Pseudogap, competing order and coexistence of staggered flux and $d$-wave pairing in high-temperature superconductors

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(Dated: January 22, 2004)

We study the $t$-$J$-$V$ model of a doped Mott insulator in connection to high-$T_c$ superconductors. The nearest neighbor Coulomb interaction ($V$) is treated quantum mechanically on equal footing as the antiferromagnetic exchange interaction ($J$). Motivated by the $SU(2)$ symmetry at half-filling, we construct a large-$N$ theory which allows a systematic study of the interplay between staggered flux order and superconductivity upon doping. We solve the model in the large-$N$ limit and obtain the ground state properties and the phase diagram as a function of doping. We discuss the competition and the coexistence of the staggered flux and the $d$-wave superconductivity in the underdoped regime and the disappearance of superconductivity in the overdoped regime.

PACS numbers: 74.25.Jb, 71.10.Fd, 74.20.Mn, 71.10.Hf

The physics of doped Mott insulators has played a central role in the study of high-$T_c$ superconductors. Traditionally, the Mott insulating state is derived from the strong onsite Coulomb repulsion and naturally accounts for the antiferromagnetic (AF) ordered state at half-filling. There is increasing evidence that, due to large quantum fluctuations in spin-1/2 systems, several exotic quantum spin liquid states are likely hidden under the AF Mott insulating ground state. These states are competitive in energy and form a basis for the resonating valence bond route to superconductivity. Several important, yet unresolved problems remain: Is the $d$-wave superconductor (dSC) the ground state when the long-range AF order is destroyed by the coherent motion of the doped holes? Does the competition between the dSC and other forms of order account for the pseudogap phenomenon in the underdoped regime? Does the physics of doped Mott insulator explain the disappearance of superconductivity in the overdoped regime?

In this paper we demonstrate that long-range Coulomb interactions, not crucial for discussing the Mott insulating state, play an important role in addressing these issues associated with doped Mott insulators. Because charge fluctuations are limited by the density of doped holes, long-range Coulomb interactions have been thought to be not important near the stoichiometric Mott limit. However, since the strength of the interaction is large compared to the Fermi energy, its effects become quickly significant with doping. We consider the microscopic $t$-$J$-$V$ model where $V$ stands for the nearest-neighbor (NN) Coulomb repulsion. As in the $t$-$J$-model, the constraint of no double occupancy leads to an insulating state at half-filling. It is well known that the $d$-wave pairing state and the staggered flux phase (SFP) are identical at half-filling owing to an $SU(2)$ gauge symmetry, two competing phases at low doping. The SFP has a plaquette flux density wave (orbital current) order with $d$-wave symmetry. It is a metallic state with hole pockets and a pseudogap of the same symmetry as the dSC. Thus the SFP serves as a candidate pseudogap phase for underdoped cuprates, much as in the $d$-density wave scenario. However, in the standard $t$-$J$-model, the ground state becomes the dSC above doping. The SFP was found to be unstable to superconductivity and only exists at finite temperatures in a very narrow regime near half-filling.

We show that the NN Coulomb interaction introduces competing and coexisting order and changes significantly the structure of the phase diagram. It is crucial to treat the $V$-term quantum mechanically, on equal footing as the exchange $J$-term, since both pairing and screening originate at the same energy scale. Motivated by the $SU(2)$ symmetry at half-filling, we construct an $SU(N,q)$ ($q =$quaternion) generalization of the $t$-$J$-$V$ model. While the $SU(2N)$ theory favors the normal state and the $SP(2N)$ theory favors the superconducting (SC) state in the large-$N$ limit, the $SU(N,q)$ theory accommodates both staggered flux (SF) and SC order, and allows a systematic study of their interplay. In the large-$N$ limit, we find that the SF order coexists with the dSC below a critical doping $x_c$ where a quantum phase transition to a pure dSC phase takes place. The SC phase is destroyed in the overdoped regime beyond $x_p > x_c$. At finite temperatures, the onset of the SF order is at $T_{SF} > T_c$, giving rise to a pseudogap SFP above the SC transition temperature $T_c$. We discuss the phase diagram, the signatures of the coexistence and the pseudogap phase.

