Staggered-flux normal state in the weakly doped *t-J* model

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A normal (nonsuperconducting) ground state of the *t-J* model may be variationally approximated by a Gutzwiller-projected wave function. Within this approximation, at small hole doping near half-filling, the normal state favors staggered-flux ordering. Such a staggered-flux state may occur in vortex cores of underdoped high-temperature cuprate superconductors. From comparing the energies of the staggered-flux state and of the superconducting state, we numerically obtain the condensation energy. Extracting the superfluid density directly from the projected superconducting wave function, we can also estimate the coherence length at zero temperature.

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Gutzwiller-projected (GP) wave functions are known to give good variational energies for the *t-J* model in the range of parameters relevant for high-temperature cuprate superconductors.[1–3] Not only do they correctly predict the *d*-wave symmetry of the superconducting pairing, but they also successfully describe properties of the superconducting state, including doping dependence of the order parameter, quasiparticle spectral weight, Drude weight, and even antiferromagnetic instability at very low doping.[4] Conceptually, use of GP wave functions for studying cuprate superconductors is tempting because of their resonating-valence-bond structure,[5] which may be relevant for such effects as topological order and spin-charge separation proposed for explaining unconventional properties of underdoped cuprates.[6,7]

If we indeed assume that GP wave functions capture the essential physics of underdoped cuprates, we may further use such wave functions for describing not only their superconducting, but also the *normal* state. While the ''pseudogap'' normal phase appears above the superconducting transition temperature and is not accessible for the variational wave function approach, the normal state also appears in vortex cores within the superconducting phase. From the available experimental evidence, the normal vortex cores are closer in their properties to the pseudogap phase than to the conventional Fermi liquid.[8,9] Lee and Wen suggested that the normal state in the vortex core is a staggered-flux state.[10] Such a state may be described by GP variational wave functions, in a manner similar to the superconducting state.

The main goal of this paper is to construct a normal ground-state wave function of the *t-J* model by projecting the doped staggered-flux state and to compare the resulting variational energy to that of the superconducting state. To make the paper self-contained, we start with a brief overview of the relations between projected staggered-flux and superconducting wave functions. This part also explains our motivation to use the staggered-flux wave function for the normal state. The second part of the paper contains the variational Monte Carlo results on the condensation energy and their implications for the doping dependence of the coherence length.

At zero doping, the staggered-flux state and the *d*-wave superconducting state yield the same variational wave function upon Gutzwiller projection (projecting onto the no-double occupancy states) due to the particle-hole symmetry.[11,12] The resulting wave function describes a spin liquid with the algebraic decay of spin correlations.[13] This spin-liquid state is not physically realized at zero doping because of the antiferromagnetic (AF) instability leading to the AF ordering. The use of GP wave functions for describing the ground state of the *t-J* model is based on the assumption that upon doping this AF Mott insulator with holes, the AF instability disappears and the spin-liquid behavior is restored.

The most used variational ansatz for the weakly doped *t-J* model is the *nearest-neighbor d-wave pairing* state involving only nearest-neighbor hopping and nearest-neighbor *d*-wave pairing on the square lattice.[2,3] For such a state, the equivalence of the staggered-flux and the *d*-wave pairing states may be extended to the case of nonzero doping, if the notion of Gutzwiller projection is modified in a SU(2)-invariant way (respecting the particle-hole symmetry away from half-filling).[14] The projected wave function has algebraic decay of spin and current correlations. The algebraic decay of correlation functions suggests that this wave function may represent a critical point and not a stable phase. In our further discussion we label this wave function as ''critical'' (CR).

It is known that the variational energy of the CR wave function may be further lowered by adding a nonzero chemical potential before projecting (in the pairing gauge).[2] In the mean-field theory, this chemical potential plays an important role for stabilizing superconductivity.[15] In the GP wave function approach, the role of the chemical potential is less transparent; here it serves only as an additional variational parameter. It shifts the nodes in the spectrum from $(\pi/2, \pi/2)$ to an incommensurate point along the diagonal of the Brillouin zone. We conjecture that a nonzero chemical potential also cuts off the algebraic behavior of the correlation functions at a finite correlation length, but this so far could not be convincingly proven by numerical calculations limited to relatively small system sizes. The GP wave function with the variationally optimized chemical potential we further denote as ''superconducting'' (SC).

