Possibility of superconductivity in the repulsive Hubbard model on the Shastry-Sutherland lattice

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(Received 9 June 2003; published 6 February 2004)

Possibility of superconductivity from electron repulsion in the Shastry-Sutherland lattice, which has a spin gap at half filling, is explored with the repulsive Hubbard model in the fluctuation-exchange approximation. We find that, while superconductivity is not favored around the half filling, superconductivity is favored around the quarter filling. Our results suggest that the Fermi-surface nesting is more important than the spin dimerization for superconductivity.

DOI: 10.1103/PhysRevB.69.054501 PACS number(s): 74.70.Kn, 74.20.Mn

Superconductivity from electron repulsion has acquired a renewed momentum from the discovery of high-T_C cuprates,[1] and the subsequent seminal proposal by Anderson[2] that the electron correlation should be at the heart of the superconductivity. An important, and still not fully understood, question dating back to the early stage along this line is the relation between the spin gap and the superconductivity. A gap in the spin excitation associated with a quantum spin liquid is, crudely speaking, favorable for a singlet-pairing formation. So one may naively expect that doping of carriers into a spin-gapped Mott insulator will show superconductivity. A clear-cut example is the *t-J* or Hubbard model on the two-leg ladder,[3] where the undoped ladder is a spin-gapped Mott insulator and the system indeed becomes superconducting when doped.

On the other hand, the spin gap is obviously not a *necessary* condition for superconductivity. The Hubbard model on the two-dimensional (2D) square lattice or the three-leg ladder[4] are examples, which are spin gapless at half filling,[3,5] but superconduct when doped.[4]

If we go back to the superconductivity from repulsive electron-electron interactions in a broader context, usual understanding is that the effective attraction between electrons is mediated by spin fluctuations.[6,7] An important difference from the superconductivity from attraction is that the effective attraction arises from pair-scattering processes across which the BCS gap function changes sign, so the effective attraction is wave-number dependent and the pairing is anisotropic (typically *d* wave as in the cuprates). Numerically, a quantum Monte Carlo calculation that takes care of the relevant energy scale[8,9] has shown an enhanced pairing correlation in the repulsive Hubbard model. Analytically, the fluctuation-exchange (FLEX) studies,[10–12] which is a kind of the renormalized random-phase approximation based on the Fermi-liquid picture, have shown *d*-wave superconductivity with a transition temperature $T_C \sim O(0.01t)$ for the repulsive Hubbard model. Notably, T_C is two orders of magnitude smaller than *t*, although T_C amounts to $\sim$100 K as in the high-T_C cuprates if we take $t \sim 0.4$ eV. We note that finite T_C's for superconductivity do not exist in purely 2D systems.[13] However, weak three dimensionality of real materials will give finite T_C. Specifically, Arita *et al.*[14] have found with FLEX that the T_C estimated for a weakly coupled stack of layers exhibits a smooth crossover to the T_C estimated for an isolated layer.

Recently, the multiband lattices having *disconnected Fermi surfaces* have been proposed as systems having much higher T_C's ($\gg 0.01t$);[15–19] while the motivation for considering disconnected Fermi surfaces is to raise the T_C, which is lowered down to $\sim 0.01t$ in ordinary lattices because the nodes in the BCS gap function intersect the Fermi surface: when the Fermi surface consists of pockets, the nodes can run in between the pockets. If we look at the proposed lattices in real space, on the other hand, we immediately notice that all of them happen to have dimerized structures in some way or other. From the spin-gap point of view one might consider this reasonable, since the dimerization can favor a spin gap when the dimerization is strong. However, we cannot identify which of the dimerization and the disconnected Fermi surface contributes to the higher T_C, since the dimerization and the disconnected Fermi surface are simultaneously satisfied in these lattices.

