Strongly correlated superconductivity: hints from the Kondo physics

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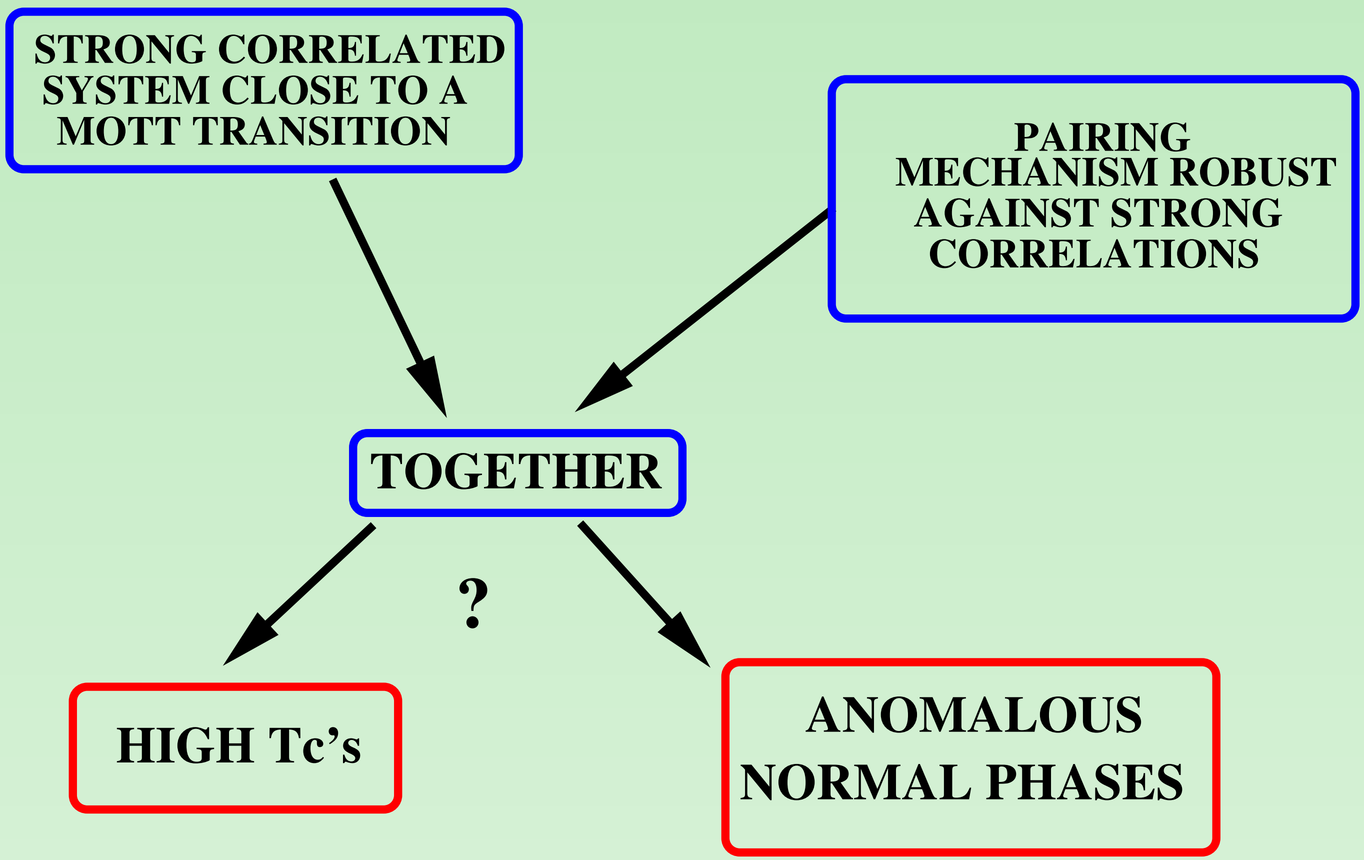
Refs. : M. Capone, M. Fabrizio, C. Castellani and E. Tosatti, Science **296**, 2364 (2002); Phys. Rev. Lett. **93**, 047001 (2004).
L. De Leo and M. Fabrizio, Phys. Rev. Lett. **94**, 236401 (2005).

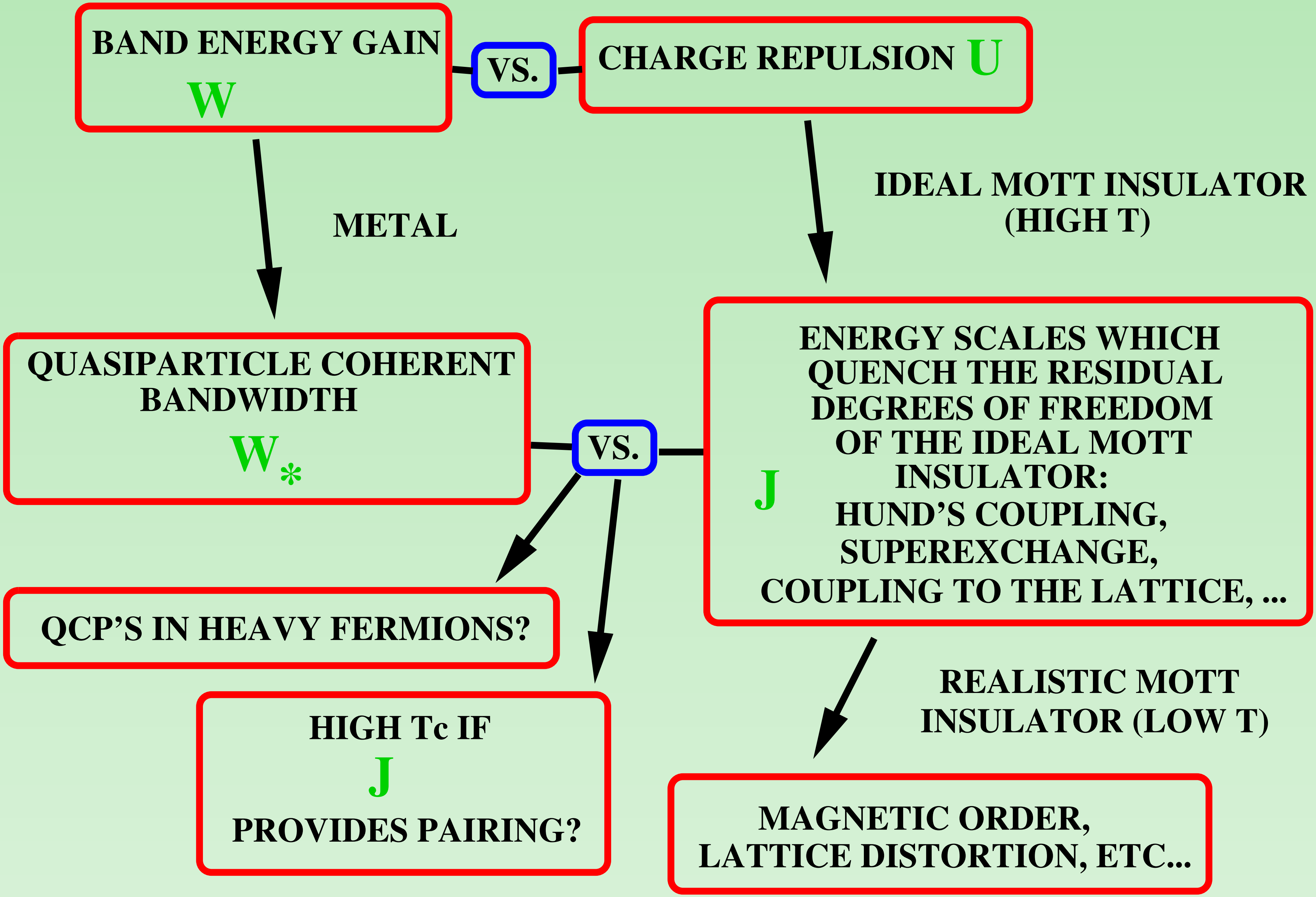
Motivation

Consider a strongly correlated system near a Mott transition. Assume that a pairing mechanism exists and it is robust against strong correlations.

What can emerge out of the interplay between these two ingredients?

