Workshop on “Heavy Fermion Physics: Perspective and Outlook”

Coexistence of Kondo screening effect with antiferromagnetic correlations in the Kondo lattice systems

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OUTLINE

- **Basic physics in heavy fermion systems**
- **Short-range antiferromagnetic metallic state in iron-based SCs**
- **Heavy Fermi liquid in the presence of AFM short-range correlations**
- **Kondo screening coexistence with AFM long-range order**
- **Conclusion**

Basic physics in heavy fermion systems

- Kondo effect in metals with dilute magnetic moments

  At low T, Kondo singlet/resonance forms → local Fermi liquid;
  At high T, free moment scatters conduction electrons → ln T resistivity.

- Heavy Fermi liquid in Kondo lattice systems

  Kondo singlets as Landau quasiparticles, leading to the large Fermi surface.

- Magnetically order states also exist in Kondo lattice systems

  RKKY interaction occurs via Kondo scatterings of conduction electrons.

- Interplay between Kondo coupling and RKKY interaction:

  Phase transitions and quantum criticality in heavy fermion systems

Heavy Fermi liquid state in the Kondo lattice model

Model Hamiltonian: $H = \sum_{k\sigma} (\varepsilon_k - \mu) c^+_{k\sigma} c_{k\sigma} + J \sum_i S_i \cdot s_i$

Fermion rep. of local moments: $\mathbf{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} f^\dagger_{i\sigma} \tau_{\sigma\sigma'} f_{i\sigma'}$ $\quad \boxed{\sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} = 1}$

$$\mathbf{S}_i \cdot \mathbf{s}_j = -\frac{1}{2} \sum_{\sigma\sigma'} f^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} f_{i\sigma'}$$

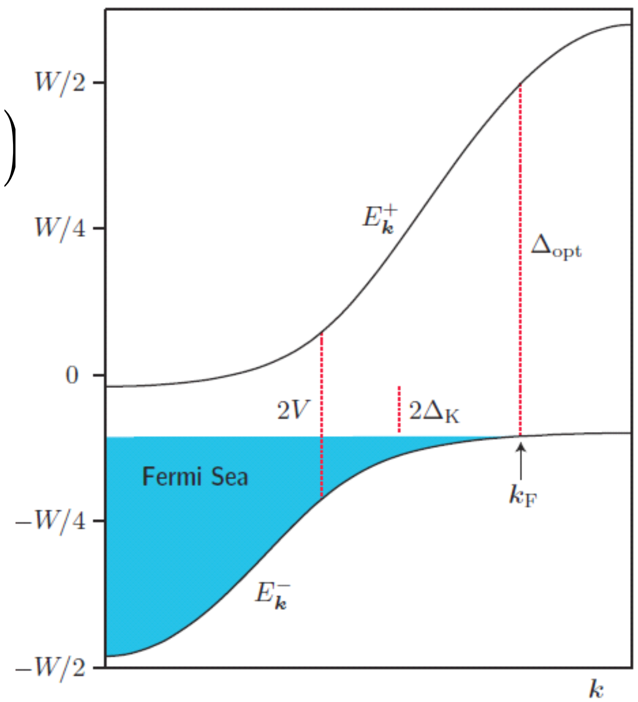
$\boxed{V = \sum_\sigma \langle c^\dagger_{i\sigma} f_{i\sigma} \rangle}$ Hybridization parameter

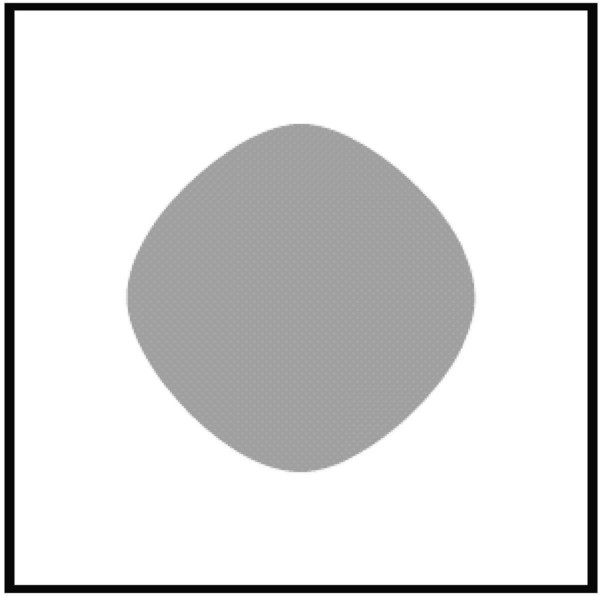
Mean field Hamiltonian:

$$H_{mf} = \sum_{\mathbf{k}\sigma} \left(c^+_{\mathbf{k}\sigma}, f^+_{\mathbf{k}\sigma} \right) \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu & -\frac{V}{2} J \\ -\frac{V}{2} J & \lambda \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} + N \left(\frac{1}{2} J V^2 - \lambda \right)$$

Renormalized band energies:

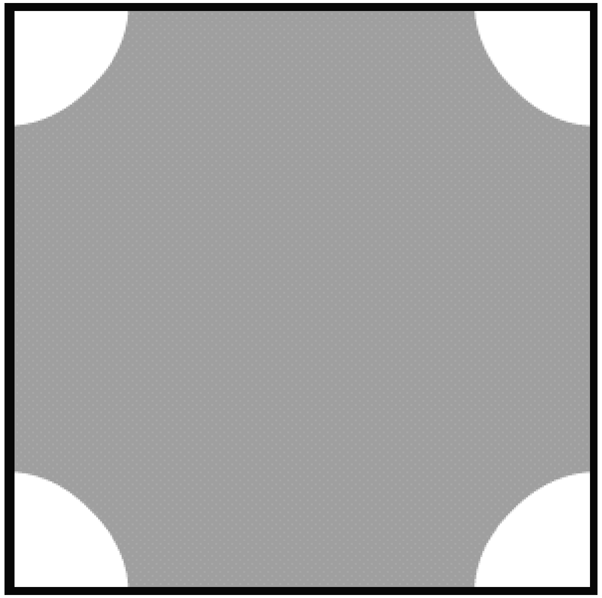
$$E^\pm_{\mathbf{k}} = \frac{1}{2} \left[\left(\varepsilon_{\mathbf{k}} - \mu + \lambda \right) \pm \sqrt{\left(\varepsilon_{\mathbf{k}} - \mu - \lambda \right)^2 + \left(J V \right)^2} \right]$$





$J = 0$

Small Fermi surface



$J \neq 0$

Large Fermi surface

Dramatic changes of Fermi surface due to the Kondo screening !

Quantum paramagnetic metallic states

epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

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EPL, **86** (2009) 37006
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Universal linear-temperature dependence of static magnetic susceptibility in iron pnictides

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Linear T susceptibility in iron-based superconductors

