Novel Orbital Physics – Unconventional BEC, Ferromagnetism, and Curie-Weiss Metal

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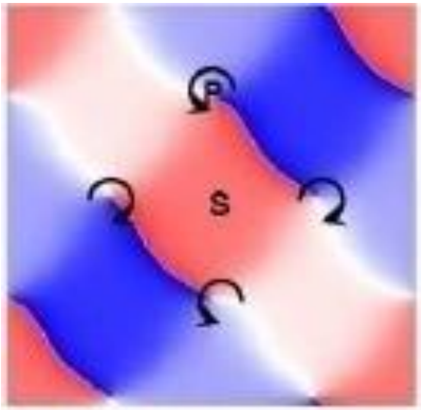

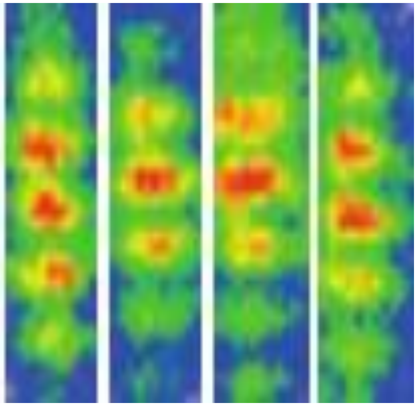

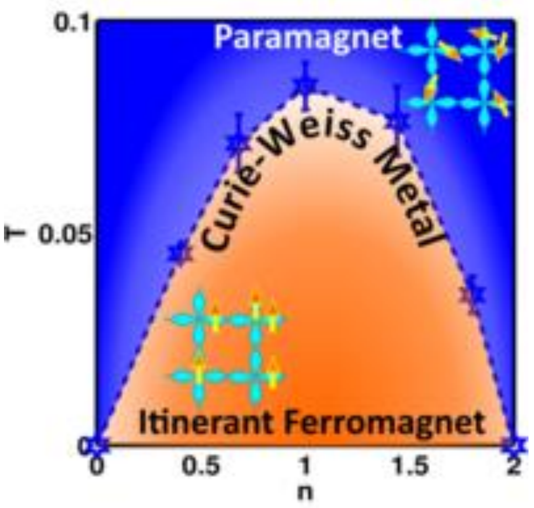

Nov 16 2017, Univ. British Columbia

Collaborators:

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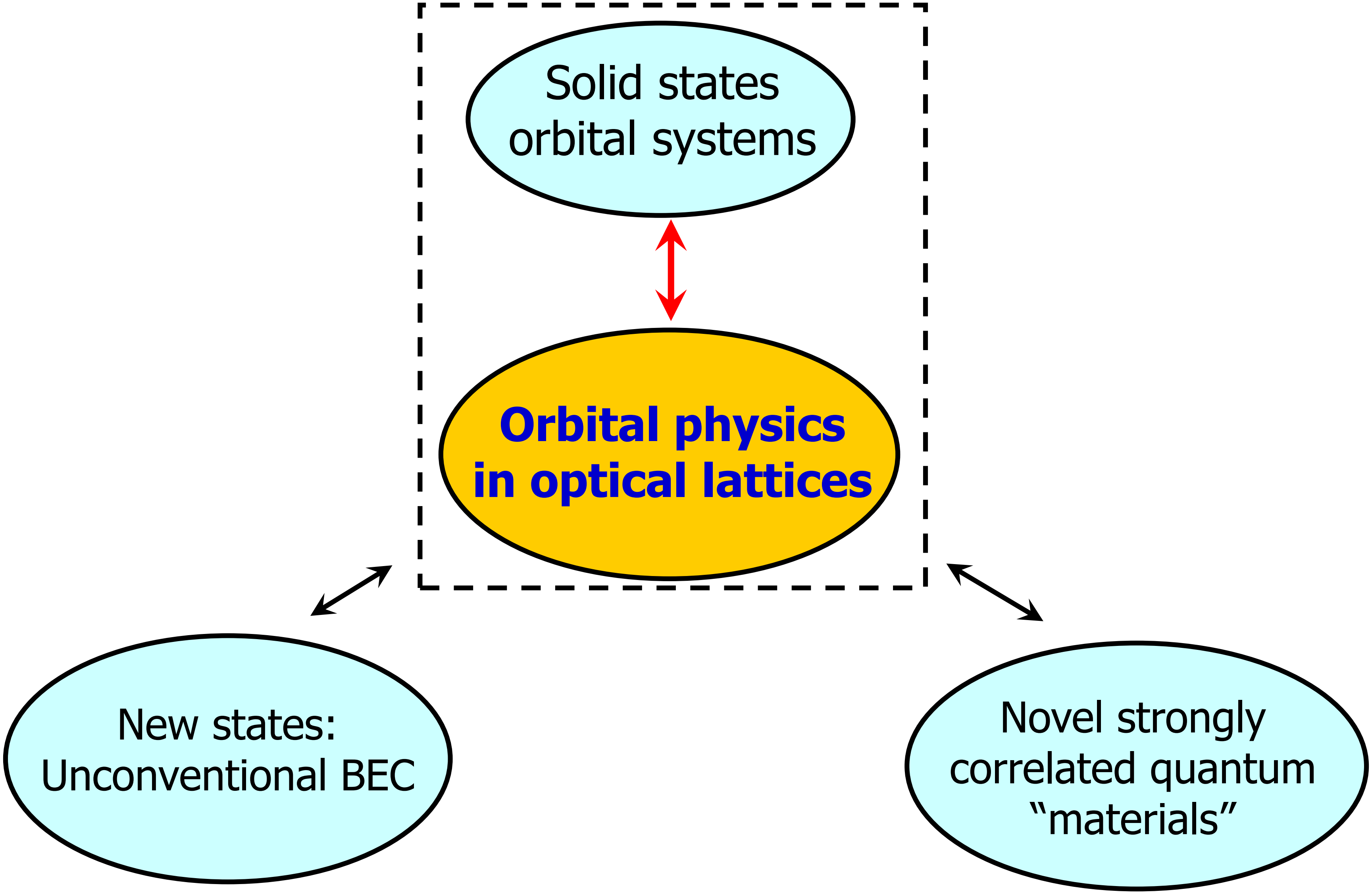
Zi Cai	(UCSD→ Innsbruck→ Shanghai Jiaotong)
Ellioit H. Lieb	(Princeton)

Thank S. Das Sarma, L. Balents, W. V. Liu for early collaborations, and G. W. Chern, H. H. Hung, R. Scalettar, C. W. Zhang, M. C. Zhang, S. Z. Zhang for collaboration on related projects.

Supported by NSF, AFOSR

Introduction

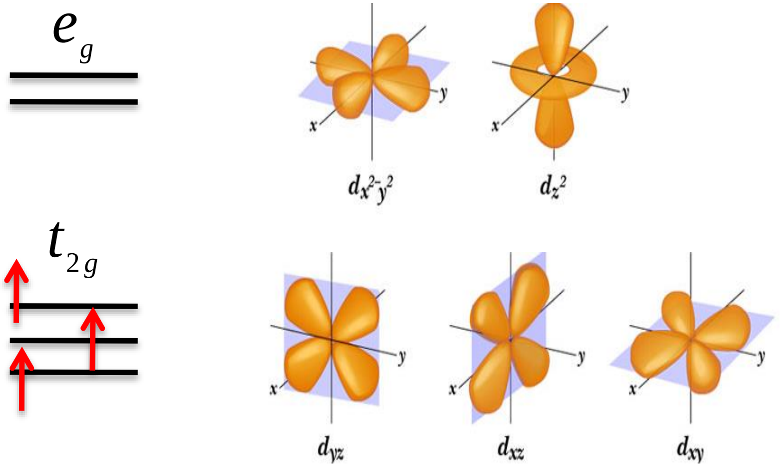


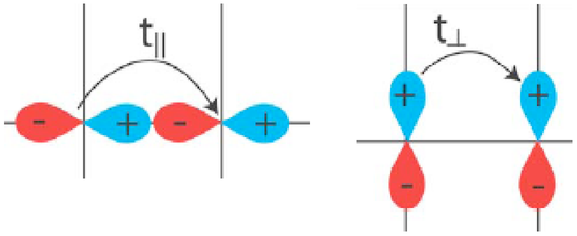
Electron orbitals: a degree of freedom independent of charge and spin

- Orbital degeneracy and **spatial anisotropy.**

d-orbitals: $d_{x^2-y^2}, d_{r^2-3z^2}, d_{xy}, d_{yz}, d_{xz}$

p-orbitals: p_x, p_y, p_z





σ-bond **π-bond**

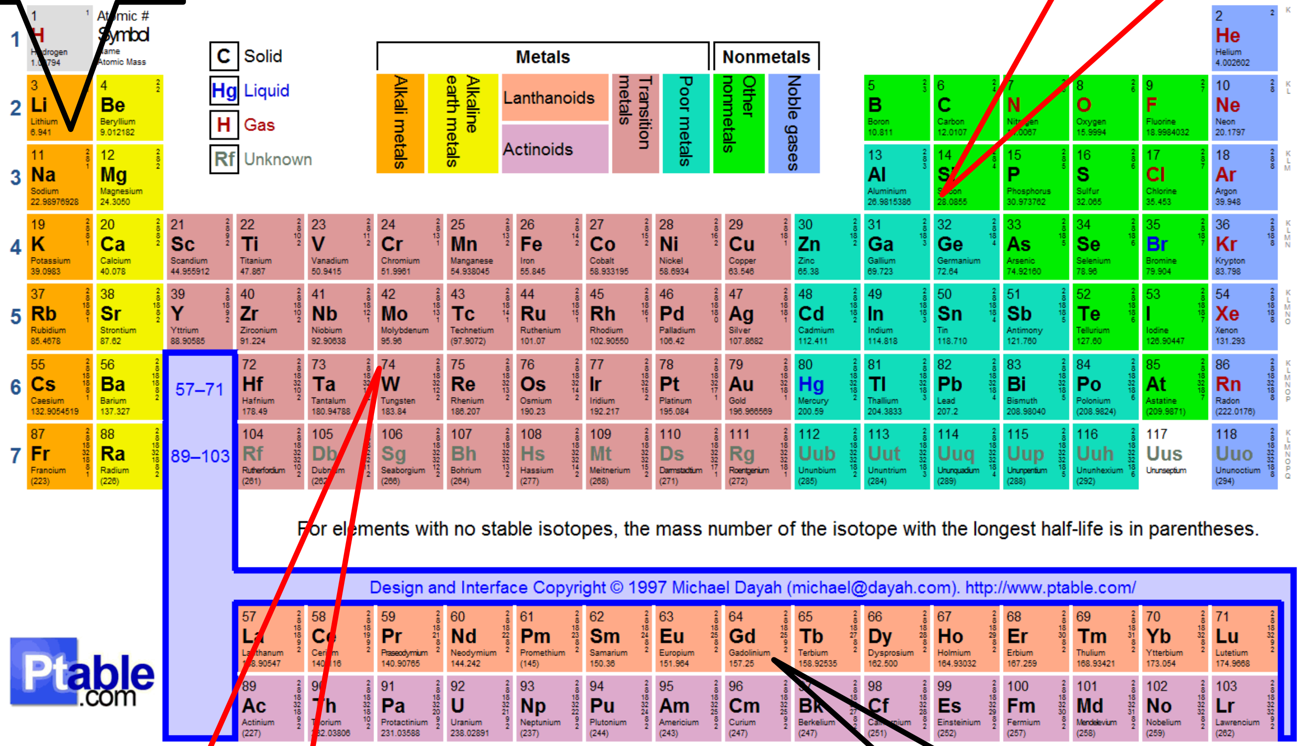
$$t_{//} >> t_{\perp}$$

Tokura, et al., science 288, 462, (2000).