In fact, both the CR and SC wave functions are superconducting in the sense that they break the U(1) electromagnetic gauge symmetry in the thermodynamic limit (at a nonzero hole doping). While this property is rather obvious for the SC state, it requires an additional clarification for the CR state. As explained in Ref. 14, the CR state may be obtained by projecting an undoped staggered-flux state wave function by means of the special ''SU(2)-invariant'' Gutzwiller projection. Since the wave function before the projection is not superconducting, one could doubt the superconducting nature of the projected wave function. However, the SU(2)-invariant Gutzwiller projection involves two species of slave bosons designed to convert both empty and doubly occupied sites into physical holes. In the thermodynamic limit, these two species of bosons form two Bose condensates. The relative phase between those condensates corresponds to the broken U(1) electromagnetic gauge symmetry.

If one attempts to design a wave function of a superconducting vortex with the use of Gutzwiller projection, the broken U(1) symmetry in the CR and SC wave functions comes into play: It is not possible to construct a smooth vortex core by a slow variation of SC or CR wave functions. A naive way to resolve this problem is to suppress the order parameter in the vortex core, as it happens in conventional superconductors. However, as pointed out in Ref. 10, such a vortex core may not require the least amount of energy. A more energetically favorable vortex core could be constructed by modifying the CR wave function into a nonsuperconducting one. For this purpose, we take the unprojected undoped staggered-flux state used in Ref. 14 for the SU(2)-invariant Gutzwiller projection and dope it until the number of fermions exactly matches the required number of physical electrons [such a doping opens Fermi pockets around the $(\pi/2, \pi/2)$ points of the Brillouin zone]. If we further apply the SU(2)-invariant Gutzwiller projection to this doped staggered-flux wave function, only one of the two species of bosons get involved (since the number of the fermions exactly matches the required number of electrons, the doubly occupied sites should not be converted into holes), and the SU(2)-invariant Gutzwiller projection in this case coincides with the usual one (prohibiting doubly occupied sites). The resulting state is obviously nonsuperconducting: It does not break the electromagnetic U(1) symmetry. Instead it breaks the time-reversal and translational symmetries, as it has static currents circulating in the staggered-flux pattern. We further denote this GP wave function as the ''staggered-flux'' (SF) state.

We schematically summarize the relationship between those three types of the GP wave functions (CR, SC, and SF) in Fig. 1. From our construction it follows that both the SC and SF states may be obtained as deformations of the CR state (with the required deformation being small at small doping). Therefore, at small doping, SC and SF states are close in energy, and this makes the SF state a good candidate for the competing ground state.

From comparing the energies of the SC state (E_{SC}) and of the SF state (E_{SF}), we can deduce the condensation energy

$$\varepsilon_c = E_{\mathrm{SF}} - E_{\mathrm{SC}}. \tag{1}$$

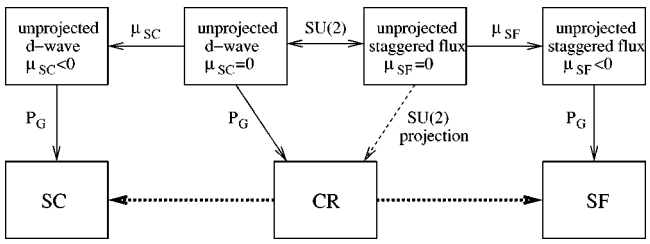

FIG. 1. A schematic illustration of the construction of the GP wave functions SC, CR, and SF. The top row of rectangles denotes unprojected wave functions. The unprojected nearest-neighbor *d*-wave and staggered-flux states at $\mu_{\mathrm{SC}}=0$ and $\mu_{\mathrm{SF}}=0$ are related by a SU(2) gauge transformation in the particle-hole space. Vertical solid arrows denote the Gutzwiller projection P_G, and the dashed arrow is the SU(2)-invariant projection as defined in Ref. 14. The dotted arrows connecting the CR state to SC and SF states are drawn to illustrate that the two latter states are continuous deformations of the CR state.

The condensation energy is involved in the energy balance determining the order parameter in nonuniform settings, e.g., in superconducting vortices. The energy of a superconducting state with a nonuniform phase of the order parameter may be written in the Ginzburg-Landau form

$$E = \varepsilon_c + \rho_s (\nabla \varphi)^2, \tag{2}$$

where φ is the phase of the order parameter, and ρ_s is the superfluid stiffness (proportional to the superfluid density). The size ξ of the vortex core may be estimated from minimizing the total energy consisting of the two parts: the core energy $\pi \xi^2 \varepsilon_c$ (up to a numerical prefactor of order one depending on the specific shape of the order-parameter profile) and the supercurrent energy $2\pi\rho_s \ln \lambda/\xi$ (where λ is the infrared cutoff). The resulting vortex size ξ (which may also be called Ginzburg-Landau coherence length at zero temperature) is