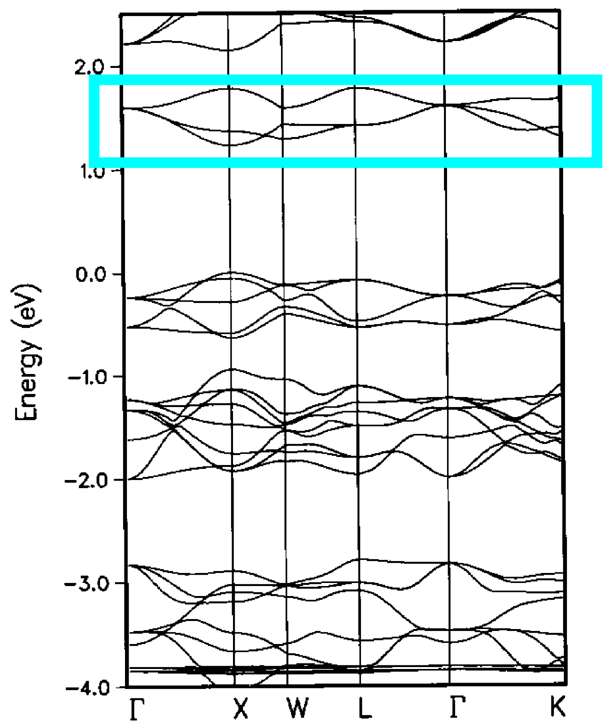


Relevant energy scales near a Mott transition



Modelling alkali doped fullerenes M_nC_{60}

BANDWIDTH $W \simeq 0.6$ eV



Doped electrons fill three narrow bands formed by the t_{1u} LUMO's of C_{60}

like atomic p-orbitals

$$c_{R\,p\sigma}, \qquad p = x, y, z, \qquad \sigma = \uparrow, \downarrow$$

$$\mathcal{H}_0 = \sum_{k\sigma} \sum_{p=x,y,z} \epsilon_p(k)\, c^\dagger_{k\,p\sigma} c_{k\,p\sigma}$$

Pairing mediated by local molecular vibrations of H_g symmetry Jahn-Teller coupled to the three orbitals

$$\boldsymbol{\mathcal{H}_{el-ph} = \sum_R \sum_{i=1}^{5} \frac{\hbar\omega_0}{2}\left(x_{R\,i}^2 + p_{R\,i}^2\right) + g\, x_{R\,i}\, c^\dagger_{R\,p\sigma}\, \mathcal{W}^{(i)}_{pq} c_{R\,q\sigma}}$$

$$\mathcal{W}^{(i)} \sim \quad (L_x\,L_y + L_y\,L_x)\,,(L_y\,L_z + L_z\,L_y)\,,(L_z\,L_x + L_x\,L_z)\,,\ \left(L_x^2 - L_y^2\right),3L_z^2 - L^2$$

Typical values: $\hbar\omega_0 \simeq \mathbf{0.13}$ **eV and** $g = \mathbf{0.05}$ **to 0.09 eV,**
$g^2/\hbar\omega_0 \simeq \mathbf{0.019}$ **to 0.057 eV**

Unretarded vibron-mediated electron-electron interaction (underestimates superconductivity)

$$\boldsymbol{\mathcal{H}^{ph}_{int} = 3\frac{g^2}{\hbar\omega_0}\sum_R \left(2\vec{S}_R\cdot\vec{S}_R + \frac{1}{2}\vec{L}_R\cdot\vec{L}_R\right) + \frac{5}{6}\left(n_R - 3\right)^2}$$

Pairing occurs in the $S = L = 0$ Cooper channel

$$\mathbf{\Delta_k} = \sum_{\mathbf{p=x,y,z}} \mathbf{c}^{\dagger}_{\mathbf{k\,p}\uparrow}\mathbf{c}_{-\mathbf{k\,p}\downarrow} + \mathbf{c}^{\dagger}_{-\mathbf{k\,p}\uparrow}\mathbf{c}_{\mathbf{k\,p}\downarrow}$$

with pairing amplitude

$$\boldsymbol{\mathcal{A}} = \mathbf{10}\frac{\boldsymbol{g}^2}{\hbar\boldsymbol{\omega}_0}, \qquad \boldsymbol{\lambda} = \boldsymbol{\rho}_0\,\boldsymbol{\mathcal{A}} \simeq \mathbf{0.38} \text{ to } \mathbf{1.06}$$

Jahn-Teller coupling is expected to be robust against strong correlations as it splits multiplets at fixed charge without moving the center of gravity

On-site Coulomb repulsion

$$\mathcal{H}_{rep} = \frac{U}{2}\sum_{R} n_R^2 - J_H \sum_{R}\left(2\vec{S}_R\cdot\vec{S}_R + \frac{1}{2}\vec{L}_R\cdot\vec{L}_R\right)$$

$$U \simeq \text{1.5 to 2.5 W}, \qquad J_H \simeq 0.05\ \text{eV}$$

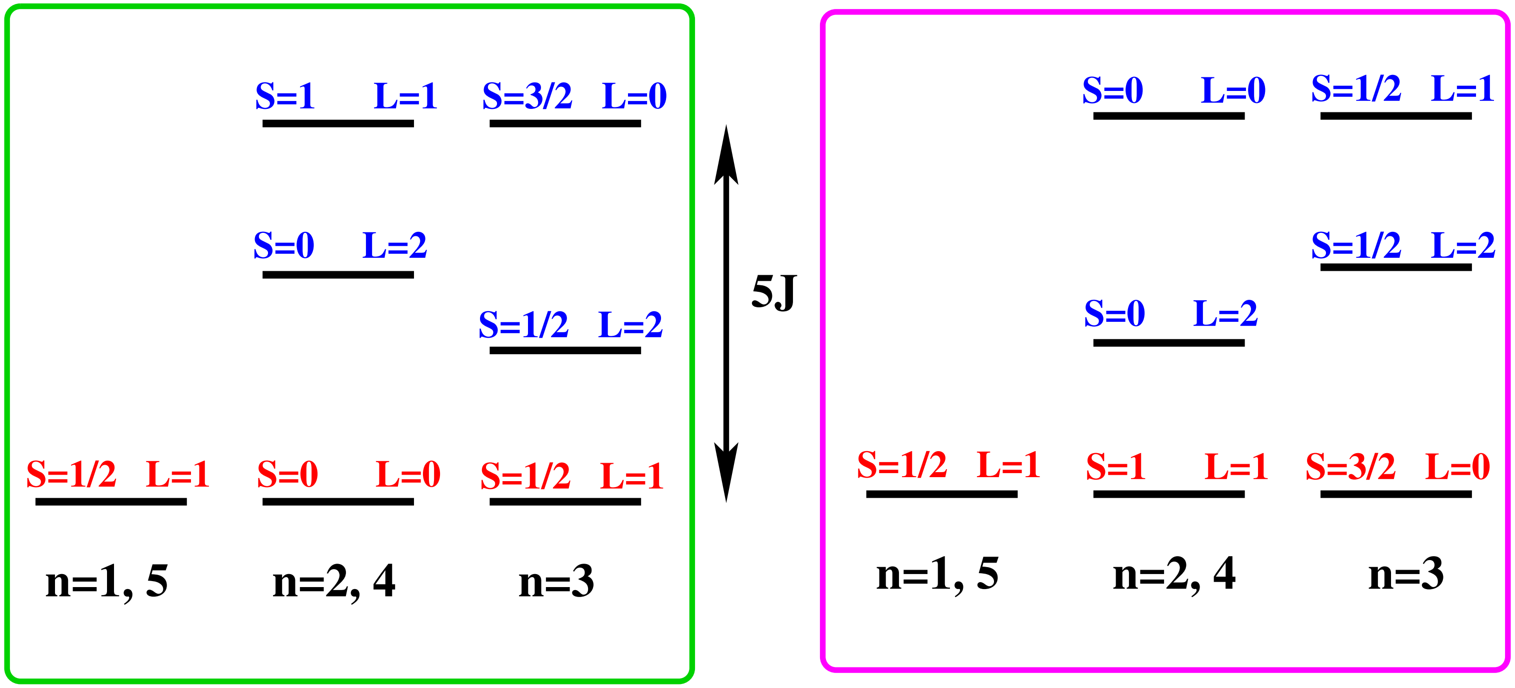
The Hund's coupling plus the Jahn-Teller one lead to the electron-electron interaction

$$\mathcal{H}_{int} = \frac{U}{2}\sum_{R} n_R^2 + J \sum_{R}\left(2\vec{S}_R\cdot\vec{S}_R + \frac{1}{2}\vec{L}_R\cdot\vec{L}_R\right)$$

with an **inverted Hund's coupling**

$$J = 3\,\frac{g^2}{\omega_0} - J_H > 0$$

Molecular levels



inverted Hund's rules conventional Hund's rules

The inverted Hund's rules act as an on-site valence-bond pairing mechanism: molecular spin-gap $\Delta E(\Delta S = 1) = 5J$. Experimentally the spin gap $\Delta E \simeq 0.07$ to 0.1 eV, pointing to a $J \simeq 0.02$ eV

Mean Field expectation on superconductivity

BCS coupling:

$$\lambda = \frac{10}{3}\rho J \simeq 0.13$$

Coulomb pseudo-potential:

$$\mu_* = \rho U \simeq 1.5 \div 2.5$$

Superconductivity is not stabilized at the mean-field level since
$$\lambda < \mu_*$$

Neglect of retardation is not very harmful since $\ln\left(W/2\hbar\omega_0\right) \simeq 0.6$

How can superconductivity appear with T$_c$ as high as 40K?
Is BCS really OK for fullerenes?

