Competing Orders and Superconductivity in the Doped Mott Insulator on the Shastry-Sutherland Lattice

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Quantum antiferromagnets on geometrically frustrated lattices often allow a number of unusual paramagnetic ground states. The fate of these Mott insulators upon doping is an important issue that may shed some light on the high \(T_c\) cuprate problem. We consider the doped Mott insulator on the Shastry-Sutherland lattice via the \(t\)-\(J\) model. The U(1) slave-boson mean field theory reveals the strong competition between different broken symmetry states. It is found that, in some ranges of doping, there exist superconducting phases with or without coexisting translational-symmetry-breaking orders such as the staggered flux or dimerization. Our results will be directly relevant to \(\text{SrCu}_2(\text{BO}_3)_2\) when this material is doped in future.

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Introduction: The understanding of the high \(T_c\) superconductivity in layered cuprates remains one of the central problems in correlated electron physics. Even though there is no consensus as to the solution of the puzzle, it is widely believed that the physics of the cuprates has much to do with the doped spin-1/2 Mott insulator. It was suggested by Anderson that the strong quantum fluctuations associated with the spin-1/2 and two dimensionality may lead to a quantum liquid of spin singlets or the resonating valence bond (RVB) state. Upon doping, it would become a superconductor when the holes are phase coherent. The undoped cuprate is, however, antiferromagnetically ordered, not a RVB liquid. Nonetheless, the hopping processes of the doped holes strongly frustrate the Néel order and the resulting spin-disordered state may have substantial correlations of the RVB state. This would be more likely the case if the RVB state were close in energy to the antiferromagnetic ground state in the undoped system.

It is, therefore, extremely interesting to identify the Mott insulators with no long-range spin order. It has been known for sometime that quantum antiferromagnets on the geometrically frustrated lattices are such examples. At the classical level, the frustration often leads to a large degeneracy of the classical ground state and the resulting fluctuations can suppress the classical long-range spin-order. Previous studies showed that various quantum paramagnetic ground states can also occur at zero temperature and they include various translational-symmetry-breaking phases as well as the RVB state. In this case, the doping of holes or electrons may naturally lead to superconductivity.

In this context, the recent discovery of superconductivity in layered cobaltates, \(\text{Na}_x\text{CoO}_2\cdot y\text{H}_2\text{O}\), deserves particular attention. It has been suggested that this system can be regarded as an electron doped Mott insulator with spin-1/2 Co ions on the triangular lattice. Recent theoretical studies of a model based on the RVB picture found a superconducting phase with the \(d + id\) pairing symmetry. While the cobaltates is in a doped state, an undoped spin-1/2 Mott insulator, \(\text{Cu}_x\text{CuCl}_4\), with Cu spins on the anisotropic triangular lattice, has been also identified. The ground state is magnetically ordered, but the system seems to be very close to the phase transition toward the RVB or spin-liquid state, as seen from the neutron scattering experiments and a large-\(N\) mean-field theory.

These discoveries raise the hope that one may be able to achieve “high \(T_c\)” superconductivity by doping frustrated magnets. Moreover, the studies of these systems may provide an insight about the role of the dynamic frustration due to the motion of doped holes in cuprates and its influence on the superconductivity, albeit it is not the same as the geometric frustration.

In this paper, we study possible superconducting states and other competing orders in the doped Mott insulator on the Shastry-Sutherland lattice. The lattice structure is shown in Fig.1. This work is strongly motivated by the discovery of the Mott insulator \(\text{SrCu}_2(\text{BO}_3)_2\) where the spin-1/2 Cu ions lie in two dimensional layers decoupled from each other. Remarkably, the topology of the nearest-neighbor antiferromagnetic exchange couplings between the Cu ions is identical to the Hamiltonian studied by Shastry and Sutherland many years ago. The model is the nearest-neighbor antiferromagnetic Heisenberg model on the Shastry-Sutherland lattice with different exchange couplings on the square lattice links \((J)\) and diagonal links \((J')\). The quantum phase diagram of this model in a wide parameter range has been extensively studied recently. Possible paramagnetic ground states include the plaquette-ordered phase, decoupled-dimer state, and the topologically ordered RVB spin-liquid phase.

