

# Ferromagnetism

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The Ohio State University

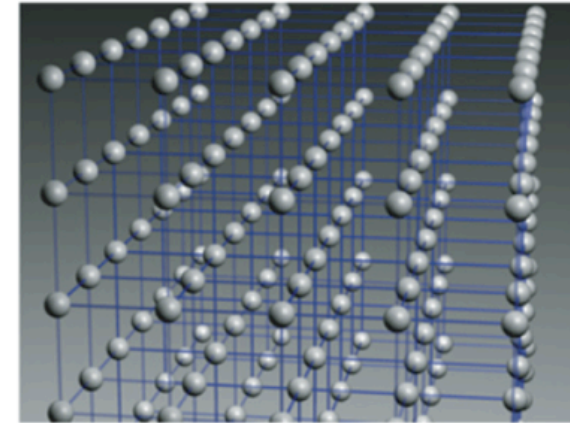
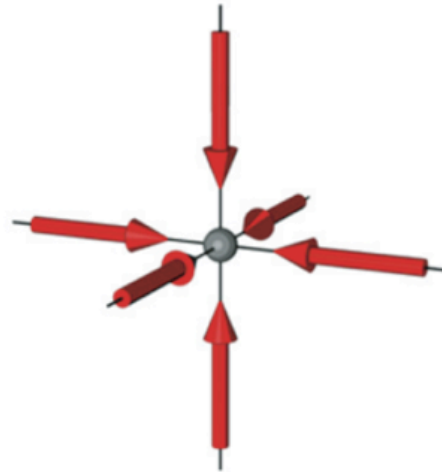
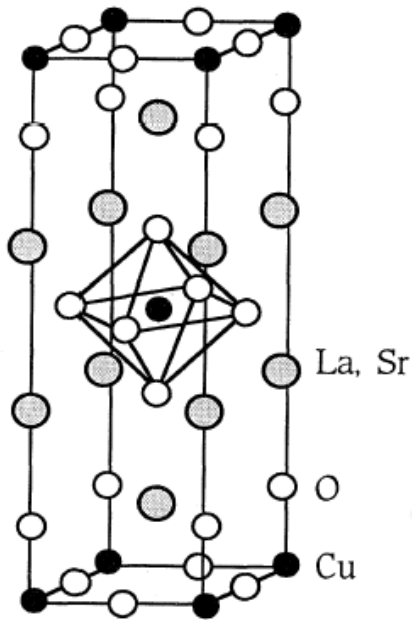
Chang, Randeria, and Trivedi, PNAS 108, 51 (2011)

O. Erten, et. al Phys. Rev. Lett. 107, 257201 (2011)



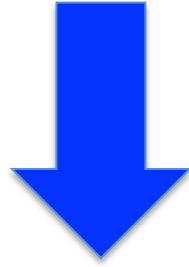
# Optical Lattice Emulator

# High T<sub>c</sub> Superconductivity → doped Mott insulator



$$\mathcal{H} = \sum_{\mathbf{k}, \sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}$$

Minimal model for this material



Minimal model for this phenomenon



# Ferromagnetism

```
graph TD; A[Ferromagnetism] --> B[Metal]; A --> C[Insulator]; B --> D["Mechanisms:  
Stoner  
Double Exchange"]; C --> E["Mechanisms:  
Superexchange"]; D --> F["Fe  
Iron Age ~ 1200 BC"]; E --> G["Fe3O4 magnetite Lodestone  
~800 BC ~28 centuries ago  
cf Superconductors ~ 100 years  
Semiconductors ~ 50 years"];
```

Metal

**Mechanisms:**  
Stoner  
Double Exchange

Fe  
Iron Age ~ 1200 BC

Insulator

**Mechanisms:**  
Superexchange

$\text{Fe}_3\text{O}_4$  magnetite Lodestone  
~800 BC ~28 centuries ago  
cf Superconductors ~ 100 years  
Semiconductors ~ 50 years

# Ferromagnetism in ultracold atomic gases

```
graph TD; A[Ferromagnetism in ultracold atomic gases] --> B[Metal]; A --> C[Insulator]; B --> D["Mechanisms:  
Stoner: hard sphere interactions;  
upper branch  
Double Exchange ?"]; C --> E["Mechanisms:  
Superexchange:  
Strongly interacting  
2 component bosons"];
```

Metal

**Mechanisms:**

**Stoner:** hard sphere interactions;  
upper branch

**Double Exchange ?**

Insulator

**Mechanisms:**

**Superexchange:**  
Strongly interacting  
2 component bosons

# Outline:

- (1) Stoner mechanism in continuum; atomic gases
- (2) Search for a minimal lattice model of ferromagnetism
  - Fe: itinerant and local moment character
  - Manganites: Double Exchange (DE)
  - Double Perovskites: Modified DE mechanism
- (3) Proposal for DE in Atomic Gases

General Theme: Searching for minimal models  
Bringing together atomic gases and condensed matter systems

## Part 1: Stoner Mechanism (in continuum)

E. Stoner (1933) Philos. Mag. **15**, 1018-1034

“Atomic moments in ferromagnetic metals and alloys with nonferromagnetic elements”

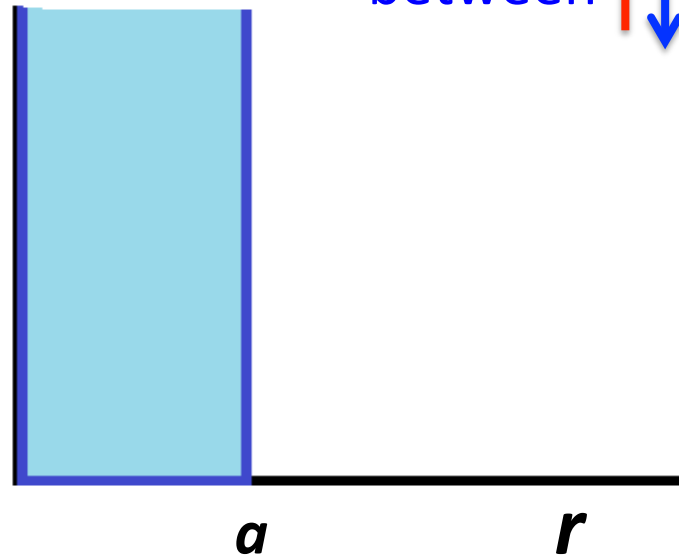
K. Huang (1987), “Statistical Mechanics” Sec. 11.7

TEXT BOOK  
PROBLEM

$$H = \sum_{i\sigma} \frac{\mathbf{p}_{i\sigma}^2}{2m} + \frac{1}{2} \sum_{i,j} V(r_{ij})$$

