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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 renormalization group 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 structure.

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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 one-dimensional (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 parameter that may be safely tuned to arbitrary values in the weak-coupling limit is the doping δ and its variation produces a sequence of states, labeled *CnSm*, with $n(m)$ gapless charge (spin) modes. For repulsive on-site Hubbard U terms, a $C1S0$ d-wave "superconducting" phase is found away from half filling ($\delta \neq 0$). Relaxing the constraint on the magnitude and on the sign of the interactions and extending their range to more distant sites allows one to promote other types of orders such as orbital antiferromagnetism (OAF).[5] This state is also known as a flux phase and was examined in the context of the two-dimensional Hubbard model.[6,7]

The question of whether orbital currents could exist in cuprate materials has received much attention. Analytical[8] and numerical[9] studies of a three-band model of the copper-oxygen planes predict that, in the large U limit, a strong Coulomb repulsion $V_{\text{Cu-O}}$ between nearest-neighbor Cu and O atoms favors such a phase. Recent experimental data seem to support that picture,[10] but more studies are needed to confirm this scenario.

We thus revisit models for ladders and include the oxygen atoms. Here, we focus on the issue of whether their presence causes any significant changes[11] and in particular whether orbital phases might exist for realistic choices of microscopic interactions, for $\delta \neq 0$.[12] We establish, in the weak coupling regime, the phase diagram as a function of hole doping of two-leg ladders whose unit cell contains both Cu and O atoms, with on-site repulsions U_{Cu} (U_{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 $\delta_{c1} < \delta < \delta_{c2}$ a fully massless phase is stabilized. The value of $\delta_{c1(c2)}$ 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 $\delta > \delta_{c1}$, an incommensurate orbital current state. It is similar to one of the patterns advocated by Varma[8] [see Fig. 1(b)]. The corresponding phase has an additional spin-density (SDW) character for $\delta < \delta_{c2}$ or charge-density wave (CDW) character for $\delta > \delta_{c2}$.

We consider the two leg ladder of Fig. 1(a) 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 difference between the Cu and O site energies. Relevant values pertaining to selected copper oxide ladders have been computed in local-density approximation,[13] and we use here $t_\perp = 1$, $\epsilon = 0.5$ in units of t. H_T is diagonalized in momentum space, and since ϵ and the various t's are of the same order, one can safely neglect the high energy orbitals. We are left with two low

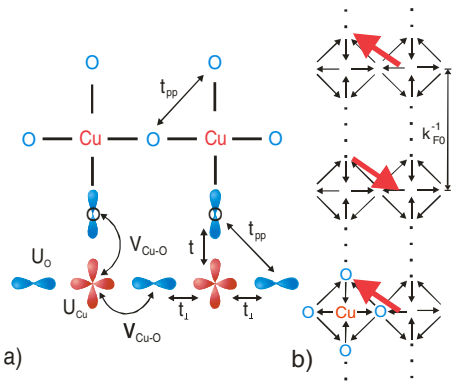

FIG. 1. (Color online) (a) Molecular structure of the unit cell showing the hopping and interaction parameters included in the Hamiltonian. (b) Orbital current pattern and SDW modulation (bold arrows) in the $C2S2$ phase. The chain direction is vertical. k_{F0} is the Fermi wave vector in the 0 band.

lying bands crossing the Fermi energy E_F, one bonding (0) and one antibonding (π) 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 ϕ for each specie. H_T is diagonal when expressed in terms of $\phi_{\mu,\nu}$ operators $\mu=c$ or s, $\nu=0$ or π in the $B_{0\pi}$ basis. The nonlinear terms of H_{int}, denoted by H_{int}^{NL}, have a simple form in the 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 B_0 basis where we introduce ϕ_λ operators with $\lambda=1,2,3,4$ (1,2 are s modes and 3,4 are c modes):

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

The matrix S which defines the rotation of the B_0 basis with respect to B_{+-} is given by

$$S=\frac{1}{\sqrt{2}}\begin{pmatrix} P_1 & Q_1 & 0 & 0 \\ -Q_1 & P_1 & 0 & 0 \\ 0 & 0 & P_2 & Q_2 \\ 0 & 0 & -Q_2 & P_2 \end{pmatrix}. \quad (2)$$

