How to remove entropy in two-channel Kondo lattice

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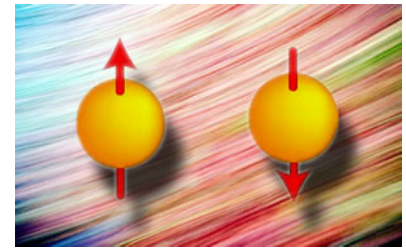
Kramers vs non-Kramers doublets

- Kramers doublet: spin or quasi-spin



$$\mathcal{T} = i\sigma_y \mathcal{K}\text{: time-reversal operator}$$

$$\mathcal{T}|\uparrow\rangle = |\downarrow\rangle, \quad \mathcal{T}|\downarrow\rangle = -|\uparrow\rangle,$$

$$\Rightarrow \mathcal{T}^2|\sigma\rangle = -|\sigma\rangle$$

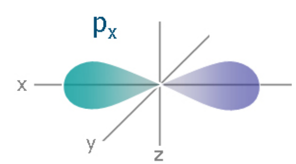
- Non-Kramers doublet: pseudo-spin

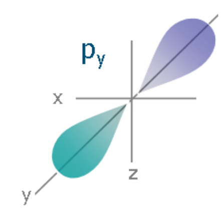
$$|p_x\uparrow, p_x\downarrow\rangle \equiv |+\rangle, \quad |p_y\uparrow, p_y\downarrow\rangle \equiv |-\rangle$$

$$\tau_x\text{: pseudo-spin flip operator}$$

$$\tau_x|+\rangle = |-\rangle, \quad \tau_x|-\rangle = |+\rangle,$$

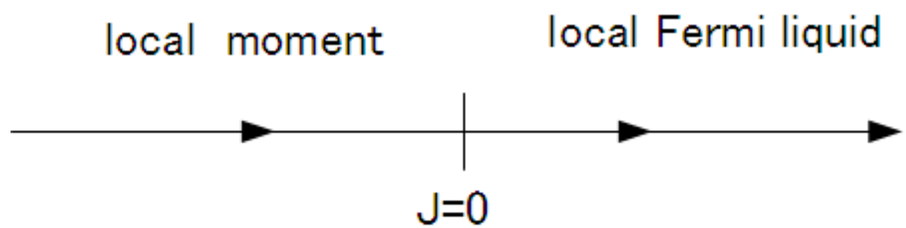
$$\Rightarrow \tau_x^2|\pm\rangle = |\pm\rangle$$



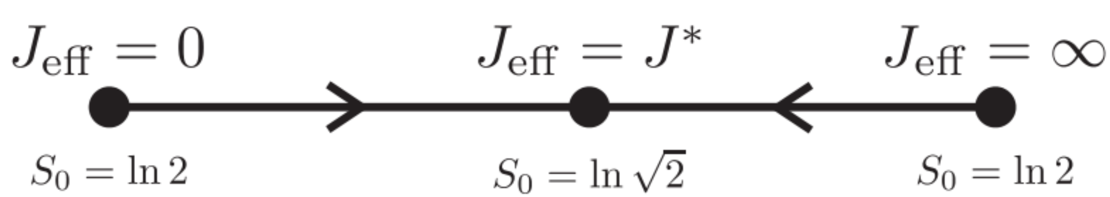


Ground states in impurity systems

- Kondo model $H_{\mathrm{int}} = J\boldsymbol{S}\cdot\boldsymbol{s}$



- Two-channel Kondo model $J\tilde{\boldsymbol{S}}\cdot(\tilde{\boldsymbol{s}}_a+\tilde{\boldsymbol{s}}_b)$



Nozieres-Blandin: 1980, D.L. Cox: 1987

Nature of residual entropy

- Size L: finite, Temperature T => 0
  - Fermionic zero mode: S = ln 2
- T: finite, L=> infinite
  - Zero mode decomposes into two Majoranas
  - One Majorana is absorbed into continuum
  - Decoupled one: S => (ln 2)/2 for $O(1/L) << T << T_K$
- What happens for the lattice?
  - Hidden symmetry: SO(5)
  - Degeneracy between different orders

Exotic orders for 2ch Kondo lattice

- Exact results in high-dimensional limit
- Non-Kramers (pseudo-)doublet
  - Composite order involving both *f* and *c* electrons
    - Diagonal

$$\Psi^z = \frac{1}{N}\sum_i \langle \tilde{\boldsymbol{S}}_i \cdot (\tilde{\boldsymbol{s}}_{ci1} - \tilde{\boldsymbol{s}}_{ci2}) \rangle$$

    - Off-diagonal

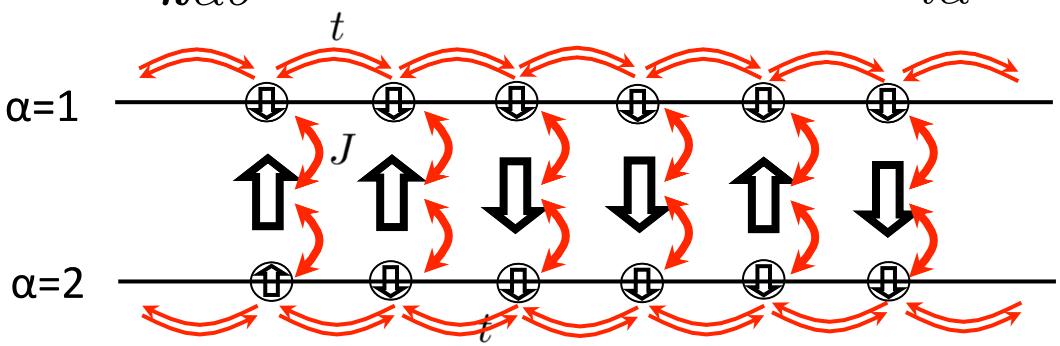
$$\Phi(\boldsymbol{Q}) = -\frac{1}{N}\sum_i \sum_{\sigma\sigma'} \exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i)\langle \tilde{\boldsymbol{S}}_i \cdot (\mathrm{i}\sigma^y \boldsymbol{\sigma})_{\sigma\sigma'} c_{i2\sigma} c_{i1\sigma'} \rangle$$

Numerical approach

- Dynamical mean-field theory (DMFT)
  - Two-sublattice generalization
  - Accurate for large number of neighbors
  - Semielliptic density of states
- Continuous-time Quantum Monte Carlo (CT-QMC)
  - Solution of the effective impurity problem

