Kondo physics and the Mott transition

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Outline of the lecture:

- **Landau-Fermi liquid theory in short**
- **ordinary Kondo physics at the Mott transition**
- **exotic Kondo physics at the Mott transition**

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Landau-Fermi liquid in short

(L. D. Landau, 1957)

- single-particle Green's function

$$G_\sigma(\tau,\mathbf{k}) = -\langle\, \mathrm{T}_\tau\Big(c_{\sigma\mathbf{k}}(\tau)\, c^\dagger_{\sigma\mathbf{k}}(0)\Big)\,\rangle = -\frac{\mathrm{Tr}\Big(\mathrm{e}^{-\beta H}\;\mathrm{T}_\tau\Big(c_{\sigma\mathbf{k}}(\tau)\, c^\dagger_{\sigma\mathbf{k}}(0)\Big)\Big)}{\mathrm{Tr}\Big(\mathrm{e}^{-\beta H}\Big)}$$

$$c_{\sigma\mathbf{k}}(\tau) = \mathrm{e}^{H\tau}\; c_{\sigma\mathbf{k}}\; \mathrm{e}^{-H\tau}$$

$$G_\sigma(i\epsilon,\mathbf{k}) = \int_0^\beta d\tau\, \mathrm{e}^{i\epsilon\tau}\; G_\sigma(\tau,\mathbf{k}) \qquad\qquad i\epsilon = (2n+1)\,\pi\, T\,, \quad n\in\mathbb{Z}$$

Landau-Fermi liquid in short

(L. D. Landau, 1957)

- assumption for ε, |**k**-**k**$_F$|,T ≪ T$_F$

$$G(i\epsilon,\mathbf{k}) \simeq G_{\text{coh.}}(i\epsilon,\mathbf{k}) + G_{\text{incoh.}}(i\epsilon,\mathbf{k}) = \frac{Z_{\mathbf{k}}}{i\epsilon-\epsilon_{\mathbf{k}}} + G_{\text{incoh.}}(i\epsilon,\mathbf{k})$$

- analytic continuation $i\varepsilon \longrightarrow z \in \mathbb{Z}$

  - $G_{\text{coh.}}(z,\mathbf{k}) \Rightarrow$ single pole on the real axis

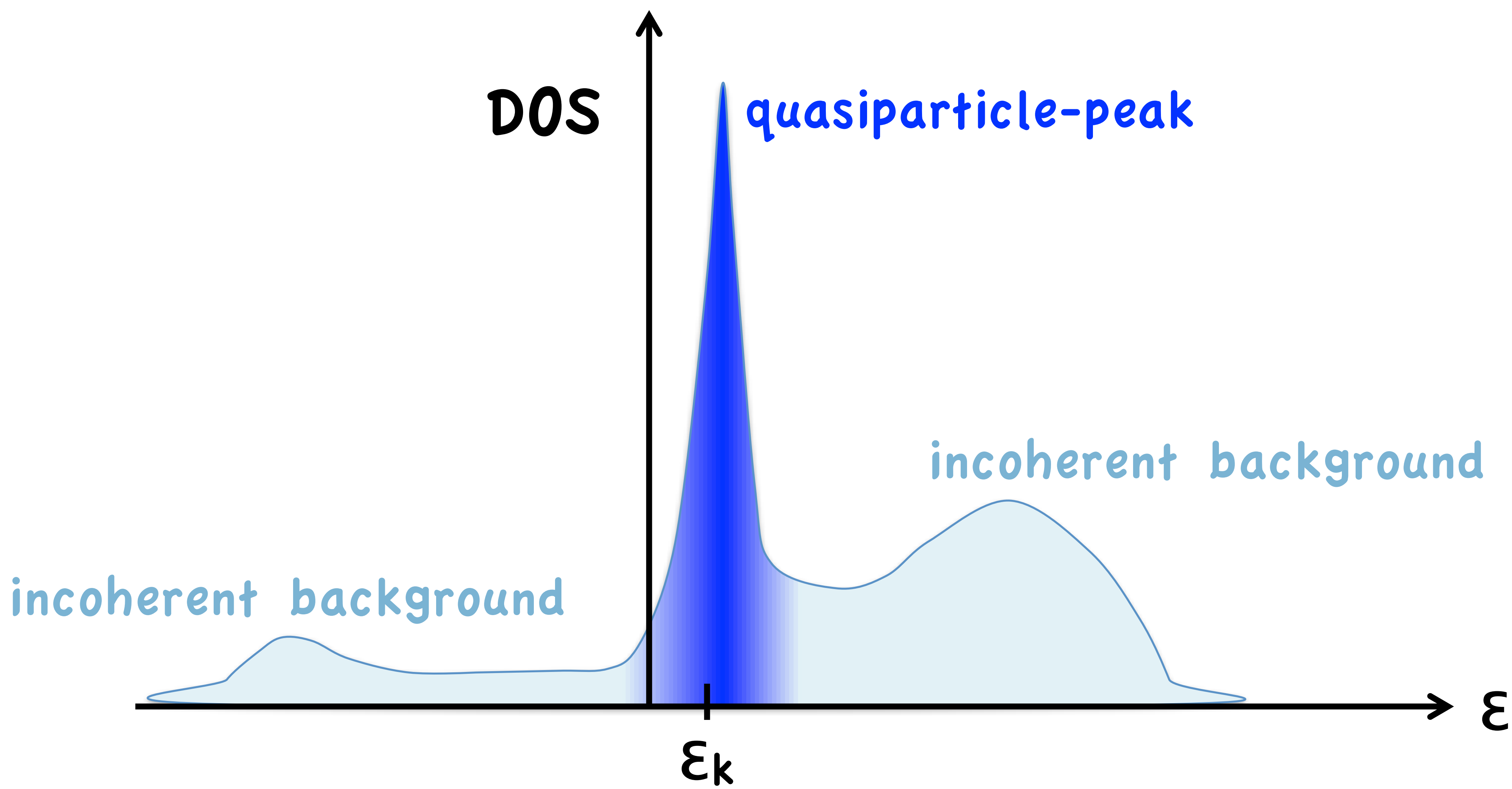
  - $G_{\text{incoh.}}(z,\mathbf{k}) \Rightarrow$ branch cut on the real axis

- **the assumption can be verified order by order in perturbation theory, though no one can guarantee that the series converges**

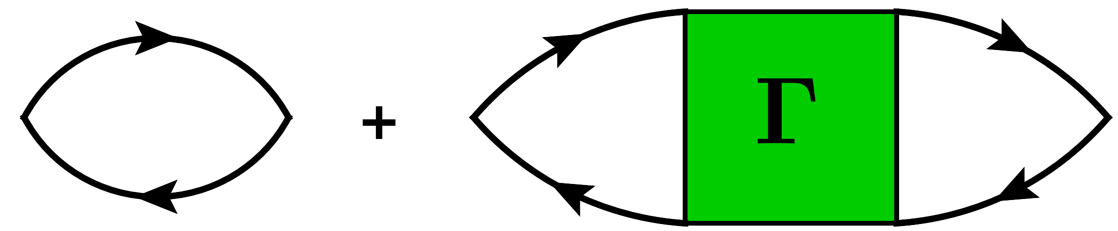
$$\boxed{G(z,\mathbf{k}) \simeq \frac{Z_{\mathbf{k}}}{z-\epsilon_{\mathbf{k}}} + G_{\text{incoh.}}(z,\mathbf{k})}$$

- single-particle density-of-states (DOS)

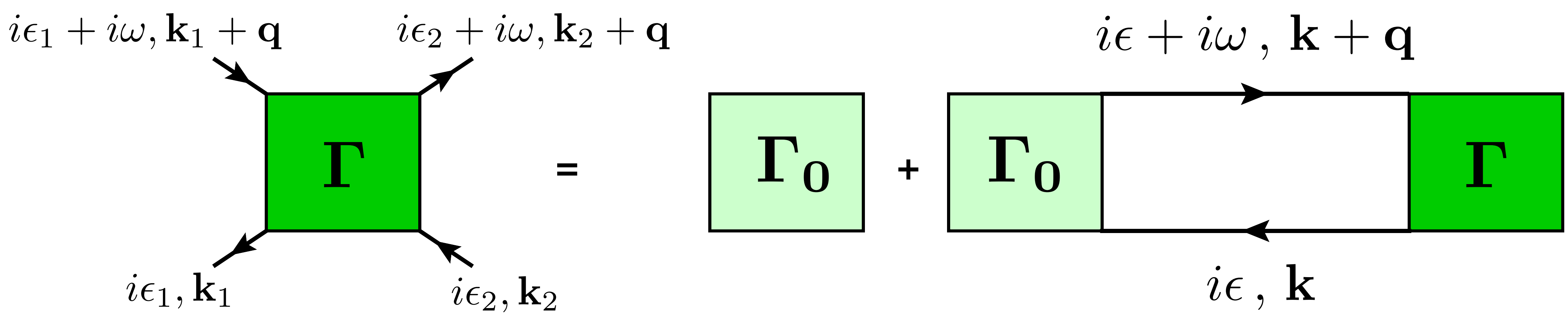
$$\mathcal{A}(\epsilon,\mathbf{k}) = -\frac{1}{2\pi}\Big(G\big(z=\epsilon+i0^+,\mathbf{k}\big) - G\big(z=\epsilon-i0^+,\mathbf{k}\big)\Big)$$
$$= Z_{\mathbf{k}}\,\delta\big(\epsilon-\epsilon_{\mathbf{k}}\big) + \mathcal{A}_{\text{incoh.}}(\epsilon,\mathbf{k})$$



• **ultimate goal: calculate physical response functions at small frequency ω and momentum q**

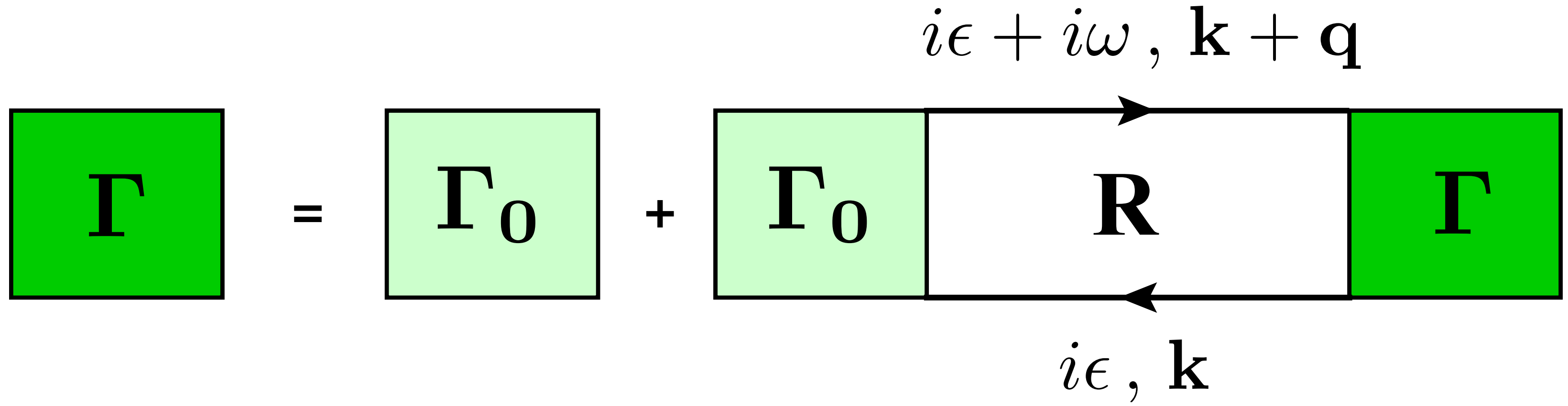
$\chi(i\omega, \mathbf{q}) =$ 

Bethe-Salpeter equation:



• **irreducible vertex in the particle-hole channel**

$$\Gamma_0 \big(i\epsilon_1 + i\omega, \mathbf{k}_1 + \mathbf{q}; i\epsilon_2, \mathbf{k}_2; i\epsilon_2 + i\omega, \mathbf{k}_2 + \mathbf{q}; i\epsilon_1, \mathbf{k}_1 \big)$$



$$
\begin{aligned}
R(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) &\equiv G(i\epsilon+i\omega,\mathbf{k}+\mathbf{q})\,G(i\epsilon,\mathbf{k})\\
&= G_{\mathrm{coh.}}(i\epsilon+i\omega,\mathbf{k}+\mathbf{q})\,G_{\mathrm{coh.}}(i\epsilon,\mathbf{k}) + R_{\mathrm{incoh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q})\\
&= R_{\mathrm{coh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) + R_{\mathrm{incoh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q})
\end{aligned}
$$

mathematical sense of a distribution

$$
R_{\mathrm{coh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) = -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\;\delta(i\epsilon)\;Z_{\mathbf{k}}^2\;\frac{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}}{i\omega-\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}}}
$$

non-analytic at the origin ω=q=0

• indeed:

$$\lim_{\omega\to 0}\lim_{\mathbf{q}\to 0} R_{\text{coh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) = \lim_{\omega\to 0}\lim_{\mathbf{q}\to 0} -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\,\delta(i\epsilon)\,Z_{\mathbf{k}}^2\,\frac{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}}{i\omega-\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}}}$$

ω-limit

$$\equiv R^{\omega}_{\text{coh.}}(i\epsilon,\mathbf{k}) = 0$$

$$\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0} R_{\text{coh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) = \lim_{\mathbf{q}\to 0}\lim_{\omega\to 0} -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\,\delta(i\epsilon)\,Z_{\mathbf{k}}^2\,\frac{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}}{i\omega-\epsilon_{\mathbf{k}+\mathbf{q}}+\epsilon_{\mathbf{k}}}$$

q-limit

$$\equiv R^{q}_{\text{coh.}}(i\epsilon,\mathbf{k}) = \frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\,\delta(i\epsilon)\,Z_{\mathbf{k}}^2$$

while by assumption:

$$\lim_{\mathbf{q}\to 0}\lim_{\omega\to 0} R_{\text{incoh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) \equiv R^{q}_{\text{incoh.}}(i\epsilon,\mathbf{k})$$

$$= \lim_{\omega\to 0}\lim_{\mathbf{q}\to 0} R_{\text{incoh.}}(i\epsilon,\mathbf{k};i\omega,\mathbf{q}) \equiv R^{\omega}_{\text{incoh.}}(i\epsilon,\mathbf{k})$$

$$\equiv R_{\text{incoh.}}(i\epsilon,\mathbf{k})$$

• therefore:

$$R^\omega(i\epsilon,\mathbf{k}) = R_{\text{incoh.}}(i\epsilon,\mathbf{k})$$
$$R^q(i\epsilon,\mathbf{k}) = R_{\text{coh.}}(i\epsilon,\mathbf{k}) + R_{\text{incoh.}}(i\epsilon,\mathbf{k})$$

• back to Bethe-Salpeter

$$\Gamma = \Gamma_0 + \Gamma_0 \odot R \odot \Gamma$$
$$\Gamma^\omega = \Gamma_0 + \Gamma_0 \odot R^\omega \odot \Gamma^\omega$$
$$\Gamma^q = \Gamma_0 + \Gamma_0 \odot R^q \odot \Gamma^q$$

$$\Gamma = \Gamma^\omega + \Gamma^\omega \odot \Big(R - R^\omega\Big) \odot \Gamma = \Gamma^q + \Gamma^q \odot \Big(R - R^q\Big) \odot \Gamma^\omega$$

$$R - R^\omega = -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\,\delta(i\epsilon)\,Z_{\mathbf{k}}^2\,\frac{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}}{i\omega - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}$$
$$R - R^q = -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}\,\delta(i\epsilon)\,Z_{\mathbf{k}}^2\,\frac{i\omega}{i\omega - \epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}}}$$

n.b. peaked at Fermi
&
not including anymore
the incoherent part

• express everything in terms of Γ^ω

$$\Gamma = \Gamma^\omega + \Gamma^\omega \odot \Big(R - R^\omega\Big) \odot \Gamma$$

$$\Gamma^q = \Gamma^\omega + \Gamma^\omega \odot \Big(R^q - R^\omega\Big) \odot \Gamma^q$$

… or rather in terms of the Landau's ***f*** parameters:

$$f_{\mathbf{k}_1\mathbf{k}_2} = Z_{\mathbf{k}_1}\, Z_{\mathbf{k}_2}\, \Gamma^\omega\big(0, \mathbf{k}_1; 0, \mathbf{k}_2; 0, \mathbf{k}_2; 0, \mathbf{k}_1\big)$$

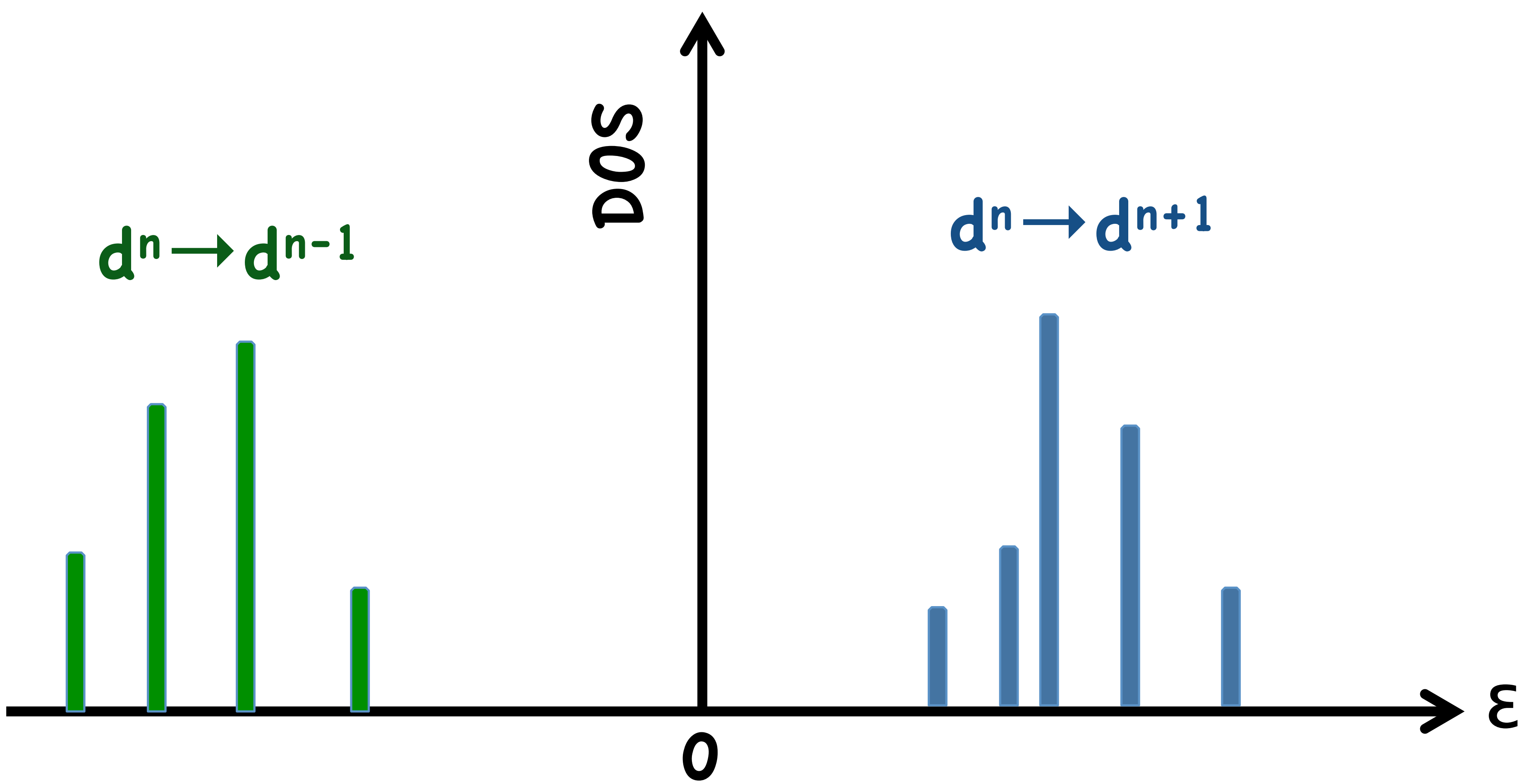
and quasiparticle scattering amplitudes:

$$A_{\mathbf{k}_1\mathbf{k}_2}(i\omega, \mathbf{q}) = Z_{\mathbf{k}_1}\, Z_{\mathbf{k}_2}\, \Gamma(\mathbf{k}_1 + \mathbf{q}, i\omega; \mathbf{k}_2, 0; \mathbf{k}_2 + \mathbf{q}, i\omega; \mathbf{k}_1, 0)$$

Exploiting Ward's identities, one can derive for any conserved quantity the known Fermi liquid expression of its response function at small ω and $\mathbf{q}$ in terms of the unknown ***f***-parameters and quasiparticle dispersion $\varepsilon_\mathbf{k}$