Now, there is an important and unresolved question of whether the spin gap associated with strong dimerization is a *sufficient* condition for superconductivity, i.e., whether the doped spin-gapped system can always become superconducting with an appreciable T_C. There are several lattices intensively studied from the viewpoint of the spin gap in the Mott-insulator phase. Among them is the Shastry-Sutherland (SS) lattice (Fig. 1), where we have a herringbone array of dimers. This lattice was first proposed by Shastry and Sutherland[20] about two decades ago. They found that the ground state in the Heisenberg model is spin-gapped when strongly dimerized, $J_2/J_1 < 0.5$, where $J_1(J_2)$ is the spin-spin interaction within (across) dimer. With the exact diagonalization method for finite clusters, Miyahara and Ueda[21] have recently obtained a more accurate critical value $J_2/J_1 \simeq 0.7$ for the appearance of the spin gap. Analytic studies such as a series expansion,[22] rigorous bounds,[23] and large-*N* theories[24] have indicated similar boundaries.

A recent impetus came from experiments on a copper compound $SrCu_2(BO_3)_2$, (Ref. 25) where the Shastry-Sutherland lattice is realized. Experimental results for magnetic susceptibility,[25,26] Cu nuclear quadrupole resonance,[25] high-field magnetization,[25] electron-spin resonance,[27] Raman

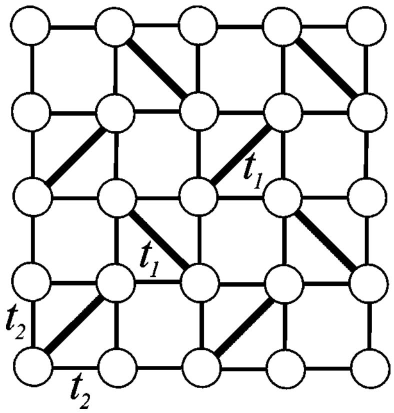

FIG. 1. The Shastry-Sutherland lattice.

scattering,[28] inelastic neutron scattering,[29] and specific heat[30] show that this compound has a dimerized ground state with a spin gap $\simeq 30$ K with no long-range magnetic order.[31]

So the SS lattice is an appropriate system for the above question of whether a spin-gapped system can superconduct when doped. A recent study[32] for the *t-J* model on the SS lattice has indeed discussed possible superconducting transition at low temperatures of $O(0.01t)$ based on RVB-type mean-field theory.[33] Usually the SS lattice is studied with the Heisenberg model, which corresponds to the half-filled Hubbard model. Here we have opted for the Hubbard model, since we can only study a finite Hubbard U, but also look at the SS lattice around quarter filling, which we propose here to be interesting. The band filling controls the shape of the Fermi surface after all, so that it should be an important parameter for studying the question at hand. Quarter-filled case is not unrealistic, since the herringbone structure of the SS lattice strongly reminds us of a class of dimerized organic crystals, where the band is often *quarter filled* rather than half filled.

So here we take the SS lattice to study superconductivity in the Hubbard model. We adopt the FLEX approximation, which has to be extended to four-band systems[16–18,34] to treat the SS lattice that has four atoms per unit cell. Superconducting transition has been examined with Eliashberg's equation.[35] We shall show that the Hubbard model, around half filling, does not exhibit superconductivity with significant T_C. So this provides an example in which a doped spin-gapped system does not guarantee an appreciable T_C. By contrast, the Hubbard model around the quarter filling exhibits superconductivity with a *d*-wave pairing when the dimerization is strong, $t_2 \ll t_1$. We shall discuss this in terms of the shape of the Fermi surface and the pair-scattering processes on it.

In the four-band version of the FLEX,[16–18,34] Green's function G, spin susceptibility χ, self-energy Σ are 4×4 matrices, e.g., $G_{lm}(\vec{k},i\epsilon_p)$ with ϵ_p being the Matsubara frequency. Here l,m refer to the four sites in a unit cell, which can be unitary transformed to band indices. We obtain the eigenvalue and the superconducting gap function ϕ_{lm} by solving the linearized Eliashberg equation.[35] For the susceptibility χ, we quote hereafter the value of the largest component when we diagonalize its matrix. In the present study, we take 32×32 k points and up to 8196 Matsubara frequencies, or 64×64 k points and up to 4096 Matsubara frequencies.