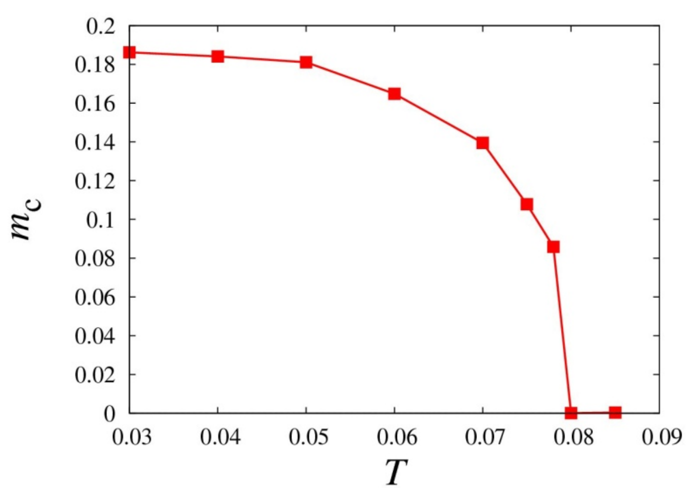
Two-channel Kondo lattice at half-filling

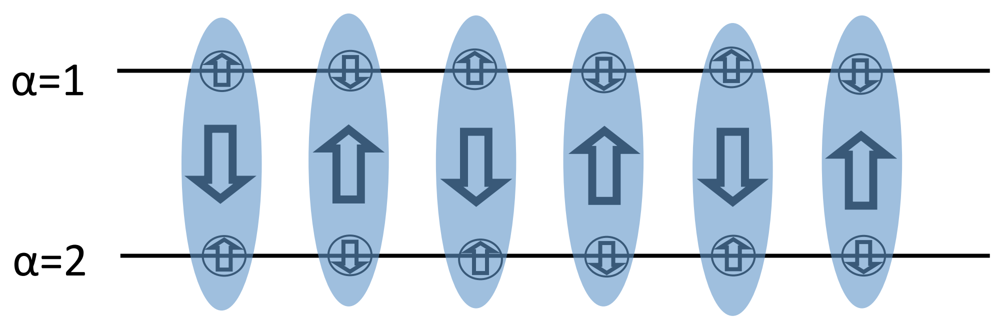
$$\mathcal{H} = \sum_{\boldsymbol{k}\alpha\sigma} (\varepsilon_{\boldsymbol{k}} - \mu) c^{\dagger}_{\boldsymbol{k}\alpha\sigma} c_{\boldsymbol{k}\alpha\sigma} + J \sum_{i\alpha} \tilde{\boldsymbol{S}}_i \cdot \tilde{\boldsymbol{s}}_{ci\alpha}$$



Singlet? Impossible!