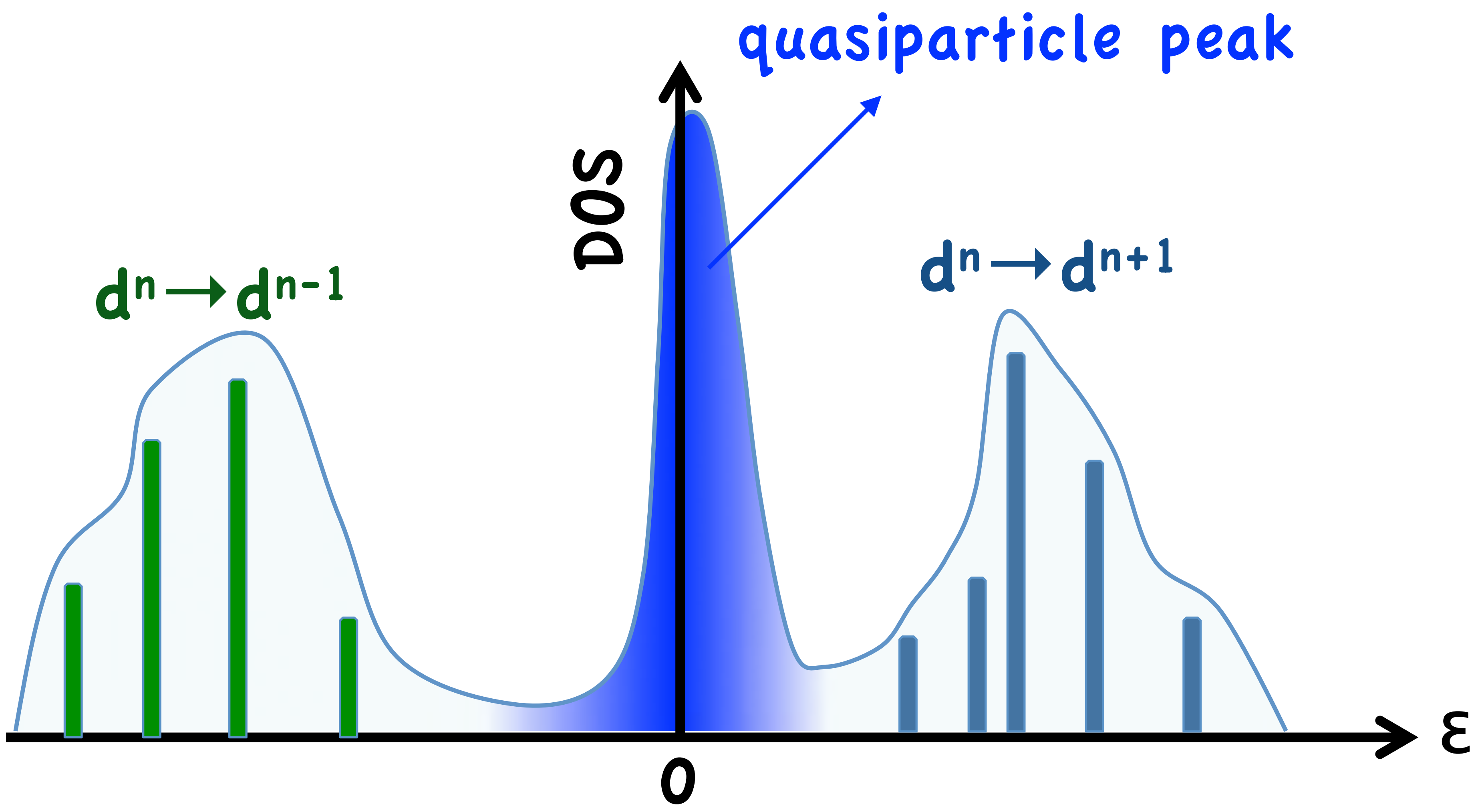
Correlated metals close to a Mott transition

- in the Mott insulator we do have a clue what $G_{incoh.}$ and thus $A_{incoh.}$ describe: the single-particle excitations of the isolated atom



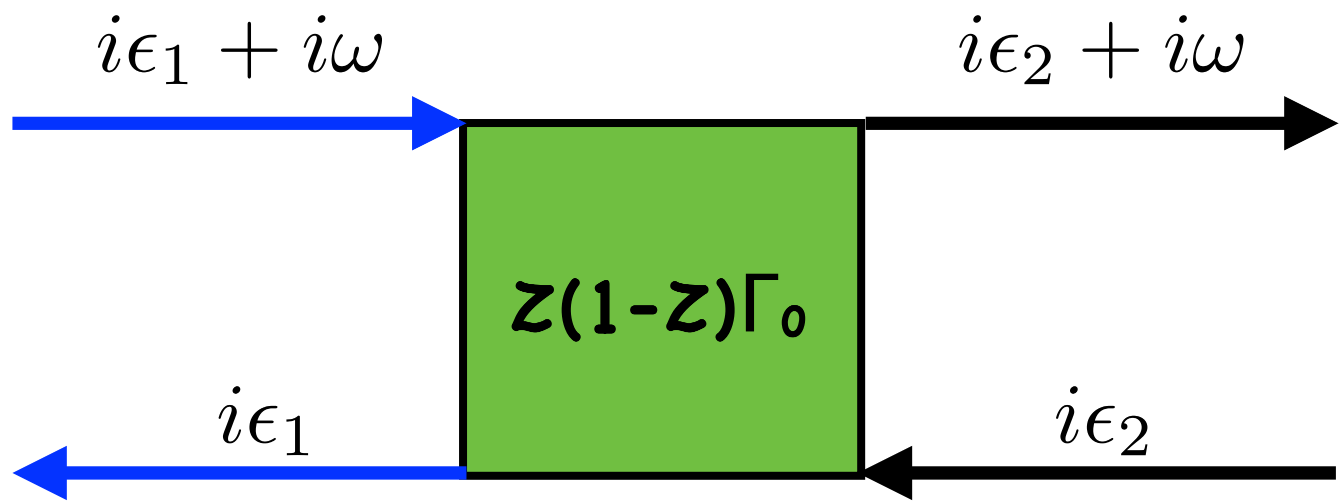
Correlated metals close to a Mott transition

- by continuity, in the metal $G_{incoh.}$ and thus $A_{incoh.}$ should still approximately describe atomic-like excitations



$G_{coh.}/Z \longrightarrow$ & $G_{incoh.}/(1-Z) \longrightarrow$ both DOS's are thus normalised to one

• scattering amplitude between quasiparticles and incoherent excitations

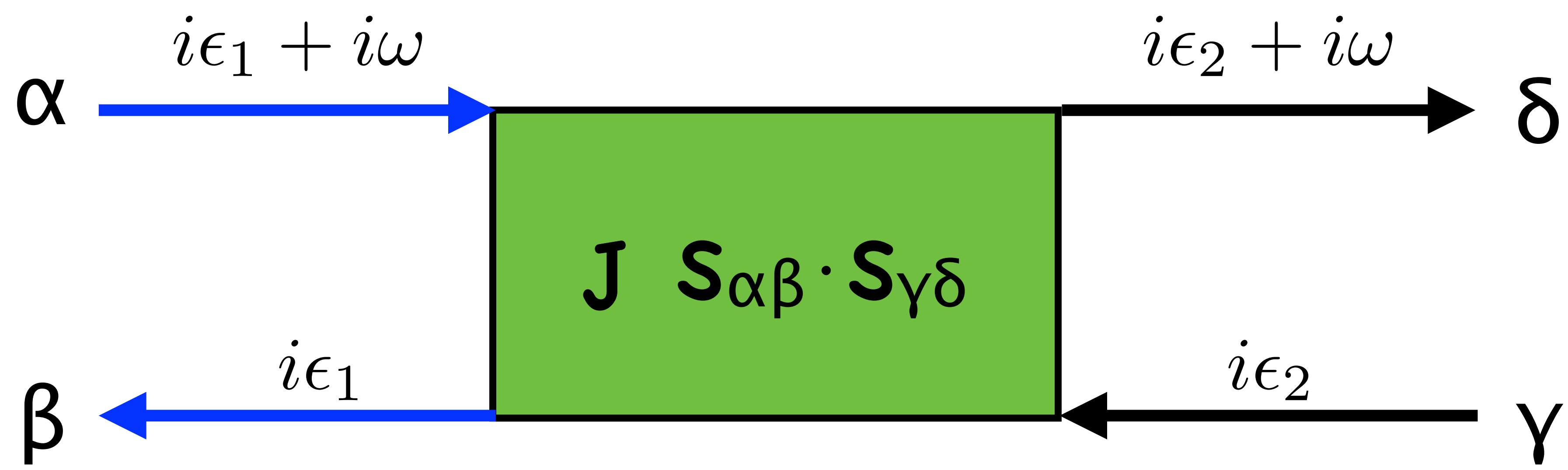


this process can transfer low energy …

• in the charge channel? **NO!**

• in the spin, orbital, spin-orbital channels? **YES!**

- e.g., in the single-band model only the spin-channel is allowed

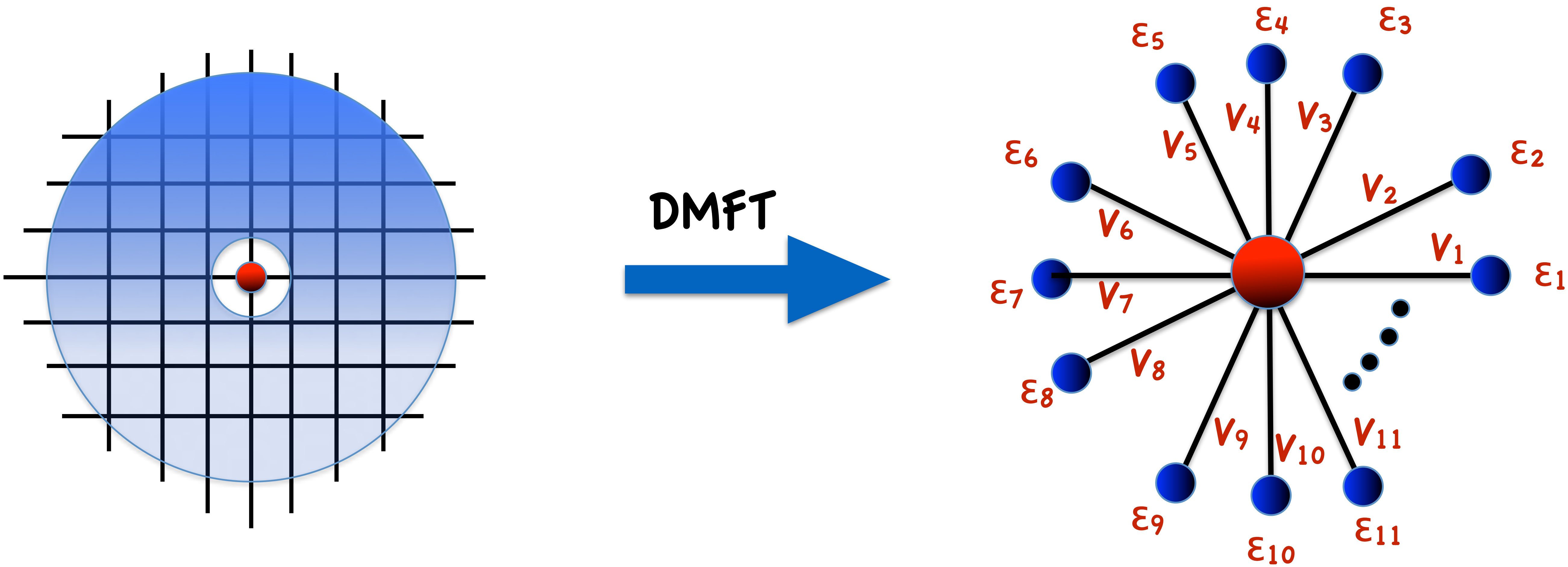


which corresponds to a model of conduction electrons coupled by a spin exchange to localised moments

Kondo-lattice model

with the exchange **J** and conduction band dispersion $\varepsilon_{\mathbf{k}}$ that are not fixed but self-consistently determined by the interacting theory

the relationship between Mott and Kondo physics becomes transparent in lattices with infinite coordination number



within DMFT a model defined on an infinitely coordinated lattice is mapped onto an Anderson impurity model **self-consistently hybridised** to a non-interacting conduction bath

e.g. Bethe lattice with infinite connectivity

$$\mathcal{G}(i\epsilon) \propto \sum_n \frac{|V_n|^2}{i\epsilon - \epsilon_n}$$

Single-band Hubbard model & single-orbital Anderson impurity

Mott transition & ordinary Kondo effect

$$H = -\frac{t}{\sqrt{z}} \sum_{<ij>\,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + H.c.\right) + \frac{U}{2} \sum_i \left(n_i - 1\right)^2$$

$$\Rightarrow\; H_{\text{AIM}} = \sum_{n\sigma} \epsilon_n\, c^\dagger_{n\sigma} c_{n\sigma} + \sum_{n\sigma} V_n \Big(d^\dagger_\sigma c_{n\sigma} + H.c.\Big) + \frac{U}{2}\left(n_d - 1\right)^2$$

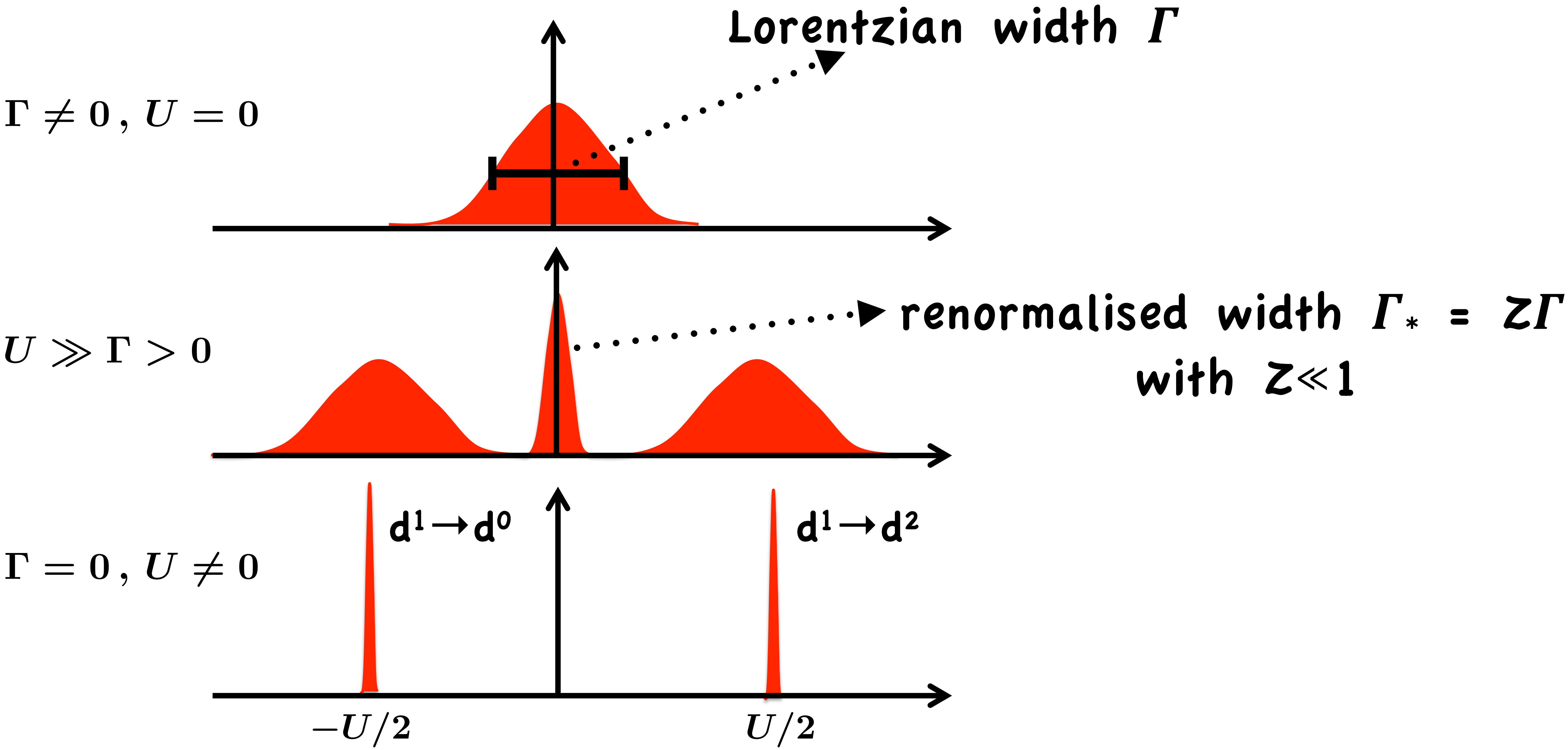
Bethe-lattice coordination number $z \to \infty$

• self-consistency:

$$-\frac{t^2}{\pi} \Im m\, \mathcal{G}\left(\epsilon + i0^+\right) \equiv \underbrace{t^2\, \mathcal{A}(\epsilon)}_{\text{impurity DOS}} = \sum_n \left|V_n\right|^2 \delta\left(\epsilon - \epsilon_n\right) \equiv \underbrace{\Gamma(\epsilon)}_{\text{hybridisation function}}$$

Ordinary Kondo effect

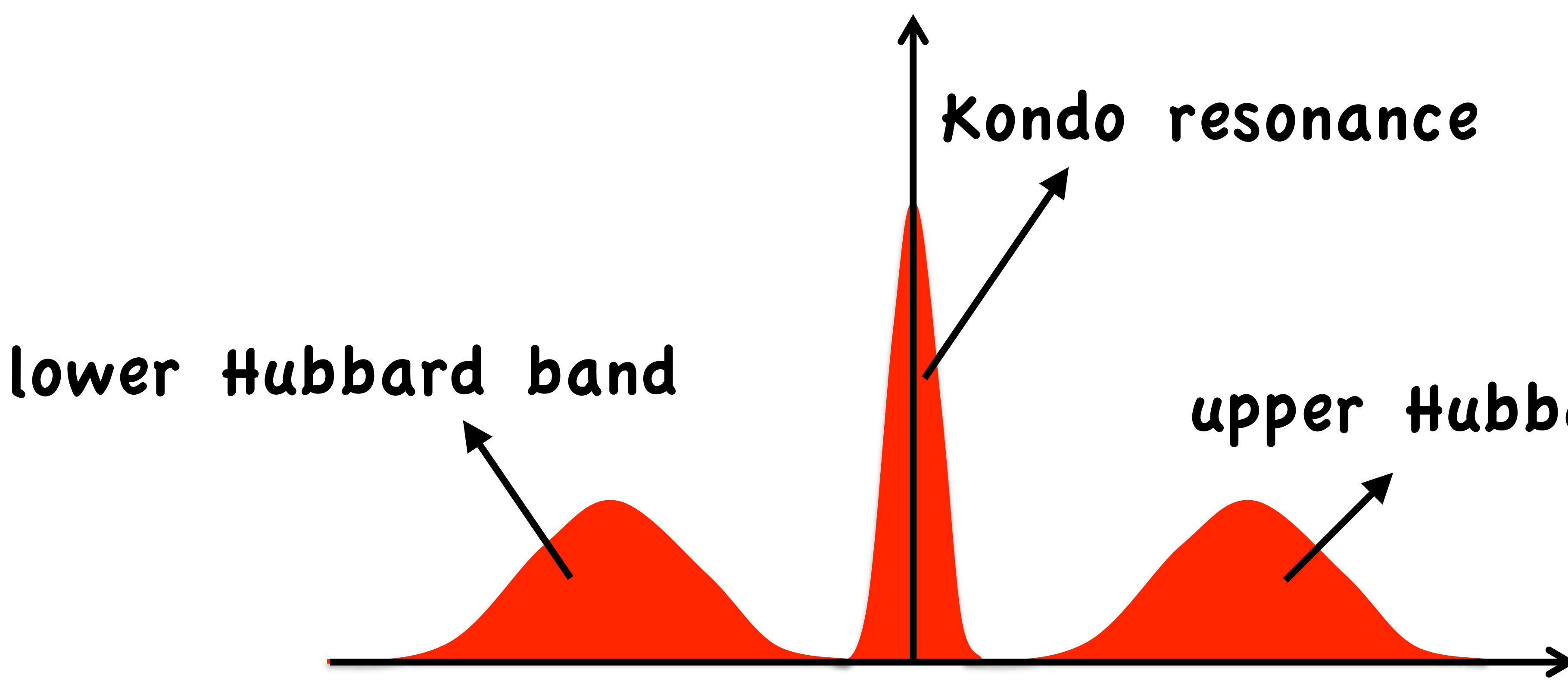
competition of U vs. $\Gamma(\epsilon = 0) \equiv \Gamma$



Without self-consistency the system always gains hybridisation energy by promoting a percentage $Z \ll 1$ of the impurity to the conduction band, and thus screening the impurity spin-1/2.

That screening is characterised by a Kondo resonance that appears at Fermi no matter how U is large, of width $\Gamma_* = Z\Gamma \ll \Gamma$, to be identified with the Kondo temperature T_K.

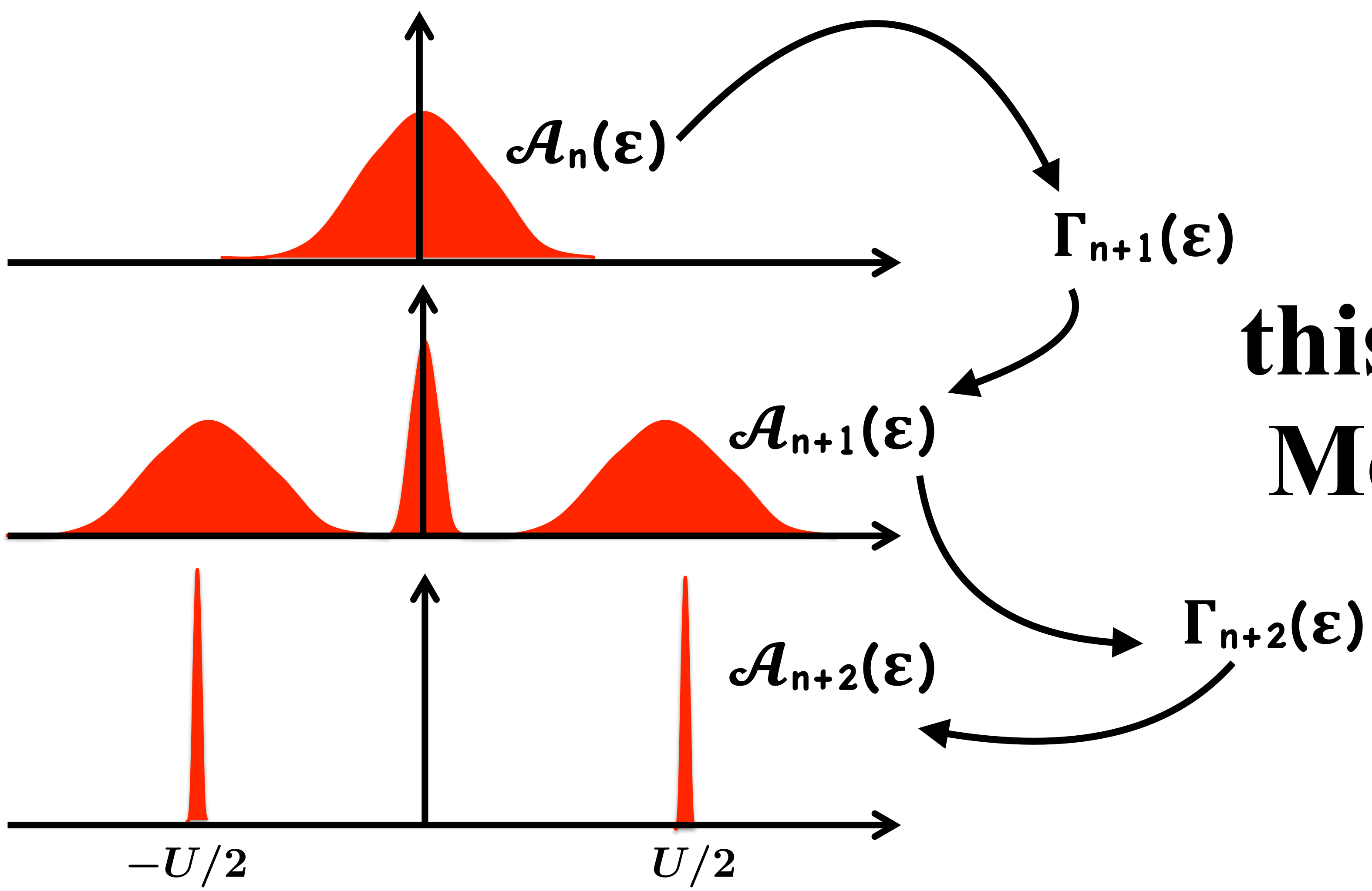
For $T \gg T_K$ the resonance is destroyed by thermal fluctuations



What is the role of self-consistency?