We start with the large-$N$ generalization of the $t$-$J$-$V$ model on a square lattice, $H = H_{tJ} + H_V$,

\begin{align}
H_{tJ} &= -\frac{t}{N} \sum_{\langle i,j \rangle} \left( c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.} \right) + \frac{J}{N} \sum_{\langle i,j \rangle} S_i \cdot S_j \\
H_V &= \frac{V}{N^2} \sum_{\langle i,j \rangle} n_i n_j, \quad V = V_c - \frac{1}{4} J.
\end{align}

The operator $c_{i,\sigma}^\dagger$ creates an electron with spin $\sigma = 1,1; \cdots; N,N$ at site $i$ under the constraint of no double occupancy for each spin flavor, $n_i = c_{i,\sigma}^\dagger c_{i,\sigma} \leq N$. The
NN Coulomb repulsion between the electrons is given by $V_c$, which is grouped together with $-(J/4)n_i n_j$ from the exchange term and represented by the $V$-term in Eq. \(2\). The usual $t$-$J$-$V$ model corresponds to $N = 1$. The projected Hilbert space can be treated in the slave boson formalism by writing $c_{iα}^\dagger = f_{iα}^\dagger a_i$, where $f_{iα}$ is a spin-carrying fermion and $b_i$ a spinless boson keeping track of empty sites, with the constraint $f_{iα}^\dagger f_{iα} + b_i^\dagger b_i = N$.

Let us introduce the pseudo-spinors, $\Psi_i = (\psi_{iσ}, \psi_{i\bar{σ}})$,

$$\psi_{iα} = \left( \begin{array}{c} f_{iα}^\dagger \\ f_{i\bar{α}}^\dagger \end{array} \right), \quad α = 1, \ldots, N,$$

and $\tilde{\psi}_i = C\psi_i$ where $C = iσ_y \otimes 1$. Here $1_{αβ}$ is the identity matrix in the flavor space and $(σ_y)_{ττ'}$ is the Pauli matrix acting on the spins. Under a unitary transformation $g_i, \psi_i \rightarrow g_i \psi_i$ and $\tilde{ψ}_i \rightarrow \tilde{ψ}_i g_i^\dagger$, provided that $g_i^\dagger C g_i = C$, i.e., $g_i \in SU(N, q)$. The $SU(N, q)$ fermion bilinear $U_{ij} = ψ_i^\dagger \Psi_j^\dagger$ transforms as $U_{ij} \rightarrow g_i U_{ij} g_j^\dagger$. To construct the large-$N$ theory, we form the flavor singlet by tracking over the flavor indices, $u_{ij} = \text{Tr} U_{ij} = \left( -\tilde{χ}_{ij}^* \Delta_{ij} \right)$, which is a quasiparticle with elements: $\tilde{χ}_{ij} = \sum_α (f_{iα}^\dagger f_{jα} + f_{i\bar{α}}^\dagger f_{j\bar{α}})$ and $\Delta_{ij} = \sum_α (f_{iα}^\dagger f_{j\bar{α}} - f_{i\bar{α}}^\dagger f_{jα})$. They represent the bond (SF) and pairing degrees of freedom. In terms of $u$, the Hamiltonian can be written as,

$$H_{ij} = -\frac{t}{2N} \sum_{(i,j)} \left[ b_i b_j^\dagger \sum_{τ} ψ_{iτ}^\dagger (1 + σ_z) ψ_{jτ} + \text{h.c.} \right] - \frac{J}{8N} \sum_{(i,j)} \text{Tr}(u_{ij} u_{ij}) + \sum_{i, τ} ψ_{iτ}^\dagger (iλ_τ - μ_f) σ_z ψ_{iτ}.$$

$$H_V = -\frac{V}{2N^3} \sum_{(i,j)} b_i^\dagger b_j^\dagger b_j b_i \text{Tr}(u_{ij} σ_z u_{ij} σ_z).$$

Here $\text{tr}$ stands for the trace in spinor space, $λ_j$ is the Lagrange multiplier enforcing the local constraints, and $μ_f$ fixes the average fermion density. Note that for general $N$, $H_V$ cannot be written solely in terms of four fermions using the constraints.

