Phase diagram of hole doped two-leg Cu-O ladders

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In the weak coupling limit, we establish the phase diagram of a two-leg ladder with a unit cell containing both Cu and O atoms, as a function of doping. We use bosonization and design a specific RG procedure to handle the additional degrees of freedom. Significant differences are found with the single orbital case; for purely repulsive interactions, a completely massless quantum critical region is obtained at intermediate carrier concentrations (well inside the bands) where the ground state consists of an incommensurate pattern of orbital currents plus a spin density wave (SDW) structure.

The challenging physics of strongly correlated systems provides a unique opportunity to test many proposals for new, unconventional quantum states of matter. In that respect, ladders constitute a particularly interesting case [1]. These 1D systems behave quite differently from single chains. One can show for instance that, for purely repulsive interactions, they favor superconductivity in their ground state. Understanding their properties – both experimentally [2] and theoretically – is thus interesting in its own right but also could help us gain valuable insight into the elusive physics of the two dimensional cuprate superconductors.

Most studies of ladder compounds model these systems with a single orbital per unit cell [3, 4]. Using a renormalization group (RG) analysis of the Hamiltonian expressed in bosonic variables, a phase diagram can be derived in the weak coupling limit. As pointed out [3], the parametrization group (RG) analysis of the Hamiltonian expressed in bosonic variables, a phase diagram can be derived in the weak coupling limit. As pointed out [3], the parametrization of the model. In contrast with the case of a single orbital ladder with a unit cell containing both Cu and O atoms, with on-site repulsions \( U_{\text{Cu}} \) (\( U_{\text{O}} \)) on the Cu (O) sites and a nearest-neighbor \( V_{\text{Cu-O}} \) Coulomb term. We use RG techniques to map out the flows for the bosonized version of the model. In contrast with the case of a single orbital ladder we find that for an intermediate range of dopings \( \delta_{\text{c1}} < \delta < \delta_{\text{c2}} \) a fully massless phase is stabilized. The value of \( \delta_{\text{c1(c2)}} \) depends on the bare magnitude of the Hubbard terms and/or the interoxygen hopping \( t_{pp} \) which we treat as tunable parameters. Furthermore, increasing \( t_{pp} \) beyond a minimum value \( t_{pp}^{min} \) promotes, for all \( \delta > \delta_{\text{c1}} \), an incommensurate orbital current state. It is similar to one of the patterns advocated by Varma [8] (see Fig. 1b). The corresponding phase has an additional SDW (CDW) character for \( \delta < \delta_{\text{c2}} (\delta > \delta_{\text{c2}}) \).

We consider the two leg ladder of Fig. 1a where the relevant hopping parameters and interactions are shown. \( H_T \) is the sum of contributions describing carrier hops plus a term proportional to \( \epsilon = E_{\text{Cu}} - E_{\text{O}} \), the differ-

FIG. 1: (Color online) (a) Molecular structure of the unit cell showing the hopping and interaction parameters included in the model. (b) Orbital current pattern and SDW modulation (bold arrows) in the C2S2 phase. The chain direction is vertical. \( k_{F0} \) is the Fermi wavevector in the 0 band.
ence between the Cu and O site energies. Relevant values pertaining to selected copper oxide ladders have been computed in LDA [13], and we use here \( t_{\perp} = 1, \epsilon = 0.5 \) in units of \( t \). \( H_T \) is diagonalized in momentum space, and since \( \epsilon \) and the various \( t \)'s are of the same order, one can safely neglect the high energy orbitals. We are left with two low lying bands crossing the Fermi energy \( E_F \), one bonding (0) and one antibonding (\( \pi \)) combination of chain states. The energy dispersion is linearized near \( E_F \). From the fermionic densities, we introduce \([14]\) charge (c) and spin boson (s) fields \( \phi \) for each specie. \( H_T \) is diagonal when expressed in terms of \( \phi_{\mu,\nu} \) operators \( \mu = c \) or s, \( \nu = 0 \) or \( \pi \) in the \( \mathbf{B}_0 \mathbf{B}_0 \) basis. The non linear terms of \( H_{\text{int}} \), denoted by \( H_{\text{int}}^{NL} \), have a simple form in the \( \mathbf{B}_+ \mathbf{B}_- \) basis, where \( \phi_{\mu,\nu} = 1/\sqrt{2} (\phi_{\mu,0} + \nu \phi_{\mu,\pi}) \), \( \nu = + \) or \( - \). When density-density interactions are included, the quadratic part of \( H \) is diagonal in the \( \mathbf{B}_0 \) basis where we introduce \( \phi_{\lambda} \) operators with \( \lambda = 1, 2, 3, 4 \) (1,2 are s modes, 3,4 are c modes):  

\[
H_0 = \sum_\lambda \int \frac{dx}{2\pi} [(u_{\lambda K}) (\pi \Pi_\lambda)^2 + \left( \frac{u_{\lambda K}}{K}\right) (\partial_x \phi_\lambda)^2] \tag{1}
\]