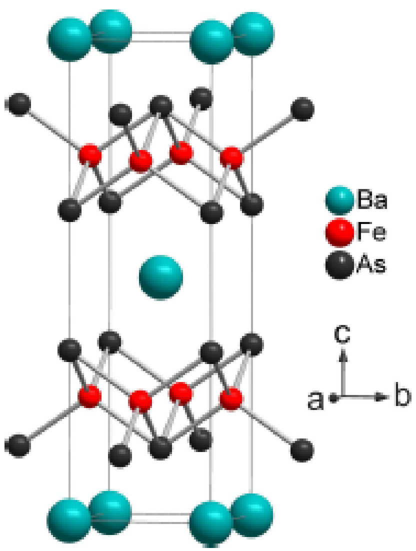
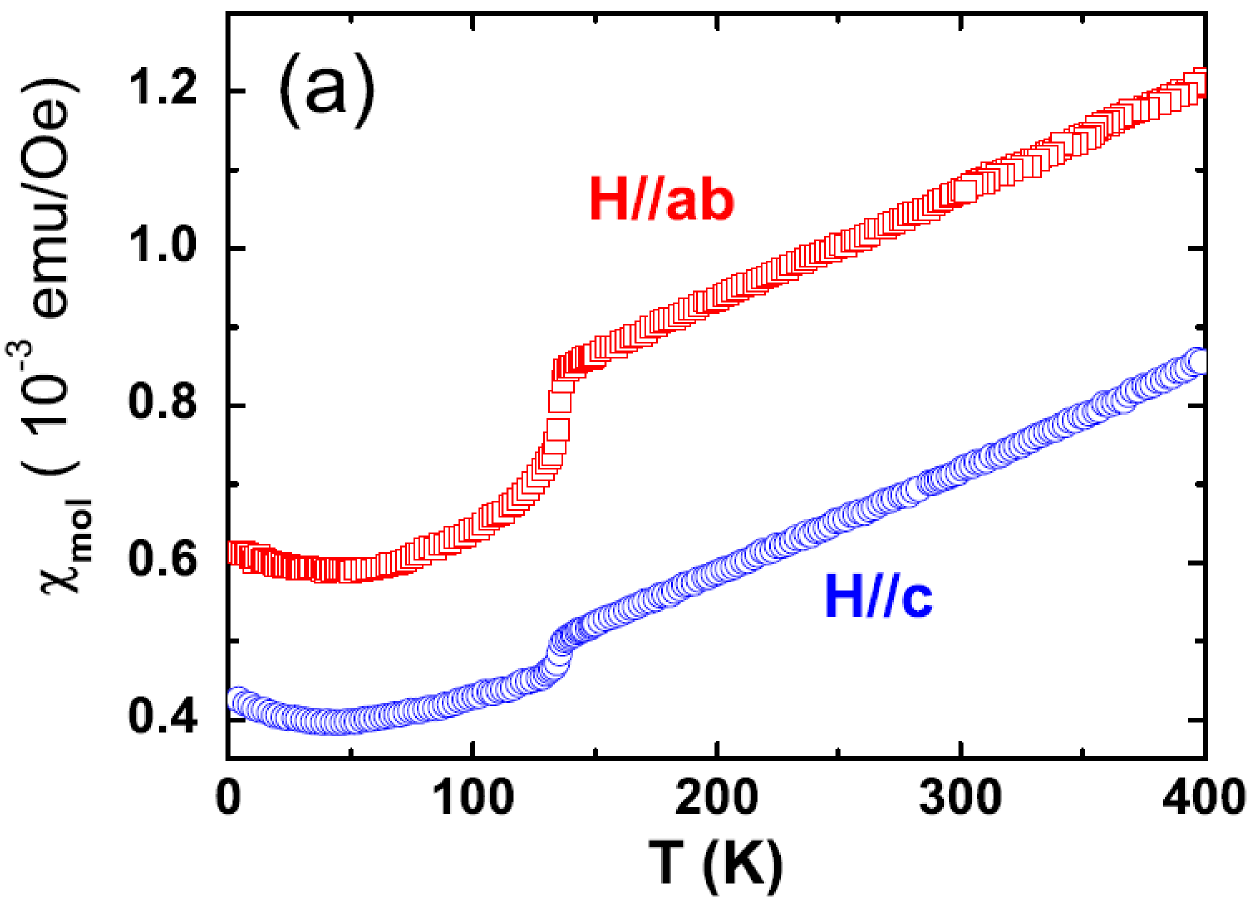


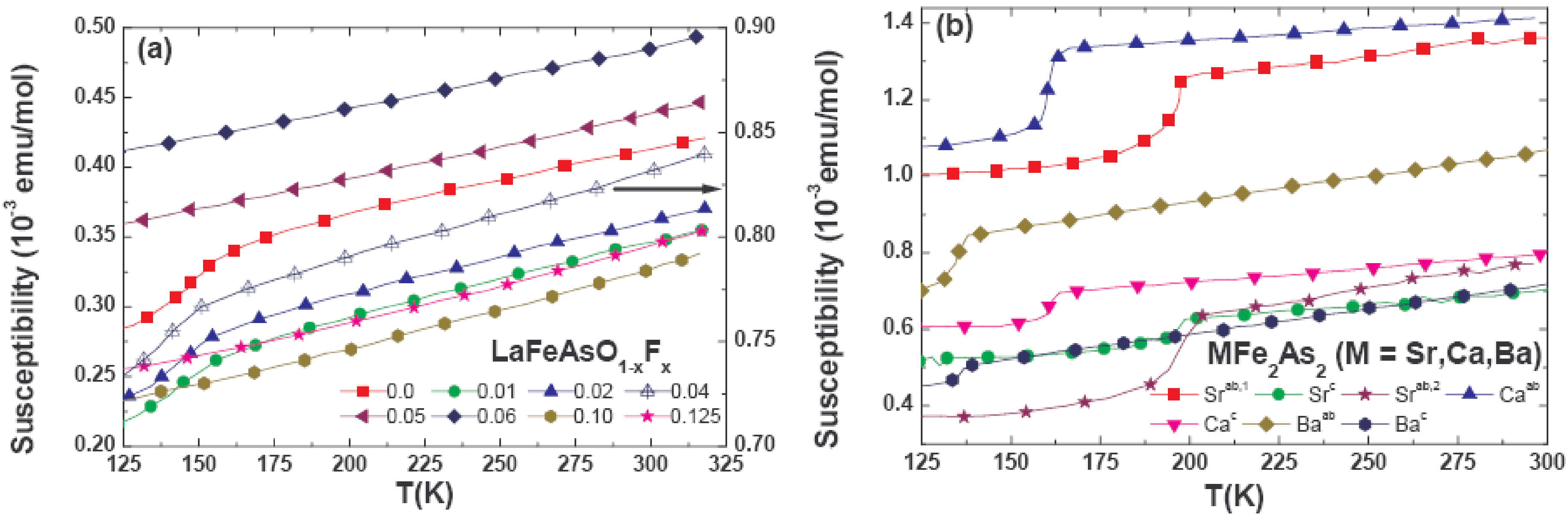
FIG. 1: Crystal structure of $BaFe_2As_2$.



$BaFe_2As_2$

X.H. Chen's group, PRL 102, 117005 (2009); arXiV:0806.2452

Universal features of the spin dynamics above T_{SDW}



- Linear T dependence of the uniform spin susceptibilities, strongly deviating from the conventional Fermi liquid theory.
- Spatial anisotropy along c-axis and 3D magnetic ordering below T_{SDW}
- **The spin dynamics for $T>T_{SDW}$ is described by an effective 2D J1-J2 AFM Heisenberg spin model.**
- **The local moment picture should be used to describe the spin physics phenomenologically.**

G.M. Zhang, et. al., EPL 86, 37006 (2009); arXiv:0809.3874

Model Hamiltonian

The minimal model effective Hamiltonian for describing the spin dynamics of the parent compounds is given by

$$H_S = J_1 \sum_{\langle i,j \rangle, a} S_{i,a} \cdot S_{j,a} + J_2 \sum_{\langle\langle i,j \rangle\rangle, a} S_{i,a} \cdot S_{j,a} + J_z \sum_{i,a} S_{i,a} \cdot S_{i,a+1},$$

In the paramagnetic state, Jz=0 can be chosen.