$$\xi = \sqrt{\rho_s/\varepsilon_c}. \tag{3}$$

The superfluid stiffness for strongly correlated systems was discussed in detail in Ref. 16. It is given by the sum of the diamagnetic term (proportional to the kinetic energy in the ground state) and of the paramagnetic term determined by the quasiparticle excitations. For our superconducting state, at the mean-field level, the low-lying quasiparticles have a Dirac-like spectrum around the nodal points. We assume that the low-lying quasiparticles preserve their mean-field structure, then the paramagnetic contribution vanishes at zero temperature.[17] Thus ρ_s is given by the diamagnetic term alone which, in our notation, equals[16]

$$\rho_s = -\tfrac{1}{16}\langle E_t \rangle, \tag{4}$$

where E_t is the hopping part of the *t-J* Hamiltonian, and the average is taken in the SC state.

Below we present our numerical results for ε_c and ρ_s (by the variational Monte Carlo method) in the *t-J* model with $t/J=3$. We start with defining the variational parameters of the wave functions. A GP wave function is constructed as

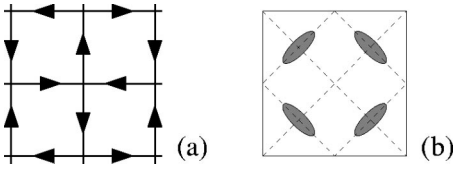

FIG. 2. (a) The vector potential in the staggered-flux state. (b) The Fermi pockets around $(\pi/2, \pi/2)$ points in the staggered-flux state.

$$\Psi_{\mathrm{GP}} = P_G \Psi_0, \tag{5}$$

where P_G is the "double" projection: First, it projects out components with doubly occupied sites (the usual Gutzwiller projection), and second, it fixes the number of particles to the required value (we shall work with finite systems where the required doping will be enforced via projection). Ψ_0 is the ground-state wave function of a BCS Hamiltonian:

$$H = \sum_{ij} \left[-\chi_{ij} c^{\dagger}_{i\alpha} c_{j\alpha} + \Delta_{ij} (c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{j\uparrow}) + \mathrm{H.c.} \right]. \tag{6}$$

χ_{ij} and Δ_{ij} are hopping and pairing amplitudes variationally adjusted to minimize the expectation value of the *t-J* Hamiltonian

$$H = P_G \left[\sum_{ij} \left[-t c^{\dagger}_{i\alpha} c_{j\alpha} + J(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j) \right] \right] P_G . \tag{7}$$

in the state Ψ_{GP}.

The CR state has χ_{ij} and Δ_{ij} nonzero only on nearest-neighbor links: $\chi_{ij} = \chi$, $\Delta_{ij} = \pm \Delta$, with $\pm$ for vertical and horizontal links, respectively. The SC state differs from the CR state only by the on-site term $\chi_{ii} = -\mu_{\mathrm{SC}}$. The SF state has $\Delta_{ij} = 0$, $\chi_{ij} = e^{i a_{ij}}$, where $a_{ij} = \pm \Phi/4$ is the vector potential defining the staggered flux pattern with the flux Φ [Fig. 2(a)]. The SF state also contains the chemical potential $\chi_{ii} = -\mu_{\mathrm{SF}}$, which is fixed to provide the required hole density and is not a variational parameter (unlike μ_{SC} in the SC state). At zero doping, all the three states coincide with $\mu_{\mathrm{SC}} = \mu_{\mathrm{SF}} = 0$, $\Delta/\chi = \tan(\Phi/4)$.

The variational parameters are μ_{SC} and Δ/χ in the SC state, and Φ in the SF state. We determine these parameters as a function of doping by minimizing the energy on the 22×22 lattice with the boundary conditions periodic in one and antiperiodic in the other direction. The results are plotted in Fig. 3(a). We find that while the gap in the superconducting state closes at around 30% doping,[18] the gap in the SF state closes at a smaller doping (around 20%).

