Quantum criticality in Quantum impurity systems and Luttinger–Friedel sum rule

~ Luttinger integral as a topological invariant ~

Curtin O. J., Nishikawa Y., Hewson A. C., Crow D. J. G. JOURNAL OF PHYSICS COMMUNICATIONS 2 (031001) 2018 :
https://arxiv.org/abs/1703.01807

Nishikawa Y., Curtin O. J., Hewson A. C., Crow D. J. G.,PHYSICAL REVIEW B 98 (104419) 2018, :
https://arxiv.org/abs/1712.08771

International Symposium in Honor of Professor Nambu for the 10th Anniversary of his Nobel Prize in Physics

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Outline of Presentation

1. Model and Systems

   General Background

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2. Method and Some Results

   Renormalized Perturbation Theory and Numerical Renormalization Group

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   Discussion

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Model and Systems

General Background

Single Impurity Anderson Model (SIAM)

$$H_{\mathrm{AM}} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} \left(V_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} + \mathrm{H.C.} \right) + \epsilon_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U \left(d^{\dagger}_{\uparrow} d_{\uparrow} \right) \left(d^{\dagger}_{\downarrow} d_{\downarrow} \right)$$

continuous energy levels
(non-interacting system)

hybridization

discrete energy level + interaction

Fig.1

Dilute magnetic alloys
(Kondo effect)

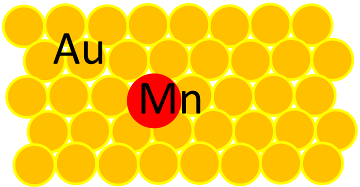


Fig.2

Scanning tunneling microscopy
(STM)

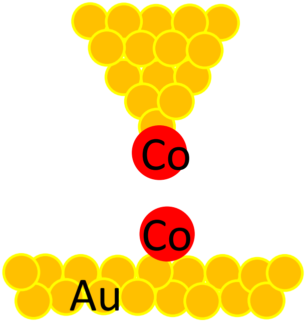


Fig.3

Quantum dot

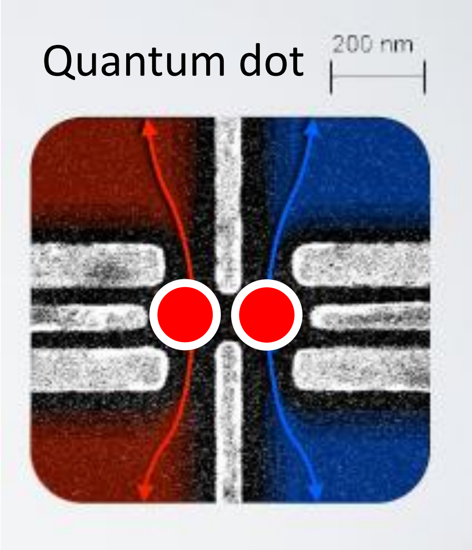


Fig.3

High-Tc superconductor
(Cuprate: YBa2Cu3O7-δ)

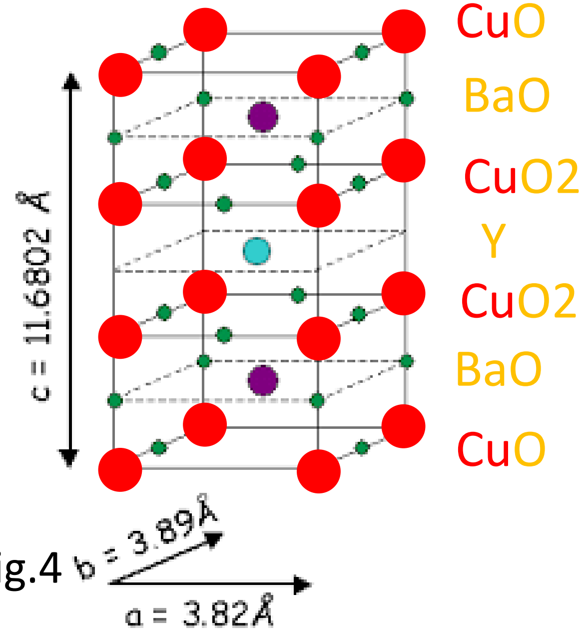
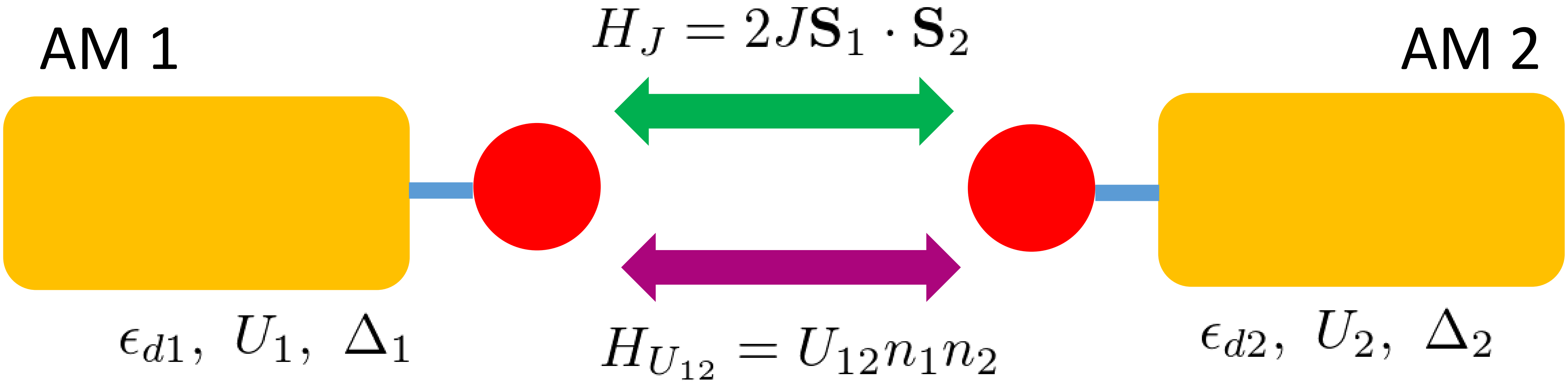


