Unconventional superconducting states on doped Shastry-Sutherland lattice

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(Dated: February 16, 2009)

PACS numbers: 71.10.Hf, 71.20.Li, 74.20.Mn

I. INTRODUCTION

Geometrically frustrated lattices have crucial impacts on the emergence of exotic electronic states in strongly correlated systems\textsuperscript{12}, examples are triangular layered cobaltates Na\textsubscript{x}CoO\textsubscript{2}\textsuperscript{3}, anisotropic triangular lattice Cs\textsubscript{2}CuCl\textsubscript{4}\textsuperscript{2} and three dimensional pyrochlore material KOs\textsubscript{2}O\textsubscript{6}\textsuperscript{5}. In particular, resonating valence bond (RVB) spin liquid or valence bond crystal may exist in frustrated quantum magnets. There is a hope that unconventional superconducting state may emerge upon doping of the frustrated magnets, it has been pointed out in the recent theoretical studies\textsuperscript{6,7,8,9,10,11}. Recent discovered two dimensional synthesized frustrated material SrCu\textsubscript{2}(BO\textsubscript{3})\textsubscript{2} is an important compound. It is topologically equivalent to the Shastry-Sutherland\textsuperscript{12,13} lattice, spin-\(\frac{1}{2}\) Cu\textsuperscript{2+} lies in two-dimensional CuBO\textsubscript{3} layers decoupled from each other by plane of Sr\textsuperscript{2+} ions, the antiferromagnetic exchange couplings between Cu\textsuperscript{2+} ions is identical to Heisenberg-hamiltonian of SS lattice and motivate us to investigate its doping properties. This lattice has been studied many years ago as a two dimensional exactly solvable\textsuperscript{14} spin model, a schematic Shastry-Sutherland lattice is illustrated in Fig.\textsuperscript{[1]}. Let \(J\) and \(J'\) be the exchange couplings along the square lattice and diagonal links, respectively. The production of valence-bond singlets on disjointed diagonal links is the exact ground state for \(J'/J > 1.47\)\textsuperscript{15,16,17}. Experiments showed that \(J'/J = 1.574\) is an optimal value\textsuperscript{18} for the insulator SrCu\textsubscript{2}(BO\textsubscript{3})\textsubscript{2}.

There are many previous investigations on the doping effect of the Shastry-Sutherland lattice and various techniques have been used\textsuperscript{19,20,21,22}. By using slave-boson mean-field theory\textsuperscript{19}, the competing orders of staggered flux state and d-wave superconducting state are investigated at a specific parameter regime. Similar results have been obtained in a recent variational Monte Carlo study\textsuperscript{22}. Based upon the analysis of \(t-J-V\) model via the bond-operator formulation, a number of superconducting states including s-wave, \((s+id)\)-wave, plaquette d-wave are found as the ground states of the doped Shastry-Sutherland lattice\textsuperscript{23}. On the other hand, exact diagonalization approaches\textsuperscript{24} have been employed to study the ground state of finite system and no superconducting order is found to be favored on doping.

In this paper, we apply the plain vanilla version of RVB theory\textsuperscript{23,24} to study the emergence of unconventional superconductivity. We define \(\eta = t'/t\) as the frustration amplitude, where \(t'\) and \(t\) are hopping integrals on diagonal links and square lattice links, respectively, and use \(t-t'-J-J'\) model to study the doping effect on the Shastry-Sutherland lattice. The competition among various superconducting states will be examined for both hole-doping and electron-doping cases. The phase diagram is depicted as functions of \(\eta\) and doping concentration \(\delta\). In particular, four distinct ground states show...
up. We classify these states in terms of relative phase of mean-field pairing amplitudes.

There are four possible ground state candidates. In certain limiting cases such as $|\eta| \ll 1$, it is well known that pairing symmetry belongs to $d_{x^2-y^2}$-wave with the superconducting order parameters on square lattice links $\Delta_x = -\Delta_y$ and the pairing parameters on diagonal links $\Delta_a = \Delta_b = 0$. Another candidate is the $s$-wave pairing symmetry with $\Delta_x = \Delta_y$ and $\Delta_a = \Delta_b$, while the relative phase shift between these two distinct links is equal to $\pi$. The third candidate state is staggered flux state, it can only be stable in negative $\eta$ and small doping. In such state, the complex particle-hole mean-field parameter is modulated alternatively by a staggered magnetic $\pm \phi$. The last candidate is normal metal with vanishing of mean-field parameters. Our calculation shows that from weak to intermediate frustration, $d$-wave state maintains in a large region of electron and hole dopings. Around the symmetric point $|\eta| = 1$, the symmetry of ground state is sensitive to the doping level since the energies of three distinct states, $d$-wave, $s$-wave pairing and staggered flux, are almost identical. For larger frustration $|\eta| > 1$, the ground state has an $s$-wave symmetry for both hole and electron doping.