Dyson-Maleev spin-wave theory

Dyson-Maleev representation:

$$S_l^- = a_l^+, \quad S_l^+ = \left(2S - a_l^+ a_l\right) a_l, \quad S_l^z = S - a_l^+ a_l, \quad l \in A$$

$$S_m^- = b_l, \quad S_m^+ = b_m^+ \left(2S - b_m^+ b_m\right), \quad S_l^z = -S + b_m^+ b_m, \quad m \in B$$

In the **linear spin-wave approximation**, we have

$$H=\sum_k\left[\eta_k\left(a_k^+a_k+b_k^+b_k\right)+\Lambda_k\left(a_kb_{-k}+a_k^+b_{-k}^+\right)\right]-2NS\left(J_2S+\lambda\right)$$

with $\eta_k=2J_1S\cos k_x+2J_2S+\lambda,\ \ \Lambda_k=2J_1S\cos\frac{k_y}{2}+2J_2S\gamma_k,\ \ \gamma_k=\cos k_x\cos\frac{k_y}{2}$

A chemical potential term for the bosons has been introduced to make the local magnetization vanish at finite temperatures:

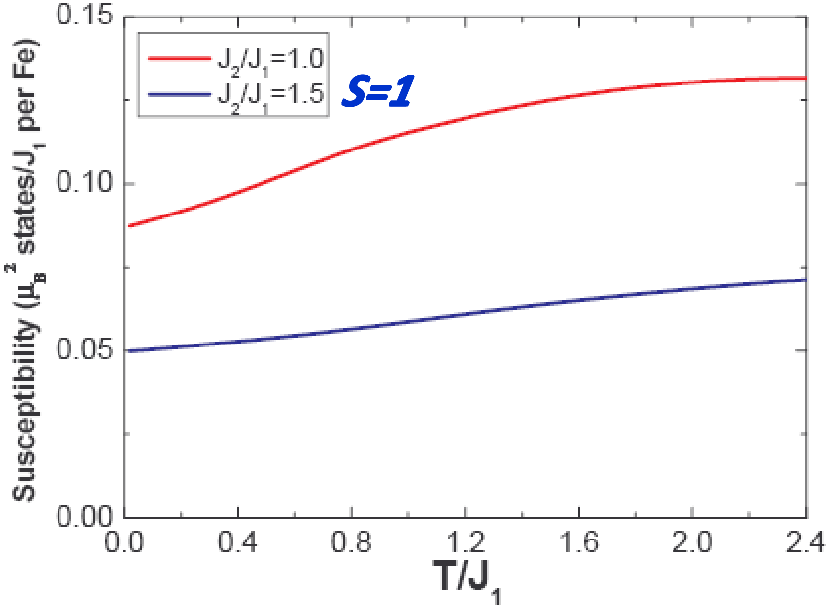
$$\left\langle S_l^z\right\rangle=0,\ \ l\in A;\qquad \left\langle \mathrm{S}_\mathrm{m}^\mathrm{z}\right\rangle=0,\ \ m\in B$$

The uniform spin susceptibility can be calculated as

$$\chi_u=\frac{(gu_B)^2}{4k_BTN}\sum_k\frac{1}{\sinh^2\left(\frac{\epsilon_k}{2k_BT}\right)}$$

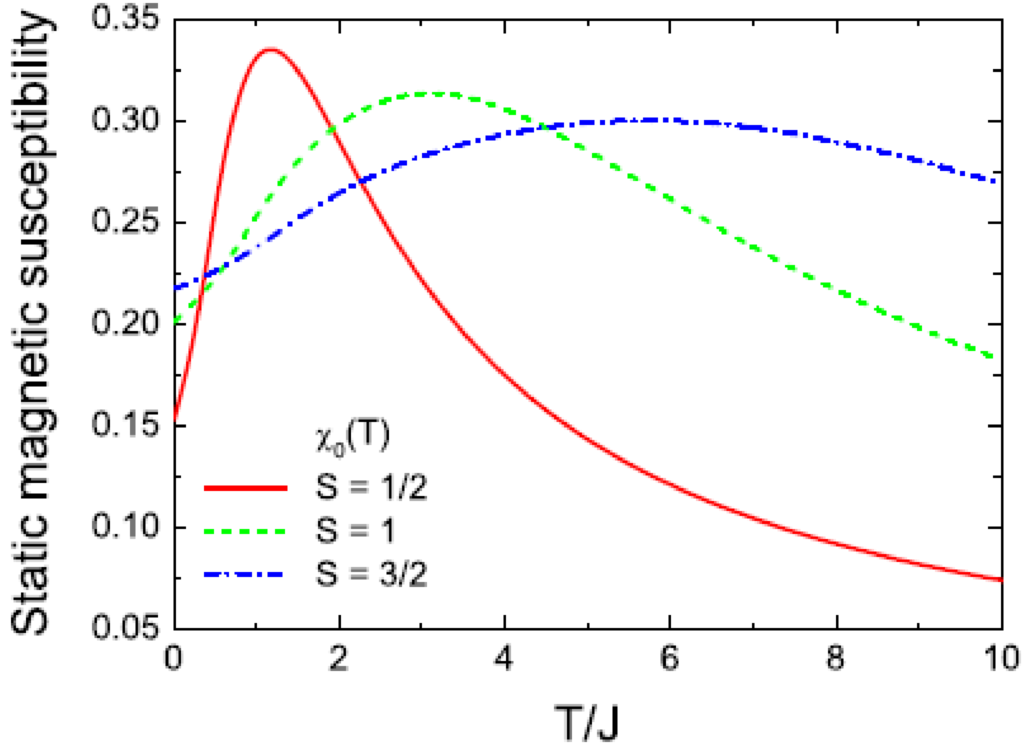
In the low T limit, we have

$$\chi_u=\chi_0\left[1+c\left(\frac{T}{J_1}\right)\right],\qquad c>0.$$



G.M. Zhang, et. al., EPL 86, 37006 (2009).

Linear spin-wave theory for 2D quantum Heisenberg antiferromagnetic model



The artifacts of those mean field /variational theories have be removed in the present linear spin-wave approximation!

Magnetic susceptibilities in metallic paramagnetic states

G.M. Zhang, et. al., EPL 86, 37006 (2009).

1. Nearly free local moments – Curie-Weiss law

$$\chi(T) = \frac{C}{T+\theta}$$

2. Weakly interacting conduction electrons – Pauli susceptibility

$$\chi(T) = const$$

3. AF fluctuating magnetic moments – Heisenberg paramagnetism

$$\chi(T) = \begin{cases} C_1 + D_1 / \ln\left(\frac{T_0}{T}\right), & \text{in 1D} \\ C_2 + D_2 T, & \text{in 2D} \\ C_3 + D_3 T^2, & \text{in 3D} \end{cases}$$

where C_n and D_n are positive constants.

What happens to the heavy Fermi liquid in the presence of short-range antiferromagnetic correlations ?

PHYSICAL REVIEW B **83**, 033102 (2011)

Lifshitz transitions in a heavy Fermi liquid driven by short-range antiferromagnetic correlations in the two-dimensional Kondo lattice model

Guang-Ming Zhang,[1] Yue-Hua Su,[2] and Lu Yu[3]

Kondo-Heisenberg lattice model in the limit of $J_K >> J_H$

$$H = \sum_{\mathbf{k},\sigma}(\epsilon_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + J_K\sum_i \mathbf{S}_i\cdot\mathbf{s}_i + J_H\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j,$$

$$\mathbf{S}_i\cdot\mathbf{S}_j = -\frac{1}{2}\sum_{\sigma\sigma'} f^\dagger_{i\sigma}f_{j\sigma}f^\dagger_{j\sigma'}f_{i\sigma'},$$

Heisenberg exchange coupling

$$\mathbf{S}_i\cdot\mathbf{s}_j = -\frac{1}{2}\sum_{\sigma\sigma'} f^\dagger_{i\sigma}c_{j\sigma}c^\dagger_{j\sigma'}f_{i\sigma'},$$

Kondo exchange coupling

MF order parameters: $\chi = -\sum_\sigma \langle f^\dagger_{i\sigma}f_{i+l\sigma}\rangle, \quad V = \sum_\sigma \langle c^\dagger_{i\sigma}f_{i\sigma}\rangle.$

