Angle dependent quasiparticle weight in heavy fermion metals

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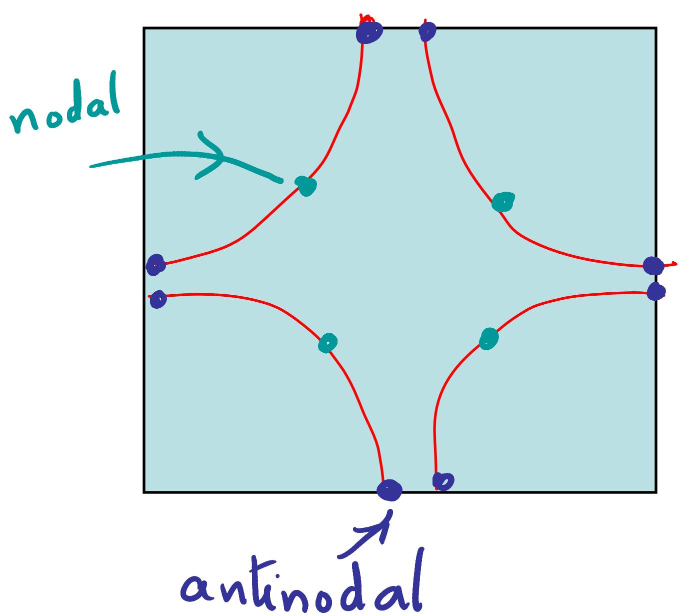
Ghaemi, TS, Phys Rev B '07 and forthcoming.

Momentum space anisotropy in the cuprate metals

Normal state of cuprates – a non-fermi liquid metal

Differences between different parts of a nominal Fermi surface



Deviation from Fermi liquid stronger on moving from nodal to antinodal direction.

(Evidence from ARPES and transport)

Strongly correlated metals

Many examples

- Normal state of cuprates
- Heavy electron metal in rare earth intermetallics
- Metals near the Mott transition (eg: organics)

Fermi liquid theory often but not always fails.

Broad questions

1. Is correlation induced momentum space anisotropy common in correlated metals?

2. How to incorporate correlation effects into a Fermi surface?

1-band Hubbard model: Interesting cluster DMFT calculations (Civelli, Parcollet, Kotliar, Georges, ...)
'04 – '07

Related simpler question

Momentum dependence of correlation effects in a Fermi liquid metal??

This talk – focus on heavy fermi liquid metals

Simple and general reasoning: strong momentum dependence of quasiparticle spectral weight

Heavy electron metal: A strongly correlated Fermi liquid

Weakly correlated conduction band coupled to correlated f-band.

- Large effective mass
- Small quasiparticle residue
- Large Fermi surface – localized f-moments dissolve into Fermi sea by Kondo singlet formation.

Simplified Anderson lattice model for heavy fermi liquids

$$H = \sum_k \epsilon_k c_k^\dagger c_k + V \sum_i \left(c_{i\alpha}^\dagger f_{i\alpha} + h.c \right)$$

$$+ \sum_k \epsilon_{kf} f_k^\dagger f_k \quad + U \sum_i \left(n_i^f \right)^2 - \mu_f \sum_i n_i^f$$

Weak-U limit : Hybridized c and f bands

Fermi volume includes both c and f electrons

but effective mass not large, and $Z \sim O(1)$.

Strong correlations: Kondo lattice

½ - filling for f-band

Large -U limit ⇒ each localized f-orbital is singly occupied.

Lattice of localized f-moments coupled to c-electrons

$$H = \sum_k \epsilon_k c_k^\dagger c_k + J \sum_i \vec{S}_i \cdot c_i^\dagger \frac{\vec{\sigma}}{2} c_i$$

$\vec{S}_i$ = f-moment ; $J \sim o(V^2/U)$

(N. Read et al, '86, Millis, Lee '86)

Slave particle formulation of Kondo lattice

Write $\vec{S}_i = f_i^\dagger \frac{\vec{\sigma}}{2} f_i$ with $f_i^\dagger f_i = 1 \ \forall i$

Important : $f_{i\alpha}$ not electrons

- neutral spin-1/2 fermions ("spinons")

$$H = \sum_k \epsilon_k c_k^\dagger c_k - J \sum_i \left(|c_i^\dagger f_i|^2 + h.c \right)$$

Constraint : $f_i^\dagger f_i = 1 \ \forall i$.