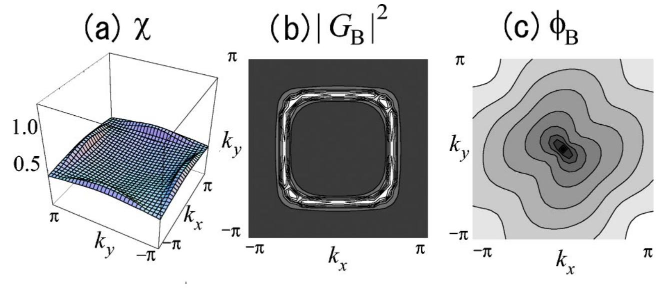

FIG. 2. Result for χ (a), $|G_B|^2$ (b), and ϕ_B (c) against k_x, k_y for the lowest Matsubara frequency for the nearly half filled $n=0.85$ with $U=7$, $t_1=1.8$, $t_2=1.0$, and $T=0.025$.

We start with the case of near half filling. Here we take the band filling n(= number of electrons/number of sites) $=0.85$, along with the on-site repulsion $U=7$ and the transfer energy within (across) dimer $t_1=\pm1.25$ ($t_2=1.0$). This value of t_1 has been adopted in Ref. 32 as appropriate to $SrCu_2(BO_3)_2$. Corresponding Heisenberg model at half filling has a spin gap because of $J_2/J_1 \sim t_2^2/t_1^2 \ll 0.7$.

The maximum eigenvalue of Eliashberg's equation λ has turned out to be much smaller than unity ($\lambda \simeq 0.43$) at low temperature ($0.01 \leq T \leq 0.04$). We have also calculated for $t_1=1.8$, which is a favorable value for the near-quarter-filled case as we shall see below, but λ is again very small ($\lambda = 0.36$, 0.37 at $T=0.04$, 0.01, respectively).

Figure 2 shows the spin susceptibility (χ), Green's function (G), and the gap function (ϕ) for the second band from the bottom (called B, which crosses the Fermi energy) for $t_1=1.8$ and $t_2=1.0$ at $T=0.025$. We see the susceptibility has no strong peaks, unlike in the square lattice which has a large antiferromagnetic peak in the susceptibility around $\vec{k} = (\pi,\pi)$ that is relevant to the superconductivity. The weak spin structure in the SS lattice should be due to the spin gap and/or the spin frustration which strongly prevent(s) the long-range spin correlation when the dimerization is strong.[36]

If we weaken the dimerization by making t_1 sufficiently smaller than t_2, the system becomes superconductive. Figure 3 shows the spin susceptibility, Green's function, and the gap

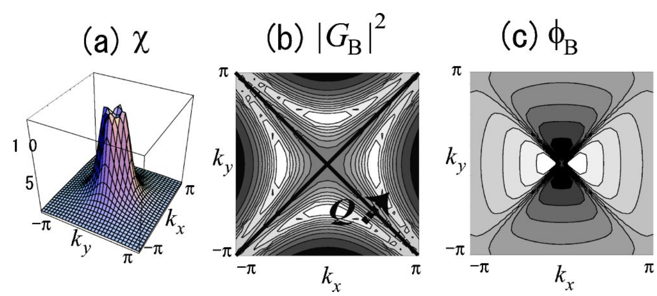

FIG. 3. The same plot as in Fig. 2 for a weaker dimerization with $t_1=0.5$. **Q** represent the nesting vector across $k_x = \pm k_y$ (solid lines).