The matrix \( S \) which defines the rotation of the \( \mathbf{B}_0 \) basis with respect to \( \mathbf{B}_+ \mathbf{B}_- \) is given by  

\[
S = \frac{1}{\sqrt{2}} \begin{pmatrix} P_1 & Q_1 & 0 & 0 \\ -Q_1 & P_1 & 0 & 0 \\ 0 & 0 & P_2 & Q_2 \\ 0 & 0 & -Q_2 & P_2 \end{pmatrix} 
\tag{2}
\]

\( P_i \) and \( Q_i \) are expressed in terms of angles \( \alpha \) for the spin part and \( \beta \) for the charge part; \( P_{1(2)} = \cos \alpha (\beta) \pm \sin \alpha (\beta) \) and \( Q_{1(2)} = \cos \alpha (\beta) - \sin \alpha (\beta) \). In the \( \mathbf{B}_+ \mathbf{B}_- \) basis \( H_{\text{int}}^{NL} \) reads:  

\[
H_{\text{int}}^{NL} = -g_{1c} \int dr \cos (2\phi_{s+}) \cdot \cos (2\theta_{e-}) + g_{1a} \int dr \cos (2\phi_{s+}) \cdot \cos (2\theta_{e-}) - g_{2c} \int dr \cos (2\theta_{e-}) \cdot \cos (2\phi_{s+}) + \ldots \tag{3}
\]

Here, we use the same convention for the Klein factors as in [13]. Subscripts 1 to 4 have the standard g-ology meaning and labels a to d refer to processes involving the 0 and/or \( \pi \) bands. The two \( g_{1d} \) terms, e.g. describe events where one right- and one left-moving fermion, both belonging to the same (0 or \( \pi \)) band, backscatter within that band. \( g_{1a} \) and \( g_{2a} \) correspond to the sum and to the difference of these “1d”-type processes respectively, and \( g_2 \neq 0 \) when the O atoms are included. The \( g_{4a} \) term has a non-zero conformal spin so that additional interactions \( G_{\mu(t)} \sim \cos(4\phi_{s-}(\theta_{e-})) \) are generated during the flow. They are included in our calculations. Since we are concerned with a priori incommensurate values of \( \delta \) we drop all umklapp terms. We renormalize the couplings in [9] following the usual RG procedure, where one integrates out high energy states. This sequence is straightforward when the quadratic part [11] is expressed in the \( \mathbf{B}_0 \) basis, since one deals with simple gaussian integrals but when we express \( H_{\text{int}}^{NL} \) in the \( \mathbf{B}_0 \) basis this involves \( P_i \) and \( Q_i \) coefficients. Each RG step then generates cross-terms in \( H_0 \), which implies a rotation of \( \mathbf{B}_0 \) with respect to the \( \mathbf{B}_+ \mathbf{B}_- \) basis. It is thus important to include the change in \( S \) during the flow. After the \( n^{\text{th}} \) iteration, we denote by \((\alpha_n, \beta_n)\) the angles between \( \mathbf{B}_0 \) and \( \mathbf{B}_+ \mathbf{B}_- \) and by \( K^{(n)} \) the parameters in the \( \mathbf{B}_0 \) basis. We perform the \((n+1)^{\text{th}}\) RG step in the \( \mathbf{B}_0 \) basis, which changes \( K^{(n)} \) (see [11]) and introduces cross-terms. We apply \( S^{-1}(\alpha_n, \beta_n) \) to \( H_0 \), which takes us back to the (fixed) \( \mathbf{B}_+ \mathbf{B}_- \) basis. Finally we determine the new angles \( (\alpha_{n+1}, \beta_{n+1}) \) which are required to make \( H_0 \) diagonal again, with new parameters \( K^{(n+1)} \).  