Hybridization mean field theory

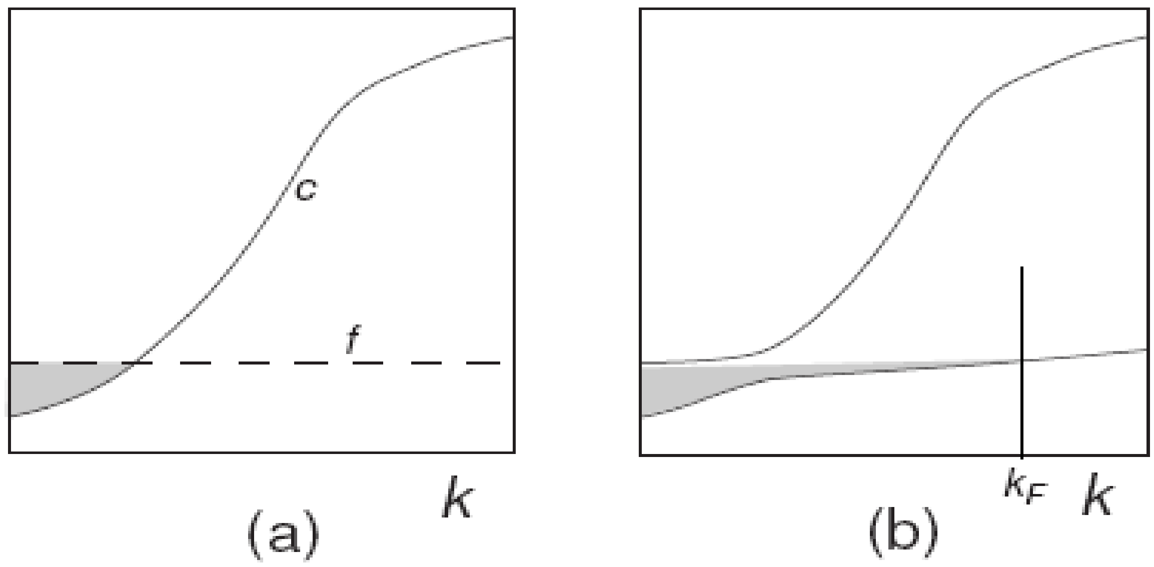
Treat Kondo exchange, constraint in mean field

$$H_{MF} = \sum_k \epsilon_k c_k^\dagger c_k + b \sum_k \left(c_k^\dagger f_k + h.c. \right) + \mu_f \sum_k f_k^\dagger f_k$$