Orbitals in solids

simple metal
(s-orbital)

semiconductor
(p-orbital)

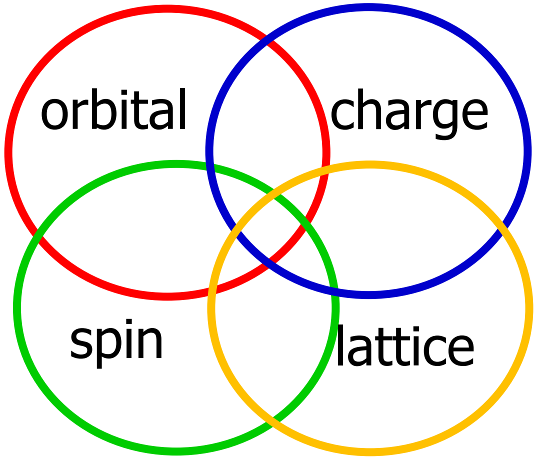


transition metal
(d-orbital)

Rare earth
(f-orbital)

Orbital physics in transition-metal oxides

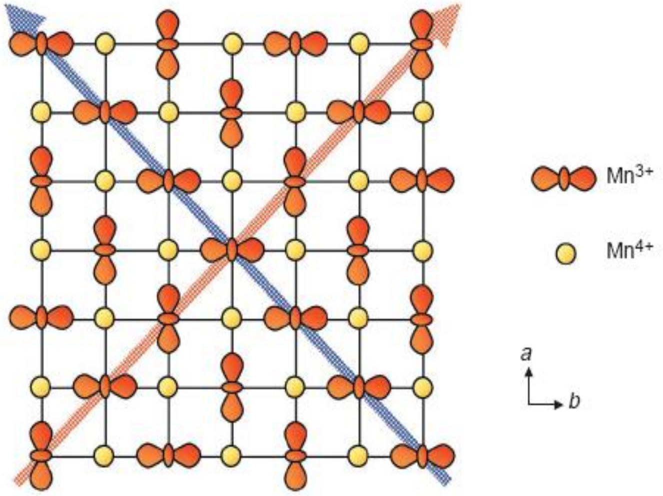
- Important to magnetism, superconductivity, and transport properties.


orbital

charge

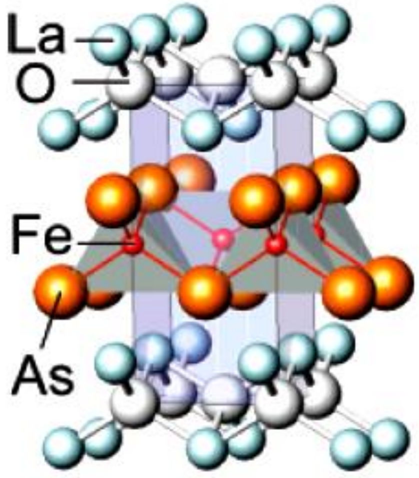
spin

lattice



Orbital stripe order:

Manganite: $La_{1-x}Sr_{1+x}MnO_4$

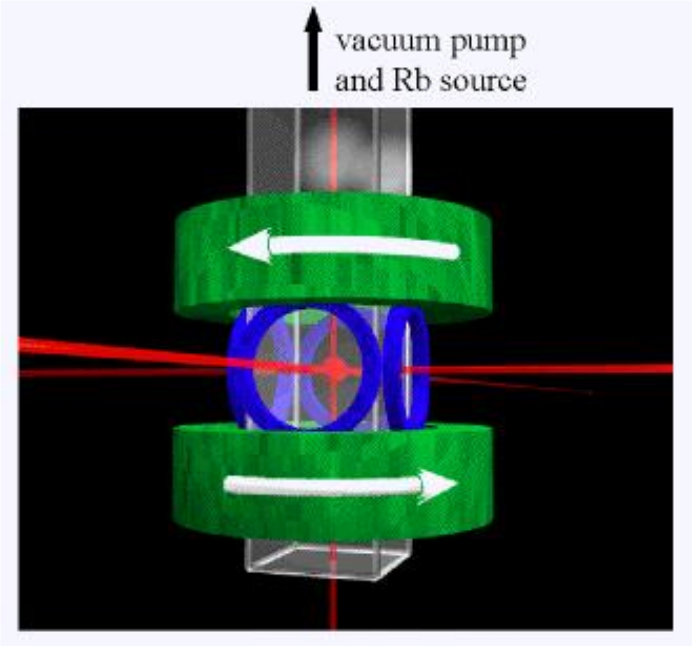


Iron-pnictide Supercond.

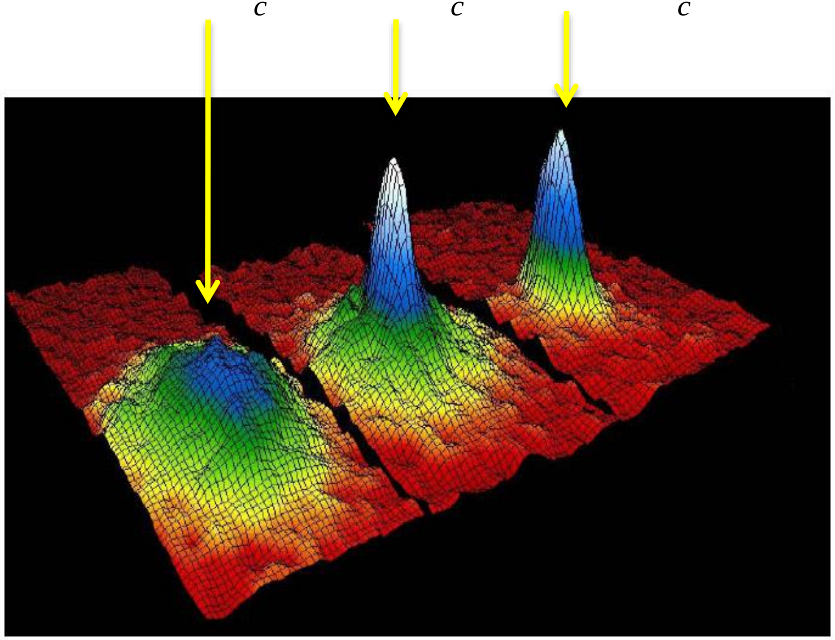
LaOFeAs

BEC of cold alkali atoms

- Dilute and weakly interacting boson systems.



$T > T_c$ $T < T_c$ $T << T_c$

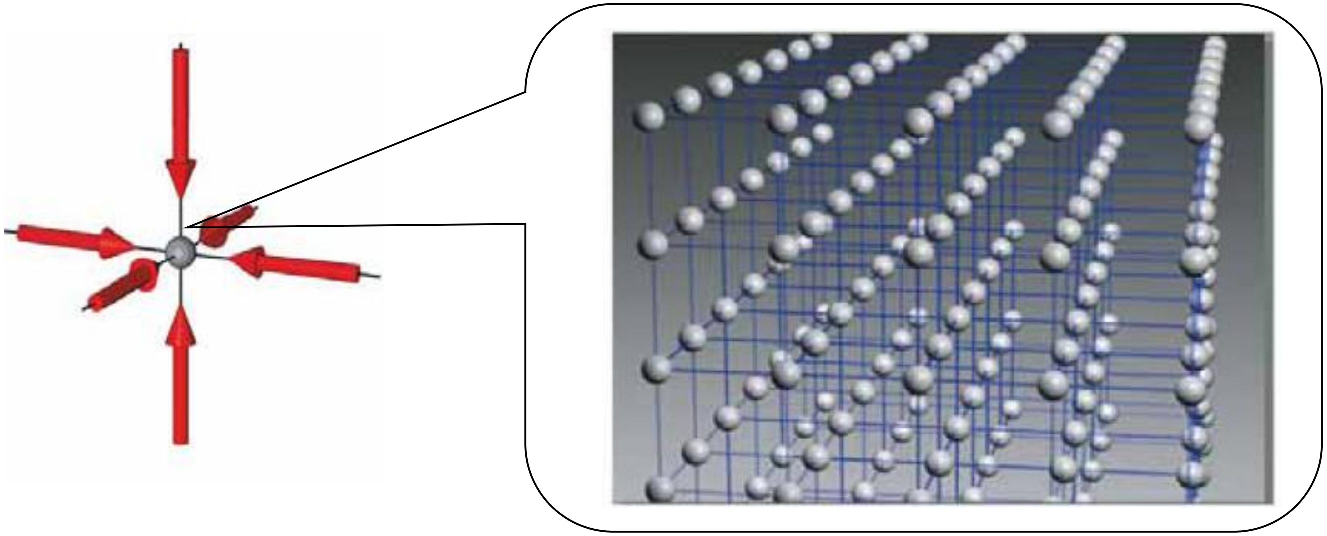


M. H. Anderson et al., Science 269, 198 (1995)

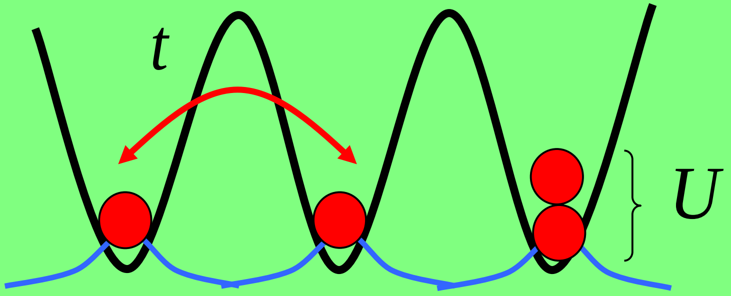
$$T_{BEC} \sim 1\mu K \quad n \sim 10^{14}\,\mathrm{cm}^{-3}$$

Time-of-flight spectra measure momentum space distribution.

Optical lattices: a new era of cold atom physics



- Interaction effects tunable by varying laser intensity.



t : inter-site tunneling
U: on-site interaction

A new direction: optical lattice orbital physics!

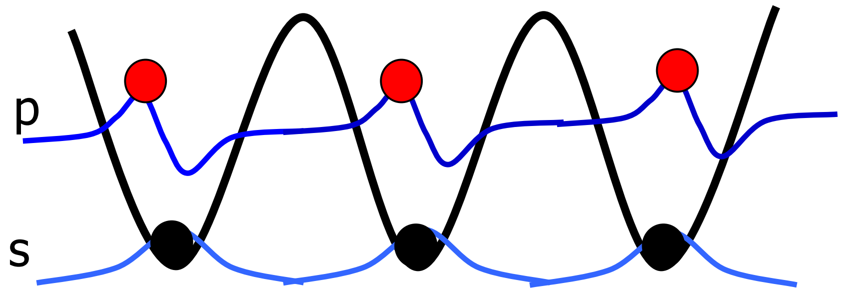
- Bosons/fermions in high-orbital bands.

Orbitals: energy levels (e.g. s, p) of each optical site.

Atoms play the role of electrons.

