How superconductivity emerges so spectacularly out of a weakly doped Mott insulator is one of the fascinating and still controversial aspects of high Tc cuprate superconductors. A novel strongly correlated superconductivity (SCS) scenario has been recently proposed [1] which deals with an ultimately related basic issue, namely the conditions under which Cooper pairing can be enhanced, rather than depressed, by strong electron repulsion. The key of the SCS proposal is the presence of pairing interaction term J, which is weak but is not suppressed by the strong short-range repulsion U. This is realized for an attraction which involves mainly spin and orbital degrees of freedom, which are not frozen near a Mott transition. In addition, close to the MIT, correlations slow down electron motion so that the effective quasiparticle bandwidth becomes eventually equal the quasiparticle bandwidth W qp < W, W being its uncorrelated value. In these conditions the pairing attraction can eventually equal the quasiparticle bandwidth J ∼ W qp. That drives the system to an intermediate-strong coupling superconducting regime where the maximum superconducting gap Δ ∼ J for given value of J is reached, as opposed to the much smaller uncorrelated BCS value Δ BCS ∼ W exp(−W/J).

A first theoretical realization of SCS was demonstrated in Ref. [1, 2] by a Dynamical Mean Field Theory (DMFT) solution of a twofold-orbital degenerate Hubbard model subject to a self-consistency condition. More recently a simpler AI with only twofold orbital degeneracy was shown by Wilson Numerical Renormalization Group (NRG) to display anomalous properties [3, 4], suggesting its lattice generalization as a new candidate for a SCS.

In this Letter we present a detailed DMFT analysis that confirms this expectation, exploiting the lower degeneracy for a wider and more revealing study. We consider an infinite coordination Bethe lattice and solve the AI by exact diagonalization. The model reads

\[ \hat{H} = -t \sum_{<ij>,\alpha,\sigma} c_{i,\alpha\sigma}^\dagger c_{j,\alpha\sigma} + H.c. + U/2 \sum_i n_i^2 + \hat{H}_J, \]  

(1)

where \( c_{i,\alpha\sigma}^\dagger \) creates an electron at site i in orbital \( \alpha = 1, 2 \) with spin \( \sigma = \uparrow, \downarrow \). Then, \( n_i = \sum_{\alpha,\sigma} c_{i,\alpha\sigma}^\dagger c_{i,\alpha\sigma} \) is the on-site occupation number. The on-site exchange is

\[ \hat{H}_J = -2J \sum_i (T_{i,x}^2 + T_{i,y}^2), \]  

(2)

where \( T_{i,\alpha} = 1/2 \sum_{\alpha,\beta} \sum_{\sigma} c_{i,\alpha\sigma}^\dagger (\tilde{\tau}_a)_{\alpha\beta} c_{i,\beta\sigma} \) are the pseudo-spin operators and \( \tilde{\tau}_a \) (\( a = x, y, z \)) the Pauli matrices. The electronic states of the isolated site with \( n \) electrons are labeled by total spin and pseudo-spin, S and T and their z-components, and have energies