P_i and Q_i are expressed in terms of angles α for the spin part and β for the charge part; $P_{1(2)}=\cos\alpha(\beta)+\sin\alpha(\beta)$ and $Q_{1(2)}=\cos\alpha(\beta)-\sin\alpha(\beta)$. In the B_{+-} basis H_{int}^{NL} reads

$$\begin{aligned} H_{int}^{NL}=&-g_{1c}\int dr\cos(2\phi_{s+})\cos(2\theta_{c-}) \\ &+g_{1a}\int dr\cos(2\phi_{s+})\cos(2\theta_{s-}) \\ &-g_{2c}\int dr\cos(2\theta_{c-})\cos(2\phi_{s-}) \\ &+g_{4a}\int dr\cos(2\phi_{s-})\cos(2\theta_{s-}) \\ &+g_1\int dr\cos(2\phi_{s+})\cos(2\phi_{s-}) \\ &+g_2\int dr\sin(2\phi_{s-})\sin(2\phi_{s+}) \\ &+g_{\|c}\int dr\cos(2\theta_{c-})\cos(2\theta_{s-}). \end{aligned} \quad (3)$$

Here we use the same convention for the Klein factors as in Ref. 15. Subscripts 1–4 have the standard *g-ology* meaning and labels a to d refer to processes involving the 0 and/or π 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 π) band, backscatter within that band. g_1 and g_2 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 nonzero conformal spin so that additional interactions $G_{p(t)}\sim\cos[4\phi_{s-}(\theta_{s-})]$ are generated during the flow. They are included in our calculations.

Since we are concerned with *a priori* incommensurate values of δ we drop all umklapp terms. We renormalize the couplings in Eq. (3) following the usual RG procedure, where one integrates out high energy states. This sequence is straightforward when the quadratic part (1) is expressed in the B_0 basis, since one deals with simple Gaussian integrals but when we express H_{int}^{NL} in the 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 B_0 with respect to the B_{+-} basis. It is thus important to include the change in S during the flow. After the nth iteration, we denote by (α_n,β_n) the angles between B_0 and B_{+-} and by $K_\lambda^{(n)}$ the parameters in the B_0 basis. We perform the $(n+1)$th RG step in the B_0 basis, which changes $K_\lambda^{(n)}$ [see Eq. (1)] and introduces cross terms. We apply $S^{-1}(\alpha_n,\beta_n)$ to H_0, which takes us back to the (fixed) 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 $K_\lambda^{(n+1)}$.

Proceeding in incremental steps gives the additional RG equations for the rotation of the B_0 basis,

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

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

$$\begin{aligned} \frac{dB_{12}}{dl}=&P_1Q_1[(g_{1a}^2+g_{\|c}^2+G_t^2)-K_1K_2(g_{1a}^2+g_{1c}^2+g_{2c}^2+G_p^2)] \\ &-K_1K_2h(P_1)g_1g_2 \\ \frac{dB_{34}}{dl}=&P_2Q_2(g_{1c}^2+g_{2c}^2+g_{\|c}^2) \end{aligned} \quad (5)$$

with $h(P_1)=[(P_1Q_1)^2+0.25(P_1^2-Q_1^2)]^{-1}$. Details of the RG equations for the various g, K and for the ratio of the Fermi velocities in the 0 and π bands will be given in a forthcoming publication.[16]

Using the above equations we establish the phase diagram for the ladder. In agreement with Ref. 3 we find that $\tilde{\alpha}=\frac{V_{Fo}+V_{F\pi}}{2V_{F_o}}$ (a ratio of Fermi velocities in the 0 and π bands) controls the behavior of the differential equation system. When $\frac{t_\perp}{t}$ is constant, $\tilde{\alpha}$ depends only on δ. 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 g terms due to the fact that the projections of the Cu and O orbitals onto the 0 and π bands have unequal amplitudes and one is the influence of the extra parameters U_O, $V_{Cu\text{-}O}$, and t_{pp}. We first investigate the impact of the asymmetry, so we set $U_O=V_{Cu\text{-}O}=t_{pp}=0$ and we choose small initial values for U_{Cu} (in the range 10^{-6}–10^{-1}).

(a) Small doping range. For small δ ($\tilde{\alpha}$), $\cot 2\alpha\to 0$ and $\cot 2\beta\to 0$ as the flow converges towards the fixed point, thus $B_0\to B_{+-}$. In this case, g_2,g_{4a},G_p,G_t are irrelevant while θ_{c-} and ϕ_{s+} are ordered ($\theta_{c-}=0$, $\phi_{s+}=0 \bmod 2\pi$). This is the $C1S0$ phase[3] where only the total (+) charge mode is massless. For the $s-$ (spin-transverse) mode, terms involving the canonically conjugated fields ϕ_{s-} and θ_{s-} are relevant and