$V(r)$

Hard Sphere interaction  
between   spins



Hard sphere diameter  
 $a = \text{range}$

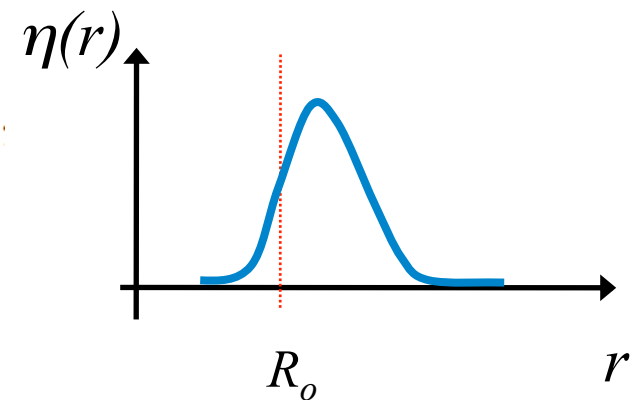
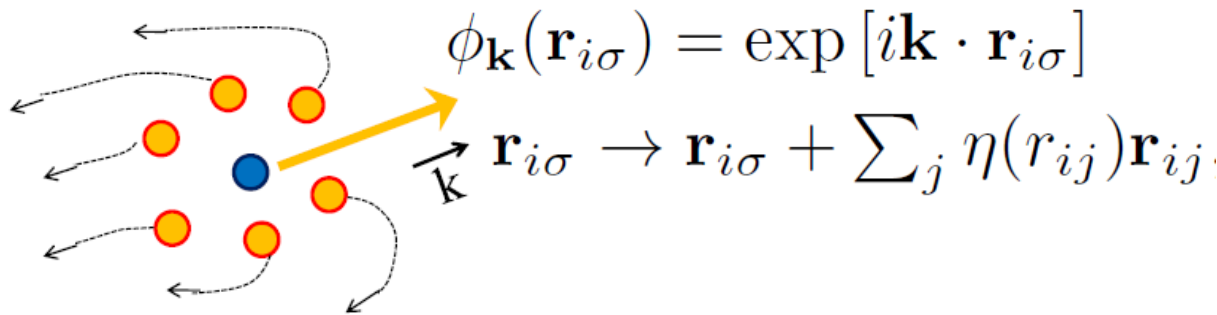
Pilati et al, PRL 105, 030405 (2010)

Chang, Randeria, and Trivedi, PNAS 108, 51 (2011)

# Quantum Monte Carlo at T=0

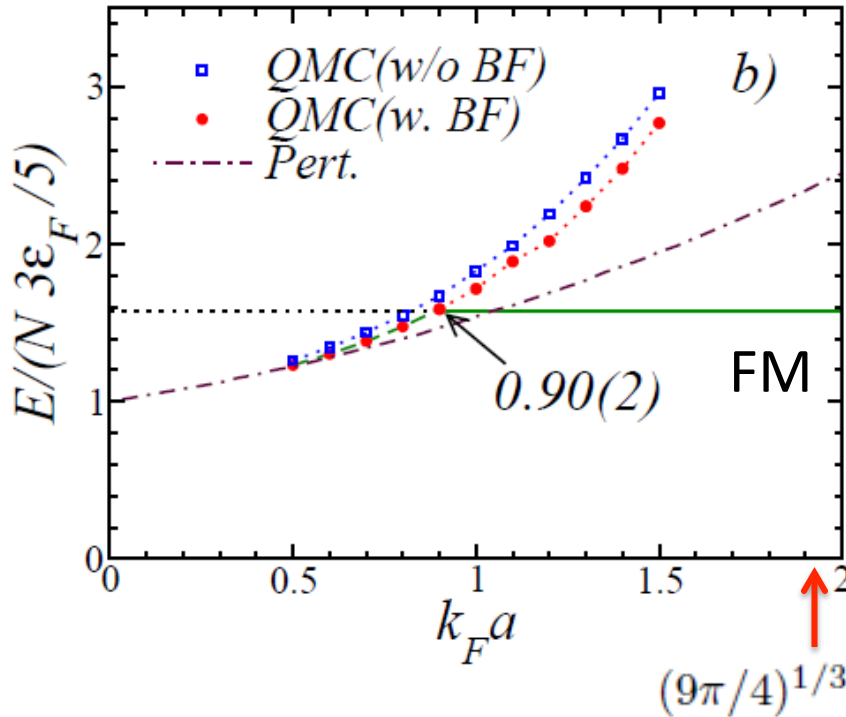
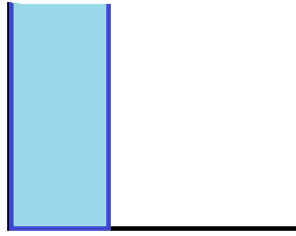
$$\Psi = \prod_{i\uparrow, j\downarrow} f(r_{ij}) \Phi_{FG\uparrow} \Phi_{FG\downarrow}$$

- **QMC essential:** MFT estimates of FM can be wrong by orders of magnitude -- electron gas
- **Jastrow:**  $f(r)$  non-zero outside hard core radius  $a$
- **Backflow** cannot be ignored *a priori*:  
not including it led to spurious FM instability in normal He-3



# Total Energy

Hard Sphere



Fermi Liquid to FM  
transition at  $k_F a = 0.9$

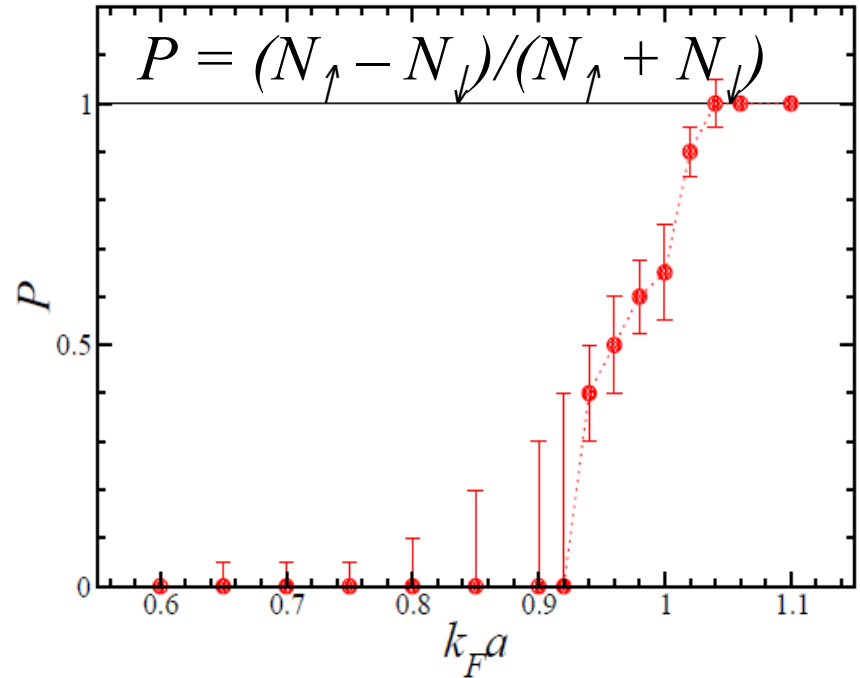
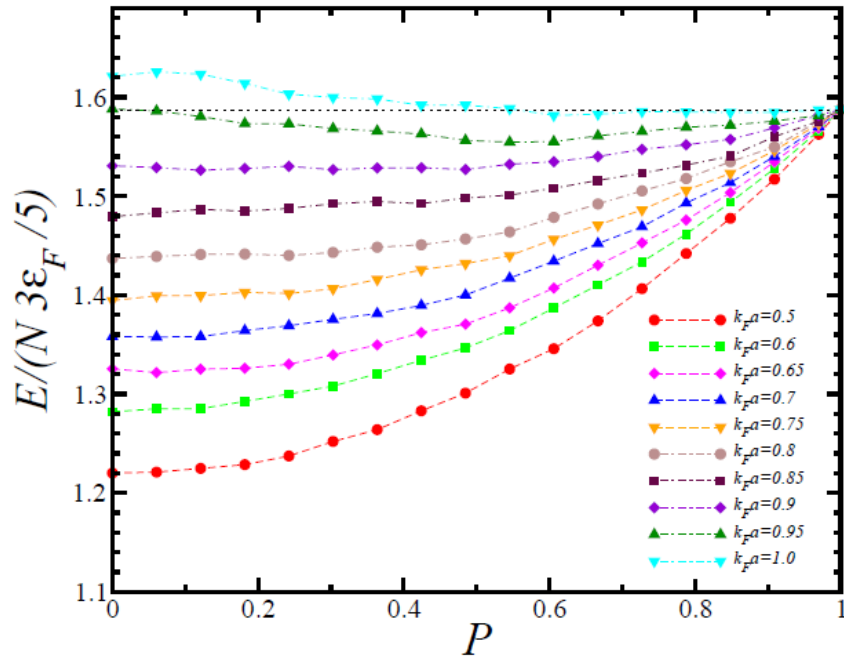
$$2^{2/3} \simeq 1.58$$