The rest of the paper is organized as follows. In Sec. II, we propose the formalism of renormalized mean-field theory to study the $t$-$t'$-$J$-$J'$ model Hamiltonian on the Shastry-Sutherland lattice. In Sec. III, we present our numerical results of renormalized mean-field theory as functions of frustration and doping level, and mean-field phase diagram as well. Finally a summary is given in Sec. IV.

II. FORMALISM

A primitive unit cell of the Shastry-Sutherland lattice includes four inequivalent sites, we consider a $t$-$t'$-$J$-$J'$ model on such lattice. The Hamiltonian can be written as

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} \bar{P}(c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \bar{P} + \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j - \mu \sum_i n_i,$$

where $c_{i\sigma}^\dagger$ is to create a hole with spin $\sigma$ at site $i$, $\vec{S}_i$ is a spin operator, $\mu$ is the chemical potential. $\langle ij \rangle$ denotes a square lattice or diagonal link on the lattice, $t_{ij}$ and $J_{ij}$ stand for the hopping integrals and antiferromagnetic exchange couplings, respectively. $t_{ij} = t$ and $J_{ij} = J$ on the square lattice links, while $t_{ij} = t'$ and $J_{ij} = J'$ on the diagonal links, as shown in Fig. 1. We use $t$ as an energy unit and set $t/J = 3$. We choose $J'/J = (t'/t)^2$ to be consistent with the superexchange relation of $J = 4t^2/U$ in the large Hubbard $U$ limit. Projection operator $\bar{P} = \prod_i (1 - n_i n_i)$ removes all the doubly occupied states.

We define particle-particle condensate mean-field as well as particle-hole condensate mean-field as,

$$\Delta_{ij} = \langle c_{i\uparrow}^\dagger c_{j\uparrow} - c_{i\downarrow}^\dagger c_{j\downarrow} \rangle_0$$

$$\xi_{ij} = \langle c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow} \rangle_0,$$

where $\langle \rangle_0$ gives expectation value corresponding to states without constraint of no double occupancy. Although the number of independent parameters in Shastry-Sutherland lattice is twelve, our calculation shows the number can be reduced to eight due to certain symmetry. The effect of the projection operator is taken into account by a set of renormalized factors $\Delta \xi$ which are determined by statistical countings. Within the Gutzwiller approximation, the energy of physical state $\psi$ can be reduced to that of state $|\psi_0\rangle$ which is free of double occupancy constraint, i.e., $\langle \psi|H|\psi\rangle = \langle \psi_0|H'|\psi_0\rangle = \langle \psi_0|\delta H_0 + g_s H_s|\psi_0\rangle$. In homogenous case the renormalized factors are self-consistently obtained for each set of frustration parameter $\eta$ and doping level $\delta$, where $\delta$ denotes the doping density. Thus, we have the effective Hamiltonian,

$$H_{eff} = \sum_{\langle ij \rangle \sigma} -g_t t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \bar{P} + \sum_{\langle ij \rangle} g_s J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$- \mu \sum_i n_i,$$

and the resulting mean-field Hamiltonian can be expressed as

$$H_{MF} = \sum_{\langle ij \rangle \sigma} -\frac{3}{8} g_s J_{ij} [\xi_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \Delta_{ij} c_{i\sigma}^\dagger c_{j\sigma} + h.c.]$$

$$-g_t t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + const,$$

with $\text{const} = \frac{1}{8} J g_s \sum_{\langle ij \rangle} |\xi_{ij}|^2 + |\Delta_{ij}|^2$. We diagonalize the mean-field Hamiltonian in momentum space, all the local order parameters and the chemical potential $\mu$ are self-consistently obtained for each set of frustration parameter $\eta$ and doping level $\delta$, with this procedures the lowest energy state can be determined.

III. NUMERICAL RESULTS OF PHASE DIAGRAM AND MEAN-FIELD THEORY

In this section, we present our numerical results of renormalized mean-field theory on the Shastry-Sutherland lattice. The mean-field order parameters depend on both frustration parameter $\eta$ and doping level $\delta$. In our calculations, we choose several typical frustration amplitude to analyze pairing symmetry for different doping levels. Larger frustration parameter $|\eta|$ corresponds to stronger interactions on the diagonal bonds, and the symmetric point $|\eta| = 1$ has the strongest frustration. We will start from the phase diagram, then provide detailed discussion of mean-field order parameters as functions of frustration parameter $\eta$ and doping level $\delta$. 

