A Hund's Rule Stabilized Nematic Magnetic State in URu_2Si_2

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Acknowledgements

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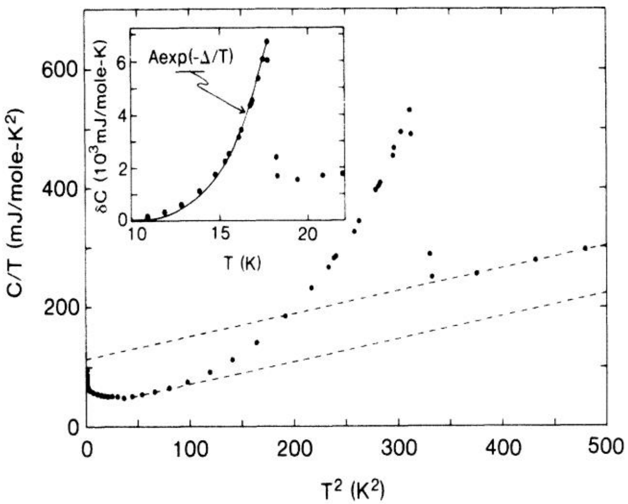
Outline

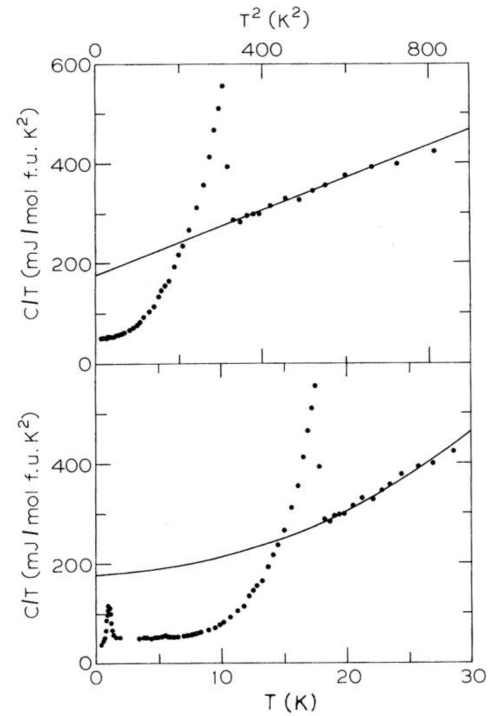
- Experiments on URu_2Si_2
- The Under-Compensated Anderson Lattice Model
- A Bare Band Structure
- The spin-rotationally invariant Coulomb interactions
- The Order Parameter
- A Mean-field Approximation
- Magnetic Nematicity
- Conclusions

The Experimental Manifestations of Hidden Order in URu_2Si_2

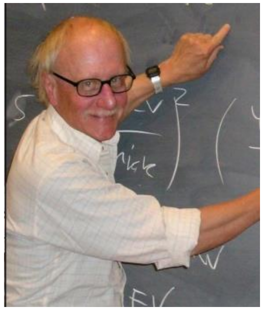
- The discovery of superconductivity at T=1.5 K and a phase transition at T=17.5 K with a large specific heat jump in the heavy-fermion material URu_2Si_2
- γ = 155 mJ/mole K^2



Maple et al. (1986)



Palstra et al. (1985)

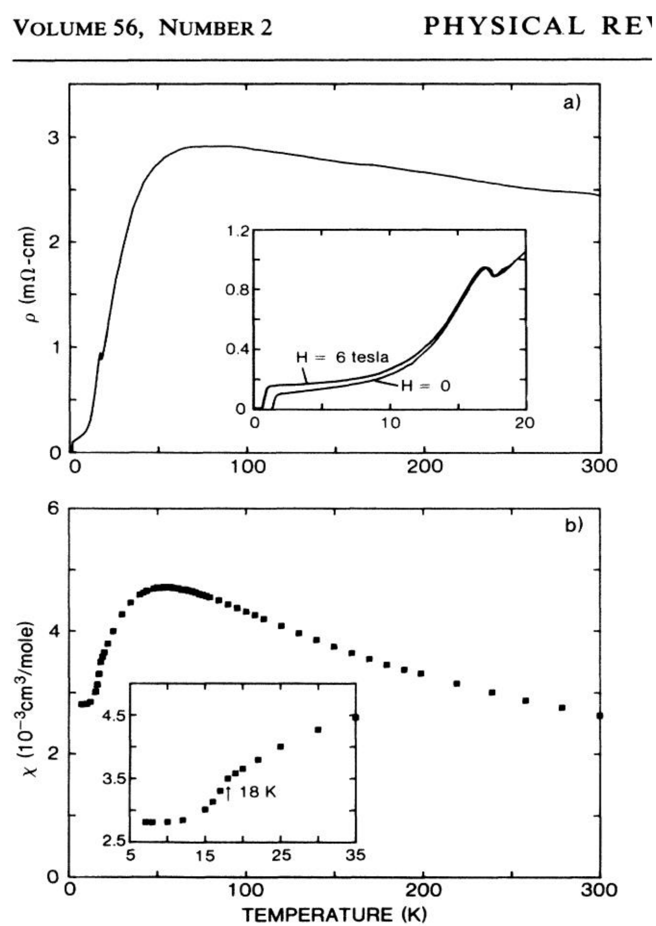


Experimental Manifestations

Maple et al. (1986)

Resistivity&Specific Heat

- Gap of ~ 10 meV
- 40% of the Fermi-Surface gapped



Direct Observation of Gaps

- Far Infrared Spectroscopy

(Reflectivity)

Bonn, Garret and Timusk (1988)

Gaps of 5 and 7.6 meV

$2\Delta/k_B T_{HO} = 3.6 - 5.1$

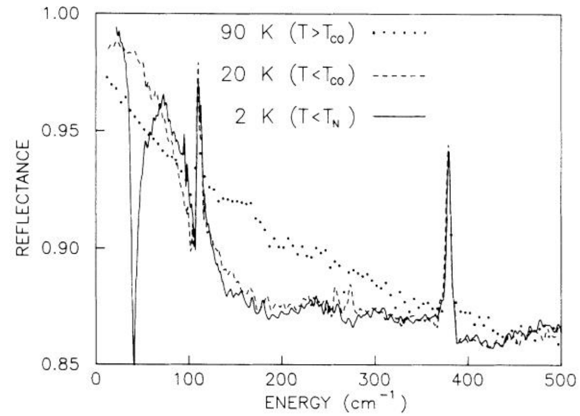
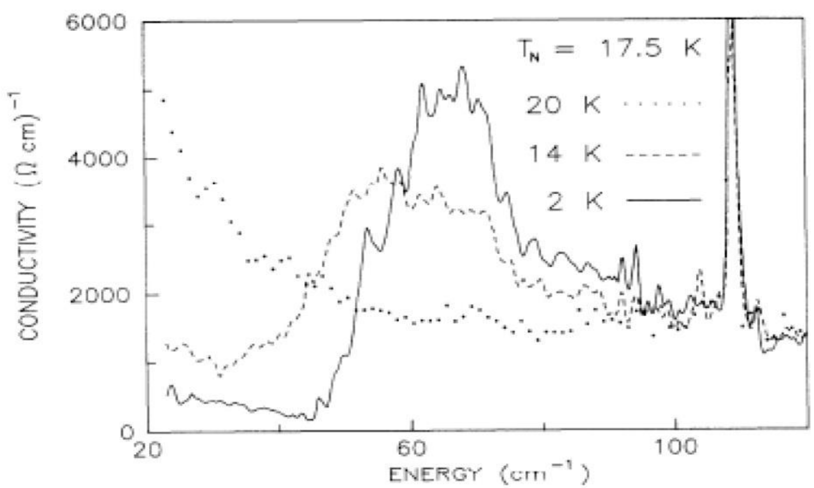


FIG. 1. The reflectance of URu_2Si_2 above the coherence temperature, below the coherence temperature, and below the Néel temperature.