Perturbation  
Theory:

$$\frac{E}{N\epsilon_F} = \frac{3}{5} + \frac{2}{3\pi}k_F a + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a)^2 + \dots$$

[Lee-Yang,  
Galitskii]

# Partially Polarized Phase: II order Phase Transition



Shallow minima in  $0.8 \leq k_F a \leq 0.96$   
Partially polarized state

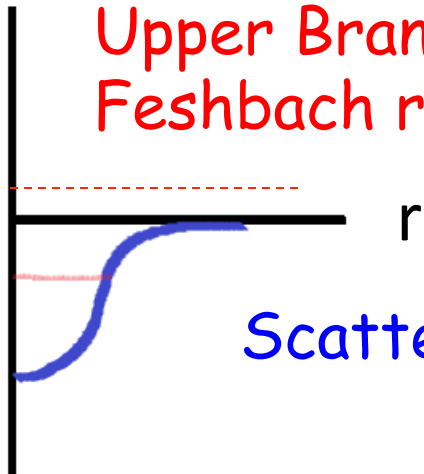


Has the Stoner transition been seen in cold atom experiments?

$$H = \sum_{i\sigma} \frac{p_{i\sigma}^2}{2m} + \frac{1}{2} \sum_{i,j} V(r_{ij})$$

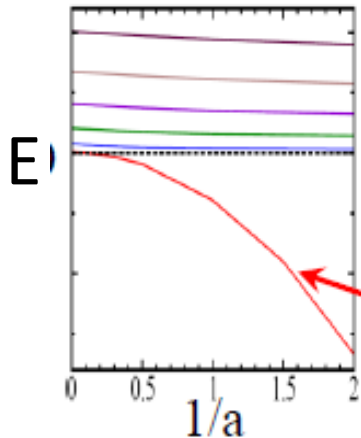
$V(r)$

Upper Branch of  
Feshbach resonance



Scattering length  
 $a > 0$

$a \gg \text{range}$

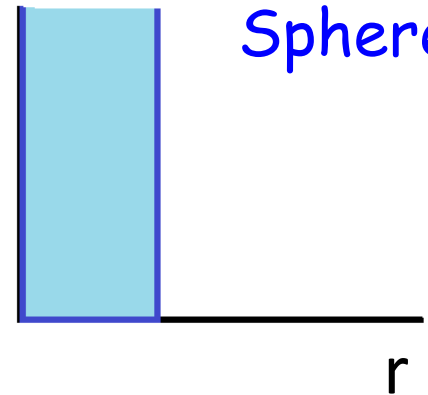


Upper Branch  
→ **effective  
repulsion**

Lower branch:  
 $E < 0$  bound state.

$V(r)$

Hard  
Sphere



Hard sphere diameter  
 $a = \text{range}$

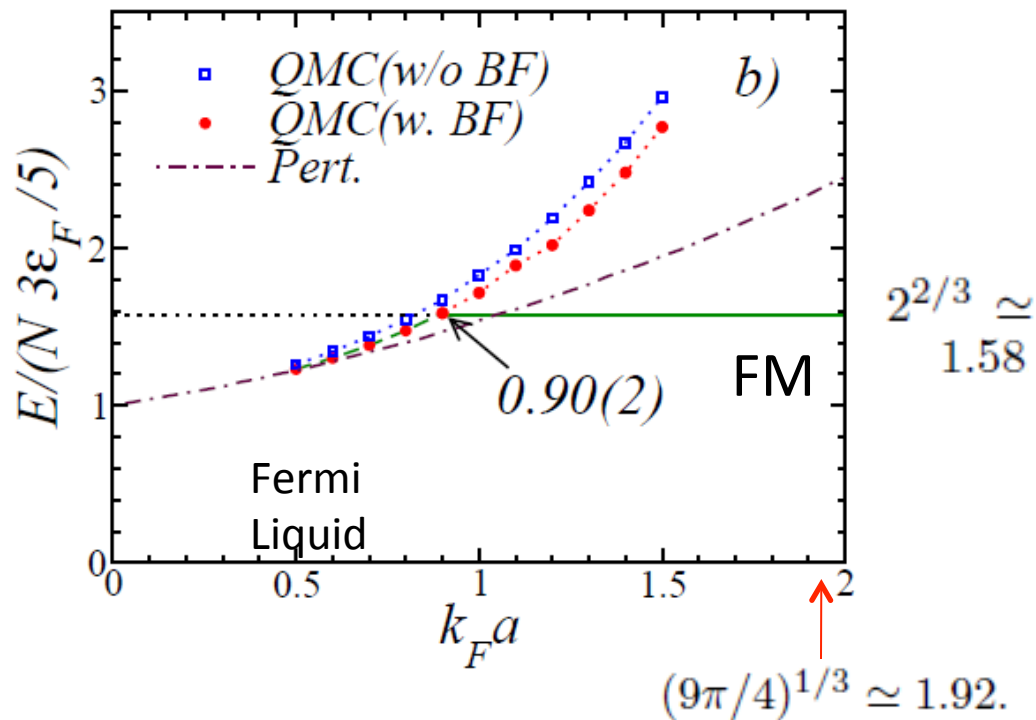
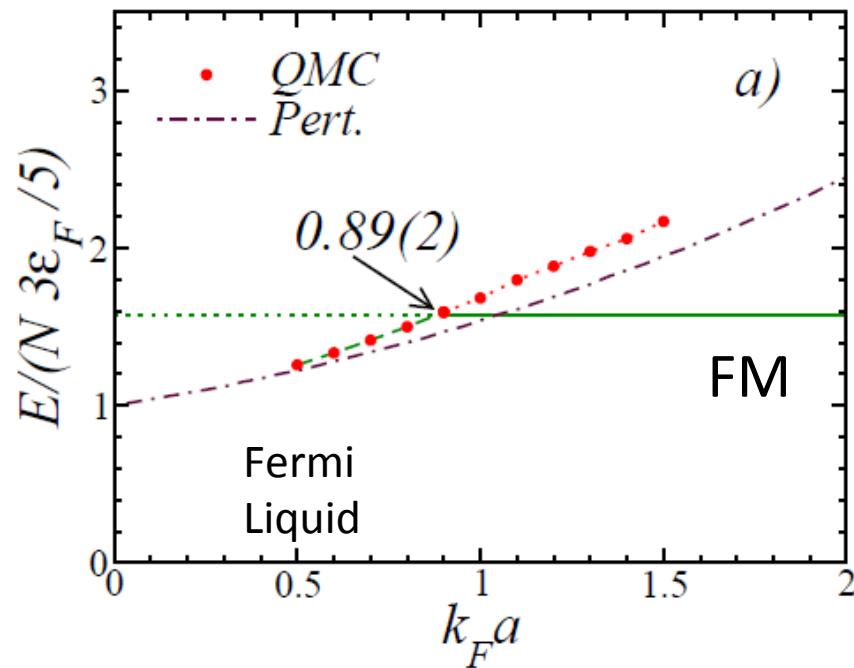
# Universality