As shown in Fig. 2, there exists four different phases in the phase diagram. It is obvious that the ground state has a $d_{x^2-y^2}$-wave or $d$-wave symmetry in the limit of $\eta \ll 1$ at finite doping. Our results show that $d_{x^2-y^2}$-wave state is stable in a wide parameter regions of $-\sqrt{0.9} < \eta < \sqrt{0.96}$ and finite doping. Previous studies have shown the robustness of $d$-wave pairing against weak frustrations on both triangular lattices and checkerboard lattices. It seems that such robustness is universal for weakly frustrated systems. At large $|\eta| > 1$, the ground state has an s-s-wave pairing symmetry with $\Delta_x = \Delta_y$ and $\Delta_a = \Delta_b$ while the relative phase between $\Delta_a$ and $\Delta_b$ is $\pi$. Recently the two families of the Fe-based superconductors are 1111 systems ReOFeAs with rare earth ions and the 122 systems AeFe$_2$As$_2$ with alkaline earth element Ae. An s-s-wave pairing symmetry was proposed as a popular candidate for the superconducting pairing symmetry of the Fe-based superconductors.

In between the above two regions, there are two non-superconducting states in such small parameter region around $|\eta| = 1$. The region around $\eta = -1$ corresponds to staggered flux state at low doping while the normal metal state prevails for $\eta \geq 1.2$ at finite doping ($\delta > 0.10$). It is interesting to find that there is an abrupt change of superconducting order parameters in between $d$-wave and s-s-wave state around $\eta = -1$ and the phase transition is first order. Around $\eta = 1$ region, phase transition from s-s-wave to d-wave state is a weakly first-order transition in which parameters change continuous at the boundary. Moreover, the phase transition between staggered-flux state and $d$-wave state is also first-order. Other phase boundary corresponds to second-order.

As we pointed out already, in the limit of weak frustration $|\eta| \ll 1$ upon doping, the model Hamiltonian may correspond to the well-known $t$-$J$ model in which the $d$-wave superconducting symmetry is the ground state. Our calculations are performed for various frustration parameter as well as doping level. In a wide range of parameter region, $d$-wave state appears to be robust as the ground state. In particular, our calculations show that $d$-wave state have lowest energy for positive $\eta$ less than $\sqrt{0.96}$. In Fig. 3, we present the amplitudes of the mean-field parameters as functions of hole density $\delta$ for $\eta = \sqrt{0.8}$ and $\eta = 1$, respectively. As shown in Fig. 3(a) for $\eta = \sqrt{0.8}$, a typical $d$-wave state is obtained and the parameter $\xi$ shows no much doping dependence. In the parameter region $0.96 < \eta \leq 1$, $d$-wave and s-s-wave superconducting state are highly competing. The mean-field order parameters of ground state are discontinuous as functions of hole density $\delta$. For better illustration, we take the symmetric point $\eta = 1$. As displayed in Fig. 3(b), the ground state has s-s-wave symmetry at small doping while the $d$-wave state prevails for larger doping level. The critical doping level corresponds to $\delta_c \approx 0.035$.

To reveal the competition between s-s-wave and $d$-wave states more clearly, we compare the mean-field order parameters, chemical potential as well as energy per site for these two states in Fig. 4 at the symmetric point $\eta = 1$. Fig. 4(a) shows parameter functions of $d$-wave, Fig 4(b) shows that for s-s-wave state in which $|\Delta_d|$ is larger than $|\Delta_{x,y}|$ where the subscript $d$ denote the diagonal bonds. For s-s-wave, all pairing parameters change non-monotonically to zero, and then metalic state emerges smoothly. We plot the parameters of s-s-wave from $\delta = 0.005$, at half filling there is no self-consistent s-s-wave solution. Fig. 4(c) shows the crossing of chemical potentials for those two competing states at the transition point $\delta \simeq 0.035$. In Fig. ref4(d), such a crossing of energy per site for those two states exhibits itself as well. It is rather clear that a zero-temperature
FIG. 4: Panels (a) and (b) describe the mean-field order parameters as functions of $\delta$ for $d$-wave and $s$-$s$-wave state for $\eta = 1$, respectively. Panels (c) and (d) correspond to the evolutions of chemical potential and energy per site as a function of $\delta$ for two competing states.

FIG. 5: Amplitudes of the mean-field order parameters as functions of $\delta$ for $\eta = -\sqrt{0.95}$. Panels (a) and (c) correspond to $d$-wave and staggered flux state, respectively. Panel (b) describes the accumulated phase of $\xi$ for staggered flux state.

first-order quantum phase transition may occur at the transition point $\delta \simeq 0.035$.

