Progress on Itinerant Electrons – Ferromagnetism, Curie-Weiss Metal, and Spin-orbit Ordering

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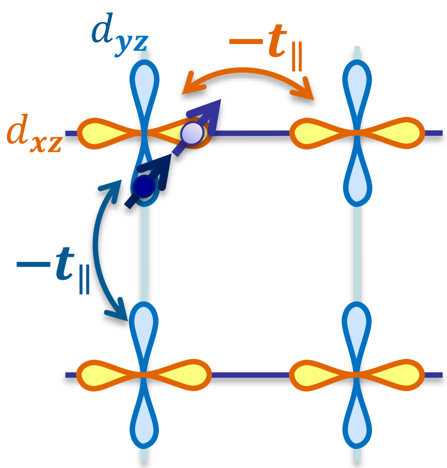

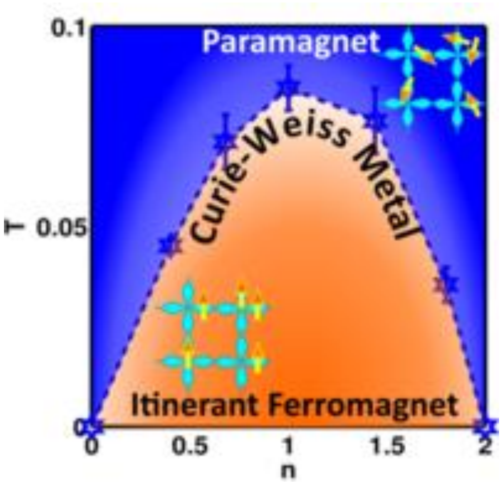

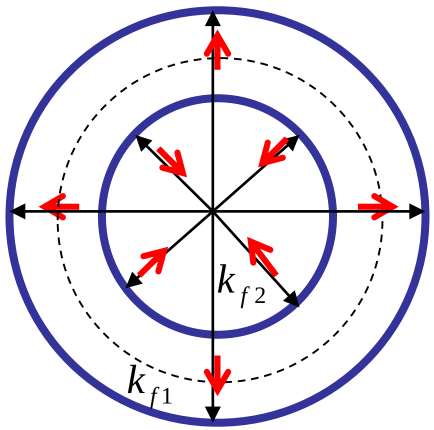

May 30, 2018, New York Univ. Shanghai

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Thank J. Hirsch, I. Schuller, S. Kivelson, Lu Yu, Tin-Lun Ho for helpful discussions.

Refs. 1) Yi Li, E. H. Lieb, C. Wu, PRL 112, 217201 (2014).
2) S. L. Xu, Yi Li, C. Wu, PRX 5, 021032 (2015).
3) Yi Li, C. Wu, PRB 85, 205126 (2012).
4) C. Wu and S. C. Zhang, PRL 93, 36403 (2004).
5) C. Wu, K. Sun, E. Fradkin, and S. C. Zhang, PRB 75, 115103 (2007).

The early age of ferromagnetism

The magnetic stone attracts iron.

慈 (ci) 石(shi) 召(zhao) 铁(tie)

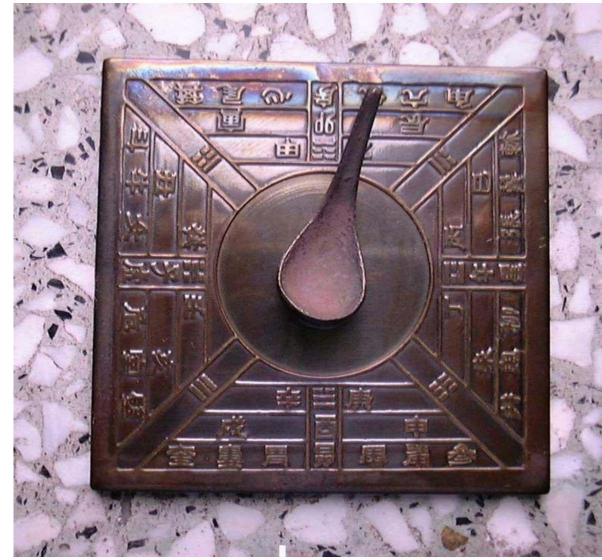
---- *Guiguzi (鬼谷子),* **(4^{th} century BC)**

慈 (loving, merciful, compassionate): the original Chinese character for magnetism

heart

磁 magnetism, magnetic

stone



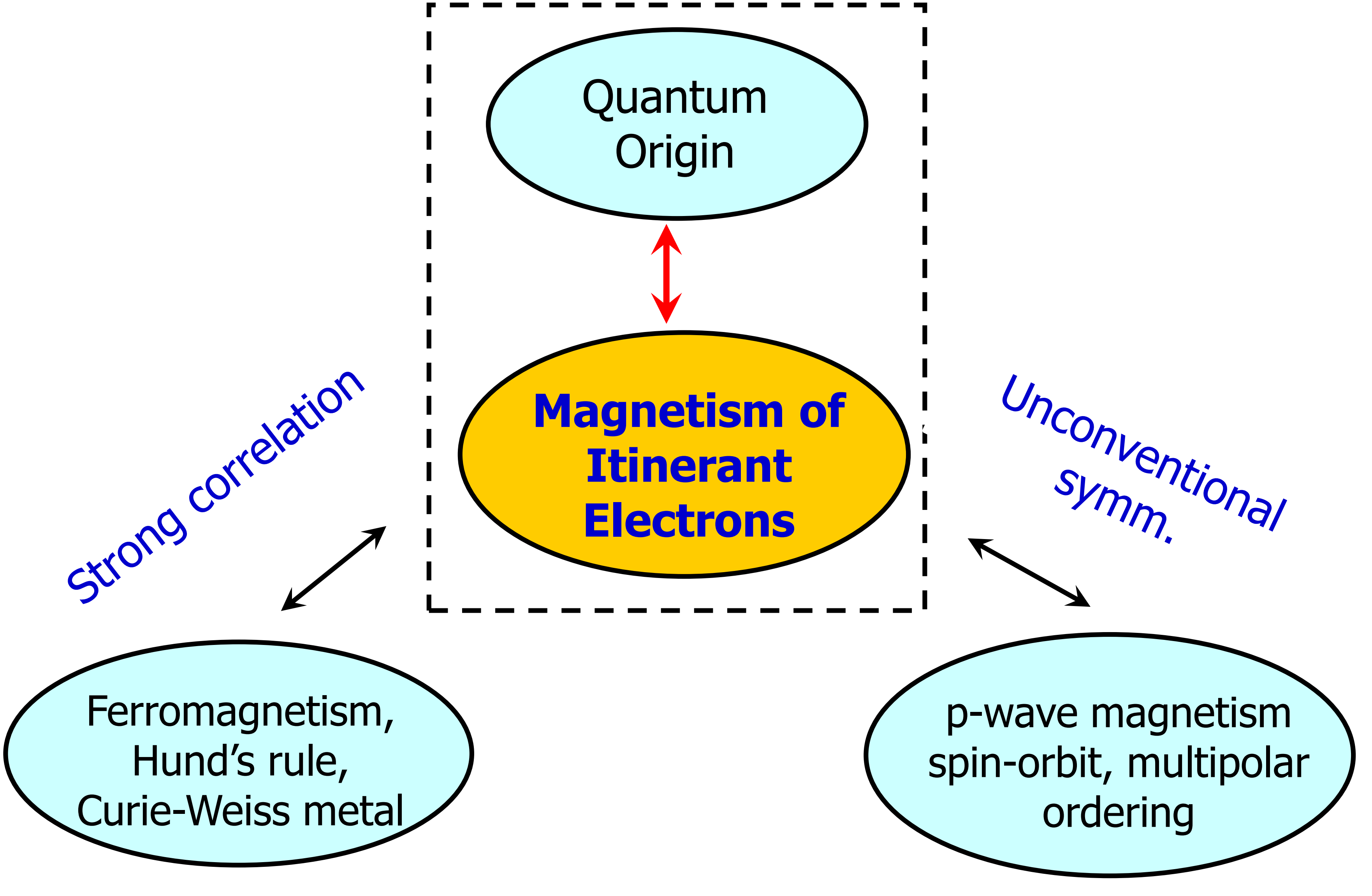
World's first compass: magnetic spoon: 1 century AD (司南 South-pointer)

Thales says that a stone (lodestone) has a soul because it causes movement to iron.

----*De Anima*, Aristotle (384-322 BC)

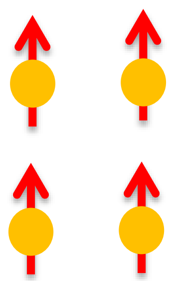
"Slightly eastward, not directly south" (常微偏东,不全南也)- Kuo Shen (沈括)(1031-1095)

Outline


Quantum Origin
Magnetism of Itinerant Electrons
Strong correlation
Unconventional symm.
Ferromagnetism, Hund's rule, Curie-Weiss metal
p-wave magnetism spin-orbit, multipolar ordering

Local moments v.s. itinerant electrons

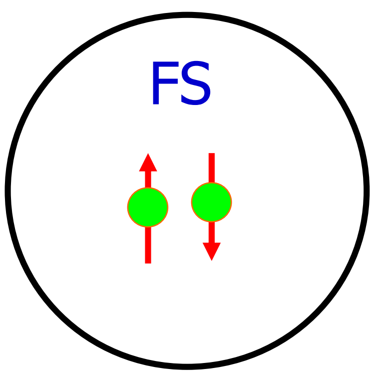
- Local moments – **not our interest!**



Curie-Weiss susceptibility

$$H = -J \sum_{ij} \sigma_i \sigma_j \longrightarrow \chi = \frac{A}{T - T_c}$$

- Itinerant electrons: Fermi surfaces – much harder to form ferromagnetism!



Pauli paramagnetism

$$\chi = N_0 \left(1 - \# \frac{T^2}{T_f^2}\right)$$

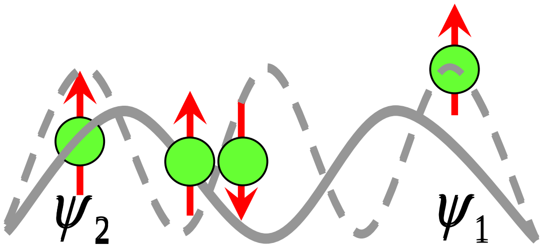
N_0: density of states at Fermi energy

N_0: density of states at the Fermi level

Itinerant ferromagnetism – Fermi statistics

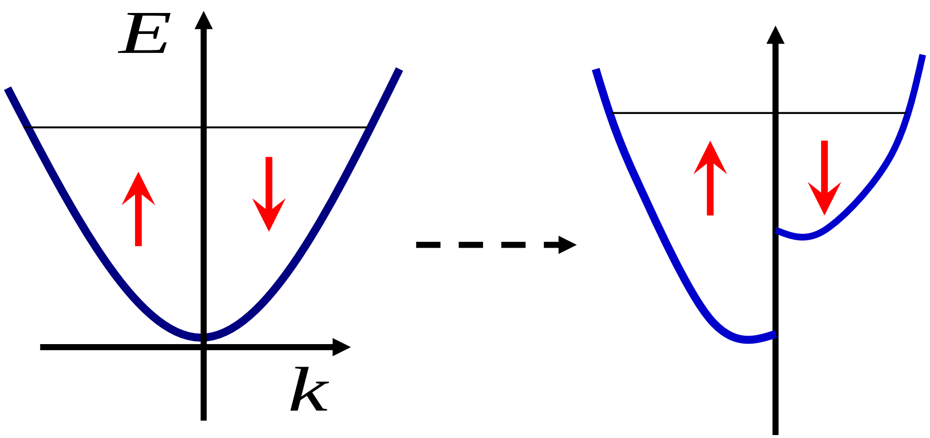
E. C. Stoner

- **Exchange due to exclusion – polarized electrons avoid each other.**



$$E_{\uparrow\uparrow} < E_{\uparrow\downarrow}$$

- **Stoner criterion: kinetic energy cost.**



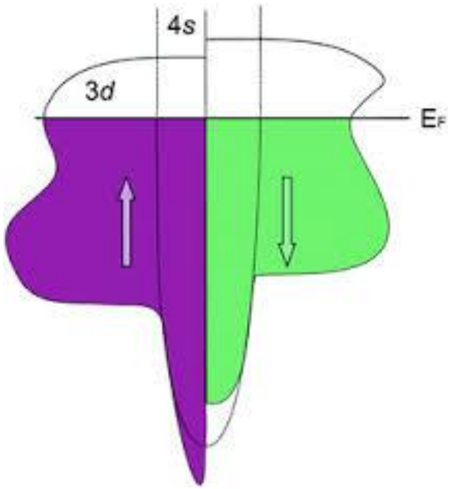
$$UN_0 > 1$$

U – average interaction strength; N_0 – density of states at the Fermi level

Kohn-Sham density functional theory – Work at Univ. California, San Diego

- Accurate on the ground state magnetizations.