■**Spontaneous symmetry breaking (CT-QMC+DMFT)**

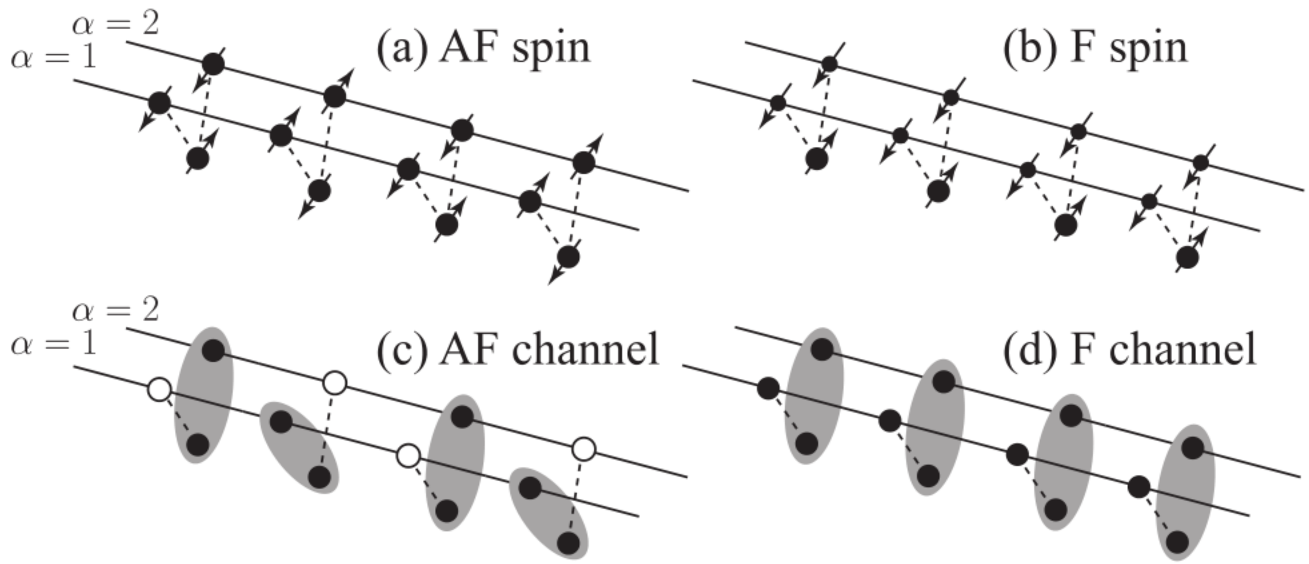




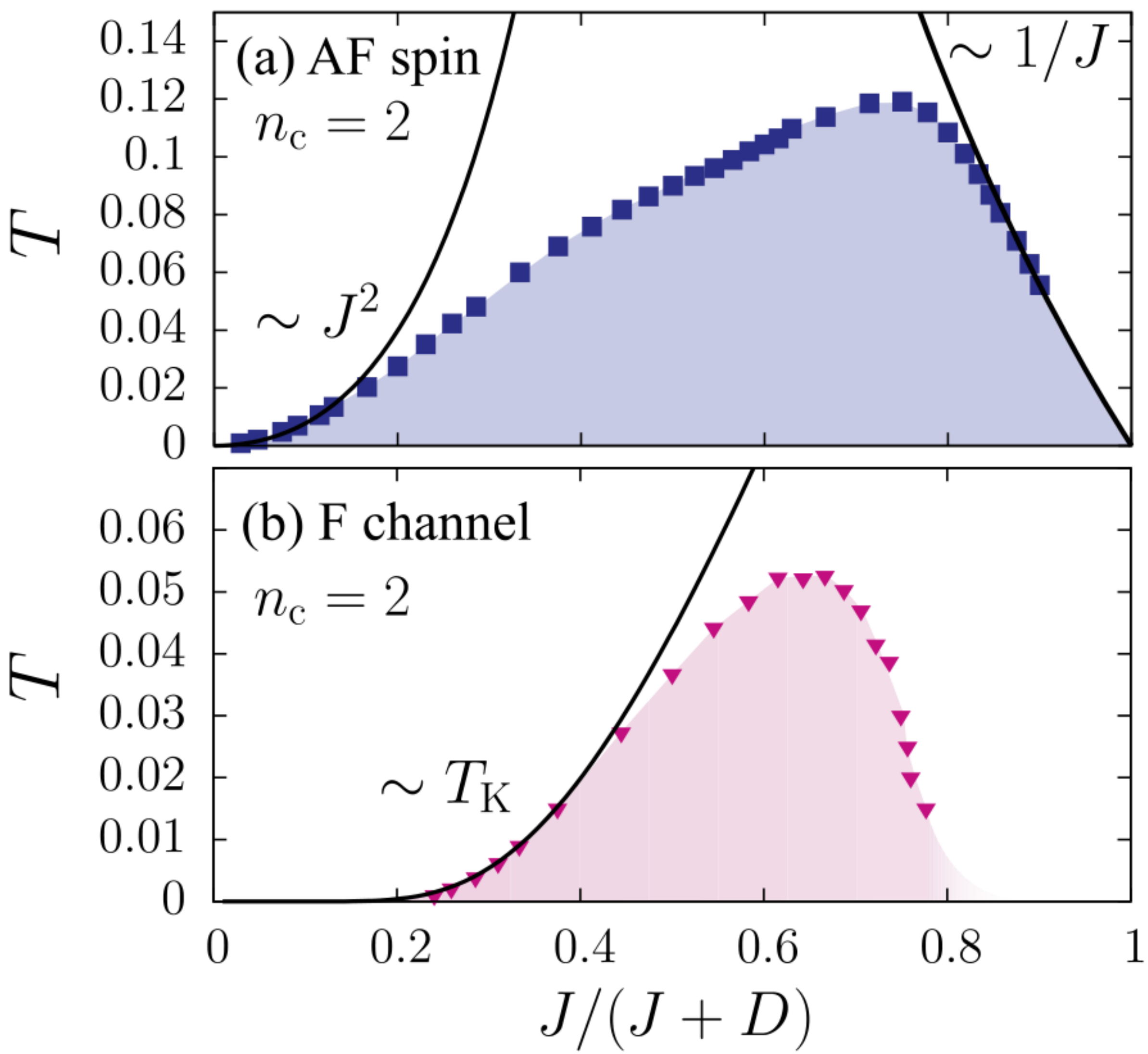
Simplest: Antiferromagnetism (of pseudo-spins)