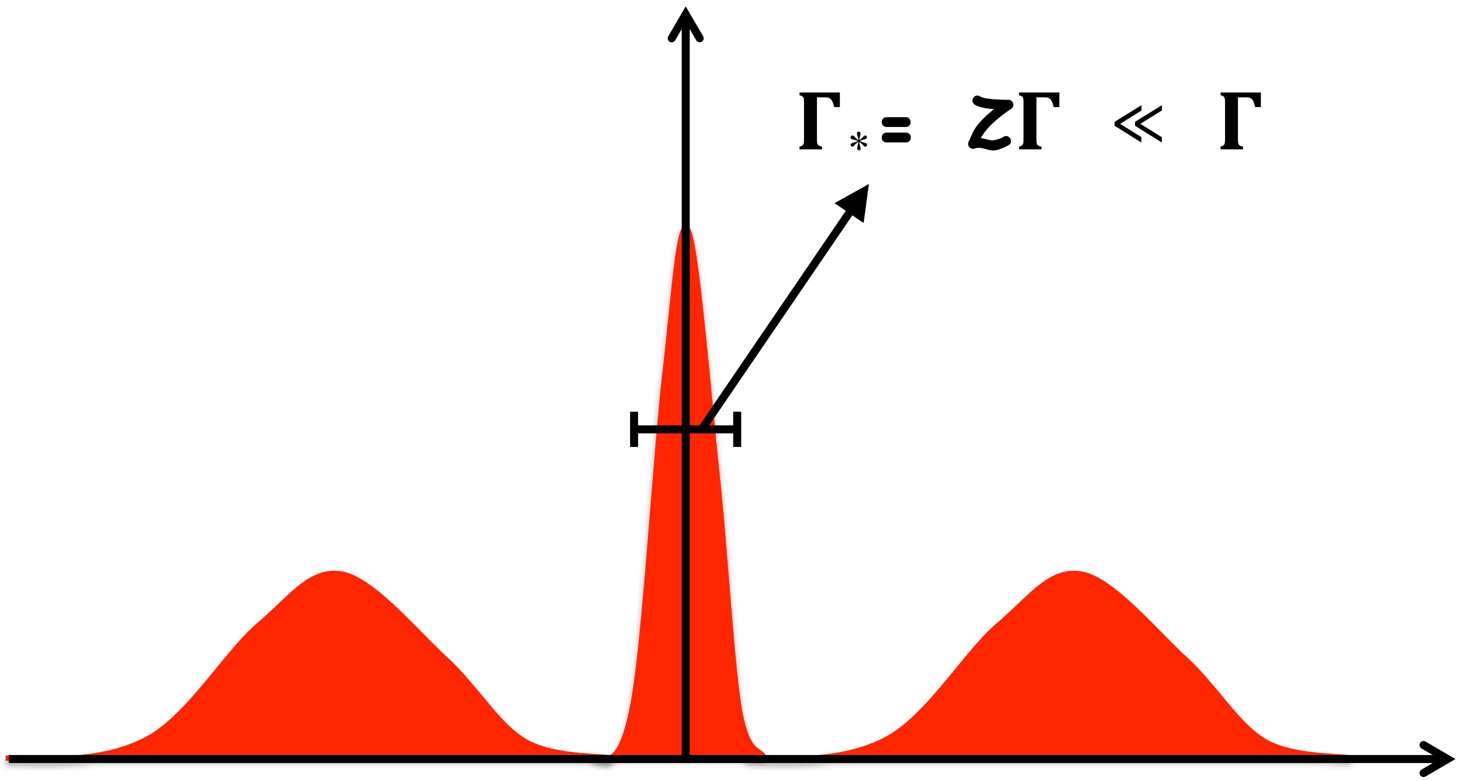
I. make the Kondo resonance disappear at finite U

$$t^2\,\mathcal{A}(\epsilon) = \Gamma(\epsilon)$$



this is precisely how the Mott transition occurs

II. turn the impurity instabilities into true bulk ones



impurity spin susceptibility

$$\chi \sim \Gamma_*^{-1} \gg 1$$

the large impurity susceptibility will transmit, through the self-consistency condition, to the bulk, making the latter unstable to magnetism. This is instead impossible in the impurity model without self-consistency.

II. turn the impurity instabilities into true bulk ones

- **the knowledge of the impurity model can thus help to anticipate, without even imposing any self-consistency condition, which instabilities are going to occur at or in proximity of the Mott transition**

- **Kondo models with exotic phases might correspond in infinitely coordinated lattices to lattice models with rich and equally exotic physics near the Mott transition**

General classification of Kondo models:

1. **screened**: number of impurity degrees of freedom = number of bath degrees of freedom

2. **overscreened**: number of impurity degrees of freedom < number of bath degrees of freedom — appealing non-Fermi-liquid properties with non-analytic thermodynamic susceptibilities

3. **underscreened**: number of impurity degrees of freedom > number of bath degrees of freedom — also appealing marginal Fermi-liquid behaviour

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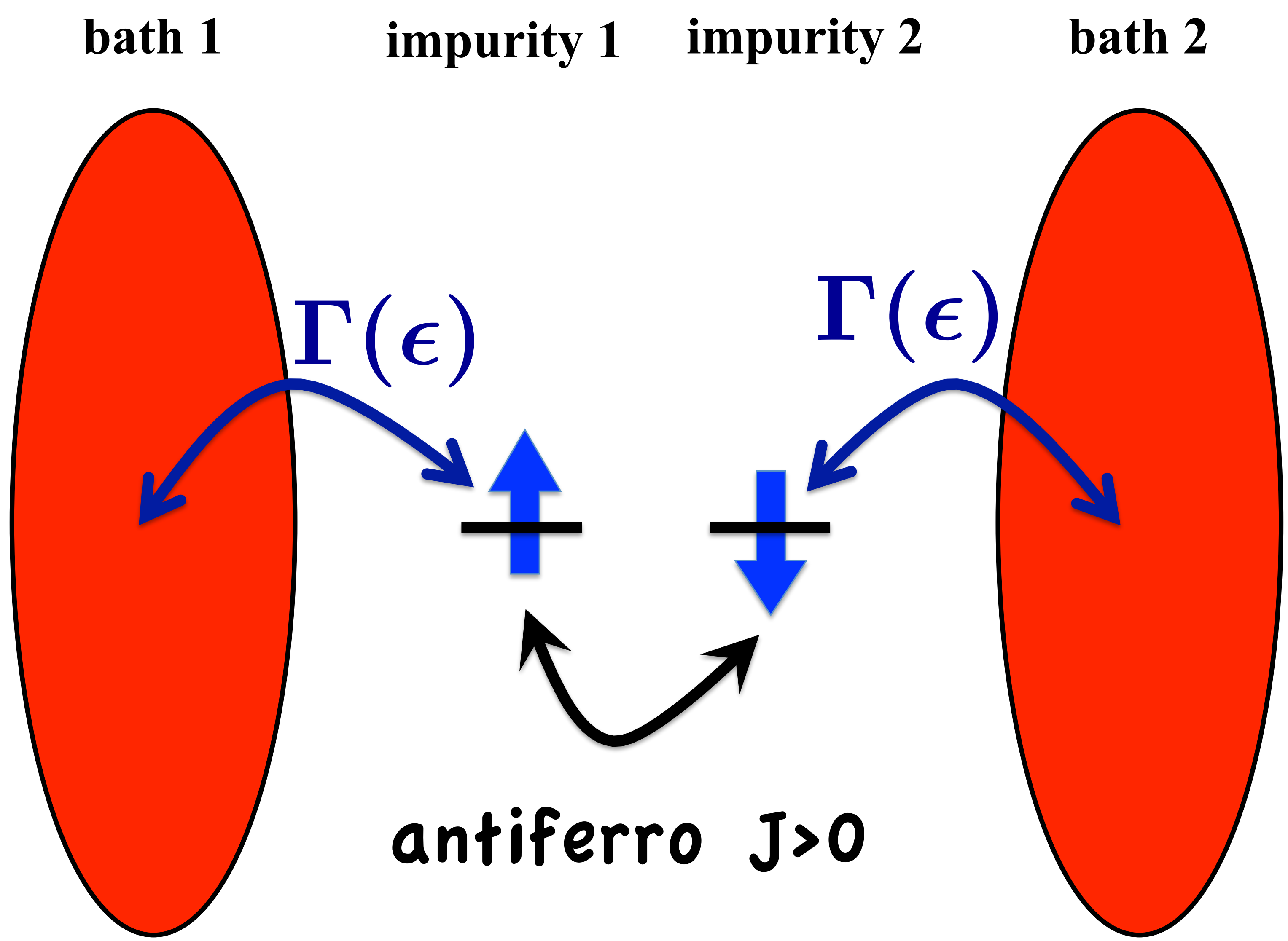
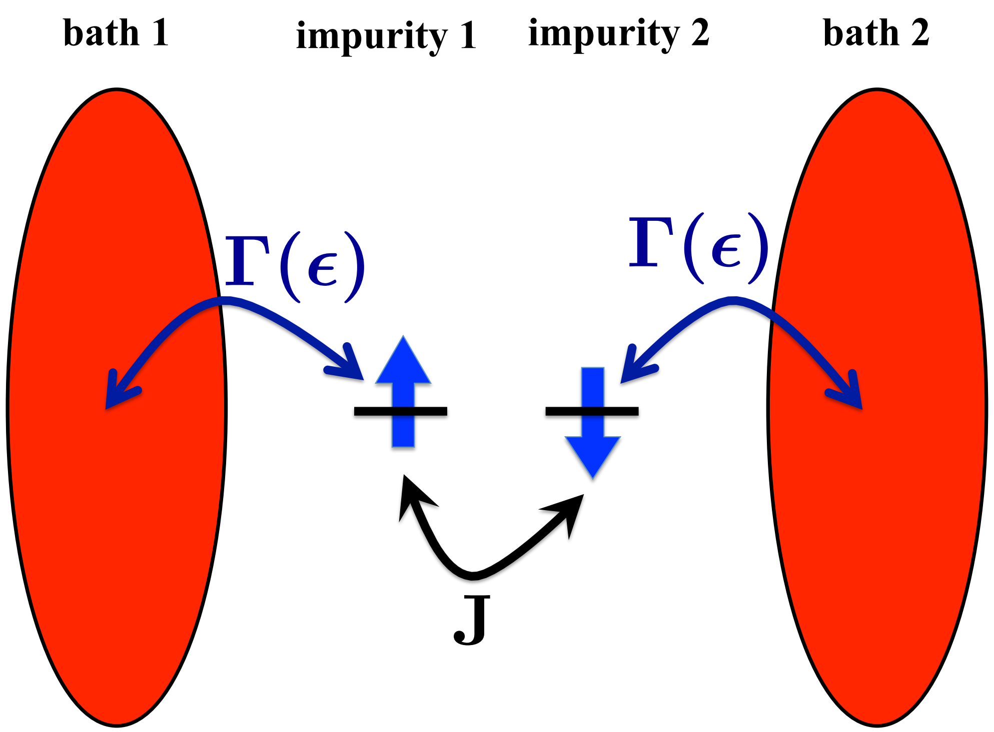
the DMFT mapping implies by construction that the impurity has the same number of degrees of freedom as the bath

Even though the impurity has the same number of degrees of freedom as the bath, still exotic Kondo physics may appear

need an impurity with internal degrees of freedom as well as with an internal mechanism able to lock the impurity into a non-degenerate state that makes Kondo screening inactive

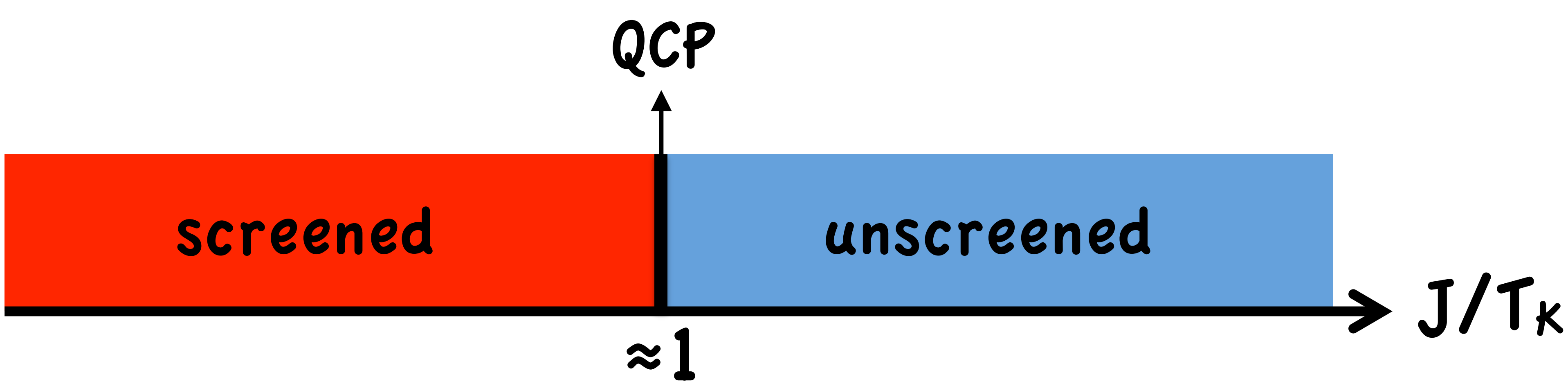
The simplest example: the two impurity model

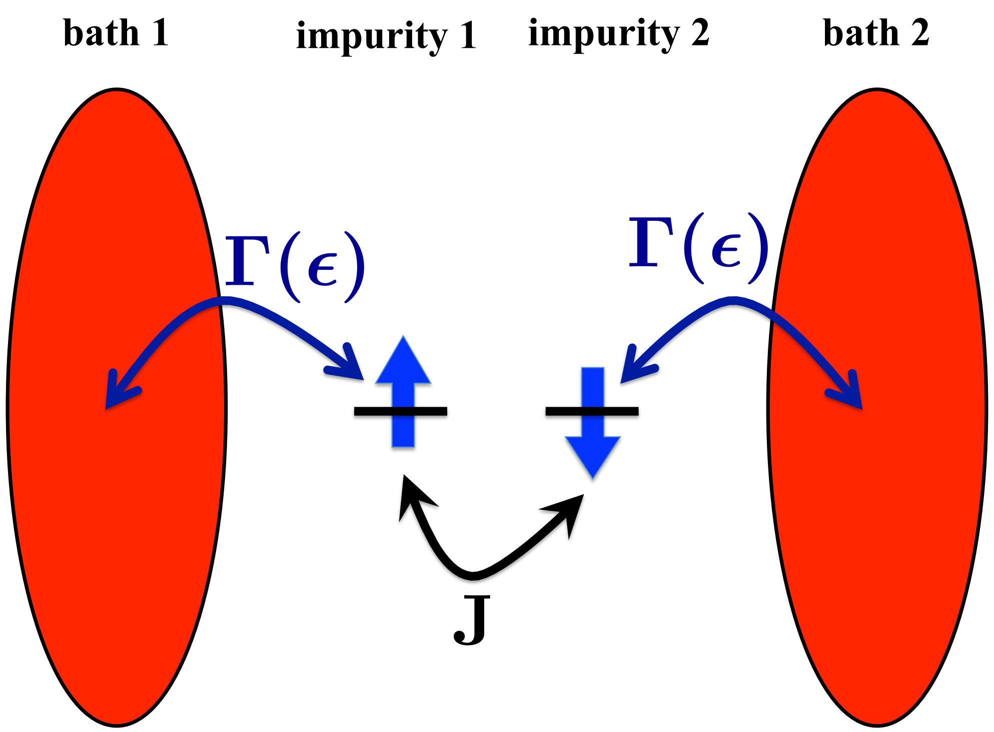




- if J=0, each impurity is Kondo screened by its own bath. The relevant energy scale is the **Kondo temperature T_K**
- if $T_K \gg J$, each impurity still remains **Kondo screened**
- if $J \gg T_K$, the two impurities lock into a spin-singlet state transparent to conduction electrons $\Rightarrow$ **no Kondo screening**

the two regimes, Kondo **screened** and **unscreened**, are separated by a true quantum critical point at $T_K \sim J$





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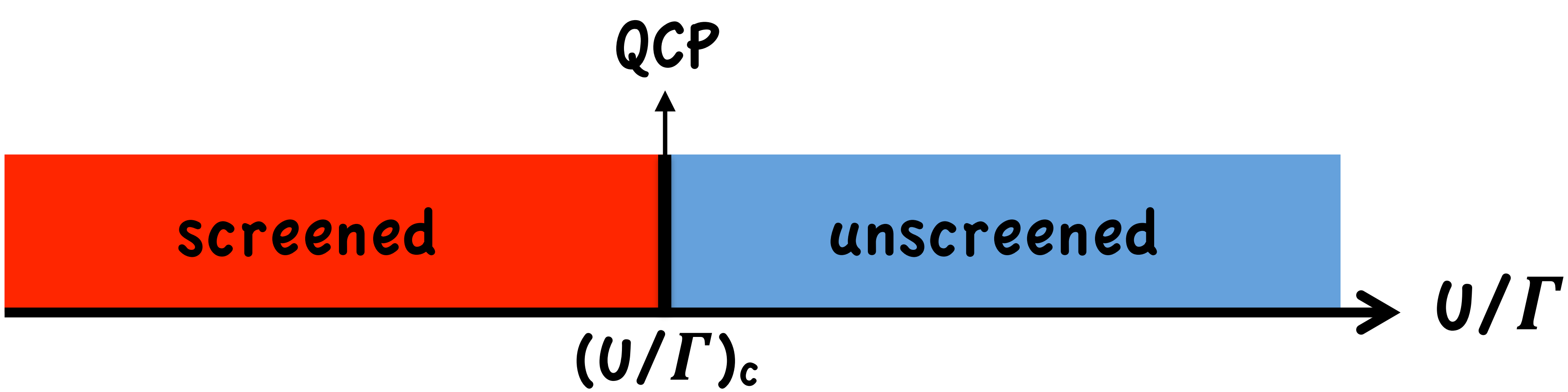
the two regimes, Kondo **screened** and **unscreened**, are separated by a true quantum critical point at $\mathbf{U/\Gamma \sim \log(U\Gamma/J^2)}$



Properties of the QCP

• instability channels Δ_i with log-diverging susceptibilities:

$$\chi_i(\omega) = \langle \boldsymbol{\Delta}_i(\omega)\, \boldsymbol{\Delta}_i^\dagger(-\omega)\rangle \sim -\ln\omega$$

• meaning of *instability*:

$$\text{if}\quad \boldsymbol{H_{2\mathrm{AIM}}} \to \boldsymbol{H_{2\mathrm{AIM}}} - \boldsymbol{h_i}\, \boldsymbol{\Delta_i}$$

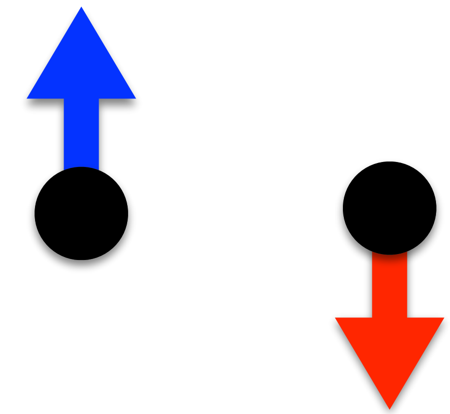
however small $\mathbf{h_i}$ is, the QCP will turn into a crossover between the screened and unscreened phases, the sharper the smaller $\mathbf{h_i}$ is

Properties of the QCP

- instability channels Δ_i with log-diverging susceptibilities:

  - "antiferromagnetic" channel

$$\vec{\boldsymbol{\Delta}}_{\mathbf{AFM}} = \vec{\boldsymbol{S}}_{\mathbf{1}} - \vec{\boldsymbol{S}}_{\mathbf{2}}$$



  - "hopping" channel

$$\boldsymbol{\Delta}_{\boldsymbol{\phi}}^{\mathbf{hyb.}} = \sum_{\boldsymbol{\sigma}} \left(\mathrm{e}^{\boldsymbol{i\phi}}\, \boldsymbol{d}_{\mathbf{1}\boldsymbol{\sigma}}^{\dagger} \boldsymbol{d}_{\mathbf{2}\boldsymbol{\sigma}} + \boldsymbol{H.c.} \right)$$