competing. *d*-type superconducting fluctuations (SCd) dominate if ϕ_{s-} is locked at 0, while OAF is favored if $\theta_{s-}=0$. 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 $B_0\to B_{0\pi}$. In this regime only $g_1\simeq -g_2$ 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 π 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 δ is just above δ_{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 π band where $\tilde{\alpha}$ is very large (in that limit, we cannot linearize the energy spectrum, but we use diagrammatic techniques).[3] This comes from the fact that for unit cells with Cu atoms only, g_2 is accidentally equal to zero. When O atoms are included (or when $V_{\mathrm{Cu\text{-}O}}\neq 0$) the initial g_2 is nonzero 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 δ approaches the critical end points δ_{c1} and δ_{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 $\delta\in(0.2;0.28)$. $\frac{d\alpha}{dl}$ and $\frac{d\beta}{dl}$ are very large and the fixed point values of β (α) just below and just above δ_{c1} (δ_{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 Eqs. (4) and (5) 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 δ_{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 Eq. (4), $|\cot 2\alpha|$ decreases to zero below δ_{c2} while above it increases to infinity. Below δ_{c2}, g_1 and g_2 are not relevant and the system flows to the $C2S2$ phase while above they are relevant, leading to the $C2S1$ phase. For δ 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 to infinity. At δ_{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 $\cos(b\phi_c)$ terms with $b=4,6,\ldots$] are irrelevant. For $\delta\in(0.2;0.28)$, all interaction terms are irrelevant and $B_{0\pi}$ (B_{+-}) 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, $K_4(K_3)$ which corresponds to the 0 (π) 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(o)] is favored. In the $C2S1$ state, $g_1\simeq -g_2<0$ 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(o) state is the slowest decaying one.

Next, we "turn on" the parameters U_{O}, $V_{\mathrm{Cu\text{-}O}}$, and t_{pp} and we examine their impact on the phase diagram. In the doping range covered by case (a), SCd becomes less dominant over OAF when we increase the (positive) bare value of U_{O} or $V_{\mathrm{Cu\text{-}O}}$ 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 $V_{\mathrm{Cu\text{-}O}}$ to cause a transition[12] to an *s*-type SC phase ($\phi_{s-}=0$, $\phi_{s+}=0$, $\theta_{c-}=\pi/2$),[15] which persists even as E_F approaches the bottom of the π band. As far as case (b) is concerned, we observe a reduction in the size of the gap for positive U_{O} and $V_{\mathrm{Cu\text{-}O}}$, while for very large attractive $V_{\mathrm{Cu\text{-}O}}$ the *s*-SC phase reenters. In case (c), increasing $V_{\mathrm{Cu\text{-}O}}$ has little effect on δ_{c2} but it shifts δ_{c1} to higher values. An unphysically large ratio $V_{\mathrm{Cu\text{-}O}}/U_{\mathrm{Cu}}\approx 5$ would be required to suppress the massless phase and to observe a reentrant $C1S0$ phase with superconducting fluctuations so that in the relevant case $V_{\mathrm{Cu\text{-}O}}<U_{\mathrm{Cu}}$ 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 δ_{c1} and δ_{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≡SDW (CDW) for the $C2S2$ ($C2S1$) regime] and it shows similarities with one of the patterns advocated by Varma[8] [see Fig. 1(b)]. This current phase is an eigenstate of the $B_{0\pi}$ 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 $t_{ij}\,\mathrm{Im}(\lambda_{i0}^{*}\lambda_{j0})$, where t_{ij} is the hopping parameter from site i to site j within the same unit cell and λ_{i0} is the overlap between the (Cu or O) wave function at site i and the 0 band eigenfunction. These quantities are of order one[16] and change by only a few percent when δ increases from δ_{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 $\mathrm{Im}(\lambda_{i\alpha}^{*}\lambda_{j\alpha})\neq 0(\alpha=0,\pi)$; otherwise, the current operator between Cu atoms has the usual interband form: $c_{o\sigma}^{\dagger}c_{\pi\sigma}$.

Our predictions could be tested by performing NMR measurements on the $Sr_{14-x}Ca_xCu_{24}O_{41}$ compound[1] where the

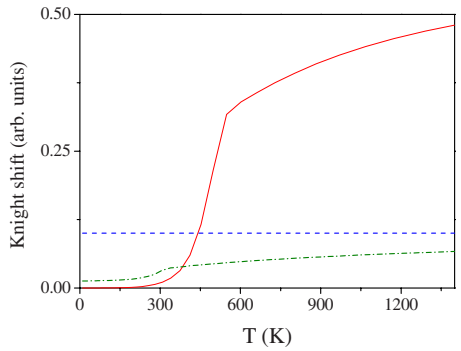

FIG. 2. (Color online) Knight shift on the outer O sites calculated for different phases: solid line $C1S0$ dashed line $C2S2$, and dash dotted line $C2S1$.

hole content can be somewhat varied, as we find very different responses of the spin modes for the Cu and O sites.[16] 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, Figure 2 shows the Knight shift predicted for the "outer" O sites (i.e., interladder bridges).

In conclusion, we have developed a 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 an 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 phase to an interladder coupling and/or to large values of the bare U are under current investigation.

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