Patterns of diagonal orders

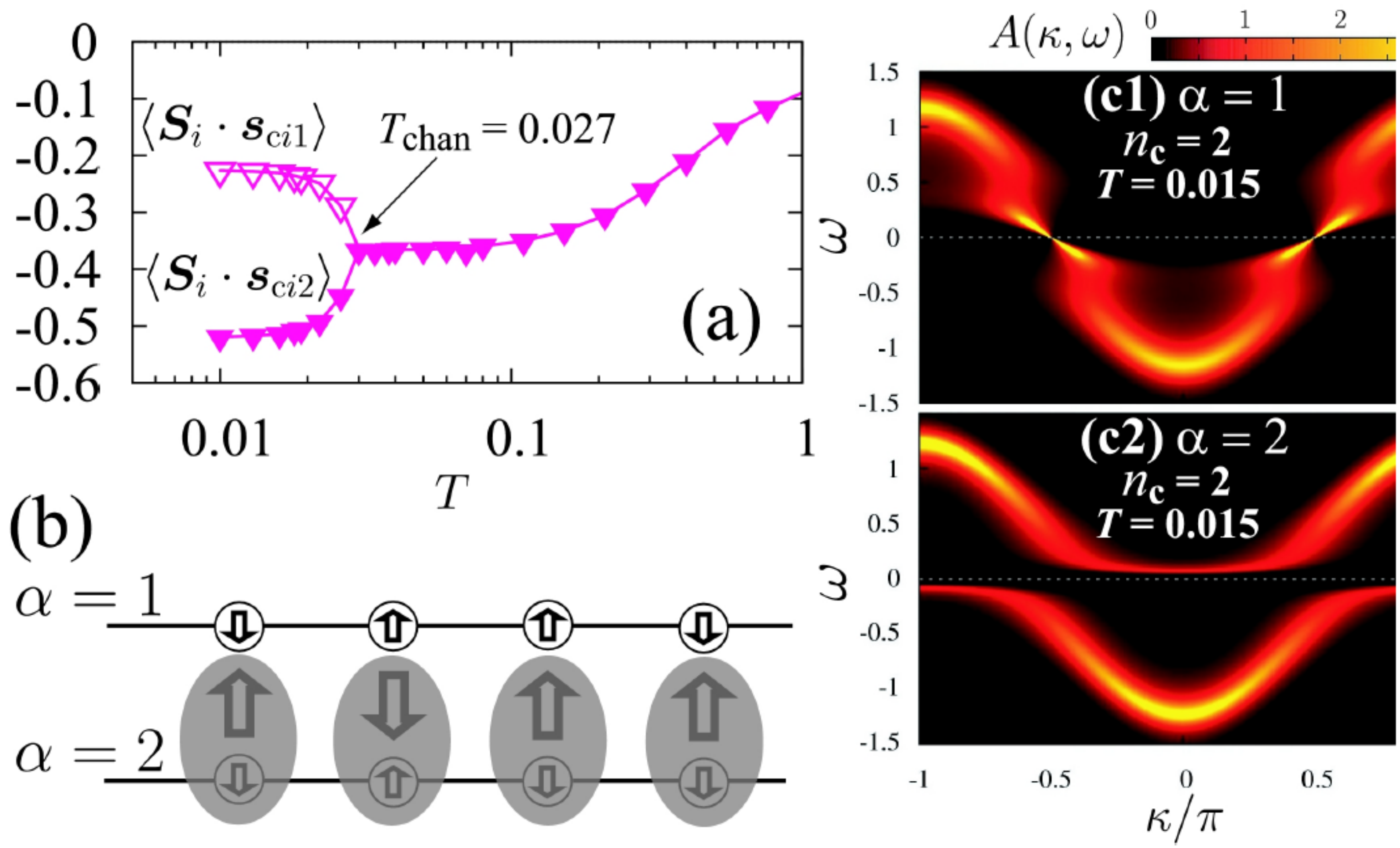
n_c=2



Ordering mechanism: different



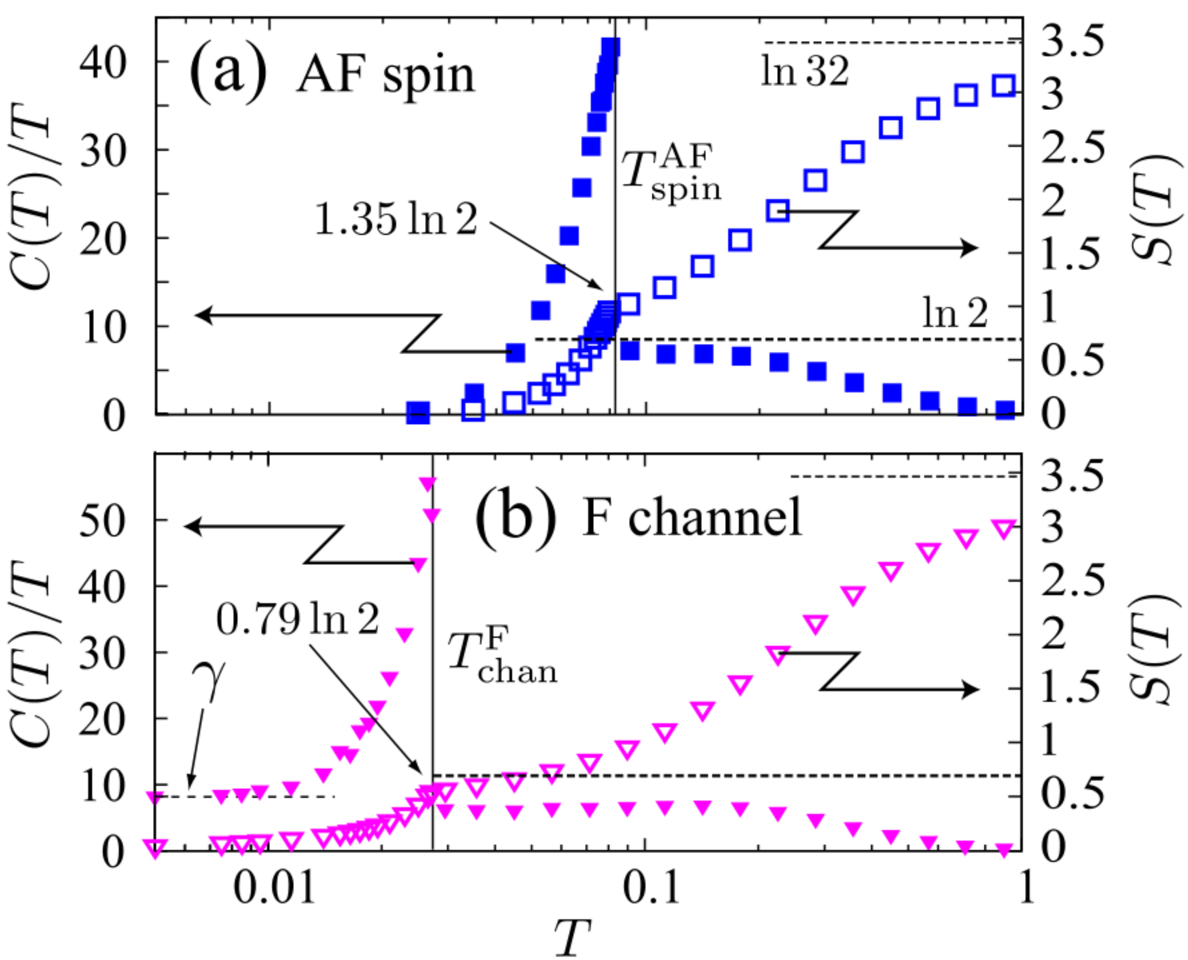
Diagonal composite order



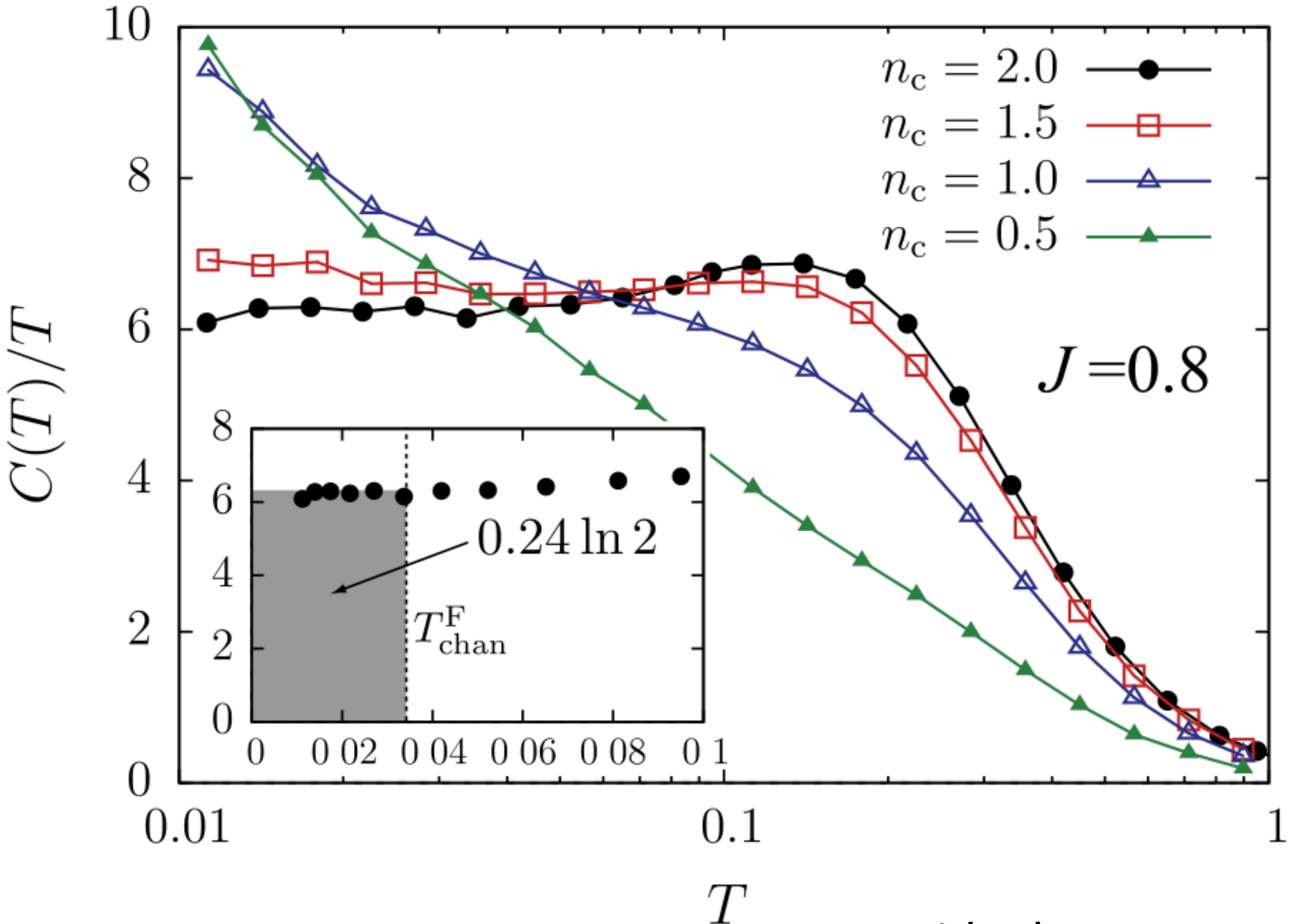
$$\Psi^z \equiv \langle \boldsymbol{S}_i \cdot (\boldsymbol{s}_{ci1} - \boldsymbol{s}_{ci2}) \rangle$$