$$b = J \langle f_k^\dagger c_k \rangle$$

$$\langle f_i^\dagger f_i \rangle = 1 .$$

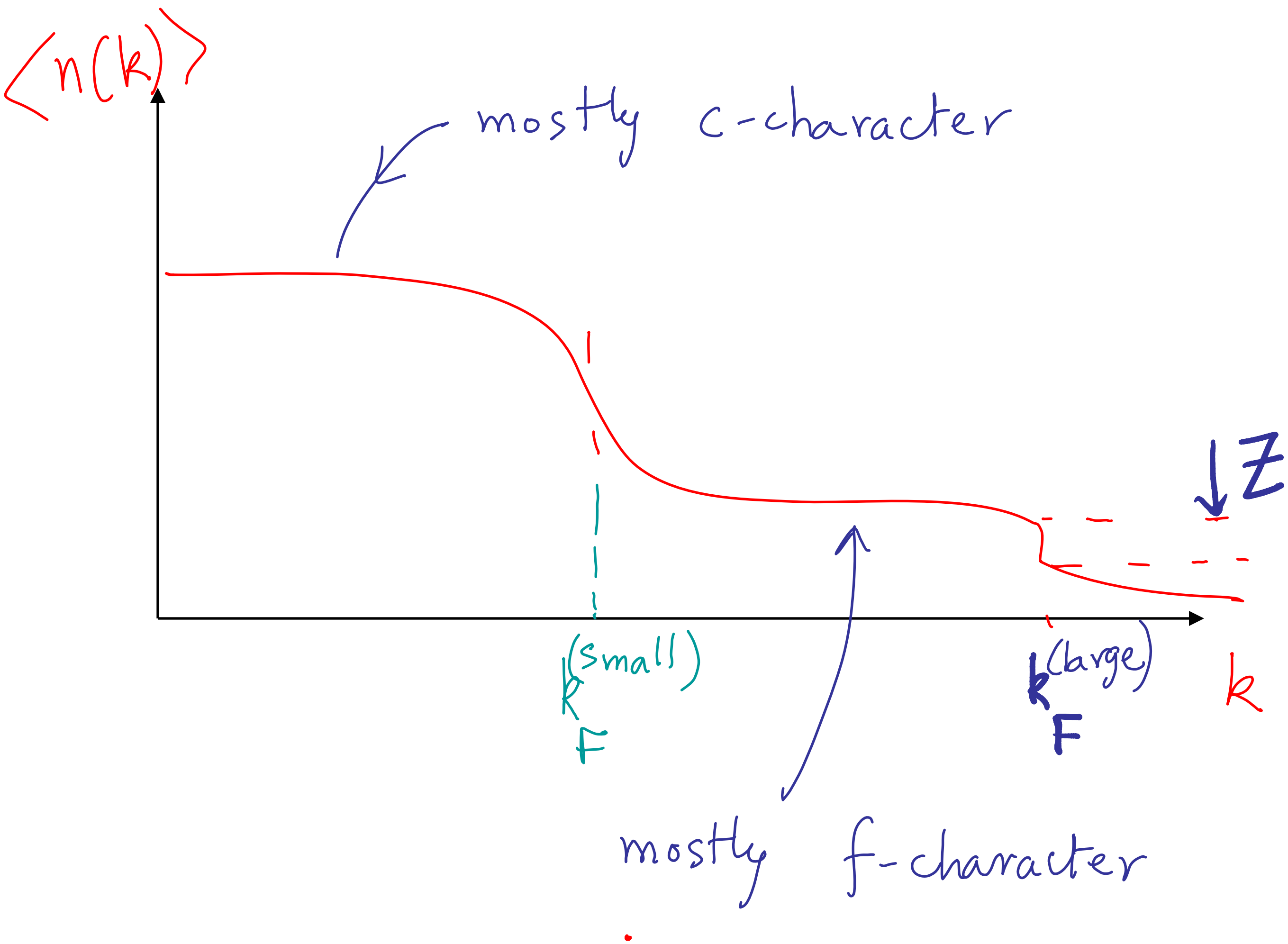
Band structure



Theory gives (i) large Fermi surface

(ii) large quasiparticle mass, etc !

Momentum distribution



Comments

1. $b \sim \langle c^\dagger f \rangle \sim$ amplitude of Kondo singlet

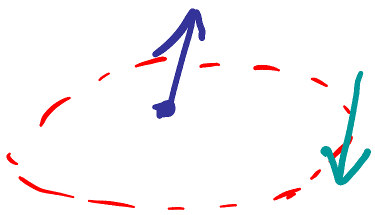
2. Heavy quasiparticles at Fermi surface

$$\approx f + b\, c$$

$$\Rightarrow \text{Quasiparticle weight } Z \sim b^2 \sim O\left(\frac{m}{m^*}\right) \ll 1$$

Real heavy fermi liquids: Kondo singlets with internal structure

Local moment in f-orbital + c-electron in (say) s-orbital

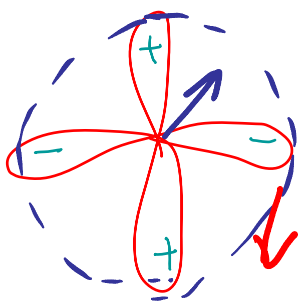


Kondo singlet "molecule" has non-trivial internal orbital structure.

