One-Dimensional Multi-Band Correlated Conductors and Anderson Impurity Physics

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A single Anderson impurity model recently predicted, through its unstable fixed point, the phase diagram of a two band model correlated conductor, well confirmed by Dynamical Mean Field Theory in infinite dimensions. We study here the one dimensional version of the same model and extract its phase diagram in this opposite limit of reduced dimensionality. As expected for one dimension, the Mott metal-insulator transition at half filling is replaced by a dimerized insulator-undimerized Mott insulator transition, while away from half filling the strongly correlated superconductivity for inverted Hund's rule exchange in infinite dimensions is replaced by dominant pairing fluctuations. Many other aspects of the one dimensional system, in particular the field theories and their symmetries are remarkably the same as those of the Anderson impurity, whose importance appears enhanced.

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Very substantial progress in our understanding of the Mott metal-insulator transition (MIT) have been made thanks to the so-called Dynamical Mean Field Theory (DMFT)[1], a quantum analogue of the classical mean-field theory which treats time correlations and is exact in infinite dimensions (∞-D). In DMFT, the approach to the MIT from the metal phase is accompanied by a net separation of energy scales between well pre-formed high energy Hubbard bands – images of the excitations in the nearby Mott insulator – and the lingering low-energy itinerant quasiparticles. This separation is in fact already contained in the isolated Anderson impurity model (AIM), where most of the spectral weight is concentrated in the high-energy sub-bands and only a small fraction – describing quasiparticles promoted into the conduction screening-bath – remains close to the chemical potential. This is of course unsurprising since in ∞-D DMFT maps the lattice model of interacting electrons onto an AIM supplemented by a self-consistency condition[1]. Irrespective of whether this mapping is merely a trick to solve the lattice model in ∞-D or whether it hides perhaps a more fundamental aspect of the physics close to a MIT, this does suggest that some of the strongly correlated lattice properties could be directly inferred by the AIM itself, even without self-consistency. This route was recently explored to anticipate the anomalous properties near the MIT of a two-band Hubbard conductor on the basis of the phase diagram and in particular of the unstable fixed point of a two-orbital AIM[2]. All the predicted properties, including strongly correlated superconductivity near the Mott transition[3] were later confirmed by full DMFT[4]. Despite that success, it would still seem hazardous to suggest that the properties of a single AIM have generally anything to do with the actual behavior of the model lattice conductor away from ∞-D, least of all in the opposite extreme of one dimension (1D). We show in this Letter that, apart from some obvious differences related to dimensionality, the phase diagram of the model does not change significantly in 1D, where therefore the AIM physics appears to remain significant.

We consider the two-band Hamiltonian near half-filling and in 1D

$$\hat{H} = -t\sum_{a=1}^{2}\sum_{i\,\sigma}\left(c^\dagger_{i,a\sigma}c_{i+1,a\sigma}+H.c.\right)+\frac{U}{2}\sum_i\left(\hat{n}_i-2\right)^2 -\frac{J}{4}\sum_{a\neq b}\sum_{i\,\sigma\,\sigma'}c^\dagger_{i,a\sigma}c^\dagger_{i,b\sigma'}c_{i,a\sigma'}c_{i,b\sigma}, \quad (1)$$