MF model Hamiltonian: $H = \sum_{\mathbf{k}\sigma}(c^\dagger_{\mathbf{k}\sigma}\ f^\dagger_{\mathbf{k}\sigma})\begin{pmatrix}\epsilon_{\mathbf{k}} - \mu & -\frac{1}{2}J_K V \\ -\frac{1}{2}J_K V & \chi_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma}\end{pmatrix} + E_0,$

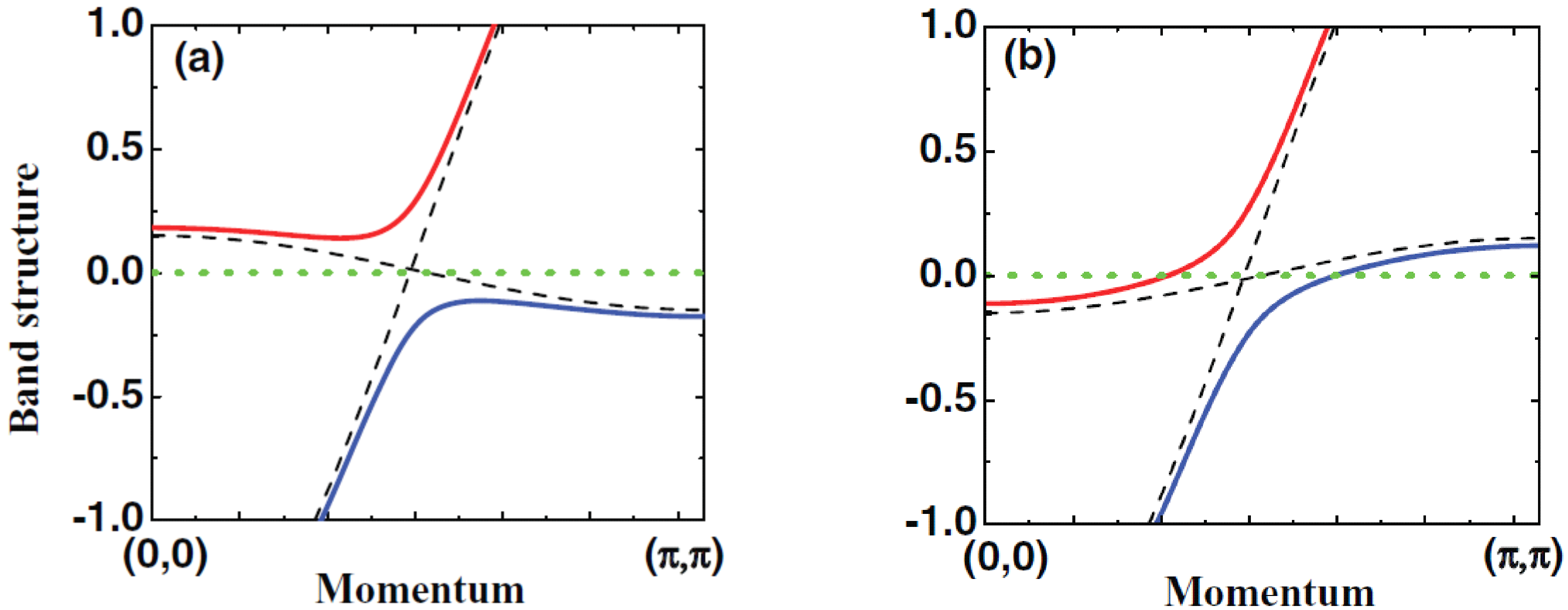
Renormalized band energies: $\varepsilon^\pm_{\mathbf{k}} = \frac{1}{2}[(\epsilon_{\mathbf{k}} - \mu + \chi_{\mathbf{k}}) \pm W_{\mathbf{k}}],$

$$W_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu - \chi_{\mathbf{k}})^2 + (J_K V)^2}$$

Two different renormalized band structures due to different types of hybridizations

On a square lattice: $\varepsilon_{\mathrm{k}} = -2t\left(\cos k_x + \cos k_y\right) + 4t' \cos k_x \cos k_y - \mu,$

$$\chi_{\mathrm{k}} = J_H \chi\left(\cos k_x + \cos k_y\right) + \lambda$$



Hybridization between c-electrons with f-holes

$\chi > 0$

Hybridization between c-electrons with f-particles

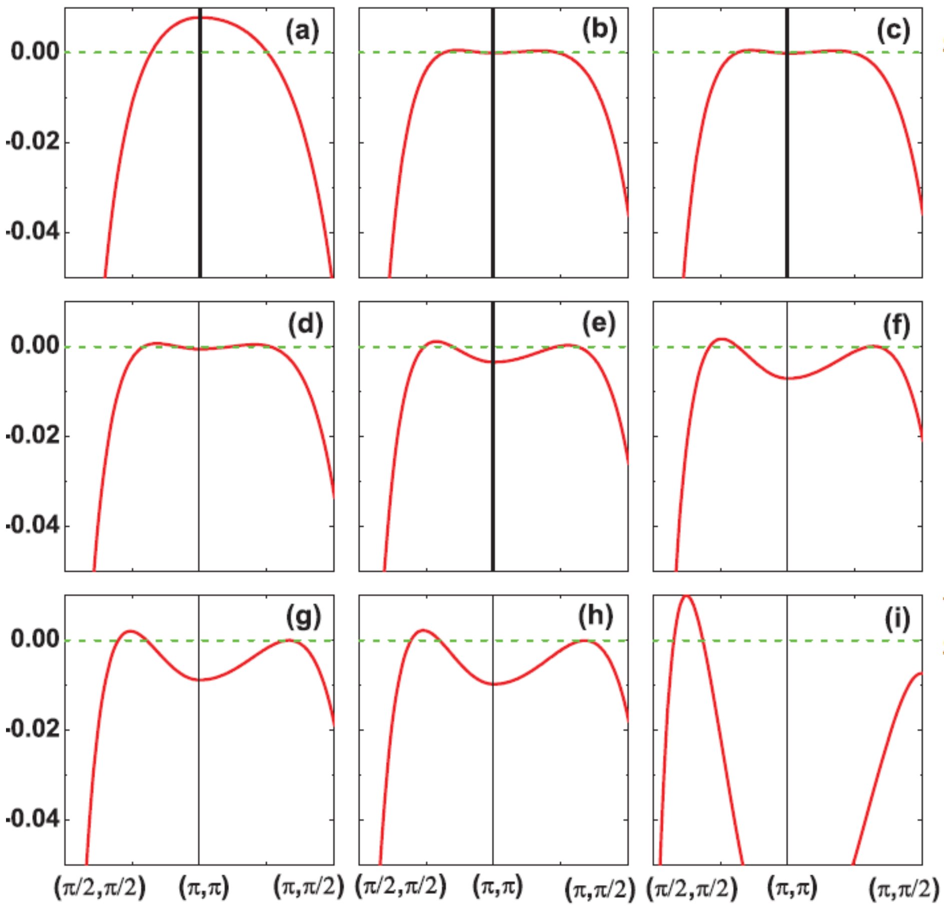
$\chi < 0$

Self-consistent MF equations:

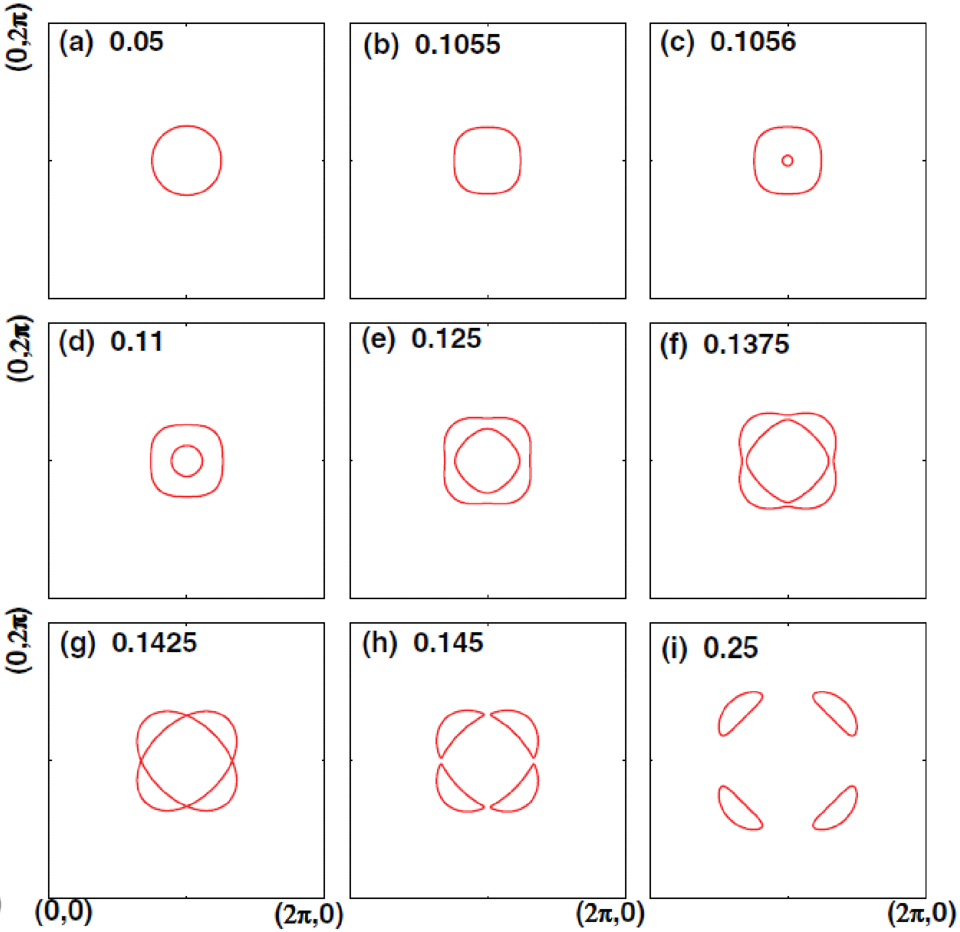
$$\frac{\partial \varepsilon_g}{\partial \chi} = 0, \quad \frac{\partial \varepsilon_g}{\partial V} = 0, \quad \frac{\partial \varepsilon_g}{\partial \lambda} = 0, \quad n_c = -\frac{\partial \varepsilon_g}{\partial \mu}. \qquad n_c = 0.9$$

For $J_K > J_H$, we always obtain the solution with $\chi > 0$.