Proceeding in incremental steps gives the additional RG equations for the rotation of the \( \mathbf{B}_0 \) basis  

\[
\frac{d}{dl} 2\cot(\beta) = \frac{((dK_{1(3)}(3) - dK_{2(4)}(4)) \tan 4\alpha + dB_{12(34)})}{K_{1(3)}(3) - K_{2(4)}(4)} \tag{4}
\]

The equations for the off-diagonal terms \( dB_{12(34)} \) are  

\[
\frac{dB_{12}}{dl} = P_1 Q_1 (g_{1a}^2 + g_{1c}^2 + G_{\pi}^2) - K_1 K_2 (g_{1a}^2 + g_{1c}^2 + 
+ 2g_{2c} + G_{\pi}^2) - K_1 K_2 (P_1) g_1 g_2 \\
\frac{dB_{14}}{dl} = P_2 Q_2 (g_{1c}^2 + g_{2c}^2 + g_{\pi}^2) \tag{5}
\]

with \( h(P_1) = ((P_1 Q_1)^2 + 0.25 (P_1^2 - Q_1^2))^{-1} \). Details of the RG equations for the various \( g \) and \( K \) for the ratio of the Fermi velocities in the 0 and \( \pi \) bands will be given in a forthcoming publication [10].  

Using the above equations we establish the phase diagram for the ladder. In agreement with [3] we find that \( \hat{\alpha} = \frac{\pi V_0 + V_\pi}{2V_F} \) (a ratio of Fermi velocities in the 0 and
\(\pi\) bands) controls the behavior of the differential equation system. When \(\frac{\Delta}{\Gamma}\) is constant, \(\delta\) depends only on \(\delta\). Two main factors may significantly affect the phase diagram that was predicted for two leg Hubbard ladders with a single orbital per site: one is the asymmetry in the charge correlations due to the fact that the projections of the \(\epsilon_{Cu}\) and \(\epsilon_{O}\) orbitals onto the 0 and \(\pi\) bands have unequal amplitudes and one is the influence of the extra parameters \(U_O, V_{Cu-O}\) and \(t_{pp}\). We first investigate the impact of the asymmetry, so we set \(U_O = V_{Cu-O} = t_{pp} = 0\) and we choose small initial values for \(U_{Cu}\) (in the range \(10^{-6} - 10^{-1}\)).

(a) Small doping range. For small \(\delta\) (\(\tilde{\alpha}\)), \(\cot 2\alpha \to 0\) and \(\cot 2\beta \to 0\) as the flow converges towards the fixed point, thus \(B_\alpha \to B_{\alpha-}\). In this case, \(g_2, g_3, G_2, G_3\) are irrelevant while \(\theta_{\alpha-}\) and \(\phi_{\alpha+}\) are ordered (\(\theta_{\alpha-} = 0, \phi_{\alpha+} = 0\) mod 2\(\pi\)). This is the \(C1S0\) phase where only the total (+) charge mode is massless. For the \(s-\) (spin-transverse) mode, terms involving the canonically conjugated fields \(\phi_{\alpha-}\) and \(\theta_{\alpha-}\) are relevant and competing, d-type superconducting fluctuations (SCd) dominate if \(\phi_{\alpha-}\) is locked at 0, while OAF is favored if \(\theta_{\alpha-} = 0\). Here, SCd is always more stable for repulsive \(U_{Cu}\). This property holds only for \(\delta < \delta_{c1} = 0.2\), where the spin and mass gaps go to zero.

(b) Large doping range. For \(\delta > \delta_{c2} = 0.28\), \(\cot 2\alpha\) and \(\cot 2\beta\) \(\to \infty\) (with opposite signs), so \(B_\alpha \to B_{\alpha+}\). In this regime only \(g_1 \approx -g_2\) are relevant and they lead to a state with one massive spin mode (in the 0 band). This is the \(C2S1\) phase. The slowest decay of correlations is observed for the CDW operator in the 0 band. Fluctuations in the \(\pi\) band favor a SDW state (when logarithmic corrections due to a marginal operator proportional to \(g_1 + g_2 > 0\) are included) but they are subdominant. If \(\delta\) is just above \(\delta_{c2}\), \(g_1\) and \(g_2\) increase very slowly during the flow and one needs to choose larger values for the bare \(U_{Cu}\) (still much smaller than \(t\)) to reach the asymptotic regime with a gap in the spin mode. In contrast with the case of a single orbital per site, the \(C2S1\) phase is stable, even for dopings such that \(E_F\) is close to the bottom of the \(\pi\) band where \(\tilde{\alpha}\) is very large (in that limit, we cannot linearize the energy spectrum, but we use diagrammatic techniques). This comes from the fact that for unit cells with \(\epsilon_{Cu}\) atoms only, \(g_2\) is second order in \(U_{Cu}\) (or when \(V_{Cu-O} \neq 0\)) the initial \(g_2\) is non-zero and \(g_2\) is always relevant. The nature of this \(C2S1\) phase is discussed in the next paragraph.