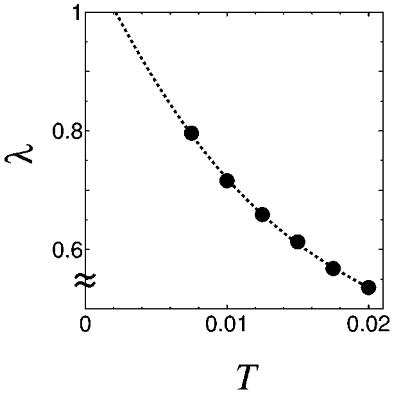

FIG. 4. For a nearly quarter-filled band ($n=0.55$) λ is plotted as a function of temperature T for $U=7$, $t_1=1.8$, and $t_2=1.0$. The dotted curve is a least-squares fit by a fourth-order polynomial. Here we take 32×32 k points and up to 8196 Matsubara frequencies. Error bars for different choice of the k-point mesh and Matsubara frequencies are $\sim10\%$ at low temperatures.

function for $t_1=0.5$ and $t_2=1.0$ at $T=0.025$, where we obtain a large $\lambda=0.94$ close to unity (λ becomes unity at lower temperature $T\sim0.02$). In the figure we see the Fermi-surface nesting across $k_x=\pm k_y$ is appreciable and the spin susceptibility has a strong peak around (0,0), which corresponds to the peak around (π,π) on the square lattice ($t_1=0$) folded. The result indicates that the dimerization (or the spin gap) is by no means a sufficient condition for very high-T_C. If we turn to the very high-T_C systems obtained in Refs. 15–19, dimerization causes the disconnected Fermi surfaces accompanied by antiferromagnetic spin fluctuations. So the present result is an example in which a dimerization works unfavorably for superconductivity in a simply connected Fermi surface. In this sense, the disconnected Fermi surfaces rather than the dimerization are essential for very high T_C in Refs. 15–19.

We have a drastically different situation when we change the band filling to quarter filling. Figure 4 shows the temperature dependence of λ at $n=0.55$ with the same parameter as those at $n=0.85$. We see λ is strongly enhanced at low temperatures.

Figure 5 shows χ, G, and ϕ for the lowest two bands (called A and B) that cross the Fermi energy for this filling. The peak in the spin susceptibility around (0,0) is much stronger than for the half filling. The spin fluctuation should mediate the pair scattering across which the gap function has opposite signs, resulting in d-wave superconductivity. How can this happen when the nesting vector is close to (0,0)? Figure 5(d) depicts the answer: the gap function has a d-wave symmetry as in the square lattice near half filling. This is physically natural because the SS lattice around quarter filling is effectively a square lattice around half filling in the strongly dimerized case $|t_1|\gg|t_2|$.

As mentioned above, it is interesting to compare the SS lattice with organic, d-wave superconductors such as κ-(BEDT-TTF)$_2$X.[37] If we assume the dimerization is sufficiently strong, the original system around quarter filling can be represented by a two-band[38,39] or a single-band[40,41] Hubbard model around half filling.[42] There, superconductivity is