where $c^\dagger_{i,a\sigma}(c_{i,a\sigma})$ creates(annihilates) an electron at site i, in orbital $a=1,2$ with spin $\sigma=\uparrow,\downarrow$, and $\hat{n}_i=\sum_{a\sigma}c^\dagger_{i,a\sigma}c_{i,a\sigma}$ is the electron density at site i, and $U\gg|J|$ is an on-site Coulomb repulsion. This Hamiltonian has recently been discussed as relevant to the novel doped metal-phthalocyanine conductors.[5] For $J=0$ Eq. (1) describes an SU(4) Hubbard model, analysed *e.g.* in Ref. [6]. A finite value of J lowers the symmetry down to U(1)×SU(2)× (U(1) × Z_2), where U(1) refers to charge, SU(2) to spin and (U(1) × Z_2) to the flavour (orbital) sector. We stress here that the single AIM shares identically this same symmetry, a point which we will return to further down. Two electrons on the same site can form either a spin triplet, with energy $J/4$, an inter-orbital singlet, with energy $-3J/4$, or two intra-orbital singlets with energy $-J/4$. Therefore $J<0$ favors the spin triplet while $J>0$ the inter-orbital singlet. Actually $J>0$, ("inverted Hund's rule exchange"), provides a pairing mechanism in the Cooper channel $c^\dagger_{i,1\uparrow}c^\dagger_{i,2\downarrow}+c^\dagger_{i,2\uparrow}c^\dagger_{i,1\downarrow}$. Pairing is impeded by the repulsion U, so that the *bare* scattering amplitude in the inter-chain singlet channel, $A=U-J/2$, is attractive only in the unrealistic case of $J>2U>0$, apparently excluding superconductivity despite the pairing mechanism provided by $J>0$. As shown in DMFT [4], this näive expection is actually wrong, at least in ∞-D. A superconducting pocket appears near the half-filled Mott insulator, $U\sim t\gg J$, moreover with a hugely enhanced superconducting gap with respect to the $U=0$ BCS gap value. This surpris-

ing result had in fact been foreshadowed by the single AIM study[2] whose phase diagram displays an unstable fixed point at $0 < J_* \simeq T_K$, where T_K is the Kondo temperature, which separates a Kondo screened phase for $J < J_*$ from an unscreened phase for $J > J_*$. Translated into DMFT, the AIM Kondo temperature becomes the quasiparticle coherent bandwidth, vanishing at the MIT. This implies that the AIM onto which the metallic lattice model maps in ∞-D must necessarily cross the unstable fixed point $J \sim T_K$ before the MIT. The speculation[2] that the lattice model would respond to the local instability by spontaneously developing a bulk order parameter in the inter-orbital singlet Cooper channel was fully confirmed by DMFT[4].

We turn now to study the same model in 1D. As usual it is convenient here to represent (1) within bosonization.[7] The Fermi fields around the right (R), $+k_F$, and left (L), $-k_F$, Fermi points are expressed as $\psi_{R(L),a\sigma}(x) \sim \exp\left[\pm i k_F x - i\sqrt{\pi}\left(\Theta_{a\sigma}(x) \mp \Phi_{a\sigma}(x)\right)\right]$, where $\Phi_{a\sigma}(x)$ and $\partial_x \Theta_{a\sigma}(x)$ are conjugate Bose fields. We introduce the linear combinations $\Phi_c = \left(\Phi_{1\uparrow} + \Phi_{1\downarrow} + \Phi_{2\uparrow} + \Phi_{2\downarrow}\right)/2$, $\Phi_s = \left(\Phi_{1\uparrow} - \Phi_{1\downarrow} + \Phi_{2\uparrow} - \Phi_{2\downarrow}\right)/2$, $\Phi_f = \left(\Phi_{1\uparrow} + \Phi_{1\downarrow} - \Phi_{2\uparrow} - \Phi_{2\downarrow}\right)/2$, and $\Phi_{sf} = \left(\Phi_{1\uparrow} - \Phi_{1\downarrow} - \Phi_{2\uparrow} + \Phi_{2\downarrow}\right)/2$, which describe respectively the total charge, the total spin, the relative charge and the relative spin density fluctuations. In this representation the interaction involves only bilinears of $\cos\sqrt{4\pi}\Phi_n$ and $\cos\sqrt{4\pi}\Theta_n$, $n = c, s, f, sf$, which in turn can be expressed as

$$\cos\sqrt{4\pi}\Phi_n = -i\frac{\pi\alpha}{2}\left(\xi_{R,n}\xi_{L,n} + \zeta_{R,n}\zeta_{L,n}\right), \quad (2)$$