Property	source	Fe (bcc)	Co (fcc)	Ni (fcc)	Gd (hcp)
M_{spin}	LSDA	2.15	1.56	0.59	7.63
M_{spin}	GGA	2.22	1.62	0.62	7.65
M_{spin}	experiment	2.12	1.57	0.55	
$M_{\text{tot.}}$	experiment	2.22	1.71	0.61	7.63

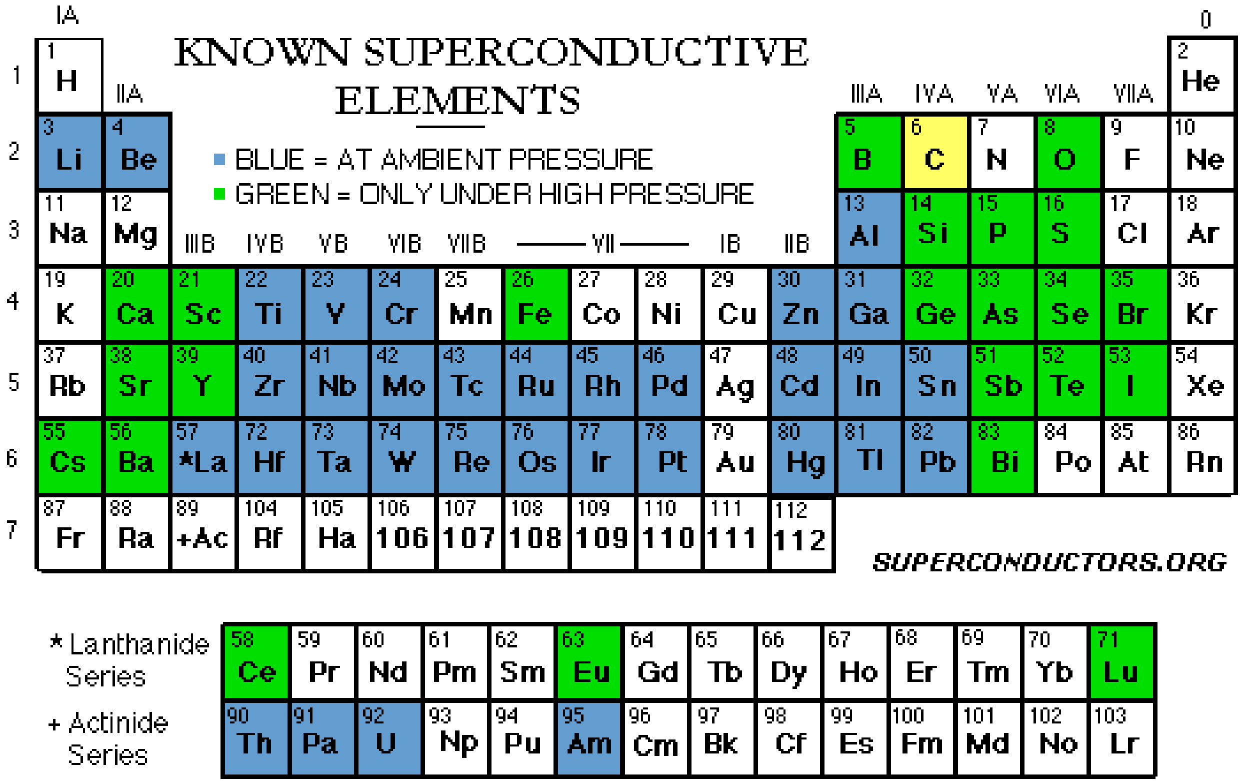


- Correlations partially contained in $V_{xc}(r)$ for energetics.

But wavefunctions remain Slater-determinant (uncorrelated) type.

- Thermal fluctuations difficult to handle – Curie temperatures overestimated.

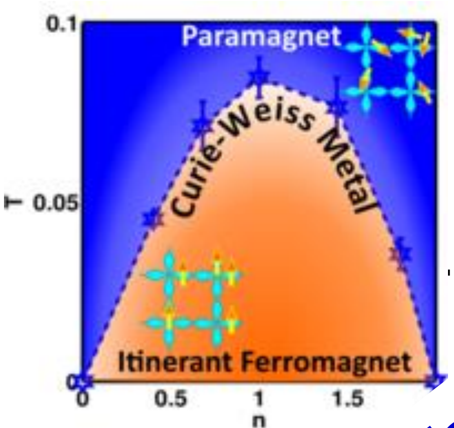
Itinerant ferromagnetism v.s. superconductivity



FM elements: Fe Co Ni Gd Dy

Outline

Quantum Origin



Strong correlation

Magnetism of Itinerant Electrons

Unconventional symm.

Ferromagnetism, Curie-Weiss metal

New states: p-wave magnetism (spin-orbit ordering)

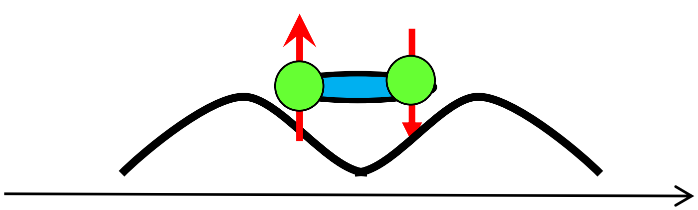
Correlations – FM is still rare!

- Electrons with opposite spins still avoid each other → **Kinetic energy advantage via correlated wavefunctions**.

- **No go!** Correlation wins: (I) two electrons, (II) 1D.

singlet (the ground state)

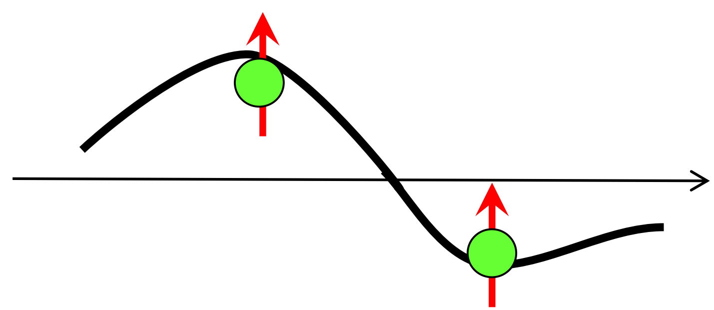
$\phi_{sym}(x_1 - x_2)$



(correlated, nodeless)

triplet

$\phi_{asym}(x_1 - x_2)$



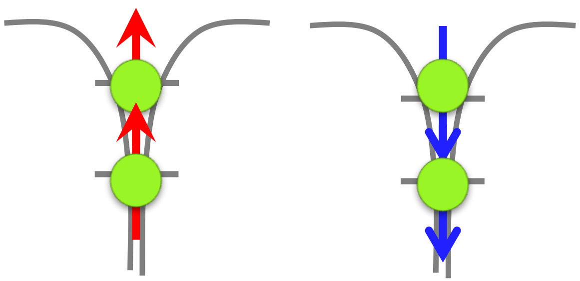
(exchange, nodal)

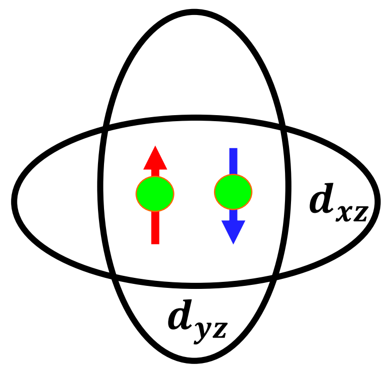
No FM in 1D – Lieb & Mattis theorem: spin singlet ground states.

Local v.s. global: Hund's coupling $\neq$ ferromagnetism

- Most ferro-metals: orbital degeneracy, Hund's coupling.

- Electron/hole spins add up – the exchange interaction.





Fermi surface

- Hund's rule usually cannot polarize the entire lattice!

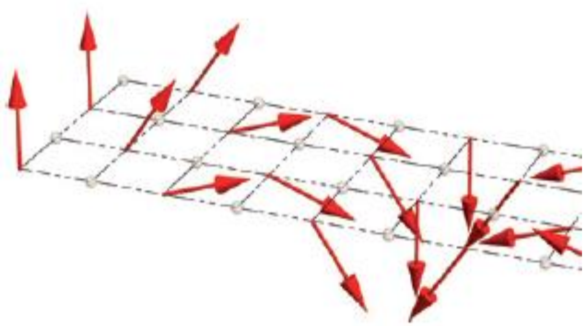
- **Under what condition, Hund's rule → global ferromagnetic coherence?**

Curie-Weiss metal ←→ high T_c pseudo-gap phase

- Curie-Weiss susceptibility: $\chi = \dfrac{A}{1 - T/T_0}$, $T_0 < T \ll T_f$

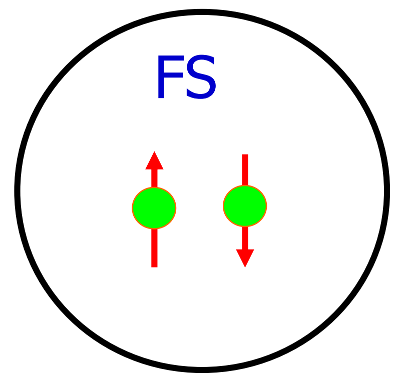
Natural for local moments but not for Fermi surfaces!

- Paramagnetic states close to T_0: domain fluctuations!



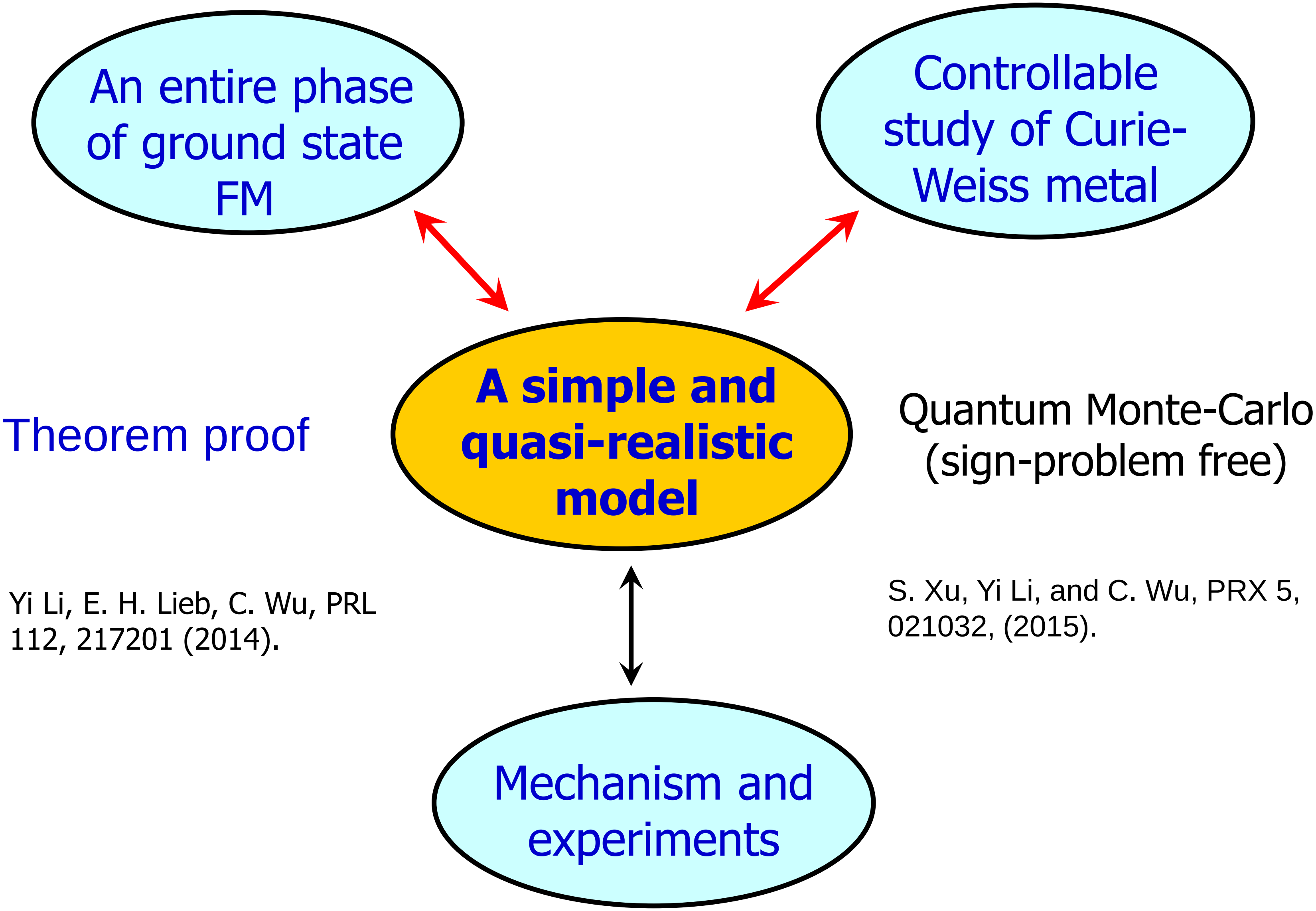
$T > T_0$

$\neq$



Stronger correlation than in the polarized FM state

Non-perturbative study on itinerant FM

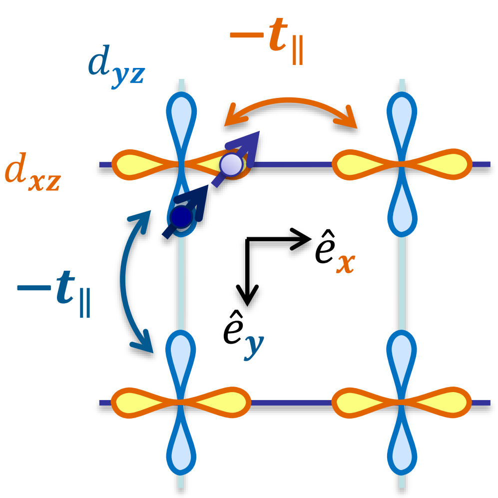


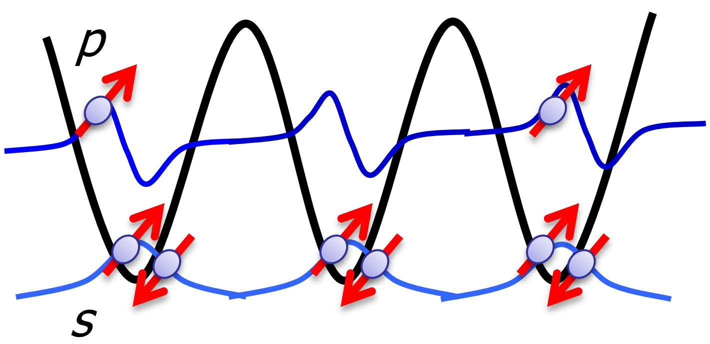
Yi Li, E. H. Lieb, C. Wu, PRL 112, 217201 (2014).