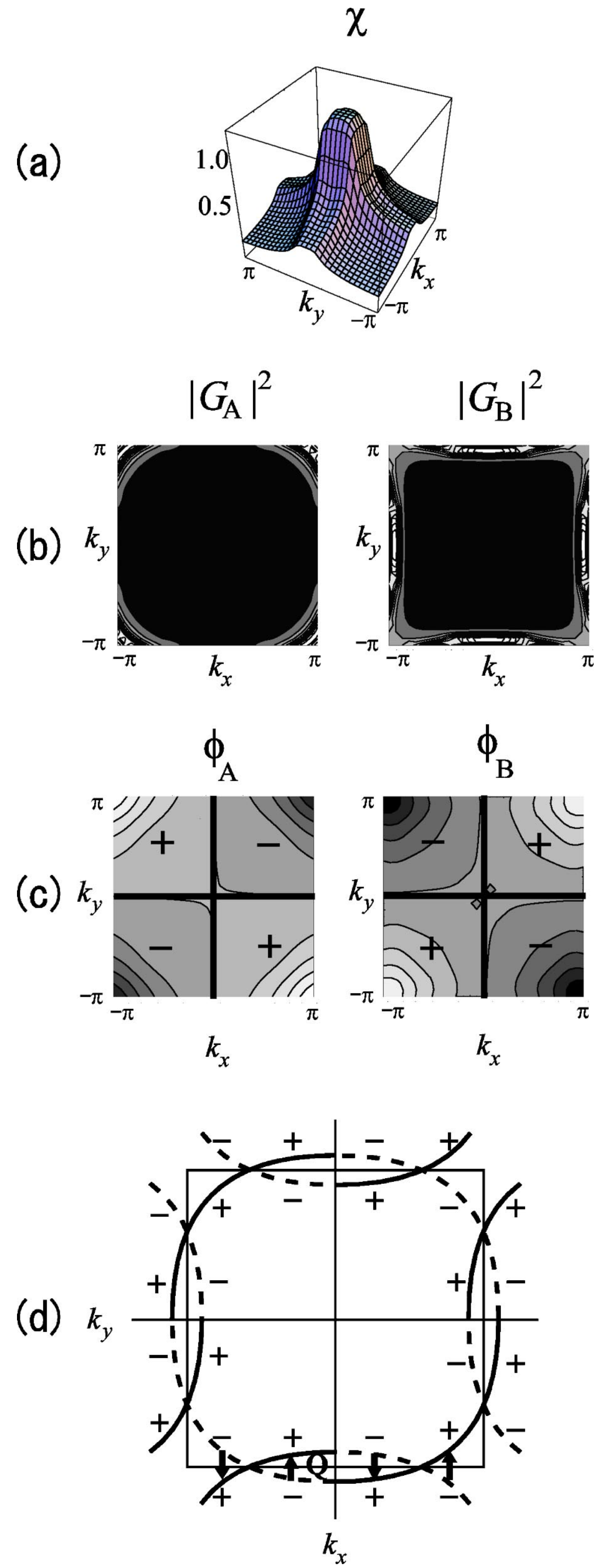

FIG. 5. For a nearly quarter-filled band ($n=0.55$) χ (a), $|G_\nu|^2$ (b), and ϕ_ν (c) ($\nu=A,B$) are plotted against k_x,k_y for the static case (lowest Matsubara frequency) for $U=7$, $t_1=1.8$, $t_2=1.0$, and $T=0.025$. (d) schematically depicts the sign of the gap function on the Fermi surface, where **Q** and arrows represent the nesting vector $\sim(0,0)$.

enhanced for $\sim 1/4$ filled band by strong dimerization as in the present study. Although organic materials that can be modeled by the SS lattice have not been known, it would be interesting to search for them.

In summary, we have studied superconductivity in the Hubbard model on the Shastry-Sutherland lattice with FLEX. Our analysis shows superconducting transition temperature, if any, is very small around half filling despite the presence of a spin gap due to the dimerization, while superconductivity is favored around quarter filling. Comparison with the RVB theory for the *t-J* model[32] is interesting because the RVB theory has shown T_C of $O(0.01t)$. While this may naively seem inconsistent with our result, the T_C of a conventional RVB theory on the SS lattice is much smaller than that $[\sim O(0.1t)]$ for the square lattice.[43,44] So the situation about the difference between T_C's is similar to this case.

This work was supported in part by a Grant-in-Aid for Scientific Research and Special Coordination Funds from the Ministry of Education of Japan. Numerical calculations were performed at the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

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weak next-nearest hopping in the square lattice does not strongly prevents the spin correlation and even enhances the superconductivity. On the other hand, the spin gap also prevents the spin correlation in many systems such as ladder systems, but does not result in very high-T_C systems.

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