$$\cos\sqrt{4\pi}\Theta_n = i\frac{\pi\alpha}{2}\left(\xi_{R,n}\xi_{L,n} - \zeta_{R,n}\zeta_{L,n}\right), \quad (3)$$

where $\xi_{R(L),n}$ and $\zeta_{R(L),n}$ are Majorana fermions and α is a cutoff distance. These fermions can be used to introduce eight two-dimensional classical Ising models, each one in principle characterized by a *mass* $m \sim (T - T_c)$, $m < 0$ and $m > 0$ meaning ordered and disordered phases, and $m = 0$ the critical point. In this way the U(1) charge sector is represented by two identical Ising models with mass m_c, the doublet $(\xi_{R,c}, \xi_{L,c})$ and $(\zeta_{R,c}, \zeta_{L,c})$; the SU(2) spin sector by three identical Ising models (mass m_s), the triplet $(\xi_{R,s}, \xi_{L,s})$, $(\zeta_{R,s}, \zeta_{L,s})$ and $(\xi_{R,sf}, \xi_{L,sf})$; the U(1) flavour sector by two identical Ising copies (mass m_f), the doublet $(\xi_{R,f}, \xi_{L,f})$ and $(\zeta_{R,f}, \zeta_{L,f})$; and finally the remaining flavour Z_2 by a single Ising model (mass m_0), the singlet $(\zeta_{R,sf}, \zeta_{L,sf})$.[8] Without interaction all Ising models are critical. The interaction induces marginally relevant couplings between them which might spontaneously generate finite masses. Indeed, by a fermion two-loop renormalization group (RG) analysis, we find that the Hamiltonian generally flows to strong coupling fixed points which allow a simple mean-field description in terms of finite average values of $\langle\xi_{R,n}\xi_{L,n}\rangle$ and $\langle\zeta_{R,n}\zeta_{L,n}\rangle$, $n = c, s, f, sf$, which preserve all continuous symmetries. Within this same description the phase diagram of (1) turns out to be characterized by simply identifying the relative signs of the masses m_i, $i = c, s, f, 0$, while the overall sign has a physical meaning only in the spontaneoulsy dimerized phase, see below.[9]

We start from half filling, $\langle\hat{n}_i\rangle = 2$, and analyse the phase diagram for increasing U/t keeping for simplicity a fixed ratio $U/|J| \gg 1$. At weak coupling, $U/t \ll 1$, the Hamiltonian flows under RG to an SO(8) Gross-Neveu model, which describes a spontaneously dimerized insulator with gaps in the whole excitation spectrum. It is known that the SU(4) Hubbard model, *i.e.* (1) with $J = 0$, dimerizes at half-filling[6, 10], and that a small $|J| \ll U$ cannot destabilize this gapped phase.[11] This phase is characterized by all masses having the same sign, with the overall sign reflecting the broken translational symmetry. Eventually, though, this dimerized phase cannot survive indefinitely for large U/t. When $U \gg t$, two electrons localize at each site in a configuration optimizing the on-site exchange J. In particular for $J < 0$, conventional Hund's rules, the model effectively reduces to a spin S=1 Heisenberg chain, still gapped everywhere in the spectrum but not dimerized[12]. For inverted Hund's rules, $J > 0$, the singlet configuration

$$\sqrt{\frac{1}{2}}\left[c^\dagger_{i,1\uparrow}c^\dagger_{i,2\downarrow} + c^\dagger_{i,2\uparrow}c^\dagger_{i,1\downarrow}\right]|0\rangle, \quad (4)$$