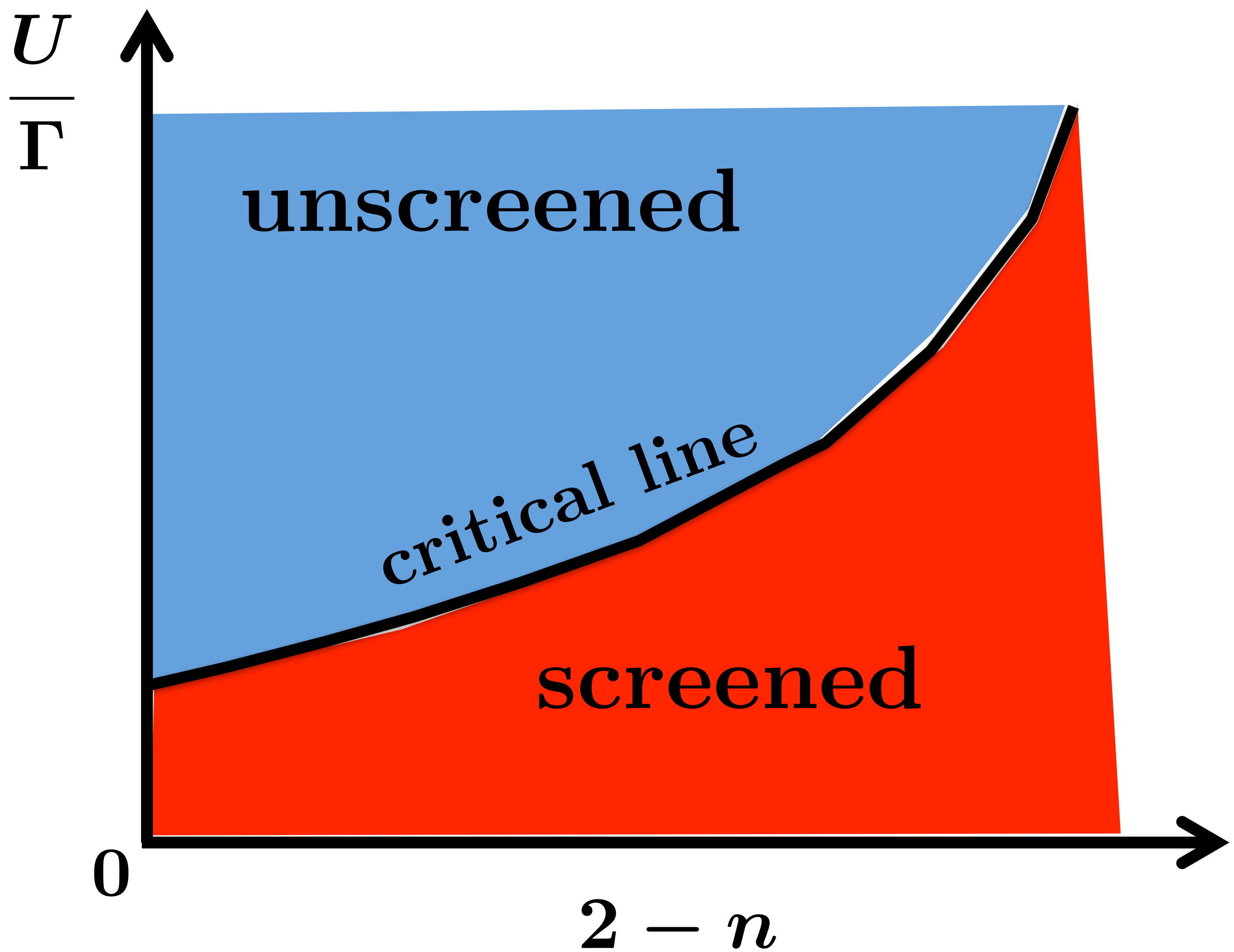
  - spin-singlet "Cooper" channel

$$\boldsymbol{\Delta}_{\boldsymbol{\phi}}^{\mathbf{SC}} = \left[\mathrm{e}^{\boldsymbol{i\phi}} \left(\boldsymbol{d}_{\mathbf{1}\uparrow}^{\dagger}\ \boldsymbol{d}_{\mathbf{2}\downarrow}^{\dagger} + \boldsymbol{d}_{\mathbf{2}\uparrow}^{\dagger}\ \boldsymbol{d}_{\mathbf{1}\downarrow}^{\dagger} \right) + \boldsymbol{H.c.} \right)\right]$$

Properties of the QCP

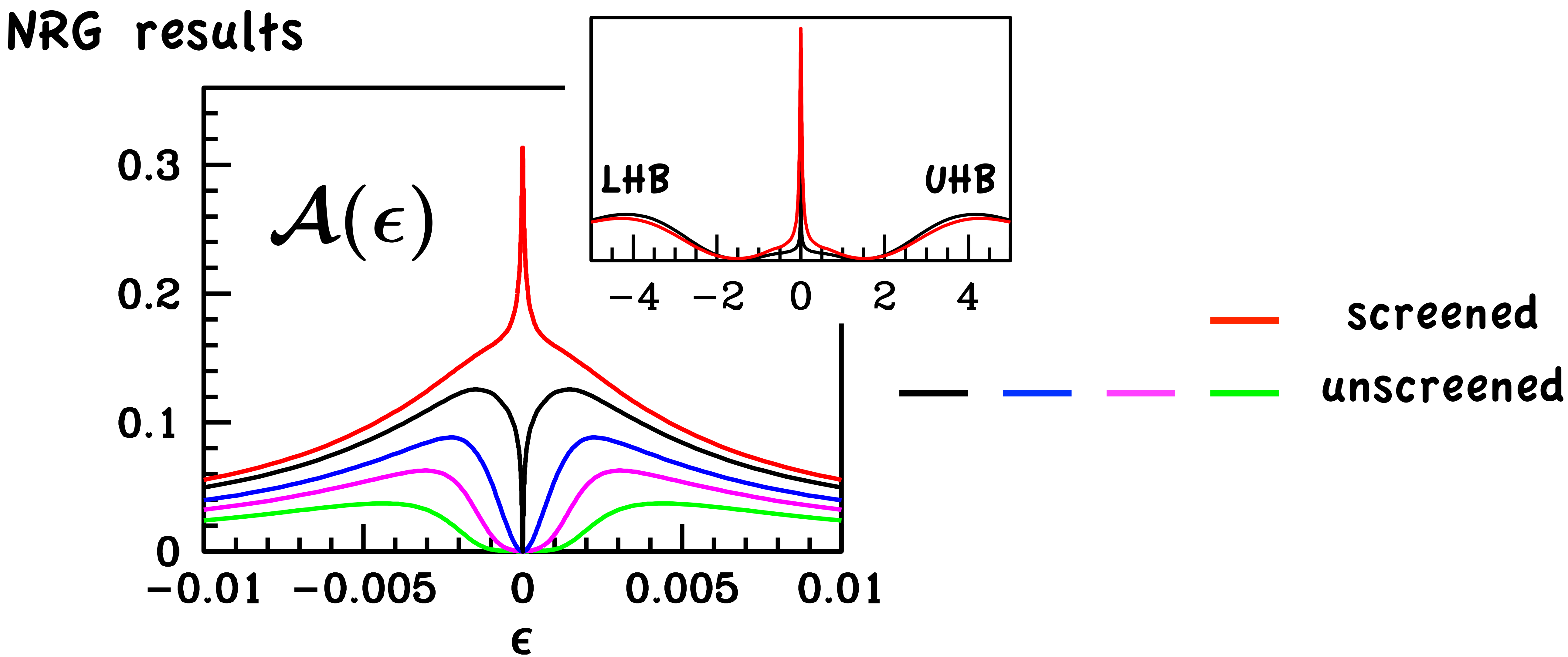
- "doping" the impurity is not an instability channel

if $\boldsymbol{H_{2\mathrm{AIM}} \to H_{2\mathrm{AIM}} + \epsilon_d\left(n_1+n_2\right) \Rightarrow \langle n_1+n_2\rangle = n \neq 2}$



the QCP at n=2 belongs to a whole critical line that bends to larger U/Γ values the higher is the doping away from half-filling

Dynamics across the QCP



across the transition from the screened to the unscreened phase the narrow Kondo resonance transforms into a narrow pseudo-gap

Dynamics across the QCP

- two energy scales

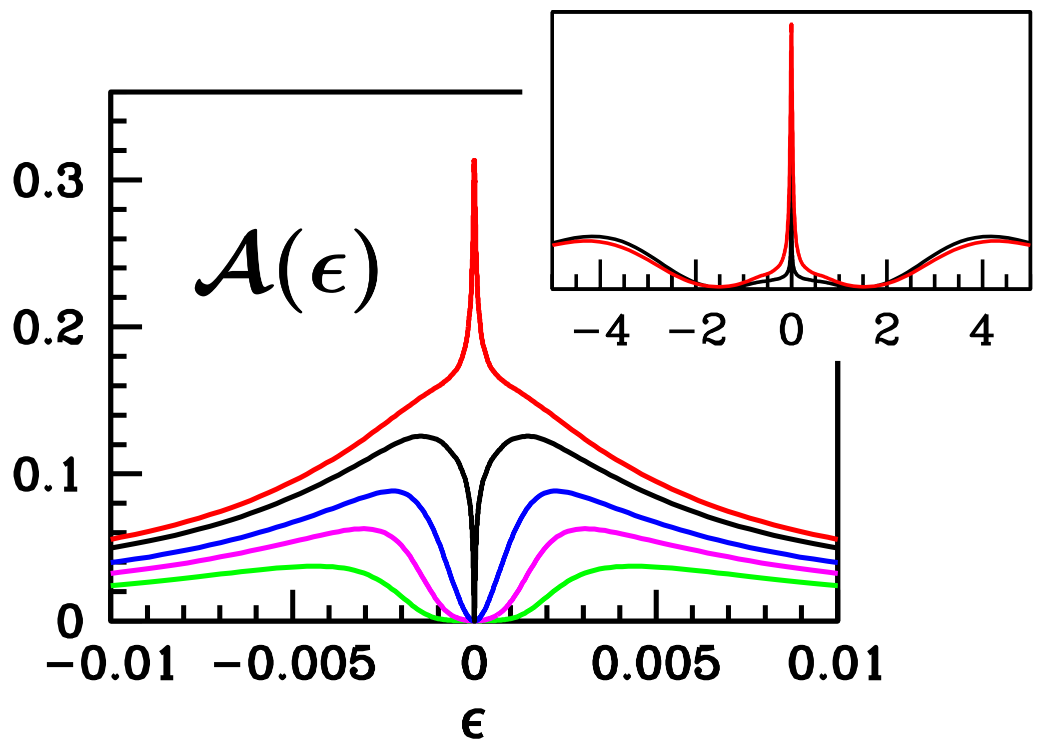
  - $T_+ \approx \max(T_K, J)$, smooth across the transition

  - T_- measuring the distance from the QCP

for instance, if both J and U are fixed and Γ varies,
the QCP occurs at $\Gamma=\Gamma_c$ and

$$T_- \sim \left(\Gamma - \Gamma_c\right)^2$$

Modelling the impurity DOS



$$T_+ \simeq \max\left(T_K, J\right)$$

$$T_- \sim \left(\Gamma - \Gamma_c\right)^2$$

- screened $$\mathcal{A}_+(\epsilon) = \frac{1}{2\pi\Gamma}\left(\frac{T_+^2}{\epsilon^2 + T_+^2} + \frac{T_-^2}{\epsilon^2 + T_-^2}\right)$$

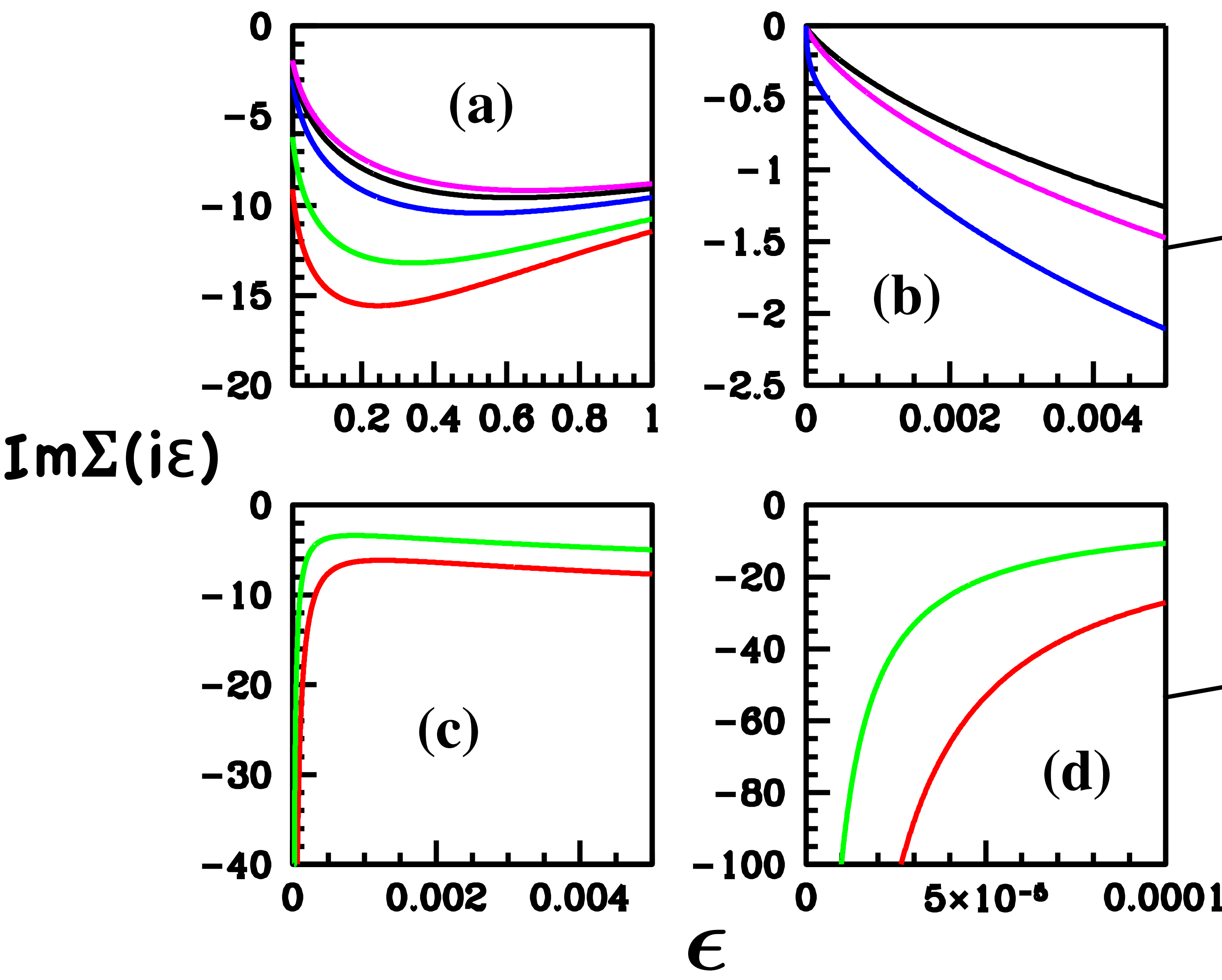
- unscreened $$\mathcal{A}_-(\epsilon) = \frac{1}{2\pi\Gamma}\left(\frac{T_+^2}{\epsilon^2 + T_+^2} - \frac{T_-^2}{\epsilon^2 + T_-^2}\right)$$

- QCP $$\mathcal{A}_{\mathrm{QCP}}(\epsilon) = \frac{1}{2\pi\Gamma}\,\frac{T_+^2}{\epsilon^2 + T_+^2}$$

Modelling the impurity DOS

$$\mathcal{G}_\pm(i\epsilon) = \frac{1}{i\epsilon + i\Gamma\,\mathrm{sign}(\epsilon) - \Sigma_\pm(i\epsilon)} \simeq \frac{1}{2\Gamma}\left(\frac{T_+}{i\epsilon + iT_+\,\mathrm{sign}(\epsilon)} \pm \frac{T_-}{i\epsilon + iT_-\,\mathrm{sign}(\epsilon)}\right)$$

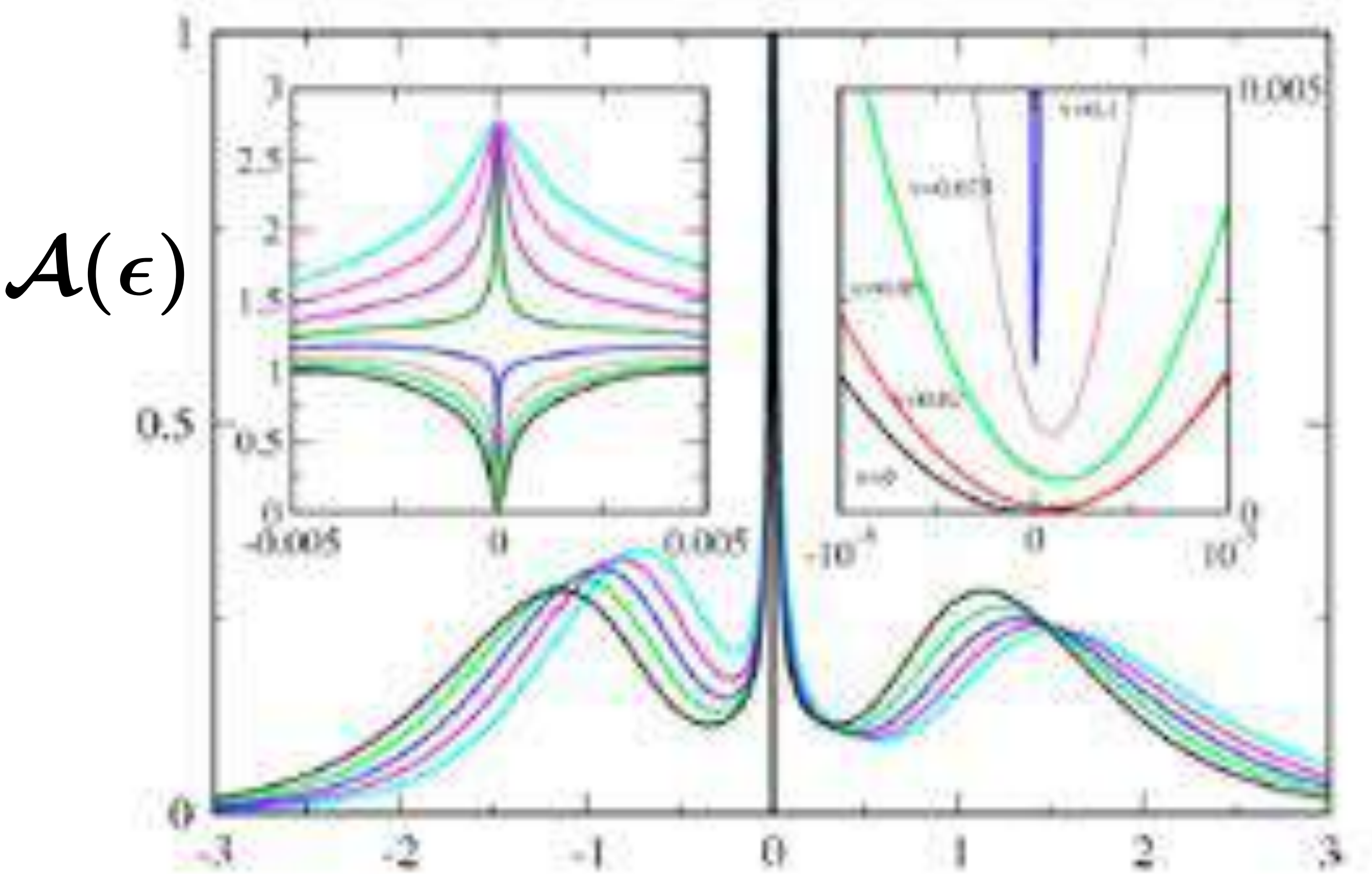
$$\Sigma_\pm(i\epsilon) \equiv i\epsilon - \frac{i\epsilon}{Z_\pm(i\epsilon)}$$