In the case of \(\text{SrCu}_2(\text{BO}_3)_2\), the values of the exchange couplings \((70 \sim 85 K)\) are much smaller than those in high-\(T_c\) cuprates (about 1500K), we therefore expect a lower superconducting transition temperature for the putative superconducting state at finite doping. The ex-
periments on the undoped system show clear spin-gap behavior and the material at ambient pressure may be in the decoupled-dimer state with the dimers on the diagonal links. This state is likely to be very close to the phase boundary of the spin-liquid state according to the large-N mean field calculation. We expect, therefore, that there will be strong competitions between different orders upon doping.

The appropriate model to describe this material at finite doping is the $t$-$J$ model on the Shastry-Sutherland lattice. This model was previously studied by Shastry and Kumar via a RVB mean-field approach where only the order parameters in the particle-particle channel were considered. As has been done in the cases of the square and triangular lattices, here we consider both the particle-hole and particle-particle channels and their mutual influence. We used the U(1) slave-boson mean field theory to get the phase diagram at zero and finite temperatures. It turns out that the consideration of the order parameters in the particle-hole channel is very important and leads to a qualitatively different phase diagram.

We start from the insulating decoupled dimer phase at the half-filling, that is appropriate for SrCu$_2$(BO$_3$)$_2$. At low temperatures, three superconducting phases appear successively as the doping is increased; a superconductor with dimerization, followed by a first order transition to a $d$-wave superconductor coexisting with the staggered flux order, and finally a uniform $d$-wave superconductor. Details of the phase diagram and other competing phases will be discussed below. We start with the description of the slave-boson mean-field theory.

**U(1) slave-boson mean-field theory:** In the U(1) slave-boson formulation, the electron operator $c^\dagger_{i\sigma}$ can be written as $c^\dagger_{i\sigma} = f^\dagger_{i\alpha} b_i (\alpha = \uparrow, \downarrow)$, where the fermion (boson) operator $f^\dagger_{i\alpha} (b_i)$ carries the spin (charge) quantum number. In this case, the constraint $f^\dagger_{i\alpha} f_{i\alpha} + b_i^\dagger b_i = 1$ should be imposed to exclude doubly occupied sites in the Hilbert space. Then the $t$-$J$ model can be written as

$$H = -\sum_{<i,j>} t_{ij} f^\dagger_{i\alpha} f_{j\beta} b_i b_j^{\dagger} + \text{h.c.}$$

$$+ \sum_{<i,j>} J_{ij} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_in_j) - \mu \sum_i f^\dagger_{i\alpha} f_{i\alpha}$$

$$+ i \sum_i \chi_i (f^\dagger_{i\alpha} f_{i\alpha} + b_i^\dagger b_i - 1),$$

where $t_{ij}$ and $J_{ij}$ are the hopping parameters and antiferromagnetic exchange couplings such that $t_{ij} = t$, $J_{ij} = J$ on the nearest-neighbor links and $t_{ij} = t'$, $J_{ij} = J'$ on the diagonal links (see Fig.1). Here $\vec{S}_i = \frac{1}{2} f^\dagger_{i\alpha} \vec{S}_{\alpha\beta} f_{j\beta}$, $n_i = f^\dagger_{i\alpha} f_{i\alpha}$, and $\lambda_i$ is the Lagrange multiplier introduced to impose the constraint.

In order to obtain the mean-field theory, we introduce the Hubbard-Stratonovitch fields $\chi_{ij}$ and $\Delta_{ij}$ to decouple the four-fermion interaction in the particle-hole and particle-particle channels, respectively. The resulting mean-field Hamiltonian can be written as

$$H_{mf} = \sum_{<i,j>} \left[ \frac{3J_{ij}}{8} (|\chi_{ij}|^2 + |\Delta_{ij}|^2) \right.$$}

$$- \chi_{ij}^2 (f^\dagger_{i\alpha} f_{j\alpha} + \frac{8t_{ij}}{3J_{ij}} b_i^\dagger b_j) - \Delta_{ij}^2 \epsilon_{\alpha\beta} f_{i\alpha} f_{j\beta} + \text{h.c.} \right]$$

$$- \mu \sum_i f^\dagger_{i\alpha} f_{i\alpha} - i \sum_i \chi_i (f^\dagger_{i\alpha} f_{i\alpha} + b_i^\dagger b_i - 1)$$

(2)

At the saddle point of the mean-field action, we get

$$\chi_{ij} = \chi_{ij} + \frac{8t_{ij}}{3J_{ij}} b_i^\dagger b_j \quad \text{with} \quad \chi_{ij} = \langle f^\dagger_{i\alpha} f_{j\alpha} \rangle$$

$$\Delta_{ij} = \langle \epsilon_{\alpha\beta} f^\dagger_{i\alpha} f^\dagger_{j\beta} \rangle.$$

(3)

Notice that $\chi_{ij}$ can be used as an alternative mean-field variables instead of $\chi_{ij}$.