Fig.4

Model

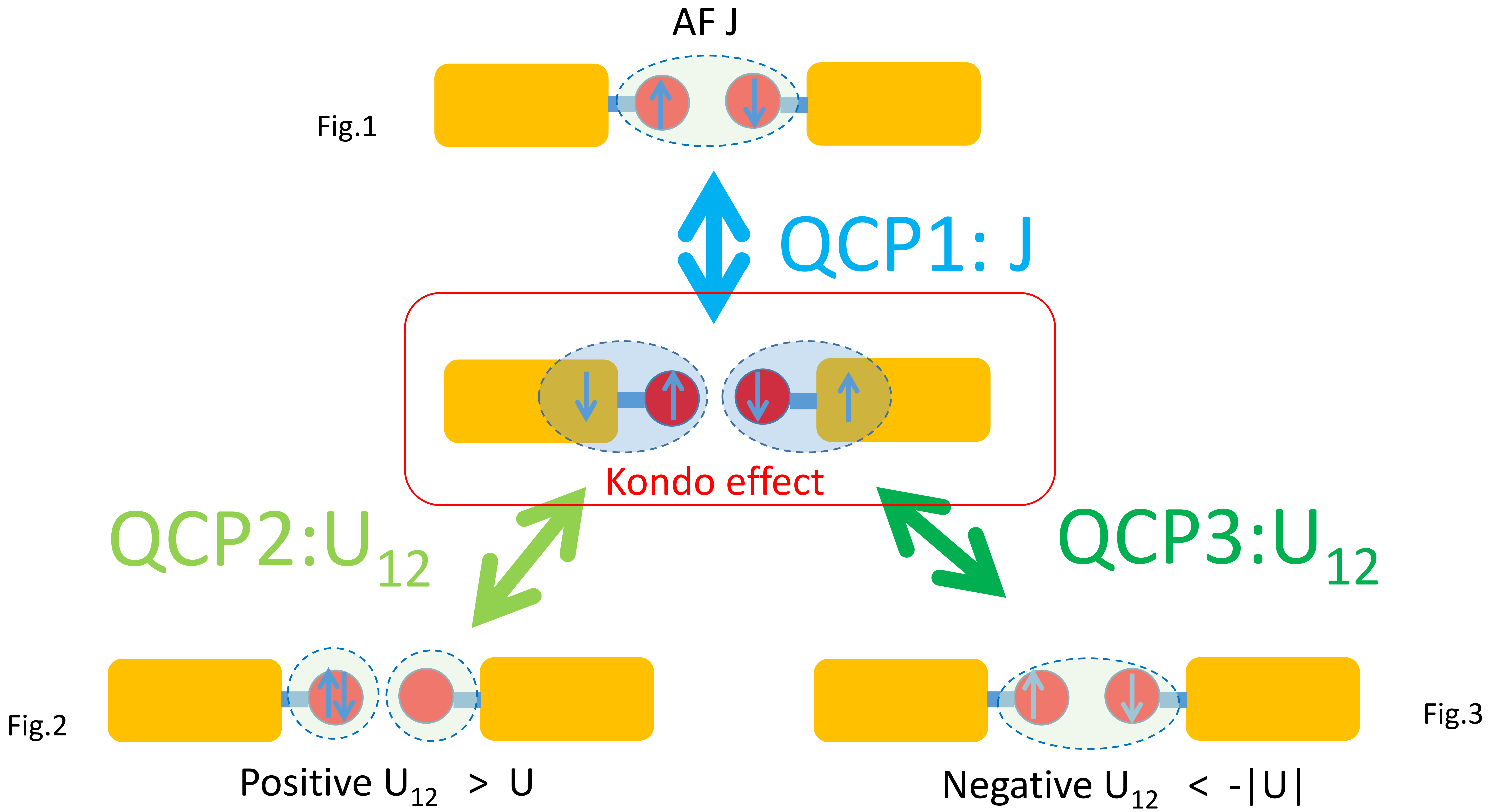
Two-Impurity Anderson Model (2IAM)

$$H_{\mathrm{2IAM}} = H_{\mathrm{AM1}} + H_{\mathrm{AM2}} + H_J + H_{U_{12}}$$



$$\epsilon_d \equiv \epsilon_{d1} = \epsilon_{d2},$$
$$U \equiv U_1 = U_2,$$
$$\Delta \equiv \Delta_1 = \Delta_2.$$

Some Quantum Critical Points



Method and Some Results

Renormalized Perturbation Theory and Numerical Renormalization Group

General assumption for low energy states (Fermi liquid)

Fermi liquid state : quasiparticles with residual renormalized interactions

Renormalized Perturbation Theory (RPT)

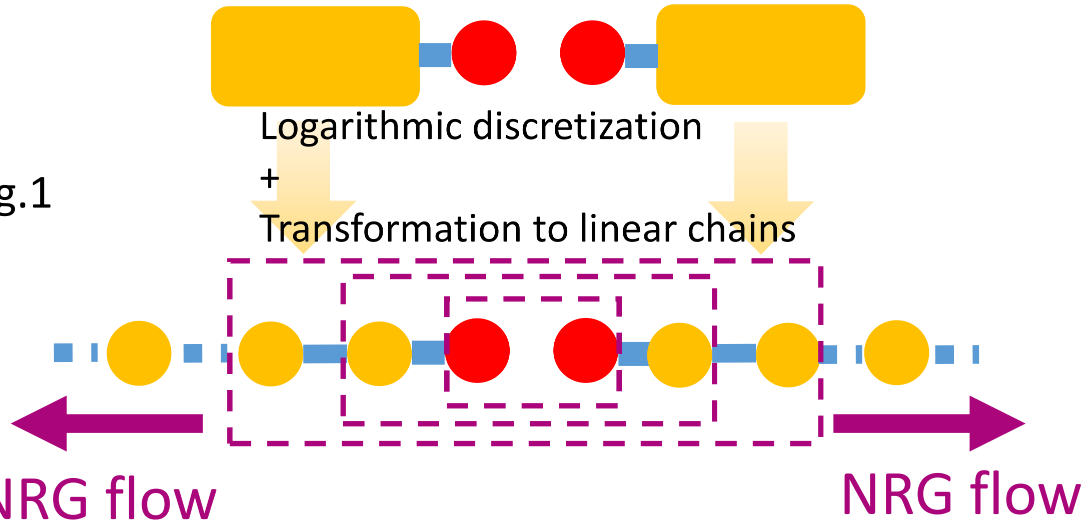
: A. C. Hewson, Phys. Rev. Lett. 70, 4007 (1993)

Perturbation expansion in powers of the renormalized interaction parameters (overcounting are avoided)

Exact expressions of some physical quantities in terms of the renormalized parameters

Numerical Renormalization Group (NRG)

Fig.1



NRG flow and NRG fixed point

Application to SIAM

Electron-hole symmetry, D→∞

Parameter space

Bethe ansatz (Exact) : special parameter

Our method : all parameters (in principle)

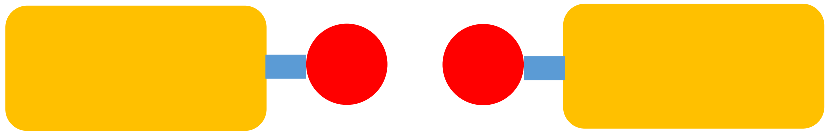
U/πΔ = 2	Wavefunction renomarization factor z = Δ~/Δ	Renormalized U~	Wilson ratio R = χ/γ
Exact (Bethe ansatz)	0.2392	0.2301	1.9620
NRG Λ=2.0	0.2389	0.2298	1.9620
NRG Λ=2.5	0.2390	0.2300	1.9621
NRG Λ=3.0	0.2390	0.2299	1.9619
NRG Λ=3.5	0.2390	0.2299	1.9620

A. C. Hewson, A. Oguri, and D. Meyer. Eur. Phys. J. B B40 177 2004

Quite good agreement

Application to 2IAM

For 2IAM, no exact results such a Bethe ansatz solution (so far).