We further use those variational parameters to determine the condensation energy ε_c. The finite-size effects are very strong in the SF state, because the Fermi pockets [Fig. 2(b)] are represented only by a small number of points in the momentum space. To estimate the magnitude of the finite-size effects, we plot ε_c for different system sizes, but with the same variational parameters, in Fig. 3(b). At small doping, ε_c grows roughly linearly with doping. This linear doping dependence is not intuitive: the mean-field theory would give $x^{3/2}$ dependence on the doping x, from the energy of the Fermi pockets. Remarkably, the same linear x dependence

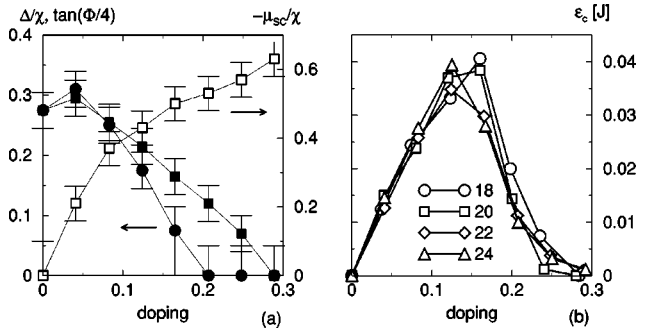

FIG. 3. (a) The gaps in the SF and SC states (solid circles and squares, respectively, scale on the left side) and μ_{SC} in the SC state (empty squares, scale on the right side) at different hole dopings. The optimization is performed on the 22×22 lattice with boundary conditions periodic in one and antiperiodic in the other direction. $t/J = 3$. (b) The condensation energy ε_c at different dopings and for different system sizes ($N \times N$ lattice with $N = 18,20,22,24$) in the units of J, per lattice site.

was obtained by Lee and Nagaosa after including the gauge-field fluctuations.[19] As a result of this linear x dependence, the core size remains finite in the small-doping limit. As the doping increases, the gaps in the SF and SC states decrease, which eventually leads to a decrease in the condensation energy ε_c. When the gaps close, the SF and SC states again coincide (with $\mu_{\mathrm{SC}} = \mu_{\mathrm{SF}}$), yielding $\varepsilon_c = 0$.

The profile of ε_c versus doping resembles the doping dependence of T_c in the cuprates. It seems reasonable to interpret the regions of increasing and decreasing ε_c as underdoped and overdoped regimes, respectively. With this interpretation, our results indicate that in the uderdoped (and possibly also in the weakly overdoped) regime the normal state inside the vortex core has a staggered-flux order. This order disappears in the strongly overdoped regime.

We further compute the superfluid stiffness ρ_s using Eq. (4). In Fig. 4(a) we plot the hopping energy E_t in the SC state as a function of doping (here we use the optimized values of Δ and μ_{SC}). The doping dependence of ρ_s is neary linear as expected.[17,20]

Combining the results for ε_c and for ρ_s, we find the

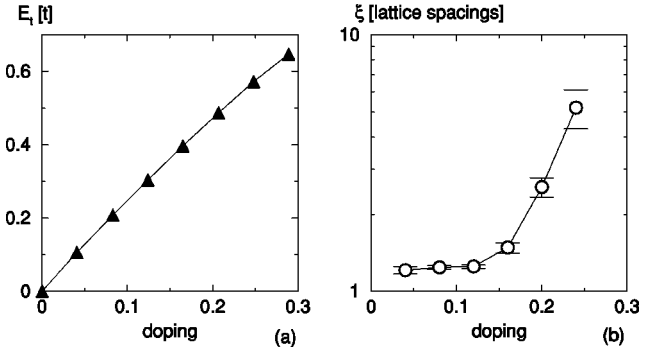

FIG. 4. (a) The hopping energy E_t in the SC state as a function of doping (in the units of t, per lattice site). The data shown are for the 22×22 lattice ($t/J = 3$). The finite-size effects and the error bars are smaller than the symbol size. (b) The coherence length ξ as a function of the doping for $t/J = 3$. Note the logarithmic scale for ξ.

Ginzburg-Landau coherence length ξ according to Eq. (3). The results are shown in Fig. 4(b).

Even though the staggered-flux core requires relatively little energy, the resulting coherence length is very short in the underdoped region. We find the coherence length of the order of one lattice spacing, which is smaller than the experimental findings.[8,9,21] Such a short coherence length must be considered a lower bound only, because SF core of the size of one lattice spacing does not make any physical sense. When we approximated the core energy by $\pi\xi^2\varepsilon_c$, we used the bulk energy density and ignored the energy requirement of the boundary between the SF and SC, i.e., the energy of smoothly connecting the two states. This assumption is correct only if the boundary is slowly varying and it surely breaks down when the distance scale is about one lattice constant.

In our treatment we neglected the possible AF order which probably plays a role at very low doping (below 0.1).[4] We expect that taking into account possible AF ordering both in the normal and in the superconducting states lowers the energy of both and only slightly modifies our results at the very low doping.

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