In the large-$N$ limit, the bosons condense at low temperatures $\langle b_i \rangle = \sqrt{N} x_i$, where $x_i$ is the local doping concentration.\[x\] Note that since charge fluctuations are suppressed, the $V$-term vanishes with vanishing boson amplitude on approaching half-filling where the $SU(2)$ symmetry is restored. The interactions are decoupled by introducing the saddle point values $x_i = \langle x_{ij} \rangle / N$ and $δ_{ij} = \langle δ_{ij} \rangle / N$. The saddle-point Hamiltonian becomes $H = \sum_{(i,j)} H_{ij} - \sum_i (μ_f - iλ_τ) x_i$,

$$H_{ij} = -t \sqrt{x_i x_j} x_{ij} - g_χ x_{ij}^2 δ_{ij} + \text{h.c.} + N(g_χ |x_{ij}|^2 + g_Δ |δ_{ij}|^2),$$

where $g_χ = J/4 + x_i x_j V$ and $g_Δ = J/4 - x_i x_j V$ are the fermion coupling constants to the bond and pairing order parameters. The effect of $V$ is to reduce pairing while enhance the SF ordering. We focus on the uniform solutions with $x_i = x$, $iλ_i = λ$, $x_i = x_1 + i(-1)^{x_{ij}} x_2$ and $δ_{ij} = δ_{i} + i(-1)^{x_{ij}} δ_{j}$, where $x_1, 2$ and $δ_{i, j}$ are real. The flux per plaquette is given by $ϕ = 4 \tan^{-1}(x_2/x_1)$. $δ_s$ and $δ_Δ$ are the $s$-wave and $d$-wave pairing order parameters, respectively. The free energy per site is obtained analytically,

$$F = -2TN \sum_{k, σ = ±} \text{ln}[2 \cosh(E_{ks}/2T)] + 2N(g_Δ |δ|^2 + g_χ |μ|^2) - Nμx,$$
t-U-V model \[14\]. (ii) The SF order develops below a critical doping \( x_c \simeq 0.1 \) and coexists with the dSC. There is a reduction of \( \Delta_d \) concomitant with the development of the SF (\( \chi_2 \)) below \( x_c \), indicative of competing order. The values of \( x_c \) and \( x_p \) depend on the band structure. A next NN hopping \( t' < 0 \) moves both to higher values. Although the \( d \)-wave pairing amplitude \( \Delta \) extrapolates to a nonzero value at half-filling, the two states are identical by invoking competing order and quantum criticality \[7\].

In Fig. 2, the phase diagram of the \( t-J \)-model is shown in the plane of temperature \( T \) versus doping \( x \). The phase boundaries are the temperatures \( T_{SF} \) and \( T_c \) at which the SF and dSC order parameters vanish, respectively. The topology of the phase diagram resembles one proposed for the cuprate high-\( T_c \) superconductors \[16\]. (ii) The SF order develops below a critical temperature \( T_{SF} \) below \( x_c \), indicative of competing order. The values of \( x_c \) and \( x_p \) depend on the band structure. A next NN hopping \( t' < 0 \) moves both to higher values. Although the \( d \)-wave pairing amplitude \( \Delta \) extrapolates to a nonzero value at half-filling, the two states are identical by invoking competing order and quantum criticality \[7\].

FIG. 1: The order parameters versus doping at \( T = 0 \).