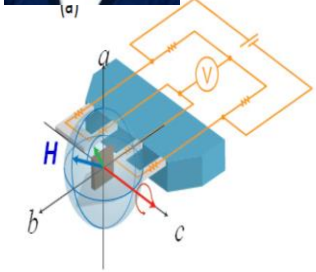


Broken Spin-Rotational Invariance

- Magnetic Torque

Okazaki et al (2011)



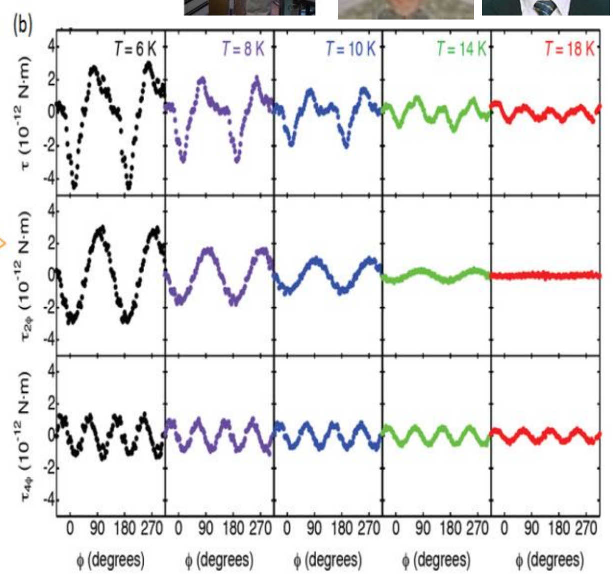


Figure 3: (a) Schematic configuration of the magnetic torque measurements for *ab*-plane field rotation by using the micro-cantilever technique. The magnetic field H (blue arrow) induces the magnetization M (green arrow) in the URu_2Si_2 crystal. The torque along the c axis (red arrow) can be detected by the change in the piezo resister, which is measured by the bridge configuration. (b) Upper panels show raw magnetic torque curves as a function of the azimuthal angle ϕ at several temperatures. All data are measured at $|\mu_0 H| = 4$ T. Middle and lower panels show twofold $\tau_{2\phi}$ and fourfold $\tau_{4\phi}$ components of the torque curves which are obtained from the Fourier analysis.

- Shubnikov-de Haas

Altarawneh et al (2011)

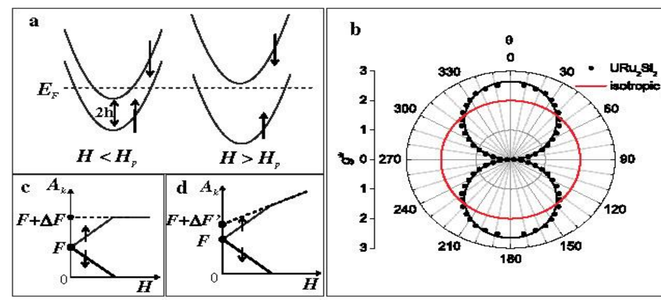


FIG. 3 (color online). (a) Schematic showing band polarization caused by Zeeman splitting, resulting in the depopulation of the minority spin component above H_p defined in Eq (1). (b) Polar plot of the measured θ-dependent effective g factor in URu_2Si_2 [19,27] (black symbols) together with a fit to $g^* = g_z \cos\theta$ (black line), where $g_z = 2.6$ (assuming $\frac{1}{2}$ pseudospins), and its comparison with an isotropic $g = 2$ (red line). (c) Schematic of the field-dependent cross-sectional areas of the up-spin and down-spin components for a single pocket, together with the "back projected" quantum oscillation frequency before F and after $F + \Delta F$ polarization. (d) The same schematic in which the frequency shift $\Delta F'$ is reduced by additional pockets acting as a charge reservoir.

The Compensated Anderson Lattice

- N-fold degenerate localized 5f atomic levels E_f
- N-fold degenerate conduction band e_k

- Hybridization V_{fd}

→ N Hybridized Bands

- Coulomb Interaction U and Hund's rule Exchange J between 5f electrons on the same atom

→ Kondo Effect with a zero magnetic moment

Localized 5f spin $S^z=N/2$ screened by a compensating cloud of conduction electrons with spin $S^z=-N/2$ (forming a spin singlet)

The Under-Compensated Anderson Lattice

- N-fold degenerate semi-localized 5f bands (small direct hopping)
- 1 (spin-only degenerate) non-degenerate itinerant conduction band

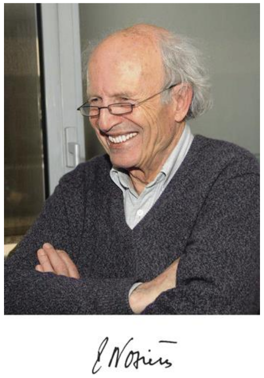
- Hybridization V_{fd}

→ Hybridized Band and (N-1) Unhybridized bands

- Coulomb Interaction U and Hund's rule Exchange J between the 5f electrons on the same atom (forms a net atomic spin)

→ Kondo Effect but also yields a net moment of (N-1)/2

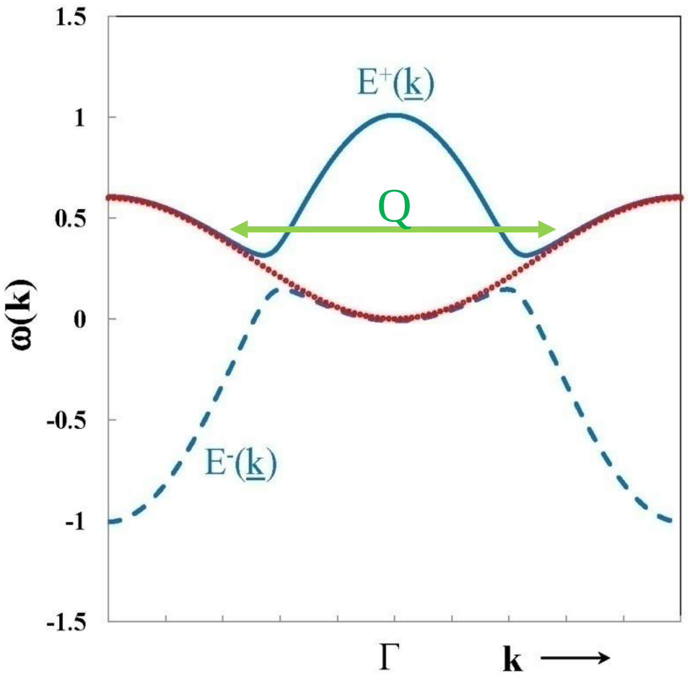
Nozieres and Blandin (1980)



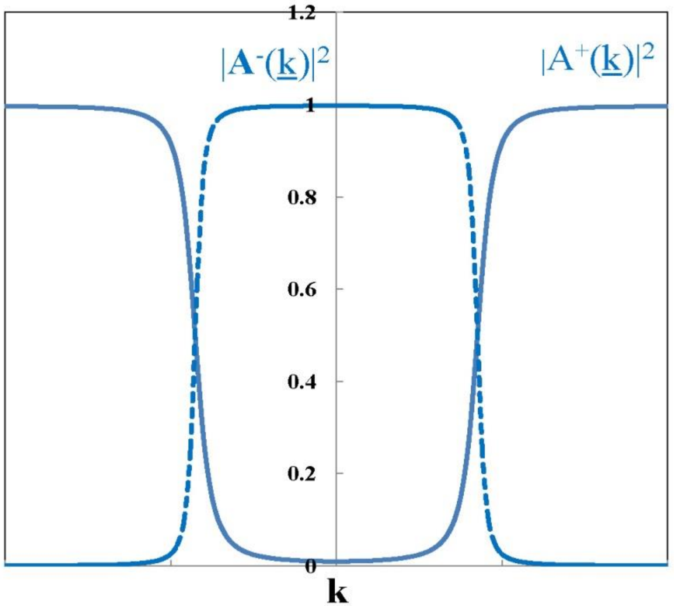
Uranium Monochalcogenides and Pnictides

Kondo Effect and Magnetic Ordering

The Bare Bands



Bands:
Two degenerate 5f bands
One conduction band
(nearest neighbour tight-binding)
Hybridization V_{fd} between the conduction and the 5f α band



5f α Characters of upper and lower hybridized bands

The 5f β band is unhybridized

Note that for most k values the α and β bands have their relative energies shifted by an amount V_{fd}^2

(Depending on μ, they have roughly the same nesting vectors, Q)

Normal State Density of States

Hybridized 5f–α states (blue)

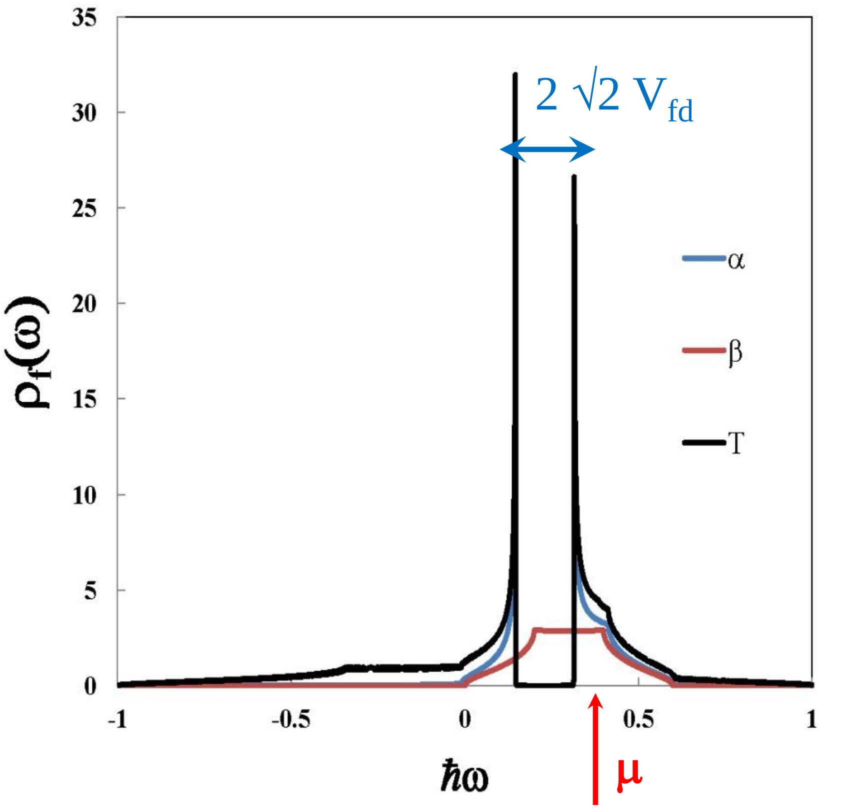
Total hybridized f α plus conduction (d) band DOS (black)

