Numerical Test of the Energy Scale of Columnar Dimerization in High-T_c Cuperate Superconductors

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Spontaneous bond dimerization (BD) was conjectured to be central to the physics of the cuperate superconductors. Based on ladder models and numerical simulations, we examine the quantitative issue of whether the energy scales involved are sufficient to influence the mechanisms of pairing, stripe formation, pseudo-gap, and quantum critical 'normal' state phenomena. We present preliminary evidence that maximum gap scales derived from BD are always too small.

A mechanism of spontaneous bond dimerization (BD) was proposed [1, 2, 3, 4] as an underlying core phenomenon in the cuperate high temperature superconducting materials. Columnar BD was proposed as the mechanism for the formation of stripes in underdoped cuprates (see Fig.1). A quantum critical point associated with BD is proposed to be responsible for certain anomalous thermodynamic and magnetic properties observed in the temperature-doping phase diagram of the cuprates. Elaborate consequences for impurity and vortex states were derived [2, 3]. Moreover, the BD is characterized by a spin gap and associated confinement of spin-$\frac{1}{2}$ excitations, and hence we note that by itself it also provides a potential mechanism of pairing.

The analysis in Refs. [1, 2, 3] focussed primarily on symmetry aspects of the BCS and BD order parameters. Here we focus on quantitative issues. In the cuprates, the maximum spin-gap in the superconducting state is $\Delta_s \equiv 2\Delta(0) \approx 800K \sim J/2$ [5], where $J$ is the antiferromagnetic exchange interaction. Pseudo-gap phenomena persist to temperatures of order 300K. Some evidence of local stripe order (incommensurate magnetism) persists up to temperatures of order 70K in some underdoped materials, where spectral signatures of incommensurate magnetism are seen up to energies of order 40meV ($\sim 450K$) [6]. Thus, for these phenomena to be associated with BD order or fluctuations, this order must generate an energy scale, say a spin gap (or spin pseudo gap), which is sufficiently large. We will adopt the lenient criterion that this energy scale must be at least of order $\Delta > 250K \approx J/6$.

Our main observation is that this aspect of the BD conjecture can be tested by numerical simulations on wide ladders (e.g., 6-leg or 8-leg). Indeed, existing numerical experiments on 4-leg ladders and on small square Heisenberg arrays will be shown to already suggest rather strongly that the energy scales derived directly from BD are considerably smaller than 250K. Pending sharper similar results in 6-leg ladders, we doubt the viability of BD as a candidate theory of pairing or stripes in the cuperate high-$T_c$ superconductors.

We stress that our analysis bares strictly on the mechanism of spontaneous BD. Associated results of the work by Sachdev and collaborators may be relevant to more general models of stripes or ladders, and hence their relevance to the cuperate superconductors may hitherto not be tied to the mechanism of spontaneous BD.

 REVIEW OF THE COLUMNAR DIMERIZATION APPROACH TO HIGH-TC

Columnar BD was introduced as a bond ordered state in 2D Heisenberg models with frustrated interactions [4]. The canonical example is the model with antiferromagnetic nearest-neighbor and next-nearest-neighbor interactions ($J$ and $J'$ respectively). The core physics can be generalized to the inclusion of further neighbor interactions. The bond ordered state is proposed to correspond to the spin gaped state which occurs when $0.4 < J/J' < 0.6$ [2, 3, 10]. The columnar BD order renders the system to be equivalent to an effective coupled 2-leg spin ladder system (see Fig.2). It is supposed that at moderate doping the BD and spin gap are retained [1, 2] which entails the confinement of spin-$\frac{1}{2}$ excitations (i.e., pairing). The spin gap is the prominent energy scale which characterizes the BD. In the spirit of the RVB doped spin liquid idea [11], pairing is inherited
from the spin liquid state of the undoped BD Heisenberg model. An analogy is drawn with the case of dimerization in one dimensional spin chains, where the spin gap can be as large as $J$ (the Majumdar-Ghosh limit). A priori, it might be that columnar BD can lead to a spin gap on the scale of weakly coupled 2-leg ladders. 

