One-Dimensional Multiband Correlated Conductors and Anderson Impurity Physics

Michele Fabrizio and Erio Tosatti

International School for Advanced Studies (SISSA), Via Beirut 2-4, I-34014 Trieste,Italy
International Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy

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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 the 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) has 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 sharp separation of energy scales between well preformed 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 an Anderson impurity model (AIM), where most of the spectral weight is concentrated in the high-energy subbands 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 nearby 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 model on the basis of the phase diagram of a two-orbital AIM [2]. All the predicted properties were later confirmed by full DMFT [3]. 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.

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

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

where $c^{\dagger}_{i,a\sigma}(c_{i,a\sigma})$ creates (annihilates) an electron at site i, in orbital $a = 1, 2$ with spin $\sigma = \uparrow, \downarrow$, $\hat{n}_i = \sum_{a\sigma} c^{\dagger}_{i,a\sigma}c_{i,a\sigma}$ 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 [4]. Moreover, it is also equivalent to two Hubbard chains with on-site repulsion U, coupled by a spin exchange J ($J > 0$ and $J < 0$ implying antiferro- and ferromagnetically coupled chains, respectively), and by a charge repulsion U. Indeed, in what follows we will often use the more familiar two-chain language [5,6] to classify the phase diagram. For $J = 0$, Eq. (1) describes an SU(4) Hubbard model, analyzed, e.g., in Ref. [7]. A finite J lowers the symmetry down to U(1) $\times$ SU(2) $\times$ (U(1) $\times$ Z_2), where U(1) refers to charge, SU(2) to spin, and (U(1) $\times$ Z_2) to the flavor (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 interorbital singlet with energy $-3J/4$, or two intraorbital singlets with energy $-J/4$. Therefore, $J < 0$ favors the spin triplet while $J > 0$ the interorbital singlet. Actually, $J > 0$ provides a pairing in the singlet 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 that 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 [3], this naïve expectation 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 $U = 0$ value. This surprising result had in fact been foreshadowed by the single AIM study [2] whose phase diagram displays an unstable fixed point at $J_* \simeq T_K$, 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 T_K of the AIM 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 interorbital singlet Cooper channel was fully confirmed by DMFT [3].

We turn now to study the same model in 1D. As usual, it is convenient to represent (1) within bosonization [8]. The Fermi fields around the right (R), $+k_F$, and left (L), $-k_F$, Fermi points are expressed as $\psi_{R(L),a\sigma}(x) \sim \exp\{\pm ik_F x - i\sqrt{\pi}[\Theta_{a\sigma}(x) \mp \Phi_{a\sigma}(x)]\}$, where $\Phi_{a\sigma}(x)$ and $\partial_x \Theta_{a\sigma}(x)$ are conjugate Bose fields. We introduce the linear combinations $\Phi_c = (\Phi_{1\uparrow} + \Phi_{1\downarrow} + \Phi_{2\uparrow} + \Phi_{2\downarrow})/2$, $\Phi_s = (\Phi_{1\uparrow} - \Phi_{1\downarrow} + \Phi_{2\uparrow} - \Phi_{2\downarrow})/2$, $\Phi_f = (\Phi_{1\uparrow} + \Phi_{1\downarrow} - \Phi_{2\uparrow} - \Phi_{2\downarrow})/2$, and $\Phi_{sf} = (\Phi_{1\uparrow} - \Phi_{1\downarrow} - \Phi_{2\uparrow} + \Phi_{2\downarrow})/2$, 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

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

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

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 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) flavor 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 Z_2 by a single Ising model (mass m_0), the singlet $(\zeta_{R,sf}, \zeta_{L,sf})$ [9]. 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 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 dimerized phase; see below [10].

We start from half filling, $\langle \hat{n}_i \rangle = 2$, and analyze 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[7,11], and that a small $|J| \ll U$ cannot destabilize this gapped phase [12]. 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 $J < 0$, the model effectively reduces to a spin $S = 1$ Heisenberg chain, still gapped everywhere in the spectrum but not dimerized [13]. For $J > 0$ the singlet configuration

$$\sqrt{\frac{1}{2}}[c^\dagger_{i,1\uparrow}c^\dagger_{i,2\downarrow} + c^\dagger_{i,2\uparrow}c^\dagger_{i,1\downarrow}]|0\rangle \tag{4}$$