\[ \varepsilon_{i,\alpha\sigma} = E_i - \frac{\Delta}{2} \sum_\alpha \varepsilon_{i,\alpha\sigma} - \frac{U}{2} n_i^2. \]
$E(n,S,S_z,T,T_z) = U n^2/2 - 2J[T(T+1) - T_z^2]$. For $n = 2$ the configurations allowed by Pauli principle are a spin triplet orbital singlet ($S = 1$ and $T = 0$) and a spin singlet orbital triplet ($S = 0$ and $T = 1$), split by $H_J$. If $J < 0$, standard Hund’s rules, the spin triplet has the lowest energy. Here we consider the less common case of $J > 0$, where the lowest energy configuration has $S = 0$, $T = 1$ and $T_z = 0$. This inversion of Hund’s rules may for instance mimic a dynamical $e \otimes E$ Jahn-Teller effect\[1,2]. Here it just represents a generic mechanism for on-site spin-singlet pairing. Indeed, for $U = 0$ and $J \ll W$, the ground state of (1) is an s-wave BCS superconductor with pairs condensed in the $S = 0$, $T = 1$ and $T_z = 0$ channel. The energy gap is $\Delta \sim W \exp(-1/\lambda)$, where $\lambda = 2JN_F$ is the dimensionless superconducting coupling, and $N_F$ the density of states (DOS) at the Fermi energy per spin and orbital. In this regime, a finite $U < W$ introduces a “Coulomb” pseudopotential $\mu_s = U N_F$ that opposes superconductivity, eventually suppressed for $U > 2J$ in favor of a normal metal ground state. For larger $U \geq U_c \sim W$, the model undergoes a MIT for all integer fillings $\langle n \rangle = 1,2,3$. We could generally expect the superconducting gap to decrease monotonically as a function of $U$, the superconductor either turning directly into a Mott insulator (for $\lambda \sim 1$), or (when $\lambda \ll 1$) first into a metal, and then into the insulator. This is indeed what we find for $\langle n \rangle = 1$ (equivalent to $\langle n \rangle = 3$ by particle-hole symmetry) and $\lambda$ ranging from 0.1 to 0.6. The picture is however richer in the half-filled $\langle n \rangle = 2$ case, as reported in Fig. 1 where the standard superconductor evolves continuously to the SCS regime if $\lambda$ is large (e.g., $J/W = 0.15$), $\Delta$ decreases with increasing $U$, as a new MIT is realized for $U \gg U_c$, until a weakly first order transition to our local-RVB insulator occurs\[3,4]. For smaller $\lambda$ however, the dependence of $\Delta$ on $U$ is non-monotonic, and the initial drop for small $U$ is followed by a rise. Finally, for the smallest values of $\lambda$, the weak-$U$ superconductor first turns into a metal but, just before the MIT, reverts back to a superconductor, as in SCS of Ref. 1. Here too the superconducting gap reaches values much larger than those attained for the same pairing attraction $\lambda$ but for $U = 0$ (compare the inset and the right-hand side of Fig. 1).

The appearance of SCS in (1) for $\langle n \rangle = 2$ supports the AI analysis\[3]. Indeed, as $U$ increases, the quasiparticle bandwidth, which is the AI effective Kondo temperature $T_K$, is gradually suppressed by the dropping quasiparticle residue $Z \ll 1$, $T_K \sim Z W$. At the same time, we expect $J$ to remain unrenormalized\[1,4]. $H_J$ splits multiplets with same $n$, and that can happen without opposing $U$, which just freezes charge fluctuations regardless of either spin or orbital degrees of freedom. As $Z$ decreases, the AI enters the critical region around its unstable fixed-point\[5,6] at a critical $T_K^{(c)} \sim J$. For $T_K > T_K^{(c)}$, the AI is in the Kondo screened regime, while for $T_K < T_K^{(c)}$, an intra-impurity singlet forms thanks to the inverted exchange $J$. At the fixed point the two effects balance exactly, leading to a residual entropy $\ln 2$. The remaining impurity degrees of freedom are quenched at a larger temperature $T_+ \sim \max(T_K, J)$. $T_- \sim |T_K - T_K^{(c)}|^2/T_K^{(c)}$ measures the deviation from the fixed point behavior. It was argued in Ref. 2 that DMFT self-consistency should turn this AI instability into a true bulk one, most likely implying superconductivity. This is now confirmed by our DMFT analysis. S-wave superconductivity opens up a new screening route which freezes the residual entropy, otherwise quenched only below $T_-$. This suggests that (a) the energy scale which controls superconductivity should be related to $T_+ - T_-$. (b) the onset of superconductivity should be accompanied by a kinetic energy gain at low frequency, as Kondo screening implies. A kinetic energy (or, more accurately, band energy) gain may be regarded as a signal of SCS (as opposed to BCS where kinetic energy rises), and that is reflected by the behavior of the Drude weight. In Fig. 2 we show for $J = 0.05$ $W$ the Drude weight of the stable superconducting solution for $0.7 \leq U/W \leq U_c$ (here the Drude weight is the strength of the superfluid peak), in comparison with that of the unstable metallic solution (obtained disallowing superconductivity), taken to represent the normal phase. Fig. 2 shows a large increase of Drude weight with superconductivity, an occurrence also predicted\[14,15] and actually observed in cuprates\[16]. Here the unstable metal Drude weight actually appears to vanish at $U_0 < U_c$. As we shall show, this reflects the opening of a pseudogap at the chemical potential before the MIT.