Exact expressions of some susceptibilities (RPT)

$$\chi_s \propto \tilde{\rho}(1+\tilde{u}-\tilde{j}) = \tilde{\rho}\eta_s$$ Spin susceptibility

$$\chi_c \propto \tilde{\rho}(1-\tilde{u}-2\tilde{u}_{12}) = \tilde{\rho}\eta_c$$ Charge susceptibility

$$\chi_s^{st} \propto \tilde{\rho}(1+\tilde{u}+\tilde{j}) = \tilde{\rho}\eta_s^{st}$$ Staggered spin susceptibility

$$\chi_c^{st} \propto \tilde{\rho}(1-\tilde{u}+2\tilde{u}_{12}) = \tilde{\rho}\eta_c^{st}$$ Staggered charge susceptibility

$$\tilde{\rho} = \frac{\tilde{\Delta}/\pi}{(\tilde{\varepsilon}_d)^2 + (\tilde{\Delta})^2}$$

Quasiparticle density of states

$$\tilde{u} = \tilde{U}\tilde{\rho}, \ \ \tilde{u}_{12} = \tilde{U}_{12}\tilde{\rho}, \ \ \tilde{j} = \tilde{J}\tilde{\rho}$$

Dimensionless renormalized interaction parameters

(Nishikawa Y., Crow D. J. G., Hewson A. C., PHYSICAL REVIEW LETTERS 108 (056402) 2012, PHYSICAL REVIEW B 86 (125134) 2012)

$\tilde{\rho} \to \infty$ @QCP

$$\chi_s \propto \tilde{\rho}\eta_s,\ \chi_c \propto \tilde{\rho}\eta_c,\ \chi_s^{st} \propto \tilde{\rho}\eta_s^{st},\ \chi_c^{st} \propto \tilde{\rho}\eta_c^{st}$$

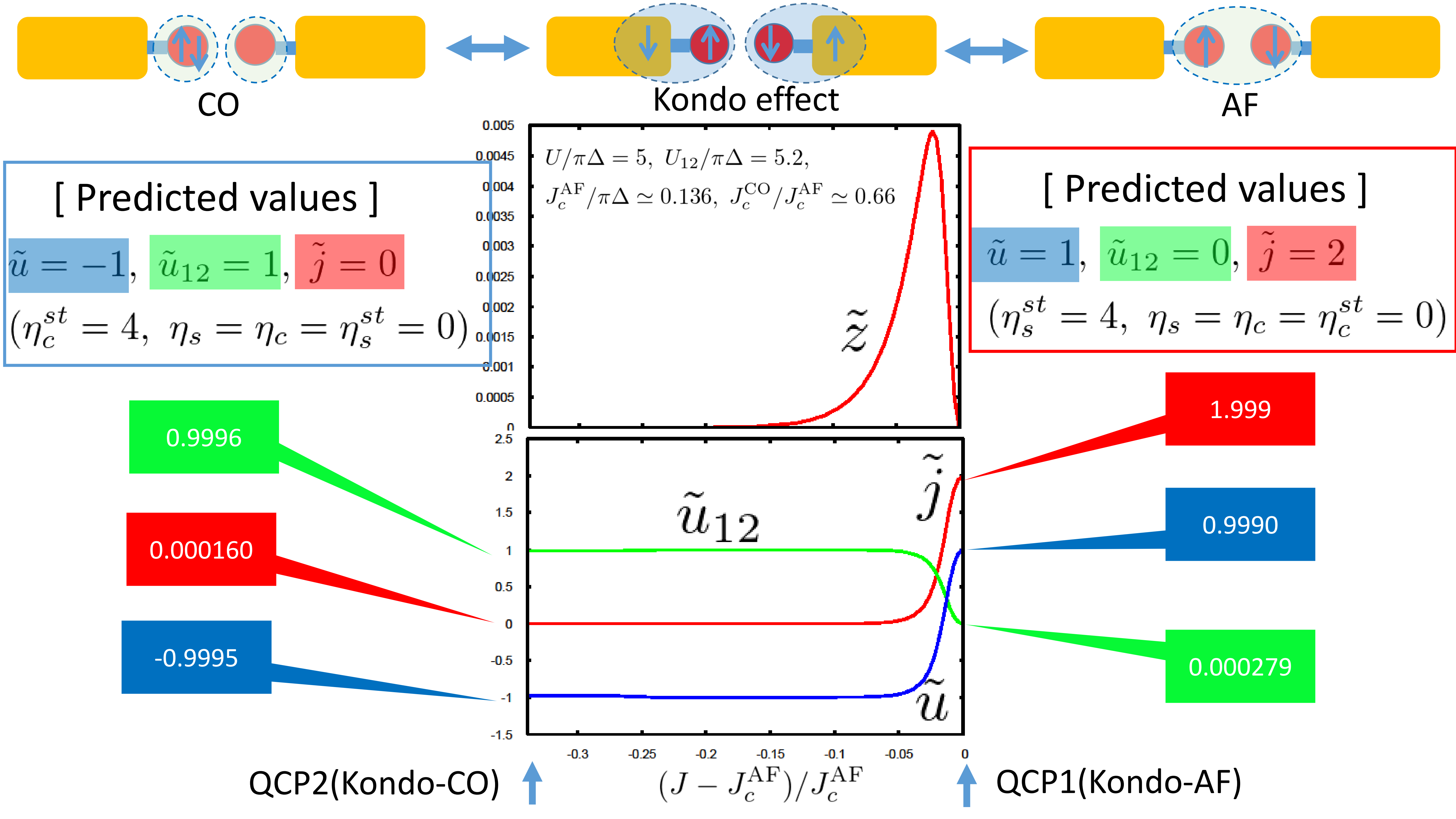
At least, one susceptibility diverges because $\eta_s + \eta_c + \eta_s^{st} + \eta_c^{st} = 4$

(assumption)
At a particular QCP, only one susceptibility associated with the QCP diverges.