Direct Hybridization Gap ~ $2\sqrt{N}\, V_{fd}$
(below Fermi energy)

Unhybridzed 5f-β states (red)
(N-1)-fold degenerate

Chemical potential μ in the upper heavy α 5f band

Model for Hidden Order
Physical Review B, 85, 165116 (2012)



Spin Rotationally Invariant Coulomb Interactions

The Coulomb interaction can be re-written in the form

$$\hat{H}_{int} = \left(\frac{U-J}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi\neq\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} \; f^{\chi}_{\underline{k},\sigma} \; f^{\dagger,\chi'}_{\underline{k}'-\underline{q},\sigma} f^{\chi'}_{\underline{k}',\sigma}$$

$$+ \left(\frac{U}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi,\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} \; f^{\chi}_{\underline{k},\sigma} \; f^{\dagger,\chi'}_{\underline{k}'-\underline{q},-\sigma} f^{\chi'}_{\underline{k}',-\sigma}$$

$$+ \left(\frac{J}{2N}\right) \sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi\neq\chi'} f^{\dagger,\chi}_{\underline{k}+\underline{q},\sigma} \; f^{\chi'}_{\underline{k},\sigma} \; f^{\dagger,\chi'}_{\underline{k}'-\underline{q},-\sigma} \; f^{\chi}_{\underline{k}',-\sigma} \qquad (7)$$

U is the direct Coulomb Interaction

J is the Hund's rule exchange (Here, N is the number of lattice sites)

$- J \, \underline{\mathbf{S}}_{\chi i} \cdot \underline{\mathbf{S}}_{\chi' i}$

As can be seen by commuting the annihilation operators, the last term is equivalent to the **spin-flip part of the Hund's rule exchange** between orbital χ and χ'

$$- J/2 \left(S^{+}_{\chi,i} \, S^{-}_{\chi',i} + S^{-}_{\chi,i} \, S^{+}_{\chi',i} \right)$$

But we view it as a spin conserving hopping process involving a spin-up electron and a spin-down electron

A Hidden Order Parameter

A possibility for the hidden order parameter is Z_Q

$$Z_Q = 1/N \sum_{k,\sigma} \sigma \ < f^{+\beta}_{k+Q,\sigma} \, f^{\alpha}_{k,\sigma} >$$

which is driven by the spin-flip part of the Hund's rule exchange J.

It only connect states with different orbital indices (α,β).

(no net spin)

(broken spin-rotational invariance, and produces an x-y anisotropy)

It can be complex (broken gauge invariance)

See also: Tanmoy Das, Scientific Reports, (2012).

A Mean-Field Approximation

- Linearize the (spin-flip Hund's rule) interactions (momentum indices supressed)

$$+ J f^{+,\beta}_{\uparrow} f^{\alpha}_{\uparrow} < f^{+,\alpha}_{\downarrow} f^{\beta}_{\downarrow} >_Q + J f^{+,\alpha}_{\downarrow} f^{\beta}_{\downarrow} < f^{+,\beta}_{\uparrow} f^{\alpha}_{\uparrow} >_Q$$
$$- J < f^{+,\beta}_{\uparrow} f^{\alpha}_{\uparrow} >_Q < f^{+,\alpha}_{\downarrow} f^{\beta}_{\downarrow} >_Q$$
$$+ \text{Hermitean conjugate}$$

What if? $< f^{+,\beta}_{\uparrow} f^{\alpha}_{\uparrow} >_Q = - < f^{+,\beta}_{\downarrow} f^{\alpha}_{\downarrow} >_Q$

(1) The energy would be lowered by ΔE compared to the normal state defined by

$< f^{+,\beta}_{\sigma} f^{\alpha}_{\sigma} >_Q = 0$, $\Delta E = - \Sigma_{\sigma} J \, | < f^{+,\beta}_{\sigma} f^{\alpha}_{\sigma} >_Q |^2$

(2) **Spin-dependent (inter-orbital) Hybridization:** (with momentum transfer Q)

$$H_{hyb} = + \Sigma_k (J < f^{+,\beta}_{\uparrow} f^{\alpha}_{\uparrow} >_Q f^{+,\alpha}_{k-Q\downarrow} f^{\beta}_{k\downarrow} + \text{H.c.})$$
$$- \Sigma_k (J < f^{+,\beta}_{\uparrow} f^{\alpha}_{\uparrow} >_Q f^{+,\alpha}_{k-Q\uparrow} f^{\beta}_{k\uparrow} + \text{H.c.})$$

A Mean-Field Approximation

$$a^{+}_{k,\uparrow} = \sqrt{½}\ (f^{+,\alpha}_{k+Q,\uparrow} + f^{+,\beta}_{k,\uparrow})$$
$$a^{+}_{k,\downarrow} = \sqrt{½}\ (f^{+,\alpha}_{k+Q,\downarrow} - f^{+,\beta}_{k,\downarrow})$$

(spin-dependent hybridized 5f bands)

Not sensitive to an (spin-independent) orbital measurement

$$½\ | \Psi^{\alpha}_{k+Q} + \Psi^{\beta}_{k} |^2 + ½ \,| \Psi^{\alpha}_{k+Q} - \Psi^{\beta}_{k} |^2$$

$$= \quad | \Psi^{\alpha}_{k+Q} |^2 + | \Psi^{\beta}_{k} |^2$$

(same result as in the normal state where there are no interference terms)

The spin-up orbital density wave is compensated by a spin down orbital density wave.

Requires Fermi-surface nesting in the normal state!

Fermi-surface Interband Nesting

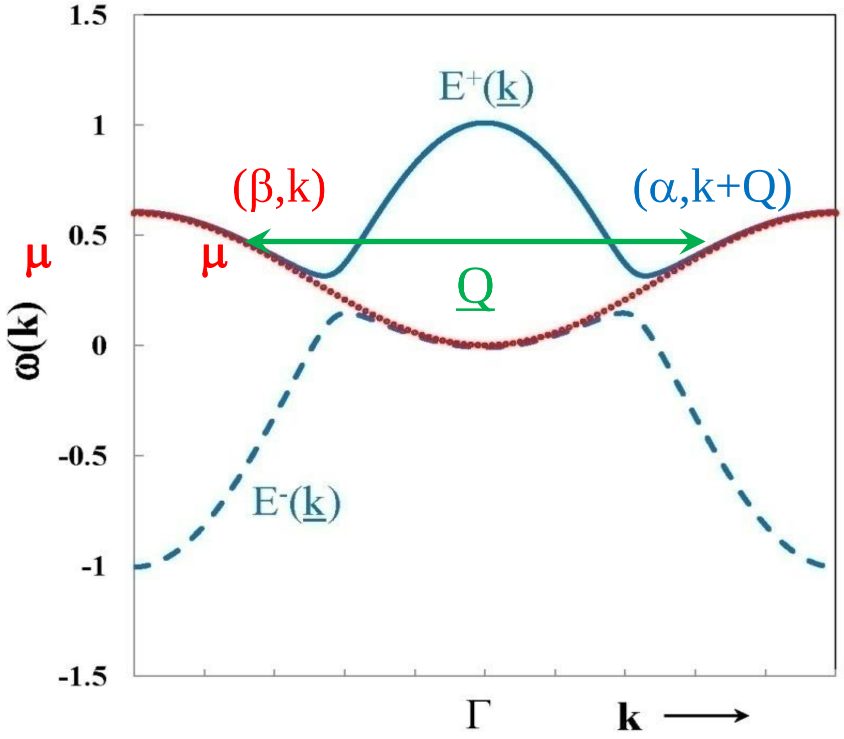
The states on the Fermi-surfaces of the α and β bands are connected by the nesting vector Q

Interband:
β–α red to blue

Intraband:
α–α blue to blue
β–β red to red

Note: The red β and blue α 5f bands are not degenerate but are shifted by a hybridization gap with a very small energy of the order V_{fd}^2/W.