The model and its DMFT analysis

$$\mathcal{H} = \sum_{\boldsymbol{k}\sigma} \sum_{p=x,y,z} \epsilon(\boldsymbol{k})\, c^{\dagger}_{\boldsymbol{k}\,p\sigma} c_{\boldsymbol{k}\,p\sigma} + \frac{U}{2} \sum_{\boldsymbol{R}} n^2_{\boldsymbol{R}} + J \sum_{\boldsymbol{R}} \left(2\vec{S}_{\boldsymbol{R}} \cdot \vec{S}_{\boldsymbol{R}} + \frac{1}{2} \vec{L}_{\boldsymbol{R}} \cdot \vec{L}_{\boldsymbol{R}} \right)$$

All relevant interactions are on-site: ideal case for DMFT

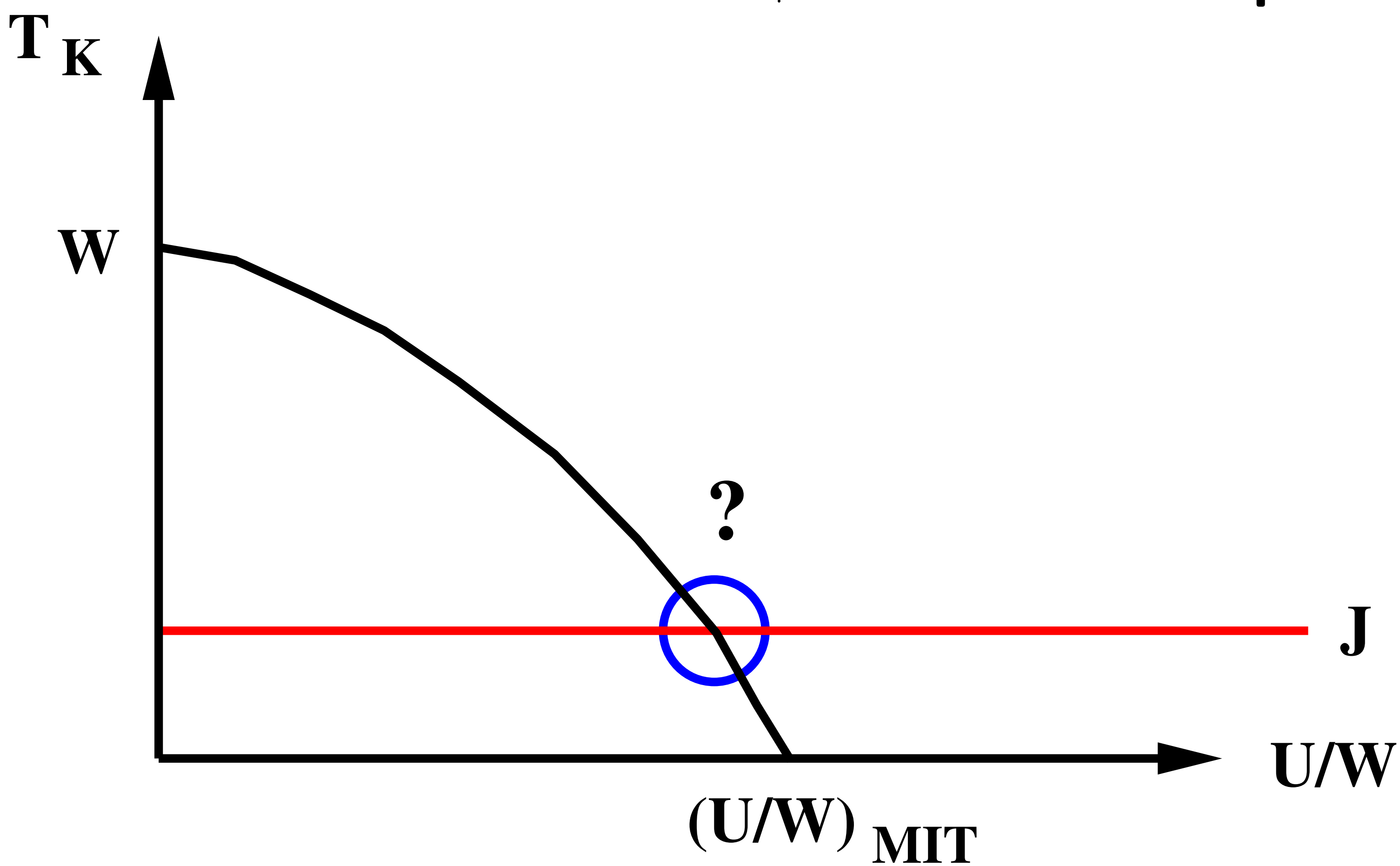
$$\mathcal{H}_{bulk} \xrightarrow{DMFT} \mathcal{H}_{AIM}$$

$$\mathcal{H}_{AIM} = \mathcal{H}_{bath} + \mathcal{H}_{hyb} + \epsilon_f\, n_f + \frac{U}{2} n_f^2 + J \left(2\boldsymbol{S}_f \cdot \boldsymbol{S}_f + \frac{1}{2} \boldsymbol{L}_f \cdot \boldsymbol{L}_f \right)$$

where $\mathcal{H}_{bath}$ and $\mathcal{H}_{hyb}$ have to be determined self-consistently.

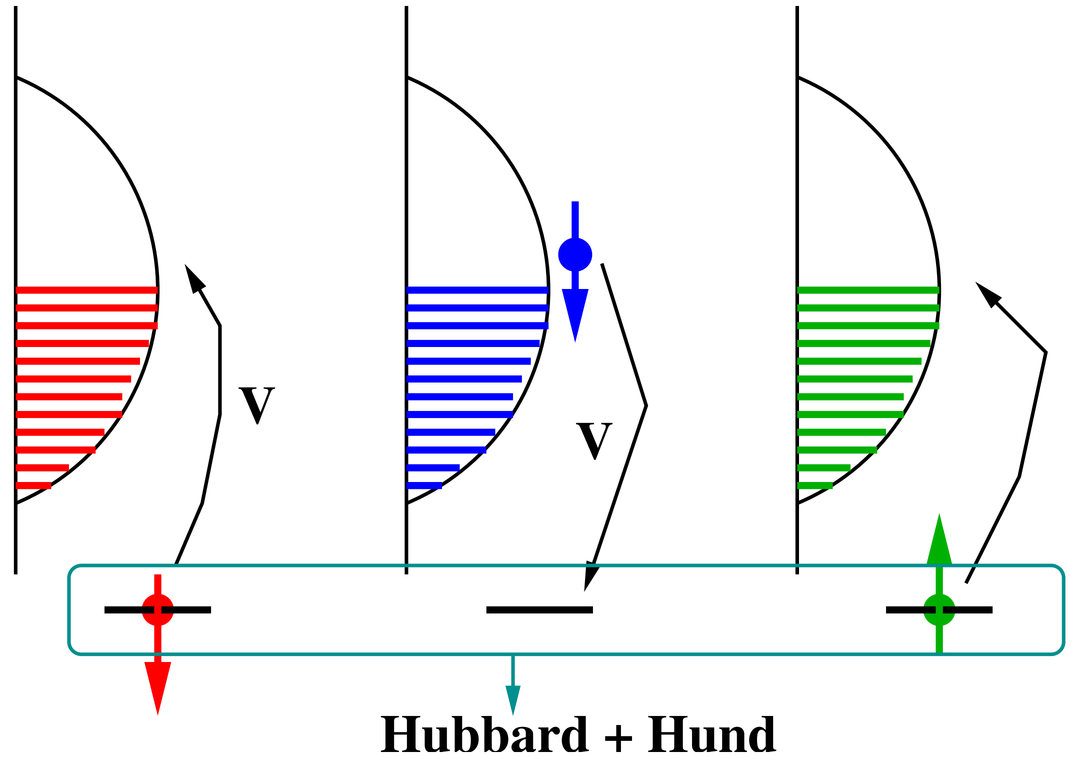
How the Mott transition translates in the AIM?

Quasiparticle coherent bandwidth W_* $\longrightarrow$ Kondo temperature T_K



J is an alternative screening mechanism competing with the conventional Kondo screening. What happens when $T_K \simeq J$?

The single impurity without self-consistency by NRG and CFT



$$\mathcal{H}_{AIM} = \sum_{k\sigma} \sum_{p=x,y,z} \epsilon_k \, c^\dagger_{k\,p\sigma} c_{k\,p\sigma} + \sum_{k\sigma} \sum_{p=x,y,z} V_k \, c^\dagger_{k\,p\sigma} f_{p\sigma} + H.c.$$

$$+\epsilon_f \, n_f + \frac{U}{2} n_f^2 + J \left(2\vec{S}_f \cdot \vec{S}_f + \frac{1}{2} \vec{L}_f \cdot \vec{L}_f \right)$$

CFT description

- CFT embedding:

$$\boldsymbol{SU(6)_1 \longrightarrow U(1)^{charge} \times SU(2)_3^{spin} \times SU(2)_8^{orbit} \times Z_3}$$