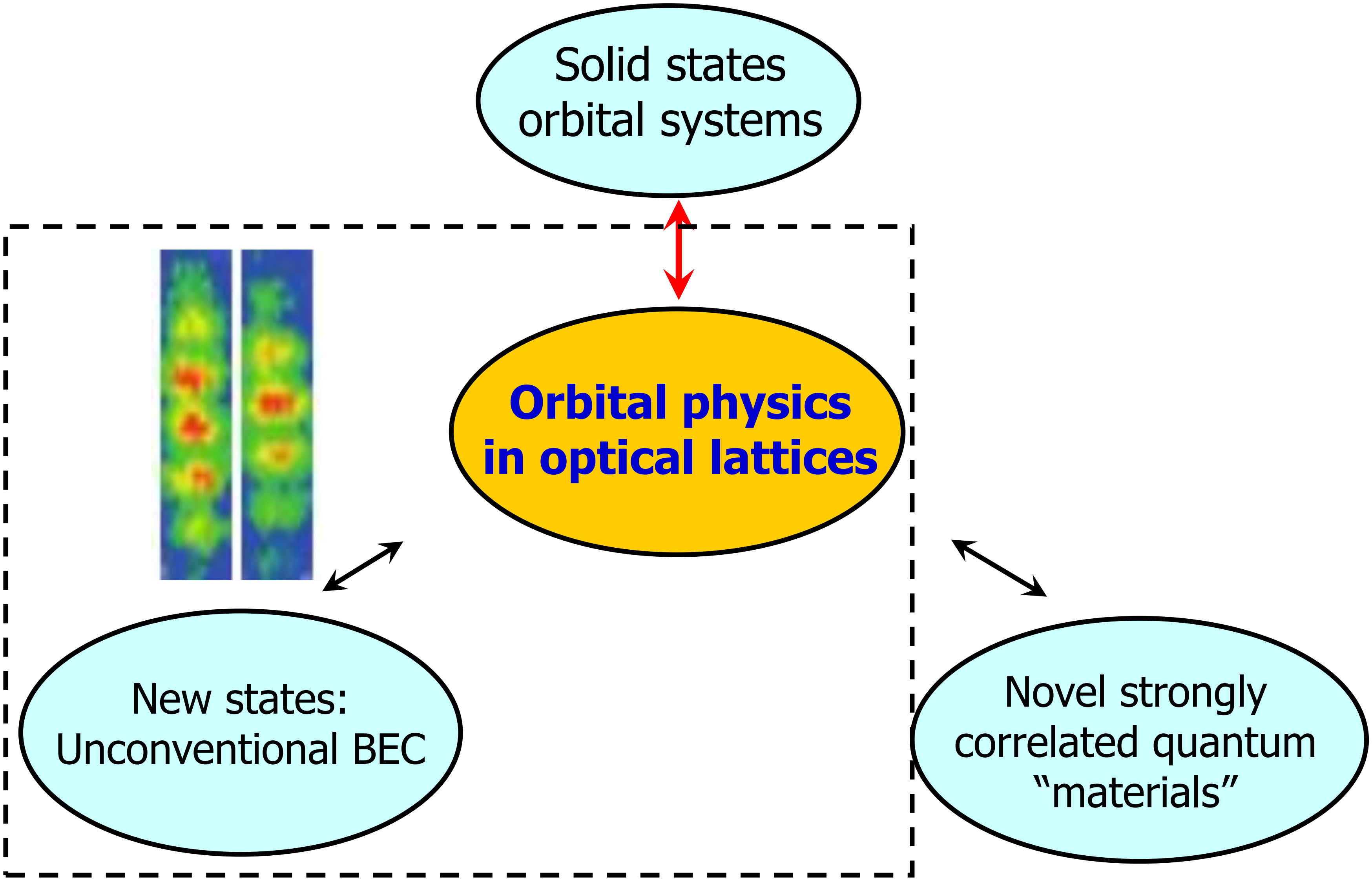
Good timing: pioneering experiments on orbital-bosons.

Square lattice (Mainz); double well lattice (NIST, Hamburg); polariton lattice (Stanford)



J. J. Sebby-Strabley, et al., PRA 73, 33605 (2006); T. Mueller et al., Phys. Rev. Lett. 99, 200405 (2007); C. W. Lai et al., Nature 450, 529 (2007).

Introduction



Solid states orbital systems

Orbital physics in optical lattices

New states:
Unconventional BEC

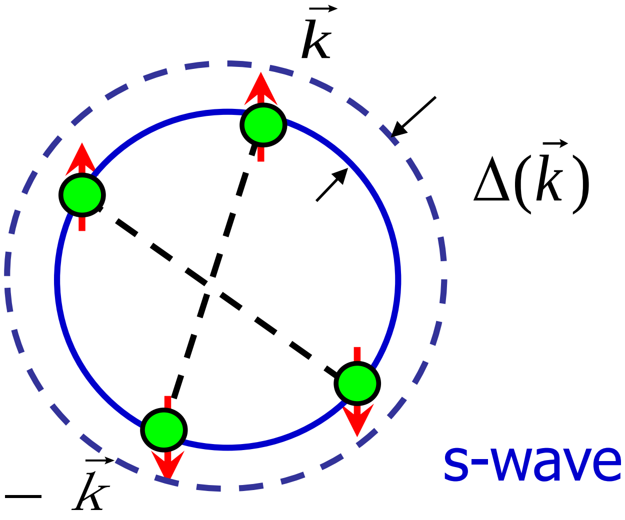
Novel strongly correlated quantum “materials”

Conventional *v.s.* unconventional superconductivity

- Cooper pair wavefunctions (WF):

$$\Psi(r_1,r_2)=\psi[(r_1+r_2)/2]\ \Delta(r_1-r_2)$$

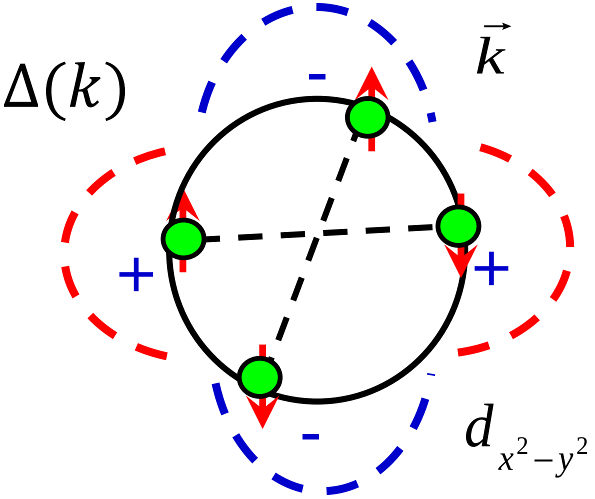
$$\Delta(r_1-r_2)=\int d\vec{k}e^{ik(\vec{r}_1-\vec{r}_2)}\Delta(\vec{k})$$



- Conventional: s-wave pairing symmetry.

- *Unconventional:* high partial wave symmetries (e.g. p, d, etc).

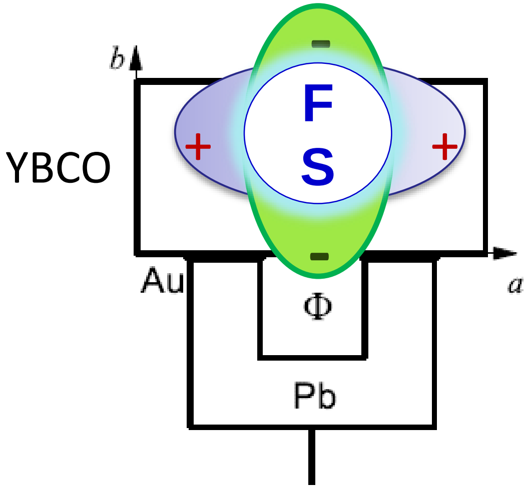
d-wave: high T_c cuprates.

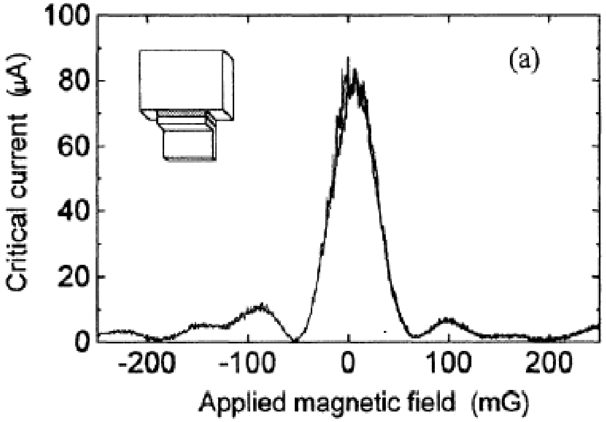


Phase-sensitive detection – interference

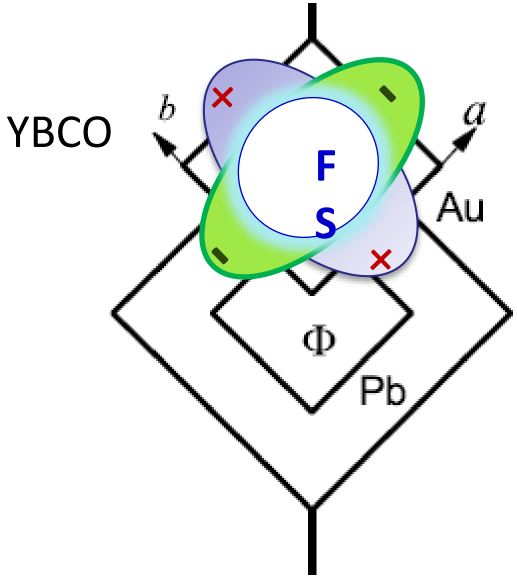
- Corner-Josephson π-junction for $d_{x^2-y^2}$

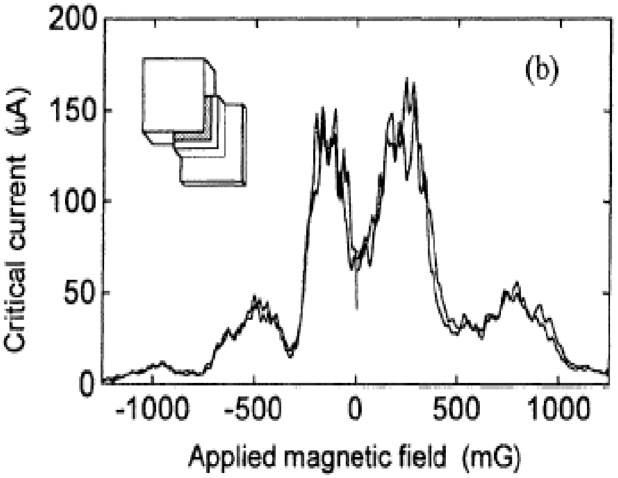
D. Van Harlingen, RMP (1995)





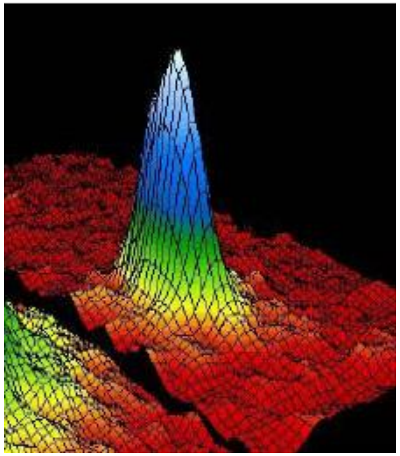
$$I_{max} = I_0 \frac{\sin(\pi\Phi/\Phi_0)}{\pi\Phi/\Phi_0}$$





$$I_{max} = I_0 \frac{\sin^2(\pi\Phi/2\Phi_0)}{\pi\Phi/\Phi_0}$$

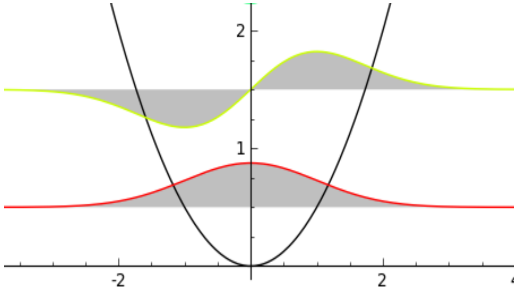
Conventional BEC: s-symmetry



- Conventional BEC (superfluid ^{4}He, cold alkali atom BEC, etc) -- **no-node, s-sym** .

- "no-node" theorem in single-particle QM.

$$\psi_G(\vec{r}) \geq 0$$

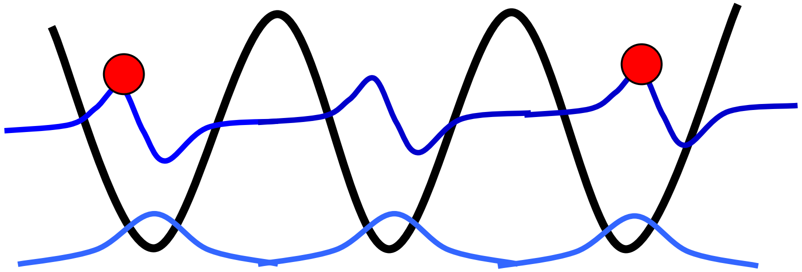


Generalization to boson many-body ground states!

- No-go! Unconventional symmetry (e.g. p, d) forbidden in ground states – requiring nodes.

Unconventional BECs in high-orbital bands

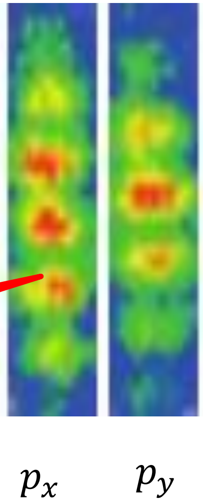
Meta-stable excited states:
Novel properties not existing in the ground states



Unconventional condensation symmetry and time-reversal symmetry breaking

C. Wu, Mod. Phys. Lett. 23, 1 (2009) (brief review).

Already seen in experiments ($p_x \pm ip_y$).