Itinerant multipoles

Entropy associated with orderings



Specific heat of disordered phase



0.79 - 0.24 = 0.55 ~ 1/2

Residual entropy ~ (ln 2)/2

Generalized superconducting order

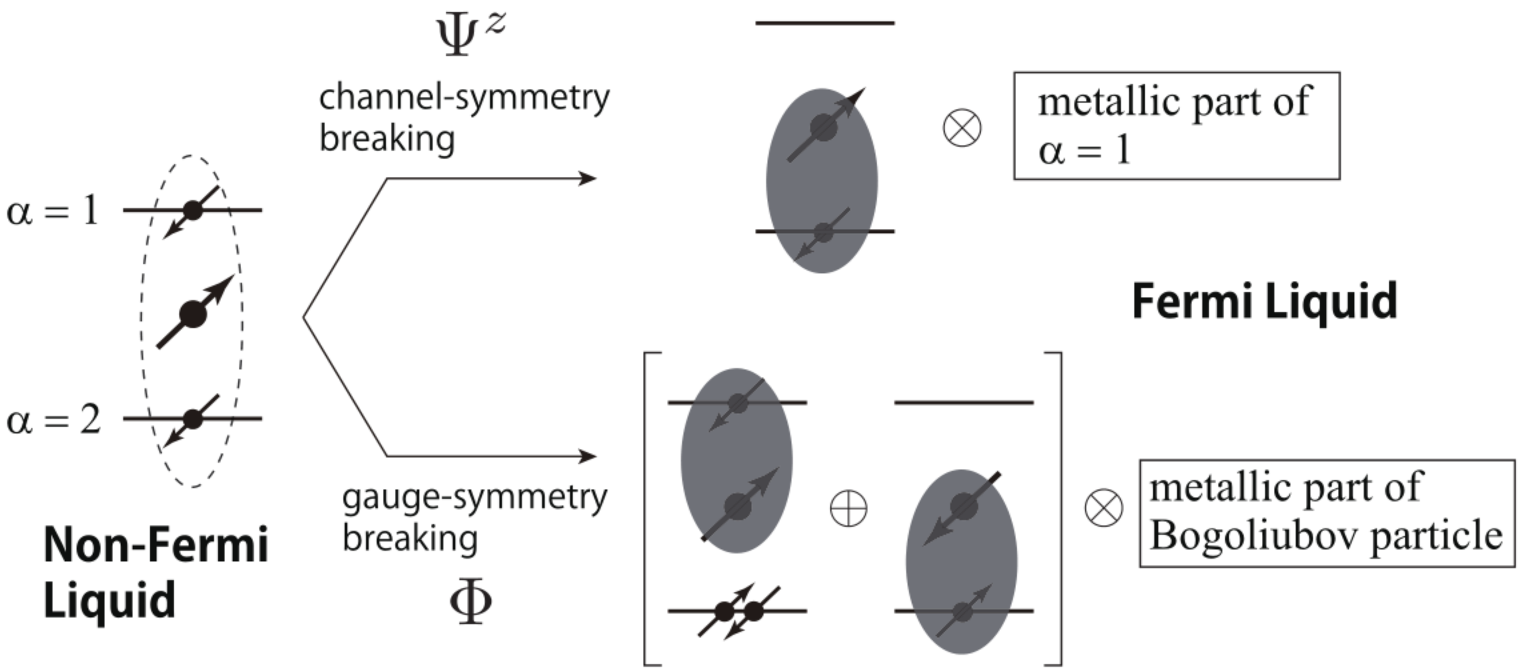
- Dynamical pairing

$$\Psi_{\alpha\beta}(\tau > 0) \equiv \langle c_\alpha(\tau) c_\beta \rangle = \psi_0 + \tau \psi_{\rm odd} + \tau^2 \psi_2 + \cdots$$

- Odd frequency order
  - zero (ordinary) order parameter: $\psi_0 = 0$
  - broken gauge symmetry if $\dot{\Psi}_{\alpha\beta}(0) = \psi_{\rm odd} \neq 0$
- Triplet s-wave etc.

Route to exotic superconductivity with use of SO(5) symmetry

Three (x,y,z) components



Two real components

Steps to off-diagonal order:

- SO(3) channel symmetry: $\Psi^{\alpha}\ (\alpha = x, y, z)$: equivalent

$$\Psi^{z} \equiv \frac{1}{N}\sum_{i}\langle \boldsymbol{S}_i \cdot (\boldsymbol{s}_{\mathrm{c}i1} - \boldsymbol{s}_{\mathrm{c}i2})\rangle$$

$$= \frac{1}{2N}\sum_{i}\sum_{\sigma\sigma'}\sum_{\alpha\beta}\langle \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c^{\dagger}_{i\alpha\sigma}\sigma^{z}_{\alpha\beta}c_{i\beta\sigma'}\rangle,$$

$$\Psi^{+} \equiv \Psi^{x} + i\Psi^{y} = \frac{1}{N}\sum_{i}\sum_{\sigma\sigma'}\sum_{\alpha\beta}\langle \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c^{\dagger}_{i1\sigma}c_{i2\sigma'}\rangle,$$

- Particle-hole symmetry
  (= Charge conjugation)

Charge conjugation $\boldsymbol{C}$ (channel index omitted)

- Sublattice-dependent phase factor

$$c_{A\uparrow} \to c^\dagger_{A\downarrow}, \quad c_{A\downarrow} \to -c^\dagger_{A\uparrow},$$

$$c_{B\uparrow} \to -c^\dagger_{B\downarrow}, \quad c_{B\downarrow} \to c^\dagger_{B\uparrow},$$

$$\text{Namely}: \quad c_{i\sigma} \to \mathrm{i}\sigma^y_{\sigma\sigma'} c^\dagger_{i\sigma'} \exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i)$$