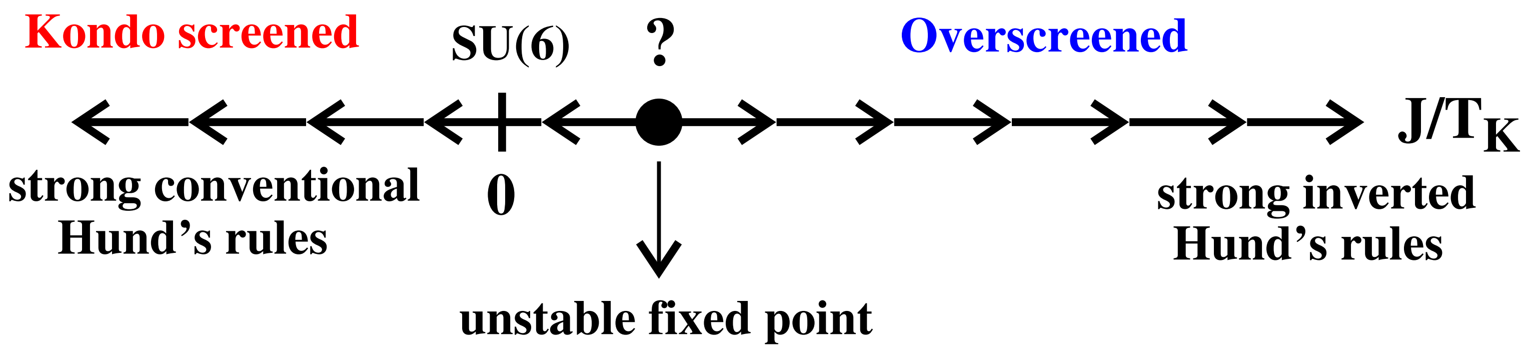
The 3-state Potts sector $\mathbf{Z_3}$ can be viewed as

$$\boldsymbol{SU(2)_3^{charge} \longrightarrow U(1)^{charge} \times Z_3}$$

The generators of the charge isospin are

$$\boldsymbol{I_z = \frac{1}{2}(n-3)\,, \quad I^+ = c^\dagger_{x\uparrow}\ c^\dagger_{x\downarrow} + c^\dagger_{y\uparrow}\ c^\dagger_{y\downarrow} + c^\dagger_{z\uparrow}\ c^\dagger_{z\downarrow}, \quad I^- = \left(I^+\right)^\dagger}$$

Strong coupling analysis $U \gg J_K \gg \ldots$ at particle-hole symmetry $\langle n_f \rangle = 3$



- **Conventional Hund's rules:**

$S = 3/2$ $L = 0$ **impurity coupled to 3 channels** $\Rightarrow$ **Perfect Kondo screening**

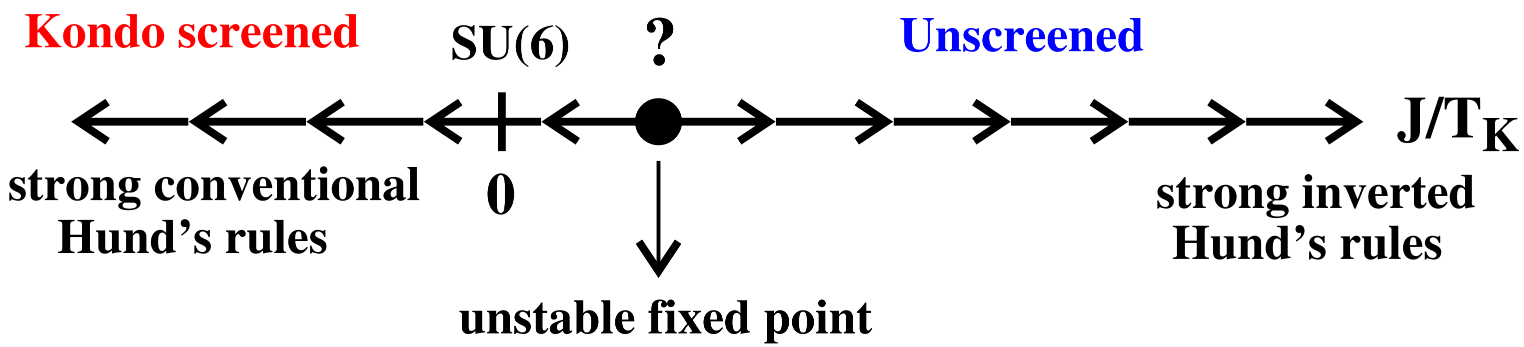
- **No Hund's rule** $J = 0$**:**

$SU(6)$ **Kondo model** $\Rightarrow$ **Perfect Kondo screening too**

- **Inverted Hund's rules:**

$S = 1/2$ $L = 1$ **impurity coupled to 3 channels** $\Rightarrow$ **Can be screened equally well by 1, 3 and 5 conduction electrons in a** $S = 1/2$ $L = 1$ **configuration** $\Rightarrow$ **Overscreened Kondo model like the three channel** $S = 1/2$**-impurity Kondo model with** $S \leftrightarrow I$**.**

Strong coupling analysis $U \gg J_K \gg \ldots$ away from particle-hole symmetry $\langle n_f \rangle = 2, 4$



• **Conventional Hund's rules:**

$\mathrm{S} = 1$ $\mathrm{L} = 1$ **impurity coupled to 3 channels** $\Rightarrow$ **Kondo screened by 4,2 electrons in the** $\mathrm{S} = 1$ $\mathrm{L} = 1$ **configuration**

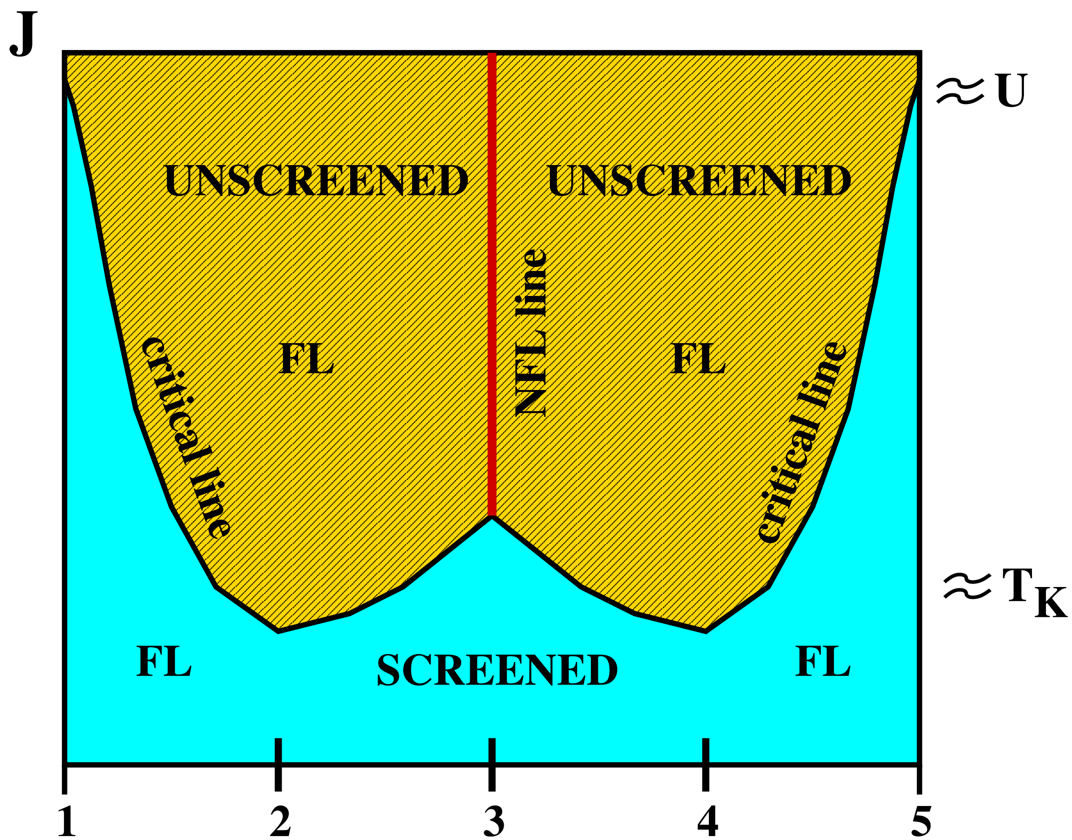
• **No Hund's rule** $\mathrm{J} = 0$**:**

$\mathrm{SU}(6)$ **Kondo model away from particle-hole symmetry** $\Rightarrow$ **Kondo screened too**

• **Inverted Hund's rules:**

$\mathrm{S} = 0$ $\mathrm{L} = 0$ **impurity** $\Rightarrow$ **Unscreened plus potential scattering**

Phase diagram



Apart from the exceptional case with perfect particle-hole symmetry, there are two Fermi liquid phases, one Kondo screened and the other unscreened, separated by a critical line with non-Fermi liquid properties