S. Xu, Yi Li, and C. Wu, PRX 5, 021032, (2015).

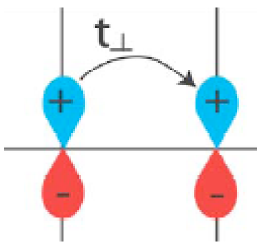
Hund's rule + quasi-1D bands (p/d-orbitals) →
2D and 3D FM in the strong interaction regime.

- d_{xz}/d_{yz} in 2D transition metal oxides
- px, py, (pz) in 2D or 3D optical lattices.





$t_{\parallel} \gg t_{\perp} \to 0$

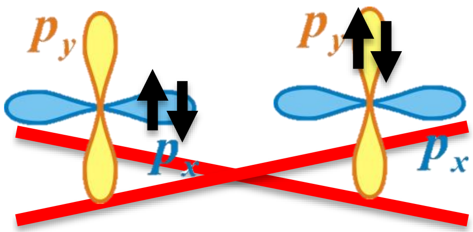


π-bond

Multi-orbital onsite (Hubbard) interactions

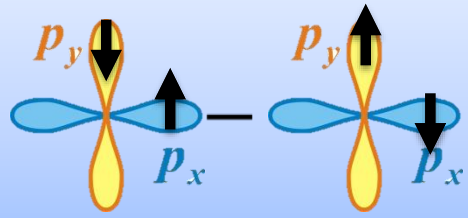
- Intra-orbital repulsion $U \to \infty$.

Intra-orbital singlet projected out



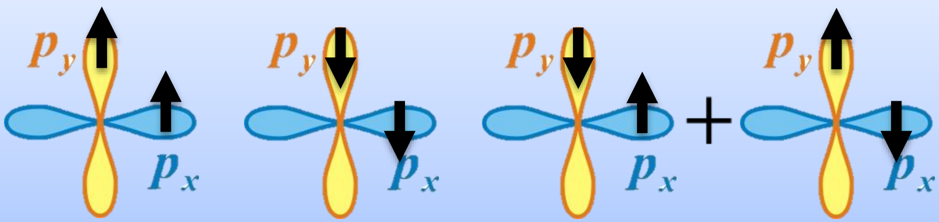
- Inter-orbital **Hund's coupling** J>0, and repulsion V.

Inter-orbital singlet



$$E = J + V$$

3-fold triplet



$$E = V$$

Theorem for a **phase** of itinerant FM

- **Theorem: FM ground states** at $U \to \infty$ (fully polarized and unique up to $2S_{tot}+1$-fold spin degeneracy).

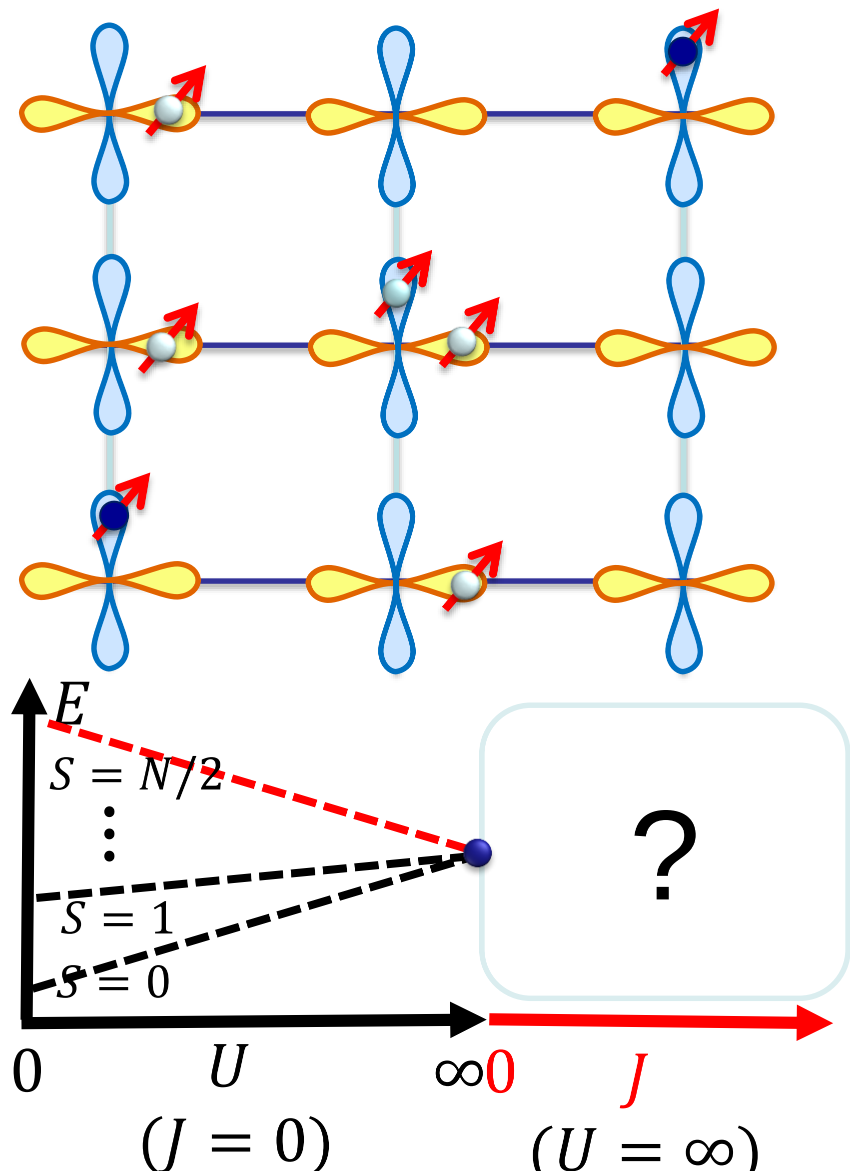
- **An entire phase**: valid at any generic filling, any value for $J>0$, and V.

- Free of quantum Monte-Carlo (QMC) sign problem at any filling – a rare case for fermions.

A reliable reference point for analytic and numeric studies of FM in multi-orbital systems

Yi Li, E. H. Lieb, C. Wu, Phys. Rev. Lett. 112, 217201 (2014)

Hund's rule assisted global FM



- Intra-chain:

Finite U: singlet ground state

$U \to \infty$: infinite degeneracy

- Inter-chain:

Hund's J lifts the degeneracy
→ global FM.

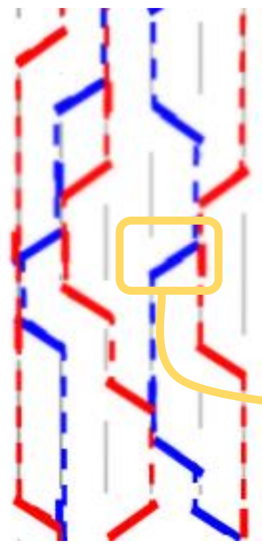
- 2D FM coherence: Total spin in each chain not conserved.

Quantum Monte Carlo (QMC)

- Stochastic method – polling the Hilbert space with importance sampling.

$$Z = Tr\left(e^{-\beta H}\right)$$

$$= \sum \left\{ \quad \right\}$$



Always Positive !

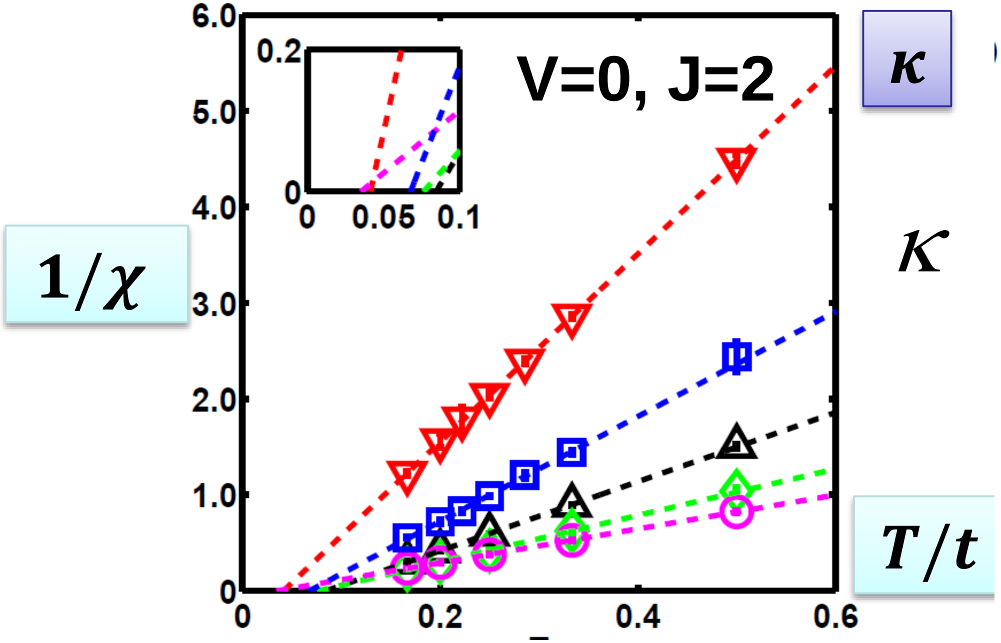
$$\langle \psi, \tau \left| (-H)^{g(b,\tau)} \right| \psi, \tau + d\tau \rangle$$

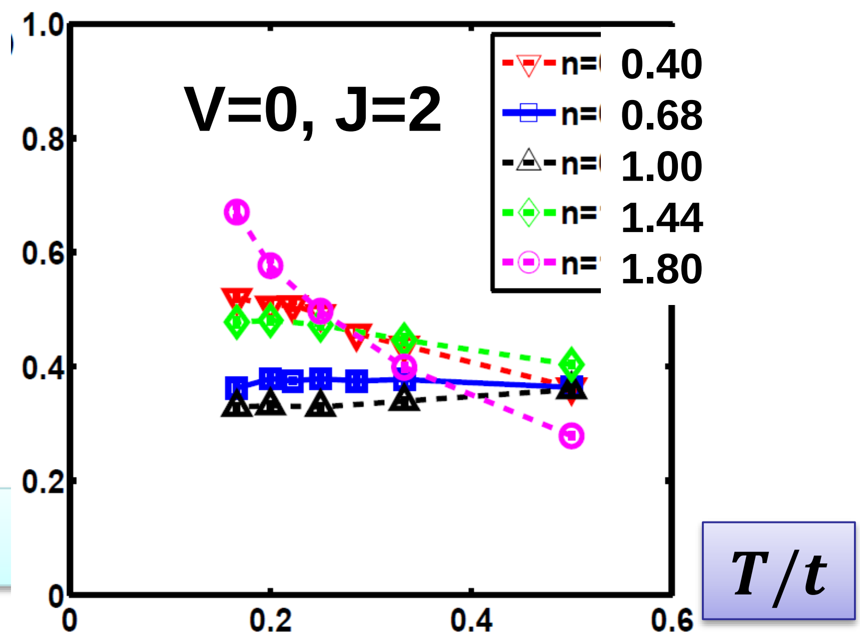
- Stochastic series expansion (SSE) + direct loop update.

- Our model is free of the sign problem – a rare case of fermion models.