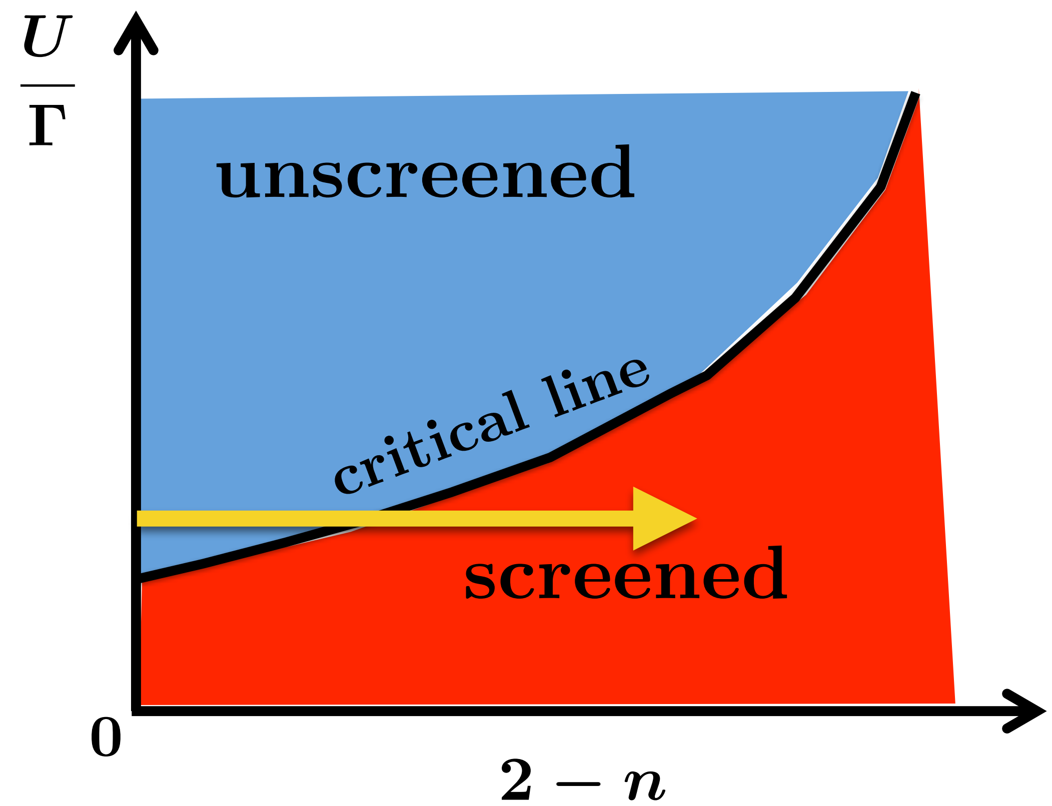


screened phase:
$\Sigma(i\varepsilon) \propto -i\varepsilon$

unscreened phase:
$\Sigma(i\varepsilon) \propto 1/i\varepsilon$

Modelling the impurity DOS away from half-filling





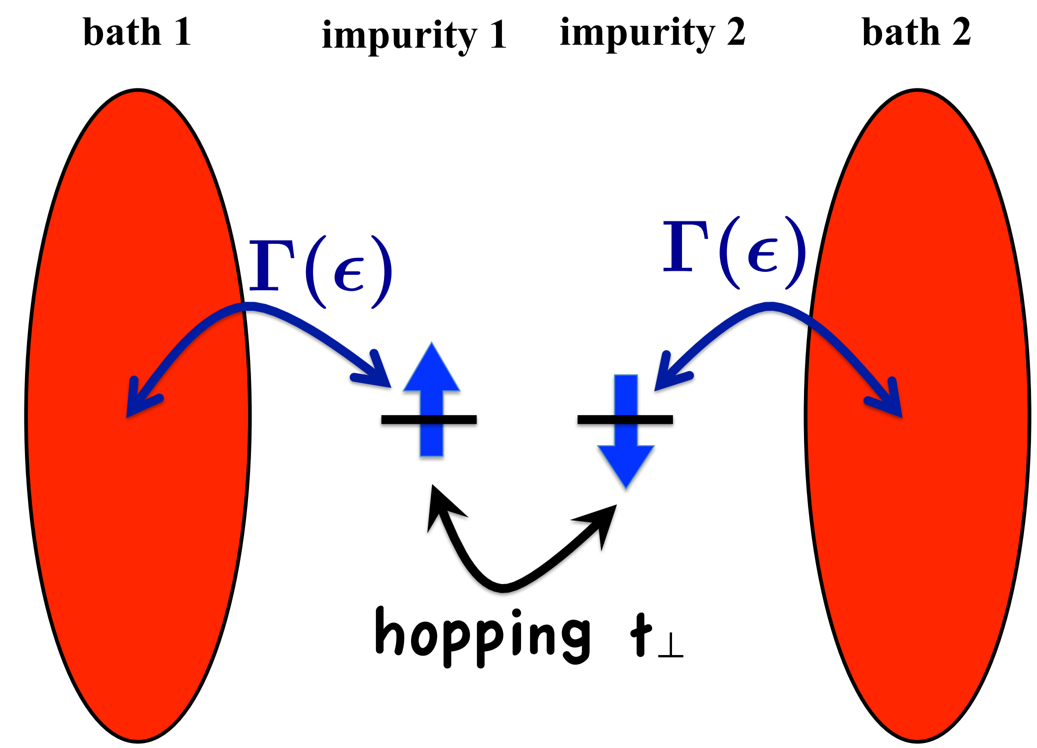
$$\mathcal{A}_{\pm}(\epsilon) = \frac{\cos^2\nu}{2\pi\Gamma}\left(\frac{T_+^2+\mu_\pm^2}{(\epsilon+\mu_\pm)^2+T_+^2} \pm \cos 2\nu\,\frac{T_-^2}{\epsilon^2+T_-^2}\right)$$

$\mu_\pm = \pm T_+ \sin(2\nu)$ measures the deviation from half-filling

the pseudo-gap is pinned at Fermi

Destabilising the QCP

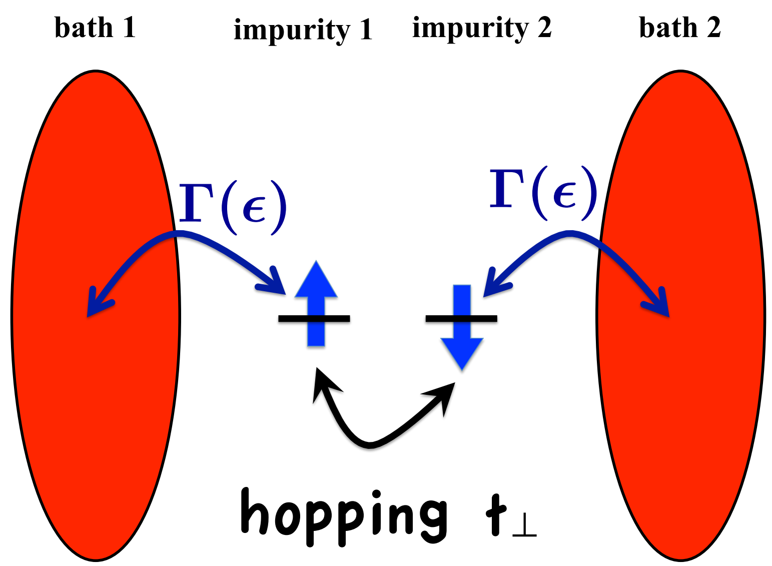
- two impurities coupled by a hopping $t_\perp$



$t_\perp$ breaks the relevant $U_f(1)$ (flavour) symmetry related to the hybridisation channel $\Delta^{hyb.}$

$$d_{1\sigma} \to \mathrm{e}^{i\phi}\, d_{1\sigma} \qquad c_{1\sigma} \to \mathrm{e}^{i\phi}\, c_{1\sigma}$$

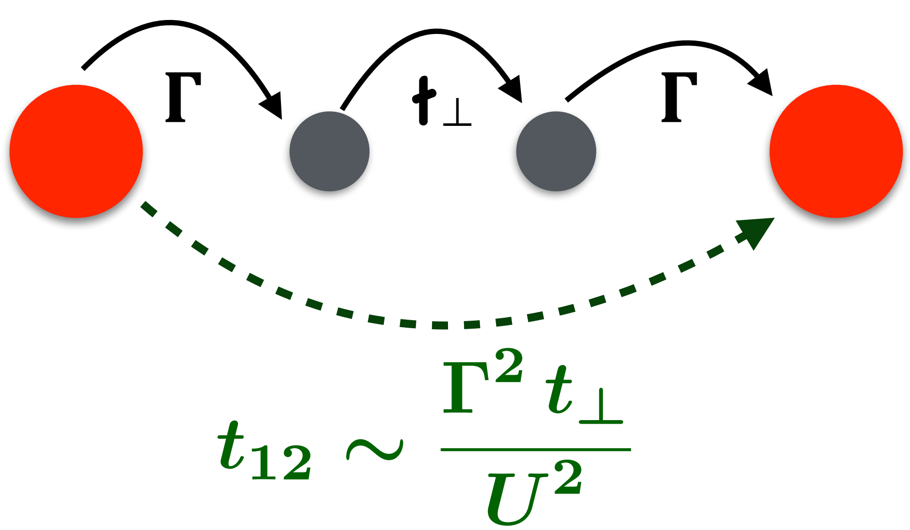
$$d_{2\sigma} \to \mathrm{e}^{-i\phi}\, d_{2\sigma} \qquad c_{2\sigma} \to \mathrm{e}^{-i\phi}\, c_{2\sigma}$$



- at leading order in $1/U$

$$t_\perp \to J = \frac{4t_\perp^2}{U}$$

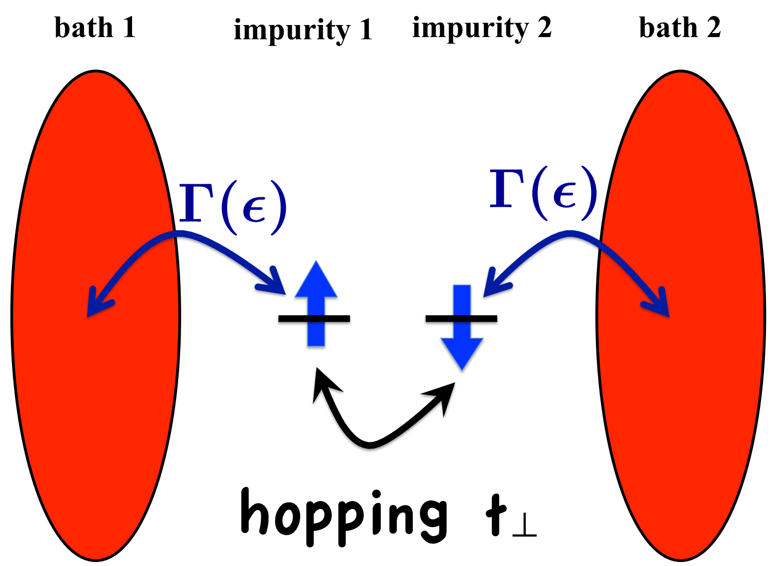
still invariant under $U_f(1)$



- next-to leading order in $1/U$

$$t_\perp \to t_{12} \sum_\sigma \left(c_{1\sigma}^\dagger c_{2\sigma} + H.c. \right)$$

only the next-to leading term breaks the $U_f(1)$ symmetry



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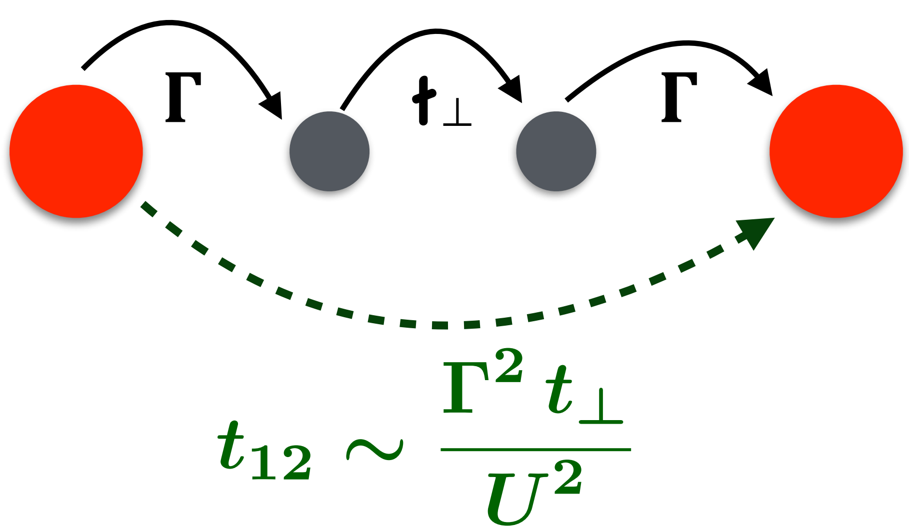
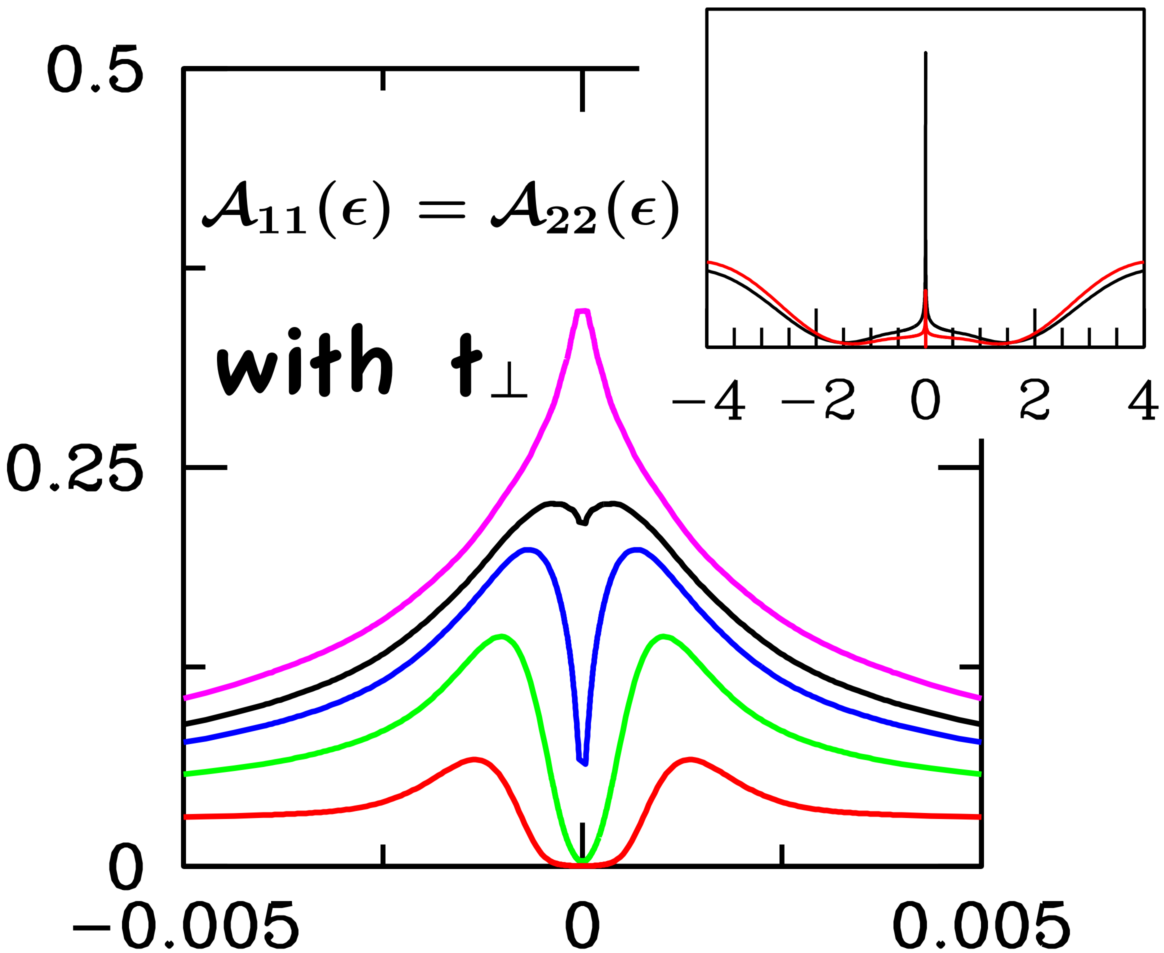
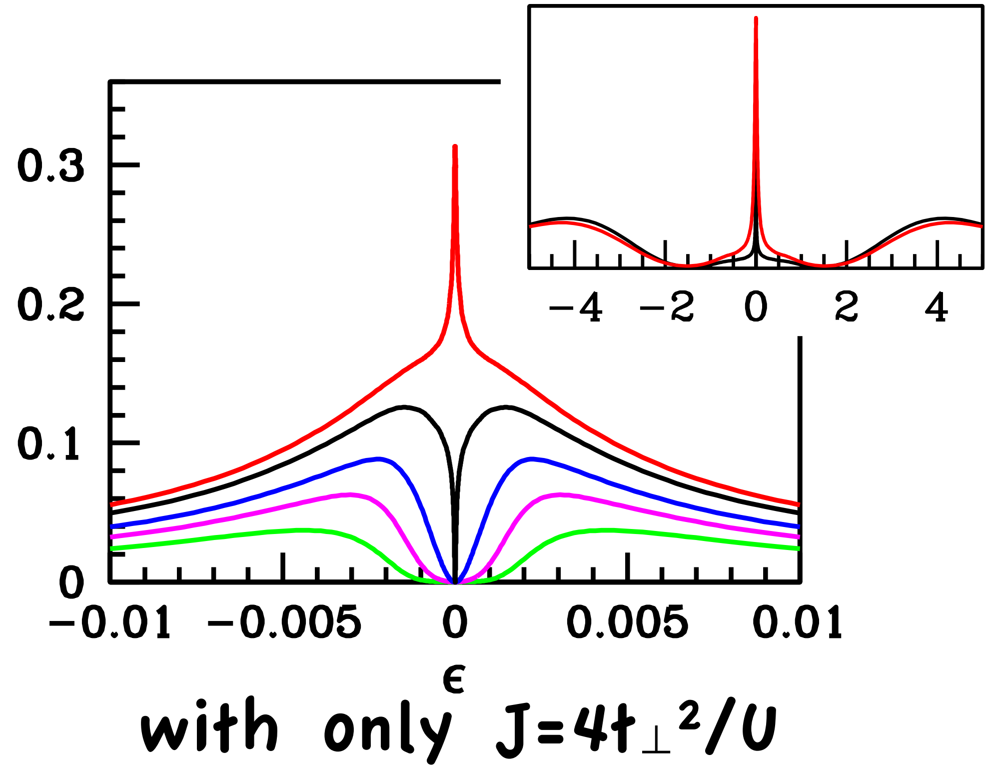


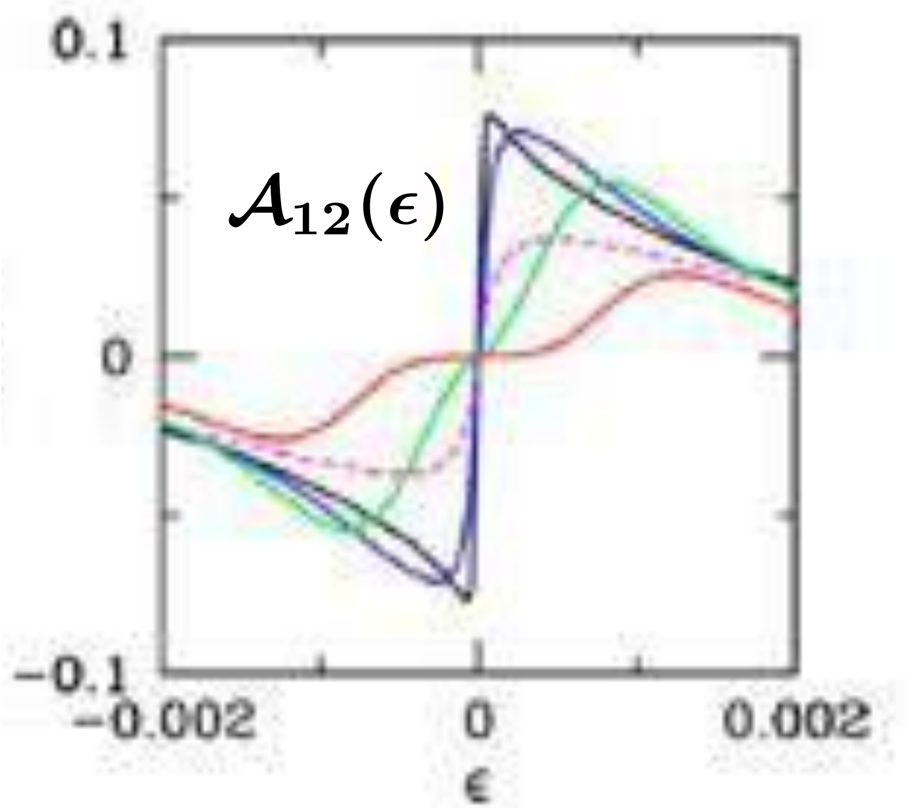
- next-to leading order in 1/U

$$t_\perp \to t_{12} \sum_\sigma \left(c^\dagger_{1\sigma} c_{2\sigma} + H.c. \right)$$

notable circumstance where $t_\perp \ll U$ generates at leading order J, which can drive the model across the QCP, but concurrently, at next-to leading order, t_{12}, which makes instead the QCP inaccessible







despite the model with $t_\perp$ is not invariant under the relevant $U_f(1)$ symmetry, yet the crossover between screened and unscreened phases is quite sharp, being $J \gg t_{12}$

Question: why approaching the QCP the system is able to respond so efficiently to a symmetry breaking term despite the vanishing quasiparticle residue Z=0?

recall that in the (local) Landau-Fermi liquid

$$A_i(i\omega) = Z^2\,\Gamma(i\omega;0;i\omega;0)$$

Answer: cancellation of vertex and self-energy corrections, $Z \to 0$ but $\Gamma \to \infty$ so that A_i is finite or even singular right at the QCP

Cancellation of vertex and self-energy corrections: physical reasons

none of the instability channels Δ_i opposes against U, but rather they all oppose against the hybridisation with the coupling Γ to the bath

their effective strength is enhanced rather than suppressed by increasing U

- without the symmetry breaking hybridisation the quasi-particle residue Z(iε) vanishes for ε→0 approaching the QCP and beyond

$$\Sigma(i\epsilon) = i\epsilon - \frac{i\epsilon}{Z(i\epsilon)} \text{ with } Z(i\epsilon) \underset{\epsilon\to 0}{\to} 0$$

- in the presence of the symmetry breaking hybridisation the self-energy acquires off-diagonal components

$$\begin{pmatrix} \Sigma(i\epsilon) & 0 \\ 0 & \Sigma(i\epsilon) \end{pmatrix} \to \begin{pmatrix} \Sigma_{11}(i\epsilon) & \Sigma_{12}(i\epsilon) \\ \Sigma_{21}(i\epsilon) & \Sigma_{22}(i\epsilon) \end{pmatrix}$$

$$\Sigma_{11}(i\epsilon) = \Sigma_{22}(i\epsilon) \qquad \& \qquad \Sigma_{21}(i\epsilon) = \Sigma_{12}(-i\epsilon)^*$$

assume cancellation of vertex and self-energy corrections and exploit what we know about weakly-disordered *s*-wave superconductors

$$\begin{pmatrix} \Sigma(i\epsilon) & 0 \\ 0 & \Sigma(i\epsilon) \end{pmatrix} \to \begin{pmatrix} \Sigma_{11}(i\epsilon) & \Sigma_{12}(i\epsilon) \\ \Sigma_{21}(i\epsilon) & \Sigma_{22}(i\epsilon) \end{pmatrix}$$

