Coexistence of Antiferromagnetism and D-wave Superconductivity in Extended t-J Model

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Abstract

We study the extended *t-J* model on a square lattice, which has the second and third-neighbor hopping terms (t' and t'', respectively) as well as the nearest-neighbor one using the slave-boson mean-field approximation. It is found that the phase diagram consistent with the experiments for multilayer high-T_c cuprates is obtained for a suitable choice of t' and t''. Temperature dependence of the uniform spin susceptibility is also calculated in the coexistence of antiferromagnetism and *d*-wave superconductivity.

Key words: coexistence, antiferromagnetism, *d*-wave superconductivity, *t-J* model
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Recently uniform coexistence of antiferromagnetism and *d*-wave superconductivity was found in multilayer high-T_c cuprate superconductors[1, 2]. This finding attracts much attention because it may give important insight into the mechanism of high-T_c superconductivity. The coexistence of antiferromagnetic (AF) and superconducting (SC) order was predicted in the two-dimensional *t-J* model using the slave-boson mean-field approximation (SBMFA)[3, 4] and the variational Monte Carlo method[5]. However, the phase diagram so obtained is not consistent with the experiments[1, 2] even qualitatively in that the Néel temperature T_N shows reentrant behavior around the tetracritical point.

In this paper we study the extended *t-J* model on a square lattice, which has the second and third-neighbor hopping terms (t' and t'', respectively) as well as the nearest-neighbor one. We treat this model using the SBMFA and show that the phase diagram consistent with the experiments[1, 2] is obtained by making a suitable choice of t' and t''.

The Hamiltonian of our model is given as

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + J\sum_{<i,j>}\mathbf{S}_i\cdot\mathbf{S}_j \quad (1)$$

where the transfer integrals t_{ij} are finite for the nearest (t), second-neighbor (t'), and third-neighbor bonds (t''), and vanish otherwise. $J(>0)$ is the antiferromagnetic superexchange interaction and $\langle i,j\rangle$ denotes the nearest-neighbor bonds. $\tilde{c}_{i\sigma}$ is the electron operator in the Fock space without double occupancy and we treat this condition using the slave-boson method by writing $\tilde{c}_{i\sigma} = b^{\dagger}_i f_{i\sigma}$, where $f_{i\sigma}$ (b_i) is a fermion (boson) operator that carries spin σ (charge e). The spin operator is expressed as $\mathbf{S}_i = \frac{1}{2}\sum_{\alpha\beta} f^{\dagger}_{i\alpha}\sigma_{\alpha\beta}f_{i\beta}$ with σ being the Pauli matrices. $\mathcal{H}$ is decoupled by introducing the following order parameters (OPs): $m = \frac{1}{2}\langle f^{\dagger}_{i\uparrow}f_{i\uparrow} - f^{\dagger}_{i\downarrow}f_{i\downarrow}\rangle e^{i\mathbf{Q}\cdot\mathbf{r}_i}$ (staggered magnetization) with $\mathbf{Q} = (\pi,\pi)$, $\chi^{(1)} = \langle\sum_\sigma f^{\dagger}_{i\sigma}f_{j\sigma}\rangle$, $\langle b^{\dagger}_i b_j\rangle$ (bond order parameter; i and j are nearest-neighbor sites), and $\Delta_\tau = \langle f_{i\uparrow}f_{i+\tau\downarrow} - f_{i\downarrow}f_{i+\tau\uparrow}\rangle$ (singlet resonating-valence-bond order parameter) with $\tau = x, y$. Here we assume that all OPs are independent of i, and consider the $d_{x^2-y^2}$-wave pairing state for Δ_τ, *i.e.*, $\Delta_x = -\Delta_y (\equiv \Delta_0)$. The SC state is characterized by $\Delta_0 \neq 0$ and $\langle b\rangle \neq 0$, while in the AF state m is finite. In the following the bosons are assumed to be Bose condensed, *i.e.*, $\langle b\rangle = \sqrt{\delta}$ and $\langle b^{\dagger}_i b_j\rangle = \delta$ with δ being the hole concentration, so that the onset of Δ_0 corresponds to that of the SC state. This assumption is valid at low T and for δ not so close to 0 ($\delta \gtrsim 0.02$). Then the self-consistency equations are obtained as[4]