S. L. Xu, Yi Li, C. Wu, Phys. Rev. X 5, 021032, (2015).

QMC: the Curie-Weiss metal





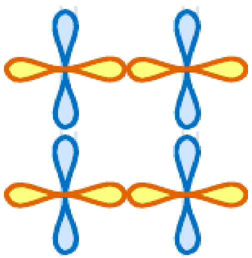
- Local moment-like spin susceptibility (spin incoherent):

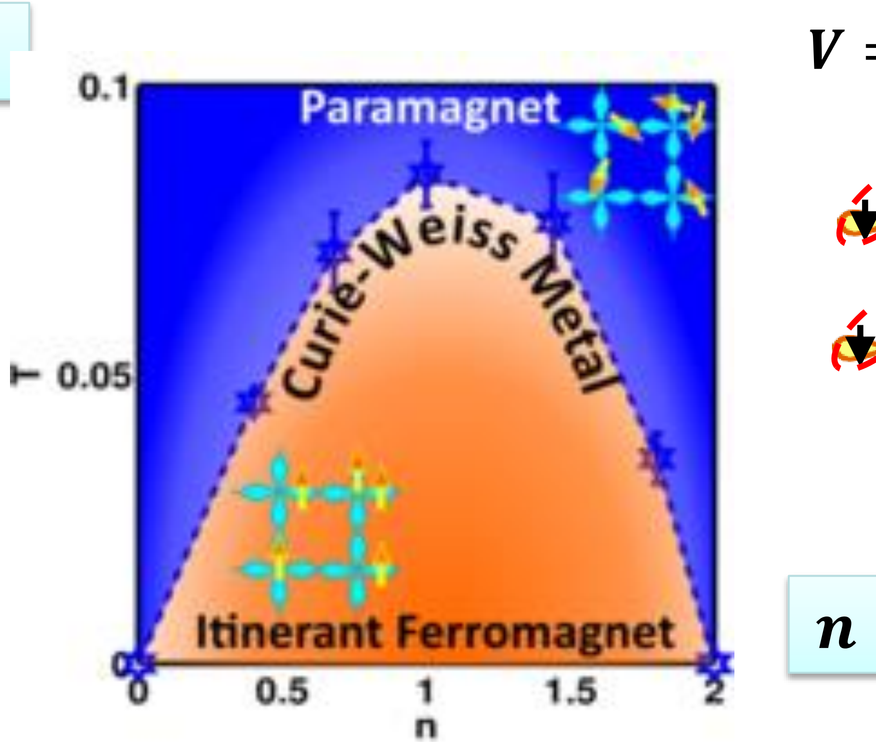
$$\chi = \frac{A}{1 - T/T_0}\,, \qquad T_0 < T < T_{ch}$$

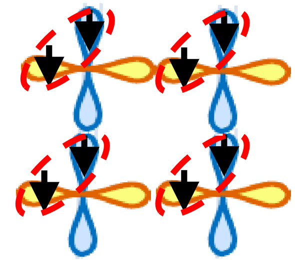
- Metalic compressibility κ :
  Saturates at $T < T_{ch}$, and $T_{ch} \sim t$ (charge itinerancy).

Curie temperatures v.s filling (V=0)

$V = 0, J = 2$







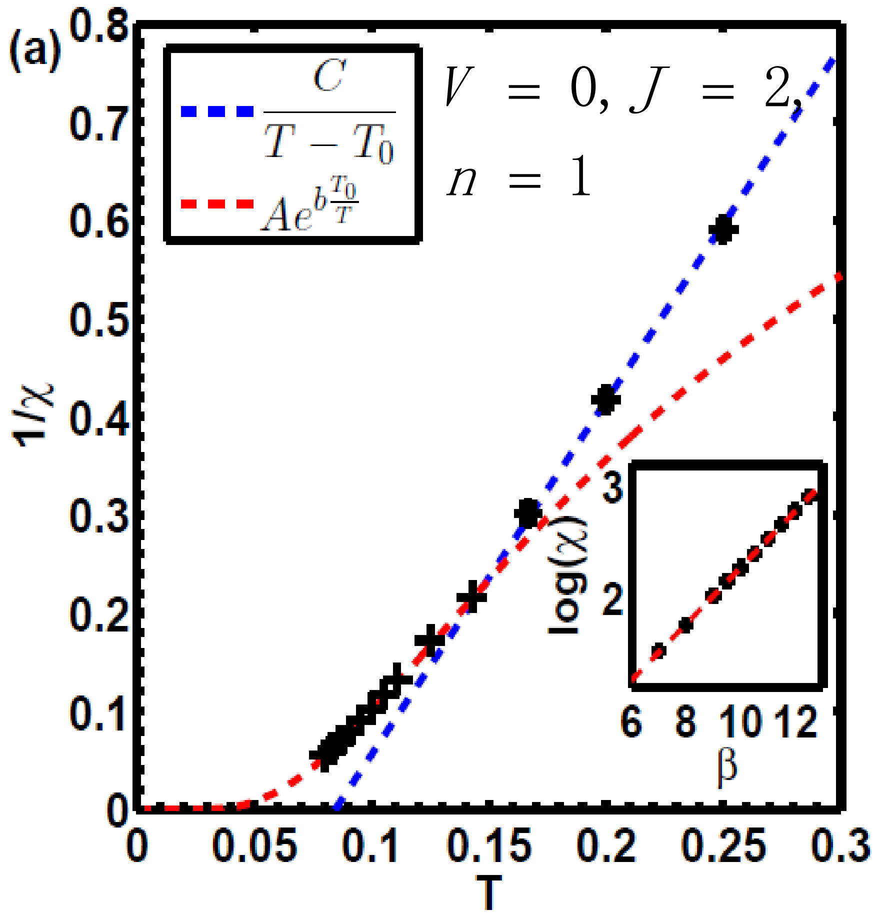
$$\chi = \frac{A}{1 - T/T_0}$$

- T_0→0 at both n→0 (particle vaccum), and

  n→ 2 (hole vaccum, spin-1 moments, no FM).

- $T_{0,max} \approx 0.08 t_{\parallel}$ at maximal itinerancy (p-h symmetry)

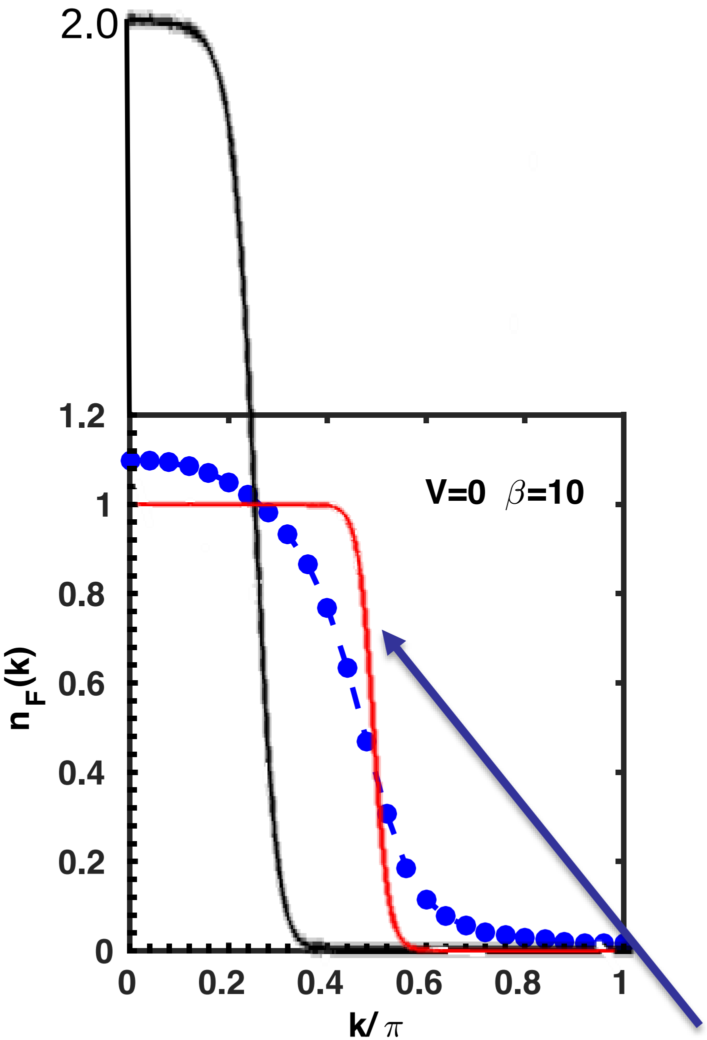
Critical ferromagnetic scaling



- **No long-range order at fintie T (Mermin-Wagner theorem)**
- **O(3) NLσ-model: FM directional fluctuations**
- **As $T < T_0$, χ crosses over into an exponential growth.**

$$\chi = \frac{C}{T - T_0} \longrightarrow \chi = Ae^{b\frac{T_0}{T}}$$

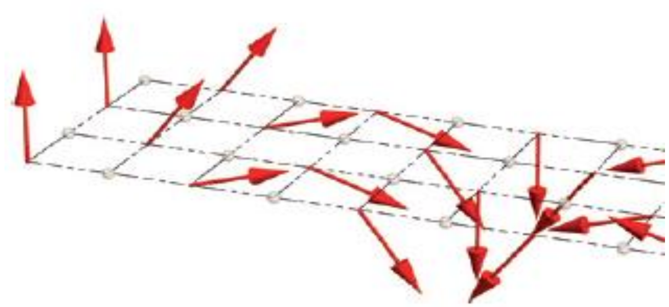
Fermi distribution $n_F(k)$



Paramagnetic Curie-Weiss metal

$$n_F(k) = n_\uparrow(k) + n_\downarrow(k)$$

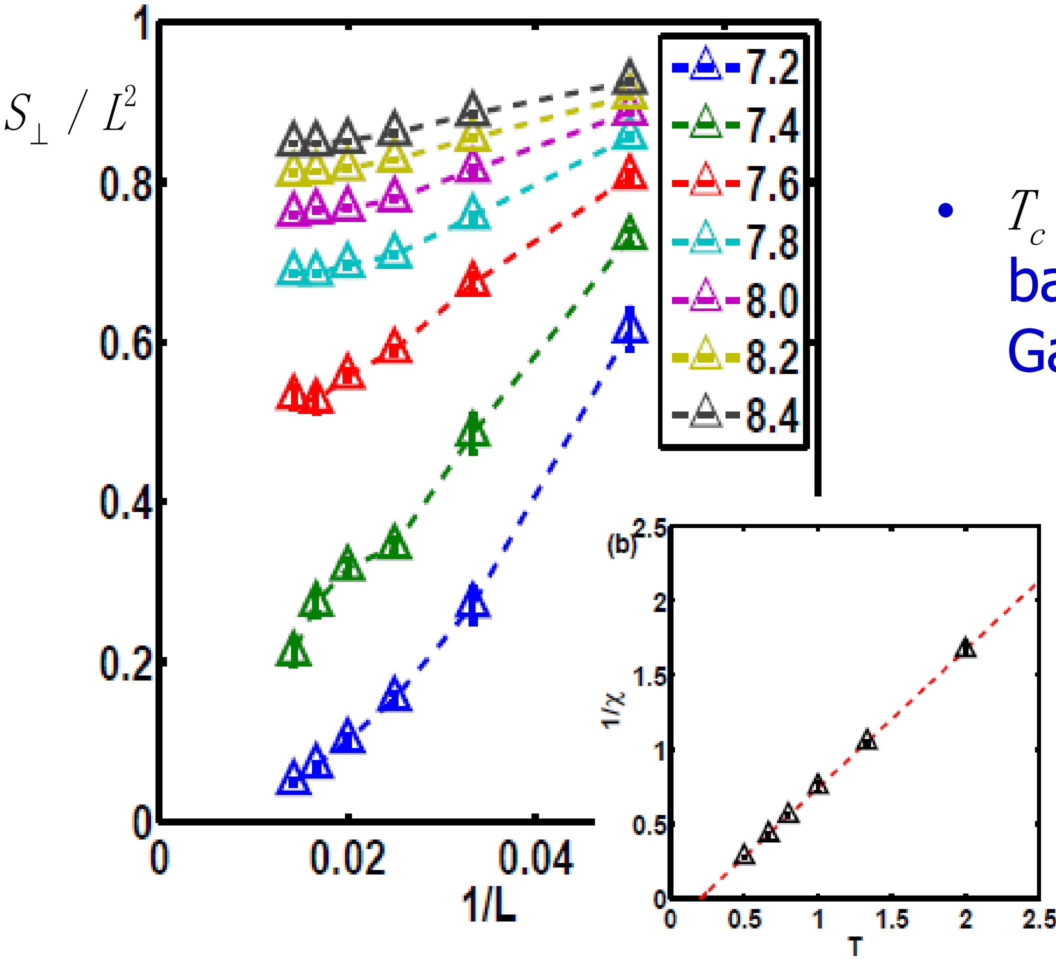
- **At k→0, $n_\uparrow(k) = n_\downarrow(k) \approx 0.54 \ll 1$**
- Large entropy (the k-space picture)
- **Strongly correlated metal phase**



Reference: **polarized fermion with $k_F^0 = \frac{\pi}{2}$**

Calculation of T_c for the Ising class!