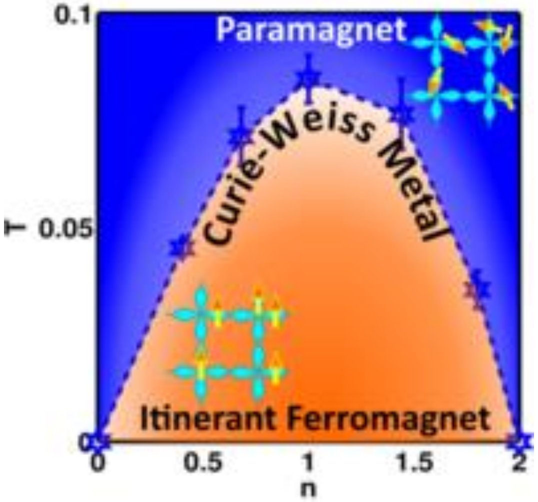
matter-wave interference

Hemmerich group Nature Physics 7, 147 (2011);
PRL 114, 115301 (2015).

Introduction

Solid states orbital systems

Orbital physics in optical lattices



New states:
Unconventional BEC

Novel strongly correlated quantum "materials"

Strongly correlated p-orbitals

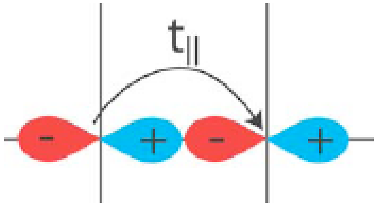
- Weakly correlated *p*-orbitals (e.g. semiconductors).

Not many *p*-orbital Mott-insulators and ferromagnets.

- p-orbitals: the strongest anisotropy.

- Combining **strong correlation + strong anisotropy** in optical lattices.

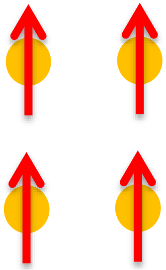
Itinerant FM,
topological states,
flat bands
unconventional Cooper pairing,
frustrated orbital exchange…



σ-bond

Magnetism: local moments vs. itinerant fermions

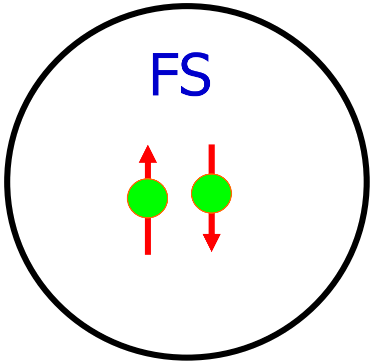
- Local Moments: non-mobile, no Fermi surfaces.



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

Curie-Weiss susceptibility

- Itinerant fermions: Fermi surfaces – much harder to form FM!

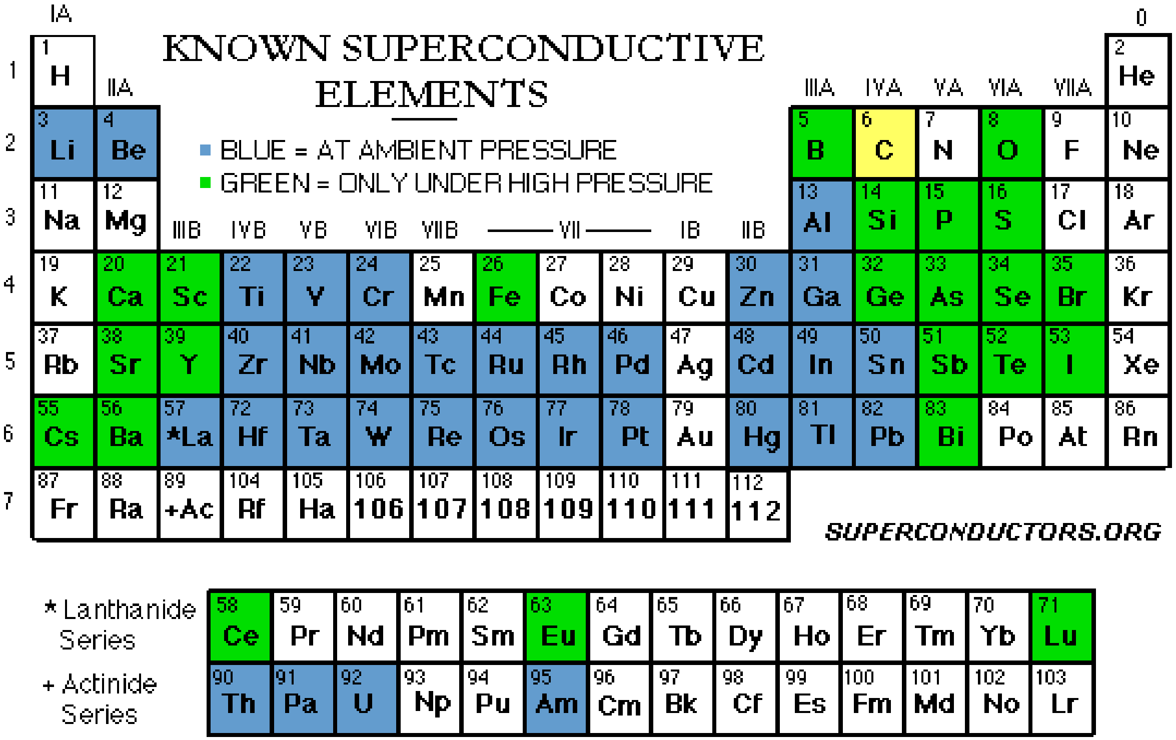


Pauli paramagnetism

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

N_0: density of states at the Fermi level

Itinerant FM v.s. superconductivity: which is rarer?



KNOWN SUPERCONDUCTIVE ELEMENTS

🟦 BLUE = AT AMBIENT PRESSURE
🟩 GREEN = ONLY UNDER HIGH PRESSURE

	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VII	VII	VII	IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
1	1 H																	2 He
2	🟦 3 Li	🟦 4 Be											🟩 5 B	🟨 6 C	7 N	🟩 8 O	9 F	10 Ne
3	11 Na	12 Mg											🟦 13 Al	🟩 14 Si	🟩 15 P	🟩 16 S	17 Cl	18 Ar
4	19 K	🟩 20 Ca	🟩 21 Sc	🟦 22 Ti	🟦 23 V	🟦 24 Cr	25 Mn	🟩 26 Fe	27 Co	28 Ni	29 Cu	🟦 30 Zn	🟦 31 Ga	🟩 32 Ge	🟩 33 As	🟩 34 Se	🟩 35 Br	36 Kr
5	37 Rb	🟩 38 Sr	🟩 39 Y	🟦 40 Zr	🟦 41 Nb	🟦 42 Mo	🟦 43 Tc	🟦 44 Ru	🟦 45 Rh	🟦 46 Pd	47 Ag	🟦 48 Cd	🟦 49 In	🟦 50 Sn	🟩 51 Sb	🟩 52 Te	🟩 53 I	54 Xe
6	🟩 55 Cs	🟩 56 Ba	🟦 57 *La	🟦 72 Hf	🟦 73 Ta	🟦 74 W	🟦 75 Re	🟦 76 Os	🟦 77 Ir	🟦 78 Pt	79 Au	🟦 80 Hg	🟦 81 Tl	🟦 82 Pb	🟩 83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 +Ac	104 Rf	105 Ha	106	107	108	109	110	111	112						

SUPERCONDUCTORS.ORG

* Lanthanide Series	🟩 58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	🟩 63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	🟩 71 Lu
+ Actinide Series	🟦 90 Th	🟦 91 Pa	🟦 92 U	93 Np	94 Pu	🟦 95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

FM elements

Fe	Co	Ni

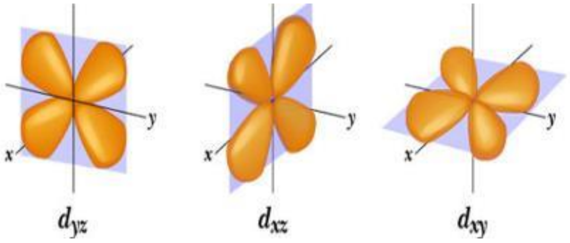
Gd

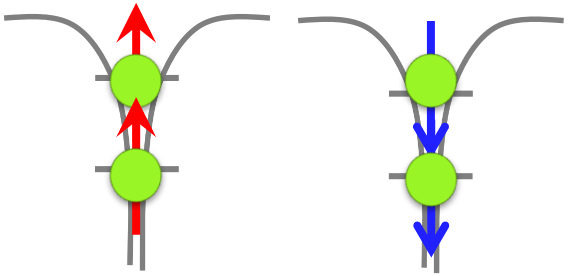
Dy

Itinerant FM: A long-standing strong correlation problem

Hund's coupling $\neq$ global FM

- Electron/hole spins add up when filling in degenerate orbitals.

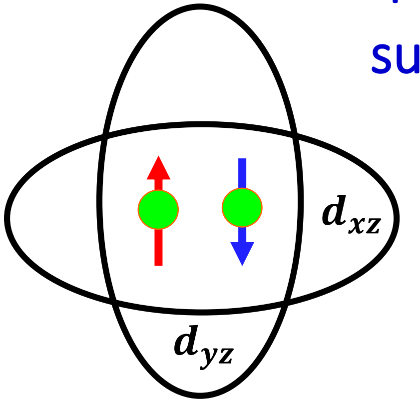




- Most FM metals have orbital degeneracy and Hund's coupling.

- Local vs. global:

Hund's rule usually cannot polarize the entire lattice!

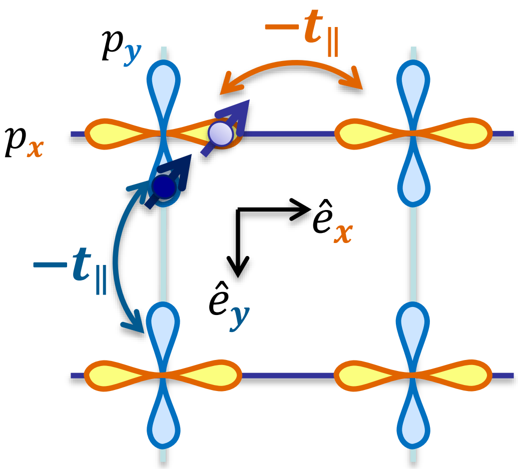


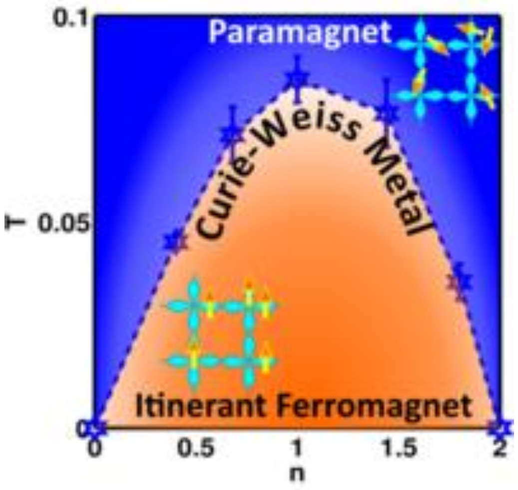
Sufficient condition for Hund’s rule assisted itinerant FM

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

theorem proofs

quan. Monte-Carlo simulations
(sign-problem free)



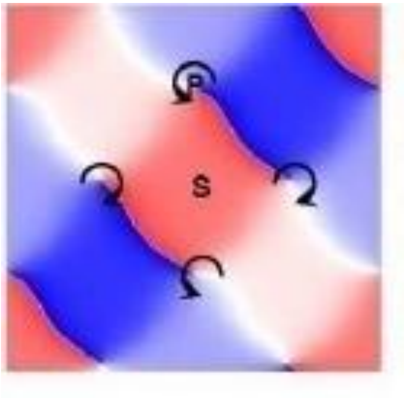


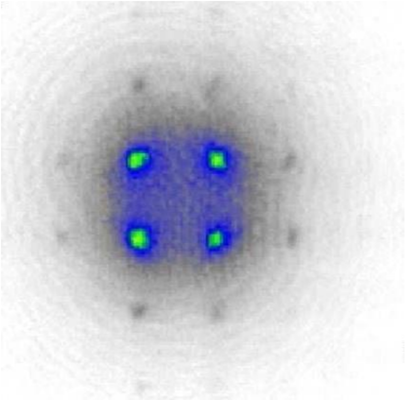
Yi Li, E. H. Lieb, C. Wu, Phys. Rev. Lett. 112, 217201 (2014).