Low renormalized band changes as J_k / J_H

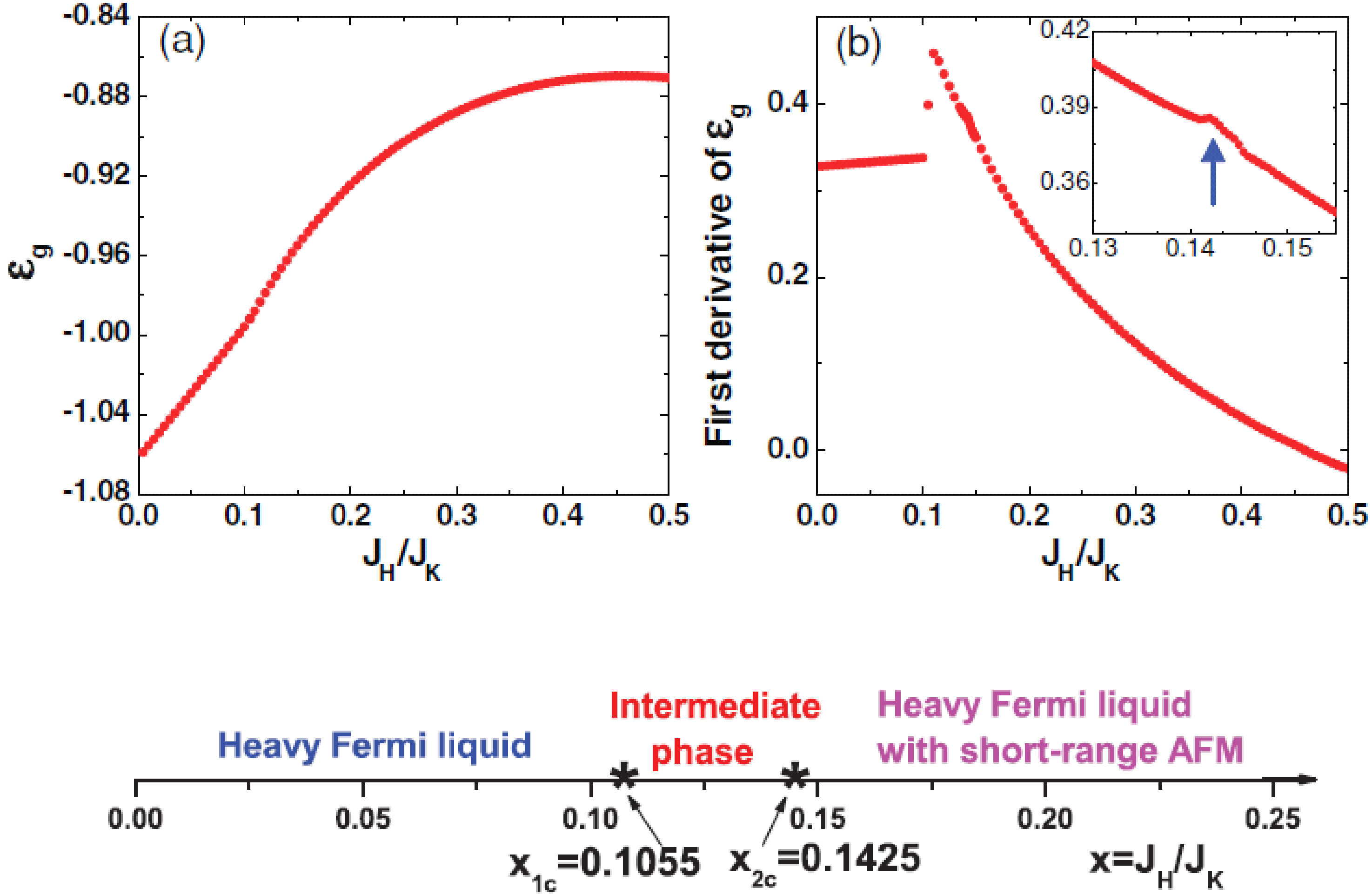


Fermi surface changes as J_k / J_H



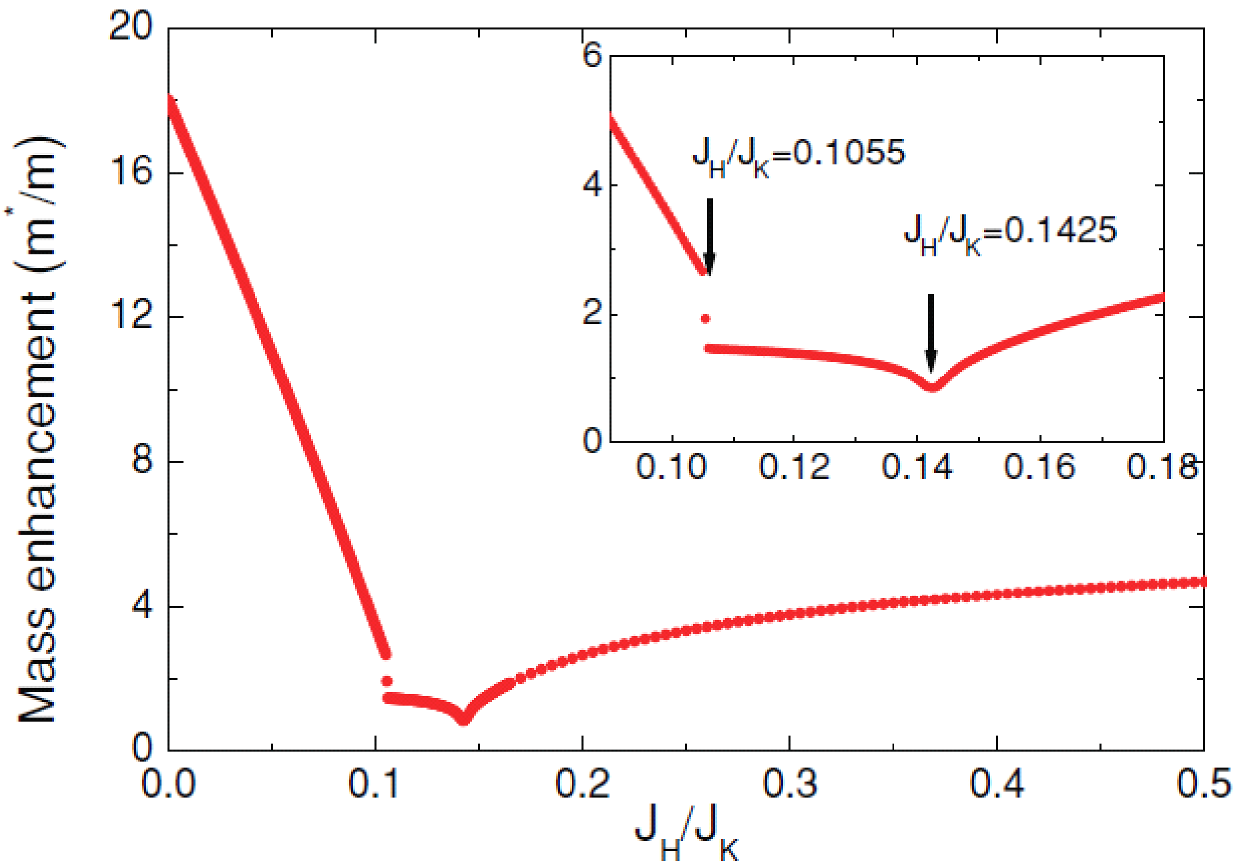
Ground state energy analysis and quantum phase transitions

$$n_c = 0.9$$

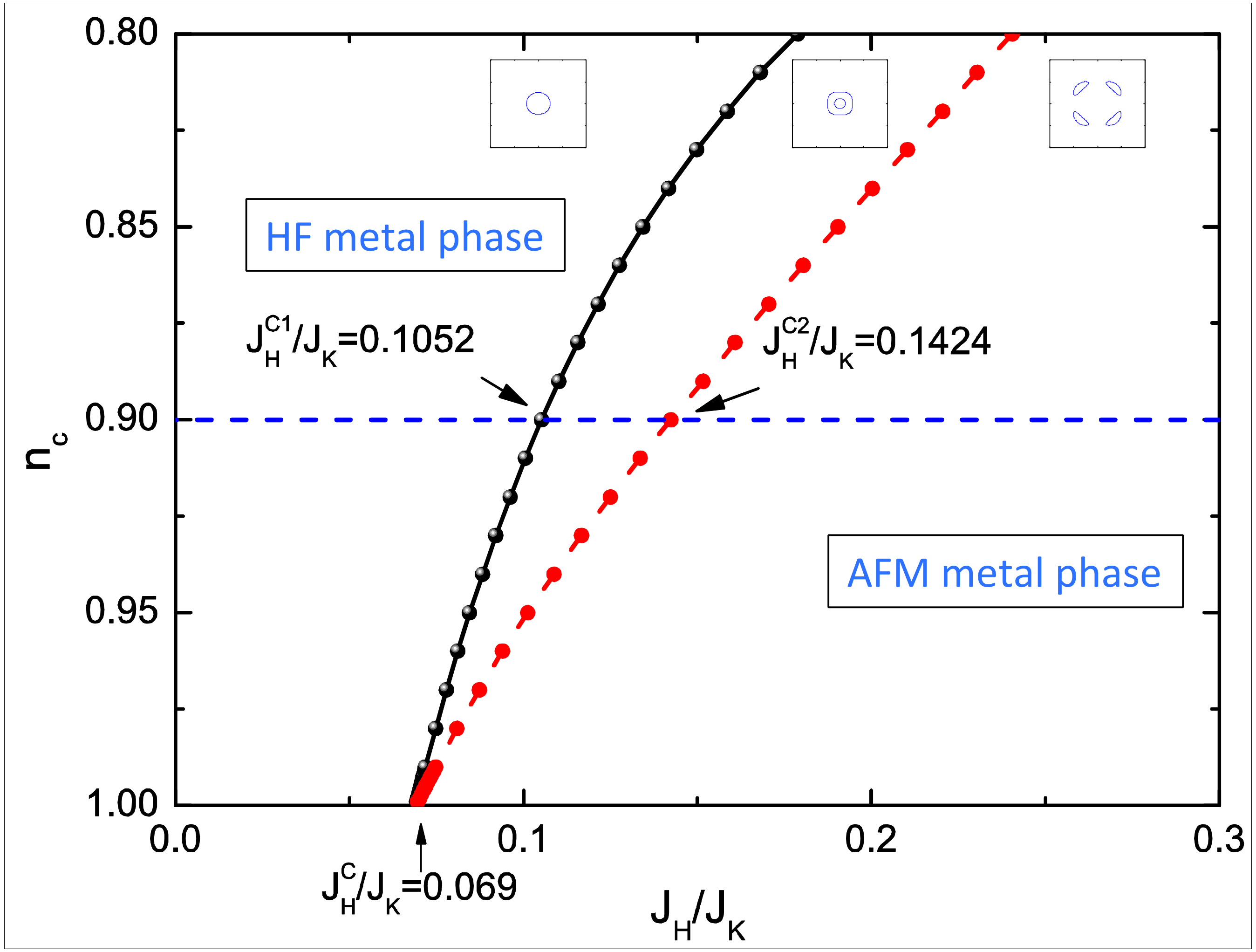


Effective mass changes

$$\frac{m}{m^*} = \left\langle \frac{\partial \varepsilon_{\mathbf{k}}^{(-)}}{\partial \epsilon_{\mathbf{k}}} \right\rangle_{\mathrm{FS}} = \frac{1}{N} \sum_{\mathbf{k}} \left[\frac{\partial \varepsilon_{\mathbf{k}}^{(-)}}{\partial \epsilon_{\mathbf{k}}} \right] \delta(\mu - \varepsilon_{\mathbf{k}}^{(-)}). \qquad n_c = 0.9$$