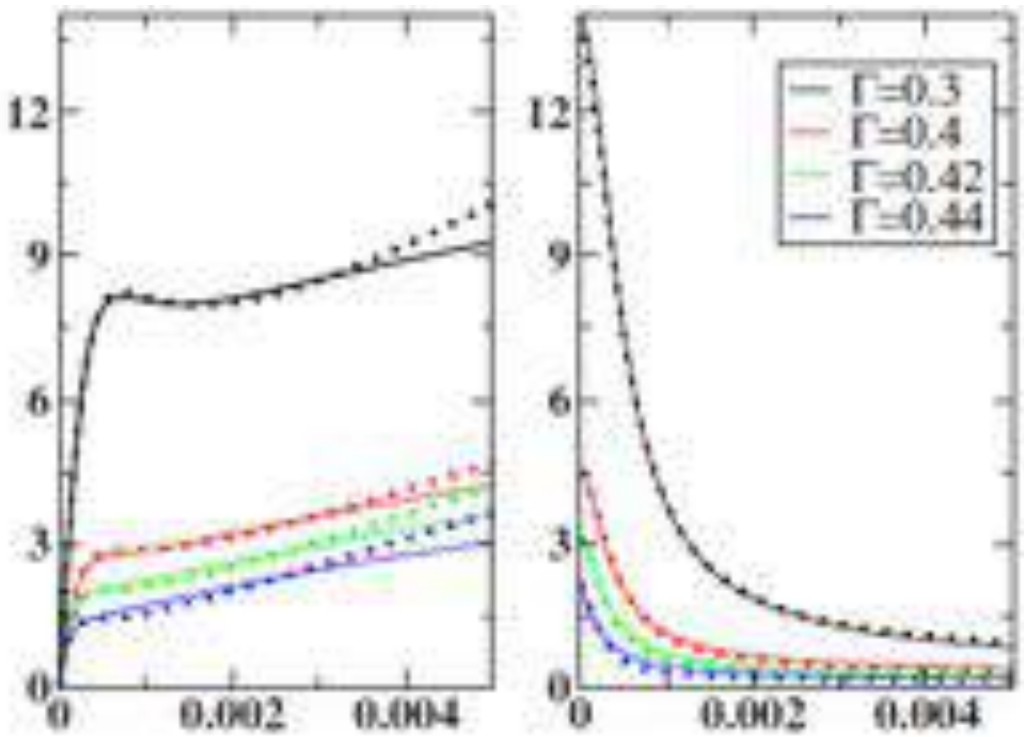
$$\Sigma_{11}(i\epsilon) = i\epsilon - \frac{i\epsilon}{Z\left(i\sqrt{\epsilon^2 + \Delta^2}\right)}$$

$$\Sigma_{12}(i\epsilon) = \frac{\Delta}{Z\left(i\sqrt{\epsilon^2 + \Delta^2}\right)}$$

Δ is a low-energy scale generated by the hybridisation that cut-offs the singularities: Fermi liquid behaviour is recovered

the assumption works extremely well at low-frequency

$\Im\mathrm{m}\Big(i\epsilon - \Sigma_{11}(i\epsilon)\Big)$ $\Re\mathrm{e}\Sigma_{12}(i\epsilon)$



ϵ

...... NRG data in the unscreened phase

—— fit with the model self-energy

$$i\epsilon - \Sigma_{11}(i\epsilon) = \frac{i\epsilon}{Z\Big(i\sqrt{\epsilon^2+\Delta^2}\Big)}$$

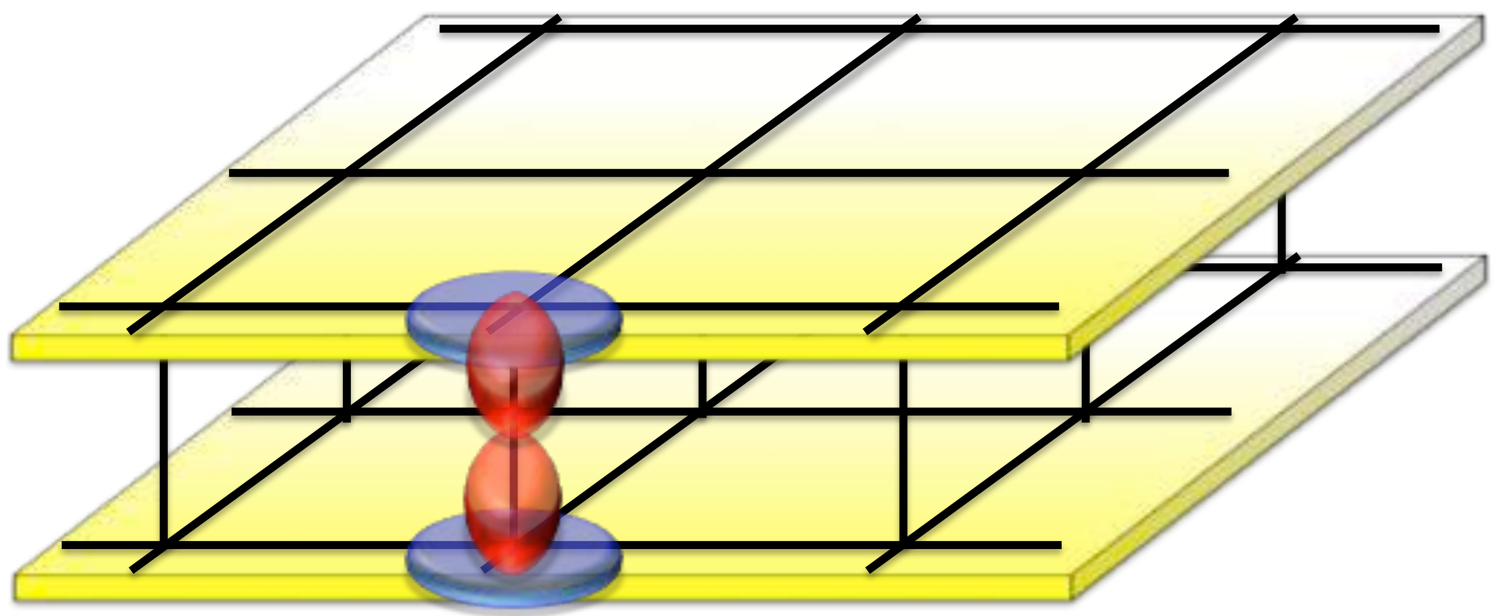
$$\Sigma_{12}(i\epsilon) = \frac{\Delta}{Z\Big(i\sqrt{\epsilon^2+\Delta^2}\Big)}$$

we thus conclude that singular self-energy and vertex corrections cancel each other

large $\Re\mathrm{e}\Sigma_{12}(0)$ in comparison with the weak symmetry breaking field

Lattice models that in infinitely coordinated lattices maps, through DMFT, onto the two-impurity model

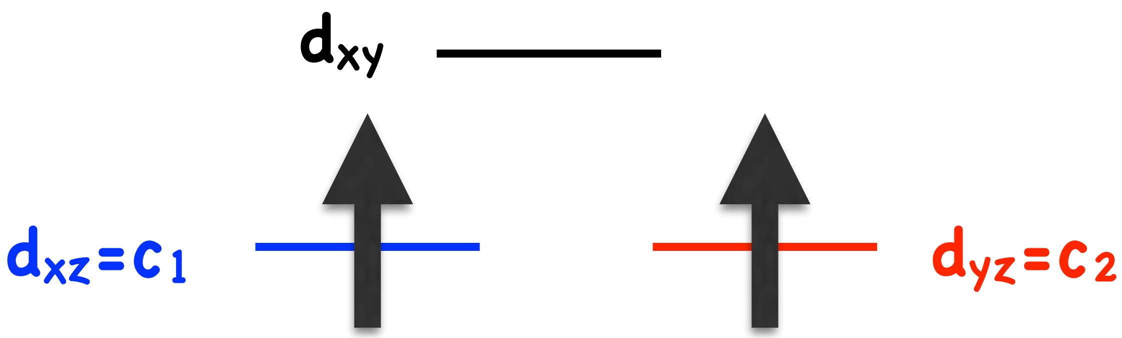
- **two-coupled Hubbard models**



$$H = -\frac{t}{\sqrt{z}} \sum_{a=1}^{2} \sum_{<ij>\sigma} \left(c^\dagger_{ia\sigma} c_{ja\sigma} + H.c. \right) + U \sum_{a=1}^{2} \sum_{i} n_{ia\uparrow} n_{ia\downarrow}$$

$$- t_\perp \sum_{i\sigma} \left(c^\dagger_{i1\sigma} c_{i2\sigma} + H.c. \right)$$

• t_{2g}^2 configuration in a square planar crystal field



$$H = -\frac{t}{\sqrt{z}}\sum_{a=1}^{2}\sum_{<ij>\sigma}\left(c^\dagger_{ia\sigma}c_{ja\sigma} + H.c.\right) + \frac{U}{2}\sum_{a=1}^{2}\sum_{i}\left(n_i - 2\right)^2$$

$$\sum_i \Big[- J_{\mathrm{H}}\,\mathbf{S}_i\cdot\mathbf{S}_i - \lambda_{\mathrm{SO}}\left(S_{ix}^2 + S_{iy}^2\right)\Big]$$

$$n_i = \sum_{a=1}^{2}\sum_{\sigma} n_{ia\sigma}$$

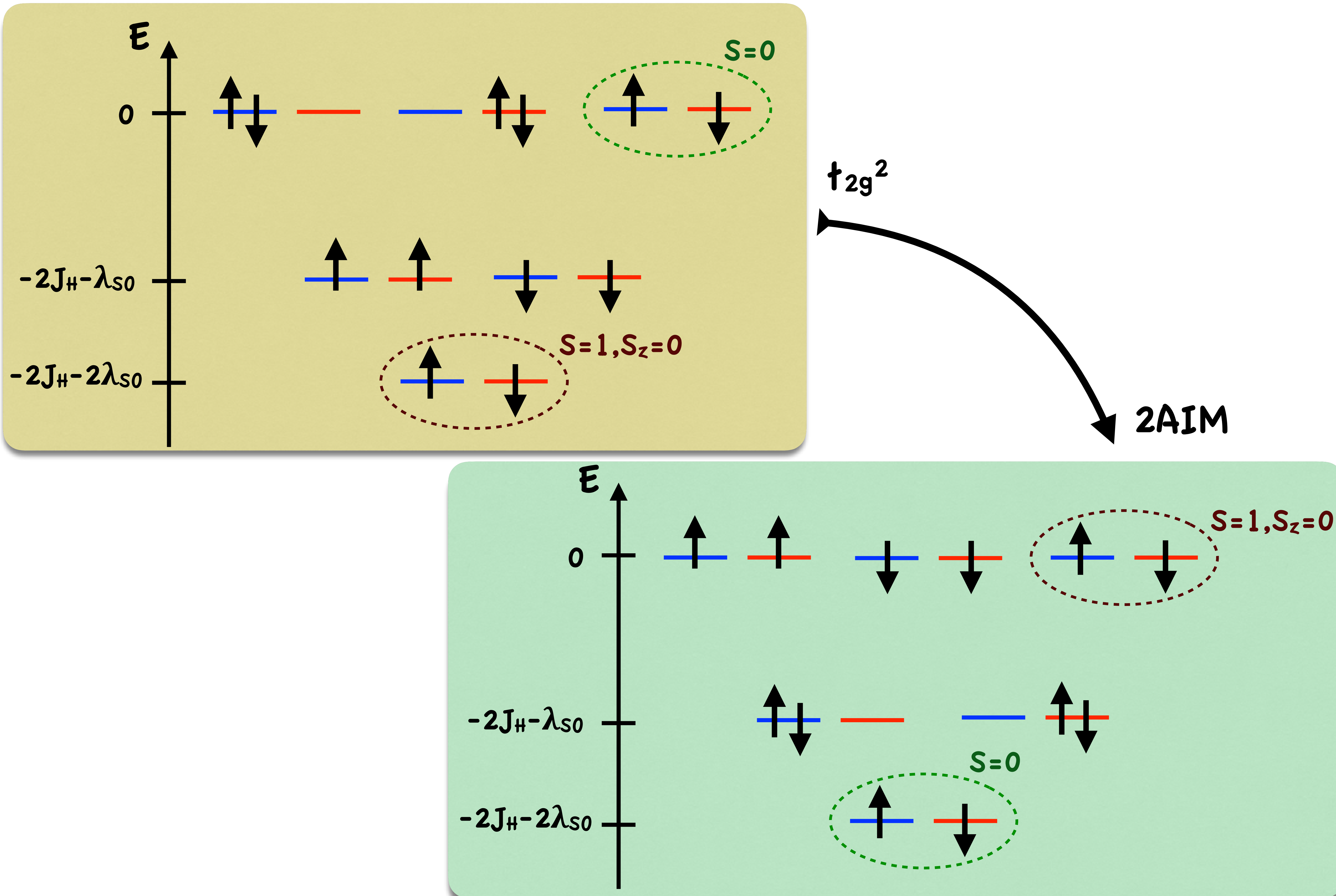
$$\mathbf{S}_i = \sum_{a=1}^{2}\sum_{\sigma\sigma'} c^\dagger_{ia\sigma}\,\mathbf{S}_{\sigma\sigma'}\,c_{ia\sigma'}$$

Hund's rule favouring
high-spin S=1

single-ion anisotropy mediated
by the spin-orbit coupling with the d_{xy}

the same physics as the 2AIM under the transformation:

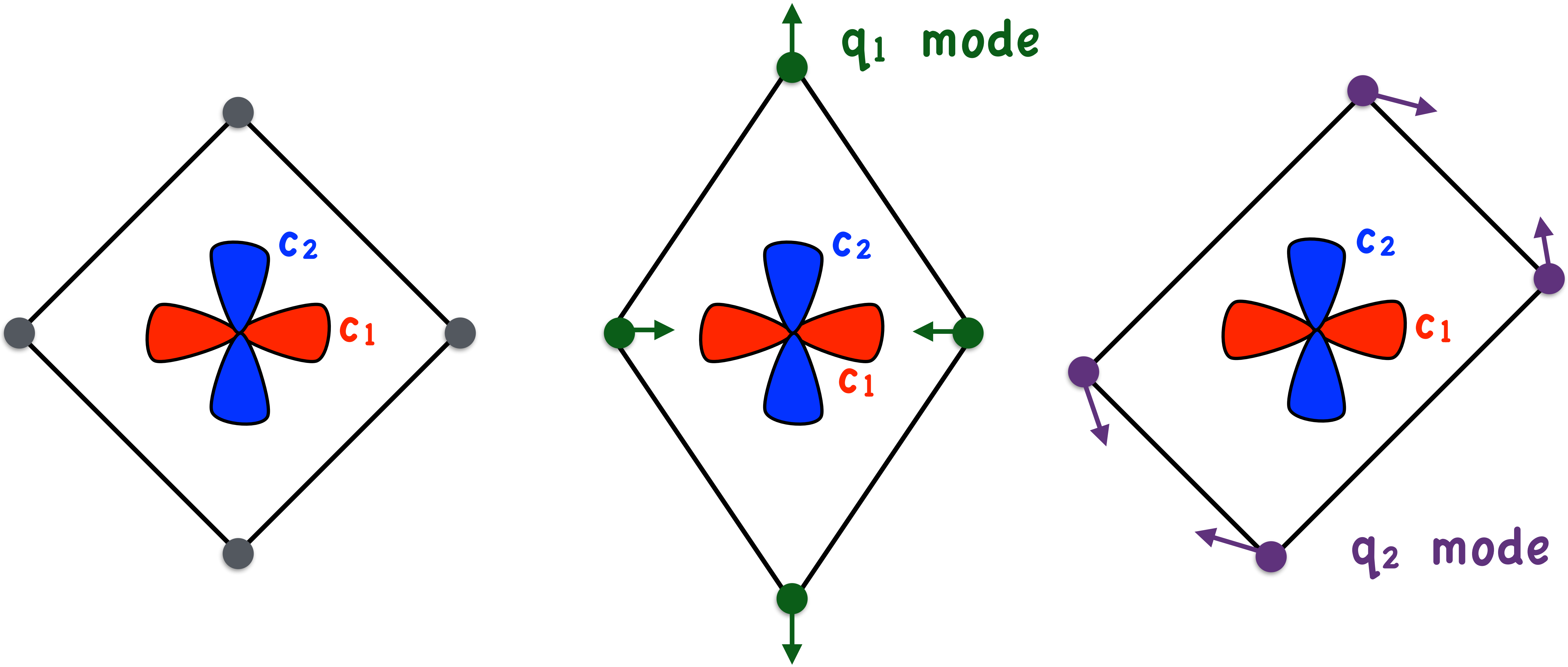
$$c_{1\uparrow} \to c_{1\uparrow} \quad c_{1\downarrow} \to c_{2\uparrow} \quad c_{2\uparrow} \to c_{1\downarrow} \quad c_{2\downarrow} \to c_{2\downarrow}$$



how do the instability channels transform?

2AIM	t_{2g}^2
$S_1^z - S_2^z$ $S_1^+ - S_2^+$ $S_1^- - S_2^-$	$S_1^z - S_2^z$ $c_{1\uparrow}^\dagger c_{2\uparrow} - c_{1\downarrow}^\dagger c_{2\downarrow}$ $c_{2\uparrow}^\dagger c_{1\uparrow} - c_{2\downarrow}^\dagger c_{1\downarrow}$
$\sum_\sigma \left[\mathrm{e}^{i\phi}\, c_{1\sigma}^\dagger c_{2\sigma} + H.c. \right]$	$\cos\phi\, S^x - \sin\phi\, S^y$
$\left[\mathrm{e}^{i\phi}\, (c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger + c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger) + H.c. \right]$	$\left[\mathrm{e}^{i\phi}\, (c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger) + H.c. \right]$

- **E×e Jahn-Teller effect**



$$H_{\mathrm{JT}} = \frac{\Omega}{2}\sum_{a=1}^{2}\left(p_a^2 + q_a^2\right) - g\sum_{\sigma}\left[q_1\left(c_{1\sigma}^{\dagger}c_{1\sigma} - c_{2\sigma}^{\dagger}c_{2\sigma}\right) + q_2\left(c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}\right)\right]$$

$$H_{\mathrm{JT}} = \frac{\Omega}{2} \sum_{a=1}^{2} \left(p_a^2 + q_a^2\right) - g \sum_{\sigma} \left[q_1 \left(c_{1\sigma}^\dagger c_{1\sigma} - c_{2\sigma}^\dagger c_{2\sigma}\right) + q_2 \left(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}\right) \right]$$

integrate out the vibrations and neglect retardation

$$H_{\mathrm{JT}}^{\mathrm{eff}} = -\frac{2g^2}{\Omega} \left(T_x^2 + T_z^2\right) \equiv -2J \left(T_x^2 + T_z^2\right) \Longrightarrow -2J \left(T_x^2 + T_y^2\right)$$

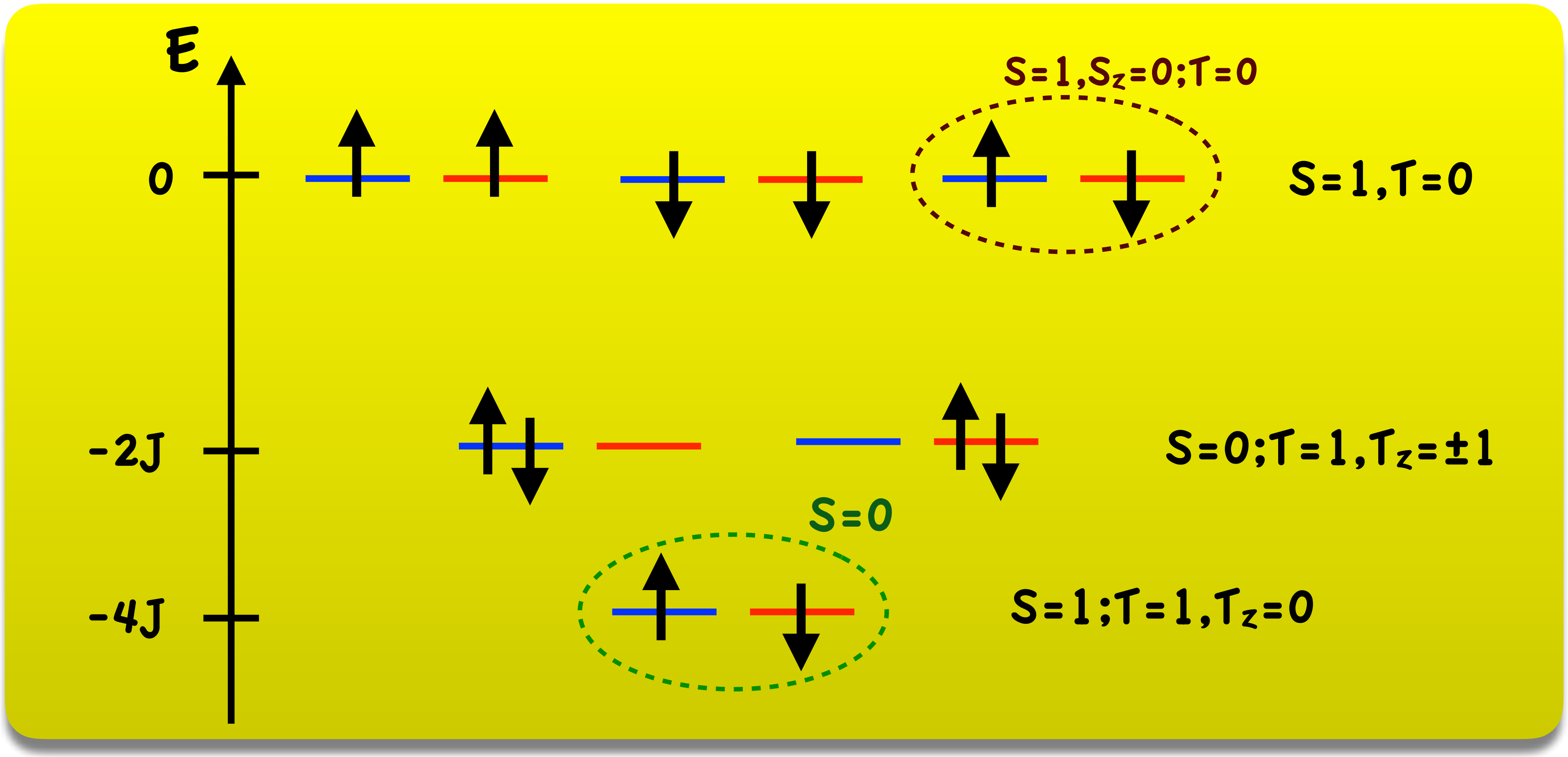
π/2 rotation around the x-axis

$$T_\alpha = \frac{1}{2} \sum_{\sigma} \sum_{a,b=1}^{2} c_{a\sigma}^\dagger \, \tau_{ab}^\alpha \, c_{b\sigma} \qquad \tau^x, \tau^y, \tau^z = \text{ Pauli matrices}$$