Properties of the critical line

- The most relevant instability is towards superconductivity in the $\mathbf{S} = \mathbf{L} = 0$ Cooper channel. The local pairing susceptibility

$$\chi_{SC}(T) \sim T^{-1/3}$$

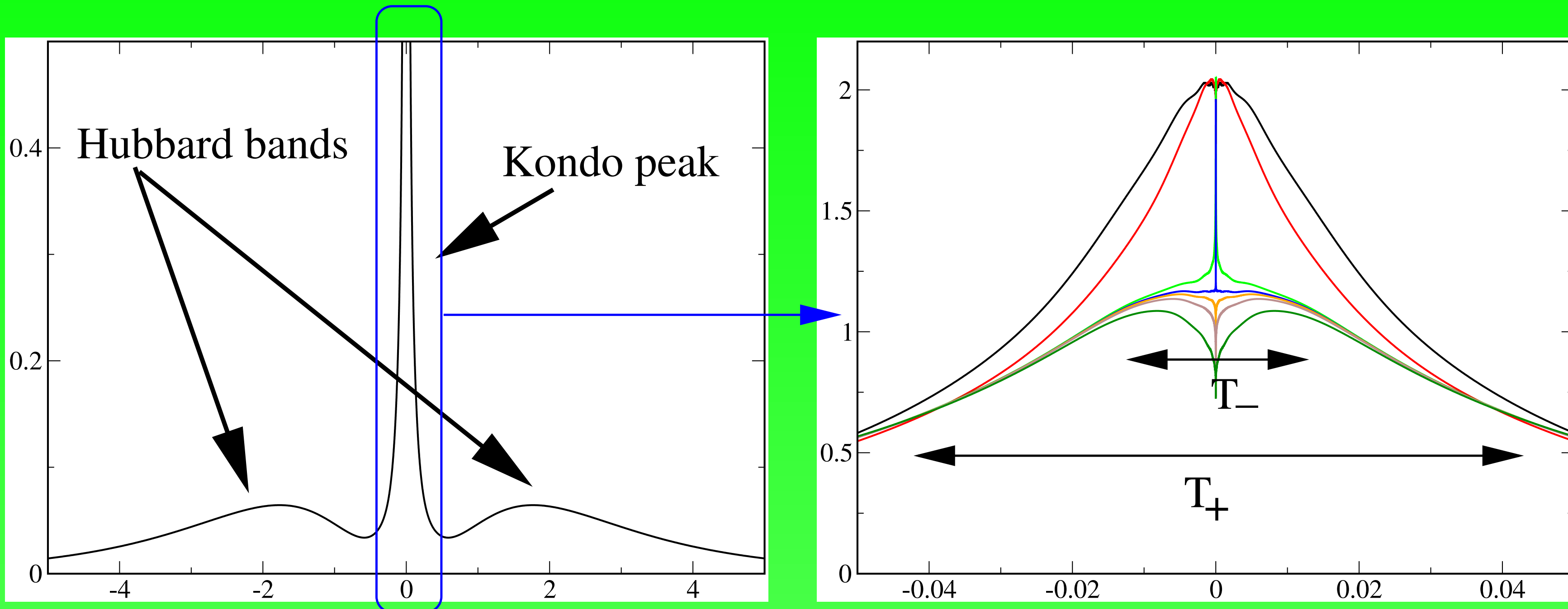
- Jahn-Teller distortion and spin/orbital splitting are less relevant.
- There is a finite residual entropy

$$S(0) = \frac{1}{2} \ln 3$$

- The deviation from the fixed point is controlled by an energy scale

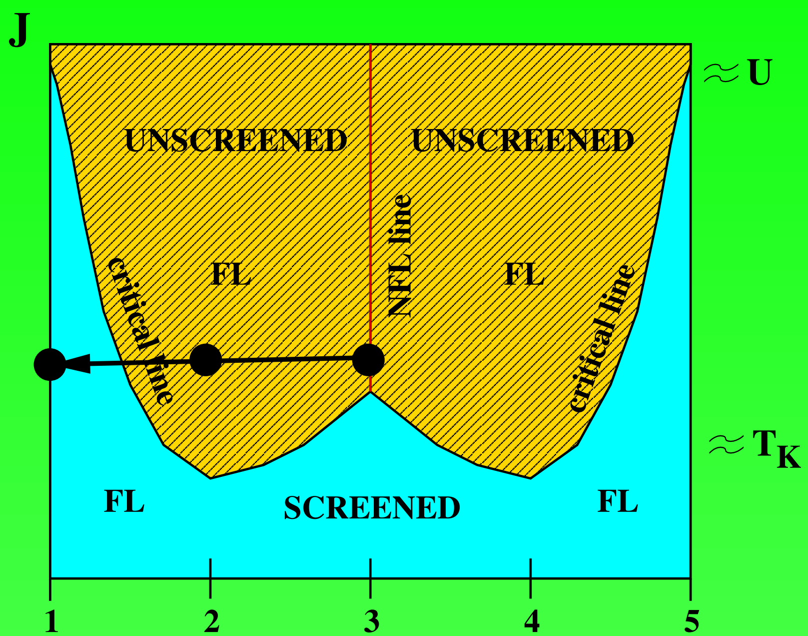
$$T_{-} \sim T_K \left| \frac{J}{T_K} - \left(\frac{J}{T_K} \right)_* \right|^3$$

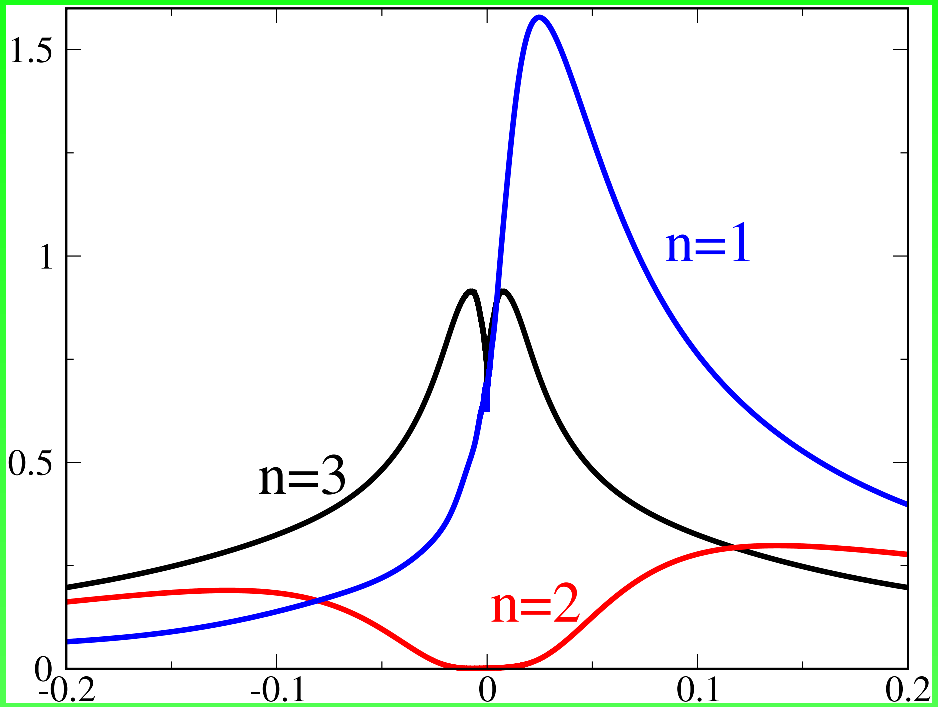
Dynamics across the critical line



The low energy dynamical behavior near the fixed point is controlled by two energy scales: T_- which measures the deviation from the fixed point J_* and $\mathrm{T}_+ \sim \mathrm{T_K} \sim \mathrm{J}_*$ which is smooth across the fixed point

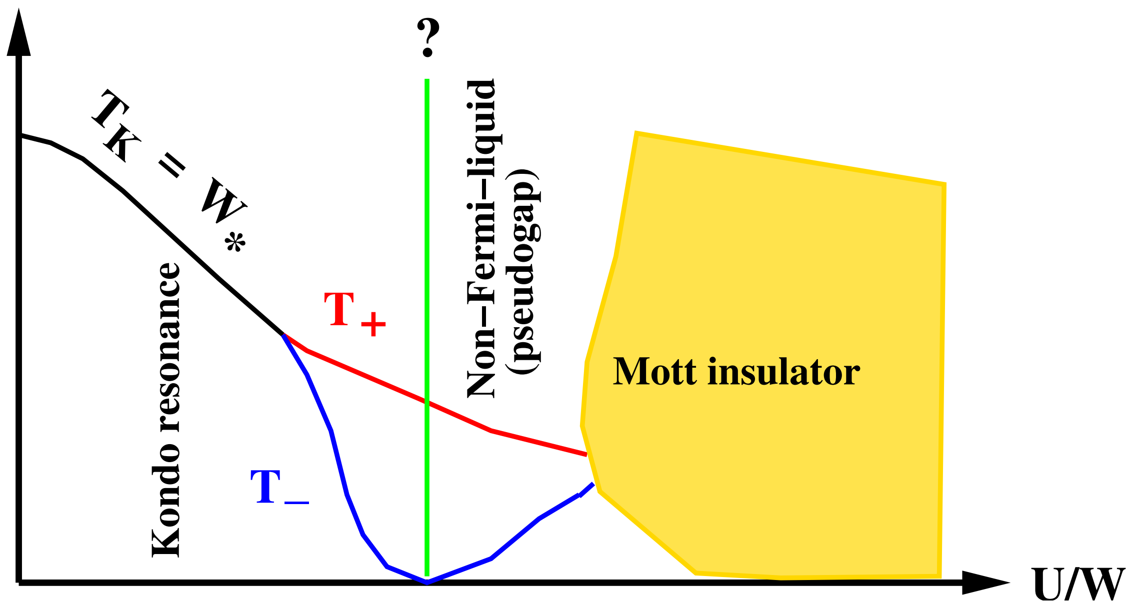
Dynamics across the critical line





The critical line can also be crossed varying the average impurity occupation

How can we translate these results in DMFT?