FIG. 2: The large-N phase diagram of the \( t-J \)-model showing a QCP at \( x_c \), a pure dSC, a coexistence phase of dSC and SF, and a finite temperature pseudogap SF phase. Inset: \( T = 0 \) single-particle gap \( \Delta_o \), condensation energy \( \Delta E_c \times 50 \), and specific heat coefficient jump \( \Delta T_c \), versus doping.

tunneling density of states (LDOS) measured by STM

\[
N(\omega) = -\text{Re} \int_0^\infty dt e^{i\omega t} \theta(t) \langle \{ c_{\sigma}^\dagger (0), c_{\sigma} (t) \} \rangle. \quad (10)
\]

In Fig. 3, we show the typical LDOS and the QP dispersion. Fig. 3(a) corresponds to the pure dSC at \( x = 0.14 \) and \( T = 0 \). The LDOS shows \( d \)-wave gap features. The two peaks near the gap edges come from the large state density at the points marked as \( X \) at \( (\pi, 0) \) and \( P \) at the nearby minimum on the dispersion, and their symmetry equivalent points. Note that the distance between neither set of peaks equals to \( 2\Delta \) where \( \Delta = 4\Delta_0 \Delta_d \) is the maximum of the \( d \)-wave gap function. One must thus be careful with extracting the SC gap from the peak-to-peak distance even with high STM resolution. The LDOS in the coexistence phase is shown in Fig. 3(c) at \( x = 0.06 \) and \( T = 0 \). Compared to Fig. 3(a) in the dSC, there is an emergent in-gap resonance peak (marked A) particle-hole reflected on both sides of zero-bias. It arises from the resonant scattering of the QP from state \( k \) to state \( k + (\pi, \pi) \) due to period doubling. A similar situation arises in the SF state around a superconducting vortex in the SU(2) formulation of the \( t-J \) model \[17\]. As shown in Fig. 3(d) for the \( s = + \) branch, at the resonant energy, the distorted ellipse at touch point \( A \), the low-energy minimum in the dispersion plotted in Fig. 3(c). These resonance peaks, albeit small in weight, are ubiquitous signatures of coexisting order and should be detectable by high resolution STM. Near the gap edges, there are four sets of peaks (two are prominent) due to the doubling of the unit cell. They are labeled by \( X_\pm \) and \( P_\pm \) and marked on the QP dispersion. It is instructive to compare these to the LDOS in the pseudogap SF at \( x = 0.06 \) and \( T = 0.08J \) shown in Fig. 3(b). The low energy resonance peaks disappear and the LDOS shifts to the unoccupied side. Interestingly, the minimum of the LDOS in the SFP coincides with the M point next to the in-gap resonance in the coexistence phase. The resonance
energy and the spectral shift depend on the band structure and doping and are on the order of $0.043J \sim 6$meV for the parameters used in Fig. 3.

An important consequence of the competing order is the emergence of two energy gaps which can be, however, difficult to observe at low temperatures [19]. In the inset of Fig. 2, the gap to single-particle excitations $\Delta_0$ obtained from the LDOS at $T = 0$ is plotted versus doping, which qualitatively agrees with the low-temperature ARPES data. It interpolates between a geometric average of the gaps associated with the SF and SC order of SF and dSC or-}


doping, which qualitatively agrees with the low temperature pseudogap SFP in the underdoped regime, and complete suppression of superconductivity beyond an overdoping. At very low doping, the phase diagram does not match that of the cuprates. The discrepancy is most obvious in the nonzero $T_c$ that extends to infinitesimal doping, whereas the SC state in the cuprates disappears at a finite doping below which a spin glass phase prevails. The lack of destruction of the dSC at low doping is because the renormalized NN Coulomb interaction must scale to zero at half-filling due to the constraint forbidding charge fluctuations. We expect the effects of doping induced inhomogeneity [21] due to poor screening of the dopant ionic potential to become very important in this regime. As a result, the local doping concentration (LDC) fluctuates dramatically and its interplay with AF may lead to the destruction of the SC state and the emergence of spin glass and insulating behaviors. Furthermore, the onset of SF order will fluctuate spatially with the LDC, smearing out the sharp finite temperature transition to the pseudogap SFP.

This work is supported in part by DOE Grants Nos. DE-FG02-99ER45747, DE-FG02-02ER63404, and ACS Grant No. 39498-AC5M.

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