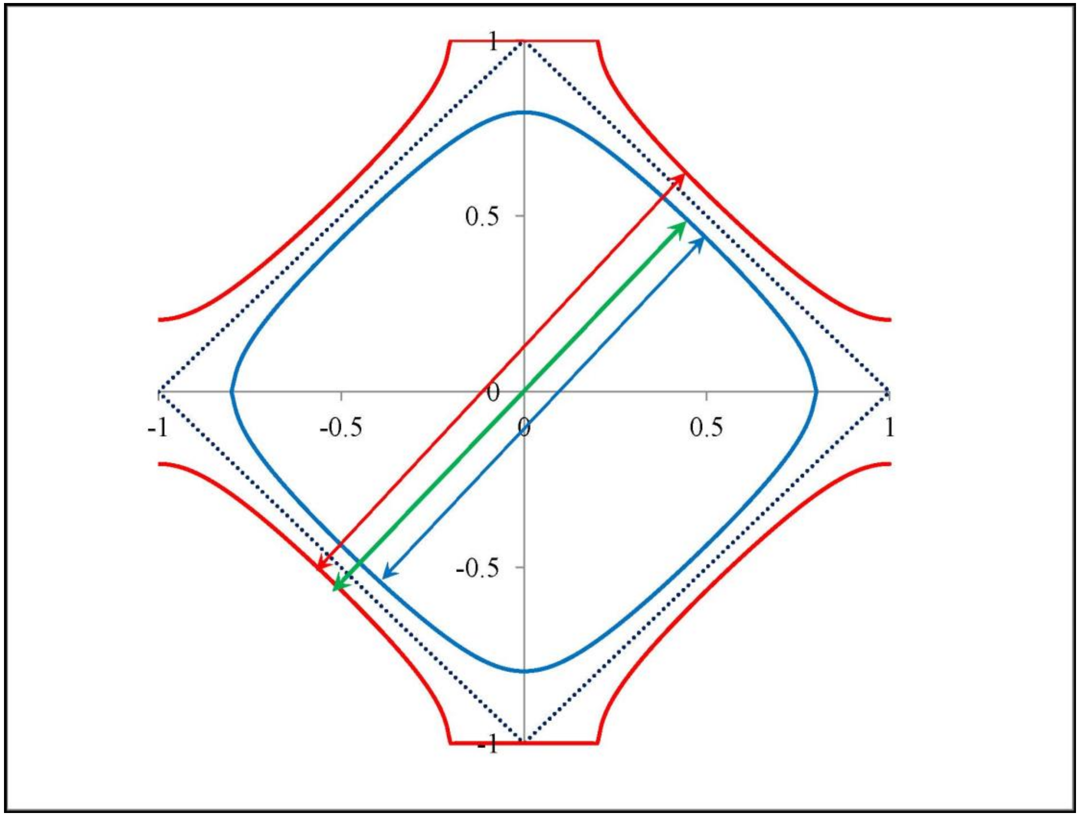
Wan-Kyu Park et al. Phys. Rev. Lett. (2012).



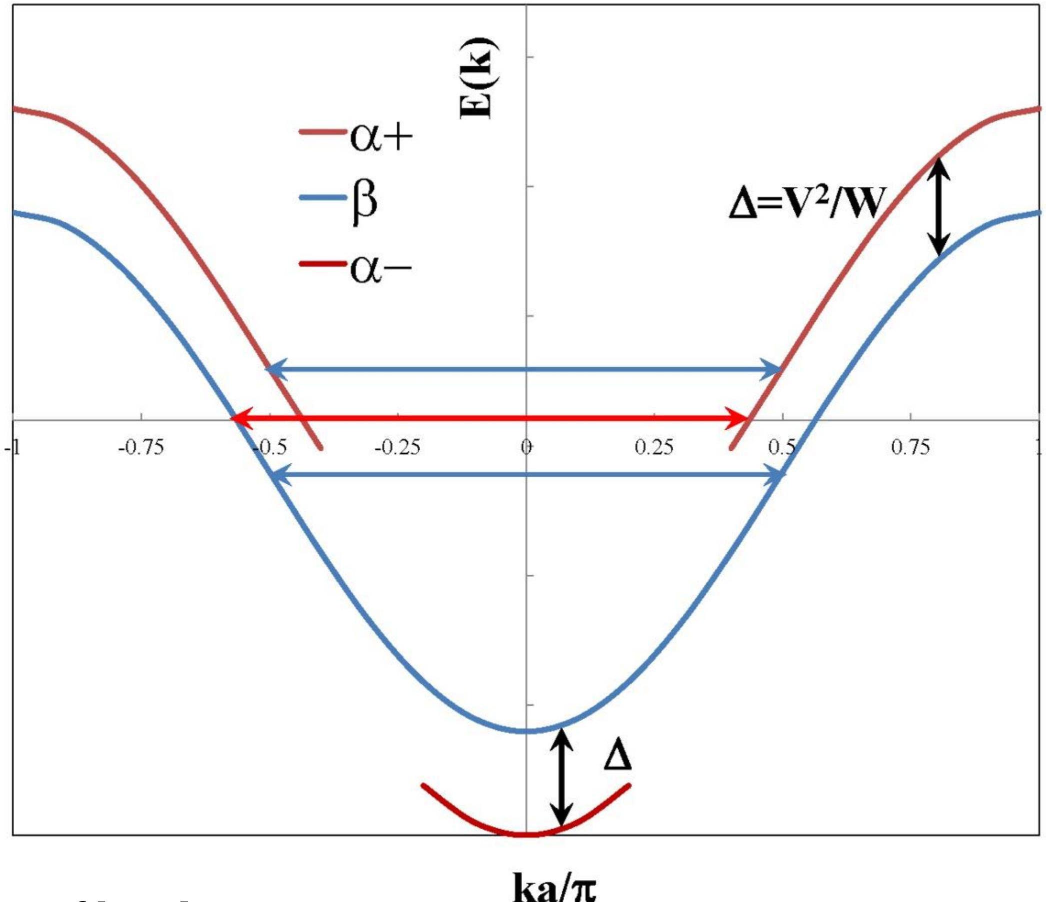
Fermi-surface Interband Nesting

- Effect of energy shift due to hybridization on inter and intraband nesting: relative shift of Fermi-energy

Schematic in 2d:



Nesting and Pressure



The red β and blue α 5f bands are not degenerate but are shifted by a very small energy of the order V_{fd}^2/W.

The Linearized Gap Equation

$$\left[1-(U-J)\chi^{\alpha,\beta,(0)}_{f,\sigma}(\underline{Q},0)\right] z^*_{\underline{Q},\sigma} = -z^*_{\underline{Q},-\sigma} J \chi^{\alpha,\beta}_{f,\sigma}(\underline{Q},0),$$

$$\left[1-(U-J)\chi^{\alpha,\beta,(0)}_{f,-\sigma}(\underline{Q},0)\right] z^*_{\underline{Q},-\sigma} = -z^*_{\underline{Q},\sigma} J \chi^{\alpha,\beta}_{f,-\sigma}(\underline{Q},0),$$

where

$$\chi^{\alpha,\beta,(0)}_{f,\sigma}(\underline{Q},0) = \frac{1}{N}\sum_{\underline{k},\pm} |A^{\pm}_{\sigma}(\underline{k})|^2 \left(\frac{f[E^{\pm}_{\sigma}(\underline{k})] - f[E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q})]}{E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q}) - E^{\pm}_{\sigma}(\underline{k})}\right).$$

1. The equations are odd in z and posses a trivial solution $z_{Q\sigma} = 0$ for $T > T_{HO}$

2. The interband susceptibility $\chi^{\alpha\beta}(Q,0)$ is positive, and **large** , if there is **inter-band nesting**.

3. The Hund's rule J exchange is enhanced by the Coulomb interaction U,

$$1 = J\,\chi^{\alpha\beta}(Q)/[1-(U-J)\,\chi^{\alpha\beta}(Q)]$$

4. At the critical temperature $T=T_{HO}$, one has an (infinitesimal) non-zero solution with $\mathbf{z_{Q,\sigma} = - z_{Q,-\sigma}}$

Nesting and Adiabatic Continuity

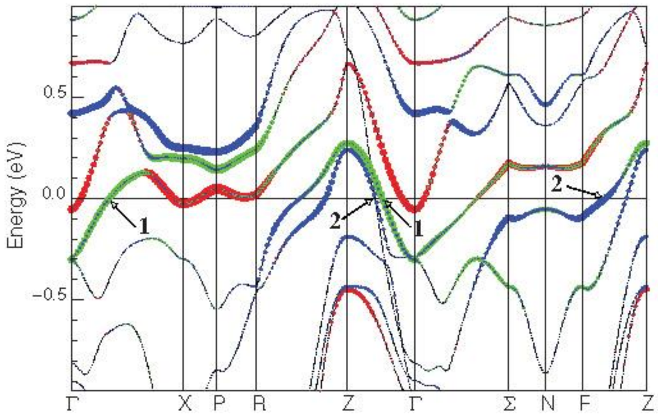


FIG. 3. (Color online) Band characters of the energy dispersions of URu_2Si_2 in the bct BZ. Green/light gray symbols illustrate the U $5f_{5/2}$ $j_z = \pm 5/2$ character, blue/dark gray symbols the $j_z = \pm 3/2$ character, and red/gray symbols the $j_z = \pm 1/2$ character (for the symmetry points used, see Ref. 35).