- Hamiltonian: invariant under $\boldsymbol{C}$

$$\text{kinetic}: \quad t c^\dagger_{A\downarrow} c_{B\downarrow} \to -t c_{A\uparrow} c^\dagger_{B\uparrow} = t c^\dagger_{B\uparrow} c_{A\uparrow},$$

$$\text{spin}: \quad c^\dagger_{i\uparrow} c_{i\downarrow} \to -c_{i\downarrow} c^\dagger_{i\uparrow} = c^\dagger_{i\uparrow} c_{i\downarrow}$$

Charge conjugation only for channel 2: *diagonal composite order => staggered superconducting order!*

$$\Psi^{+} = \frac{1}{N}\sum_{i}\langle \boldsymbol{S}_i \cdot \boldsymbol{\sigma}_{\sigma\sigma'} c^{\dagger}_{i2\sigma} c_{i1\sigma'} \rangle$$

$$\Rightarrow -\frac{1}{N}\sum_{i}\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i)\langle \boldsymbol{S}_i \cdot (\mathrm{i}\sigma^{y}\boldsymbol{\sigma})_{\sigma\sigma'}\, c_{i2\sigma} c_{i1\sigma'} \rangle$$

$$\equiv \Phi(\boldsymbol{Q}) \sim -\frac{1}{N}\sum_{i}\exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i)\mathrm{i}\sigma^{y}_{\sigma\sigma'}\langle c_{i2\sigma}\dot{c}_{i1\sigma'} \rangle$$

Even-frequency composite = odd-frequency pair

Spin-singlet, channel-singlet

Even and odd pairing susceptibilities

$$\chi_{ij}^{\ell}(\tau_1,\tau_2,\tau_3,\tau_4) = \langle T_\tau O_i^{\ell}(-\tau_2,-\tau_1)^\dagger O_j^{\ell}(\tau_3,\tau_4)\rangle$$

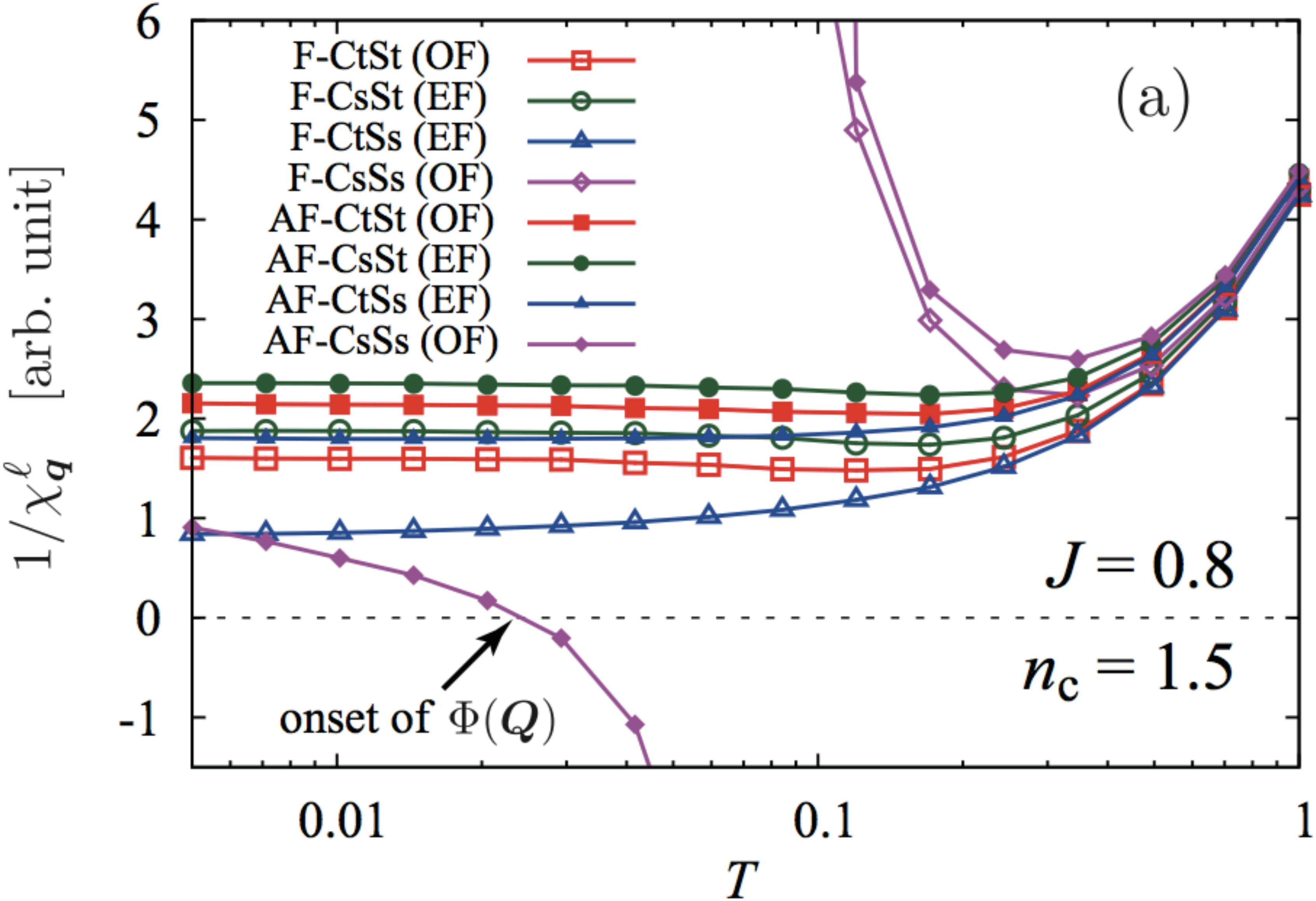
$$\chi_{\boldsymbol{q}}^{\ell}(\mathrm{i}\varepsilon_n,\mathrm{i}\varepsilon_{n'}) = \frac{1}{N\beta^2}\sum_{ij}\int_0^\beta \mathrm{d}\tau_1\cdots\mathrm{d}\tau_4\ \chi_{ij}^{\ell}(\tau_1,\tau_2,\tau_3,\tau_4)$$
$$\times\,\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j)}\mathrm{e}^{\mathrm{i}\varepsilon_n(\tau_2-\tau_1)}\mathrm{e}^{\mathrm{i}\varepsilon_{n'}(\tau_4-\tau_3)},$$

$$\chi_{\boldsymbol{q}}^{\ell\mathrm{EF}} = \frac{1}{\beta}\sum_{nn'}\chi_{\boldsymbol{q}}^{\ell\mathrm{EF}}(\mathrm{i}\varepsilon_n,\mathrm{i}\varepsilon_{n'}),$$

$$\chi_{\boldsymbol{q}}^{\ell\mathrm{OF}} = \frac{1}{\beta}\sum_{nn'}g_n g_{n'}\chi_{\boldsymbol{q}}^{\ell\mathrm{OF}}(\mathrm{i}\varepsilon_n,\mathrm{i}\varepsilon_{n'})$$