At the half-filling, the original Hamiltonian has a hidden SU(2) symmetry. Upon doping, this symmetry is broken down to U(1) and there exist a number of equivalent mean-field states that can be transformed into each other under the U(1) gauge transformation: $f^\dagger_{i\sigma} \rightarrow e^{i\phi_i} f^\dagger_{i\sigma}$, $b_i^\dagger \rightarrow e^{i\phi_i} b_i^\dagger$, $\chi_{ij} \rightarrow \chi_{ij} e^{i(\phi_i - \phi_j)}$, and $\Delta_{ij} \rightarrow \Delta_{ij} e^{i(\phi_i + \phi_j)}$. Therefore, the mean-field states should be classified using the the gauge-invariant quantities. It will prove useful to utilize $\chi_{ijk}$ on each plaquette and $\chi_{ijk}$ on each triangular loop. The phases of these products can be interpreted as the “flux” of the U(1) gauge field going through a plaquette or a triangle. If the “flux” away from half-filling does not equal to $\pi$ or 0, it will generate the staggered orbital current proportional to $\text{Im}(\langle b_i^\dagger b_j \rangle - \chi_{ij}^2)$ running through the plaquette or triangle. The superconductivity requires the condensation of the bosons $b_i^\dagger b_i$ as
with $d$-wave superconductivity. In this phase, we have $|\chi_1| = |\chi_2| = \bar{\chi}$, $|\bar{\chi}_1| = |\bar{\chi}_2| = \bar{\chi}$, $\Delta_1 = -\Delta_2 = \Delta$, and $\Delta_1 = \Delta_2 = 0$. Moreover, the product of the $\chi$ fields has a non-trivial phase factor (or “flux”) $\pm \phi$ on the plaquette and $\pm \phi/2$ on the triangle in a staggered fashion where $0 < \phi < \pi$. There exists a finite staggered orbital current circulating around the plaquette, and no current along the diagonals. It is worthwhile to notice that the staggered flux phase coexisting with $d$-wave superconductivity was not discovered in the slave-boson mean-field theories of the pure $t$-$J$ model on the square and triangular lattices [17, 18, 19] (except for the large-$N$ SU($N$) study where only the $\chi_{ij}$ field is considered [12]).

As the doping is increased, the staggered flux order decreases and vanishes at $\delta = 0.12$ where the ground state undergoes a continuous transition to the uniform $d$-wave superconducting state where $|\chi_1| = |\chi_2| = \bar{\chi}$, $|\bar{\chi}_1| = |\bar{\chi}_2| = \bar{\chi}$ with $\bar{\chi}$ and $\bar{\chi}$ being comparable to each other, and $\Delta_1 = -\Delta_2 = \Delta$, $\Delta_1 = \Delta_2 = 0$. There is no flux or orbital current in this phase. This phase is similar to the $d$-wave superconducting phase found in the pure $t$-$J$ model on the square lattice [13, 17] except that we have nonzero diagonal $\chi$ fields.

When the doping reaches $\delta = 0.22$, the superconducting order vanishes and the ground state becomes a normal Fermi liquid [12, 14]. In this phase, all the $\Delta$ fields are zero, and the $\chi$ fields are real with $\chi_1 = \chi_2 = \bar{\chi}$, $\bar{\chi}_1 = \bar{\chi}_2 = \bar{\chi}$. Also, the magnitude of $\chi_1$ is comparable to that of $\bar{\chi}_1$.

**Finite temperature phase diagram:** The phase diagram at finite temperatures as a function of doping and temperature (in unit of $t'$) is plotted in Fig.3. The thick solid line represents the first order phase transition. To the right, finite $d$-wave order parameter $\Delta$ starts to develop below the dashed line ($T_{RVB1}$). Also, the $\chi_{ij}$ fields have a nontrivial flux below the long dashed line. To the left of the first order transition line, the particle-particle dimer order parameter $\Delta$ is finite below the dot-dashed line ($T_{RVB2}$). Below the solid line ($T_{BEC}$), the bosons are condensed. The superconducting transition temperature $T_{SC}$ is the smaller of the $T_{RVB1}$ (or $T_{RVB2}$) and $T_{BEC}$ [13, 17]. In order to get nonzero bose-condensate at finite temperatures, we introduced a small kinetic energy term along the $c$-axis whose precise value is not important for the phase diagram.