$$\begin{aligned}
m &= \frac{1}{N}\sum_k \frac{Jm}{D_k}\Big(\frac{\eta^+_k}{\lambda^+_k}\tanh\frac{\lambda^+_k}{2T} - \frac{\eta^-_k}{\lambda^-_k}\tanh\frac{\lambda^-_k}{2T}\Big)\\
\chi^{(1)} &= -\frac{1}{2N}\sum_k \frac{\xi^-_k}{D_k}(\cos k_x + \cos k_y)\\
&\quad\times\Big(\frac{\eta^+_k}{\lambda^+_k}\tanh\frac{\lambda^+_k}{2T} - \frac{\eta^-_k}{\lambda^-_k}\tanh\frac{\lambda^-_k}{2T}\Big)\\
\Delta_0 &= -\frac{1}{2N}\sum_k(\cos k_x - \cos k_y)\Big(\frac{\Delta_k}{\lambda^+_k}\tanh\frac{\lambda^+_k}{2T} + \frac{\Delta_k}{\lambda^-_k}\tanh\frac{\lambda^-_k}{2T}\Big)\\
\delta &= \frac{1}{N}\sum_k\Big(\frac{\eta^+_k}{\lambda^+_k}\tanh\frac{\lambda^+_k}{2T} + \frac{\eta^-_k}{\lambda^-_k}\tanh\frac{\lambda^-_k}{2T}\Big).
\end{aligned} \quad (2)$$

Here $\lambda^{\pm}_k = \sqrt{(\eta^{\pm}_k)^2 + \Delta^2_k}$, $\eta^{\pm}_k = \xi^+_k \pm D_k$, $D_k = \sqrt{(\xi^-_k)^2 + (2Jm)^2}$, $\xi^{\pm}_k = (\xi_k \pm \xi_{k+Q})/2$, $\xi_k = -2(t\delta + \frac{3}{8}J\chi^{(1)})(\cos k_x + \cos k_y) - 4t'\delta\cos k_x\cos k_y - 2t''\delta(\cos 2k_x + \cos 2k_y)$ and $\Delta_k = -\frac{3}{4}J\Delta_0(\cos k_x - \cos k_y)$. T, N and μ represent temperature, the total number of lattice sites and the chemical potential, respectively, and the $\mathbf{k}$ sum is over the region $|k_x| + |k_y| \leq \pi$.

We solve the above self-consistency equations numerically to obtain the phase diagram in the plane of T and δ. In Fig.1 the result for $t/J = 4$, $t'/t = 0.12$ and $t''/t = -0.06$ is shown. Curves (a) and (c) denote the Néel temperature T_N and the SC transition temperature T_c, respectively; (b) is the T_c when the AF order is assumed to be absent. The region below both

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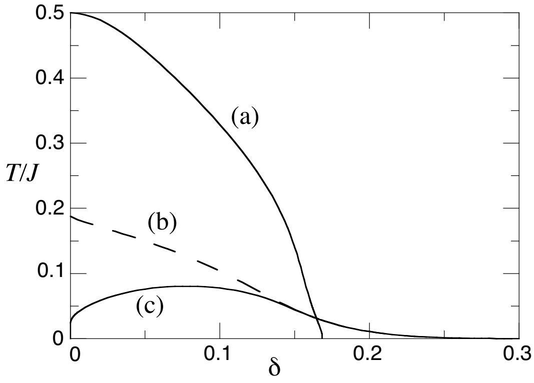

Figure 1: Phase diagram in the plane of T and δ for $t/J = 4$, $t'/t = 0.12$ and $t''/t = -0.06$. (a) Néel temperature T_N. (c) SC transition temperature T_c; note that T_c becomes zero at half filling, which however is not visible, and finite once carrier is doped. If AF order is absent, T_c would follow the curve (b).

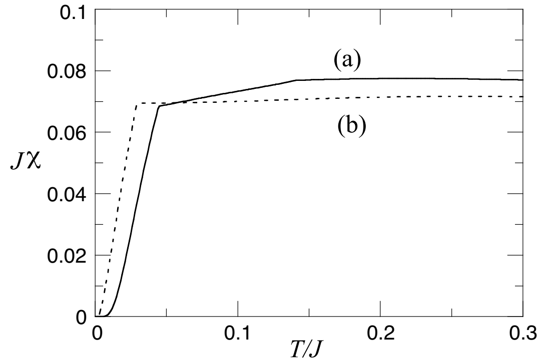

Figure 2: Uniform spin susceptibility χ as a function of T for (a) $\delta = 0.15$ and (b) $\delta = 0.167$.