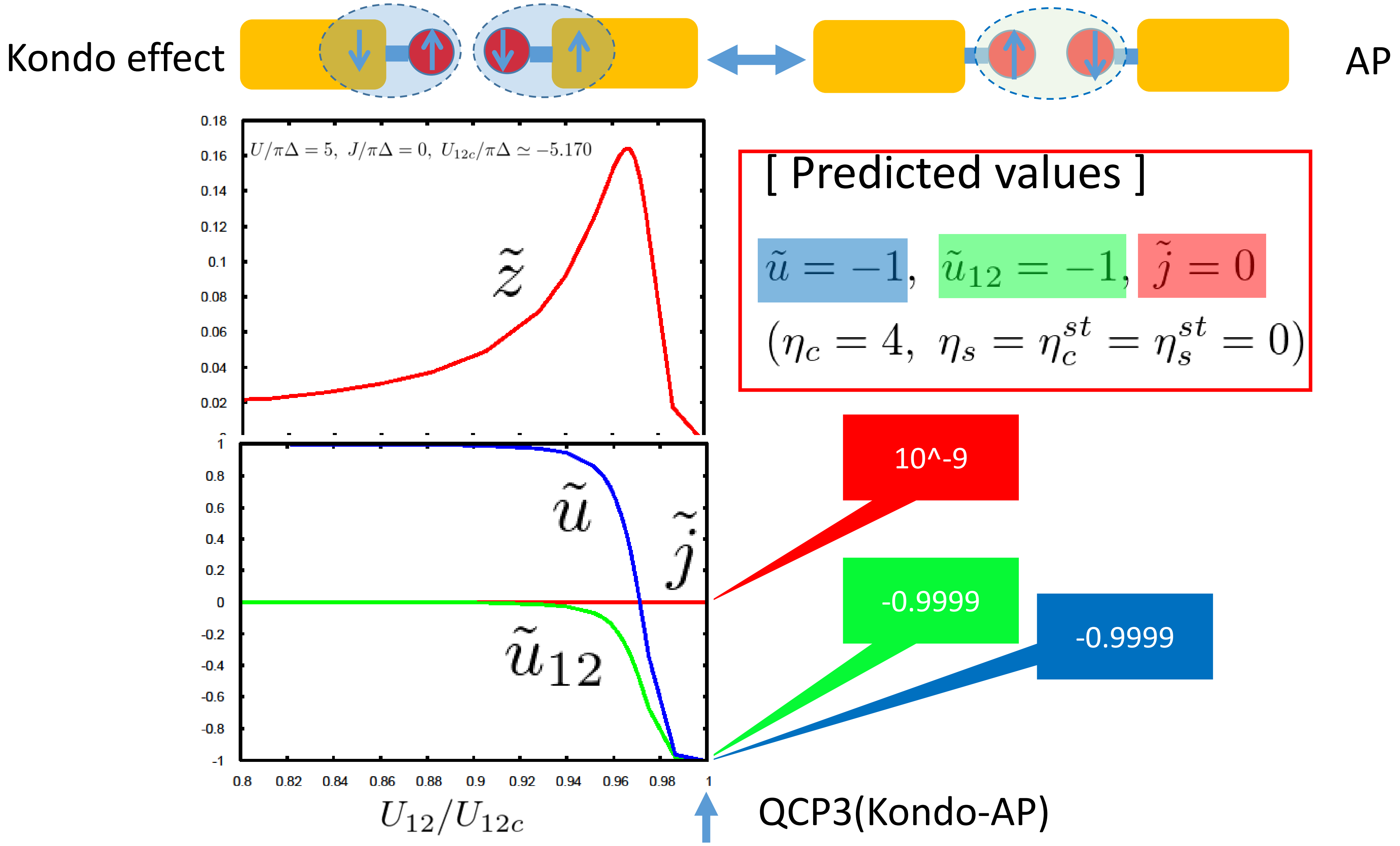
(necessary condition for the assumption)
⇒ one η → 4 and the other η s → 0.

It enables us to predict the values of the renormalized interaction parameters at the QCP using the following equations.

$$\tilde{u} = \frac{\eta_s + \eta_s^{st} - 2}{2} \qquad \tilde{j} = \frac{-\eta_s + \eta_s^{st}}{2} \qquad \tilde{u}_{12} = \frac{-\eta_s - 2\eta_c - \eta_s^{st} + 4}{4}$$



CO
Kondo effect
AF
[Predicted values]
$\tilde{u}=-1$, $\tilde{u}_{12}=1$, $\tilde{j}=0$
$(\eta_c^{st}=4,\ \eta_s=\eta_c=\eta_s^{st}=0)$
[Predicted values]
$\tilde{u}=1$, $\tilde{u}_{12}=0$, $\tilde{j}=2$
$(\eta_s^{st}=4,\ \eta_s=\eta_c=\eta_c^{st}=0)$
$U/\pi\Delta=5,\ U_{12}/\pi\Delta=5.2,$
$J_c^{\rm AF}/\pi\Delta\simeq 0.136,\ J_c^{\rm CO}/J_c^{\rm AF}\simeq 0.66$
$\tilde{z}$
$\tilde{u}_{12}$
$\tilde{j}$
$\tilde{u}$
0.9996
0.000160
-0.9995
1.999
0.9990
0.000279
$(J-J_c^{\rm AF})/J_c^{\rm AF}$
QCP2(Kondo-CO)
QCP1(Kondo-AF)



[Predicted values]

$\tilde{u} = -1,\ \tilde{u}_{12} = -1,\ \tilde{j} = 0$

$(\eta_c = 4,\ \eta_s = \eta_c^{st} = \eta_s^{st} = 0)$

Our method is reliable for 2IAM.