Structure factor scaling



- Reduce symm to the Ising class.

$$J_{//} = 2, J_\perp = 4$$

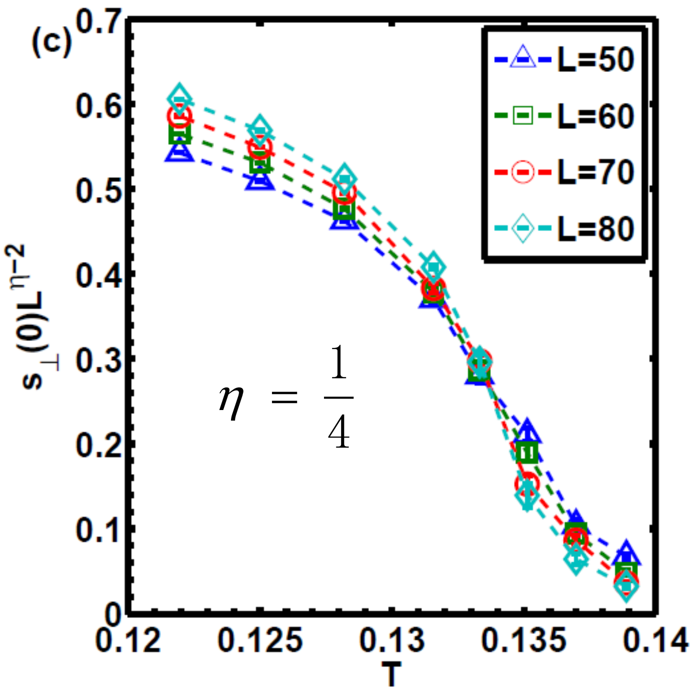
- T_c is be suppressed from T_0 based on CW-law by non-Gaussian fluctuations.

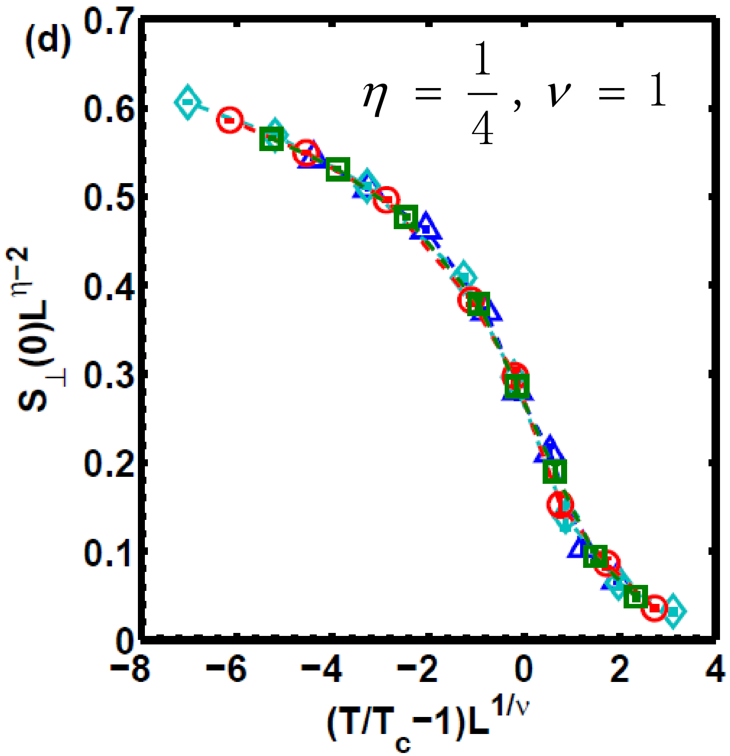
$$T_c = \frac{1}{\beta_c} = \frac{1}{7.6} \approx 0.132,$$

$$T_0 \approx 0.2$$

Critical scaling and data collapse: 2D Ising class

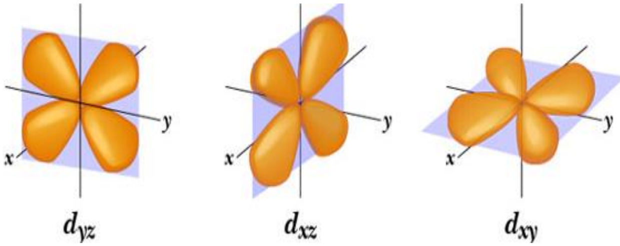
Data crossing: $S_{\perp}(0)L^{-2+\eta}$ $v.s.$ T $\qquad$ $S_{\perp}(0)L^{-2+\eta} = f((T/T_c - 1)L^{1/\nu})$





$T_c \approx 0.134,$

Apply to the $LaAlO_3/SrTiO_3$ interface



- d_{xz}, d_{yz}: quasi-1D bands, higher energy.
- d_{xy}: quasi-2D band, lower energy.

- Our theorem to $\boldsymbol{d_{xz}}$, $\boldsymbol{d_{yz}}$ bands: quas-1D + Hund's coupling + strong intra-orbital repulsion for 3d-orbitals.

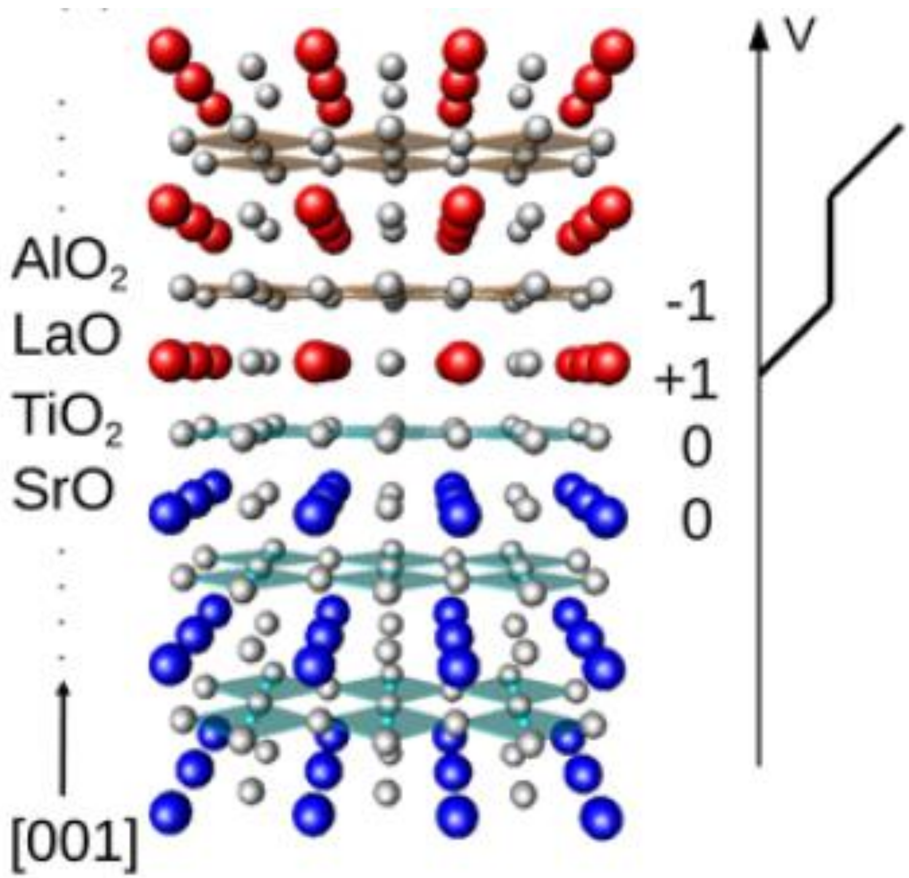
- The FM d_{xz}, d_{yz} -bands polarize the paramagnetic d_{xy} - band.

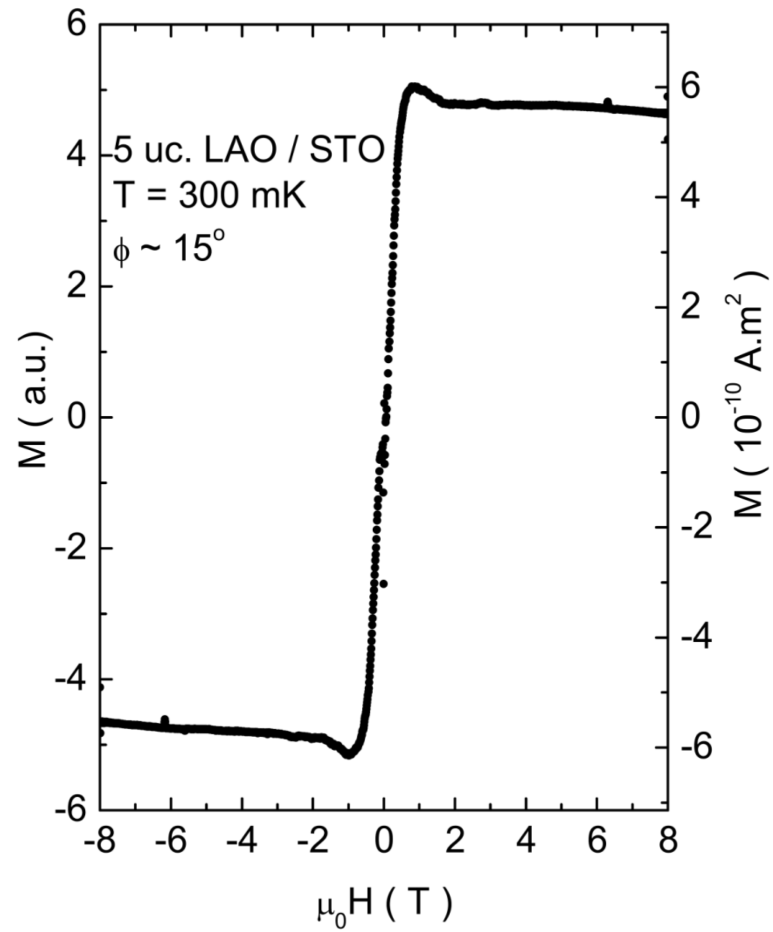
- No local moments needed! Different from double exchange.

A similar proposal by Chen and Balents based on mean-field treatment of the coupling between dxz/dyz-bands.

Lu Li et al, Nat. Phys 2011, Bert et al, Nat. Phys 2011

FM at the interface of $SrTiO_3/LaAlO_3$





Lu Li et al, Nat. Phys 2011, Bert et al, Nat. Phys 2011

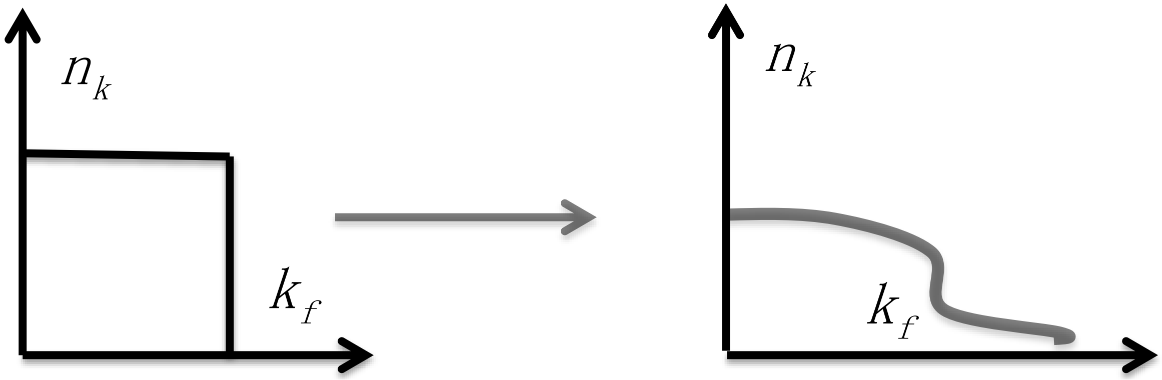
Why is ferromagentism difficult?

- Large kinetic energy cost to polarize the ideal Fermi distribution.

- Hund J is the key, but by itself, it is insufficient!

- Hubbard U mostly favors anti-FM, but brutal enough to distort the Fermi distribution.