Higher angular momentum Kondo liquids

Nontrivial Fermi surface variation in heavy
Fermi liquid

Eg: Toy model of d-wave Kondo liquid
(Ghaemi, TS '07)



Similar theoretical discussion of gapless
Kondo insulators

- Ikeda, Miyake '96
Moreno, Coleman '00

Illustrate: Kondo lattice model for a cubic Ce-based heavy fermi liquid

Ce f^1 ion in cubic environment:

spin orbit + crystal field $\Rightarrow$ low energy Kramers doublet occupied by f-electron.

Kramers doublet (label $M = 1, 2$)

Kondo lattice model for a cubic Ce-based heavy fermi liquid (cont'd)

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + J \sum_{\vec{R}} \sum_{\vec{k}} \sum_{\substack{M\sigma \\ M'\sigma'}} \langle \vec{k}\sigma | k M \vec{R} \rangle \langle k \vec{M}' R | \vec{k}\sigma' \rangle f^\dagger_{M\vec{R}} c_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma'} f_{M'\vec{R}}$$

$$+ \text{ constraint } \sum_M f^\dagger_{M\vec{R}} f_{M\vec{R}} = 1$$

$|k M \vec{R}\rangle$ = partial wave centered at site $\vec{R}$

Mean field theory: angle dependent hybridization

$$H_{MF} = \sum_{\vec{k}\sigma} \epsilon_k\, c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \mu_f \sum_{M\vec{R}} f^\dagger_{M\vec{R}} f_{M\vec{R}}$$

$$+ \, b \sum_{\vec{k}M\sigma} \left(\langle \vec{k}\sigma | kM \rangle\, c^\dagger_{\vec{k}\sigma} f_{\vec{k}M} + h.c \right)$$

Hybridization matrix

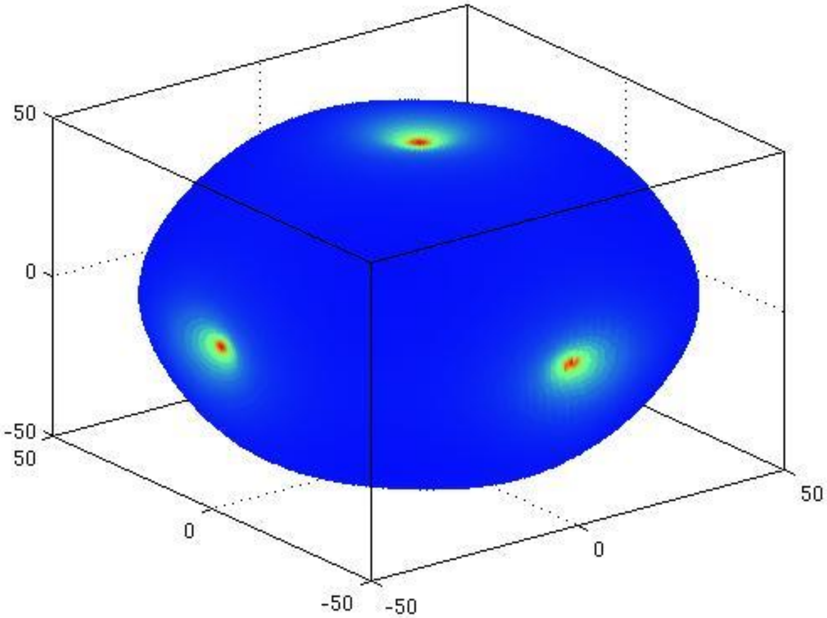
$b \langle \vec{k}\sigma | kM \rangle$: Strong dependence on $\vec{k}$-direction

Vanishes along (100) & related directions.