is favored and the ground state is akin to a collection of local singlets, a kind of local valence-bond Mott insulator, still gapped but not dimerized. We conclude that upon increasing U/t the dimerization must disappear for either sign of J. In fact, whereas at weak coupling at for $J = 0$ the dimerization-induced gaps in the spin and flavour sectors follow the BCS-like behavior of the charge gap, the latter continues to increase monotonically as U increases while the former gaps reach a maximum, approximately when $U \sim 5t$, and then start dropping as t^2/U for $U \gg t$[6, 10]. This decoupling of charge from spin and orbital modes is a 1D remnant of the MIT and seems quite sharp[6]. The weak exchange $|J|/U \ll 1$, irrelevant in the weak coupling dimerized phase, eventually turns in strong coupling to a relevant perturbation able to suppress dimerization. Thus one might expect that this could occur only for very large U, when the spin gap induced by dimerization becomes small of order $|J|$. However it cannot be excluded that the demise of dimerization could even take place for smaller U, say for $U < 5t$. The two-loop RG equations moreover suggest for $J < 0$ a $c = 3/2$ spin-SU$(2)_2$ critical point where the triplet mass m_s changes sign[13], signaling a transition from the dimerized insulator to the Haldane spin-1 chain Mott insulator. For $J > 0$ the transition is instead predicted to occur through a $c = 1/2$ Ising critical point where the singlet mass m_0 crosses zero, signaling the transition from a dimerized to the valence-bond Mott insulator, see Fig. 1.

Let us introduce doping, moving away from half filling. Dropping the Umklapp terms from the weak coupling

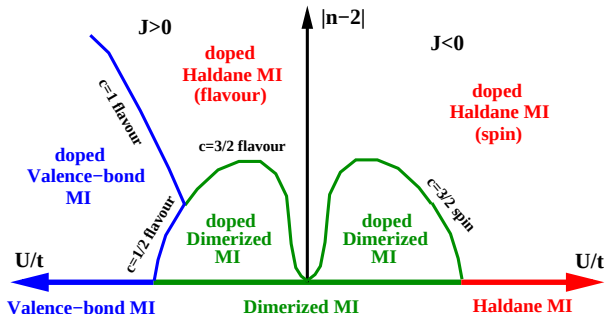

FIG. 1: Phase diagram of model (1) near half-filling as a function of doping $|n-2|$ and of U/t at fixed $|J|/U \ll 1$ for $J<0$ (right panel) and $J>0$ (left panel). At half-filling the system is always insulating and displays by increasing U/t an Ising transition ($c=1/2$ flavour) from a Dimerized Mott insulator (MI) to a Valence-bond MI for $J>0$; and a $c=3/2$ transition to a S=1 Haldane MI for $J<0$ where the spin is gapless ($c=3/2$ spin). All the insulating phases evolve upon doping into metal with gaps in all noncharge sectors. For the doped Haldane MI the additional label (flavour) or (spin) indicates that the phase can be viewed as the natural evolution away from half-filling of a Haldane chain built of either spin or flavour triplets. The transition lines bewteen each different metallic phase are identified by the central charge c and by the sector involved, spin or flavour.

RG equations, the interaction flows, for either sign of J, towards a fixed point

$$\hat{H}_{int} \to -g_* \int dx\, \Delta^\dagger(x)\, \Delta(x), \tag{5}$$

where

$$\Delta^\dagger = \psi^\dagger_{R,1\uparrow}\psi^\dagger_{L,2\downarrow} + \psi^\dagger_{L,2\uparrow}\psi^\dagger_{R,1\downarrow} - \psi^\dagger_{L,1\uparrow}\psi^\dagger_{R,2\downarrow} - \psi^\dagger_{R,2\uparrow}\psi^\dagger_{L,1\downarrow} \tag{6}$$