(independent of details of interaction potential)

# Total Energy

Upper Branch

Hard Sphere



Perturbation Theory:

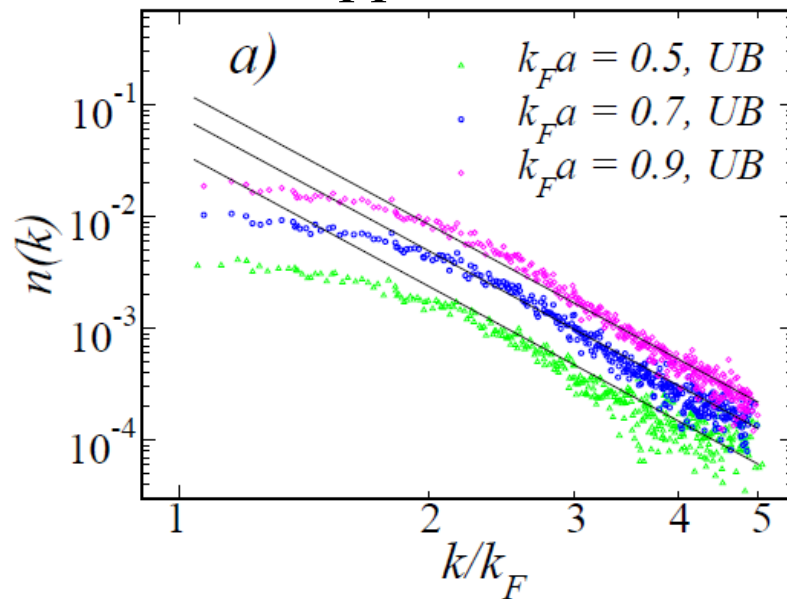
$$\frac{E}{N\epsilon_F} = \frac{3}{5} + \frac{2}{3\pi}k_F a + \frac{4}{35\pi^2}(11 - 2\ln 2)(k_F a)^2 + \dots$$

[Lee-Yang, Galitskii]

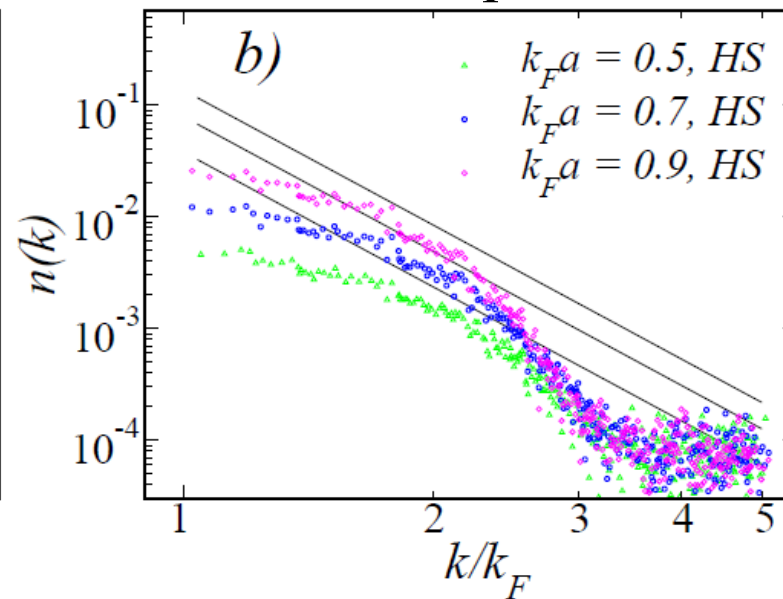
Fermi Liquid to FM transition at  $k_F a = 0.9$

# Contact Physics: $\lim_{k \rightarrow \infty} n(k) = C/k^4$

Upper Branch



Hard Sphere



EOS

$$C = \frac{2}{5\pi} \frac{d \left( \frac{E}{N 3\epsilon_F / 5} \right)}{d \left( -\frac{1}{k_F a} \right)} k_F^4$$

## Upper branch; life time effects

If three-body processes leading to molecule formation can be suppressed, there may be a window of time-scales where equilibrium physics in the upper branch would be observed

- [1] G. Jo, et al, Science **325**, 1521 (2009).
- [2] A. Sommer, M. Ku, G. Roati, and M. W. Zwierlein, Nature **272**, 201 (2011).
- [3] C. Sanner, E. J. Su, W. Huang, A. Keshet, J. Gillen, and W. Ketterle, arXiv:1108.2017
- [4] E. Taylor, S. Zhang, W. Schneider, and M. Randeria, arXiv:1106.4245.