To the left of the first order transition line (thick solid line), the phase I represents the superconducting phase defined by $T < \min(T_{BEC}, T_{RVB2})$ with $\Delta \neq 0$, $\bar{\chi} \neq 0$, and $< b_i > \neq 0$ and it is the same dimer superconductor discussed in the zero temperature case. The phase II can be a dimer phase without superconducting order when $T_{BEC} < T < T_{RVB2}$ with $\Delta \neq 0$, $\bar{\chi} \neq 0$, and $< b_i > = 0$. In the rest of the region II, there is no dimerization nor superconducting order.

The phase III is the $d$-wave superconductor coexisting with the staggered flux order. Absence of the bose-

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**FIG. 2:** Zero temperature phase diagram. The magnitudes of the order parameters $\chi$, $\bar{\chi}$, $\Delta$, $\bar{\Delta}$ (defined in the text and in unit of $t'$) are plotted as a function of doping $\delta$. The thin dot-dashed curve denoted by “Flux” is the value of $\phi$ (phase factor) of the plaquette product of $\chi$-fields (in unit of $\pi$).

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The bosons are condensed and there exist four different phases as shown in Fig.2. At the half-filling, the ground state is an insulator with the dimerization only on the diagonal bond: $\Delta_1 = \Delta_2 \neq 0$, others $= 0$ or $\bar{\chi}_1 = \bar{\chi}_2 \neq 0$, others $= 0$. Notice that the equivalence between the $\Delta$ and $\bar{\chi}$ dimer states is a consequence of the SU($2$) symmetry at the half-filling. This dimer ground state at the half-filling was also found in previous studies [12, 14]. Away from half-filling, however, this symmetry is broken and we find the phase with $|\bar{\chi}_1| = |\bar{\chi}_2| = \bar{\chi} \gg |\Delta_1| = |\Delta_2| = \Delta$, $\bar{\chi} \gg |\chi_1| = |\chi_2| = \chi$, and $\Delta_1 = \Delta_2 = 0$ is the ground state up to $\delta < 0.023$. There is no flux from the $\chi$ field. In this phase, since both $\Delta \neq 0$ and $< b_i > \neq 0$, it is a superconducting phase where Cooper pairs are dimer singlets living on the diagonals [14].

At $\delta = 0.023$, there is a first order transition from the dimer phase to the staggered flux phase coexisting...
condensation ($b_1 = 0$) in the phase IV leads to the staggered flux order without superconductivity, but with $d$-wave spin gap. As the doping is increased at low temperatures, the staggered flux order disappears and only pure $d$-wave superconductivity (with uniform $\chi$) remains in the phase V. Upon increasing temperature, superconductivity disappears in the phase VI, but $d$-wave spin gap survives. The phase VII is the Fermi liquid phase and the phase VIII is the “strange metal” phase with uniform $\chi$-field discussed in previous studies of the $t$-$J$ model on the square and triangular lattices.

Summary and Discussion: We investigated possible superconducting phases and other competing orders of the doped Mott insulator on the Shastry-Sutherland lattice within the slave-boson mean-field theory of the $t$-$J$ model. One of the most interesting discoveries is the $d$-wave superconducting state with coexisting staggered flux order or the staggered orbital current at relatively lower doping as well as the pure $d$-wave superconductor at higher doping. The coexisting phase was not discovered in the pure $t$-$J$ model on the square and triangular lattices. Perhaps more interestingly, we found two different “pseudogap” phases; one of them has the staggered flux order (staggered orbital current) and the $d$-wave spin gap. The other has only the $d$-wave spin gap without orbital current. It is intriguing to see the emergence of two different pseudogap phases on the Shastry-Sutherland lattice in view of the fact the long-range orbital antiferromagnetic order and the $d$-wave spin gap with only the short-range orbital antiferromagnetic correlations have been suggested as the origin of the pseudogap in cuprates. Clearly the geometric frustration is responsible for the complexity and competition shown in the phase diagram. Whether the dynamic frustration due to the motion of holes in cuprates leads to similar physics is an important question that needs to be investigated in future. Moreover, our results provide directly relevant predictions for the doped version of the Mott-insulator SrCu$_2$(BO$_3$)$_2$ that may be available in future.

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