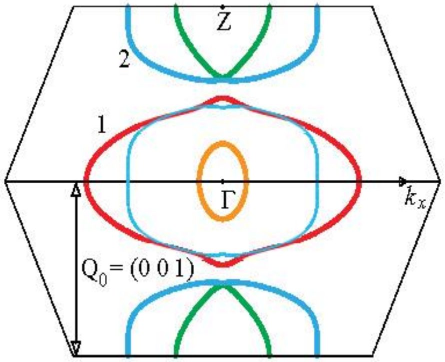


FIG. 2. (Color online) Cross section of the bct BZ displaying an imperfect nesting of the FS sheets No. 1 and 2 at Q_0. FS sheet No. 2 has additionally been shifted by Q_0, shown by the thin curve, to illustrate the imperfect nesting. The cross section is spanned by the k_z and k_x axes. Cross sections of two other existing FS pockets are shown at the Γ and Z points.

LDA Peter Oppeneer (2011)

Two nesting vectors in URu_2Si_2: One is Commensurate and one is Incommensurate.

dHvA Hassinger (2010)

Q_0=(0,0,1)

Hidden Ordering,

Q_0=(0,0,1)

Magnetic Ordering

Adiabatic Continuity?

- Change μ (fixed V_{fd})

Criterion for Instability (U=J)

$1/U = \chi^{\alpha\alpha}(Q,0) + \chi^{\beta\beta}(Q,0)$

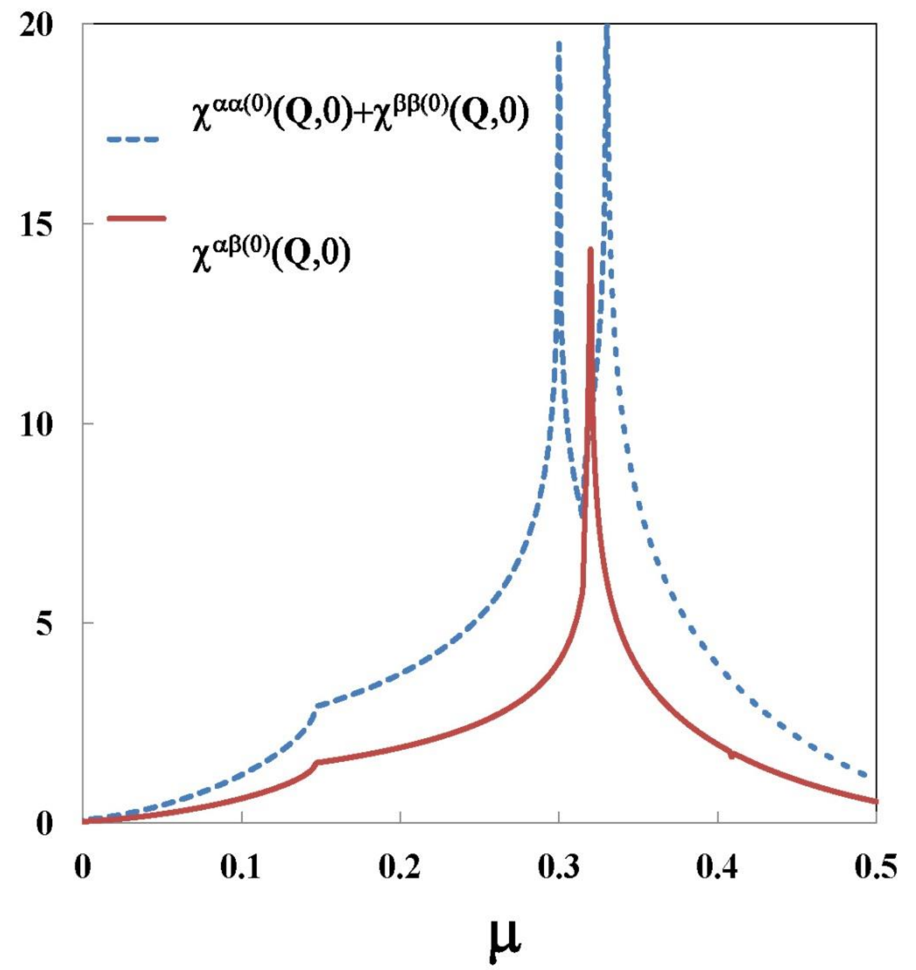
Antiferromagnetism

Hidden Order

$1/U = \chi^{\alpha\beta}(Q,0)$

Antiferromagnetism

(separated by μ the order of V_{fd}^2/W)



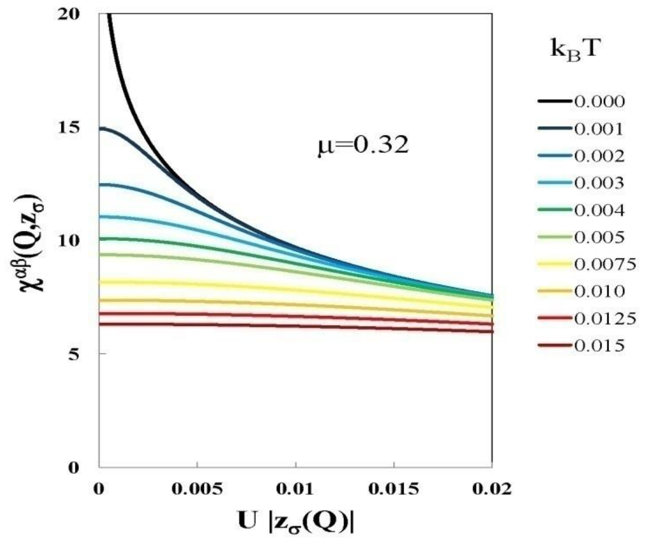
- Adiabatic Continuity:

either $V_{fd} \rightarrow 0$ or W increases

AF and HO instabilities become degenerate

The Gap Equation

$$z^*_{\underline{Q},\sigma} \; = \; - \, \frac{1}{N} \, \sum_{\underline{k}} \, \Bigg[\, \int_C \, \frac{d\omega}{2 \pi i} \, f(\omega) \, G^{\beta,\alpha}_{ff,\sigma}(\underline{k}+\underline{Q},\underline{k},\omega) \, \Bigg]$$ [2]



The Hartree-Fock f band dispersion relation $E^{\chi}_{f,\sigma}(\underline{k})$ is given by

$$E^{\chi}_{f,\sigma}(\underline{k}) \; = \; E^{\chi}_{f}(\underline{k}) \; + \; \sum_{\chi'} \, \Bigg(\, (U-J) \; n^{\chi'}_{f,\sigma} \; (1 - \delta^{\chi,\chi'}) \; + \; U \; n^{\chi'}_{f,-\sigma} \Bigg)$$

and the gap parameter $\kappa_{\underline{Q},\sigma}$ is defined as the complex number

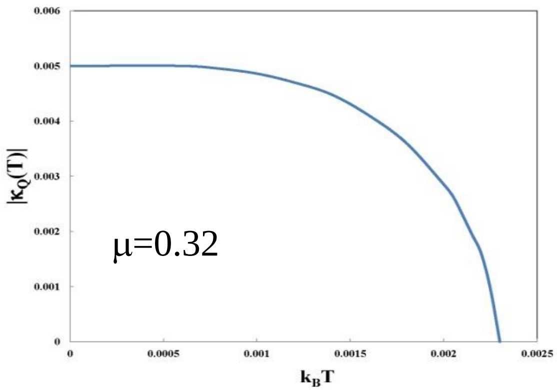
$$\kappa_{\underline{Q},\sigma} \; = \; J \; z_{-\underline{Q},-\sigma} \; - \; (\; U \; - \; J \;) \; z_{-\underline{Q},\sigma}$$