# Outline:

(1) Stoner mechanism in continuum; atomic gases

(2) Search for a minimal lattice model of ferromagnetism

➤ Fe: itinerant and local moment character

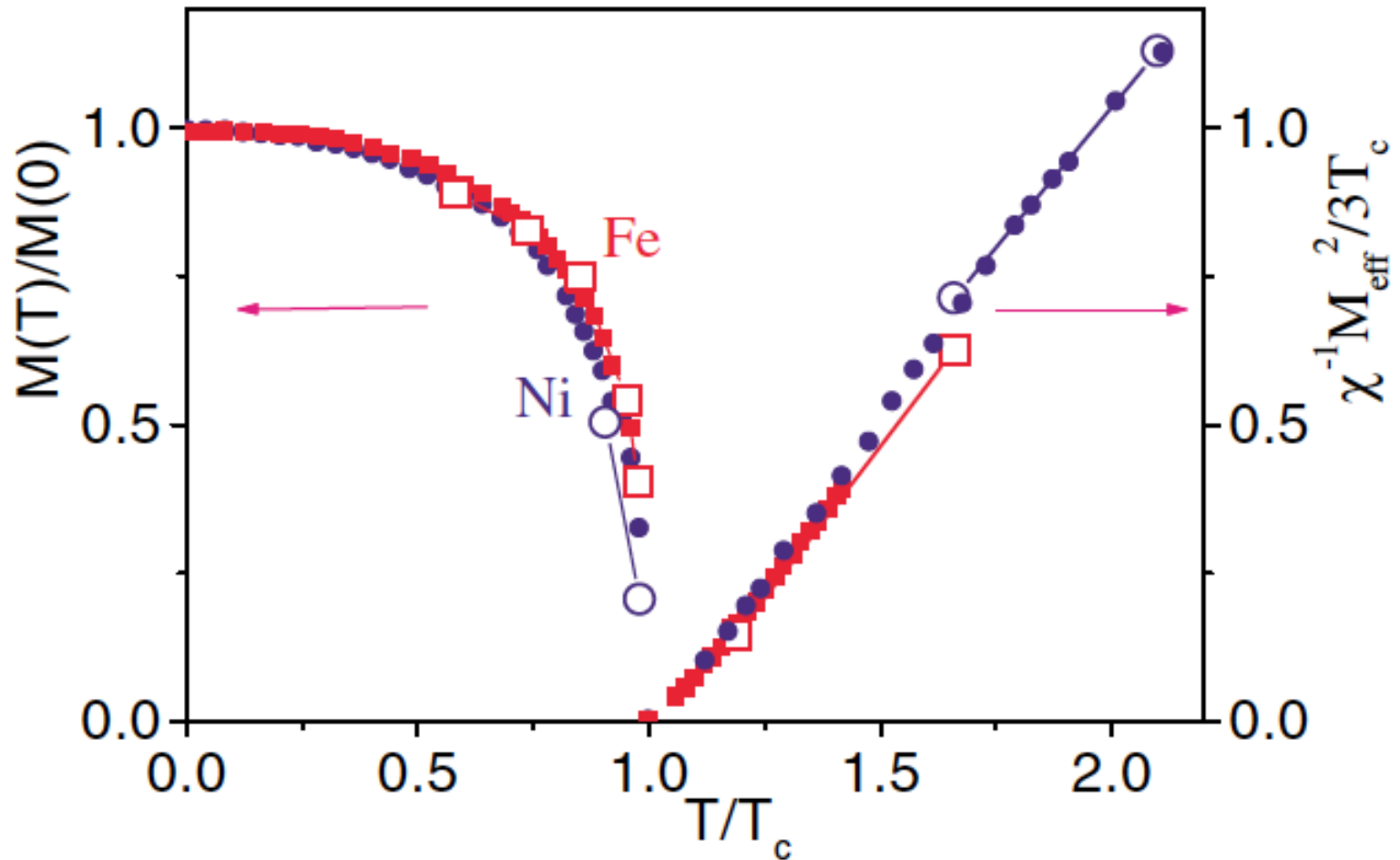
➤ Manganites: Double Exchange (DE)

➤ Double Perovskites: Modified DE mechanism

(3) Proposal for DE in Atomic Gases

Why is the problem of FM of Fe  
a difficult theoretical problem?





Local Moments exist above  $T_c$  concomitantly with a Fermi surface

S. V. Vonsovsky, Magnetism, vol.2 (1974);  
Ferromagnetic materials, vol. 1, ed. by E.P. Wolfarth (1986).

(a) Fe: no clean separation between  
local moment vs itinerant character

Analogy:

band SDW to Heisenberg Local moments

BCS to BEC

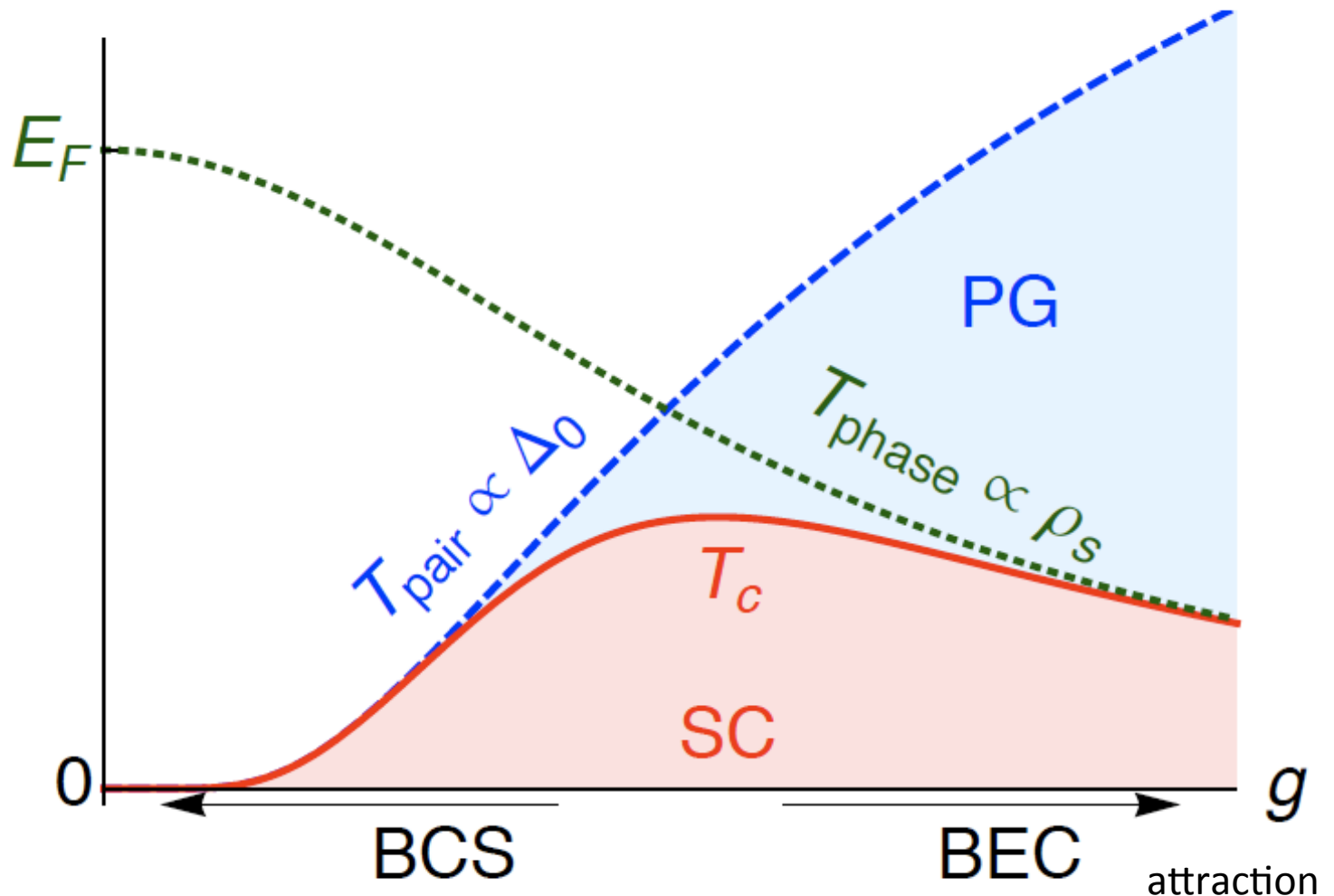
(b) Manganites:

Some separation between local moment  
and itinerant carriers

(c) Double Perovskites:

Clear separation of local moment  
and itinerant carriers

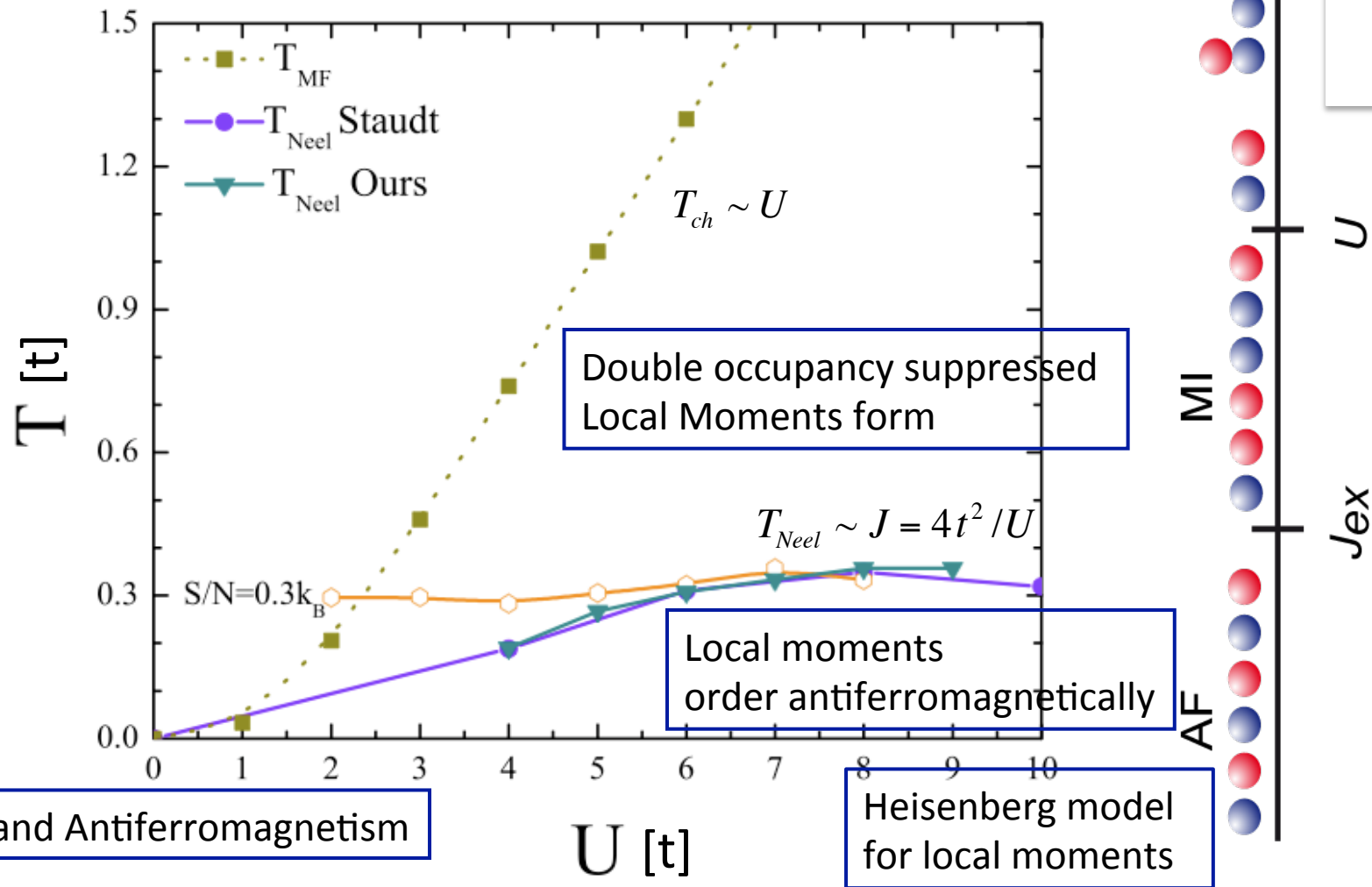
# Role of amplitude and phase fluctuations:



$$T_c = \min(\Delta_0, \rho_s)$$

# 3D Repulsive U Hubbard model

$$N_{\uparrow} = N_{\downarrow}; N_{\text{fermions}} = N_{\text{sites}}; d = 3$$



Energy in units of  $t$

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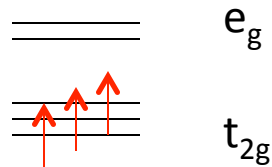
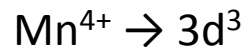
(3) Proposal for DE in Atomic Gases

# What is a minimal lattice model that shows FM?

## Guidance from Condensed matter systems

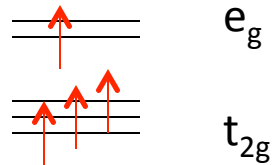
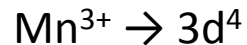
- **Narrow band width**
  - Enhances Coulomb correlations
- **Multi degenerate and orthogonal orbitals**
  - Hund's coupling
  - Local moment on an atom
- **Ordering of Local moments**

# Double-Exchange in Manganites



## Ingredients:

- Large Hund's coupling: Spins are aligned
- Cubic crystal field:  $t_{2g}$  and  $e_g$  orbitals



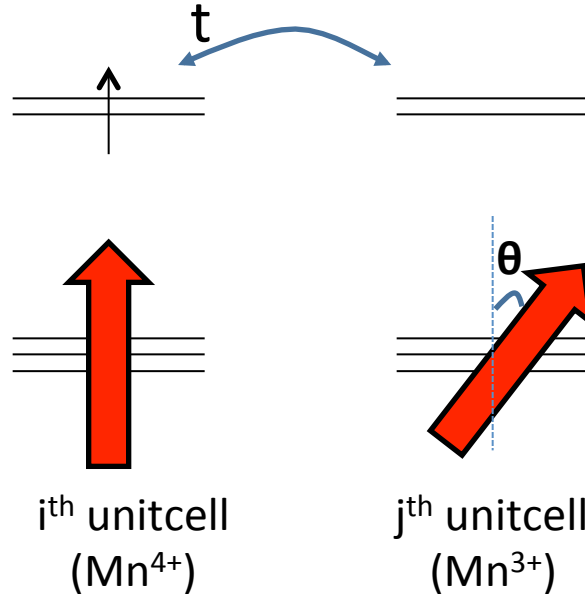
## Outcome:

- $3e^-$  in  $t_{2g}$  forms a large spin  $S=3/2$   
→ treat classically
- $\text{Mn}^{3+}$  the extra  $e^-$  delocalizes in  $e_g$   
→ treat quantum mechanically

Zener, Phys. Rev. 82 403 (1951)

Anderson & Hasegawa, Phys. Rev. 100 675 (1955)

# Double-Exchange in Manganites



QM rotation of axis of quantization

$$|\uparrow i\rangle = \cos(\theta/2)|\uparrow j\rangle + \sin(\theta/2)|\downarrow j\rangle$$

Then calculate the matrix elements

$$\langle \uparrow i | H | \uparrow j \rangle = \cos(\theta/2)t \quad \leftarrow \text{Zener}$$