- The approach to the Mott transition is not controlled by a single energy scale $T_K = W_*$, but actually by two scales T_- and T_+
- If we prevent any symmetry breaking within DMFT, before the Mott transition the effective impurity model will cross its unstable fixed point $T_- = 0$. Both at this point and after it, the impurity self-energy and consequently the bulk one are non-Fermi liquid

$$\Sigma(i\omega_n) \sim i\Gamma \mathrm{sign}(\omega_n),\ \frac{\Gamma}{i\omega_n}$$

What we expect if symmetry broken phases are allowed

The most-singular local-susceptibility around the unstable fixed point is the pairing one in the $S = L = 0$ Cooper channel. The only scale controlling this singularity is $T_+ \simeq T_K \simeq J$

$$\Downarrow$$

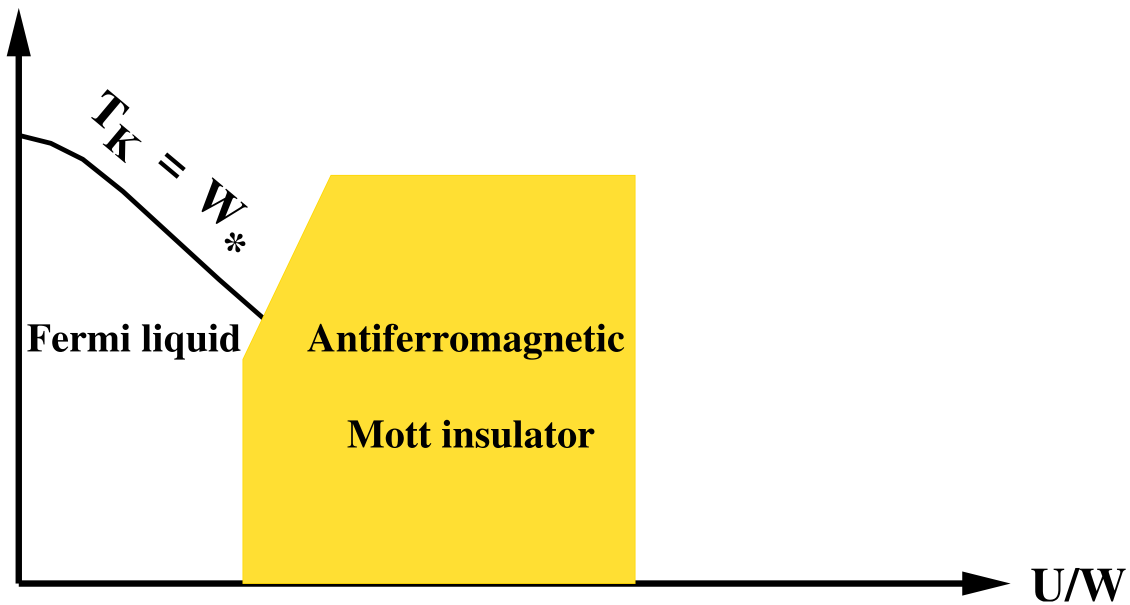
Within DMFT the irreducible scattering vertex of the bulk model in that channel is singular too on the scale $W_* \simeq J$. Since the Cooper bubble is always log-diverging

$$\Downarrow$$

A superconducting pocket might emerge around the $T_- = 0$ point with a critical temperature T_c corresponding to quasiparticles of bandwidth $W_* \sim T_+$ with a pairing amplitude J of similar strength – the maximum T_c at a given attraction

Phase diagram at half-filling?

At half-filling, $\langle n \rangle = 3$ the Cooper instability competes with other particle-hole instabilities. Since the Mott insulator is formed by local moments with $S = 1/2$ and $L = 1$, it has to magnetically and orbitally order at low-temperature. Therefore either this insulating phase hides completely the superconducting one,



Phase diagram at half-filling?

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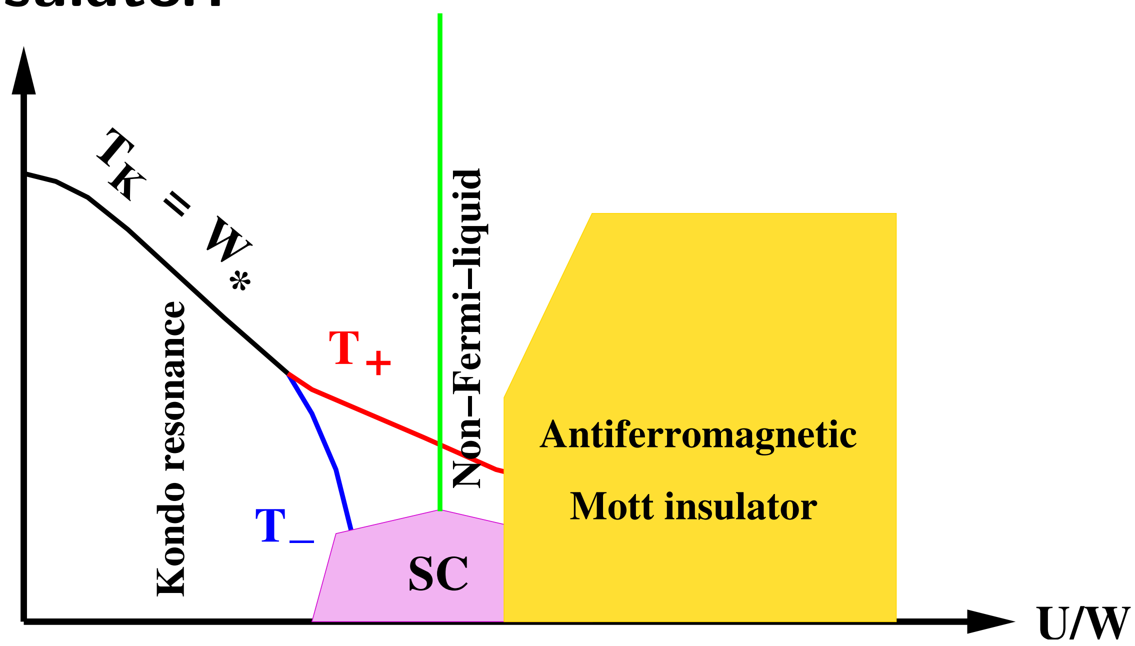
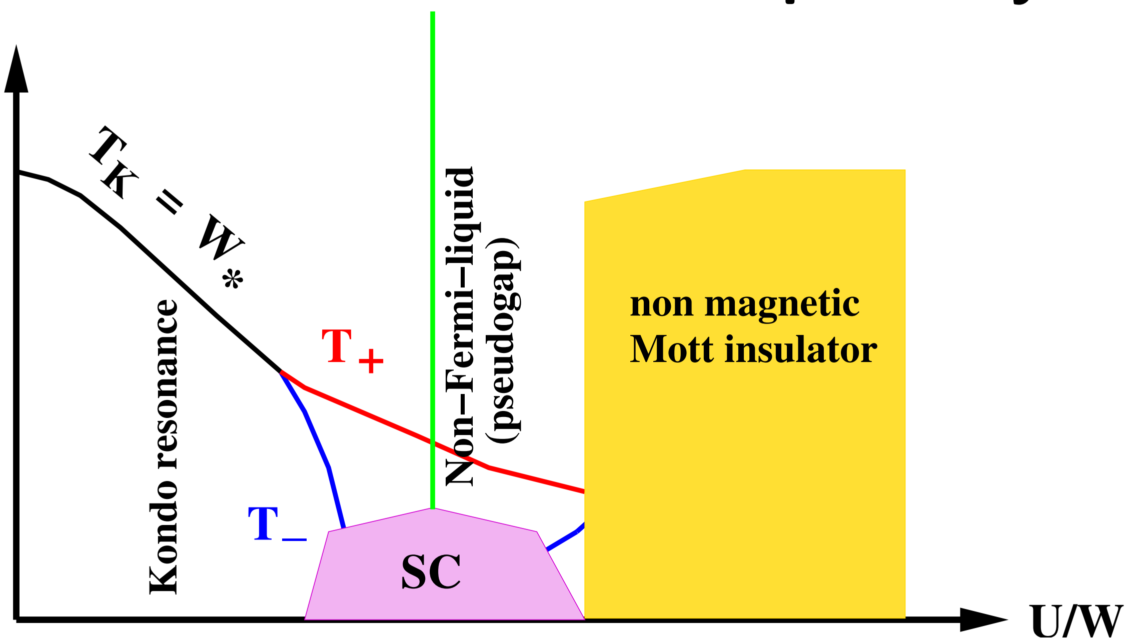


Phase diagram at $\langle n \rangle = 4, 2$?