(c) Massless regime in the \((\delta_{c1}, \delta_{c2})\) range. As \(\delta\) approaches the critical end points \(\delta_{c1}\) and \(\delta_{c2}\) respectively from below (in the \(C1S0\) phase) and from above (in the \(C2S1\) phase), gaps in the spin and/or in the charge sectors go to zero. All spin and charge modes are massless in the entire range of dopings \(\delta \in (0.2; 0.28)\). \(\frac{d\phi_{\alpha-}}{d\delta}\) and \(\frac{d^2\phi_{\alpha+}}{d\delta^2}\) are very large and the fixed point values of \(\beta\) (\(\alpha\)) just below and just above \(\delta_{c1}\) (\(\delta_{c2}\)) are significantly different. So we approach the critical points from the massive phases at both ends; we discard couplings which flow to zero and thus obtain a simpler set of equations. Next we single out terms in \(u_{10}\) which produce large values of the derivatives in this range and determine the fixed point value of \(\cot 2\alpha (\beta)\). It allows us to write down a minimal set of differential equations for the couplings and to determine those which are relevant in the doping range \((\delta_{c1}, \delta_{c2})\). We first consider dopings close to \(\delta_{c2}\). This corresponds to an initial value of \(\cot 2\alpha\) equal to one. The signs of \((dK_1 - dK_2)\) and \(dB_{12}\) are the same and positive whereas the sign of \((K_1 - K_2)\) is negative so that, according to \(u_{10}\), \(\cot 2\alpha\) decreases to zero below \(\delta_{c2}\) while above it increases to infinity. Below \(\delta_{c2}\), \(g_1\) and \(g_2\) are not relevant and the system flows to the \(C2S2\) phase above while they are relevant, leading to the \(C2S1\) phase. For \(\delta\) close to \(\delta_{c1} = 0.2\), \((dK_3 - dK_4)\) and \(dB_{34}\) have opposite signs. Depending on which of the two terms dominates, \(\cot 2\beta\) goes to zero or infinity. At \(\delta_{c1}\) they are exactly equal, \(\cot 2\beta\) \(\to \infty\), for \(\delta > \delta_{c1}\), but, since \(0.5 < K_4 < 1\), one finds that all interband couplings (as well as higher order \(\cos(b\phi_{\alpha})\) terms with \(b = 4, 6, . . .\)) are irrelevant. For \(\delta \in (0.2; 0.28)\), all interaction terms are irrelevant and \(B_{\alpha}(\phi_{\alpha+})\) is the eigenbasis for the charge (spin) modes. A numerical solution of the full set of RG equations confirms this statement. The existence of this massless regime is essential to maintain spin rotational symmetry in this doping range. The nature of the \(C2S2\) phase can be determined in the framework of the Luttinger liquid description. In that phase, \(K_3 (K_3)\) which corresponds to the 0 (\(\pi\)) band is smaller than (around) one. Dominant fluctuations occur in the 0 band, and this case is equivalent to treating a single chain problem. The only marginal couplings are \(g_1\) and \(g_2\) \((g_1 > g_2)\). Including logarithmic corrections allows us to identify the slowest decaying correlation function and we find that in the \((\delta_{c1}, \delta_{c2})\) doping range, a SDW in the 0 band (SDW(0)) is favored. In the \(C2S1\) state, \(g_1 \approx -g_2 < 0\) are relevant which gives a gap in the spin sector of the 0 mode. In that regime, fluctuations in the 0 band dominate, and one finds that the CDW(0) state is the slowest decaying one.