"Hybridization nodes"

Fermi surface structure

Along "hybridization nodes" large Fermi surface is within original small c-electron Fermi surface.

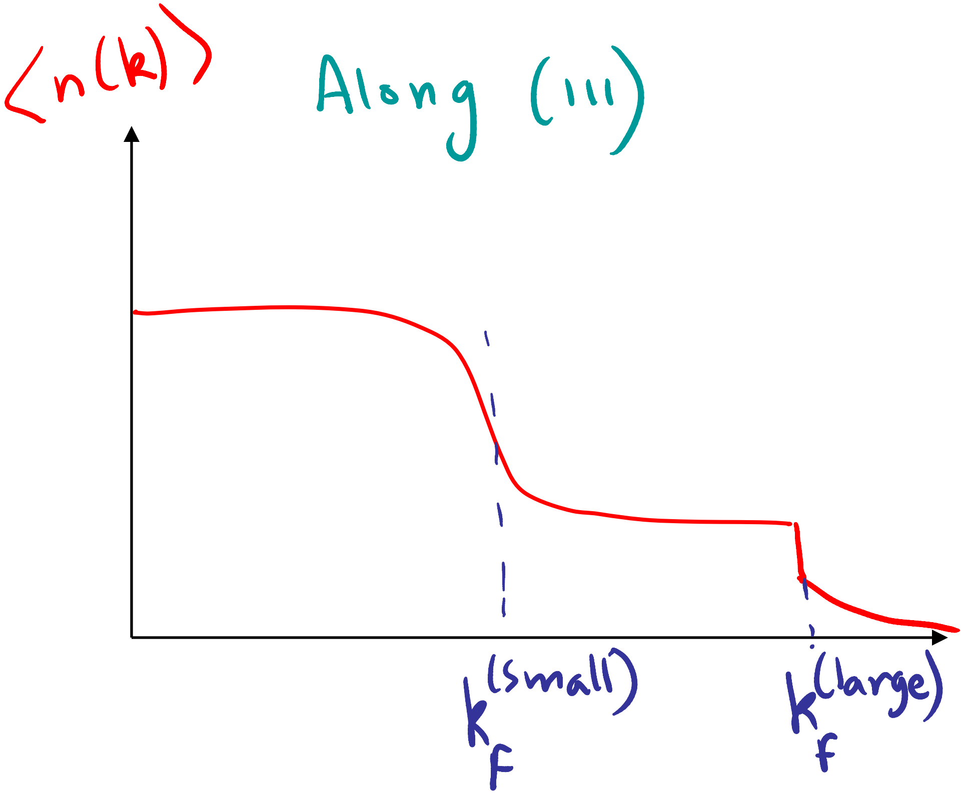


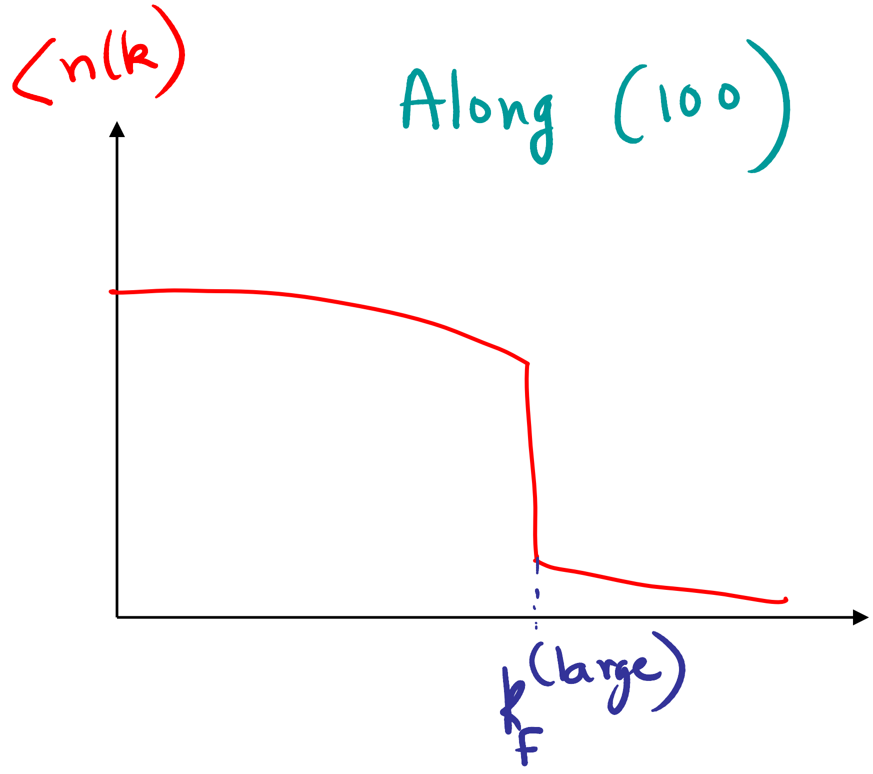
Angle dependence of c-character

Along hybridization node directions, quasiparticles essentially c-like but become essentially f-like further away

$\Rightarrow$ Strong angle dependence of c-character.

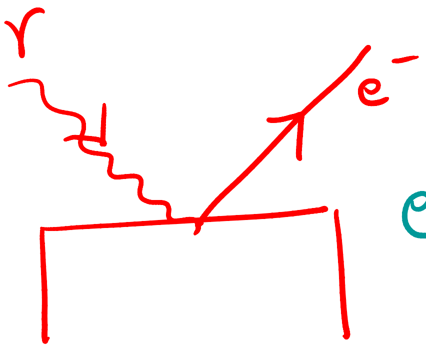
Momentum distribution





Probe in photoemission ?

Photoemission theory for Kondo lattices



For Anderson lattice model,

extracted electron $\psi_{k\sigma} \sim c_{k\sigma} + \sum_{M} \alpha_{M\sigma k} f_{kM}$

Strong correlation limit: Changing f-occupation costs energy $o(U)$

At low energy

$$\psi_{\vec{R}\sigma} \approx c_{\vec{R}\sigma} + \frac{V}{U} \sum_{MM'R'} a_{MM'\sigma} \underbrace{f_{\vec{R}M} f^{\dagger}_{\vec{R}M'}}_{\text{preserves on-site f-occupancy.}} c_{R'\sigma}$$