(a) and (c) corresponds to the coexistence of AF and SC order, and there is a tetracritical point at $(\delta, T) = (\delta_{\rm tetra}, T_{\rm tetra})$ ($\delta_{\rm tetra} \approx 0.165, T_{\rm tetra} \approx 0.031J$) where the normal, AF, SC and coexistent states touch. This phase diagram is in qualitative agreement with that obtained experimentally[2].

The coexistence of AF and SC order was already predicted in the previous works[3, 4, 5]. However, the Néel temperature shows the reentrant behavior around the tetracritical point in contradiction to the experimental findings[2]. The difference between the present and the previous works resides in the different choices of the long-range transfer integrals t' and t'', which lead to different shapes of the Fermi surface. In the present paper t' and t'' are chosen in such a way that the nesting of the Fermi surface for the wave vector $\mathbf{Q}$ occurs near $\delta \approx \delta_{\rm tetra}$ though the system is away from half-filling. This results in a divergence of the static spin susceptibility $\chi(\mathbf{q})$ at $\mathbf{q} = \mathbf{Q}$ and thus the commensurate AF order is induced, while it is not the case for the choices of t' and t'' in Ref.3 and 4, leading to the reentrant behavior around the tetracritical point. From the above argument one may expect that the phase diagram may be determined by the shape of the Fermi surface irrespective of the values of t' and t''. In order to check this, we have examined the different values of t' and t'' which lead to almost the same Fermi surface ($t'/t = -1/6$, $t''/t = -1/5$). The resulting phase diagram becomes indeed almost the same as in the case of $t'/t = 0.12$ and $t''/t = -0.06$.

Next we study the uniform spin susceptibility $\chi(\mathbf{0}) = \chi$. In Fig.2 we show χ as a function of T for different values of δ. At high temperatures ($T > T_c$, T_N) χ is almost independent of T when δ is not so small ($\delta \gtrsim 0.15$). At lower T, χ shows qualitatively different behavior for $\delta > \delta_{\rm tetra}$ and $\delta < \delta_{\rm tetra}$. When $\delta < \delta_{\rm tetra}$, χ gradually decreases as T passes T_N ($\approx 0.14J$), and then sharply drops when the superconducting order sets in at $T = T_c$ ($\approx 0.045J$). On the other hand for $\delta > \delta_{\rm tetra}$, χ does not show a noticeable change at T_N ($\approx 0.017J$). This is because χ decreases rapidly below T_c ($\approx 0.03J$) due to the opening of the gap in the excitation spectrum and the change at $T = T_N$ is hard to be distinguished.

The coexistence of AF and SC order has not been observed in LSCO (single layer) and YBCO (bilayer) systems, and the AF state is realized only near half-filling ($\delta \lesssim 0.02$ for LSCO[6], $\delta \lesssim 0.055$ for YBCO[7]), though the superexchange interaction within the CuO_2 plane, J, is almost material independent. This may be understood as follows. In genuine two-dimensional systems the AF order cannot occur due to the Mermin-Wagner theorem. The weak three dimensionality, which is always present in real systems, may stabilize the AF order, but it would be easily hindered by such extrinsic effects as randomness. In single-layer and bilayer systems the effect of fluctuations due to low dimensionality may be strong and the AF order will be easily destroyed. On the contrary the SC order can occur as the Kosterlitz-Thouless (KT) transition at finite T even in genuine two-dimensional systems. Thus the SC order is expected to be more robust than the AF order, which may explain why the SC order is observed in a similar doping region in both multilayer and single-layer systems. (Note that the critical phenomena near T_c in real systems are not KT like, but three dimensional because of the weak three dimensionality.)

The coexistence of AF and SC order was observed only in multilayer systems. Nevertheless we expect that the present mean-field analysis based on the single-layer model may capture the essential features of the phase diagram including the coexistent state, because the condition for the occurrence of the coexistence is essentially determined by the shape of the Fermi surface, in particular, the condition for the nesting. However, the precise and quantitative arguments should be given by employing the multilayer *t-J* model, which is under way.

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