- **Apply J on top of U → FM with less kinetic energy cost and even gain kinetic energy.**



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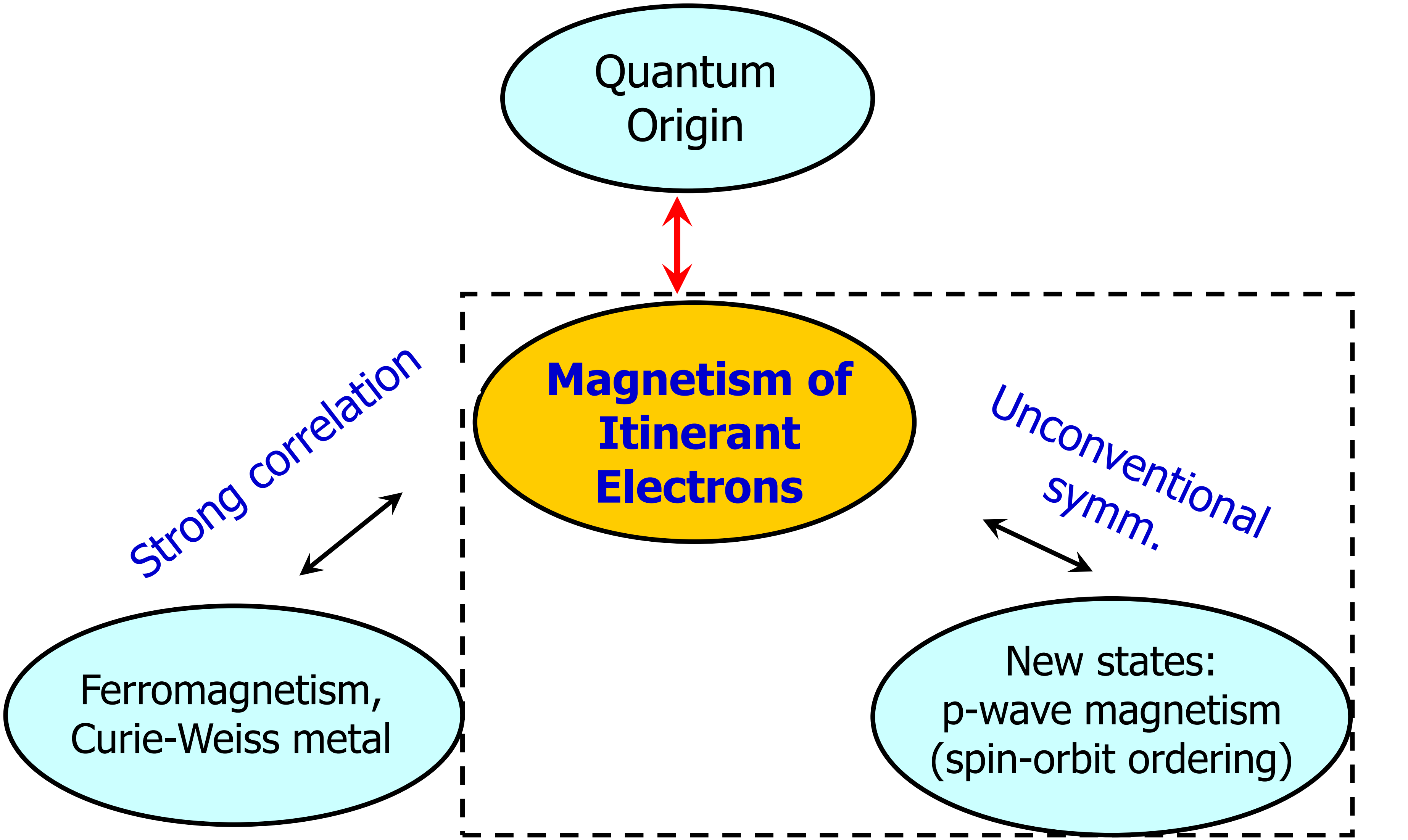

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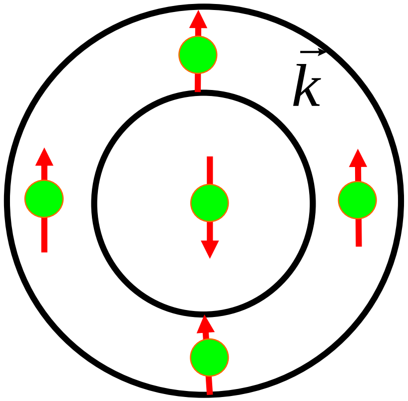
Itinerant ferromagnetism: ***s*-wave**

- Spin rotational symmetry is broken.

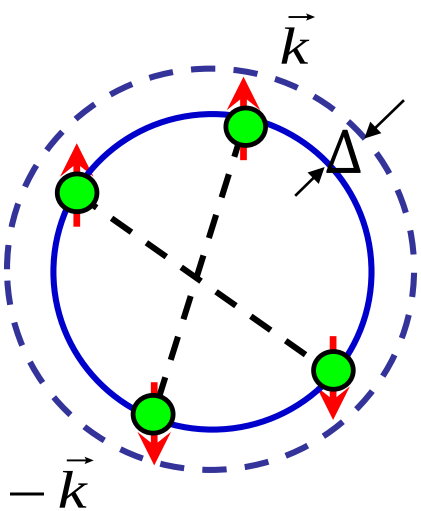


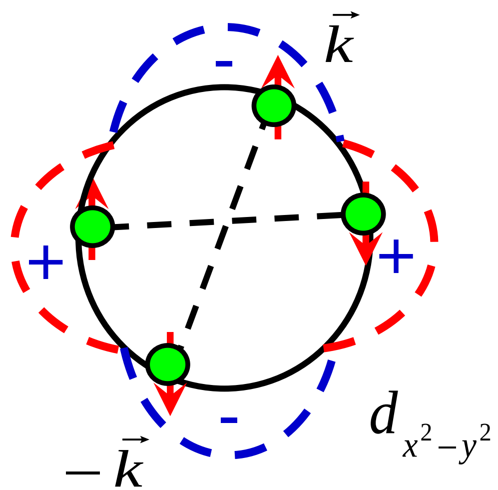
- Orbital rotational symmetry is **NOT** broken:
spin polarizes along **a fixed direction**.

- *cf.* Conventional superconductivity (s-wave)

Unconventional superconductivity (e.g. d-wave high T_c cuprates)

s -wave

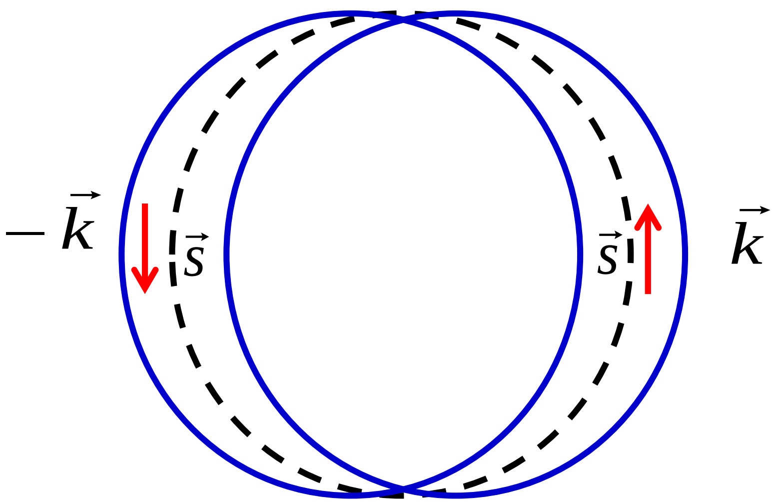




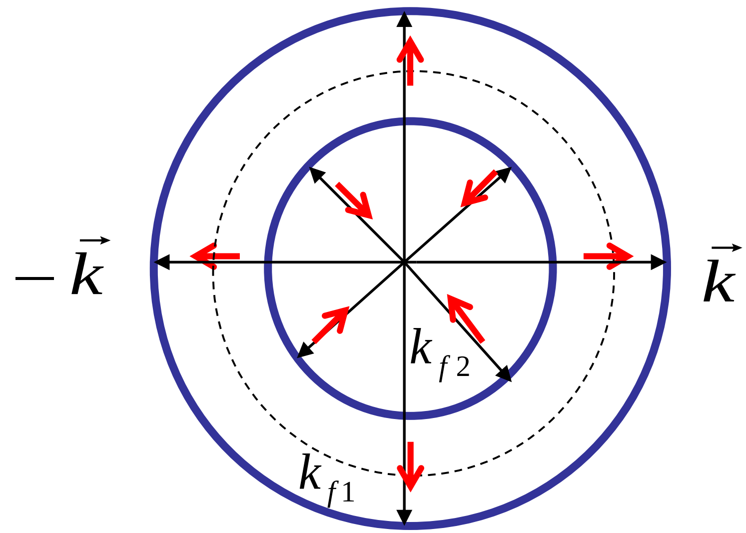
New states of matter: **unconventional magnetism**!

- High partial-wave channel magnetism (e.g. *p, d-wave*…) .

- Multi-polar spin distribution over the Fermi surface.



anisotropic *p*-wave state

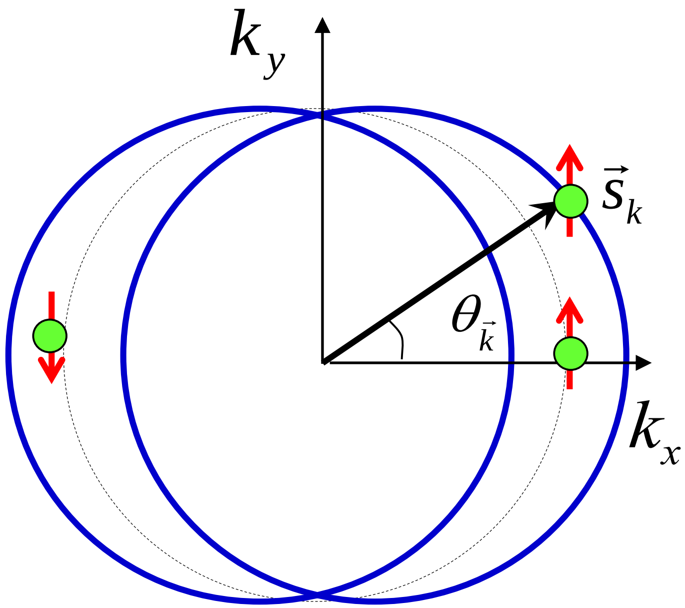


isotropic *p*-wave state

spin-split state by J. E. Hirsch, PRB 41, 6820 (1990); PRB 41, 6828 (1990).

spin flips the sign as $\vec{k} \to -\vec{k}$

Anisotropic unconventional magnetism: spin nemetic liquid phases!



anisotropic *p*-wave magnetic phase

- *p*-wave distortion of the Fermi surface.
- Spin dipole moment in momentum space (not in coordinate space).

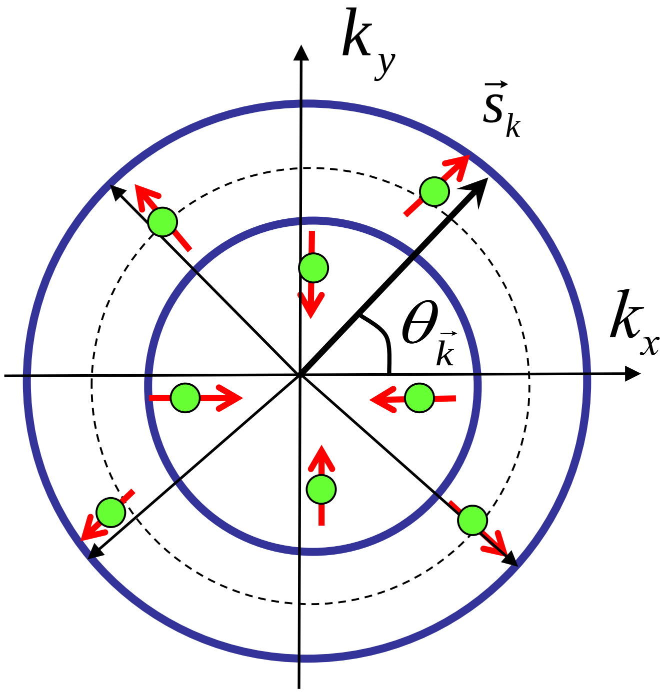
$$\vec{n}_1 = \sum_{\vec{k}} \vec{s}_k \cos\theta_k \neq 0$$

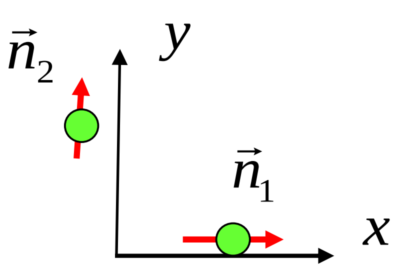
- Both orbital and spin rotational symmetries are broken.

spin-split state by J. E. Hirsch, PRB 41, 6820 (1990); PRB 41, 6828 (1990).

V. Oganesyan, et al., PRB 64,195109 (2001). C. Wu et al., PRL 93, 36403 (2004); Varma et al., Phys. Rev. Lett. 96, 036405 (2006)

The isotropic *p*-wave magnetic phase





- Helicity $\vec{\sigma}\cdot\vec{k}$ is a good quantum number.

- No net spin-moment; spin dipole moment in momentum space.

$$\vec{n}_1 = \sum_{\vec{k}} \vec{s}_k \cos\theta_k, \quad \vec{n}_2 = \sum_{\vec{k}} \vec{s}_k \sin\theta_k$$

- **Isotropic phase with SO coupling.**

$$H_{MF} = H_0 + \bar{n}\sum_k \psi^{+}_{\alpha}\vec{\sigma}_{\alpha\beta}\cdot\vec{k}\,\psi_{\beta}$$

$$\bar{n} = |\vec{n}_1| = |\vec{n}_2|$$

C. Wu et al., PRL 93, 36403 (2004);
C. Wu et al., PRB PRB.75, 115103 (2007). .

Dynamic generation of spin-orbit (SO) coupling!

