high temperature, the compound enters a pseudogaped state [6] in which the density of states (DOS) near the Fermi level is partially suppressed. The pseudogap (PG) resides at the antinodal regions in reciprocal space. A cuprate in the pseudogaped regime possesses various kinds of the above mentioned inhomogeneities. A coherent d-wave superconductivity (dSC) is the last to appear in the course of the lowering of temperature.

The superconducting cuprates are narrow band systems, which may be modeled by the Hubbard type models, or in the strong repulsion limit by the t–J type models [7–11]. The Gutzwiller projected [12,13] t–J models are often taken as minimal models for the cuprates [14–16]. There is always a tendency toward an intralayer phase separation (PS) in UD t–J models, regardless of the methodologies in the studies [17,18]. A heuristic argument based on a slave boson (SB) mean field theory (MFT) [19–21] for the PS may be given below. We argue that when the band filling or particle density n is varied, the chemical potential μ does not monotonically depend on n. Consider a simple monolayered t–J model with only a first nearest neighbor (NN) hopping and an AF Heisenberg coupling. The hopping and exchange integrals are taken as $t=-1$ and $J=1/3$ respectively. The AF gap at half band filling (HBF) is $J=1/3$. The renormalized bandwidth B_δ for a nonmagnetic state at a doping density $\delta=1-n=0.15$ is estimated as $B_\delta \simeq 8\delta = 1.2$. Assuming a constant DOS, the chemical potential μ at this doping density is estimated as $\mu \simeq -\delta B_\delta/2 \simeq -0.1$, which is within the AF gap at HBF. Therefore, we have argued that a chemical potential may simultaneously correspond to a nonmagnetic state at a high doping density, and a magnetic state at a low doping density. This multiple correspondence is due to the large AF gap at HBF, and the small renormalized bandwidth at nonvanishing doping densities.

Another noteworthy feature in a t–J model with a hole-like FS is the suppression of dSC by AFM [22]. The is due to the location of both of the gaps of the AFM and dSC are at the antinodal regions of the Fermi surface (FS), and an AFM is more effective in lowering the energy of a system at near HBF.

The PS instability in the t–J model may be related to the inhomogeneities in the UD cuprates. Analogous to an intralayer PS, in this paper we show that an interlayer phase lamination (PL) can occur in a bilayered t–J model with a weak interlayer coupling. A PS occurs with an intralayer interphase boundary, whereas a PL occurs with an interlayer interphase boundary. In a bilayered t–J model, the competition between the dSC and AFM may be avoided via a PL, leading to a rise in the superconducting transition temperature.

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Section 2 presents the model and our formulation. Section 3 presents the phase diagram of a bilayered t–J model on an n–T plane, the constant volume specific heat capacity, and the low excitation DOS. Section 4 discusses the result and relates it to the superconducting cuprates.

2. Models and formulation

We consider a t–J model defined on a bilayer of square lattices. The Hamiltonian reads

$$\hat{H} = \hat{H}_{\parallel} + \hat{H}_{\perp} + \hat{H}_c, \tag{1}$$

where

$$\hat{H}_{\parallel} = \sum_{\alpha} \sum_{\mathbf{i},\mathbf{j},\sigma} t_{\mathbf{ij}} \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{j}\sigma} + \sum_{\alpha} \sum_{\langle \mathbf{i},\mathbf{j}\rangle} J \left(\hat{\mathbf{S}}_{\alpha\mathbf{i}} \cdot \hat{\mathbf{S}}_{\alpha\mathbf{j}} - \frac{\hat{n}_{\alpha\mathbf{i}} \hat{n}_{\alpha,\mathbf{j}}}{4} \right) \tag{2}$$

and

$$\hat{H}_{\perp} = \sum_{\mathbf{i},\sigma} t_{\perp} \left(\hat{c}^{\dagger}_{A\mathbf{i}\sigma} \hat{c}_{B\mathbf{i}\sigma} + \text{H.c.} \right) + \sum_{\mathbf{i}} J_{\perp} \left(\hat{\mathbf{S}}_{A\mathbf{i}} \cdot \hat{\mathbf{S}}_{B\mathbf{i}} - \frac{\hat{n}_{A\mathbf{i}} \hat{n}_{B\mathbf{i}}}{4} \right). \tag{3}$$

$\hat{H}_{\parallel}$ and $\hat{H}_{\perp}$ describe the intralayer and interlayer electronic dynamics respectively. Within a layer, we consider NN, second nearest neighbor, and third nearest neighbor hopping with bare hopping integrals t, t', and t'' respectively; and a NN AF Heisenberg coupling with an exchange integral J. The intralayer electronic dynamics in the two layers are identical. Between the layers, we consider a perpendicular hopping with a bare hopping integral $t_{\perp}$, and a perpendicular AF Heisenberg coupling with an exchange integral $J_{\perp}$. We consider a t–J model as a Hubbard model in the strong repulsion limit.