Angle dependent quasiparticle weight

In mean field $\psi_k \approx c_k + b_k f_k$

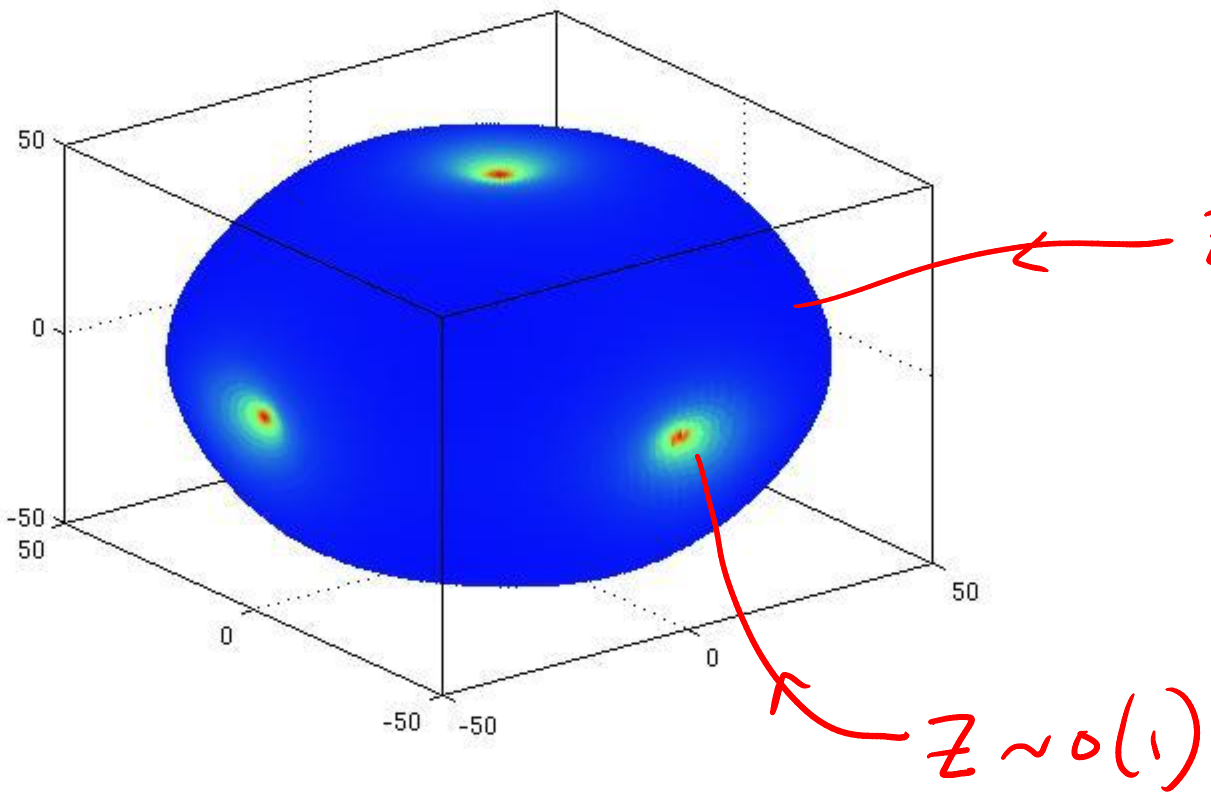
Along hybridization nodes $\psi_k \approx c_k$

$\Rightarrow$ $Z \sim o(1)$ as quasiparticles are c-like

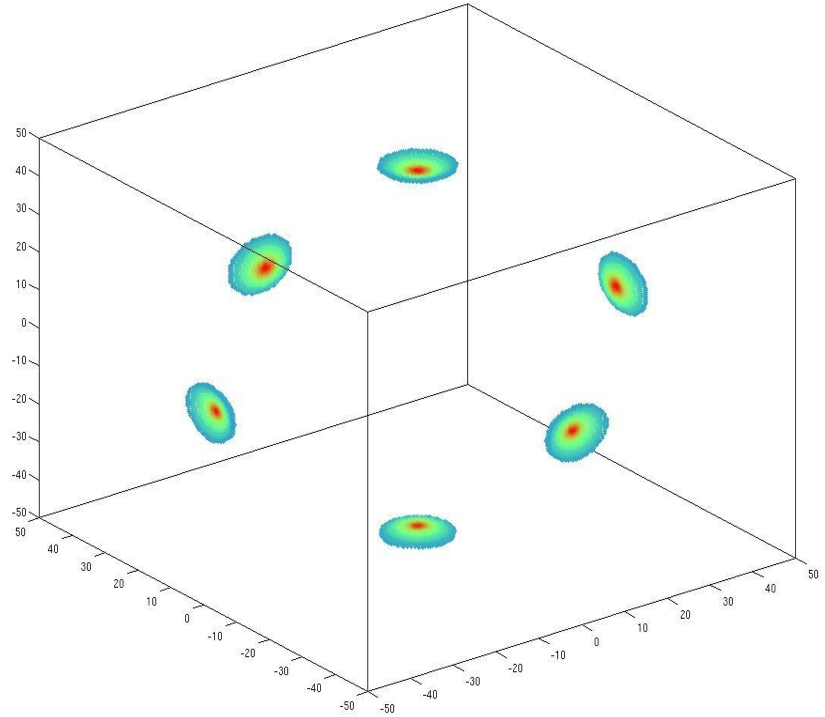
Further away $Z \sim o(b_k^2) \ll 1$

$\Rightarrow$ Strong angle dependent Z

Z on the Fermi surface



Apparent ``open" Fermi patches in ARPES



Small Z regions may be missed in experiment!