Results and Discussion

Luttinger – Friedel sum rule

- Luttinger's theorem

The volume inside the Fermi surface is invariant by the interaction.
(If the number N of particles is held fixed.)

$$N = \sum_{\alpha} (1 - \theta(\tilde{\varepsilon}_{\alpha})) = \sum_{\alpha} \Big(1 - \theta(\varepsilon^{(0)}_{\alpha})\Big) \qquad (1)$$

- Friedel sum rule

$$n_{d\alpha} = \tilde{n}_{d\alpha} \equiv \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\tilde{\varepsilon}_{d\alpha}}{\tilde{\Delta}_{\alpha}}\right) \ \left(\neq n^{(0)}_{d\alpha} \right) \qquad (2)$$

$$\longrightarrow 1 - \theta(\tilde{\varepsilon}_{d\alpha}), \text{(4)} \ (\tilde{\Delta}_{\alpha} \overset{\text{(3)}}{\rightarrow} 0)$$

Violation of Luttinger –Fridel sum rule 1

$J > J_c$

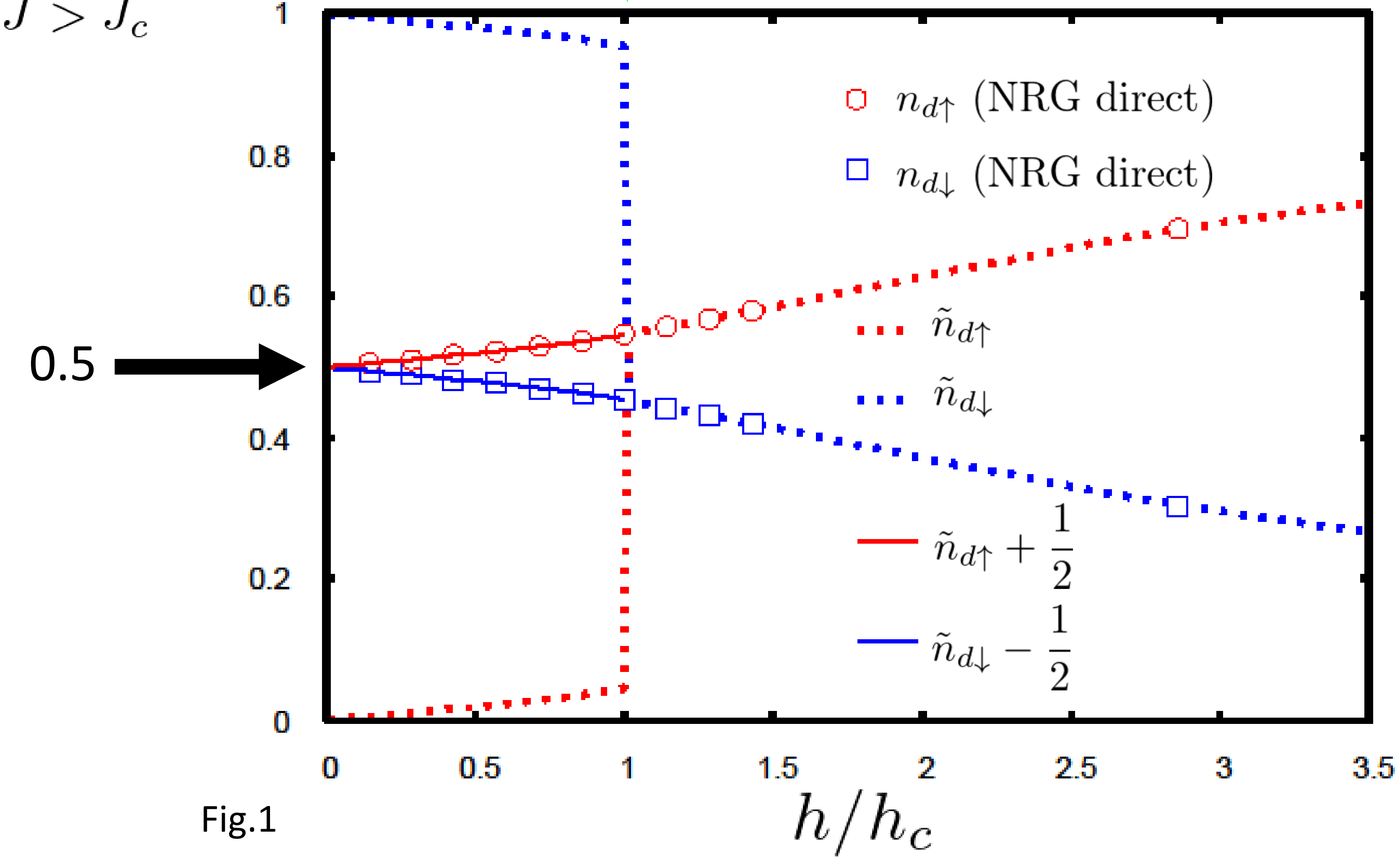
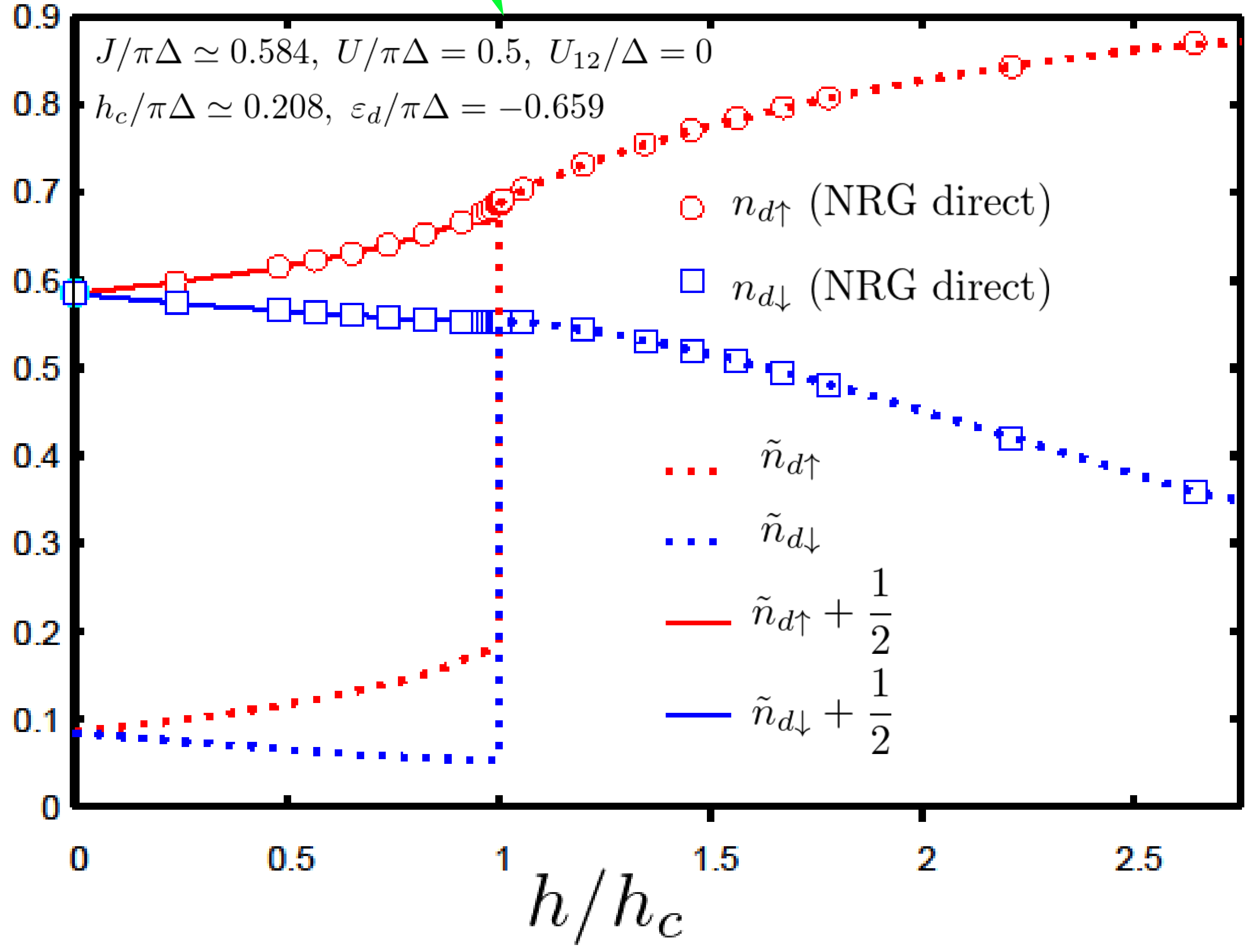