which is a spin-singlet, flavour-singlet but space-odd pairing operator[11, 14]. This fixed point interaction has a dynamically enlarged SU(4) symmetry[9, 11], unlike the original model (1), and realizes a doped Haldane chain, the two 1/2-spin constituents forming singlet bonds, one to its right and the other to its left.[15] Moving from $J<0$ to $J>0$ interchanges the spin sector and the flavour sector, which includes the doublet and the singlet forming a degenerate triplet, again a dynamically enlarged $SU(2)_2$ flavour symmetry. The Ising masses satisfy $m_c=0$, $m_f\, m_0>0$ but $m_s\, m_f<0$. The pairing correlation function $\langle\Delta(x)\Delta^\dagger(0)\rangle \sim (1/x)^{1/2K_c}$ where K_c is the Luttinger liquid exponent of the gapless U(1) charge sector. There are also power-law decaying $4k_F$ correlation functions with exponent $2K_c$ which involve the density-wave operators $\exp\left(\pm i4\, k_F\, x \pm i\sqrt{4\pi}\Phi_c\right)\cos\sqrt{4\pi}\Phi_{s(f)}$ and $\exp\left(\pm i4\, k_F\, x \pm i\sqrt{4\pi}\Phi_c\right)\cos\sqrt{4\pi}\Theta_{sf}$. If $K_c>1/2$ the superconducting fluctuations dominate over the $4k_F$ density-wave ones, and the opposite for $K_c<1/2$. Since the model has an insulating phase at quarter filling[16], by standard arguments[17] we expect $K_c \geq 1/4$. Hence the pairing susceptibility in channel (6) always diverges faster than for free fermions.

Revealing as it is, this weak coupling analysis is not fully satisfying as it implies an unphysically abrupt change of sign of m_s at the slightest density deviation from half-filling. A better approach near half filling may be a two-cutoff RG scheme, namely running at first the RG as if for half filling until reaching an energy scale of the order of the chemical potential shift, and only at this point dropping the Umklapp terms. Doing this we find that the doped dimerized Mott insulator turns to a metallic phase, $m_c=0$, all other masses retaining their sign. Here the dimer order parameter is zero but its correlation function decays slowly with a power-law exponent $K_c/2$. This agrees with a similar analysis by Boulat[10] and leads us to propose the phase diagram of Fig. 1 where the doped dimerized insulator transform into the doped Haldane phase by a $c=3/2$ critical line[13] which involves the spin or the flavour sector for $J<0$ and $J>0$, respectively. In addition we expect, by similar arguments, that the valence bond Mott insulator at large U/t with $J>0$ transforms upon doping to a metal phase, with $m_c=0$, $m_s\, m_f>0$ but $m_0\, m_f<0$. This phase is identified by a fixed point interaction of exactly the same form as (5) with the pairing operator corresponding to the singlet configuration (4), namely

$$\Delta^\dagger = \psi^\dagger_{R,1\uparrow}\psi^\dagger_{L,2\downarrow} + \psi^\dagger_{L,2\uparrow}\psi^\dagger_{R,1\downarrow} + \psi^\dagger_{L,1\uparrow}\psi^\dagger_{R,2\downarrow} + \psi^\dagger_{R,2\uparrow}\psi^\dagger_{L,1\downarrow}, \tag{7}$$

which is still a spin-singlet but it is now no longer invariant under the flavour SU(2). The pairing correlation function in this channel still decays with exponent $1/2K_c$, and again there are competing $4k_F$ density wave fluctuations with exponent $2K_c$. Therefore we argue that the Ising critical point at half-filling for $J>0$ and large U/t extends to a critical $c=1/2$ line away from half-filling, as in Fig. 1. This line should merge into the $c=3/2$ flavor $SU(2)_2$ critical line, out of which a $c=1$ U(1) critical line must emerge. Along this line the flavor doublet mass, m_f, changes sign. This scenario is compatible with our expectation far away from half-filling. Indeed, if we keep the ratio $J/U>0$ fixed and increase U/t we arrive at a situation where $J \gg t$. Here, whenever two electrons occupy the same site, they are forced into the singlet configuration (4). This constraint can be implemented by a projector leading to a model which was numerically analysed in Ref. [18] close to quarter filling. The numerical results are compatible with the existence of the doped valence-bond phase. Since the weak coupling phase is instead the doped Haldane chain, we conclude that there is a transition by increasing U/t at fixed $J/U>0$ whose criticality belongs to the U(1) universality class. Out of all these arguments we finally draw the qualititative phase diagram of Fig. 1.

