Stability of inhomogeneous superstructures from renormalized mean-field theory of the $t-J$ Model

Didier Poilblanc$^{1,2}$

$^1$ Laboratoire de Physique Théorique, Université Paul Sabatier, F-31062 Toulouse, France
$^2$ Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, BSP 720, CH-1015 Lausanne, Switzerland

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Using the $t-J$ model (which can also include Coulomb repulsion) and the “plain vanilla” renormalized mean-field theory of Zhang et al. (1988), stability of inhomogeneous $4a \times 4a$ superstructures as those observed in cuprates superconductors around hole doping 1/8 is investigated. We find a non-uniform $4a \times 4a$ bond order wave involving simultaneously small ($\sim 10^{-4}$) inhomogeneous staggered plaquette currents as well as a small charge density modulation similar to pair density wave order. On the other hand, no supersolid phase involving a decoupling in the superconducting particle-particle channel is found.

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Although the global phase diagram of high-Tc cuprate superconductors seems, at first sight, to contain only three homogeneous phases, antiferromagnetic, superconducting and metallic phases, a closer inspection reveal a striking complexity with some form of local electronic ordering around 1/8 hole doping. For example, recent scanning tunneling microscopy/spectroscopy (STM/STS) experiments of under-doped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ in the pseudogap state have shown evidence of real-space modulations of the low-energy density of states (DOS) with period close to four lattice spacings. Spatial variation of the electronic states has also been observed in the pseudogap phase of Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$ single crystals ($x=0.08 \sim 0.12$) by similar STM/STS techniques. In the same material, signatures of this unusual $4a \times 4a$ checkerboard charge-ordered state have been found in Angular Resolved Photoemission Spectroscopy (ARPES) experiments. How this local ordering could be explained on theoretical grounds is a topic of intense ongoing investigation.

In the Resonating Valence Bond (RVB) theory, one of the early approach to understand strongly correlated HTC superconductors, a simple variational Ansatz is constructed from a BCS paired superconducting state $|\Psi_{BCS}\rangle$ by a Gutzwiller projection of the high energy configurations with doubly occupied sites. At half-filling, this procedure generates a highly correlated wavefunction $P_G|\Psi_{BCS}\rangle$ where the spins are paired up in singlet bonds to form a quantum spin liquid with short range antiferromagnetic correlations. In fact, due to a SU(2) electron-hole symmetry, the RVB state can take various forms like the half-flux state which can be mapped onto free electrons on a lattice experiencing half a flux quantum per plaquette.

The main difficulty to deal with such wavefunctions is to treat correctly the Gutzwiller projection. Exact Variational Monte Carlo (VMC) calculations on large clusters show that the magnetic energy of the variational RVB state at half-filling is very close to the best exact estimate. It also provides, at finite doping, a semi-quantitative understanding of the phase diagram of the cuprate superconductors and of their experimental properties. Another route to deal with the Gutwiller projection is to use a “renormalized mean-field (MF) theory” in which the kinetic and superexchange energies are renormalized by different doping-dependent factors $q_1$ and $q_J$ respectively. As emphasized recently by Anderson and coworkers, the procedure consists in searching for an effective MF Hamiltonian that determines a function $\langle \Psi \rangle$ to be projected as $P_G|\Psi\rangle$. Crucial, now well established, experimental observations such as the existence of a pseudo-gap and nodal quasi-particles and the large renormalization of the Drude weight are remarkably well explained by this early MF theory.

Away from half-filling, “commensurate flux phases” have also been proposed as another class of competitive projected wavefunctions. Such time reversal symmetry broken states, generalizing Affleck-Marston 1/2-flux phase away from half-filling, are made out of orbitals solving a fictitious Hofstadter problem of free particles under a (fictitious) magnetic flux. Within this class of wavefunctions, the lowest energy is obtained when the flux per unit cell equals exactly the filling fraction $\nu = \frac{1}{2}(1-x)$ (x being the hole doping) suggesting that doping induces a (scalar) chirality of the spin background. This scenario also emerges naturally within a renormalized MF theory although the stability condition (self-consistency) leads to a more complex one-body effective MF Hamiltonian with inhomogeneous flux. For example, at filling $\nu = p/q$, diagonal “stripe” modulations of supercell $qa/\sqrt{2} \times \sqrt{2}a$ ($a$ is the lattice spacing) are found. In this Letter, we generalize the MF approach of Ref. to allow for non-uniform densities (and also include off-diagonal pairing). We determine under which conditions a $4a \times 4a$ superstructure might be stable for hole doping close to 1/8.