The interlayer Heisenberg coupling is much smaller than the intralayer Heisenberg coupling, but it can have a nonnegligible effect such as the finite temperature AF phase transition in the superconducting cuprates. It is also relevant to some of the results in our discussion (Sec. 3).

The t–J Hamiltonian in Eq. (1) is defined to act on a Gutzwiller projected Fock space, in which there are no doubly occupied sites. In a SB MFT [19–21], the nonholonomic constraint due to the Gutzwiller projection is transformed into a holonomic constraint and treated in a mean field manner. This leads to the substitutions

$$t_{\mathbf{ij}} \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{j}\sigma} \to \sqrt{\delta_{\alpha\mathbf{i}} \delta_{\alpha\mathbf{j}}}\, t_{\mathbf{ij}} \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{j}\sigma}, \tag{4}$$

and

$$t_{\perp} \hat{c}^{\dagger}_{A\mathbf{i}\sigma} \hat{c}_{B\mathbf{i}\sigma} \to \sqrt{\delta_{A\mathbf{i}} \delta_{B\mathbf{i}}}\, t_{\perp} \hat{c}^{\dagger}_{A\mathbf{i}\sigma} \hat{c}_{B\mathbf{i}\sigma}, \tag{5}$$

where $\delta_{\alpha\mathbf{i}} = 1 - \langle n_{\alpha\mathbf{i}} \rangle$ is a site doping density. The substitutions reflect the reduction of the kinetic energy due to the no-double occupancy constraint. The quartic interacting terms are decoupled in all channels into quadratic terms. The Heisenberg coupling is decoupled as

$$\begin{aligned}
\hat{\mathbf{S}}_{\alpha\mathbf{i}} \cdot \hat{\mathbf{S}}_{\beta\mathbf{j}} &= \frac{1}{4} \sum_{k=x,y,z} \sum_{\mu,\nu,\gamma,\delta=1}^{2} \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \sigma_k^{\mu\nu} \hat{c}_{\alpha\mathbf{i}\nu} \cdot \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \sigma_k^{\gamma\delta} \hat{c}_{\beta\mathbf{j}\delta} \\
&\to \frac{1}{4} \sum_{k=x,y,z} \sum_{\mu,\nu,\gamma,\delta=1}^{2} \sigma_k^{\mu\nu} \sigma_k^{\gamma\delta} \\
&\quad \Big(\langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}_{\alpha\mathbf{i}\nu} \rangle \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \hat{c}_{\beta\mathbf{j}\delta} + \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}_{\alpha\mathbf{i}\nu} \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \hat{c}_{\beta\mathbf{j}\delta} \rangle \\
&\quad - \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}_{\alpha\mathbf{i}\nu} \rangle \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \hat{c}_{\beta\mathbf{j}\delta} \rangle \\
&\quad + \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \rangle \hat{c}_{\beta\mathbf{j}\delta} \hat{c}_{\alpha\mathbf{i}\nu} + \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \langle \hat{c}_{\beta\mathbf{j}\delta} \hat{c}_{\alpha\mathbf{i}\nu} \rangle \\
&\quad - \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \rangle \langle \hat{c}_{\beta\mathbf{j}\delta} \hat{c}_{\alpha\mathbf{i}\nu} \rangle \\
&\quad - \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}_{\beta\mathbf{j}\delta} \rangle \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \hat{c}_{\alpha\mathbf{i}\nu} - \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}_{\beta\mathbf{j}\delta} \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \hat{c}_{\alpha\mathbf{i}\nu} \rangle \\
&\quad + \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\mu} \hat{c}_{\beta\mathbf{j}\delta} \rangle \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\gamma} \hat{c}_{\alpha\mathbf{i}\nu} \rangle \Big),
\end{aligned} \tag{6}$$

where $\sigma_k^{\mu\nu}$ is the (μ, ν) element in Pauli matrix σ_k. The charge density interaction is decoupled as

$$\begin{aligned}
\hat{n}_{\alpha\mathbf{i}} \hat{n}_{\beta\mathbf{j}} &= \sum_{\sigma,\sigma'=\uparrow,\downarrow} \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{i}\sigma} \cdot \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\beta\mathbf{j}\sigma'} \\
&\to \sum_{\sigma,\sigma'=\uparrow,\downarrow} \Big(\langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{i}\sigma} \rangle \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\beta\mathbf{j}\sigma'} \\
&\quad + \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{i}\sigma} \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\beta\mathbf{j}\sigma'} \rangle - \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\alpha\mathbf{i}\sigma} \rangle \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\beta\mathbf{j}\sigma'} \rangle \\
&\quad + \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \rangle \hat{c}_{\beta\mathbf{j}\sigma'} \hat{c}_{\alpha\mathbf{i}\sigma} + \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \langle \hat{c}_{\beta\mathbf{j}\sigma'} \hat{c}_{\alpha\mathbf{i}\sigma} \rangle \\
&\quad - \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \rangle \langle \hat{c}_{\beta\mathbf{j}\sigma'} \hat{c}_{\alpha\mathbf{i}\sigma} \rangle - \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\beta\mathbf{j}\sigma'} \rangle \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\alpha\mathbf{i}\sigma} \\
&\quad - \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\beta\mathbf{j}\sigma'} \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\alpha\mathbf{i}\sigma} \rangle + \langle \hat{c}^{\dagger}_{\alpha\mathbf{i}\sigma} \hat{c}_{\beta\mathbf{j}\sigma'} \rangle \langle \hat{c}^{\dagger}_{\beta\mathbf{j}\sigma'} \hat{c}_{\alpha\mathbf{i}\sigma} \rangle \Big).
\end{aligned} \tag{7}$$