Fig.1

Violation of Luttinger –Fridel sum rule 2

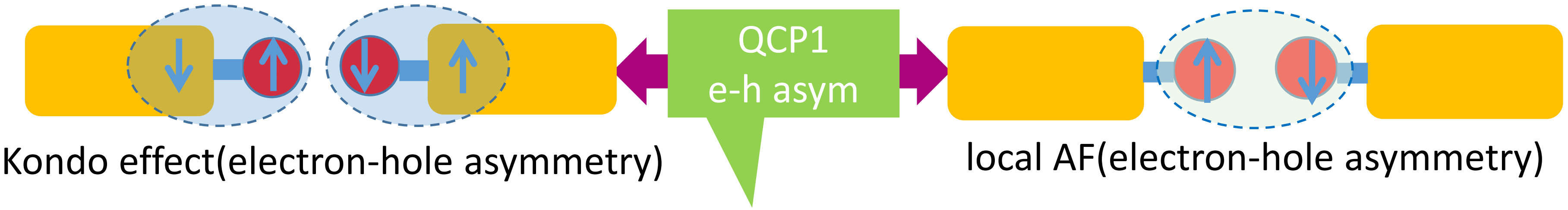
local AF (electron-hole asymmetry)

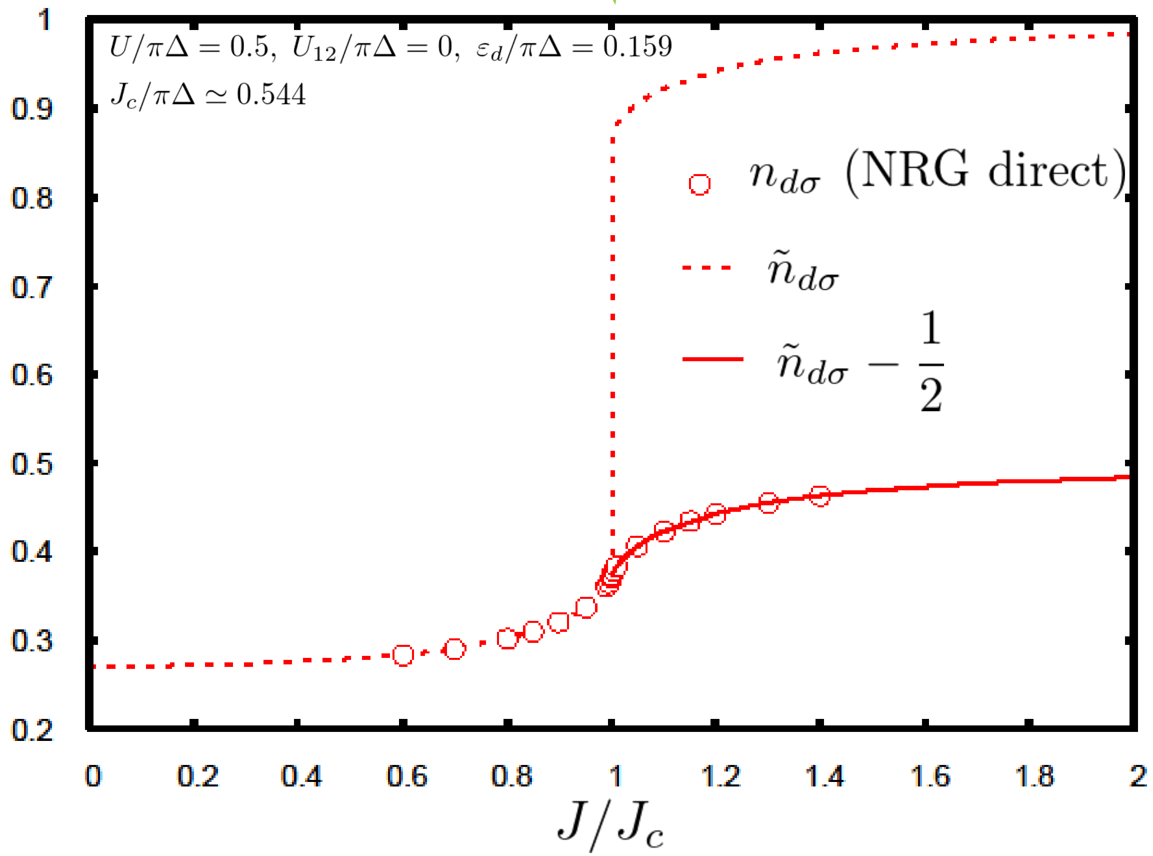
$J > J_c$



Nishikawa Y., Curtin O. J., Hewson A. C., Crow D. J. G.,PHYSICAL REVIEW B 98 (104419) 2018