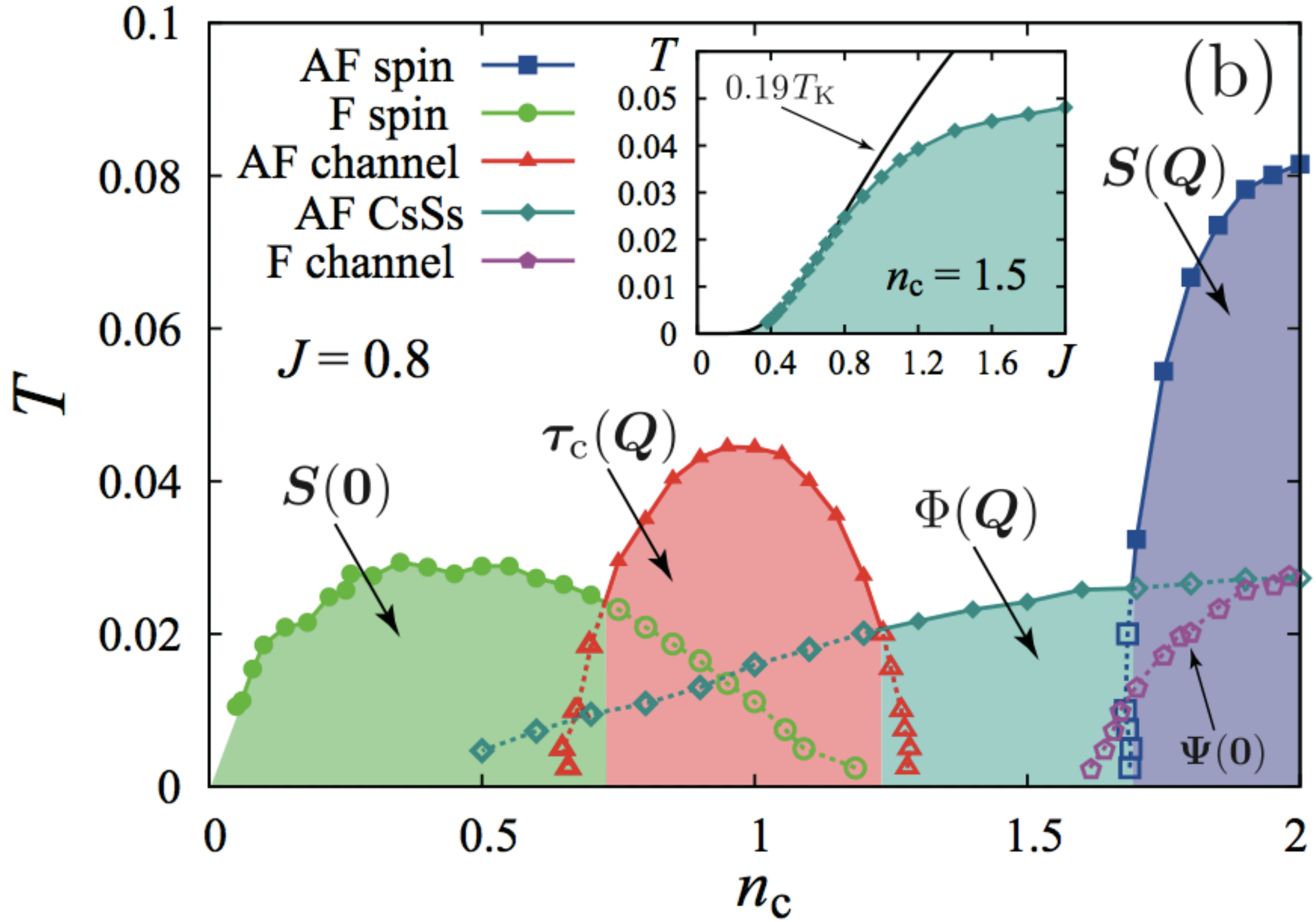
where $g_n = \operatorname{sgn}\varepsilon_n$

Even (EF) and odd (OF) susceptibilities



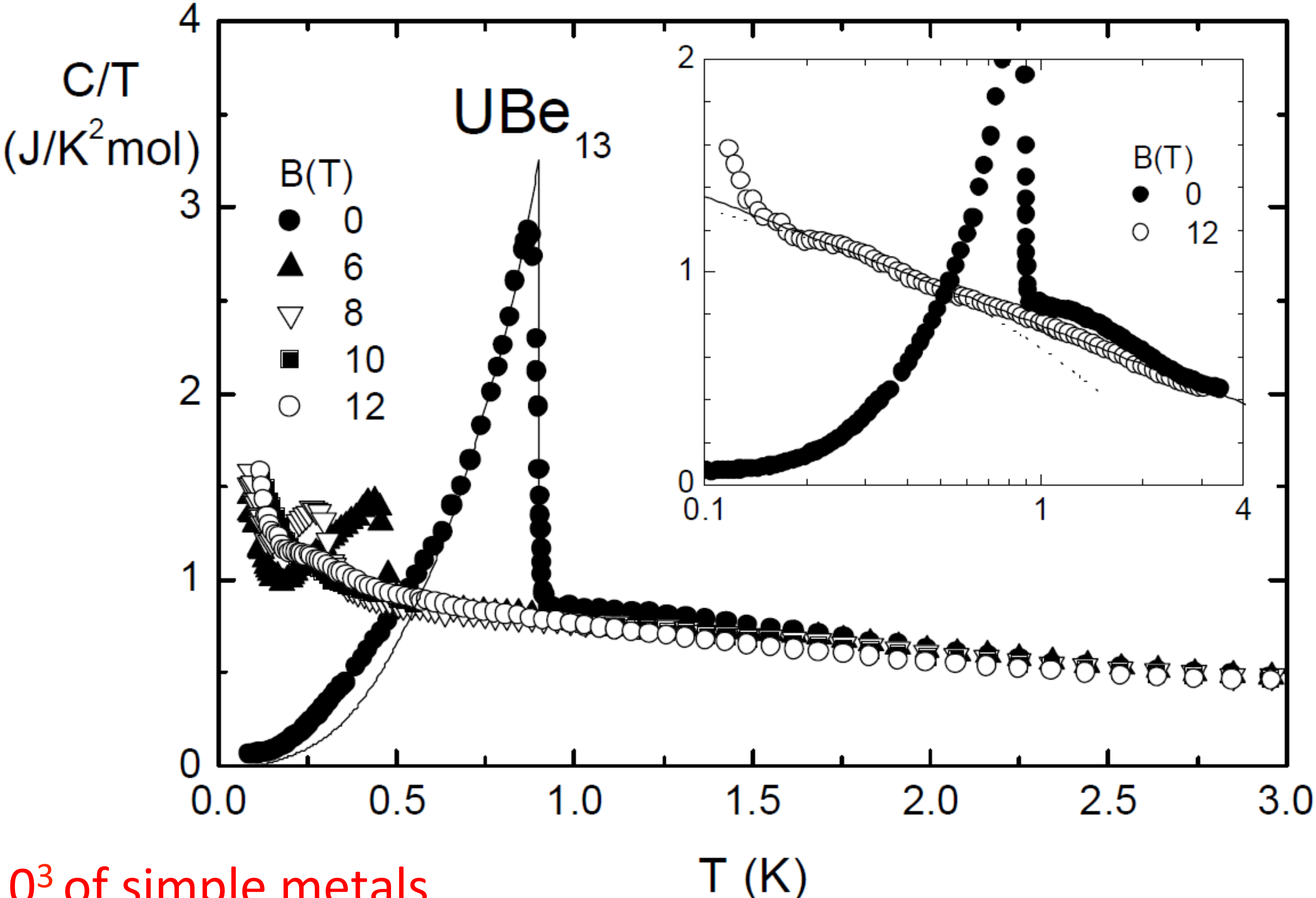
Phase diagram (Φ: superconductivity)