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, dimerization must disappear for either sign of J. In fact, whereas at weak coupling and for $J = 0$ the dimerization-induced gaps in the spin and flavor sectors follow the BCS-like behavior of the charge gap, the latter continues to increase monotonically as U increases while the spin gaps reach a maximum, approximately when $U \sim 5t$, and then start dropping as t^2/U for $U \gg t$ [7,11]. This decoupling of charge from spin and orbital modes is a 1D remnant of the MIT and seems quite sharp [7]. 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. One might expect that this could occur only for 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 moreover suggests for $J < 0$ a $c = 3/2$ spin-SU(2)$_2$ critical point where the triplet mass m_s changes sign [14], 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 move away from half filling. Dropping the umklapp terms from the RG equations, the interaction flows,

for either sign of J, towards a fixed point

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

where $g_* > 0$ and

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

which is a spin singlet, flavor singlet, but space-odd pairing operator [12,15]. In the two-chain language it corresponds to a singlet d_{xy}-wave Cooper pair, odd under space inversion or chain permutation. This fixed point is the natural evolution upon doping of a Haldane chain, built with spin or flavor triplets when $J < 0$ or $J > 0$, respectively, the two 1/2-spin constituents forming singlet bonds, one to its right and the other to its left [16]. 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 $\exp(\pm i4k_F x \pm i\sqrt{4\pi}\Phi_c)\cos\sqrt{4\pi}\Phi_{s(f)}$ and $\exp(\pm i4k_F x \pm i\sqrt{4\pi}\Phi_c)\cos\sqrt{4\pi}\Theta_{sf}$. 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 [17], by standard arguments [18] 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 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. By doing this, we find that the dimerized insulator turns into a charge-density-wave metal (CDW), $m_c = 0$, 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 [11] and leads us to propose the phase diagram of Fig. 1 where the CDW phase transforms into a quasi-long-range-ordered superconducting phase, with d_{xy}-wave symmetry in the two-chain language, through a $c = 3/2$ critical line [14]. 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, in the two-chain language the 1D analog of a $d_{x^2-y^2}$-wave superconductor [10], 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 the same form as (5) with the pairing operator corresponding to the singlet configuration (4), namely

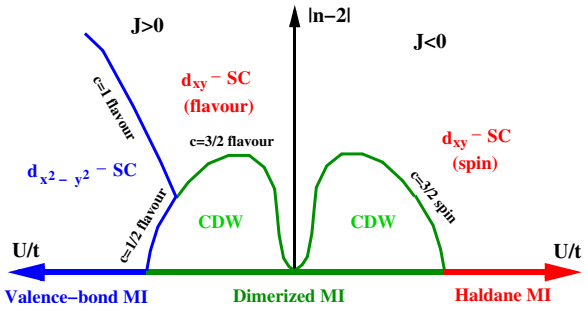

FIG. 1 (color online). Phase diagram of model (1) near half filling as a function of doping $|n-2|$ and of U/t at fixed $|J|/U \ll 1$ for $J < 0$ (right panel) and $J > 0$ (left panel). At half filling the system is always insulating and displays by increasing U/t an Ising transition from a dimerized Mott insulator (MI) to a valence-bond MI for $J > 0$ and a $c = 3/2$ transition to an $S = 1$ Haldane MI for $J < 0$ where the spin is gapless. All the insulating phases evolve upon doping into metals with gaps in all noncharge sectors, a charge-density-wave metal (CDW) and, in the two-chain language, the 1D analogues of d_{xy}-wave (d_{xy}-SC) and $d_{x^2-y^2}$-wave ($d_{x^2-y^2}$-SC) superconductors. For the d_{xy}-SC, the additional label (flavor) 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 flavor triplets. The transition lines between different metallic phases are identified by the central charge c and by the sector involved, spin or flavor.

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

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 analyzed in Ref. [19] close to quarter filling. The numerical results are compatible with the existence of the $d_{x^2-y^2}$-superconducting (SC) phase. Since the weak coupling phase is instead the d_{xy}-SC phase, we conclude that there is a U(1) transition by increasing U/t at fixed $J/U > 0$. Out of all these arguments we finally draw the overall 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 flavor 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 turn implies that increasing U effectively enhances pairing fluctuations.

Finally we consider the competition between Cooper pairing and $4k_F$ density-wave fluctuations in the SC 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 $\cos\sqrt{4\pi}\Phi_c \times \cos\sqrt{4\pi}\Phi_s(\cos\sqrt{4\pi}\Phi_f)(\cos\sqrt{4\pi}\Theta_{sf})$. Since the spin and flavor sectors remain gapped away from half filling, one is tempted to conclude that $K_c \to 1$ on approaching half filling [18]. This agrees with the numerical evidence 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 $K_c \simeq 1/4$ (the critical value for a purely-charged $8k_F$ umklapp [7]) to $K_c = 1$. Hence we conclude that sufficiently close to the MIT the Cooper pairing dominates over $4k_F$ fluctuations.

We can finally return to our original motivation and discuss differences or analogies with the phase diagram of the same model in ∞-D 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 bandlike 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 CDW to a $d_{x^2-y^2}$-SC phase with singular pairing susceptibility. This is the exact analog of what was found in ∞-D. Even more surprising is the role of the 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 just uncovered in 1D. It is now clear that both the 1D and the single impurity analyses make use of the same field theoretical scheme, the non-Abelian bosonization, where the Ising sector emerges naturally from embedding the flavor $SU(2)_2$ into U(1). In addition, it is well established that there is a link between 1D electron models with current-current interactions and impurity models [20], as well as between the latter and lattice models in ∞-D [1]. Therefore, it is not surprising, although suggestive, that the phase diagrams of (1) in one 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 or temperature scales before full bulk coherence settles in.

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