Violation of Luttinger –Fridel sum rule 3





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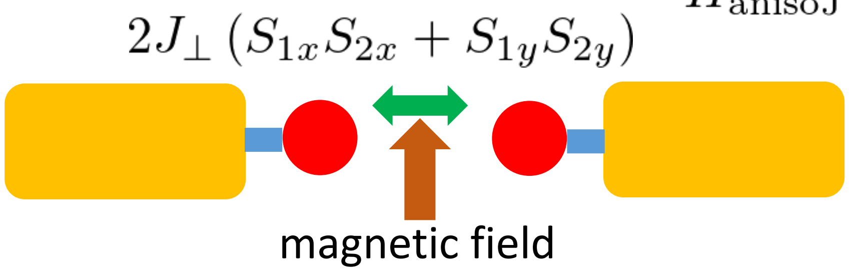
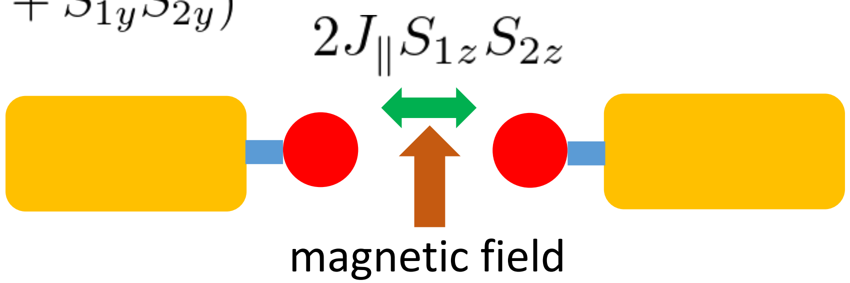
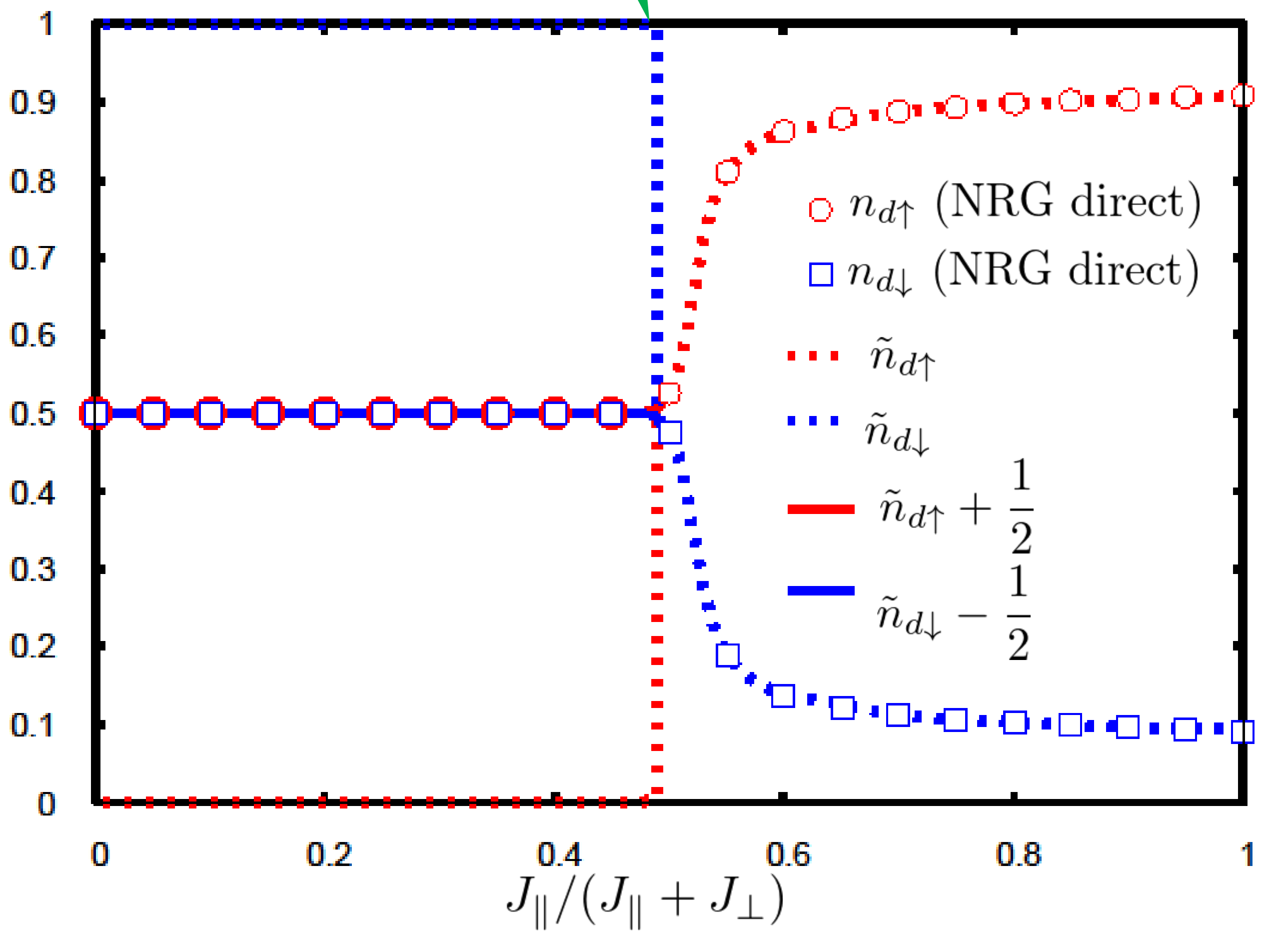
The local AF QCP (QCP1) is robust against parameter perturbations
(magnetic field, electron-hole asymmetry, (geometric asymmetry), and some of them)

Violation of Luttinger –Fridel sum rule 4

$$H_{\mathrm{anisoJ}} = 2J_{\parallel} S_{1z} S_{2z} + 2J_{\perp} \left(S_{1x} S_{2x} + S_{1y} S_{2y} \right)$$







Discussion

$$n_{d\alpha} = \frac{1}{2} - \frac{1}{\pi}\arctan\left(\frac{\tilde{\varepsilon}_{d\alpha}}{\tilde{\Delta}_\alpha}\right) + I_{L,\alpha} \quad (1)$$

1. Long-lived quasiparticle excitation at the Fermi level

$$I_{L,\alpha} = 0$$

2. Adiabatic continuous

[Luttinger integral]

$$I_L \equiv -\frac{1}{\pi}\int_{-\infty}^{0} d\omega \mathrm{Im}\left\{G_{d\alpha}(\omega_+)\frac{\partial\Sigma_{d\alpha}(\omega_+)}{\partial\omega}\right\} \quad (2)$$

Constant in a phase

$$I_{L,\alpha} = \mathrm{Const.}$$

Quantized

$$I_{L,\alpha} = 0,\ \pm\frac{1}{2}$$

Robustness of the QCP against some perturbations

Luttinger integral as a Topological invariant

- characterizing the two Fermi liquid phases
- induced by electron correlations

Luttinger's theorem…. something topological…

For example,

[1] M.Oshikawa, PHYSICAL REVIEW LETTERS 84 (3370) 2000 : https://arxiv.org/abs/cond-mat/0002392

Q1. " a Fermi liquid which violates Luttinger's theorem can exist? "

⇒

● (Local) Fermi liquid states violating Luttinger's theorem (Luttinger-Friedel sum rule).

● Deviations from Luttinger-Friedel sum rule are quantized.