Next, we “turn on” the parameters \(U_O, V_{Cu-O}\) and \(t_{pp}\) and we examine their impact on the phase diagram. In the doping range covered by case (a), SCd becomes less important over OAF when we increase the (positive) bare value of \(U_O\) or \(V_{Cu-O}\) at fixed \(t_{pp}\) but it is still the phase with the lowest free energy. One would need to assume a very large attractive bare \(V_{Cu-O}\) to cause a transition to an s-type SC phase \((\phi_{\alpha-} = 0, \phi_{\alpha+} = 0, \theta_{\alpha-} = \pi/2)\) which persists even as \(E_F\) approaches the bottom of the \(\pi\) band. As far as case (b) is concerned, we observe a reduction in the size of the gap for positive \(U_O\) and \(V_{Cu-O}\), while for very large attractive \(V_{Cu-O}\) the s-SC phase re-enters. In case (c), increasing \(V_{Cu-O}\) has little effect on \(\delta_{c2}\) but it shifts \(\delta_{c1}\) to higher values. An un-
physically large ratio $V_{Cu-O}/U_{Cu}$ $\approx 5$ would be required to suppress the massless phase and to observe a renentrant $C1S0$ phase with superconducting fluctuations so that in the relevant case $V_{Cu-O} < U_{Cu}$ the intermediate massless phase does exist.

The interoxygen hopping has a more significant effect. Increasing the value of $t_{pp}$ causes a concomitant decrease of $\delta_{c1}$ and $\delta_{c2}$. For $t_{pp} = 0.5$ -a value pertaining to $Cu - O$ ladders $^{13}$- their values are about half that quoted for $t_{pp} = 0$. If $t_{pp} > t_{pp}^{min}$, a new phase is favored when $\delta > \delta_{c1}$. This state has both orbital current and DW fluctuations ($DW \equiv SDW$ ($CDW$) for the C2S2 ($C2S1$) regime) and it shows similarities with one of the patterns advocated by Varma $^{8}$ (see Fig. 1). This current phase is an eigenstate of the $B_{0x}$ basis (it is invariant under the exchange of the two legs) in contrast with the other Varma pattern or with the usual OAF. The pattern has an incommensurate spatial periodicity $\sim k_{F0}^{-1}$. The amplitude of this order parameter is a sum of current operators between links of the $Cu-O$ loops, of the form $t_{ij} Im(\lambda^*_\alpha \lambda_{\alpha})$, where $t_{ij}$ is the hopping parameter from site $i$ to site $j$ within the same unit cell and $\lambda_\alpha$ is the overlap between the $(Cu$ or $O$) wavefunction at site $i$ and the $0$ band eigenfunction. These quantities are of order one $^{10}$ and change by only a few percent when $\delta$ increases from $\delta_{c1}$ to the bottom of the band. Due to current conservation, the weakest link between atoms determines the maximal current, and we find that, for $t_{pp}^{min} \approx 0.3$, the “Varma” state dominates the DW($o$).

The presence of the $O$ sites insures that $Im(\lambda^*_\alpha \lambda_{\alpha}) \neq 0$ ($\alpha = 0, \pi$); Otherwise, the current operator between $Cu$ atoms has the usual interband form: $c_{i\sigma} c_{i\pi \sigma}$.

Our predictions could be tested by performing NMR measurements on the $Sr_{14-x}Ca_xCu_{24}O_{41}$ compound $^{11}$ where the hole content can be somewhat varied, as we find very different responses of the the spin modes for the $Cu$ and $O$ sites $^{10}$. Knight shifts $K$ and relaxation rates $T^{-1}_1$ can be evaluated in all three regimes. For low doping we find an activated behavior of $K$ (and also $T^{-1}_1$) and $K(T = 0) = 0$; for high doping the temperature dependance is similar but $K(T = 0) \neq 0$; finally, at intermediate dopings the usual high temperature behavior $K \sim T^0$ (saturation to the LL value) extends to $T \rightarrow 0$. For instance, Fig. 2 shows the Knight shift predicted for the “outer” $O$ sites (i.e. interladder bridges)

In conclusion, we have developed a new RG method to handle correlation effects in the weak coupling limit for two leg Hubbard ladders at generic filling, when oxygen atoms are included in the unit cell. We have found a ground state phase diagram where the $C1S0$ and $C2S1$ phases are present at small and large dopings, as for the single orbital ladder, but also a new intermediate phase $C2S2$ which is completely massless. Dominant fluctuations in the $C2S2$ and $C2S1$ states correspond to orbital currents preserving the mirror symmetry of the ladder structure on top of a SDW($o$) and CDW($o$) respectively. The stability of this new phase to an interladder coupling and/or to large values of the bare $U$ are under current investigation.

Acknowledgments. The authors are indebted to T. Becker and to C.M. Varma. This work was supported in part by the Swiss NSF under MaNEP and Division II and by an ESRT Marie Curie fellowship.

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