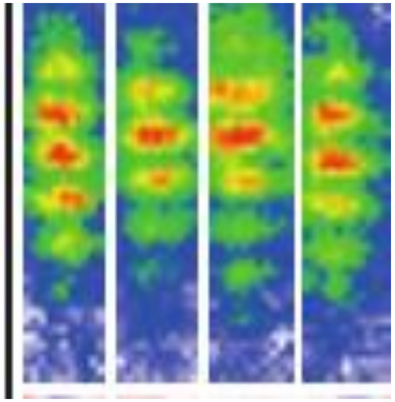
S. Xu, Yi. Li, and C. Wu, Phys. Rev. X 5, 021032, (2015).

Outline

- Orbital bosons (unconventional **symmetry**): $p_x \pm ip_y$ BECs beyond the “no-node” theorem **– already observed!**







- Orbital fermions: Itinerant FM, a long-standing problem – a **non-perturbative** study.

The “no-node” theorem (Perron-Frobenius)

- Many-body **ground-state wavefunctions** of bosons are **positive-definite**.

$$\psi(r_1, r_2, \ldots r_n) \geq 0$$

- A general property of the ground states:

Laplacian kinetic energy (no rotation).

Arbitrary single-particle potential (with lattice or not) .

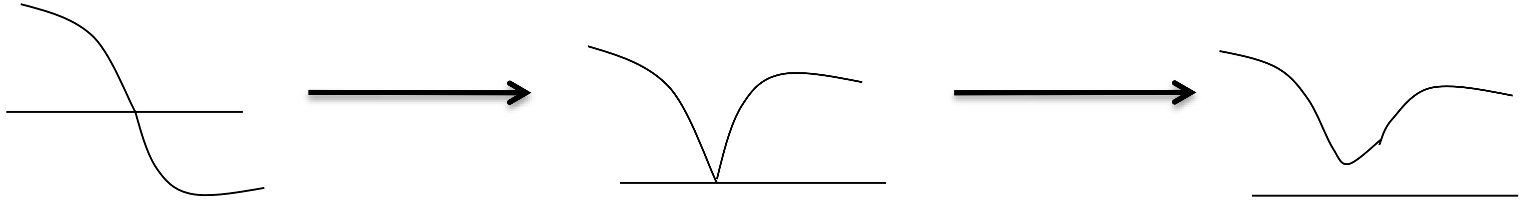
Coordinate-dependent interactions.

$$H = \sum_{i=1}^{N} -\frac{\hbar^2 \nabla_i^2}{2M} + \sum_{i=1}^{N} U_{ex}(\vec{r}_i) + \sum_{i<j}^{N} V_{\text{int}}(\vec{r}_i - \vec{r}_j)$$

Proof

Feynman, Statistical Mechanics

$\psi(r_1, r_2, \ldots r_n)$ $\qquad$ $|\psi(r_1, r_2, \ldots r_n)|$ $\qquad$ $\phi(r_1, r_2, \ldots r_n) > 0$



$$\langle \psi | H | \psi \rangle = \int dr_1 \ldots dr_n \ \frac{\hbar^2}{2m} \sum_{i=1}^{n} \ |\nabla_i \psi(r_1, \ldots r_n)|^2 + |\psi(r_1, \ldots r_n)|^2 \sum_{i=1}^{n} U_{ex}(r_i)$$

$$+ |\psi(r_1, \ldots r_n)|^2 \sum_{i<j} V_{\text{int}}(r_i - r_j)$$

- Generally speaking not for fermions, but possible under certain conditions.

“no-node” consequences

- Valid for superfluid, Mott states, super-solids, etc.

- Constraint on bosons: Time-reversal symmetry cannot be spontaneously broken!

Complex-valued wavefunctions → positive-definite distr.

TR: $\Psi(r_1, r_2 \ldots, r_n) \rightarrow \Psi^*(r_1, r_2 \ldots, r_n)$

- Goal: Seek for unconventional BECs beyond “no-node” paradigm and breaking TR symmetry!

C. Wu, Mod. Phys. Lett. 23, 1 (2009).

Unconventional (UBEC) – metastable states

- The condensate $\Psi(r)$ possesses a non-s-wave symmetry → Nodal lines or points beyond "no-node".

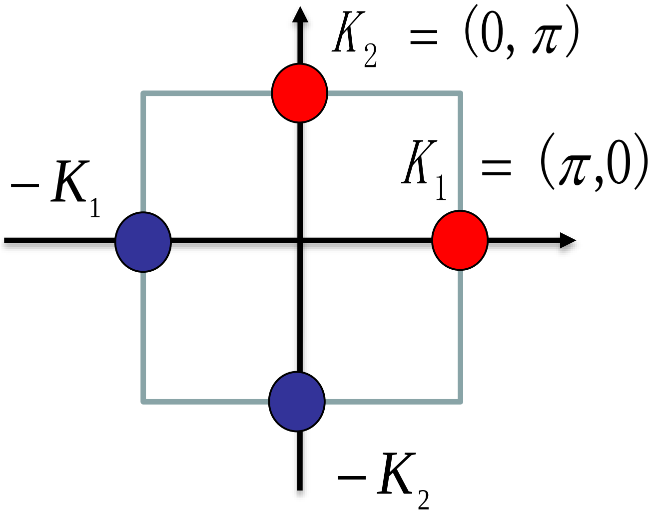
- Complex, spontaneous time-reversal symmetry breaking.

- e.g. the *p*-orbital bands with degenerate minima.

$$\Psi(\vec{r}) = \Psi_{K1}(\vec{r}) + i\Psi_{K2}(\vec{r})$$

$$R_{90^0}\Psi(\vec{r}) = \Psi_{-K_2}(\vec{r}) + i\Psi_{K_1}(\vec{r}) = -\Psi_{K_2}(\vec{r}) + i\Psi_{K_1}(\vec{r})$$

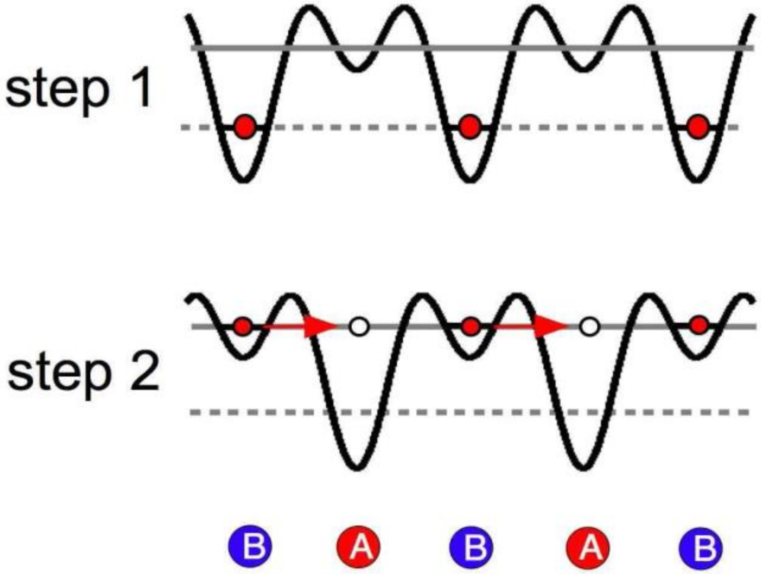
$$= i(\Psi_{K_1}(\vec{r}) + i\Psi_{K_2}(\vec{r}))$$



C. Wu, Mod. Phys. Lett. 23, 1(2009).
W. V. Liu and C. Wu, PRA 2006.

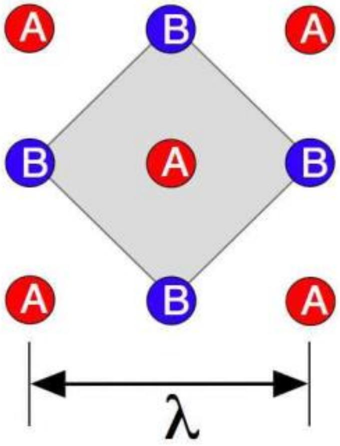
p+ip UBEC:

Observed! Double-well lattice experiment

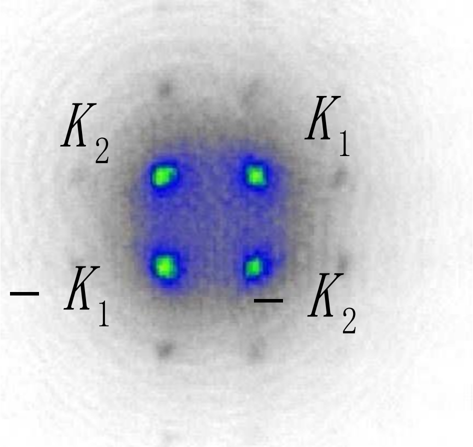


$$\theta < \frac{\pi}{2}$$

$$\theta > \frac{\pi}{2}$$



- Condensate wavecters (K_1, K_2): half values of reciprocal lattice vectors.

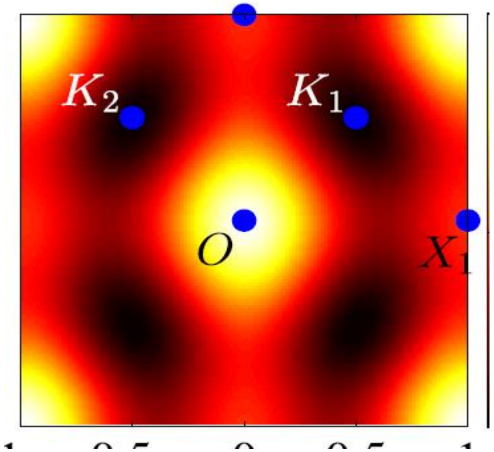


Wirth, Oelschlaeger, **Hemmerich,** Nature Physics 7, 147 (2011).

Experiment lattice – shallow (weakly interacting)

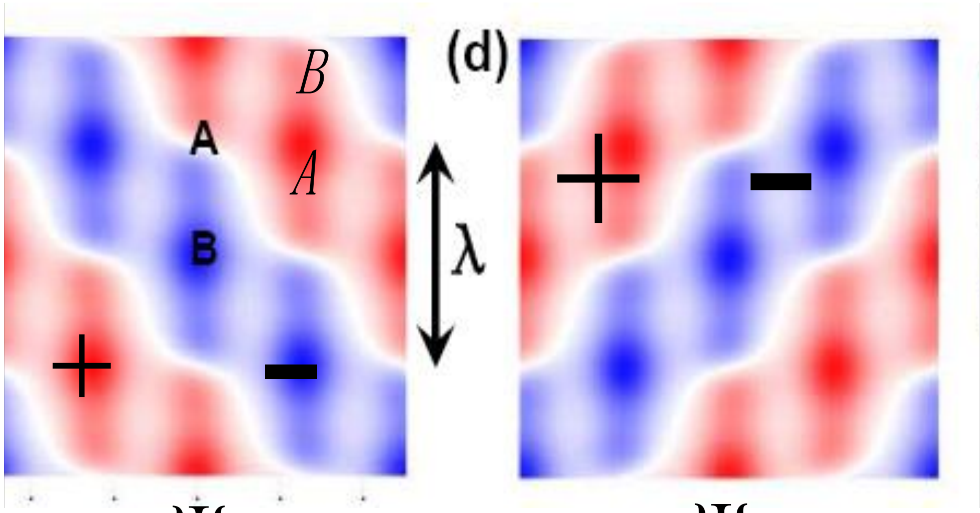
- Energy minima $K_{1,2} \equiv -K_{1,2}$ --- (mod reciprocal lattice vectors).