Additional physical insight is gained by analyzing the DOS in the strongly correlated region $U/W > 0.7$. FIG. 1: Superconducting gap for $\langle n \rangle = 2$ as a function of Hubbard repulsion for fixed coupling $J = \lambda/(2N_F)$. Increasing repulsion spoils superconductivity at large coupling. At weak coupling superconductivity is instead strongly enhanced close to the Mott transition. The inset shows the weak coupling regime on an expanded scale, showing a much smaller gap at small $U$ compared with SCS at large $U$.
FIG. 2: Drude weight as function of $U$ at $J = 0.05W$. SCS points: lowest energy superconducting solution; unstable metal points: metastable solution with superconducting order parameter forced equal to zero. Note the very large Drude weight increase in the SCS pocket (magnified in the inset).

Within DMFT, the DOS in this region of parameters displays three features: Two high-energy Hubbard bands and a low-energy feature associated to quasiparticles. Fig. 3 displays the evolution of the DOS of the normal state solution in this regime, and shows that a pseudogap opens within the low-energy peak. A similar pseudogap appeared also in the NRG solution of the AI of Ref. [7], where it was argued that the low-energy DOS around the unstable fixed point is well described by

$$
\rho(\omega) = \frac{\rho_0}{2} \left( \frac{T_+^2}{\omega^2 + T_+^2} \mp \frac{T_-^2}{\omega^2 + T_-^2} \right),
$$

where $\rho_0$ is the non-interacting DOS, and plus/minus refers to the Kondo screened/unscreened phase. We find that (3) fits well also the low-frequency behavior of the DMFT results [8]. Eq. (3) implies that at the chemical potential $\rho(0) = \rho_0$ in the Kondo screened regime, compatible with a Fermi-liquid with $\text{Im} \Sigma(\omega) \sim \omega^2$. On the contrary, the DOS values at $T_- = 0$, $\rho(0) = \rho_0/2$, and in the pseudogap phase, $\rho(0) = 0$, imply a singular behavior of the self-energy, i.e., a non-Fermi liquid. The best-fit values of $T^+$ and $T^-$ for $J = 0.05 W$ are shown in Fig. 4 and compared with the superconducting gap $\Delta$. The maximum of $\Delta$ almost coincides with the vanishing of $T_-$, which corresponds to the AI unstable fixed point. Fig. 4 suggests a scenario which shares similarities to the quantum critical point [9] and the gauge theory-slave boson [10] pictures of cuprates. For temperatures $T$ above $T_\ast$ (presumably of order $\Delta$), but below $T_-$, the normal phase is a Fermi-liquid for $U < U_\ast$, and a non Fermi-liquid pseudogap phase for $U_\ast > U > U_c$. For $T_- < T < T_\ast$, both the narrow Fermi-liquid quasiparticle peak and the pseudogap should be washed out, leaving a broader resonance reflecting the properties of the non Fermi-liquid AI unstable fixed point. The resonance will eventually disappear above $T_\ast$. Close to the MIT, the unstable metallic solution and the stable superconductor have almost the same energy and very similar DOS, but for the presence of a very small superconducting gap. From this point of view, the pseudogapped unstable phase plays a role similar to the staggered flux phase within the SU(2) invariant slave-boson description of the $t$-$J$ model, and may therefore be thought as a phase with broken symmetry in the particle-hole or in the particle-particle channels, where the full symmetry is restored by fluctuations [11]. We note here that (a) superconductivity is not an accidental route which the lattice system takes to rid itself of competition among other phases, but is one of the pre-determined instabilities of the AI; (b) attempts to uncover the fixed point by suppressing superconductivity would likely spoil the fixed point or unveil other instabilities of the lattice model.

The analogy with high $T_c$ cuprates becomes even more

FIG. 4: Behavior of the relevant energy scales (defined in the text) close to the MIT for $J/W = 0.05$ as function of $U/W$. 
suggestive when we analyze the phase diagram away from half-filling, and follow the fate of superconductivity upon doping. SCS extends (Fig. 5) into a superconducting pocket away from \( n = 2 \) at \( J = 0.05 \) W. The think vertical line marks the singlet Mott insulator. The inset shows, for \( U = 0.92 \) W, the superconducting gap \( \Delta \) divided by a factor \( 10^{-3} \) and Drude weight \( D \) (normalized to the non-interacting value) as functions of doping \( \delta \).

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\[ \text{FIG. 5: Phase diagram as function of } U/W \text{ and doping } \delta = n - 2 \text{ at } J = 0.05 \text{ W. The think vertical line marks the singlet Mott insulator. The inset shows, for } U = 0.92 \text{ W, the superconducting gap } \Delta \text{ divided by a factor } 10^{-3} \text{ and Drude weight } D \text{ (normalized to the non-interacting value) as functions of doping } \delta. \]

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