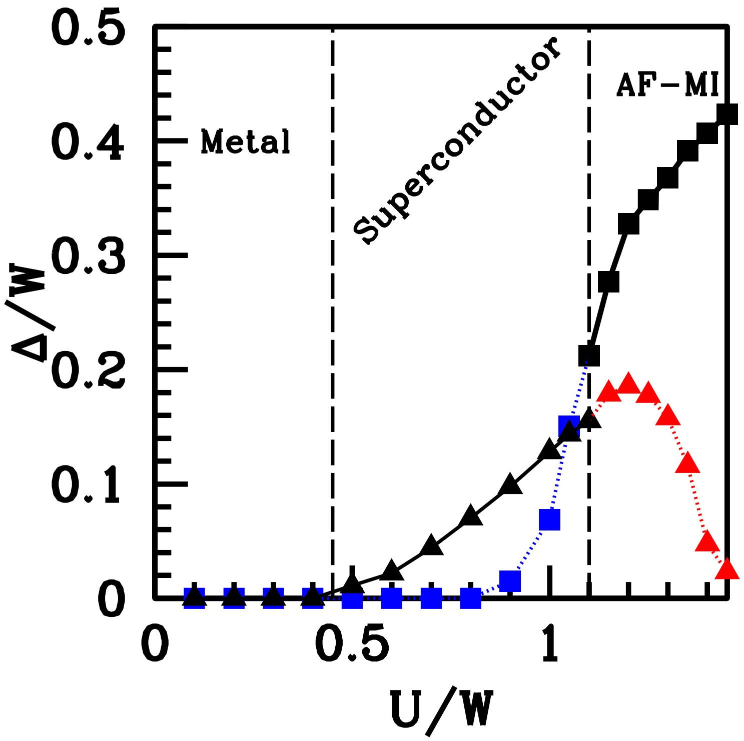
On the contrary, for $\langle n \rangle = 4, 2$, the Mott insulator is somehow a local version of a valence-bond insulator, each site being in a configuration with $S = L = 0$. In this case a continuous transition between the superconductor and the Mott insulator is perfectly allowed.



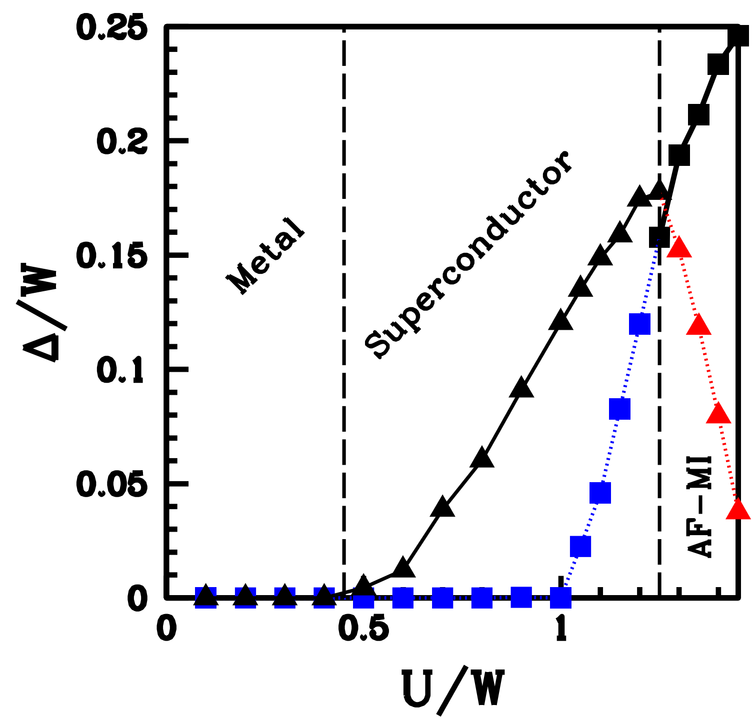
DMFT results for $\langle n \rangle = 3$

Anomalous superconducting zero-frequency self-energy vs. antiferromagnetic one for $J = 0.05W$