- Conventional wisdom**:**

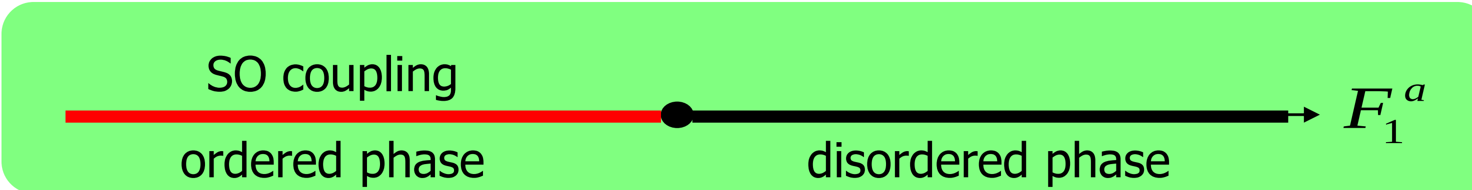
  A **single-body** effect inherited from the Dirac equation

- New mechanism **(many-body collective effect):**

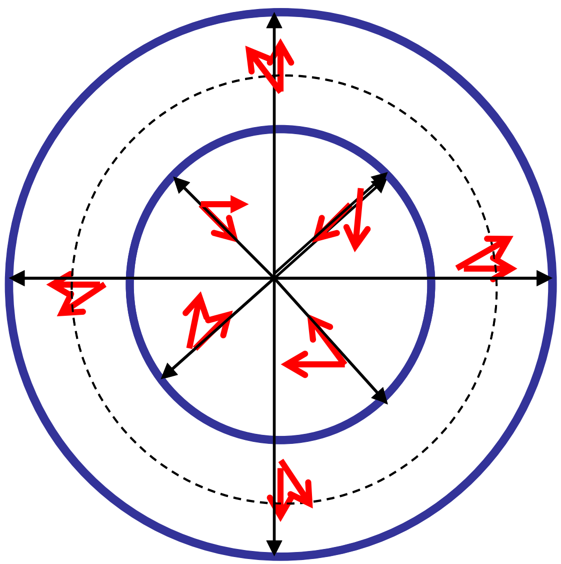
Generate SO coupling through **unconventional magnetic phase transitions.**

- **Advantages**: tunable SO coupling by varying temperatures;
  new types of SO coupling.

The subtle symmetry breaking pattern

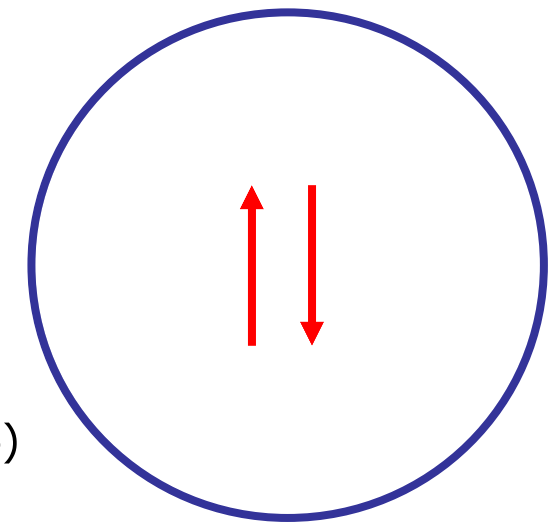


- $\vec{J}$ is conserved , but $\vec{L}, \vec{S}$ are not separately conserved.
- **Independent** orbital and spin rotational symmetries.



$$\vec{J} = \vec{L} + \vec{S}$$

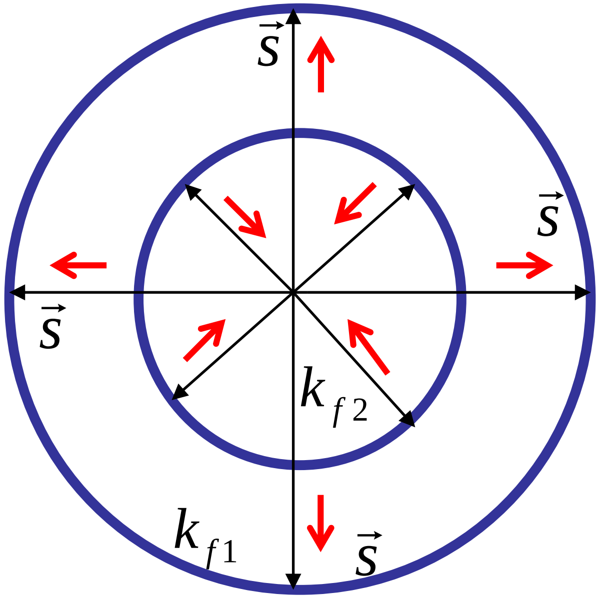
Leggett, Rev. Mod. Phys **47**, 331 (1975)



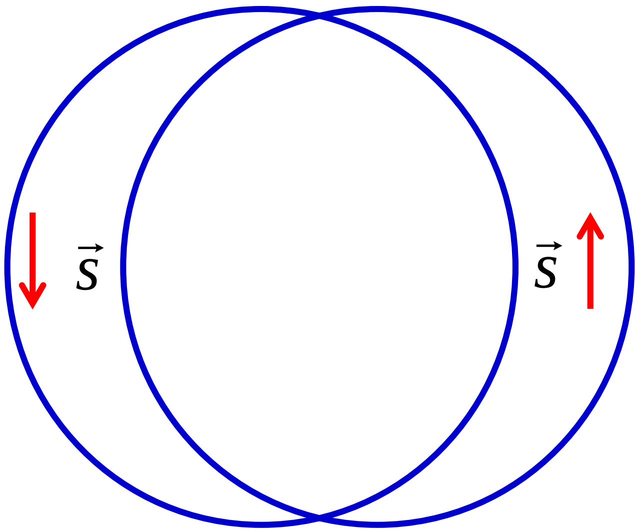
- **Relative spin-orbit** symmetry breaking.

Unconventional magnetism: Pomeranchuk instability in the spin channel

F_1^a



$\beta-$phase

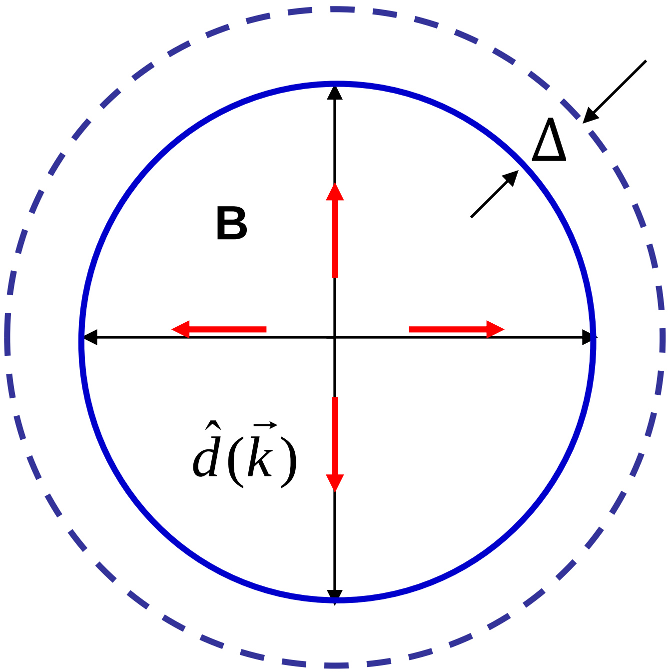


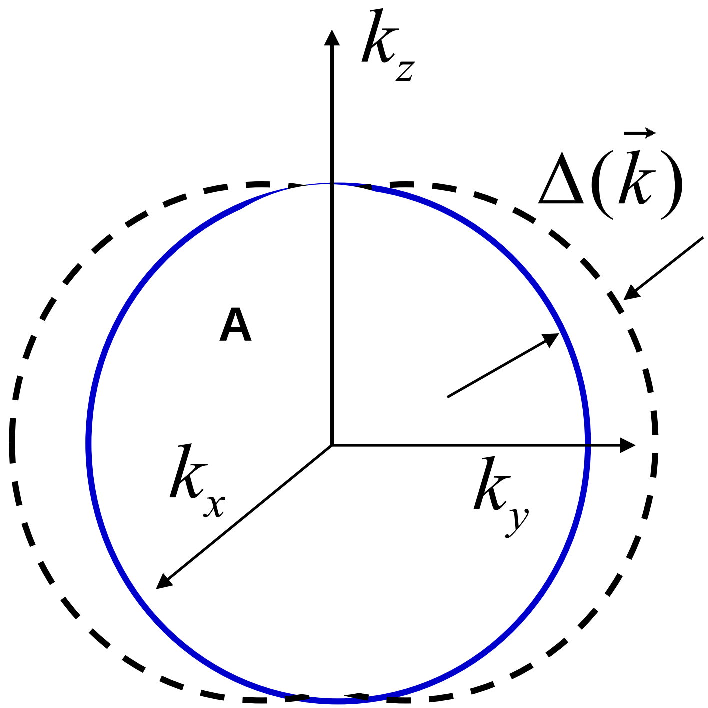
$\alpha-$phase

- An analogy to superfluid ^{3}He-B (isotropic) and A (anisotropic) phases.

cf. Superfluid ^{3}He-B, A phases

- *p*-wave triplet Cooper pairing.





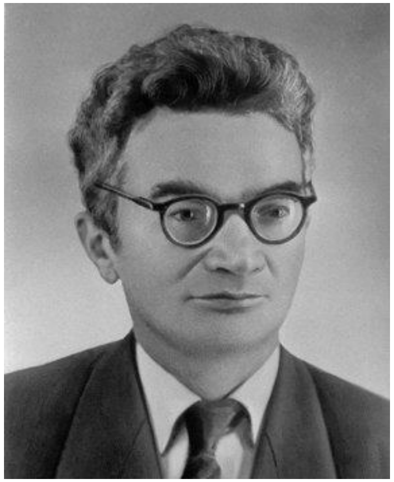
$$\vec{\Delta}(\vec{k}) = \Delta\hat{d}(\vec{k}) = \Delta\hat{k}$$

$$\vec{\Delta}(\vec{k}) = \Delta\hat{d}(\hat{k}_x + i\hat{k}_y)$$

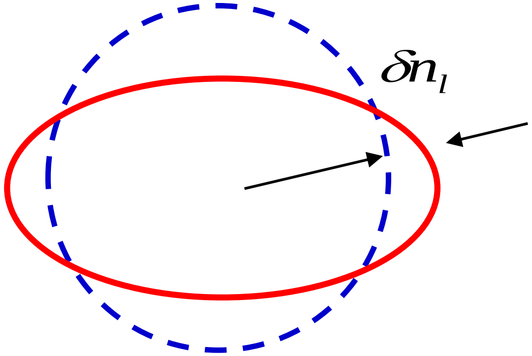
- ^{3}He-B (isotropic) phase.
- ^{3}He-A (anisotropic) phase.

A. J. Leggett, Rev. Mod. Phys 47, 331 (1975)

Pomeranchuk instability



I. Pomeranchuk



- Fermi surface: elastic membrane.
- Stability:

$$\Delta E_K \propto (\delta n_l^{s,a})^2$$

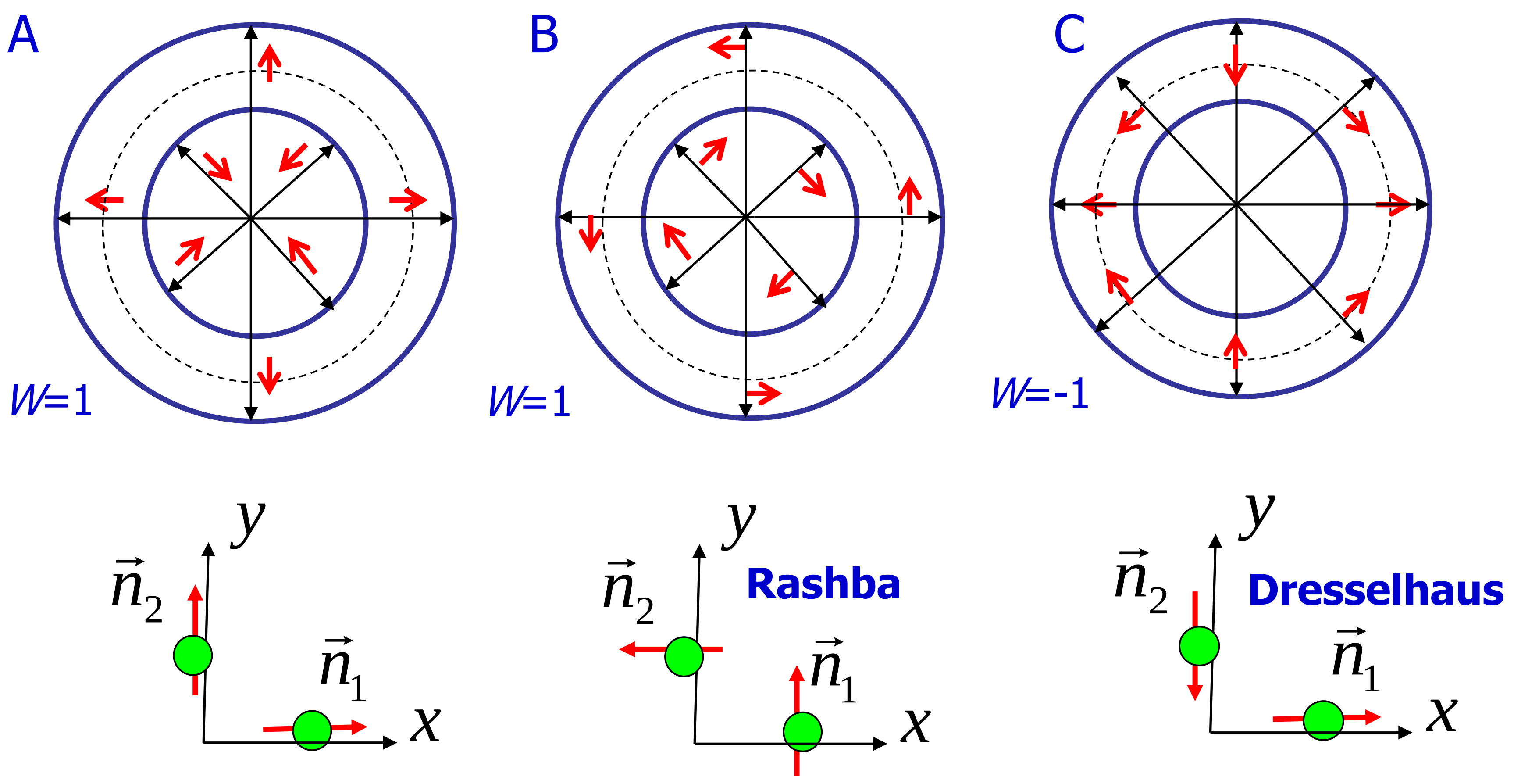
$$\Delta E_{\text{int}} \propto \frac{F_l^{s,a}}{2l+1} (\delta n_l^{s,a})^2$$

- Surface tension vanishes at:

$$F_l^{s,a} < -(2l+1)$$

- Ferromagnetism: the F_0^a channel.
- Nematic electron liquid: the F_2^s channel.