The electron filling factor dependence of the phase transitions

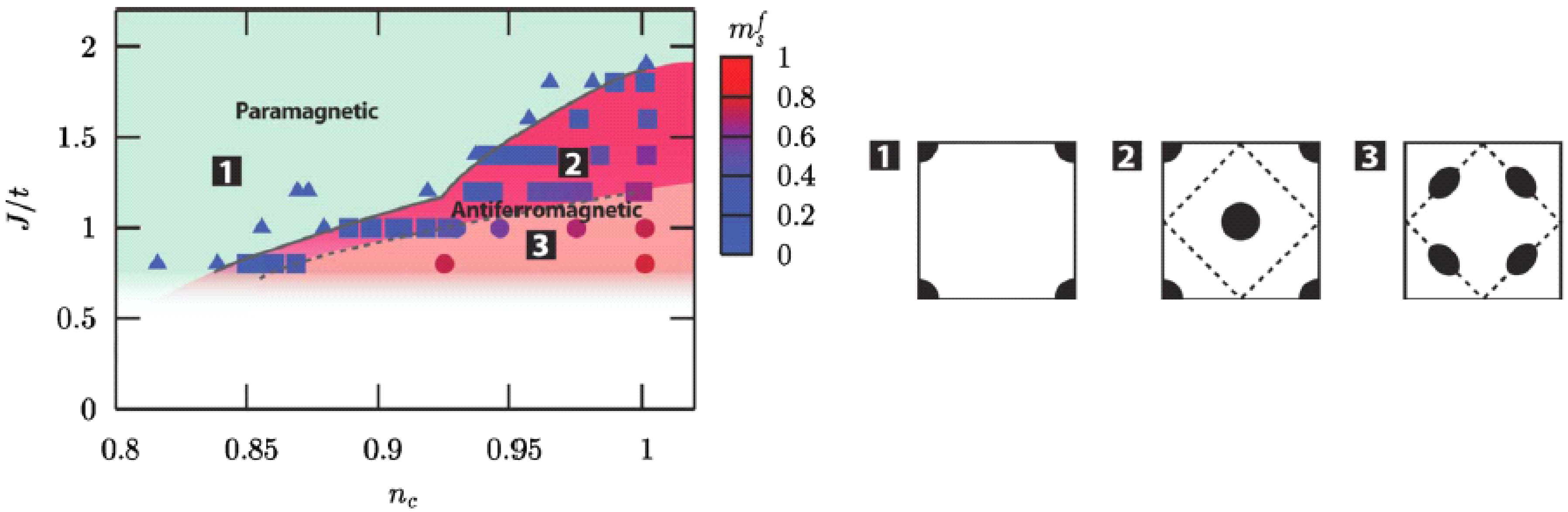


PHYSICAL REVIEW B **82**, 245105 (2010)

Fermi surface topology of the two-dimensional Kondo lattice model: Dynamical cluster approximation approach

L. C. Martin, M. Bercx, and F. F. Assaad

We report the results of extensive dynamical cluster approximation calculations, based on a quantum Monte Carlo solver, for the two-dimensional Kondo lattice model. Our particular cluster implementation renders possible the simulation of spontaneous antiferromagnetic symmetry breaking. By explicitly computing the single-particle spectral function both in the paramagnetic and antiferromagnetic phases, we follow the evolution of the Fermi surface across this magnetic transition. The results, computed for clusters up to 16 orbitals, show clear evidence for the existence of three distinct Fermi surface topologies. The transition from the paramagnetic metallic phase to the antiferromagnetic metal is continuous; Kondo screening does not break down and we observe a backfolding of the paramagnetic heavy-fermion band. Within the antiferromagnetic phase and when the ordered moment becomes *large* the Fermi surface evolves to one which is adiabatically connected to a Fermi surface where the local moments are frozen in an antiferromagnetic order.



Can Kondo screening coexist with AFM long-range order?

PHYSICAL REVIEW B VOLUME 62, NUMBER 1 1 JULY 2000-I

Kondo singlet state coexisting with antiferromagnetic long-range order: A possible ground state for Kondo insulators

Guang-Ming Zhang[1] and Lu Yu[2,3]

Focus on the half-filled Kondo lattice model

$$H=\sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + H_{\parallel} + H_{\perp} ,$$

$$H_{\parallel}=\frac{J_{\parallel}}{4}\sum_{i} (d^{\dagger}_{i\uparrow}d_{i\uparrow}-d^{\dagger}_{i\downarrow}d_{i\downarrow})(c^{\dagger}_{i\uparrow}c_{i\uparrow}-c^{\dagger}_{i\downarrow}c_{i\downarrow}), \qquad H_{\perp}=\frac{J_{\perp}}{2}\sum_{i} (d^{\dagger}_{i\downarrow}d_{i\uparrow}c^{\dagger}_{i\uparrow}c_{i\downarrow}+d^{\dagger}_{i\uparrow}d_{i\downarrow}c^{\dagger}_{i\downarrow}c_{i\uparrow}),$$

AFM order parameters: $m_c=-\frac{1}{2}\langle c^{\dagger}_{i\uparrow}c_{i\uparrow}-c^{\dagger}_{i\downarrow}c_{i\downarrow}\rangle e^{-i\mathbf{Q}\cdot\mathbf{r}_i}$ $\qquad m_d=\frac{1}{2}\langle d^{\dagger}_{i\uparrow}d_{i\uparrow}-d^{\dagger}_{i\downarrow}d_{i\downarrow}\rangle e^{-i\mathbf{Q}\cdot\mathbf{r}_i},$

Kondo screening: $\left\langle c^{+}_{i\uparrow}d_{i\uparrow} + d^{+}_{i\downarrow}c_{i\downarrow}\right\rangle = \left\langle c^{+}_{i\downarrow}d_{i\downarrow} + d^{+}_{i\uparrow}c_{i\uparrow}\right\rangle = -V$

$$H_{11} \ : \ \frac{J_{\parallel}}{2}\left[m_d\sum_{i} e^{i\mathbf{Q}\cdot\mathbf{r}_i}(c^{\dagger}_{i\uparrow}c_{i\uparrow}-c^{\dagger}_{i\downarrow}c_{i\downarrow})-m_c\sum_{i} e^{i\mathbf{Q}\cdot\mathbf{r}_i}(d^{\dagger}_{i\uparrow}d_{i\uparrow}-d^{\dagger}_{i\downarrow}d_{i\downarrow})\right]+J_{\parallel}m_c m_d\mathcal{N},$$

$$H_{\perp} \ : \ \frac{J_{\perp}V}{2}\sum_{i\sigma} (c^{\dagger}_{i\sigma}d_{i\sigma}+d^{\dagger}_{i\sigma}c_{i\sigma})+\frac{J_{\perp}}{2}V^2\mathcal{N},$$

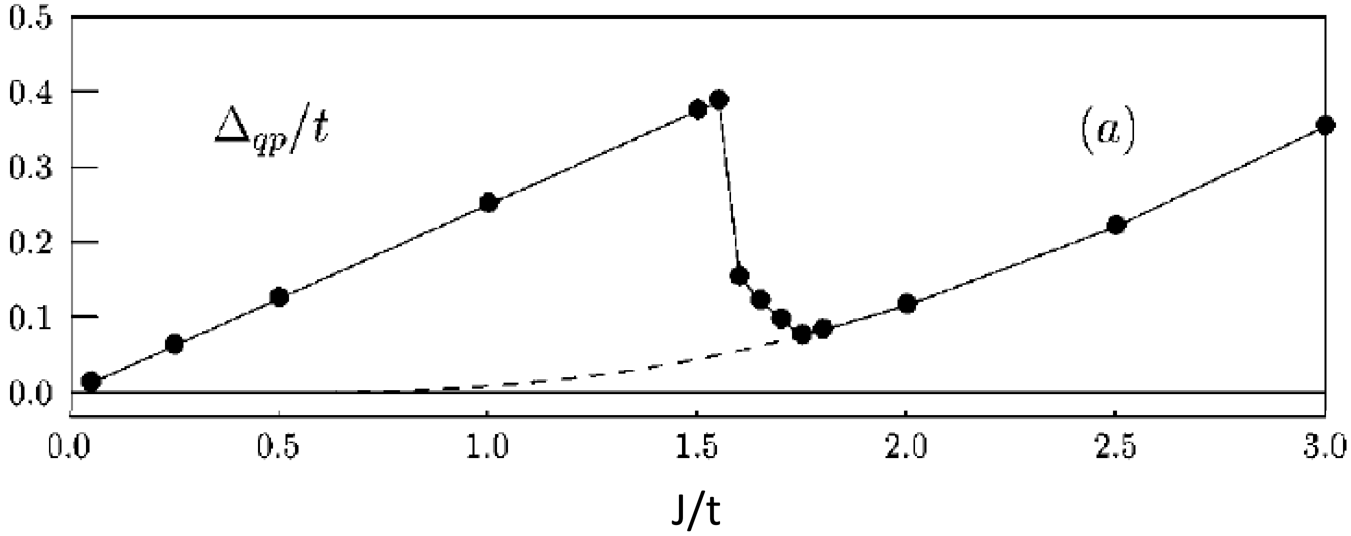
Renormalized bands energies:

$$E_{\pm\pm}(\mathbf{k})=\pm\frac{1}{\sqrt{2}}\sqrt{\epsilon^2_{\mathbf{k}}+J^2_{\parallel}(m^2_c+m^2_d)/4+J^2_{\perp}V^2/2\pm E'(\mathbf{k})},$$

$$E'(\mathbf{k})=\left\{[\epsilon^2_{\mathbf{k}}+J^2_{\parallel}(m^2_c+m^2_d)/4+J^2_{\perp}V^2/2]^2-\frac{1}{4}(J^2_{\parallel}m_c m_d+J^2_{\perp}V^2)^2-J^2_{\parallel}m^2_c\epsilon^2_{\mathbf{k}}\right\}^{1/2}.$$