From Fig. 2 one can see that near $\eta = -1$, a staggered-flux state may appear in a small parameter region. For instance, we plot the mean-field parameters of $d$-wave state and staggered-flux state for $\eta = -\sqrt{0.95}$ in Fig. 5(a),(c) respectively. Calculation shows that for staggered flux state $\xi_{ij}$ is a complex value. The phase of $\xi_d$ is $\pi$, and the accumulating phase of $\xi_{ij}$ on a plane is independent of $\eta$ and reduces linearly with increasing doping, as shown in Fig. 5(b). At half-filling, it is hard to obtain self-consistent solution. For $\eta$ less than 0.04, the staggered flux state is stable, while in high doping level $d$-wave state has lower energy. For $\eta < -1$ $s$-$s$-wave state emerges with introduce of mobile charge, and have favorable energy than the staggered flux state.

For large frustrated amplitude, the interactions on diagonal bonds may play a dominate role in determination of superconducting pairing symmetry. When $\eta$ takes a value slightly larger than 1, as the superconducting pairing symmetry may change from $s$-$s$-wave to $d$-wave and mean-field parameters varies rather smoothly. This transition is weakly first order. In Fig. 6(a), it shows that $\Delta_d$ varies nonmonotonically to zero and ground state evolves from $s$-$s$-wave state to $d$-wave state with increasing doping for $\eta = \sqrt{1.005}$. Precise calculation of pairing parameters shows that around the critical point $\Delta_{x,y} \neq 0$. This is illustrated in the inset picture of Fig. 6(a), and indicates that this is a weakly first order phase transition. Fig. 6(b) presents the mean-field parameter as functions of $\delta$ for $\eta = \sqrt{1.08}$. We find that a larger $\eta$ corresponds to a smaller amplitude of $\Delta_{x,y}$ of $d$-wave state. For $\eta \geq 1.4$, amplitude of the $d$-wave state is vanished and metal state follows the $s$-$s$-wave.

For large frustrated amplitude, $s$-$s$-wave state is the ground state for both positive and negative $\eta$. Fig. 7(b) takes $\eta = \sqrt{2}$ as an illustration. By increasing doping to a considerable high level, both $|\Delta_{x,y}|$ and $|\Delta_d|$ approach zero. However they do not reach zero simultaneously and $\Delta_{x,y}$ decreases more rapidly. It implies that superconducting order parameter may exist only on diagonal bonds in some cases. As positive $\eta$ becomes larger, no metal state will appear since the pairing parameters of $s$-$s$-wave state may have finite amplitude at high doping level. For negative larger frustration amplitude cases, $s$-$s$-wave state is ground state at all doping level. Amplitude of $\Delta_d$ is larger comparing to that of correspond-
ing positive case, since the negative $t'$ frustrated hopping thus enhance pairing amplitude. It indicates that superconductivity favors electron doping. This has been shown in Fig. 7(a). It should be pointed out that for larger frustrated case, our mean field theory cannot obtain the exact dimer ground state at half-filling.

IV. SUMMARY

We have employed the renormalized mean-field theory to study the $t$-$t'$-$J$-$J'$ model on the geometrically frustrated Shastry-Sutherland lattice for both hole and electron doping cases. Our calculation shows that the ground state of the doped system depends on the frustration amplitude $\eta$ and doping level $\delta$. For weak frustration $\eta << 1$, $d$-wave state is stable in a large parameter region in agreement with the case of $t$-$J$ model on square lattice. For strong frustration $\eta > 1$, $s$-$s$-wave state dominates in a wide range of parameter region. This feature has also been found in the doped triangular and checkerboard antiferromagnets. When approaching the most frustrated point $\eta = 1$, $d$-wave state competes with $s$-$s$-wave state, the phase transitions are first-order, the parameters change suddenly at critical point. Near $\eta = -1$, staggered flux state dominates. For frustrated amplitude is not very large, as doping increasing ground state changes from $s$-$s$-wave state to $d$-wave state via the weakly first-order transition. Moreover, we have found the enhancement of superconducting order parameter for negative $\eta$ because the negative $t'$ may introduce frustration in kinetic energy and result in the enhancement of the pairing amplitude. Our theoretical predications might be examined in future experiments on doped SrCu$_2$(BO$_3$)$_2$.

V. ACKNOWLEDGMENTS

H.X.H. would like to thank Profs. F.C. Zhang, Y.Q. Li and Y. Jiang for helpful discussions. This work was supported by the National Natural Science Foundation of China (Grants No. 10747145 and No. 10874032) and the State Key Programs of China (Grant No. 2009CB929204). Y.C. acknowledges the support from Shanghai Municipal Education Committee.

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