The weakly doped antiferromagnet is described here...
by the renormalized $t-J$ model Hamiltonian,

$$H = -t \sum_{\langle ij \rangle \sigma} \langle c^\dagger_{i, \sigma} c_{j, \sigma} + h.c. \rangle + J g_{\perp} \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$  \hspace{1cm} (1)

where the local constraints of no doubly occupied sites are replaced by statistical Gutzwiller weights $g_{\perp} = 2x_i/(1 + x_i)$ and $g_{\parallel} = 4/(1 + x_i)^2$. We shall assume a typical value of $t/J = 3$ hereafter.

Decoupling in both particle-hole and (singlet) particle-particle channels can be considered simultaneously leading to the following MF hamiltonian,

$$H_{\text{MF}} = -t \sum_{\langle ij \rangle \sigma} g_{\perp,i,j} \langle c^\dagger_{i, \sigma} c_{j, \sigma} + h.c. \rangle - \mu \sum_{i \sigma} n_{i, \sigma}$$

$$-\frac{3}{4} J \sum_{\langle ij \rangle \sigma} g_{\parallel,i,j} (\chi_{ij} c^\dagger_{i, \sigma} c_{j, \sigma} + h.c. - |\chi_{ij}|^2)$$

$$-\frac{3}{4} J \sum_{\langle ij \rangle \sigma} g_{\parallel,i,j} (\Delta_{ij} c^\dagger_{i, \sigma, j, -} + h.c. - |\Delta_{ij}|^2),$$

where the previous Gutzwiller weights have been expressed in terms of local fugacities $z_i = 2x_i/(1 + x_i)$ ($x_i$ is the local hole density), $g_{\perp,i,j} = \sqrt{z_i z_j}$ and $g_{\parallel,i,j} = (2 - z_i)/(2 - z_i)$, to allow for small non-uniform charge modulations. The Bogoliubov-de Gennes self-consistency conditions are implemented as $\chi_{ij} = \langle c^\dagger_{i, \sigma} c_{i, \sigma} \rangle$ and $\Delta_{ij} = \langle c_{i, -\sigma} c_{j, \sigma} \rangle$.

Assuming an homogeneous system, the RVB theory of Refs. [4, 9] is recovered leading to a $d_{x^2-y^2}$ RVB superconducting (for $x > 0$) ground state (GS). $\Delta_{i,i+x} = \Delta$, $\Delta_{i,i+y} = -\Delta$ and $\chi_{ij, \sigma} = \chi$. When doping $x \rightarrow 0$, $\Delta = \chi \approx 0.169$, giving a magnetic energy per bond of $\sim 0.339J$ and a kinetic energy per hole of $\sim -2.71t$ (within MF). $\Delta$ is physically the pseudo-gap while the superconducting temperature scales like $g_{\parallel}J/\Delta \propto x$.

Our aim here is to investigate inhomogeneous solutions of these equations which might a priori break translation symmetry. However, searching for the global energy minimum in a completely unconstrained variational space is a formidable task owing to the non-linear nature of the MF equations. Therefore, guided by experimental observations, for an average hole density of $x \approx 1/8$, we shall restrict ourselves to a $4a \times 4a$ superstructure (which could, as well, accommodate a smaller spatial periodicity) with a natural $C_4$ rotation symmetry, hence naturally restricting the number of non-equivalent bonds and sites to 6 and 3, respectively. Within these restrictions, MF equations are solved on finite clusters (with periodic boundaries) of sizes ranging from 16×16 to 48×48.

We first consider non-superconducting solutions i.e. $\Delta_{ij} = 0$ on all bonds. Starting with an initial set of $\chi_{ij}$ which simultaneously (i) corresponds to a uniform (fictitious) flux (per plaquette) equal to the filling fraction $\nu = 7/16$ and (ii) fulfills the above symmetry requirements within the supercell, we then solve the self-consistent equations iteratively [17]. A typical MF solution is shown schematically in Fig. 1. As shown in Table I, the bond parameters $\chi_{ij}$, here obtained e.g. on a 48×48 cluster [18], show strong spatial modulations leading to a bond order wave (BOW) in both spin-spin correlations $\langle \chi_{ij}^2 \rangle$ and charge hoppings $2g_{\parallel,i,j} \text{Real} \{\chi_{ij}\}$. At first sight, such a state could be seen as an extension of the bond-centered stripe [19] or 4×4 plaquette [20] solutions found in some $SU(2N)/Sp(2N)$ mean field theories. However, in our case, $\chi_{i,j}$ exhibit imaginary parts (as in staggered [21] and commensurate flux states) producing a time-reversal symmetry broken state and small plaquette charge currents $2g_{\parallel,i,j} \text{Im} \{\chi_{ij}\}$ (see Table I). The current pattern is similar to the alternating distribution of the staggered flux state although the amplitude of the current loops is not uniform. As shown on the first line of Table I such a state also exhibits a small charge density wave (CDW) component.