Zi Cai, C. Wu, PRA, 84,033635 (2011)



$$K_{1,2} = (\pm\frac{\pi}{2a}, \frac{\pi}{2a})$$

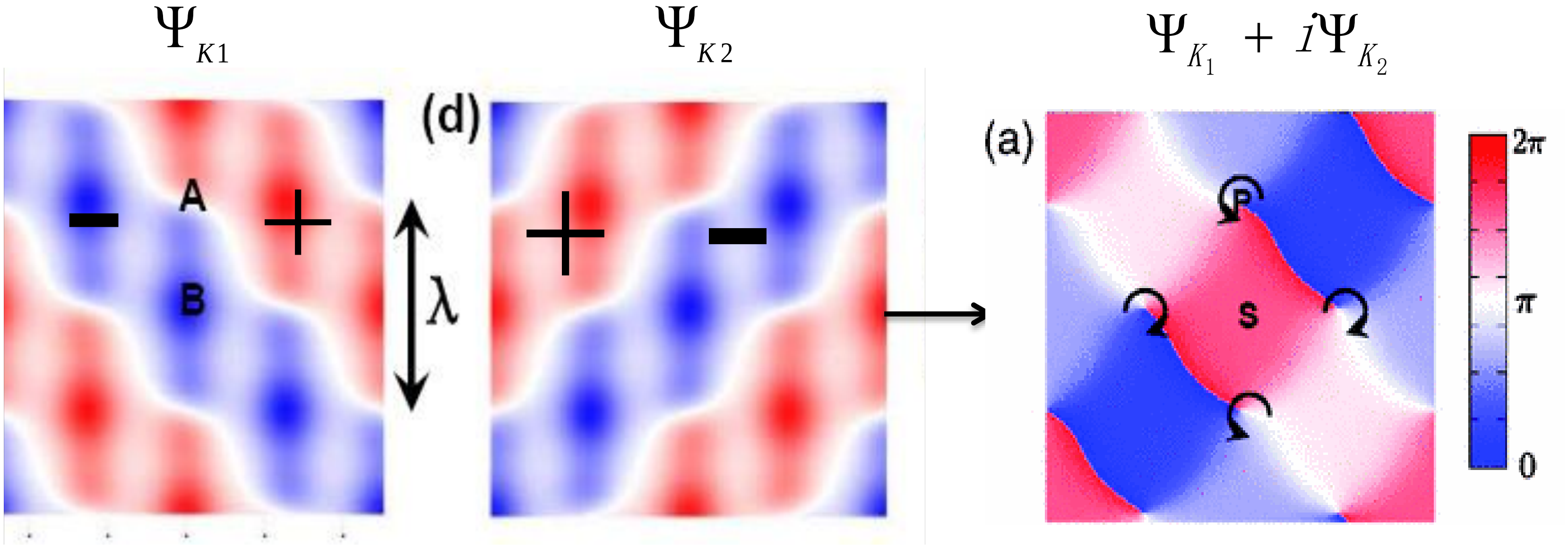
- Real space distribution of $\Psi_{K_{1,2}}(r)$



Ψ_{K1} Ψ_{K2}

- Standing waves (real).
- Nodal lines pass A-sites (p).
- Antinode B-sites (s).

Nodal points (complex) v.s. lines (real)



- Real $\Psi_{K_1} \pm \Psi_{K_2}$: nodal **lines**

- **Complex $\Psi_{K_1} \pm i\Psi_{K_2}$**: nodal **points** at crossings → **more uniform (favored by repulsive interaction)**

- Phase winding: **vortex-anti-vortex lattice.**

- Spontaneous TR symmetry breaking.

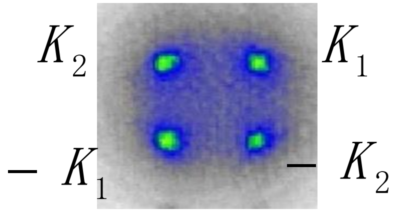
See the "i" -- Matter-wave interference

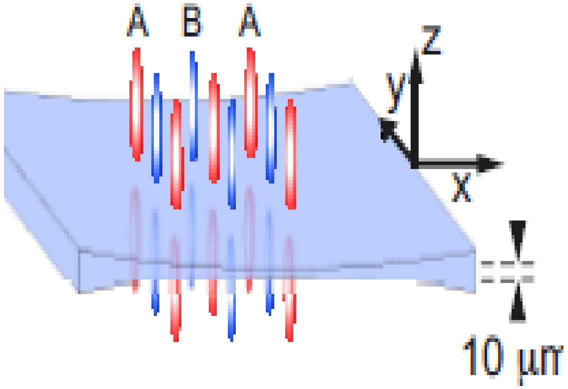
Hemmerich group PRL 114, 115301 (2015).

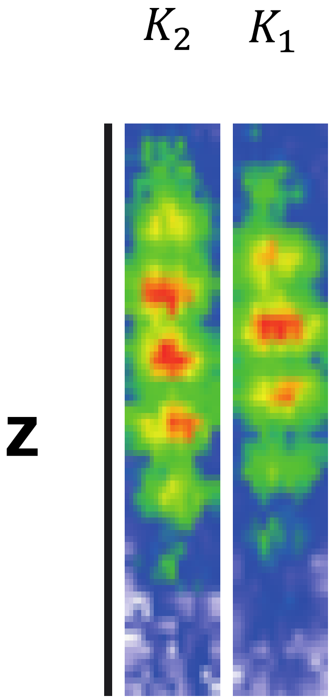
25ms expansion
Interference along the z-axis

Upper space

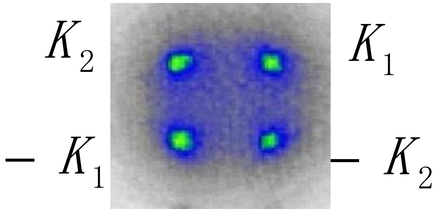
$$\Psi_{K_1} + i\Psi_{K_2}$$







$$\Psi_{K_1} - i\Psi_{K_2}$$



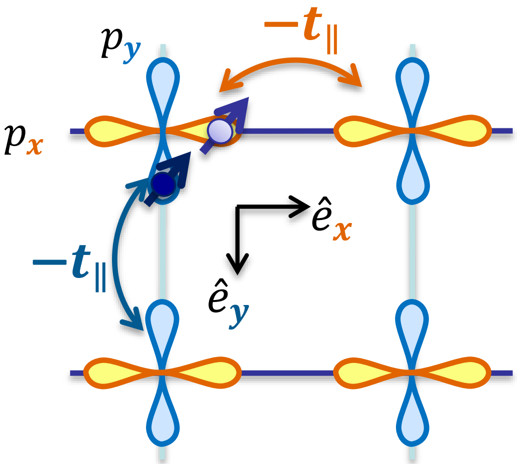
Lower space

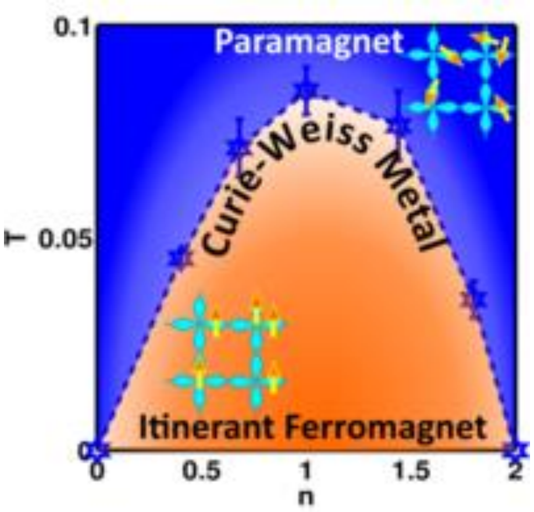
XY

Outline

- Orbital bosons (unconventional symmetry): p_x+ip_y BECs beyond the "no-node" theorem – already observed!

- Orbital Fermions (strong **correlation**): Itinerant FM, a long-standing problem – a **Non-perturbative** study.





The early age of ferromagnetism

The magnetic stone attracts iron.

慈 (ci) 石(shi) 召(zhao) 铁(tie)

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

慈 (loving, kind, merciful, gentle): 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.

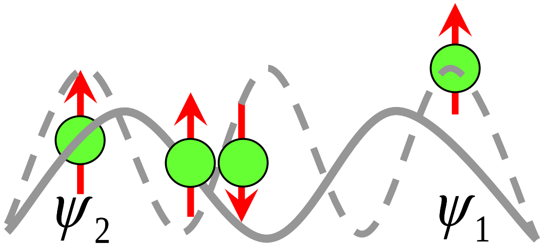
----*De Anima*, Aristotle (384-322 BC)

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

Origin of itinerant FM – fermion exchange

E. C. Stoner

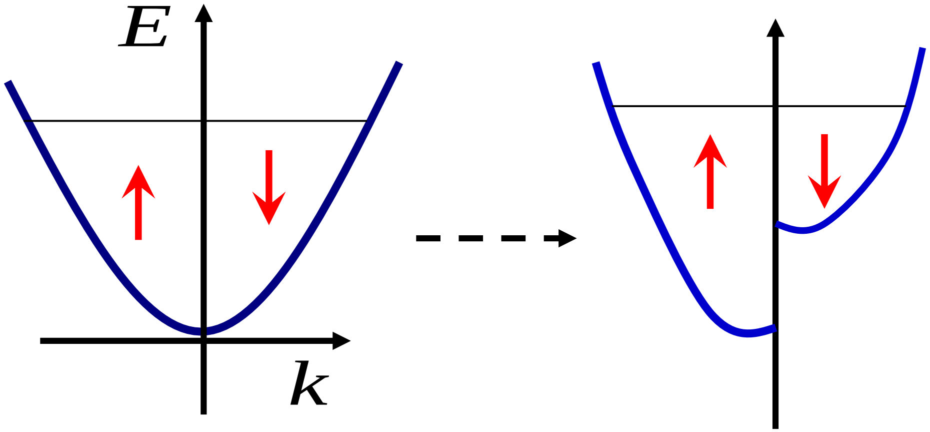
- **Fermi statistics → Slater determinant-like wavefunction → direct exchange.**



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

- **Stoner criterion:**

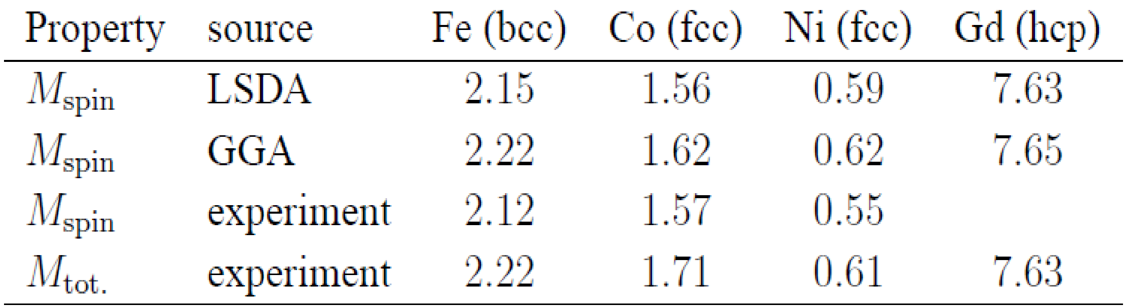
$$UN_0 > 1$$



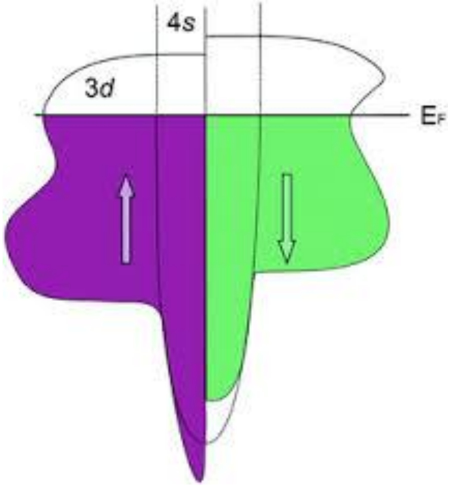
U – average interaction strength; N_0 – density of states at the Fermi level

Density functional (Kohn-Sham) theory

- Accurate on ground state magnetic polarization.



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	
$M_{\mathrm{tot.}}$	experiment	2.22	1.71	0.61	7.63



- Correlations partially contained in $V_{xc}(r)$, but wavefunctions remain Slater-determinant type.

- Thermal fluctuations difficult to handle -- Curie temperatures overestimated.