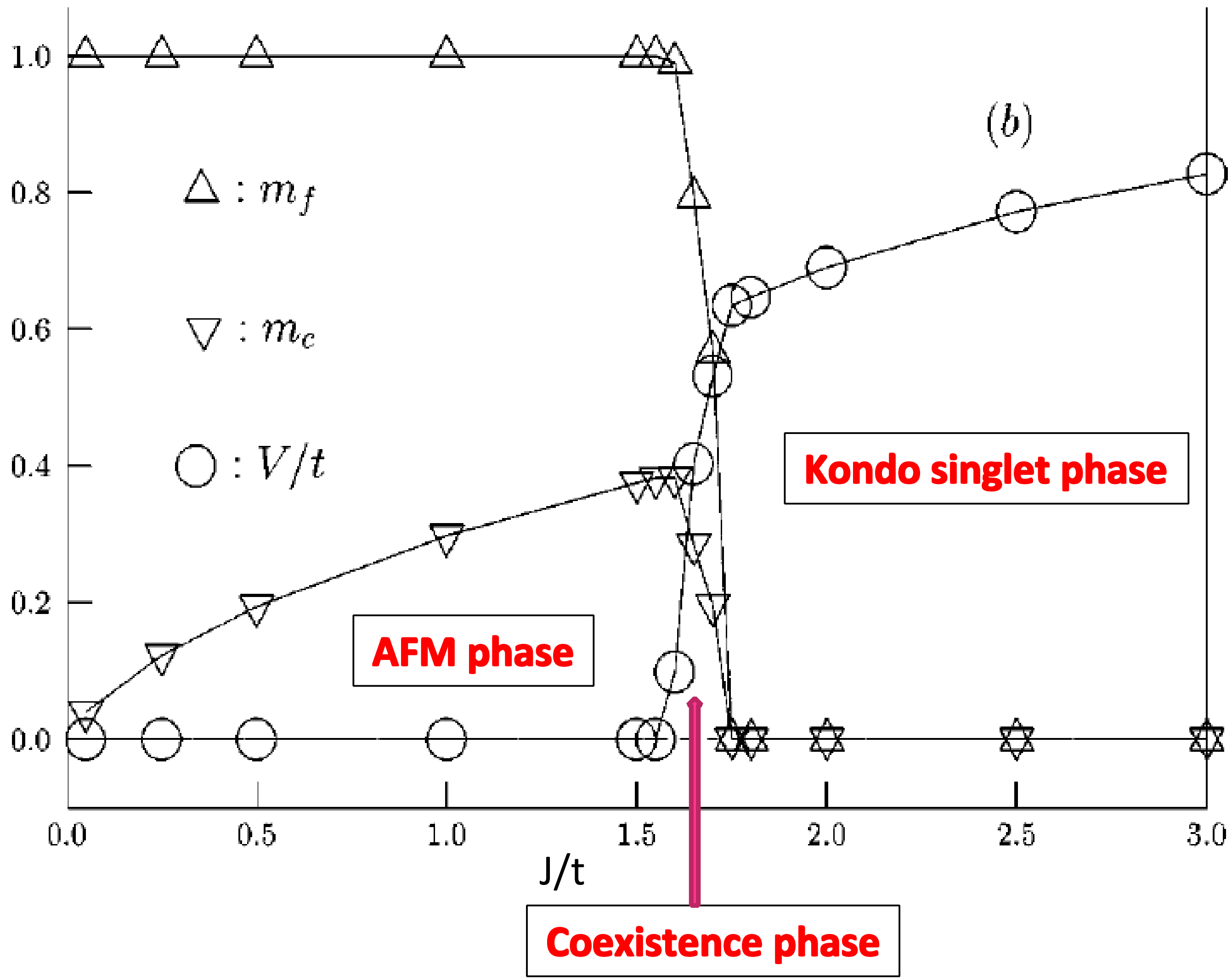
The ground state energy: $E_g = 2\sum_{\mathbf{k}}{}' [E_{--}(\mathbf{k}) + E_{-+}(\mathbf{k})] + \mathcal{N}\left(J_{\parallel} m_c m_d + \frac{J_{\perp} V^2}{2} \right)$

The numerical calculations are performed on a square lattice with $J_{11} = J_{\perp} = J$.



A finite quasiparticle gap implies the Kondo correlated insulating state!

Order parameters for the half-filled Kondo lattice model



Coexistence of Kondo screening and AFM long-range order is confirmed by QMC !

PHYSICAL REVIEW B, VOLUME 63, 155114

Spin and charge dynamics of the ferromagnetic and antiferromagnetic two-dimensional half-filled Kondo lattice model

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(Received 26 October 2000; published 30 March 2001)

Abstract

We present a detailed numerical study of ground state and finite temperature spin and charge dynamics of the two-dimensional Kondo lattice model with hopping t and exchange J. Our numerical results stem from

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from its strong-coupling form with spin gap at $\vec{q}=(\pi,\pi)$ to a spin-wave form. For $J>0$, the single-particle spectral function $A(\vec{k},\omega)$ shows a dispersion relation following that of hybridized bands as obtained in the noninteracting periodic Anderson model. In the ordered phase this feature is supplemented by shadows, thus allowing an interpretation in terms of the coexistence of Kondo screening and magnetic ordering. In contrast,

Conclusions

- **Multiply quantum phase transitions can be driven by AFM short-range correlations within the heavy Fermi liquid phase in the Kondo lattice systems**
- **Kondo screening coexisting with the AFM long-range order can be a ground state of the Kondo insulating phase**
- **Kondo screening can also coexist with the FM long-range order in Kondo lattice model**

PHYSICAL REVIEW B **81**, 094420 (2010)

Kondo screening coexisting with ferromagnetic order as a possible ground state for Kondo lattice systems

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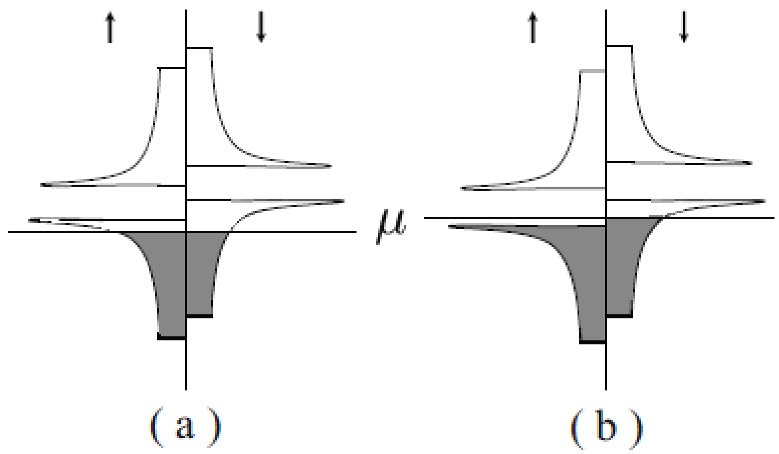
Lu Yu

Schematic renormalized local density of states:



Phase diagram