![FIG. 1: (Color on-line). Schematic pattern of the bond $\chi_{ij}$ distribution. Non-equivalent bonds (labelled from 1 to 6) are indicated by different types of lines whose widths qualitatively reflect the magnitudes of $\chi_{ij}$. Arrows indicate the directions of the small charge currents. Numerical values for $t/J = 3$ are given in Table I](image)

### Table I: Numerical values of the bond amplitudes $|\chi_{ij}|$, the bond spin-spin correlations and the bond average hoppings and currents (in units of $t$) in the normal phase MF solution obtained on a 48×48 cluster for $t/J = 3$ and 2022 fermions on 48×48 sites ($x \approx 1/8$). Note the current conservation at the lattice sites, in particular “2+6”=“3+4”.

| Bond # | 1 | 2 | 3 | 4 | 5 | 6 |
|--------|---|---|---|---|---|---|
| $|\chi_{ij}|$ | 0.2579 | 0.1871 | 0.2595 | 0.2259 | 0.1887 | 0.1639 |
| $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ | −0.3456 | −0.1720 | −0.3131 | −0.2359 | −0.1637 | −0.1249 |
| hoppings | 0.0554 | 0.0571 | 0.1188 | 0.1063 | 0.0915 | 0.0725 |
| currents | 0.0453 | 0.0373 | 0.0370 | 0.0305 | 0.0228 | 0.0302 |
We now turn to superconducting solutions allowing pair order parameter \( \Delta_{ij} \neq 0 \). We repeat the previous procedure adding to \( \chi_{ij} \) arbitrary initial values for \( \Delta_{ij} \), only requesting \( |\Delta_{ij}| \) to have s-wave symmetry w.r.t. the center of the central plaquette (defined by bonds #1). Within this restriction, we have looked for 3 candidates compatible with a \( 4a \times 4a \) cell, exhibiting (i) \( d_{x^2-y^2}+is \), (ii) \( d_{x^2-y^2}+id_{xy} \) or (iii) \( d_{x^2-y^2}+d_{x^2-y^2} \) symmetries. Note that we allow again inhomogeneous solutions so that the minimization of the MF energy w.r.t. the set of \( \Delta_{ij} \) is performed indeed on 6 independent complex parameters. However, for a doping around 1/8 and all cluster studied, no modulated solution was found. On the contrary, the iteration procedure always converges towards the standard \( d_{x^2-y^2} \) RVB superconductor, a state particularly rigid w.r.t. the establishment of spontaneous modulations.

Next, we investigate the role of a Coulomb repulsion,

\[
H_V = \frac{1}{2} \sum_{i,j} \Delta_{ij} (n_i - n)(n_j - n),
\]

that we treat within a simple decoupling scheme, i.e. replacing the density-density interaction by \( \langle n_i \rangle n_j + \langle n_j \rangle n_i \) and Cst. We assume here both long range \( V_{i,j} = V/r_{ij} \) and screened \( V_{i,j} = V' \exp(-r_{ij}/l)/r_{ij} \) potentials (with a screening length set to \( l = 4a \)). To minimize finite size effects, we also use the "periodic distance" \( r_{ij} \) on the torus. As shown in Table II we find that moderate values of \( V \) (or \( V' \)) \( \sim t \) affects only slightly the form of the CDW. Moreover, the pattern for both spin-spin correlations and effective hoppings remains qualitatively similar to \( V = 0 \) (see Table III). Note that the charge current magnitude tends to increase (decrease) with \( V \) on the central, (outer) plaquette, i.e. on bonds #1 (#5). As expected, results do not depend drastically on the long-distance part of \( V_{i,j} \).