Tunneling?

Mass enhancement also strongly anisotropic

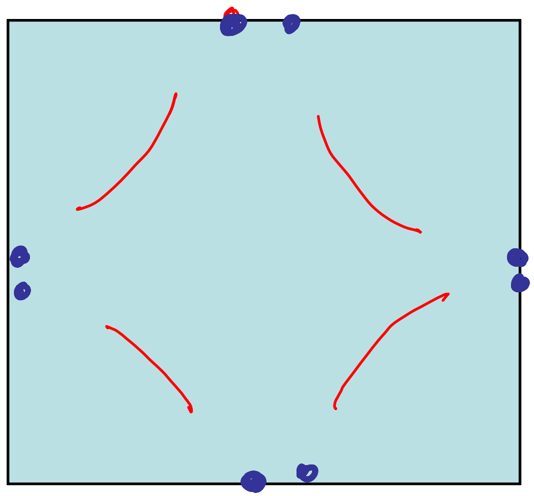
Along (100) $\frac{m^*}{m_e} \sim o(1)$

but along (111), $m^*/m_e \sim \frac{1}{b_k^2} \gg 1$

Tunneling density of states

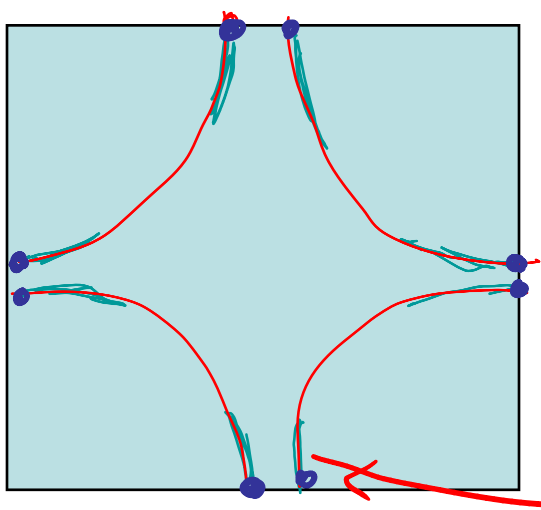
$$\sim \int d\Omega \, \frac{Z(\Omega)}{v_F(\Omega)}$$ <u>not</u> enhanced.

Similar in cuprates?



Underdoped cuprates :

Mysterious gapless Fermi arcs in pseudogap normal state.



Could there really be a large Fermi surface with $Z \sim o(1)$ along arcs but small near antinode ?

small Z ??

Similar in cuprates?

Heavy fermions: small Z regions $\Longleftrightarrow$ large effective mass.

Cuprates: Density of states decreases on cooling into pseudogap phase!

In general $Z \neq \frac{m_e}{m^*}$;

$\Rightarrow$ In cuprates, small antinodal Z with no mass enhancement?

Could the pseudogap phase actually have a LARGE Fermi surface with strongly angle dependent low energy electron spectral weight?

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Many appealing features !

Consistency with high field quantum oscillations through low-T density wave transition of large Fermi surface.

Summary

1. Strong angle dependent quasiparticle weight in heavy electron metals due to orbital structure of Kondo singlet.

2. Angle dependent Z correlated with angle dependent m^*

(Heavy Fermi liquid not uniformly heavy).

Summary (cont'd)

Possibility of "hybridization nodes":

1. Kondo-Heisenberg models: Vanishing Z at isolated points on Fermi surface.

   Should we call these Fermi liquids?

2. Heavy fermion SC driven by f-pairing (a'la RVB)

   Pairing structure of physical SC order parameter?