Anderson-Hasegawa calculated for 2 unit cells

$$H = t \sqrt{\frac{1 + S_i \cdot S_j}{2}}$$

Maximizing KE drives the core spins to align ferromagnetically



# Outline:

(1) Stoner mechanism in continuum; atomic gases

(2) Search for a minimal lattice model of ferromagnetism

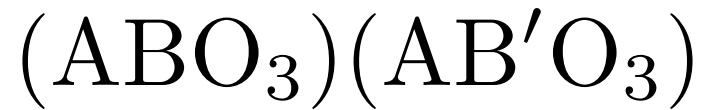
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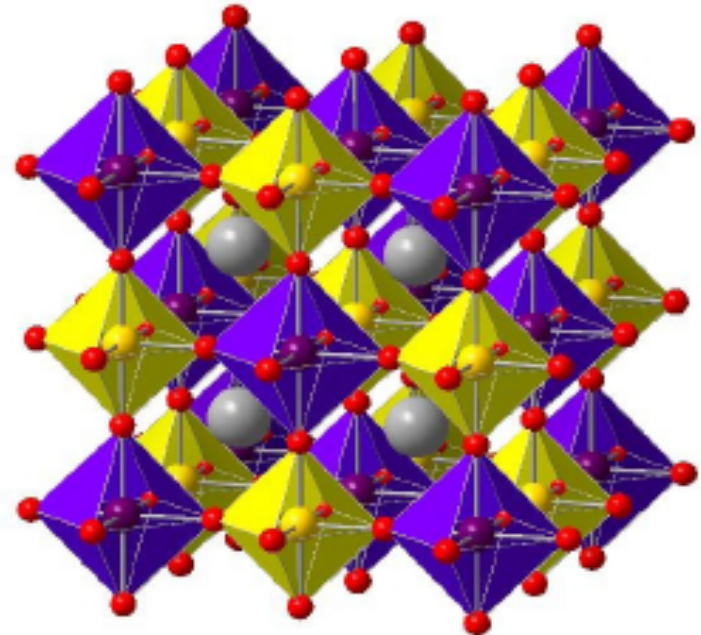
(3) Proposal for DE in Atomic Gases

# Double Perovskites



|    | 6  | 7  | 8  |     |
|----|----|----|----|-----|
| 3d | Cr | Mn | Fe | $B$ |
| 4d | Mo | Tc | Ru |     |
| 5d | W  | Re | Os |     |

$B'$



*Tunability....*



- Half-metal
- Ferrimagnet
- $T_c = 420 \text{ K}$

O. Erten, O. N. Meetei et al,  
 "Theory of half-metallic ferrimagnetism in double perovskites"  
 Phys. Rev. Lett. 107, 257201 (2011)

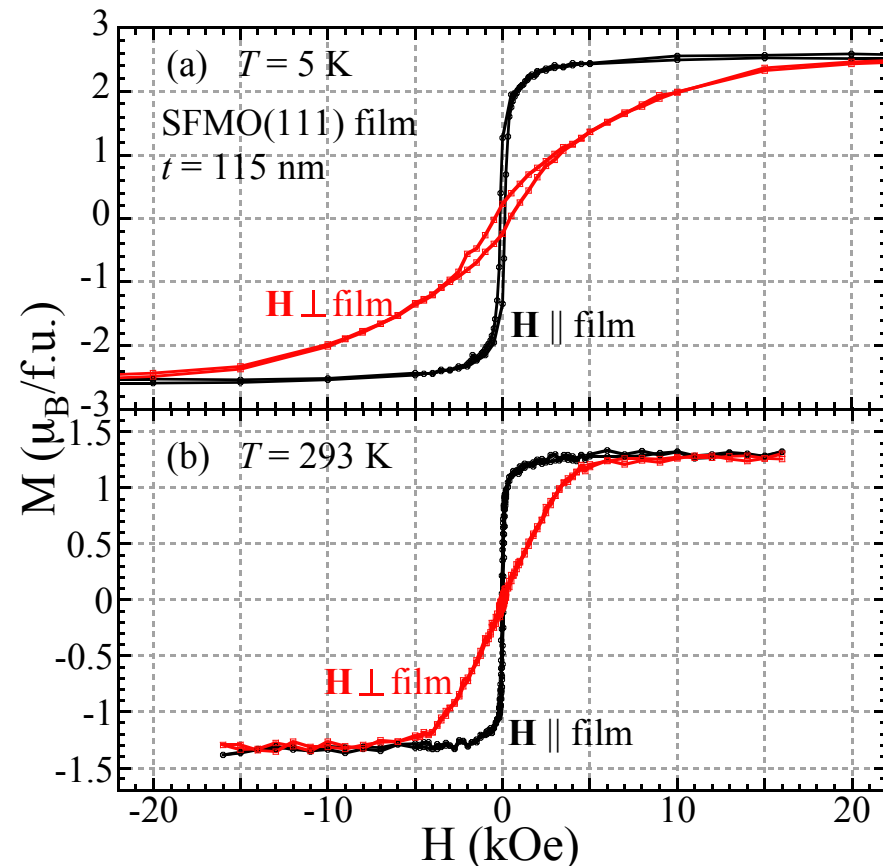
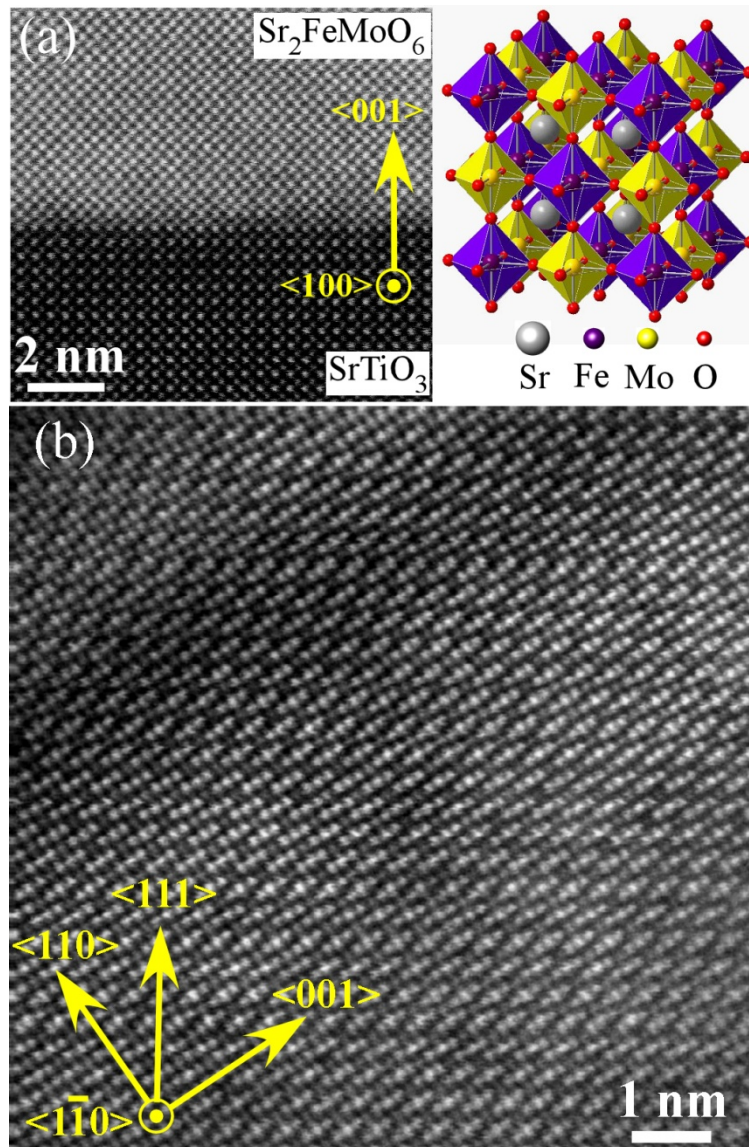