The mixed character 5f Green's function is given by

$$G^{\beta,\alpha}_{ff,\sigma}(\underline{k},\underline{k}',\omega) \;\; = \;\; \frac{\kappa^*_{\underline{Q},\sigma} \; (\omega - \epsilon(\underline{k}+\underline{Q})) \; \delta^{\alpha,\chi'} \, \delta_{\underline{k}+\underline{Q},\underline{k}'}}{D_\sigma(\underline{k}+\underline{Q},\omega)}$$

where the denominator is given by

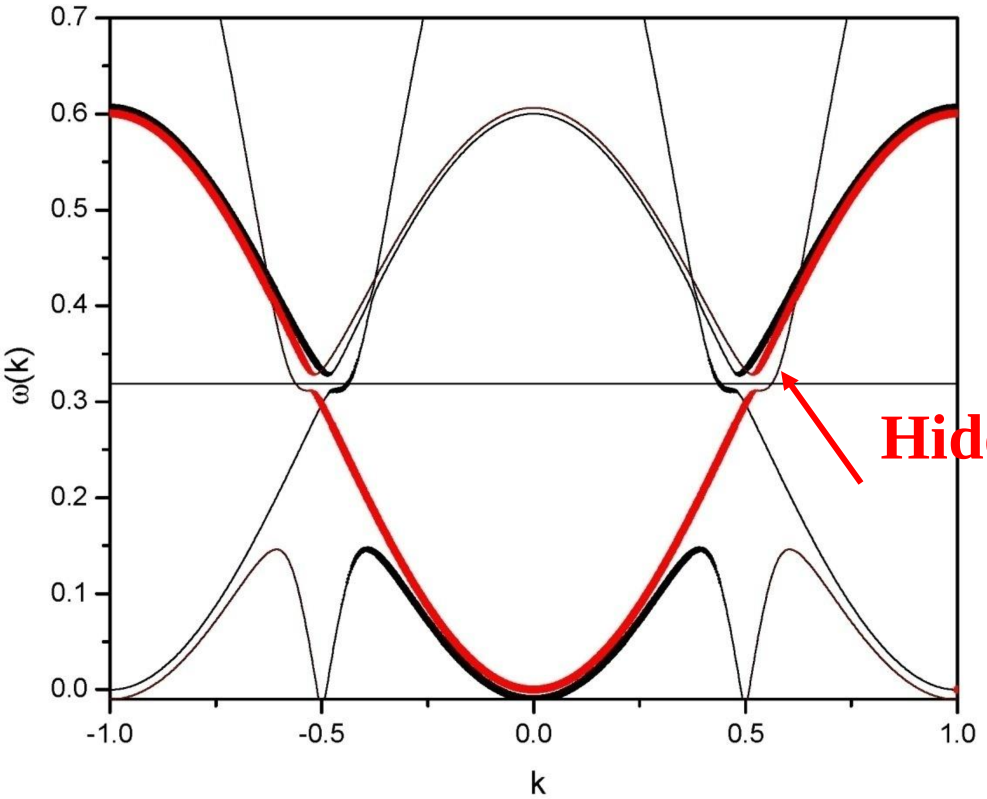
$$D_\sigma(\underline{k},\omega) \;\; = \;\; \Bigg[\, \Bigg(\omega - E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q}) \Bigg) \Bigg(\omega - E^{\alpha}_{f,\sigma}(\underline{k}) \Bigg) - \; |\kappa_{\underline{Q},\sigma}|^2 \, \Bigg] \; \Bigg(\omega - \epsilon(\underline{k}) \Bigg) \; - \; |V_\alpha(\underline{k})|^2 \, \Bigg(\omega - E^{\beta}_{f,\sigma}(\underline{k}+\underline{Q}) \Bigg)$$



$2|\kappa(0)|/k_B T_c = 4.54$

f- Quasiparticle Bands

Fermi Energy μ



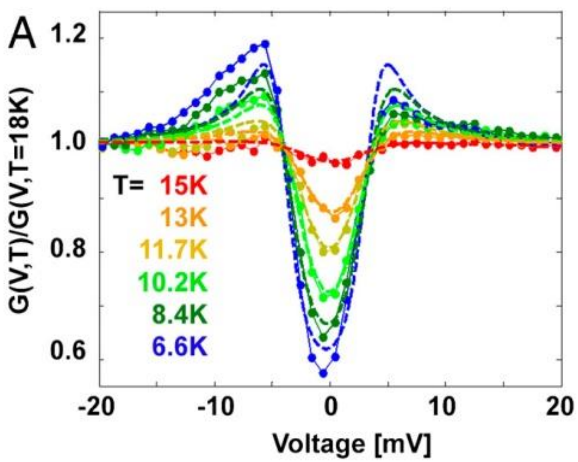
Hidden Order Gaps

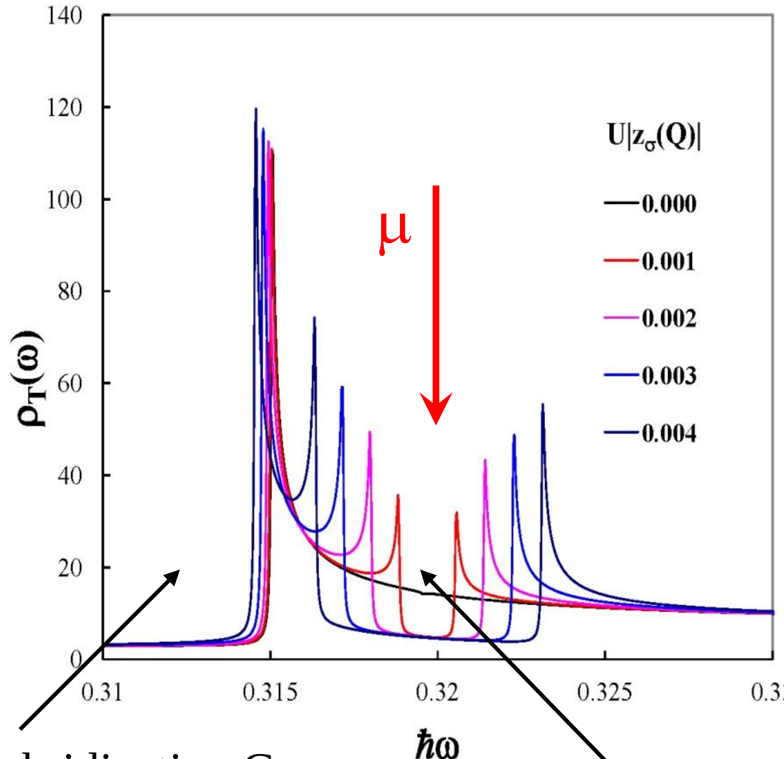
Asymmetric HO Gap in DOS

Anayajian et al. (2010)

60% Fermi Surface Gapped

Asymmetric HO Gap





Direct Hybridization Gap

Hidden Order PseudoGap

The Hidden Order Transition produces a pseudo-gap in the DOS.

Magnetic Nematicity

- Broken Spin Rotational Invariance (V=0)

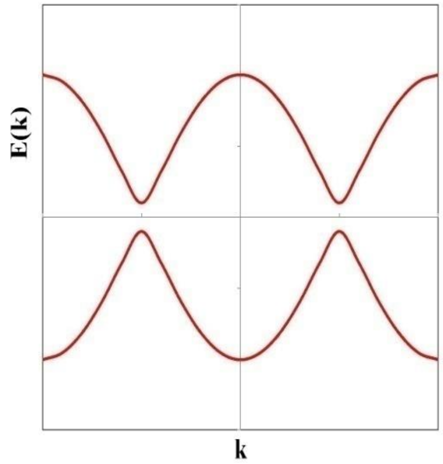
upper gap edge state (unoccupied)

$(\Psi^{\alpha}_{k+Q\uparrow} + \Psi^{\beta}_{k\uparrow})/\sqrt{2}$ $\quad$ $(\Psi^{\alpha}_{k+Q\downarrow} - \Psi^{\beta}_{k\downarrow})/\sqrt{2}$

lower gap edge state (occupied)

$(\Psi^{\alpha}_{k+Q\uparrow} - \Psi^{\beta}_{k\uparrow})/\sqrt{2}$ $\quad$ $(\Psi^{\alpha}_{k+Q\downarrow} + \Psi^{\beta}_{k\downarrow})/\sqrt{2}$

Band Gap $\quad$ $2 J |z_\sigma|$



- Zeeman Interaction (orientational dependence wrt to the z axis)

Parallel $\quad$ $-\mu_B H^z \sigma^z$

Matrix elements between occupied and unoccupied states are zero

No field dependence of the Energy $\quad$ **$\therefore \chi = 0$**

Perpendicular $\quad$ $-\mu_B H^x \sigma^x$

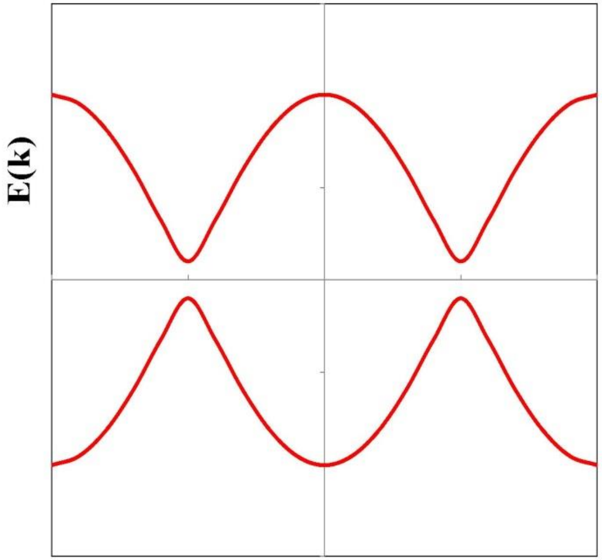
Matrix elements between occupied and unoccupied states are unity