t' = 0

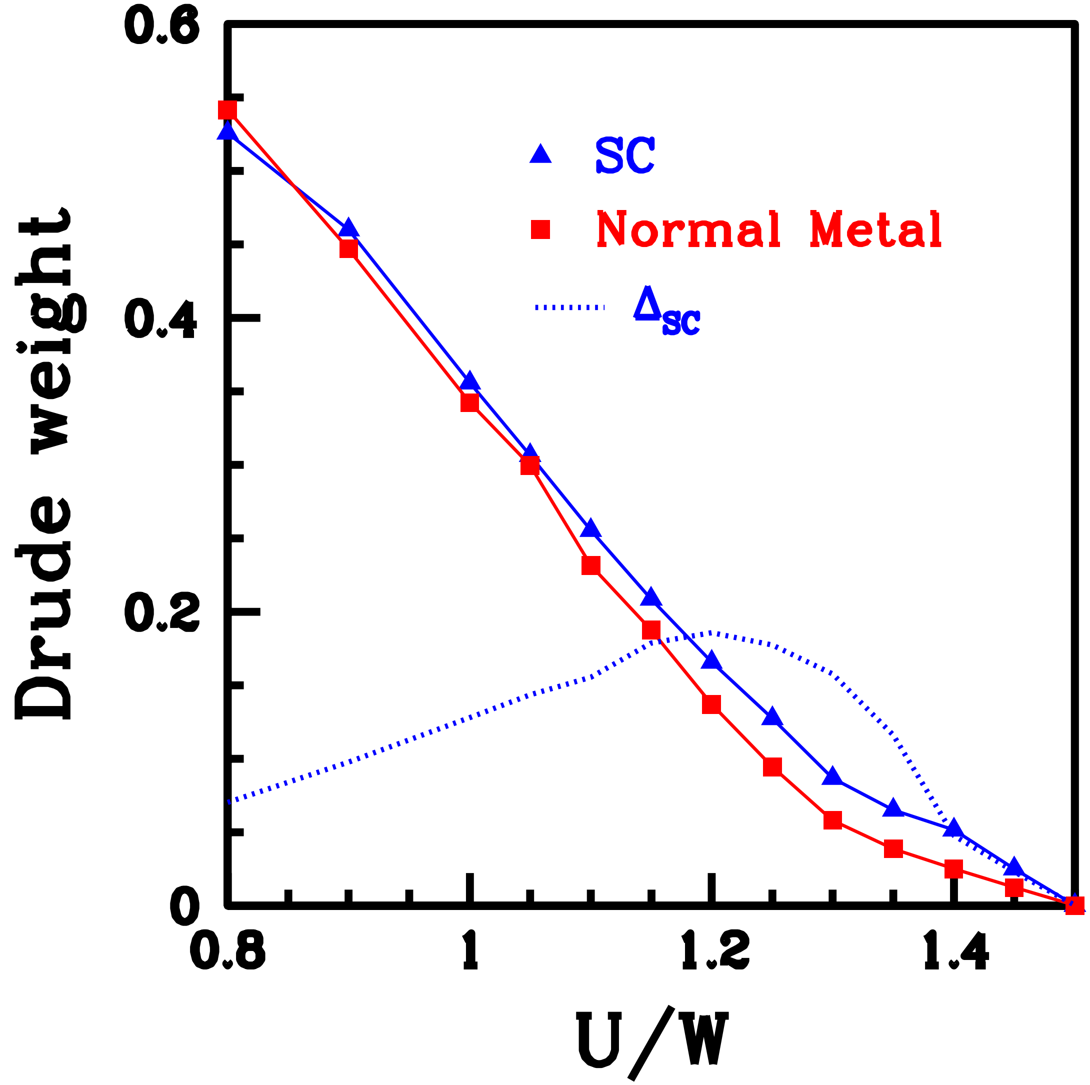


t' = 0.3



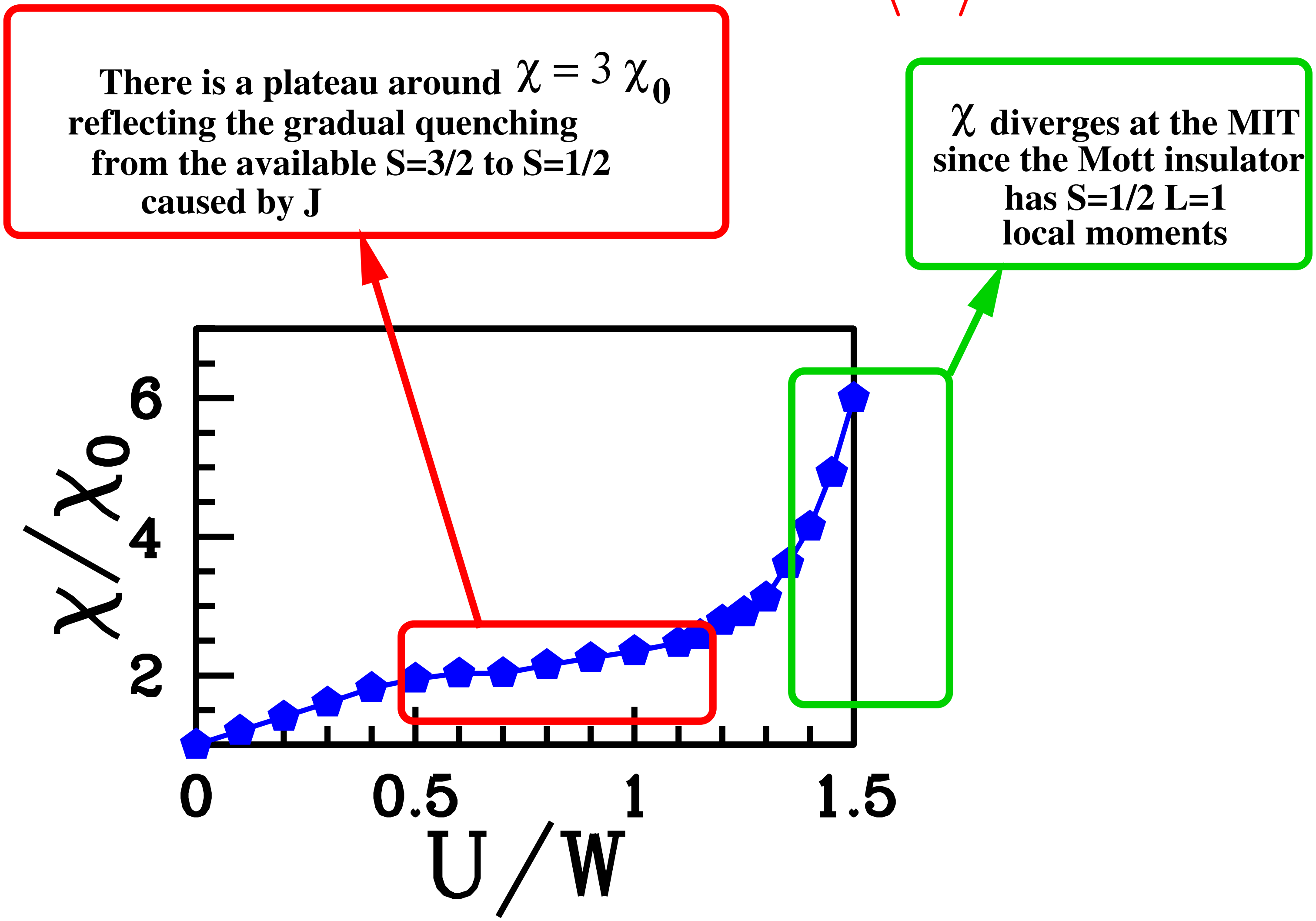
$$J = 0.05\ W \;\rightarrow\; \lambda = 0.21 \;\rightarrow\; 2\,\Delta_{BCS} = 0.0089\ W$$

DMFT results for $\langle n \rangle = 3$



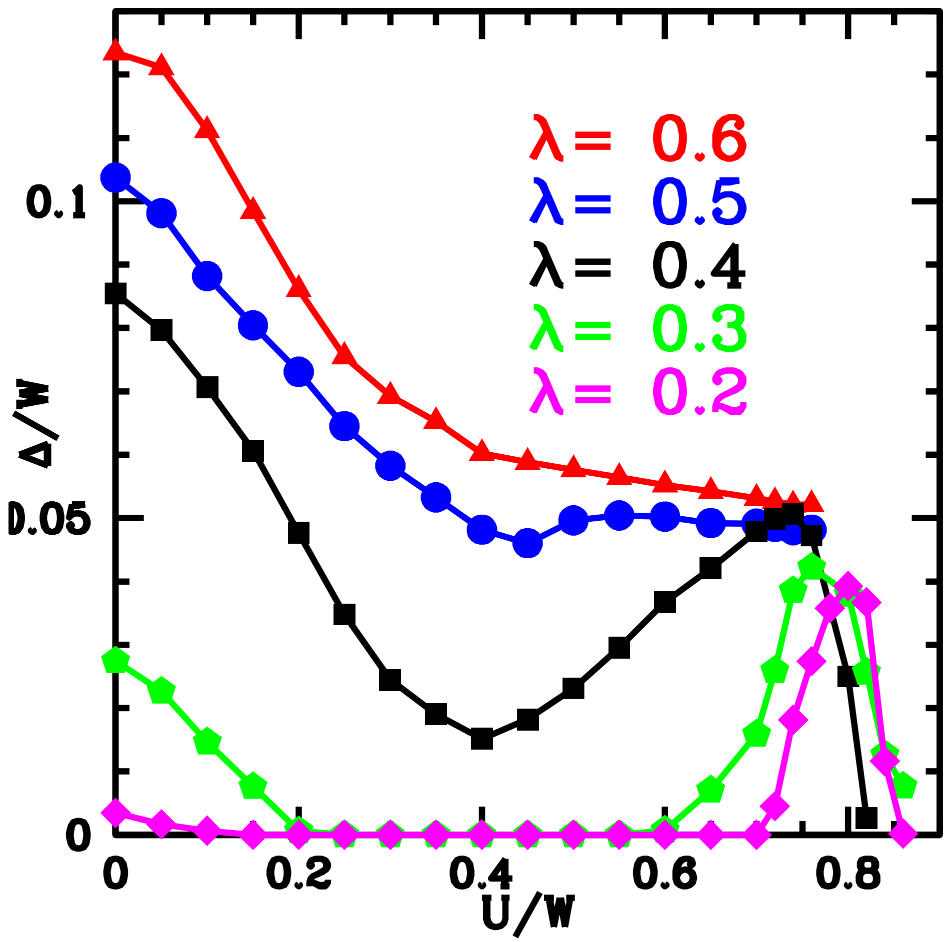
The on-set of superconductivity is accompanied by a band-energy gain!

DMFT results for $\langle n \rangle = 3$



Since the maximum of superconductivity occurs in the plateau region, one might be tempted to conclude that quasiparticles are weakly correlated, $m_* \sim 3m$. This is wrong as the energy scale of quasiparticles actually vanishes around this point and, after that, quasiparticles do not even exist.

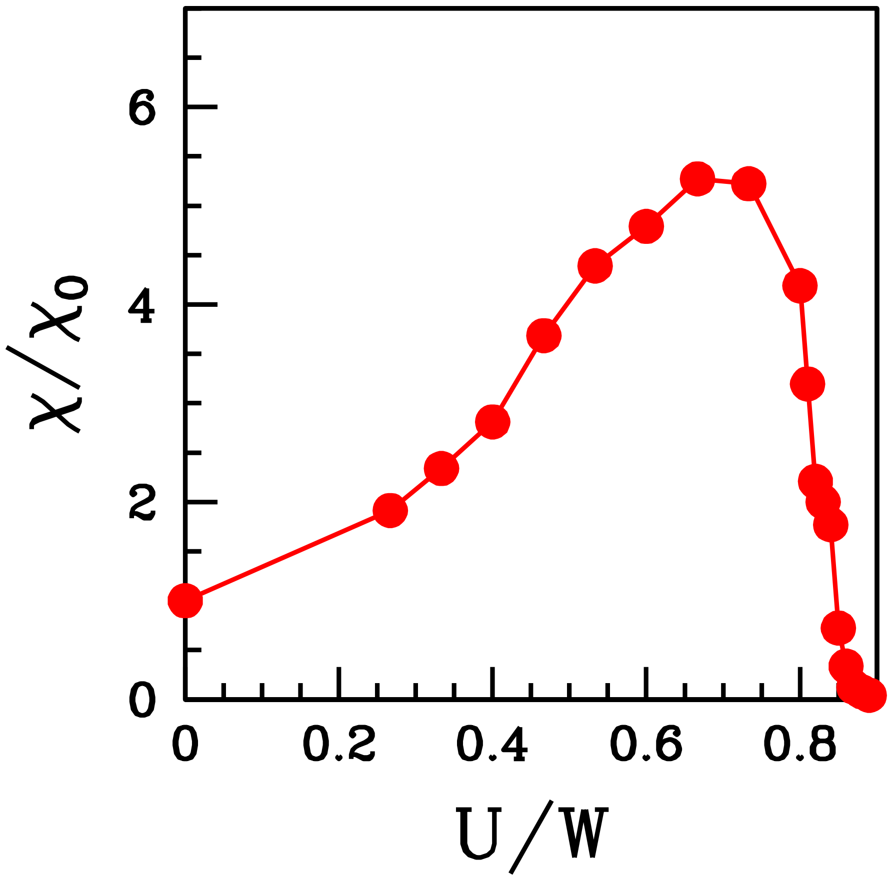
DMFT results for $\langle n \rangle = 2, 4$



For small λ's superconductivity re-emerges just before the Mott transition with a hugely amplified gap.

The transition to the Mott insulator is continuous.

DMFT results for $\langle n \rangle = 2, 4$



The Mott transition for $\langle \mathrm{n} \rangle = 2, 4$ is accompanied by the vanishing of the magnetic susceptibility. The Mott insulator is therefore non magnetic, as observed in M_4C_{60}'s.

Conclusion

- **The proximity to a Mott transition can strongly amplify a pairing mechanism able to survive in the Mott insulator**
- **This pairing can induce a superconducting region before the Mott transition with the highest T_c attainable with the "bare" pairing amplitude**
- **The normal phase in this region is non-Fermi liquid and commonly the DOS has a pseudo-gap**
- **The Mott transition is accompanied by more than a single energy scale. Hence the Brinkman-Rice picture of the Mott transition turns out to be incomplete**
- **If alkali doped fullerenes happen to be in that parameter range, it also implies that conventional BCS theory is inadequate for them**