The β-phases: vortices in momentum space



- Perform global spin rotations, A→ B→ C.

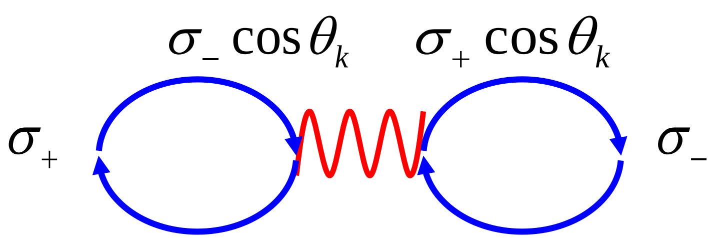
L. Fu's(PRL2015): gyro ferroelectric muti-polar

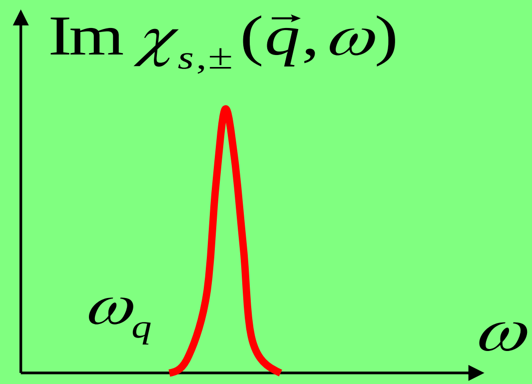
Neutron spectra (The α-phase)

- No *elastic* Bragg peaks.

- $\vec{n}_{1,2}$ couple with spin dynamically **at $T < T_c$** -- coupling between Goldstone modes and spin-waves.

$$L = (\vec{n}_1 \times \partial_t \vec{n}_1 + \vec{n}_2 \times \partial_t \vec{n}_2) \cdot \vec{S}$$
$$\rightarrow \bar{n}\,(S_y \partial_t n_{1x} - S_x \partial_t n_{1y})$$





$$\mathrm{Im}\,\chi_{s,\pm}(\vec{q},\omega) \approx N_0 \omega_q^2 \delta(\omega^2 - \omega_q^2)$$

- *In-elastic*: **resonance peaks** develop **at $T<T_c$**.

A natural generalization of ferromagnetism

- The driving force is still exchange interactions, but in **non-s-wave** channels.

	s-wave	*p*-wave	*d*-wave
SC/SF	Hg, 1911	^{3}He, 1972	high T_c, 1986
magnetism	Fe, ancient time	?	?

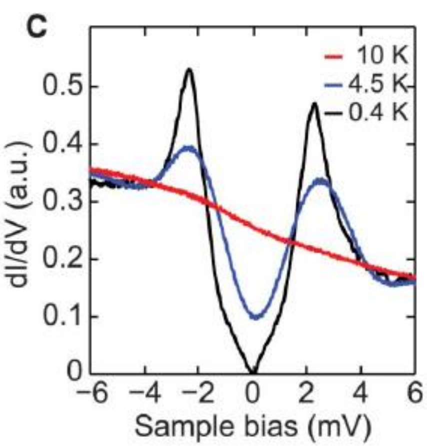
- Optimistically, unconventional magnets may already exist.

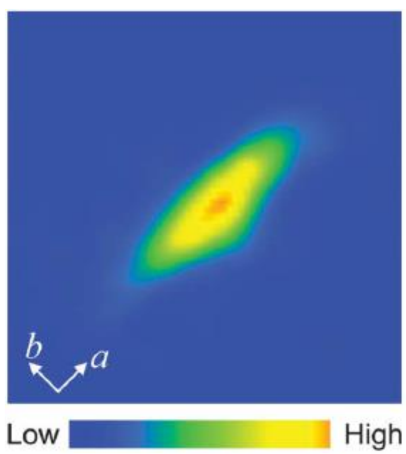
cf. Antiferromagnetic materials are actually very common in transition metal oxides. But they were not well-studied until neutron-scattering spectroscopy was available.

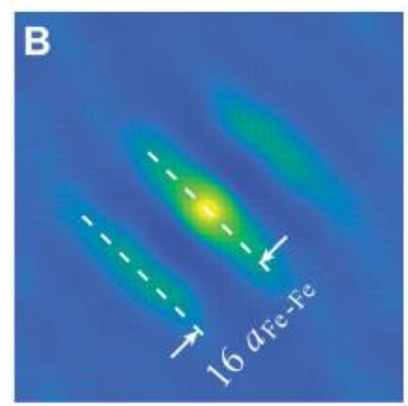
Direct Observation of Nodes and Twofold Symmetry in FeSe Superconductor

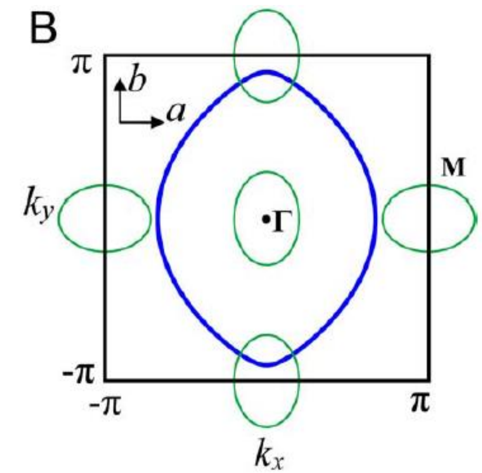
Science 332, 1410 (2011)

Can-Li Song,[1,2] Yi-Lin Wang,[2] Peng Cheng,[1] Ye-Ping Jiang,[1,2] Wei Li,[1] Tong Zhang,[1,2] Zhi Li,[2] Ke He,[2] Lili Wang,[2] Jin-Feng Jia,[1] Hsiang-Hsuan Hung,[3] Congjun Wu,[3] Xucun Ma,[2*] Xi Chen,[1*] Qi-Kun Xue[1,2]





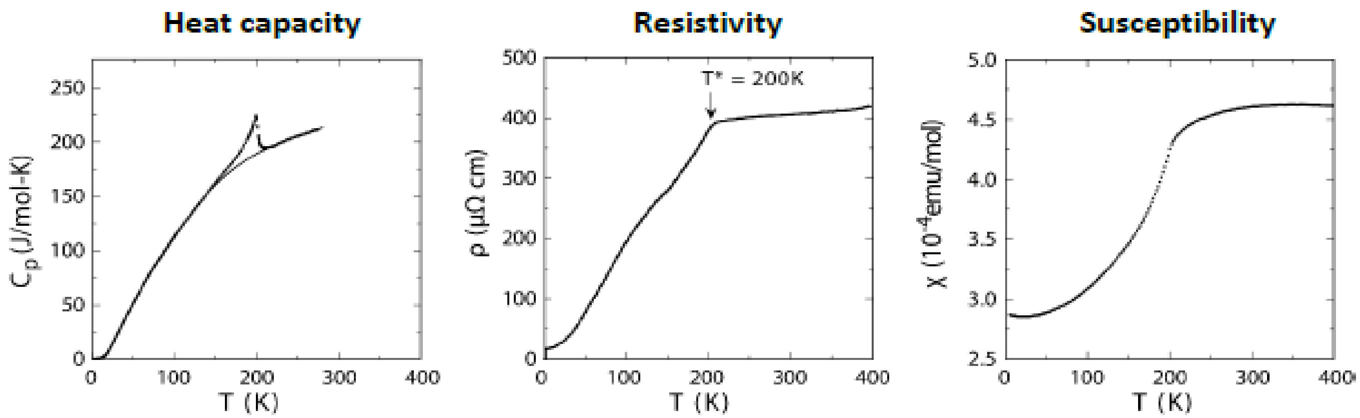




- Consistent with orbital ordering between dxz/dyz orbitals.

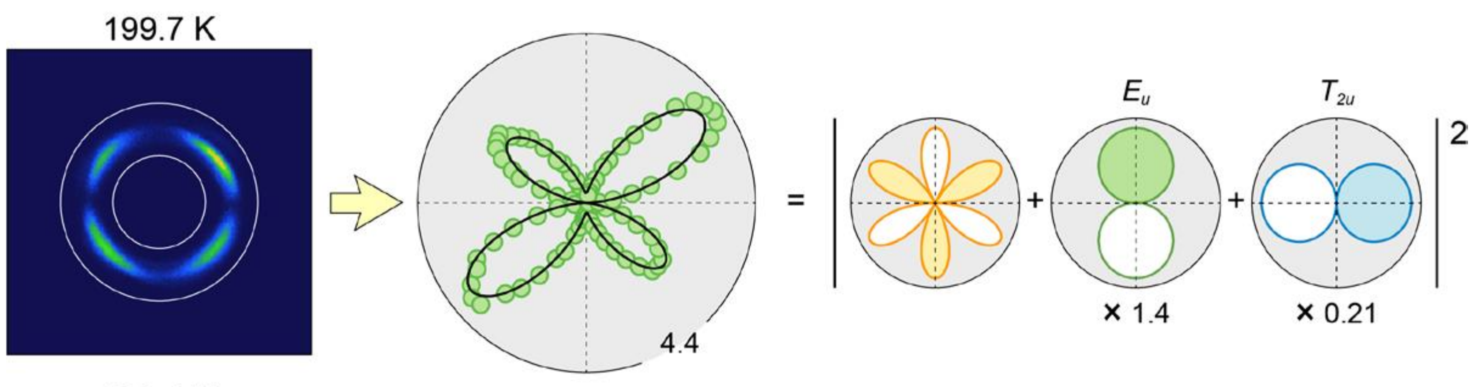
H. H. Hung, C. L. Song, Xi Chen, Xucun Ma, Q. K. Xue, C. Wu, Phys. Rev. B 85, 104510 (2012).

Parity breaking nematic phase in Cd_2ReO_7



Jin *et al.*, *J. Phys.: Condens. Matter* **14**, L117 (2002).

- Signature of parity breaking through 2nd harmonic generation method.



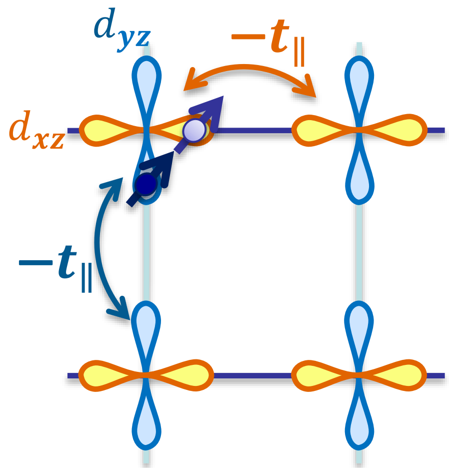
J. W. Harter, Z. Y. Zhao, J. Q. Yan, D. G. Mandrus, and D. Hsieh, Science 356， 295-299 (2017).

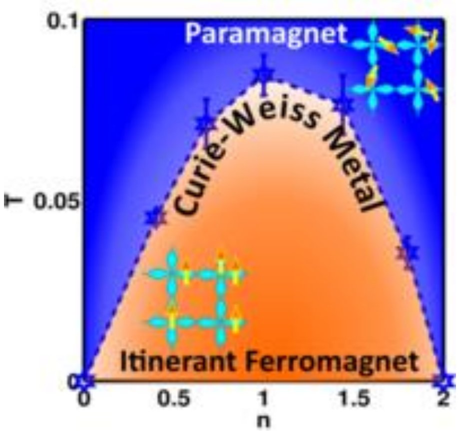
Summary: Itinerant magnetism (ferro and beyond)

- Non-perturbative study on itinerant FM and Cuire-Weiss metals

Hund's rule + quasi 1D + strong correlation

Sign-problem QMC simulations.

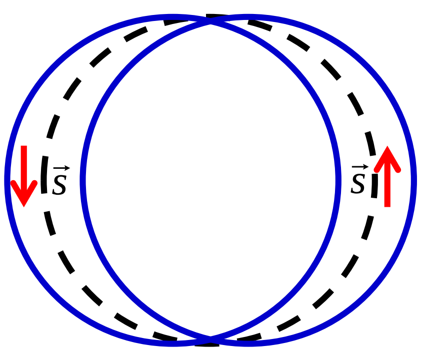




- New states of matter: p-wave magnetism

Spontaneous generation of spin-orbit ordering.

α-phase



β-phase