Applying the substitutions in Eqs. (4), (5), (6), and (7) to Eqs. (2) and (3) reduces $\hat{H}_{\parallel}$ and $\hat{H}_{\perp}$ to SB MF Hamiltonians $\hat{H}^{\text{mf}}_{\parallel}$ and $\hat{H}^{\text{mf}}_{\perp}$ respectively.

While the short range Coulomb interaction has been taken into account by the low energy effective J and $J_{\perp}$ terms, the long range Coulomb interaction has to be included when there is charge inhomogeneity. As at the interface of a semiconductor heterostructure, the long range Coulomb interaction leads to a capacitive field between the layers when there is an imbalance of charge in the layers. This field tends to restore the equality of the layer charge densities, and this effect is to be described by $\hat{H}_c$.

We confine our discussion to an uniform charge distribution in a layer with $\langle \hat{n}_{\alpha\mathbf{i}} \rangle = n_{\alpha}$, and include an uniform capacitive field between the layers. We approximate $\hat{H}_c$ by a mean field Hamiltonian

$$\hat{H}^{\text{mf}}_c = \sum_{\alpha} \sum_{\mathbf{i}} \varepsilon^c_{\alpha} \hat{n}_{\alpha\mathbf{i}}, \tag{8}$$

where the layer potentials are given by $\varepsilon^c_A = -\varepsilon^c_B = V_c(n_A - n_B)/2$. The parameter V_c is related to a particular cuprate by $V_c = e^2 c / 2\varepsilon_r \varepsilon_0 ab$, where a and b are the intralayer lattice constants, c is the interlayer lattice constant, e is the electronic charge, ε_0 is the permittivity in vacuum, and ε_r is the relative permittivity for the interstitial space between the CuO_2 layers. The electric fields due to the ionic background in the two layers cancel each other for they are equal in strengths but opposite in directions. For $|t| = 0.3$ eV and lattice constants $a = b = 3.85$ Å, and $c = 3.4$ Å, the dimensionless parameter $V_c/|t| \simeq 140/\varepsilon_r$. In the literature, $80 \lesssim \varepsilon_r \lesssim 250$ has been used to fit measurement data from the cuprates.

The Hamiltonian $\hat{H}$ is hence reduced to a mean field Hamiltonian $\hat{H}^{\text{mf}} = \hat{H}^{\text{mf}}_{\parallel} + \hat{H}^{\text{mf}}_{\perp} + \hat{H}^{\text{mf}}_c$. A chemical potential μ is introduced to control the particle number, and we will solve a grand canonical Hamiltonian $\hat{H}^{\text{mf}} - \mu \hat{N}$, where $\hat{N} = \sum_{\alpha} \sum_{\mathbf{i}} \hat{n}_{\alpha\mathbf{i}}$. We consider only real valued order parameters, and uniform and isotropic intralayer order parameters. Let the particle density $\langle \hat{n}_{\alpha\mathbf{i}} \rangle = n_{\alpha}$, AF spin moment $\langle \hat{S}^z_{\alpha\mathbf{i}} \rangle = (-1)^{i_x + i_y} m_{\alpha}$, where $\hat{S}^z_{\alpha\mathbf{i}} = (\hat{n}_{\alpha\mathbf{i}\uparrow} - \hat{n}_{\alpha\mathbf{i}\downarrow})/2$, and d-wave singlet superconducting pairing amplitude $\langle \hat{\Delta}^s_{\alpha,\mathbf{i};\alpha,\mathbf{i}+\hat{x}} \rangle = -\langle \hat{\Delta}^s_{\alpha,\mathbf{i};\alpha,\mathbf{i}+\hat{y}} \rangle = \Delta^s_{\alpha}$, where $\hat{\Delta}^s_{\alpha,\mathbf{i};\alpha,\mathbf{i}+\mathbf{d}} = \hat{c}_{\alpha\mathbf{i}\uparrow} \hat{c}_{\alpha,\mathbf{i}+\mathbf{d},\downarrow} - \hat{c}_{\alpha\mathbf{i}\downarrow} \hat{c}_{\alpha,\mathbf{i}+\mathbf{d},\uparrow}$. The particle density in layer α is n_{α}, and the average particle density or band filling is $n = (n_A + n_B)/2$. The doping density in layer α is $\delta_{\alpha} = 1 - n_{\alpha}$, and the average doping density in a bilayer is