orbital pseudo-spin 1/2

- **lattice model**

$$H = -\frac{t}{\sqrt{z}} \sum_{<i,j>\sigma} \sum_{a=1}^{2} \left(c^\dagger_{ia\sigma} c_{ja\sigma} + H.c. \right) + \frac{U}{2} \sum_i \left(n_i - 2 \right)^2$$
$$- 2J \sum_i \left(T_x^2 + T_y^2 \right)$$



like in the 2AIM the ground state is a non-degenerate spin-singlet

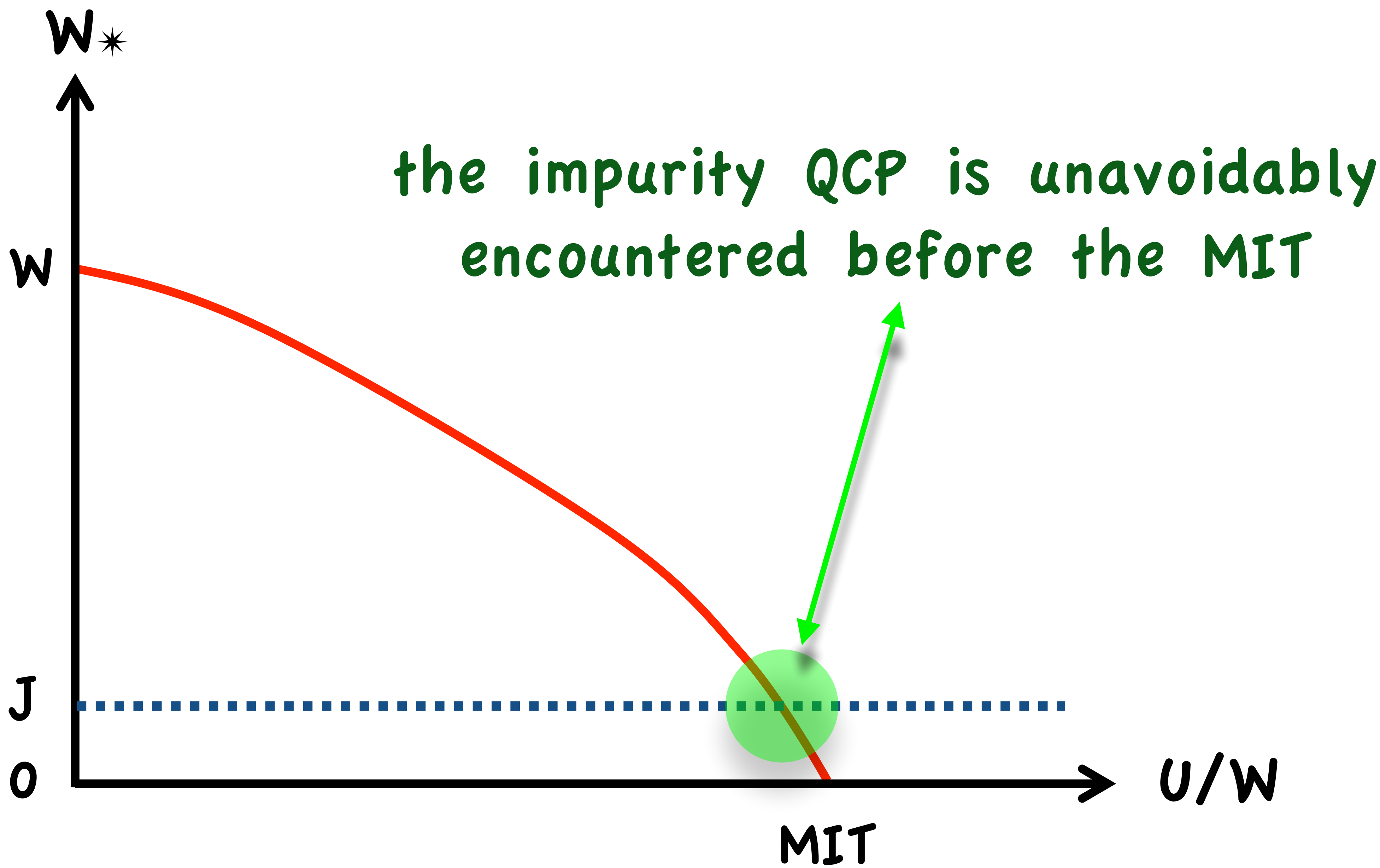
in all those three lattice models, the ground state in the atomic limit is non-degenerate and it is stabilised with respect to the other excited states by an on-site term of strength **J**

in the impurity models onto which those lattice models map by DMFT, **J** tends to lock the impurity into a non-degenerate state and thus competes with the Kondo effect, whose energy scale is the Kondo temperature $\mathbf{T_K}$

What shall we expect?

- bandwidth = W and J≪W

$$W_* = \mathrm{Z}\, W \Rightarrow T_{\mathrm{K}}$$

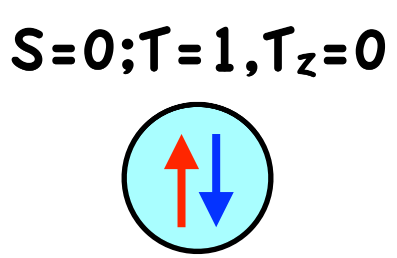


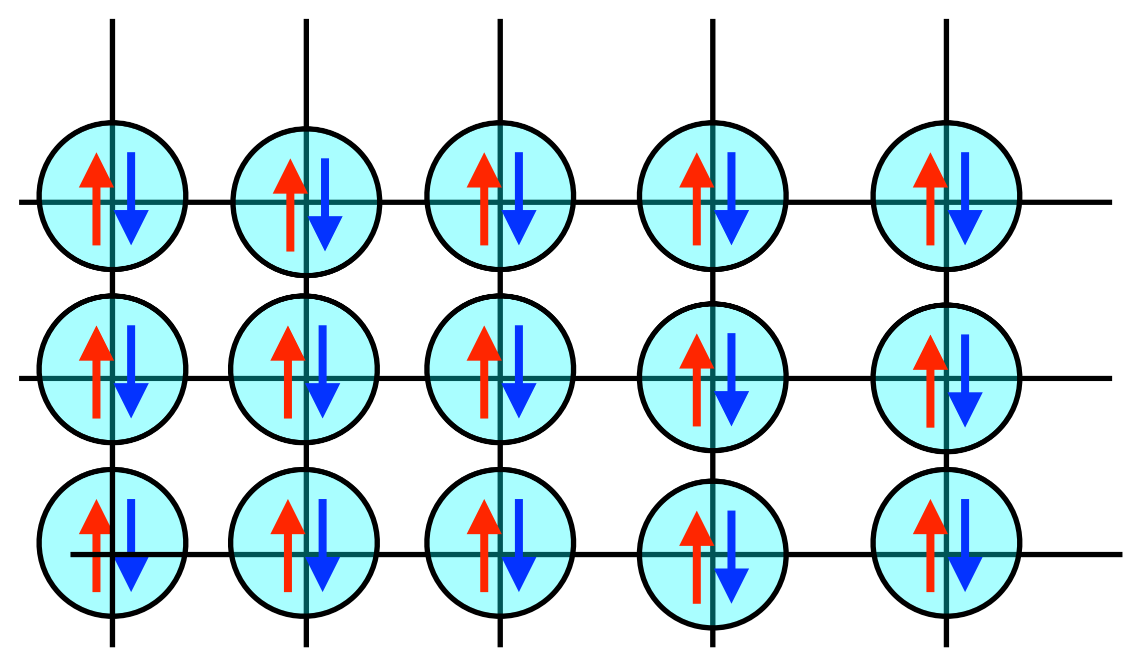
Explicit DMFT calculation: the E×e Jahn-Teller model

$$H = -\frac{t}{\sqrt{z}} \sum_{<i,j>\sigma} \sum_{a=1}^{2} \left(c^\dagger_{ia\sigma} c_{ja\sigma} + H.c. \right) + \frac{U}{2} \sum_i \left(n_i - 2 \right)^2 - 2J \sum_i \left(T_x^2 + T_y^2 \right)$$

- **atomic limit ≈ Mott insulator**

each site will freeze in the non-degenerate atomic ground state with S=0, T=1 and T_z=0: the on-site version of a valence-bond crystal





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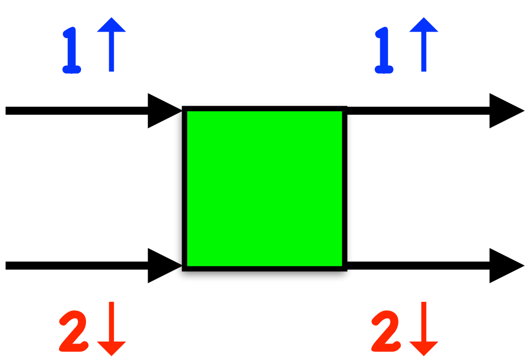
$$H = -\frac{t}{\sqrt{z}} \sum_{<i,j>\sigma} \sum_{a=1}^{2} \left(c^{\dagger}_{ia\sigma} c_{ja\sigma} + H.c. \right) + \frac{U}{2} \sum_{i} \left(n_i - 2 \right)^2 - 2J \sum_{i} \left(T_x^2 + T_y^2 \right)$$

- **weak-coupling U≪W**

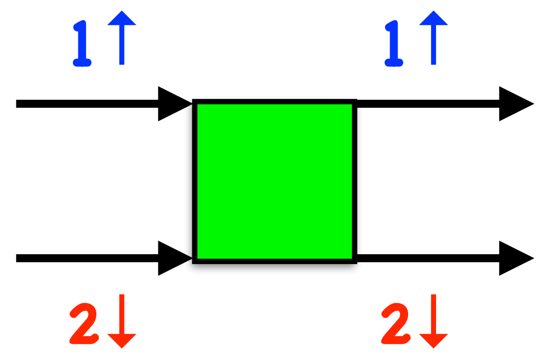
half-filled two-band metal with pairing channel:



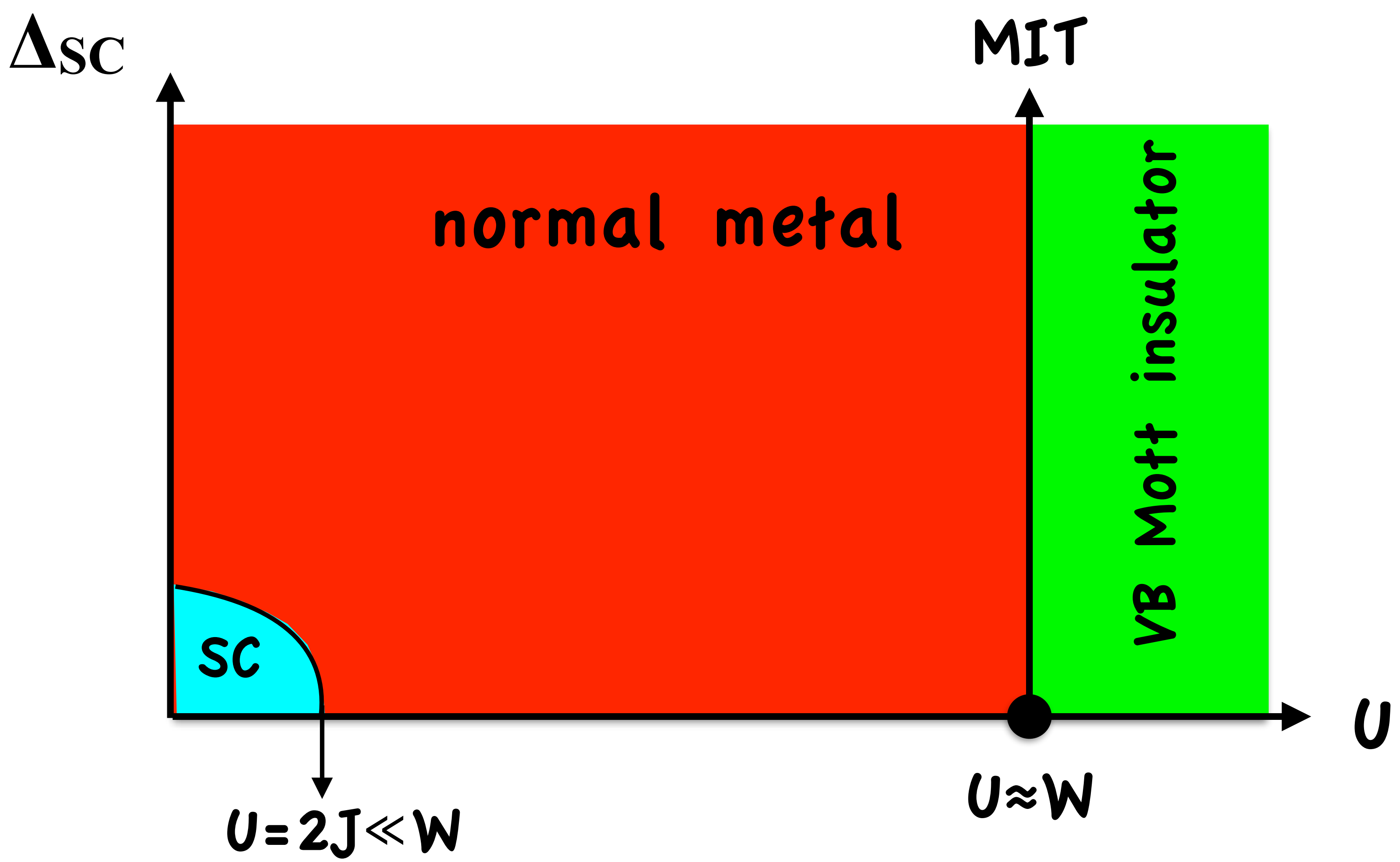
$= - (2J - U) = - \rho^{-1} (\lambda - \mu_{*})$

- if U<2J the metal is unstable towards s-wave superconductivity
- if U>2J the vertex is repulsive and the system is a normal metal