Since the undoped cuprates have a quasi long range antiferromagnetic ground state, the applicability of a BD model to the cuprates is not straight forward. The mechanism implied by the phase diagram (Fig.1) is the following. The microscopic degrees of freedom and interactions in the cuprate superconductors are capture by a one band generalized t-J model (e.g., $t$-$t'$-$J$-$J'$) plus coulomb interactions. The bare parameters values are such that groundstate of the undoped system is the Neel state as described by Chakravarty et al. With the introduction of holes, the holes dynamics enhances the effective range of parameters 0.4 < $J_2/J_1$ < 0.6. It appears that, unlike the one dimensional spin chain case where the spin gap can be as big as $\Delta = J_1$ (the Majumdar-Ghosh limit), the effective model ladders are columnar BD (see images). One might conjecture that by fine tuning some additional further interactions $(J_3, J_4, ...)$ one might conjure higher gap values, that would not constitute a robust model. Since the square $J_1 - J_2$ Heisenberg model is the effective model system which is at the origin of the BD mechanism proposed by Sachdev, the results presented in Fig.3 already put in serious doubt the basic conjecture which underlies the introduction of spontaneous BD as responsible for phenomena at energy scale $\Delta \geq J/6$ in the cuprate high temperature superconductors.

Even leg ladders are an ideal testing ground for t-J model physics. Numerical simulations of doped t-J model ladders show groundstate pairing correlations in agreement with effective columnar BD (see Fig.4). Therefore, ladders seem to be a favorable system for BD. It is worth noting that the appearance of columnar pairing correlations in ladders may also be a simple consequence of geometrical anisotropy and boundary conditions. Yet, such knowledge is not essential to our arguments in this paper. We argue that the key issue...
FIG. 4: DMRG results for the real space singlet pairing expectation values on nearest-neighbor sites \[^{15}\]. Pair correlations on doped 4-leg ladder seem to manifest columnar dimerization.

FIG. 5: DMRG results for the real space singlet pairing expectation values on nearest-neighbor sites \[^{15}\]. Pair correlations on doped 4-leg ladder seem to manifest columnar dimerization.

is the size of the spin gap.

Numerical simulations by CORE method on doped 4-leg ladders already seem to indicate that the spin gap of the doped ladder does not get bigger than that of the undoped ladder (see Fig. 5). But there is an ambiguity between open and periodic boundary conditions. Apparently, the spin gap of 4-leg ladders \(\Delta_0 \approx J/5\) is to begin with too large to draw sharp conclusions from. On the other hand, as we elaborate below, similar calculations for 6-leg ladders are all that is needed to make the point.

Undoped 6-leg t-J ladder models have a small spin gap \(\Delta_0 \approx J/20\). Upon doping, the ground state still has a spin gap and enhanced pairing correlations. We propose to examine a 6-leg ladder model with the same bare t-J-J' model parameters as are assumed for the C-O planes of the cuprate superconductors (e.g., bare ring exchange interaction may need to be included \[^{14}\]). The generation of effective interactions due to the holes dynamics is a local process which qualitatively and quantitatively we expect to be the same in wide ladders (e.g., 6-leg or 8-leg ladders) as in a 2D plane. Consequently, what ever is the potential for BD in the 2D C-O plane, it should manifest itself with the same strength already in wide ladder models.

The spin gap in undoped and doped 6-leg \(t-J\) ladders can be deduced from the energy gap to the first \(S = 1\) spin excitation. Examples of such a calculation were done for a 2-leg and 4-leg ladders by both DMRG and CORE methods \[^{12,13}\]. For spontaneous BD to be a mechanism relevant at energy scales of order \(\Delta \approx 250K\), it is required that the size of the spin gap for the doped system will be on the order of \(\Delta_s \approx 250K\), i.e., 4 times bigger than that of the undoped 6-leg ladder!!

In summary, bond dimerization (BD) is seen to occur, to some extent, in doped even-leg ladders. Thus, aspects of the resulting physics can be directly studied by numerical investigations of such ladders. Specifically, we have proposed testing whether the energy scales involved are sufficiently large to be relevant to a host of properties of the cuprates (such as pairing and stripes). The experimental phenomenology is sufficiently complicated that detailed quantitative comparisons are certainly premature, but we believe there is a significant theoretical distinction between the maximum spin-gap energy scales \(\Delta_s \approx J/8\) found in BD magnets \[^{10}\], and the minimum necessary magnitudes \(\Delta_s > J/6\). More directly, if the BD mechanism fails to produce a high spin gap energy scale in doped 6-leg and 8-leg ladder systems (as is our prediction) then its prospects as the root cause of pairing, stripe formation, or normal state properties in the cuprate superconductors are in serious doubt. Of course, we cannot rule out the possibility that additional well adjusted interactions, such as the electron-phonon interaction, could increase the stability of the BD state and hence manage to overcome this objection. Yet, such elements are not part of the framework currently presented by \[^{1,2,3,4}\].

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