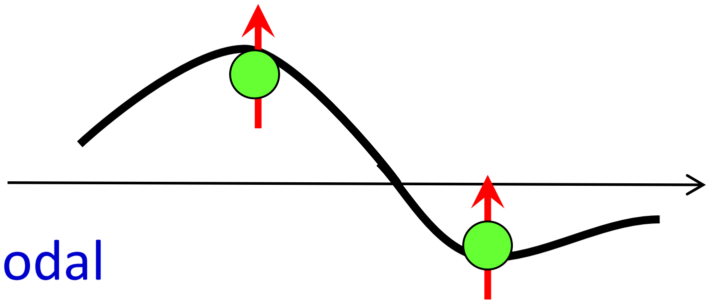
Correlations – Non-perturbative studies desired!

- Unpolarized but correlated WFs → less kinetic energy cost.

- **No go**! Two-electron ground states are non-magnetic.

triplet

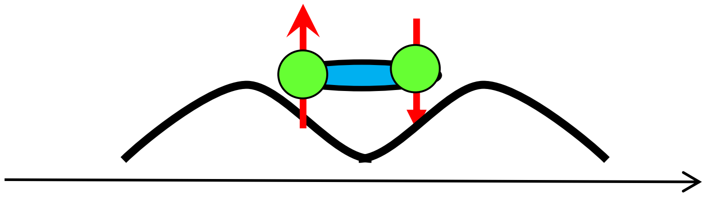
$\phi_{asym}(x_1 - x_2) \otimes |\uparrow\rangle_1 |\uparrow\rangle_2$



nodal

singlet

$\phi_{sym}(x_1 - x_2) \otimes (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$



(ground state) nodeless

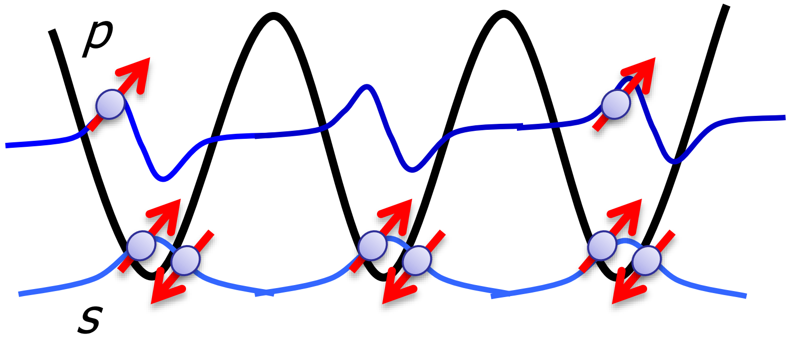
- **No go!** Absence of itinerant FM in 1D – Lieb & Mattis theorem.

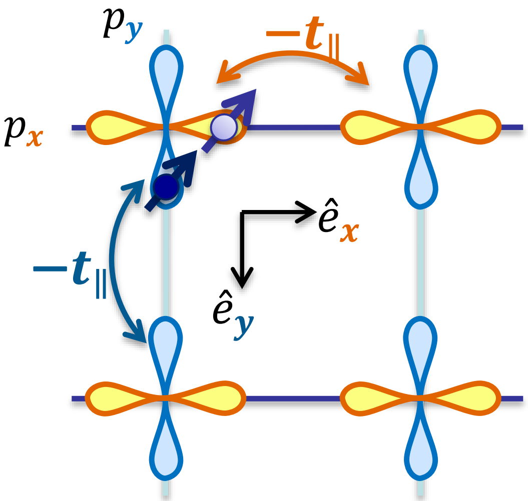
Previous exact results (e.g. Nagaoka FM, flat-band FM) do not really set up a stable phase of itinerant FM.

We need a **simple** and **quasi-realistic** model:

- A ground state FM **phase** of **itinerant fermions without ambiguity.**
- A controllable reference point for studying the **Curie-Weiss metal phase**.
- Hint for the driving force of itinerant FM?

Prediction for test: FM in p-orbitals (or d_{xz}/d_{yz})

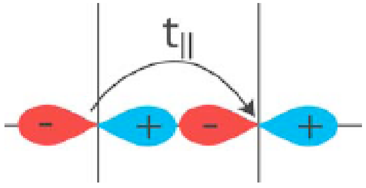




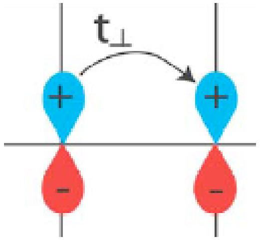
- p-orbital band: 1d-like band structure.
- Tunable interactions

$$t_\parallel \gg t_\perp$$

- Our prediction: itinerant FM phase appears at $t_\perp = 0$ in the strong coupling regime.



σ-bond

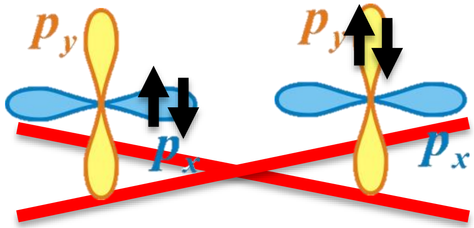


π-bond

Multi-orbital onsite (Hubbard) interactions

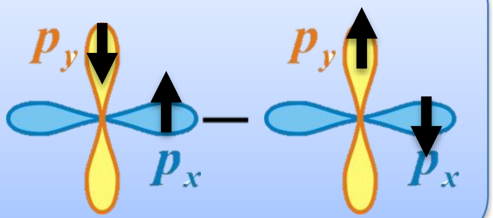
- Intra-orbital repulsion $U \to \infty$.

Intra-orbital
singlet projected out



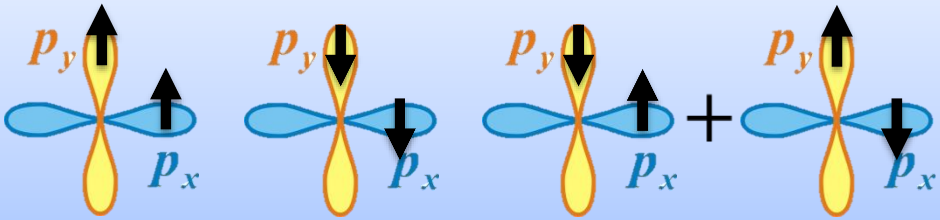
- Inter-orbital **Hund's coupling** J>0, and repulsion V.

Inter-orbital
singlet



$$E = J + V$$

3-fold
triplet



$$E = V$$

The orbital-assisted Itinerant FM

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

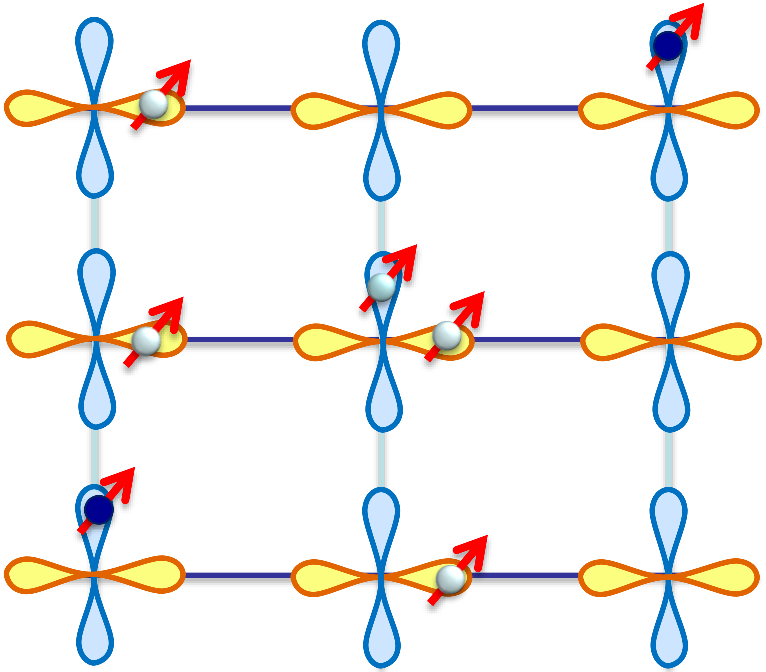
- **An entire FM phase**: valid at any generic filling, any value for J>0, and V.

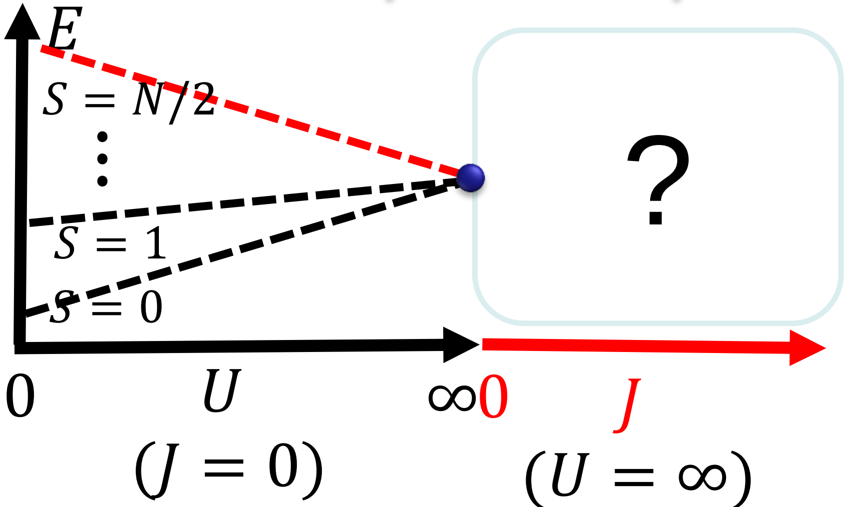
- Free of quantum Monte-Carlo (QMC) sign problem at any filling – a rare case for fermions.

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

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

Hund’s rule assisted global FM





- Intra-chain physics at $U \to \infty$: infinite degeneracy.

- Inter-chain physics (J): Hund’s coupling lifts the degeneracy by aligning spins → global FM.

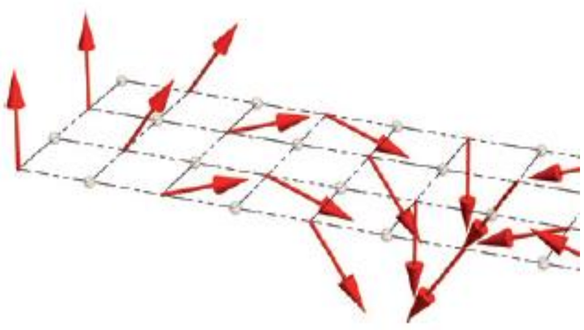
- 2D FM coherence in spite of 1D band structure (the total spin in each chain is not conserved).

Open question: Curie-Weiss metal

Local-moment-like: Unnatural for metals with **Fermi surfaces.**

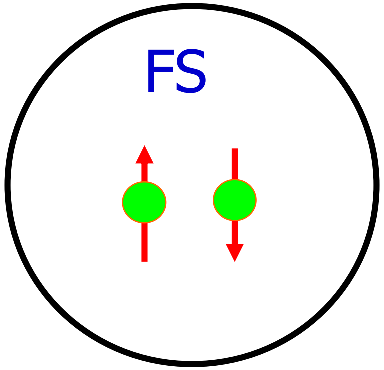
$$\chi = \frac{A}{1 - T / T_0} \qquad T_0 < T \ll T_F$$

- The paramagnetic phase is NOT simple: domain fluctuations!