Field dependence of the Energy

$$-(\mu_B H^x)^2 / 2 J |z_\sigma|$$

Magnetic Nematicity

- **Perpendicular susceptibility** V



Matrix elements $\mu_B J z / \sqrt{(\varepsilon(k)^2 + J^2 z^2)}$

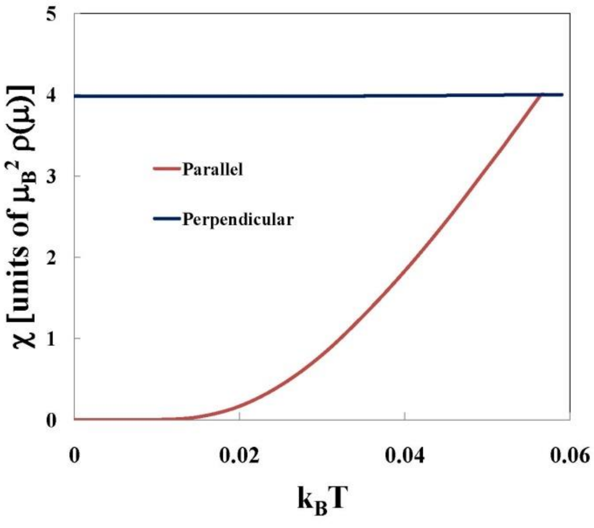
Gap $2 \sqrt{(\varepsilon(k)^2 + J^2 z^2)}$

Susceptibility

$$\mu_B^2 \int d\varepsilon \, \rho(\mu) \frac{J^2 z^2}{(\varepsilon^2 + J^2 z^2)^{3/2}}.$$

Nominally proportional to order parameter squared, but

$$\chi \sim 4 \mu_B^2 \rho(\mu)$$



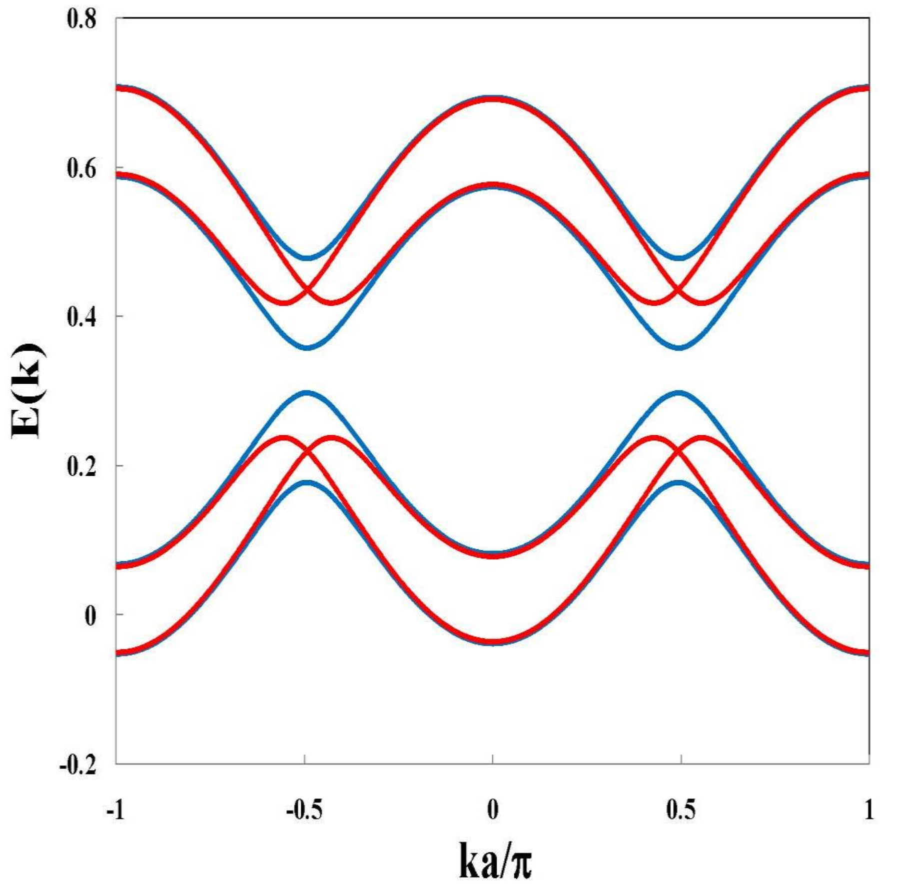
Magnetic Nematicity

- Quasiparticle Dispersion Relations in Field (V=0)
- Field Parallel to z $2\mu_B H^z$

Spin Split Bands

- Field Perpendicular to z

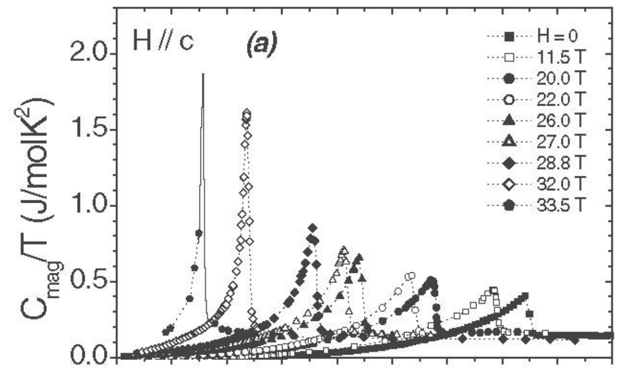
Coupled Bands



Quantum Critical Point?

Continuous Transition ends with a line of First-order Transitions?

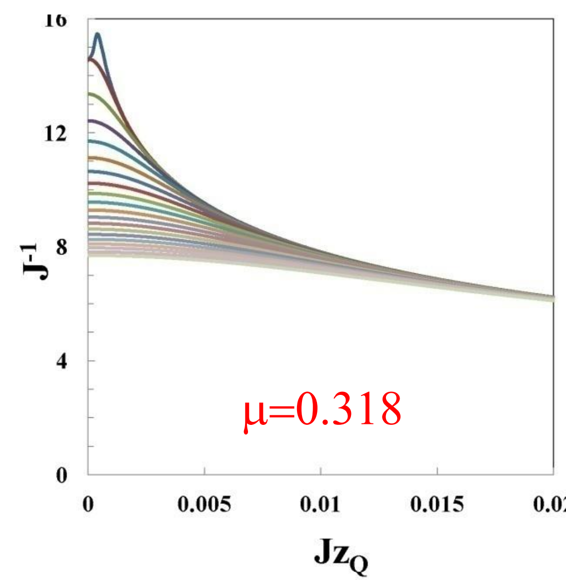
Marcelo Jaime et al. (2002).



On decreasing J one expects to reach a **Quantum Critical Point**. However:

Self consistency conditions for the gap as a function of U^{-1} for different T, for μ slightly off from the ideal nesting value

$$U^{-1}=\chi^{\alpha\beta}(T,z_Q)$$



U^{-1}<14 Second-order
U^{-1}>14 First-order

Riseborough&Magalhaes

QCP &Discontinuous Transition

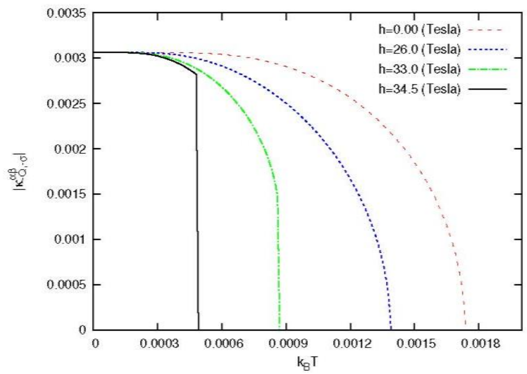


Figure 4: The gap $\kappa^{\alpha\beta}_{-Q,-\sigma}$ as function of k_BT for $J = 0.075$, $D = 0.60$ and different intensities of the magnetic field h.