[2]

Curtin O. J., Nishikawa Y., Hewson A. C., Crow D. J. G. JOURNAL OF PHYSICS COMMUNICATIONS 2 (031001) 2018 : https://arxiv.org/abs/1703.01807

Nishikawa Y., Curtin O. J., Hewson A. C., Crow D. J. G.,PHYSICAL REVIEW B 98 (104419) 2018, : https://arxiv.org/abs/1712.08771

Other example :

[3]

G. G. Blesio, L. O. Manuel, P. Roura-Bas, A. A. Aligia, PHYSICAL REVIEW B 98 (195435) 2018 : https://arxiv.org/abs/1805.11518

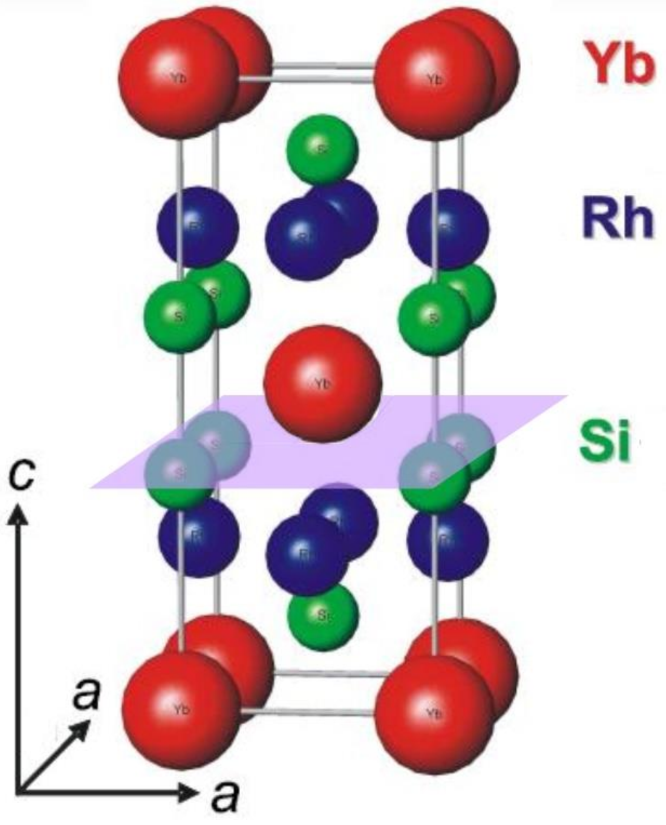
Q2. the topological understanding

⇒ ●Winding number

[4] K. Seki, S. Yunoki, PHYSICAL REVIEW B 96 (085124)2017 : https://arxiv.org/abs/1708.00986

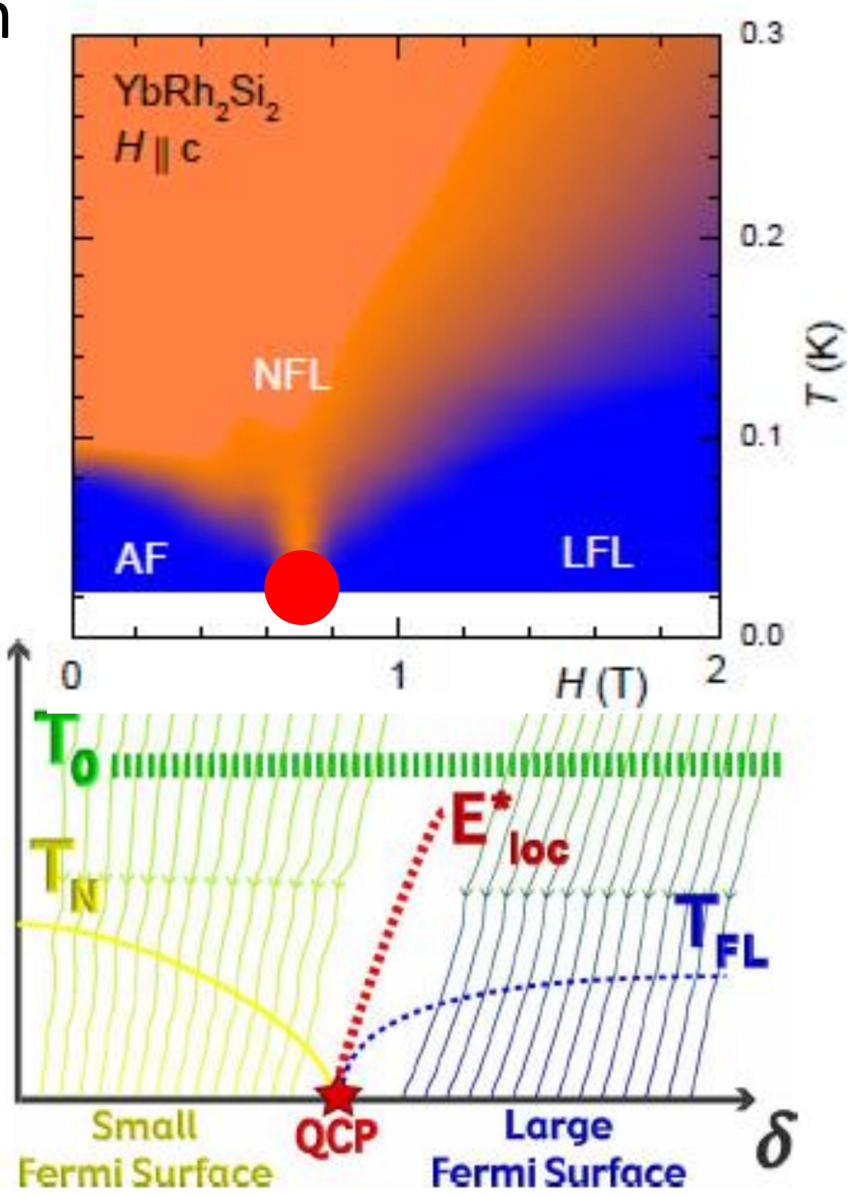
Related experiment : heavy fermion system

Fig.2



http://www2.cpfs.mpg.de/~wirth/rec/stm4.html

Fig.1



Philipp Gegenwart, Qimiao Si, Frank Steglich,
Nature Physics volume 4, 186–197 (2008)

Summary and Conclusion

- Quantum criticality in two impurity Anderson model
- Method : RPT and NRG
- Violation of Luttinger-Friedel sum rule in some Fermi liquid states
- Luttinger integral as a topological invariant

  Characterizing the two fermi liquid phases separated by the QCP

  Induced by electron correlations
- Related experiment on a heavy fermion metal, YbRh2Si2

Thank you for your attention.