We note the presence throughout the phase diagram (except of course at half filling) of a singular spin-singlet Cooper pairing susceptibility either in channel (6), within the doped Haldane insulator, or in channel (7), within the

doped valence-bond insulator. The latter, as discussed at the beginning, is most unexpected, emerging only for sufficiently strong repulsion U. We note that, if $0 < J \ll t$ were fixed, we still would expect at $U = 0$ singular pairing susceptibilities below an exponentially small energy scale of the order of the spin and flavour gaps. Remarkably, we find that the role of a large U is to raise this energy scale by increasing the magnitude of the gaps, which in turns implies that U effectively enhances pairing fluctuations.

Finally we consider the competition between Cooper pairing and $4k_F$ density-wave fluctuations in the doped valence bond and in the Haldane phases as we approach the Mott insulator at half filling. The insulating behavior is driven at weak coupling by $4k_F$-Umklapp terms of the form $\cos\sqrt{4\pi}\Phi_c \cos\sqrt{4\pi}\Phi_s \left(\cos\sqrt{4\pi}\Phi_f\right)\left(\cos\sqrt{4\pi}\Theta_{sf}\right)$. Since the spin and flavour sectors remain gapped away from half filling, one is tempted to conclude that $K_c \to 1$ on approaching half filling[17]. However, both Haldane and valence bond Mott insulators require a large U/t, and the above weak-coupling argument might not be correct. One may argue that the decoupling of charge from the other sectors as U/t increases may be modelled by adding an $8k_F$-Umklapp $\cos\sqrt{16\pi}\Phi_c$[6]. If alone this term would rather suggest a MIT at half filling with $K_c \to 1/4$. However it was found numerically that in the half-filled SU(4) Hubbard model the charge-2 Majorana fermions, $\xi_{R(L),c}$ and $\zeta_{R(L),c}$, remain coherent excitations even at large U, even though their energy is only slightly below the two-particle continuum, merging into the latter only for $U/t \to \infty$. This suggests that K_c tends always to 1 as the density approaches half filling, even though a larger U implies a sharper crossover from $K_c \simeq 1/4$ to $K_c = 1$. Hence we conclude that sufficiently close to the MIT the Cooper channel pairing dominates over $4k_F$ fluctuations.

We can finally return to our original motivation and discuss differences/analogies with the phase diagram of the same model suggested by the AIM and verified by DMFT in infinite dimensions for $J > 0$. At half filling we always find in 1D an insulator because of perfect nesting, generally absent in higher dimensions. Hence the MIT of ∞-D is replaced in 1D by an Ising transition between two insulators, the band-like dimerized insulator (driven by nesting) and the strong-coupling undimerized valence-bond Mott insulator. Upon doping, we still expect by increasing U/t an Ising transition from a doped dimerized insulator into a doped valence-bond insulator, the latter characterized by a singular pairing susceptibility. This is the exact analog of what was found in infinite dimensions. Even more surprising is the role of the singlet Ising sector $(\zeta_{R,sf}, \zeta_{L,sf})$ which becomes critical at the transition. As previously mentioned, the behavior of the lattice model in ∞-D is controlled near the MIT by the unstable fixed point of the AIM onto which the lattice model maps. In turn this unstable fixed point can be interpreted as the free boundary condition fixed point separating the two fixed boundary conditions just in the same Ising sector, and that is the natural generalization to a boundary problem of the Ising critical point which we uncovered in 1D. It is now clear that both the 1D and the single impurity analysis make use of the same field theoretical scheme, the non-abelian bosonization, where the Ising sector emerges naturally from embedding the flavour $SU(2)_2$ into U(1). Suggestively, this appears to be the reason why the behavior in one dimension and in infinite dimensions are so similar. At this stage we cannot say whether this similarity is a mere accident or not. It certainly does encourage the speculation that the physics of a single AIM may play a more fundamental role in the description of strongly correlated metals in any dimensions, at least at intermediate energy/temperature scales before full bulk coherence settles in.

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