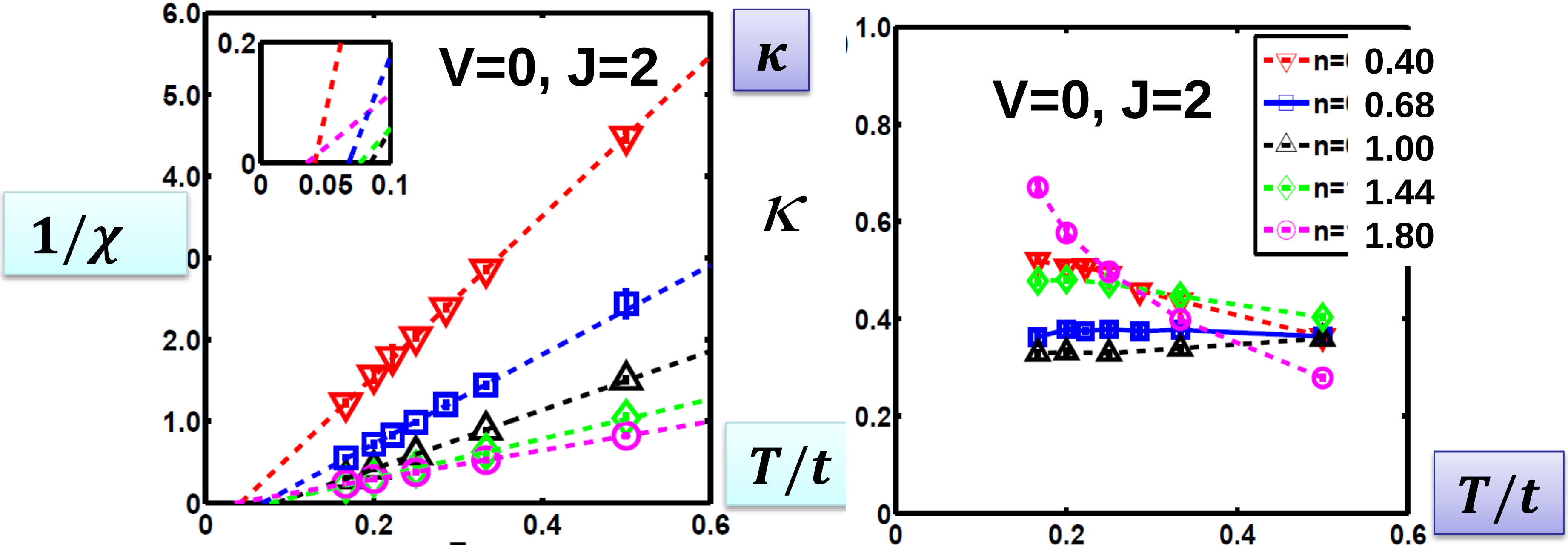
$T > T_0$

$\neq$



- Non-perturbative study – sign-problem free QMC simulations, asymptotically exact.

The Curie-Weiss metal



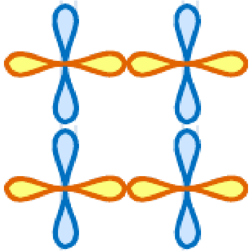
- Local moment-like: Curie-Weise (spin incoherent).

$$\chi = C/(T - T_0) \qquad T_0 << T_{ch}$$

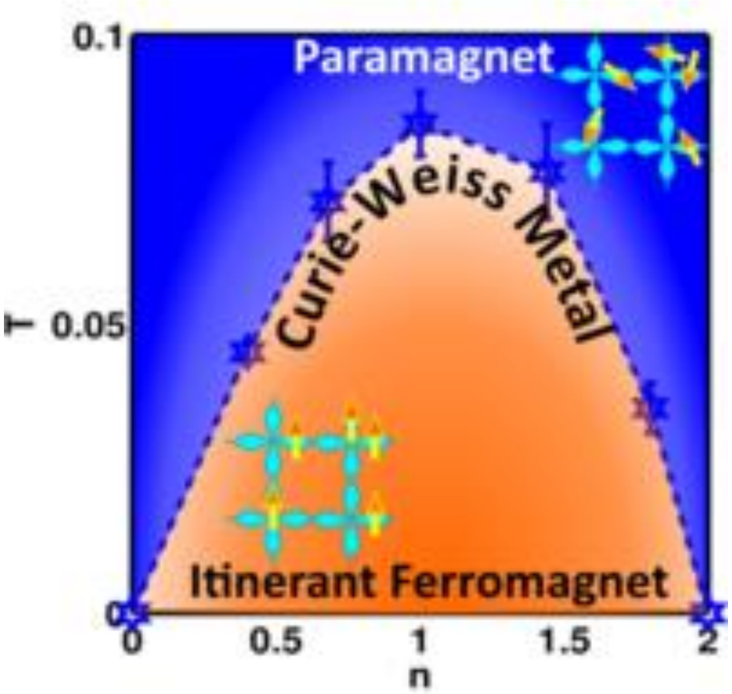
- Metalic (itinerancy): κ satures at $T < T_{ch}$, T_{ch} is roughly the kinetic energy scale.

QMC: Curie-Weiss temperature v.s filling (V=0)

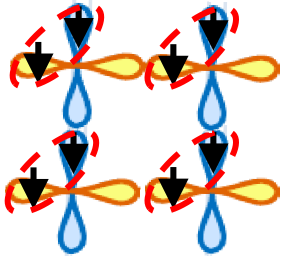
T_0



$$\chi = \frac{C}{T - T_0}$$



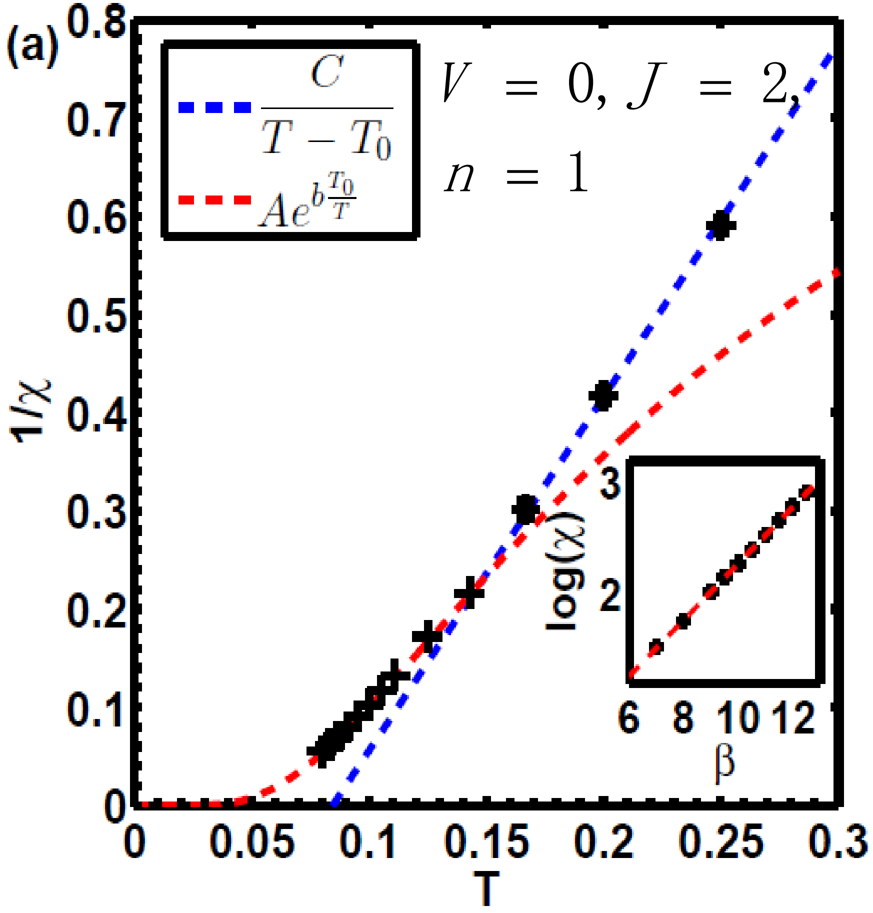
V=0, J=2



n

- T_0→0 at both n→0 (particle vaccum), and n→ 2 (hole vaccum).
- T_0 reaches the maximum at n~ 1 : $T_{0,max} \approx 0.08 t_{\parallel}$.

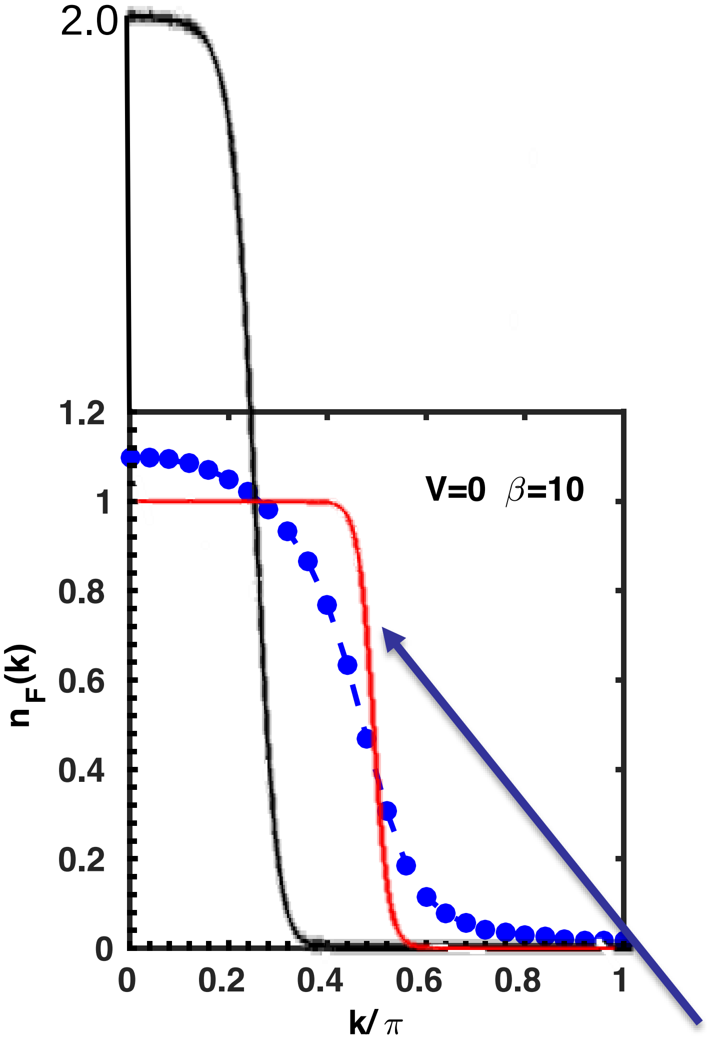
Deviation from the Curie-Weiss law (critical region)



- **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.**

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

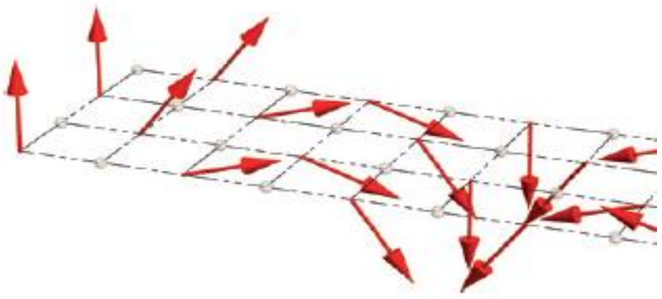
Fermi distribution $n_F(k)$ – non-pertubative result



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 Curie-Weiss metal phase**



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

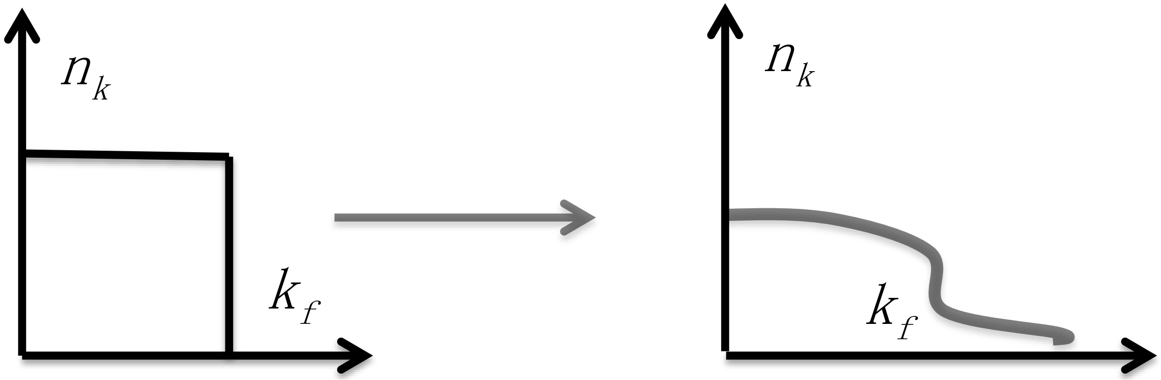
Hints for mechanism for itinerant FM

- Why is FM 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 (c.f. J. Hirsch's works).**



Summary: orbital physics with cold atoms

- Novel orbital physics not easily accessible in solid state systems.
- Unconventional BEC beyond the “no-node” theorem.
- A novel system for itinerant ferromagnetism – a non-perturbative study.