S. Hoshino and YK: PRL 112, 167204 (2014)



Heavy electrons in UBe_{13}

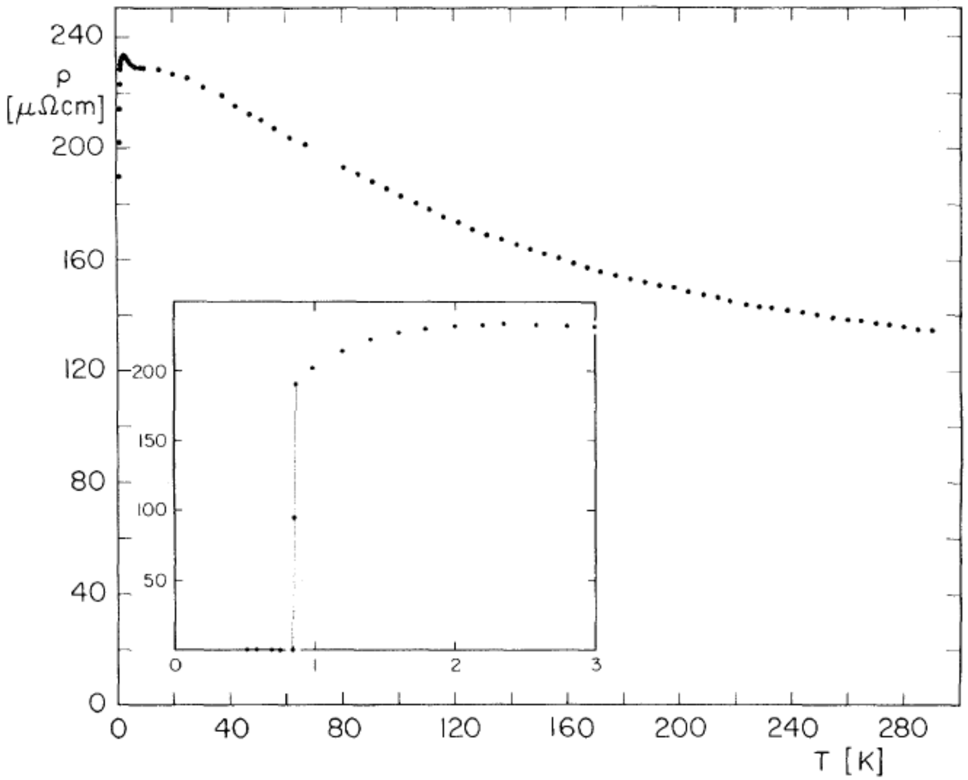
P. Gegenwart et al: Physica C 408-410, 157 (2004)



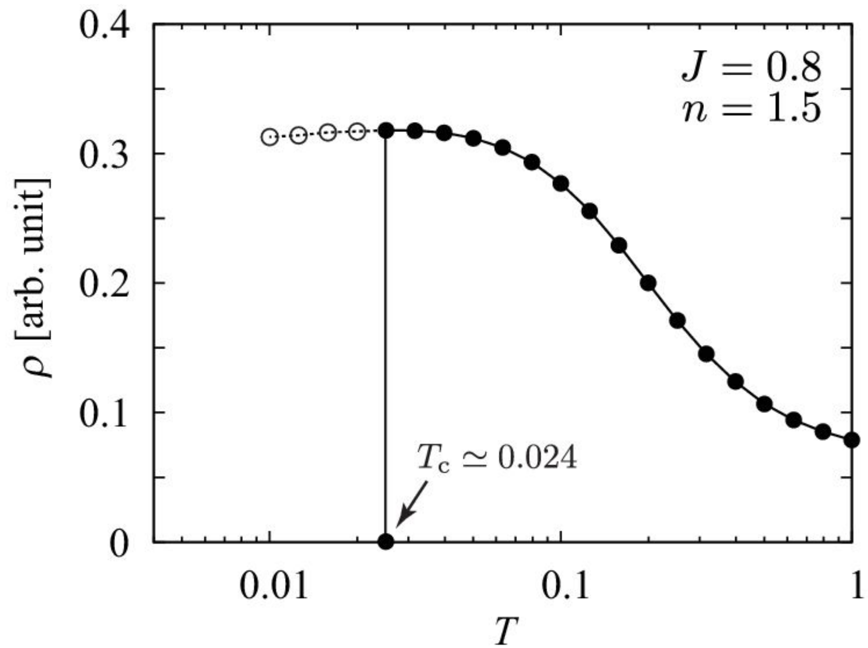
~10^3 of simple metals

UBe_{13}

Ott et al; PRL (1983)



Two-channel Kondo lattice
by DMFT



Possible detection of staggered pairs
cf. Hoshino: arXiv:1406.1983

- Thermodynamics
  - Gapless superconductivity
  - Weak Meissner effect
- Microscopic probes
  - Charge Goldstone mode at $\boldsymbol{Q}$ (cf. plasmon)
  - Staggered field gradient => NQR

Summary

- Residual entropy removed by ordering
  – About 1.5 (ln2)/2 at the transition
- Kondo-induced diagonal order: homogeneous
  – Itinerant multipoles
- Kondo-induced Off-diagonal order: staggered
  – Composite (or odd-frequency) superconductivity
- Actual systems?
  – Staggered pairing should be probed!