• naïve expectation

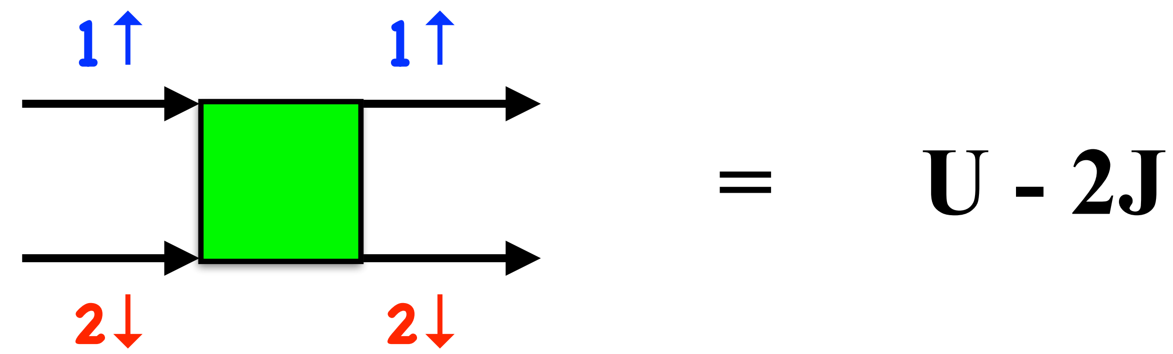


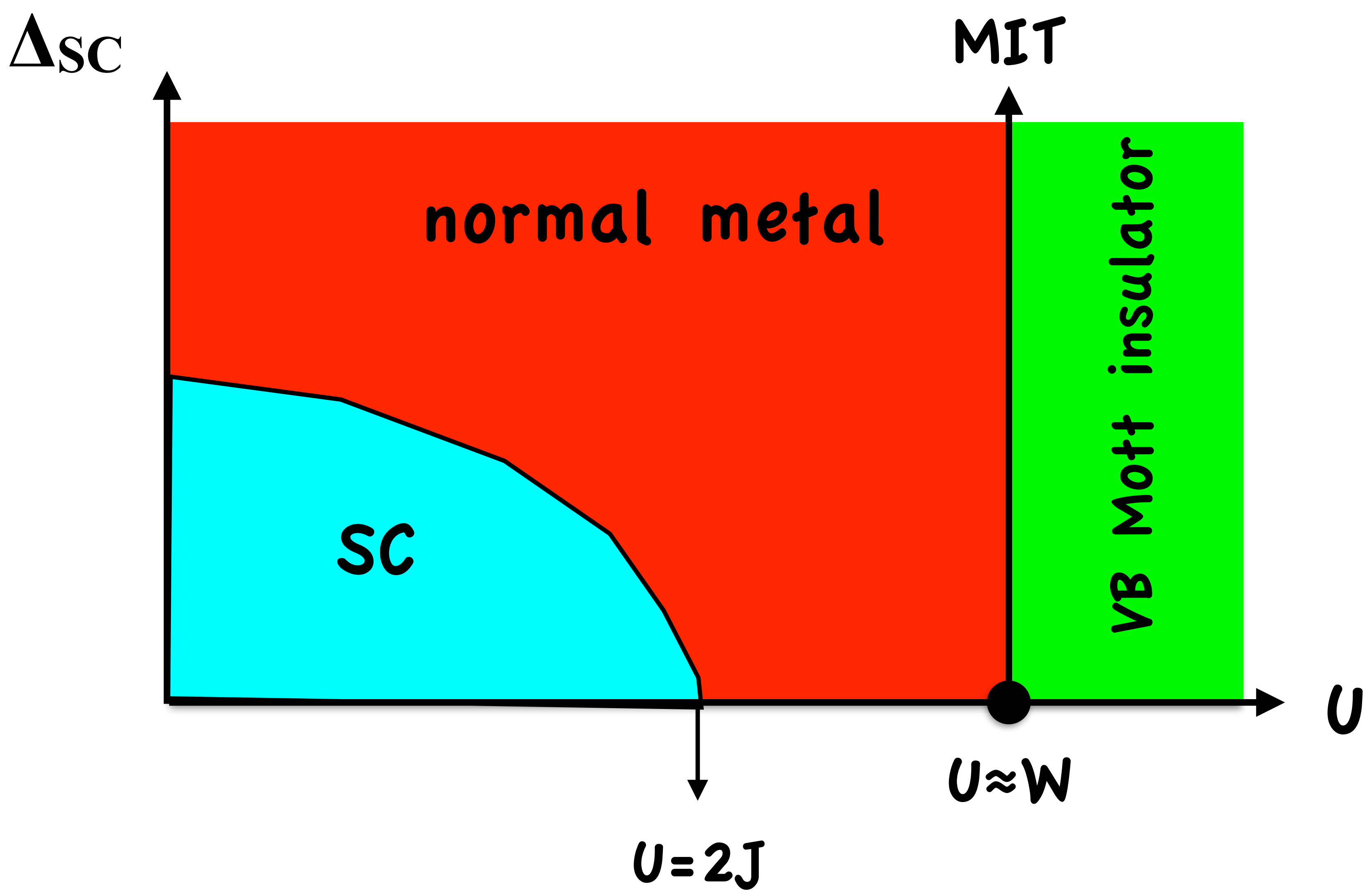
$= \quad U - 2J$



if J is much smaller than the bandwidth

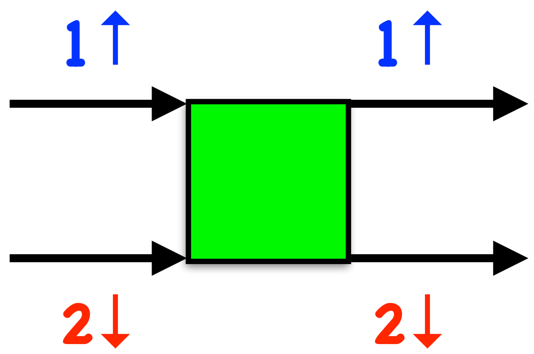
• **naïve expectation**



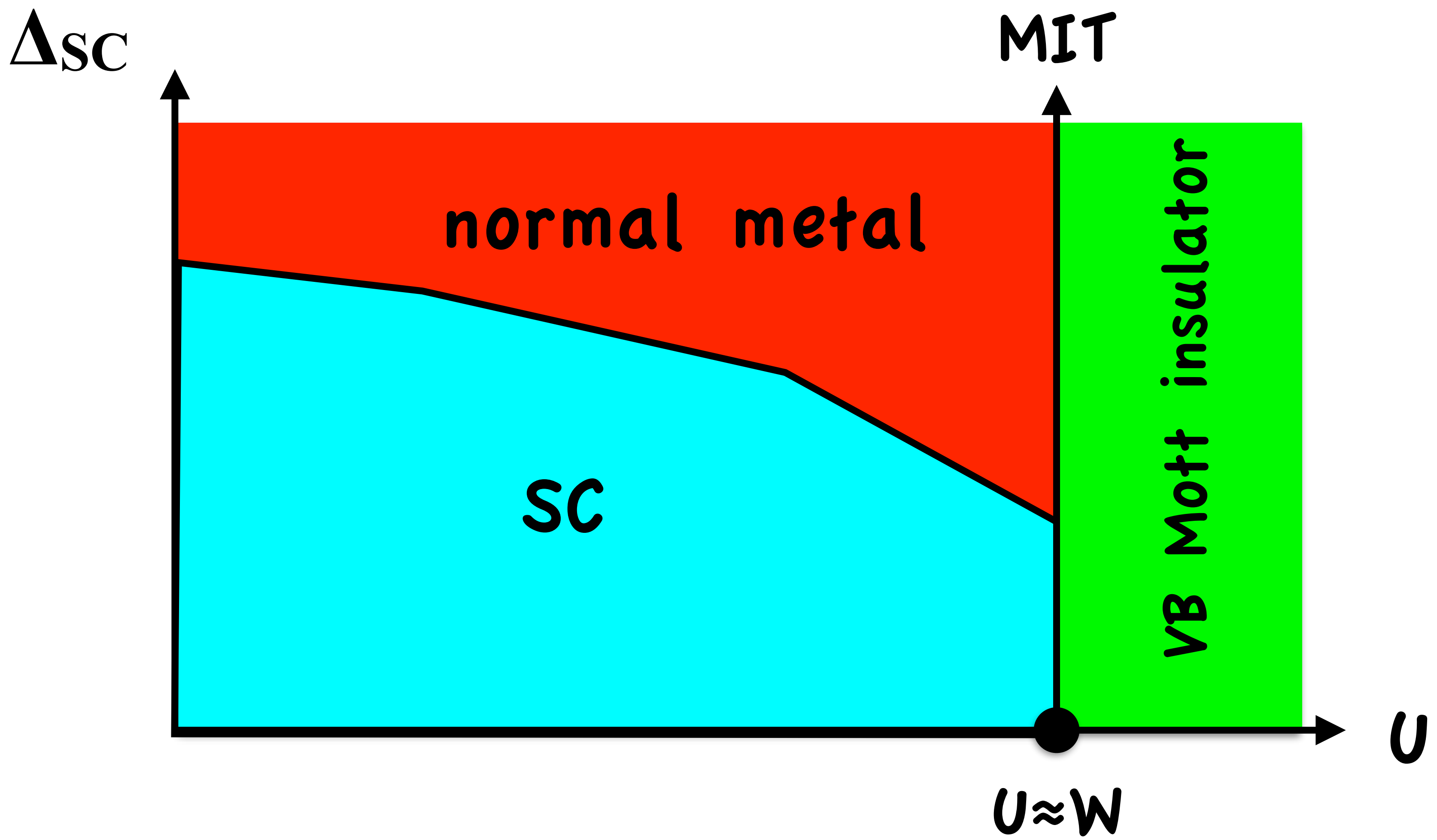


then J increases

• **naïve expectation**

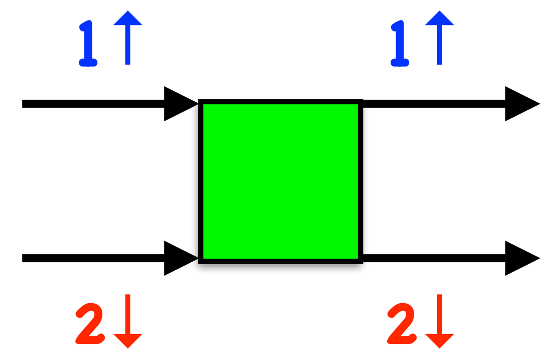


$= \quad U - 2J$

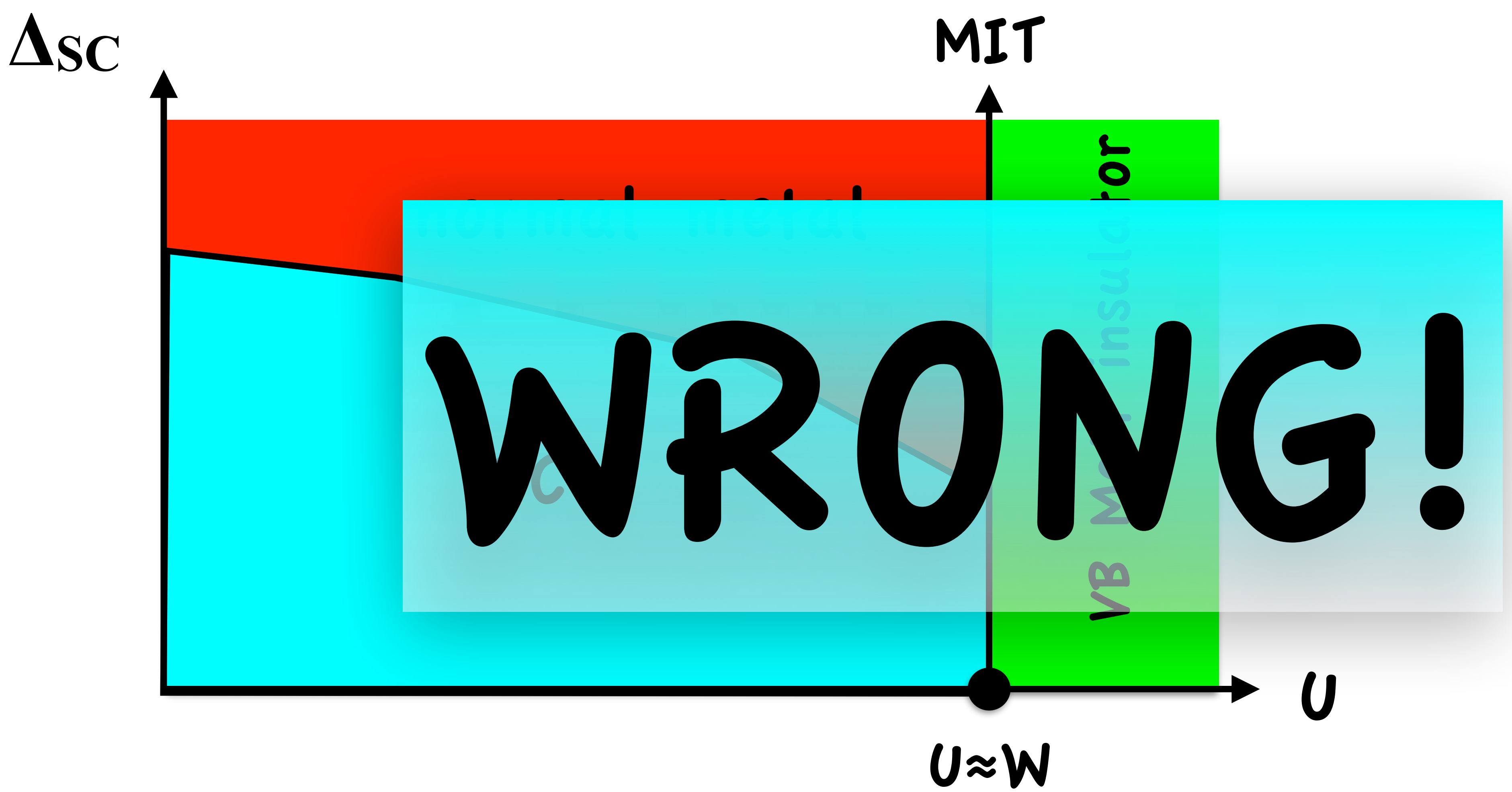


till it becomes comparable with the bandwidth

• **naïve expectation**

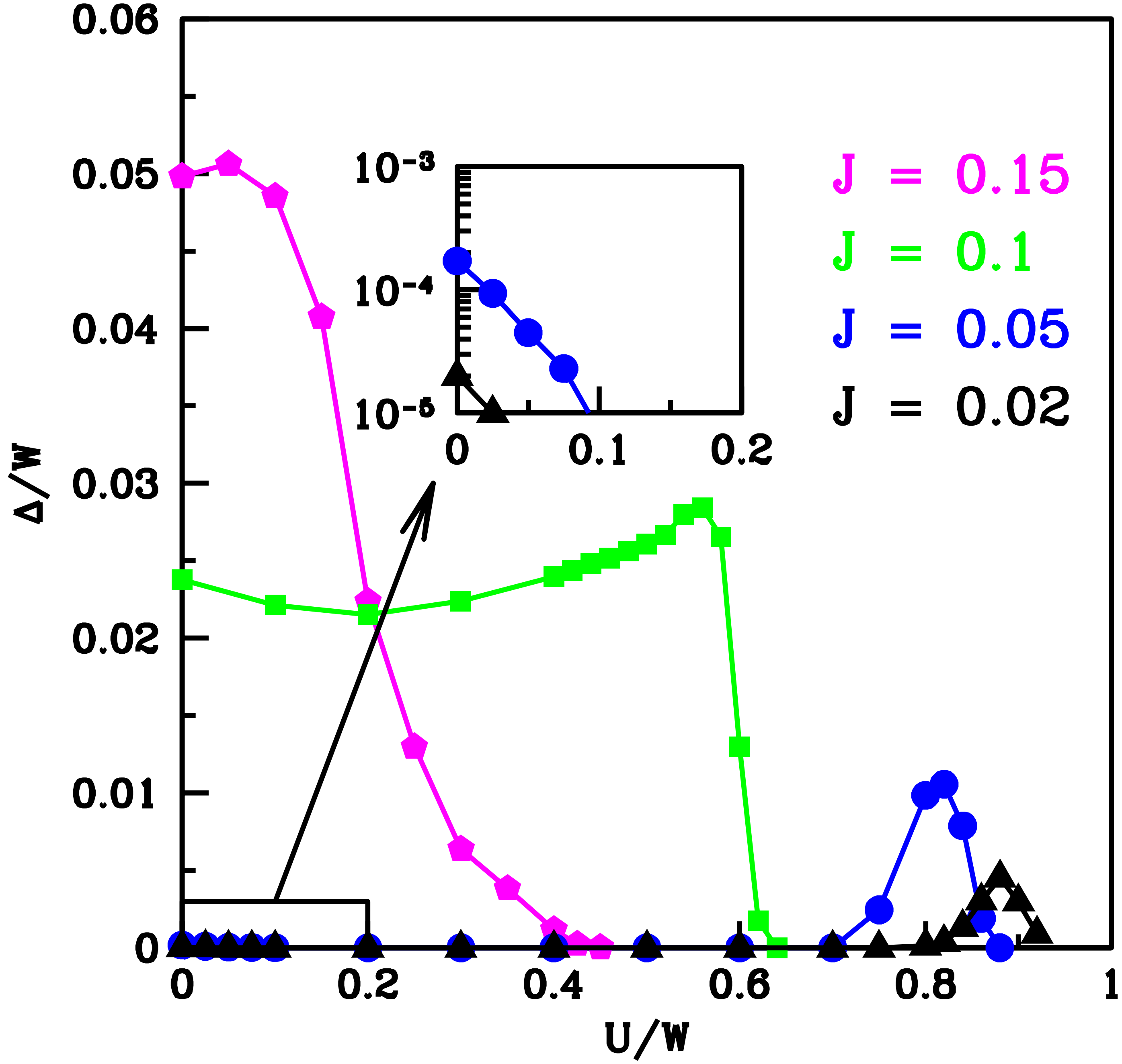


$= \quad U - 2J$



till it becomes comparable with the bandwidth

True DMFT phase diagram

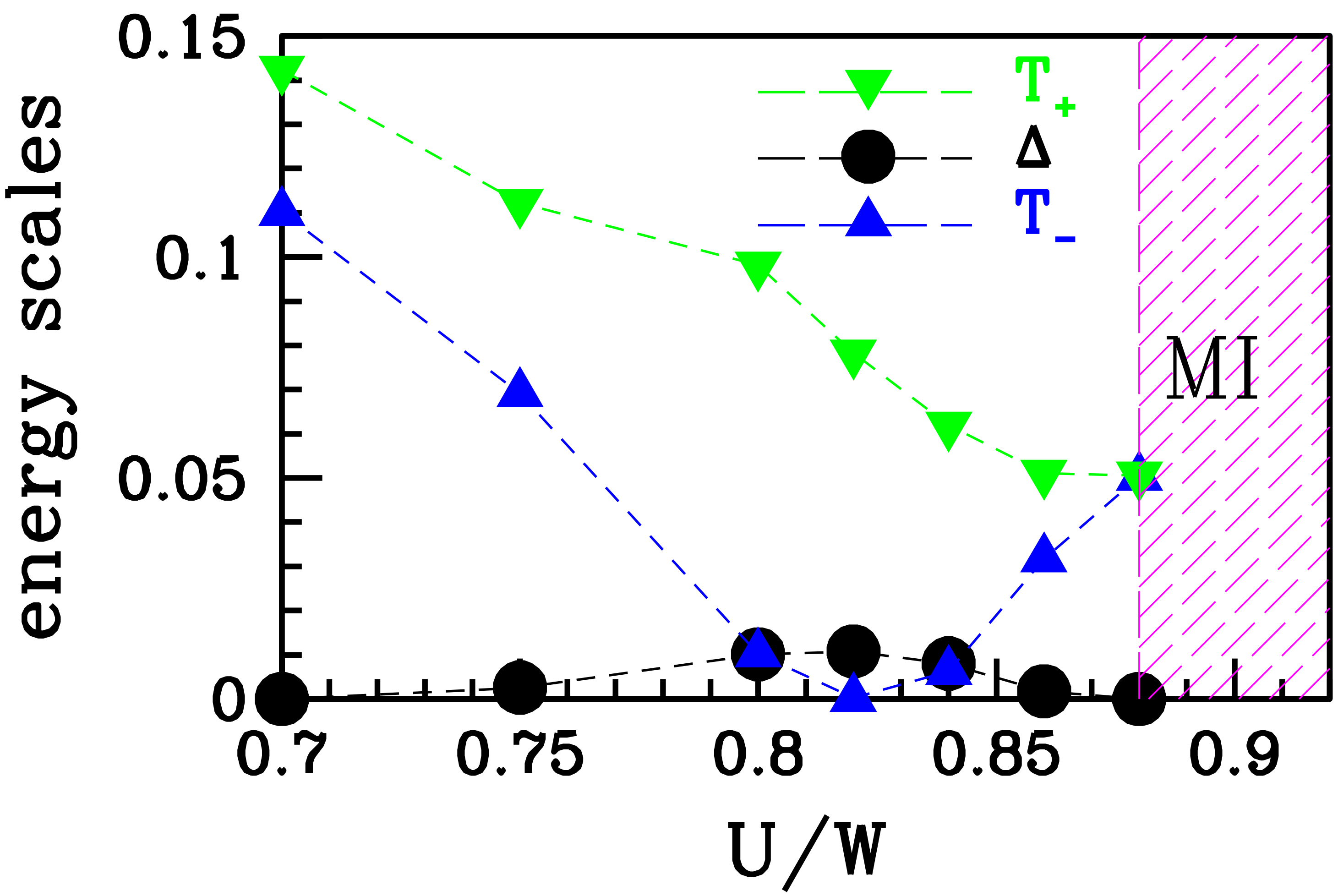


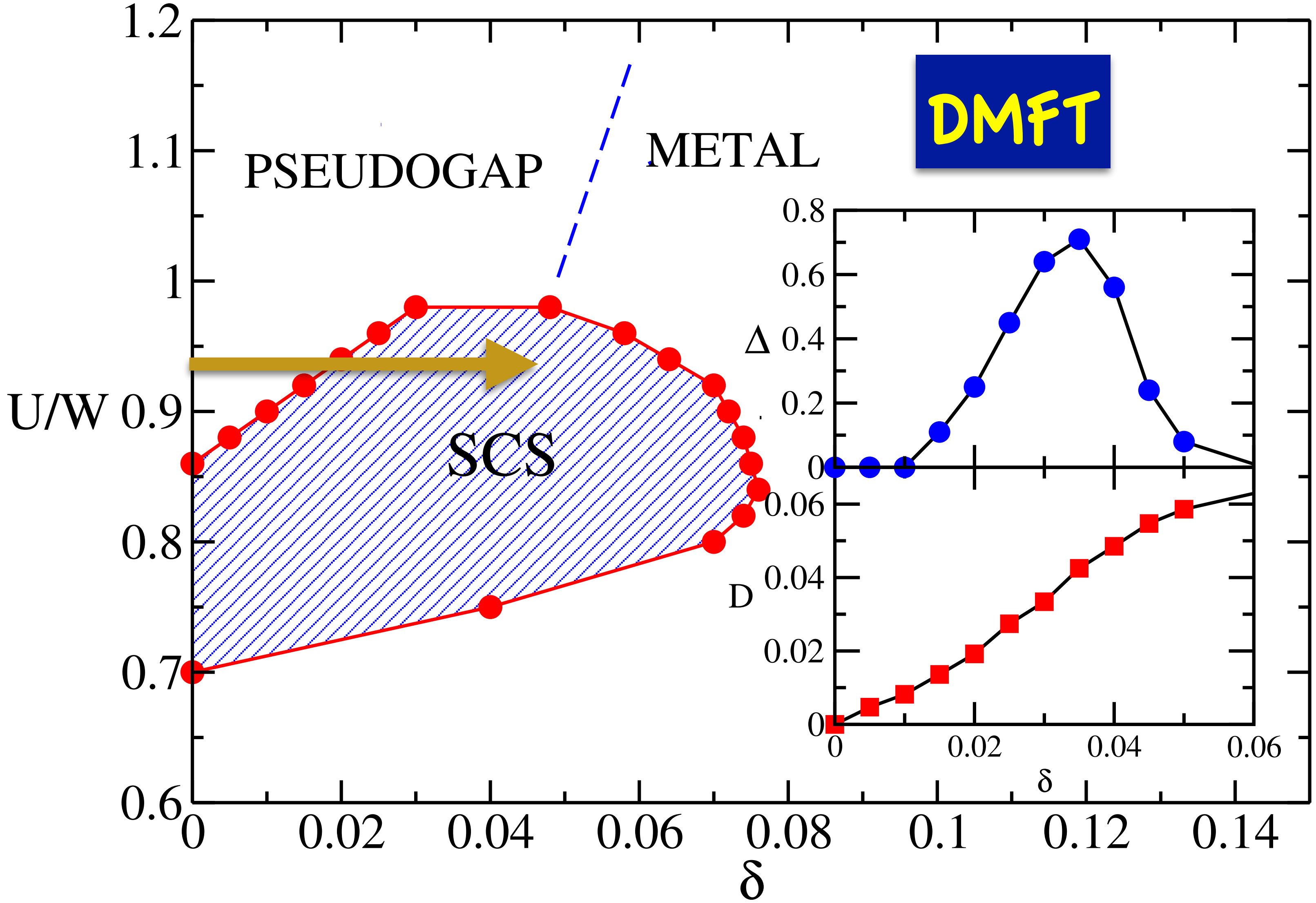
for small J a superconducting dome appears right before the MIT with a Δ_{SC} much bigger than at U=0: this is just the mere manifestation of the impurity QCP

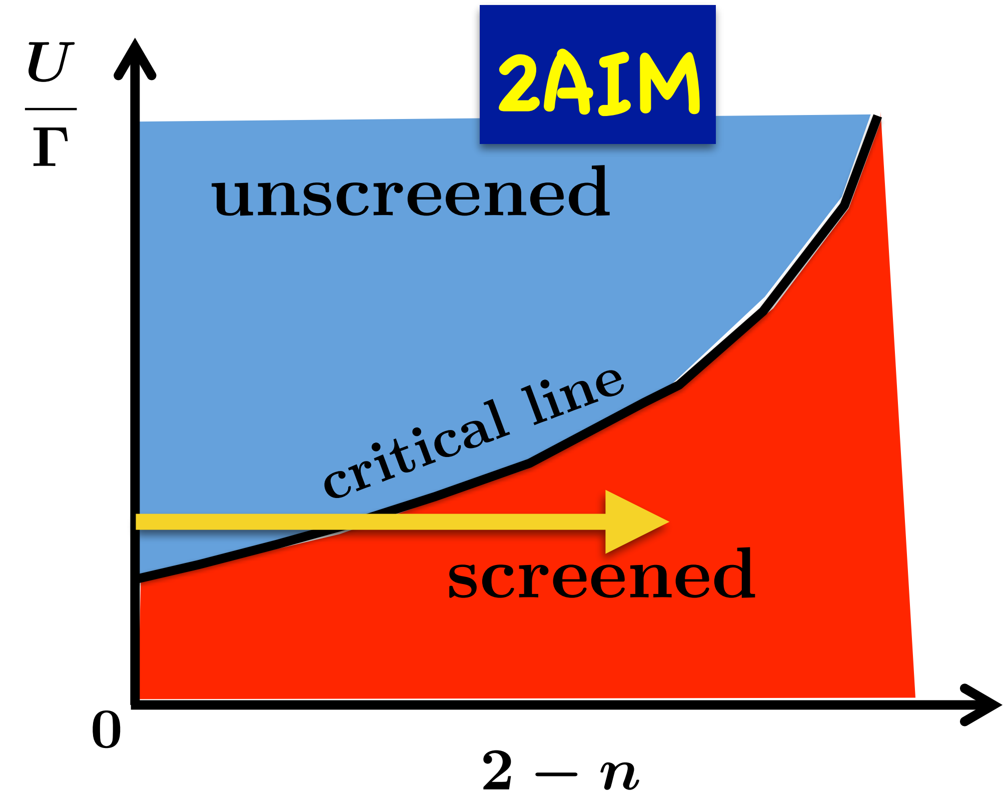
… indeed the low-frequency fit of the putative T=0 normal phase, obtained by not allowing anomalous components of the Green's function in DMFT, with

$$\mathcal{G}_{\pm}(i\epsilon) = \frac{1}{i\epsilon + i\Gamma\mathrm{sign}(\epsilon) - \Sigma_{\pm}(i\epsilon)} \simeq \frac{1}{2\Gamma}\left(\frac{T_+}{i\epsilon + iT_+\,\mathrm{sign}(\epsilon)} \pm \frac{T_-}{i\epsilon + iT_-\,\mathrm{sign}(\epsilon)}\right)$$

works extremely well and provides estimates of T_+ and T_-







the physics of the isolated impurity emerges overwhelmingly also in the behaviour away from half-filling

Take-home message

- **The physics of the Anderson impurity might be very useful in interpreting and even anticipating the behaviour of correlated models next to a Mott transition.**

- **This is indeed the case in infinitely coordinated lattices.**

- **In realistic lattices with finite coordination, Fermi liquid theory suggests that part of the Kondo physics may still survive — to what extent is so far unclear.**

Final warning...

- in most examples relevant to DMFT, one encounters impurity models H_{AIM} with no true quantum critical point, but rather with a sharp crossover, like the model of two impurities coupled to each other by $t_\perp$

- in this case it might be convenient to find the underlying impurity model $H^{(0)}_{AIM}$, which is invariant under a larger symmetry group that allows the critical point to exist.

- afterwards, one should regard the original model H_{AIM} as the higher-symmetry one $H^{(0)}_{AIM}$ plus a relevant symmetry breaking perturbation δH_{AIM}, i.e.

$$H_{AIM} = H^{(0)}_{AIM} + \delta H_{AIM}$$

POSTDOCTORAL POSITIONS AVAILABLE IN SISSA

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