TABLE II: Numerical values of charge densities in the normal phase obtained on a \( 48 \times 48 \) cluster for \( t/J = 3 \) and doping \( x \approx 1/8 \) and different Coulomb repulsions. Average density, magnetic bond energy, kinetic energy per hole and energy per site are provided in the 4 last columns. Last line: same data obtained for the d-wave RVB superconductor on a \( 32 \times 32 \) cluster for \( \mu = -0.4 \) (leading to \( \chi \approx 0.192 \) and \( \Delta \approx 0.120 \)).

| Site # | 1 | 2 | 3 | n | \( \langle S_i \cdot S_j \rangle \) | \( E_K/t \) | \( c_0/J \) |
|---|---|---|---|---|---|---|---|
| V = 0 | 0.925 | 0.864 | 0.857 | 0.8776 | -0.220 | -2.660 | -1.438 |
| V/t = 0.5 | 0.894 | 0.913 | 0.783 | 0.8759 | -0.227 | -2.588 | -1.425 |
| V/t = 0.8 | 0.876 | 0.940 | 0.760 | 0.8769 | -0.232 | -2.396 | -1.367 |
| \( V'/t = 0.8 \) | 0.850 | 0.932 | 0.786 | 0.876 | -0.222 | -2.559 | -1.406 |
| RVB | 0.876 | 0.876 | 0.876 | 0.8762 | -0.243 | -2.730 | -1.500 |

Let us now turn to the issue of the relative stability of the BOW/CDW state w.r.t. the RVB superconductor. For \( V = 0 \) the latter has a slightly lower energy. However, a moderate repulsion can easily stabilize the BOW/CDW state whose energy is only weakly affected by \( V \) (or \( V' \)). On the contrary, the pairing amplitude of the RVB superconductor is expected to be quite sensitive to the Coulomb potential. Indeed, a decoupling in the particle-particle channel of e.g. the nearest neighbor repulsion \( V_{ij}n_{i\uparrow}n_{ij} \) term generates a positive contribution \( \propto V_{ij}|\Delta_{ij}|^2 \) which tends to strongly reduce the pairing amplitude. Therefore, the BOW/CDW state is expected to become stable when \( x \sim 1/8 \).

TABLE III: Same as Table II but for a screened Coulomb potential \( V'/t = 0.8 \) (\( l = 4a \)). 2016 fermions on \( 48^2 \) sites \( (x = 1/8) \).

| Bond # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| \( \chi_{ij} \) | 0.2297 | 0.2015 | 0.2741 | 0.1917 | 0.2166 | 0.2020 |
| \( \langle S_i \cdot S_j \rangle \) | -0.2395 | -0.1984 | -0.3952 | -0.1700 | -0.1909 | -0.2146 |
| hopplings | 0.1105 | 0.0637 | 0.0547 | 0.0773 | 0.1524 | 0.0403 |
| currents | 0.0459 | 0.0366 | 0.0436 | 0.0251 | 0.0109 | 0.0321 |

Lastly, we would like to discuss similarities and differences of our findings with previous theoretical suggestions to explain the \( 4a \times 4a \) patterns experimentally observed e.g. in BiSCO. First, we should stress that the state found in this work is quite different from an ordinary CDW or Wigner solid which, for a doping around 1/8, is expected to have a \( \sqrt{8} \times \sqrt{8} \) supercell. As a matter of fact, the BOW is not primarily stabilized by Coulomb repulsion. Secondly, we notice that it bears some similarities (in addition to the common \( 4a \times 4a \) periodicity)
with the insulating Pair density Wave (PDW) state \[22\] which also does not exhibit \(U(1)\) phase coherence. For example, it shows a higher hole density on a given plaquette within the supercell (which, incidently, carries the minimum value of the current). Like the PWD state, the BOW differs from the stripe state in terms of the rotational symmetry. In addition, in contrast to PDW and stripe states, it breaks time-reversal symmetry. However, an experimental observation of its manifestation i.e. the plaquette orbital currents might be quite tedious due to their small magnitudes. We note that the current pattern is, at first glance, staggered (in fact, incommensurate with a wave vector close to \((\pi, \pi)\)), a finding consistent with exact diagonalisations of doped Hubbard and \(t-J\) clusters showing enhancement of staggered chiral correlations under doping \[23\]. Finally, we observe that recent VMC calculations of staggered flux states \[21\] suggest an instability towards phase separation. A modulated structure like the one found here is in fact an alternative scenario.

In conclusion, using renormalized meanfield theory of the \(t-J\) model, \(4a \times 4a\) BOW states are found for doping around \(1/8\). We suggest that such states might be relevant to explain the spatial modulations of the DOS in STM experiments of underdoped cuprates superconductors. They carry small (almost staggered) plaquette currents and are stable for moderate Coulomb repulsion.

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