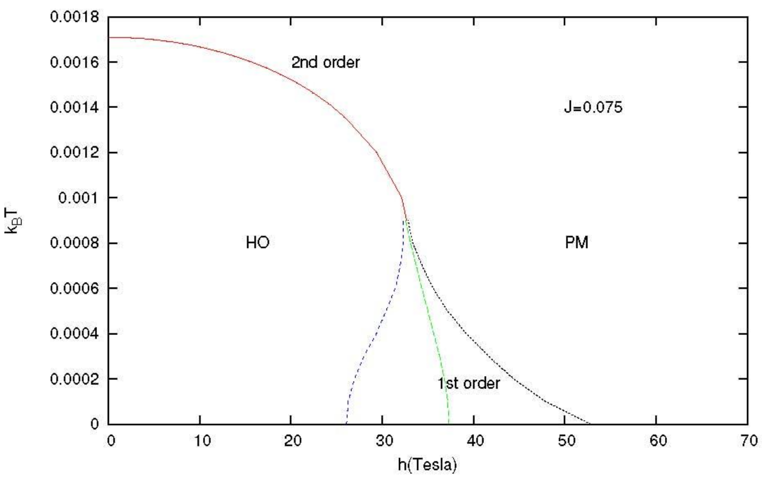
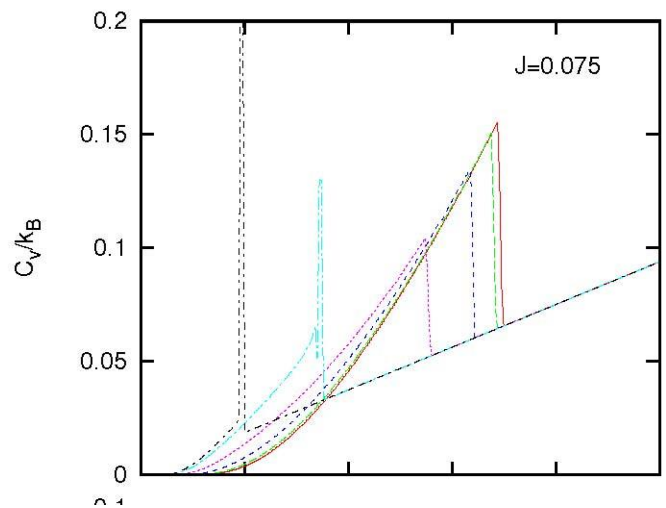


Figure 5: Phase diagram as function of the magnetic field h.



Eleonir Joao Calegari

Conclusions

- For systems with more than one occupied 5f band, there may be order parameters corresponding to the spontaneous (spatially inhomogeneous) mixing of the 5f bands, i.e.

$$\Sigma_{k,\sigma}\ \sigma < f^{+\beta}_{k+Q,\sigma}\ f^{\alpha}_{k,\sigma} > \ \neq 0$$

- The transition has broken spin-rotational invariance but doesn't have a staggered moment.

  (Magnetic Nematicity)

- The Hund's rule exchange J may stabilize an inter-orbital spin density wave

$$\Sigma_{k,\sigma}\ \sigma < f^{+\beta}_{k+Q,\sigma}\ f^{\alpha}_{k,\sigma} > \ \neq\ 0$$

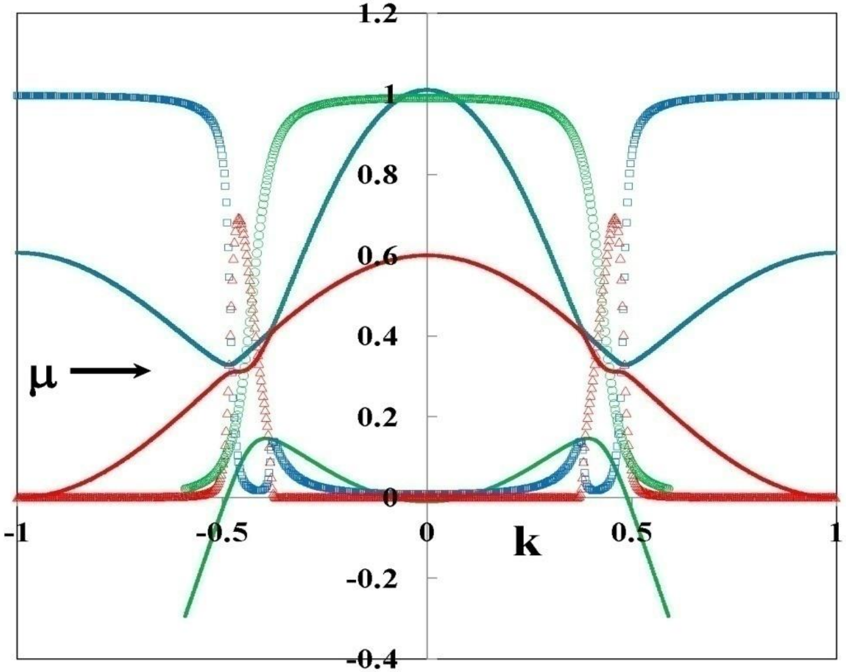
- The pseudogap in the DOS has a magnitude of U $z_{Q,\sigma}$

- The Hund' rule mechanism could equally apply to transition metals.

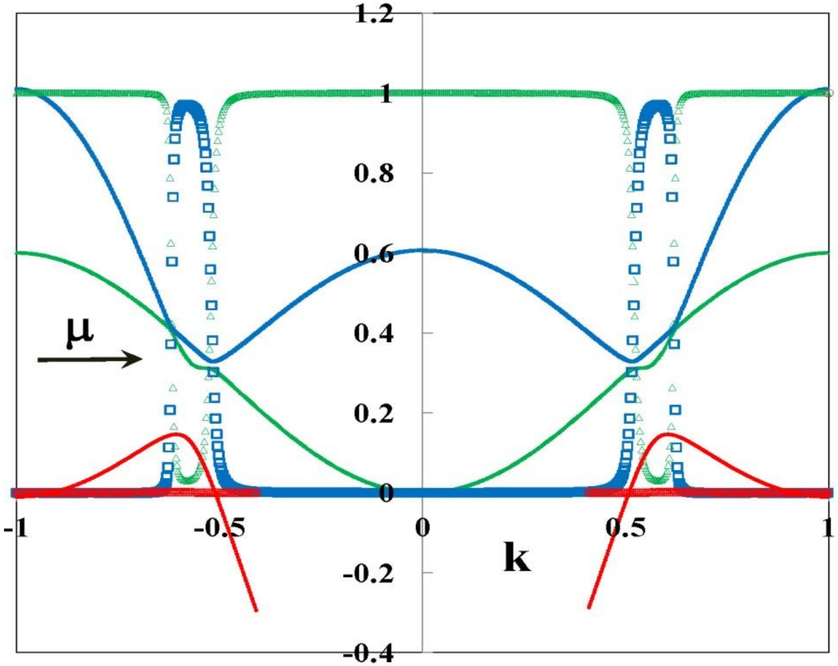
  (eg Fe-pnictides, especially where there is magnetic nematicity.)

f Quasiparticle Bands

Weights and Dispersion

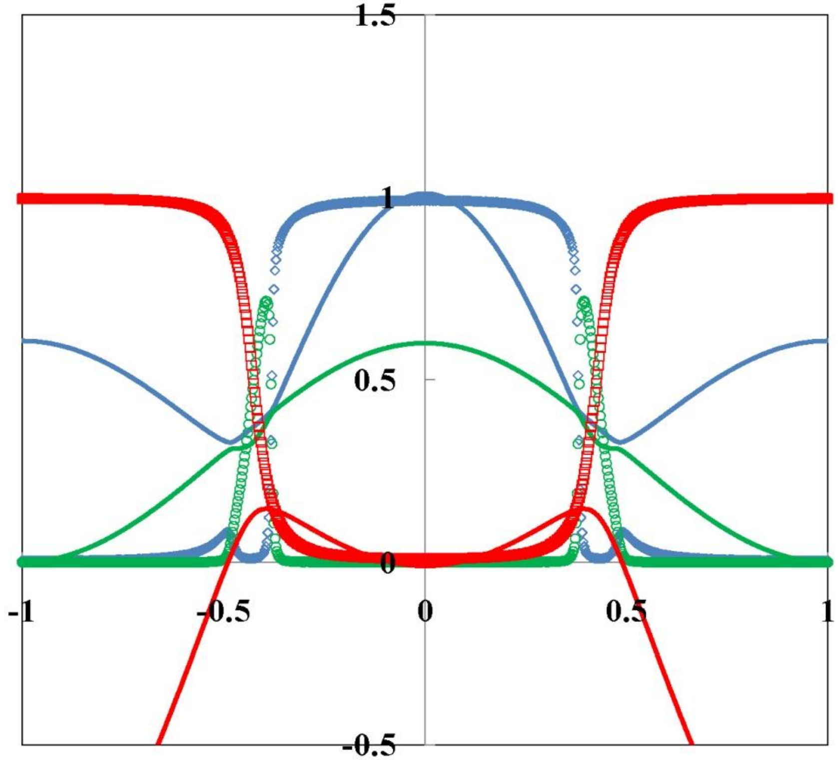


5f bands of α character



5f bands of β character

Quasiparticle Conduction Bands



Bands and weights with d character