- Mott insulator
- Ferrimagnet
- $T_c = 720 \text{ K}$

O. N. Meetei, O. Erten et al,  
 (to be submitted)

|    | 6  | 7  | 8  |
|----|----|----|----|
| 3d | Cr | Mn | Fe |
| 4d | Mo | Tc | Ru |
| 5d | W  | Re | Os |

# Sputter deposited $\text{Sr}_2\text{FeMoO}_6$ films



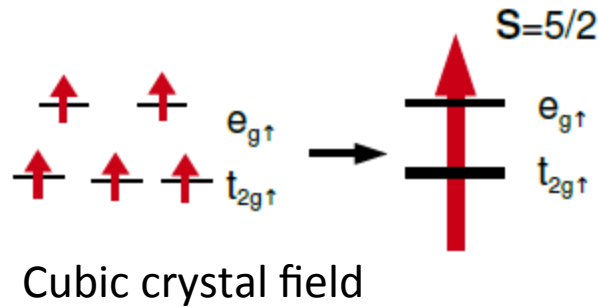
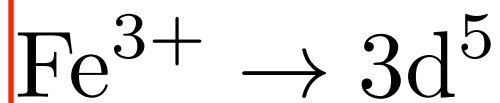
RBS:  $\text{Sr}_2\text{Fe}_{0.94}\text{Mo}_{1.06}\text{O}_6$

XRD:  $a = 7.909 \text{ \AA}$  (out of plane)

Fe/Mo Order parameter:  $\xi = 86\%$  (99%)

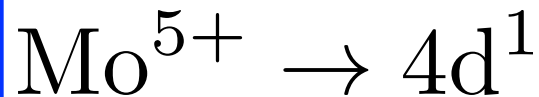
$T_C = 380 \text{ K}$

$M_{\text{sat}} = 2.6 \mu_B / \text{f.u.}$



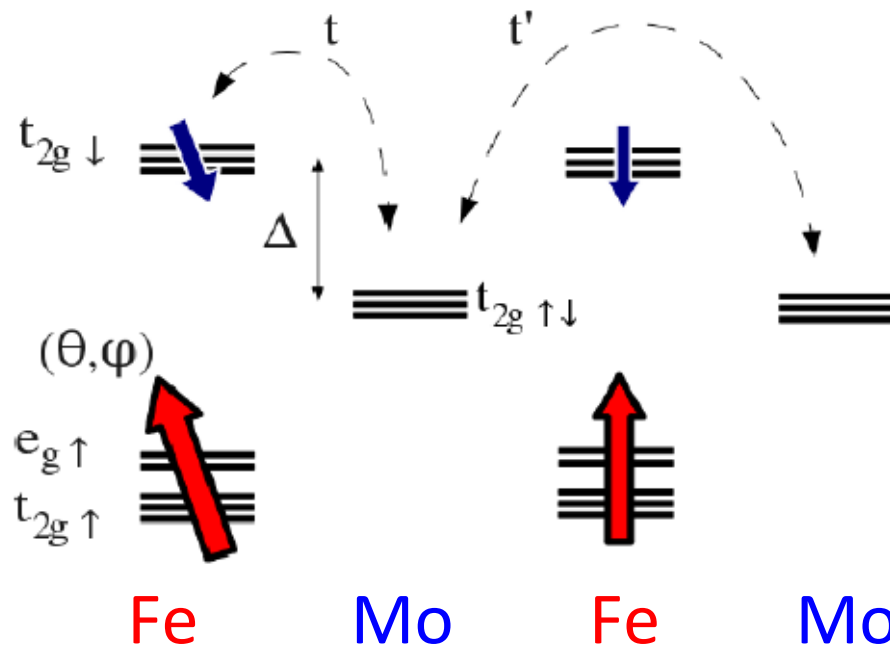
large  $J_H$  )

$S = 5/2$   
spins



Itinerant electrons

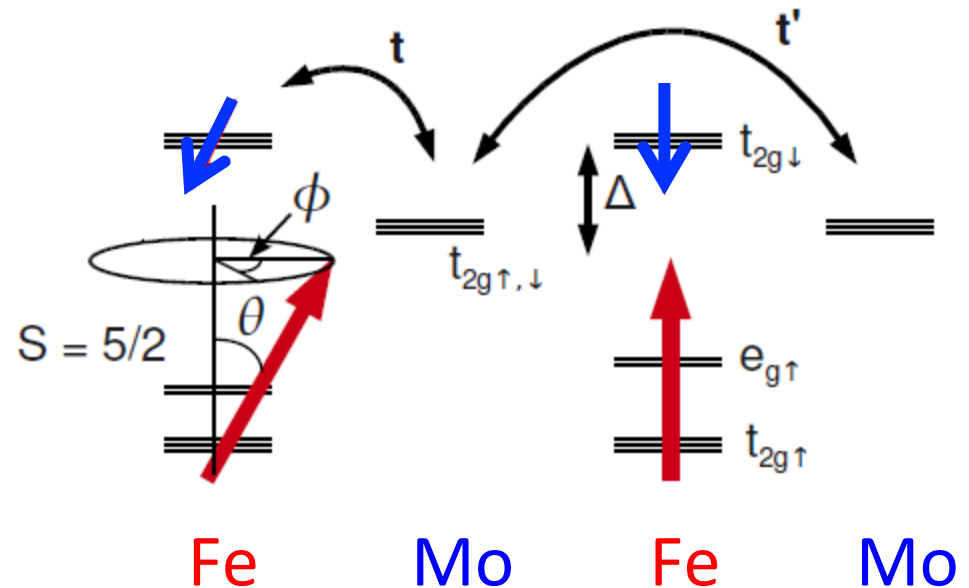
in  $t_{2g}$  orbitals



Quantum electrons  
+ Classical Fe Spins

# Quantum electrons + Classical Fe Spins

- el-spin anti-parallel to Fe spin
- “double exchange”



$$H = - \sum_{\langle ij \rangle, \sigma} \left( t_{ij\sigma} d_{i\downarrow}^\dagger c_{j\sigma} + h.c. \right) + \Delta \sum_i d_{i\downarrow}^\dagger d_{i\downarrow} \\ - t' \sum_{\langle\langle ij \rangle\rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right)$$

$$t_{ij\uparrow} = -t e^{i\phi_i/2} \sin(\theta_i/2)$$

$$t_{ij\downarrow} = t e^{-i\phi_i/2} \cos(\theta_i/2)$$

# Solving the Full Hamiltonian

## "Slow" variables

Localized

$S=5/2$  Fe spins

→ Classical  $\mathbf{S} \rightarrow (\theta, \phi)$

→ Monte Carlo (MC)

## "Fast" variables:

Itinerant electrons ("Mo")

→ Quantum

→ Exact

Diagonalization (ED)

**"ED+MC" method**

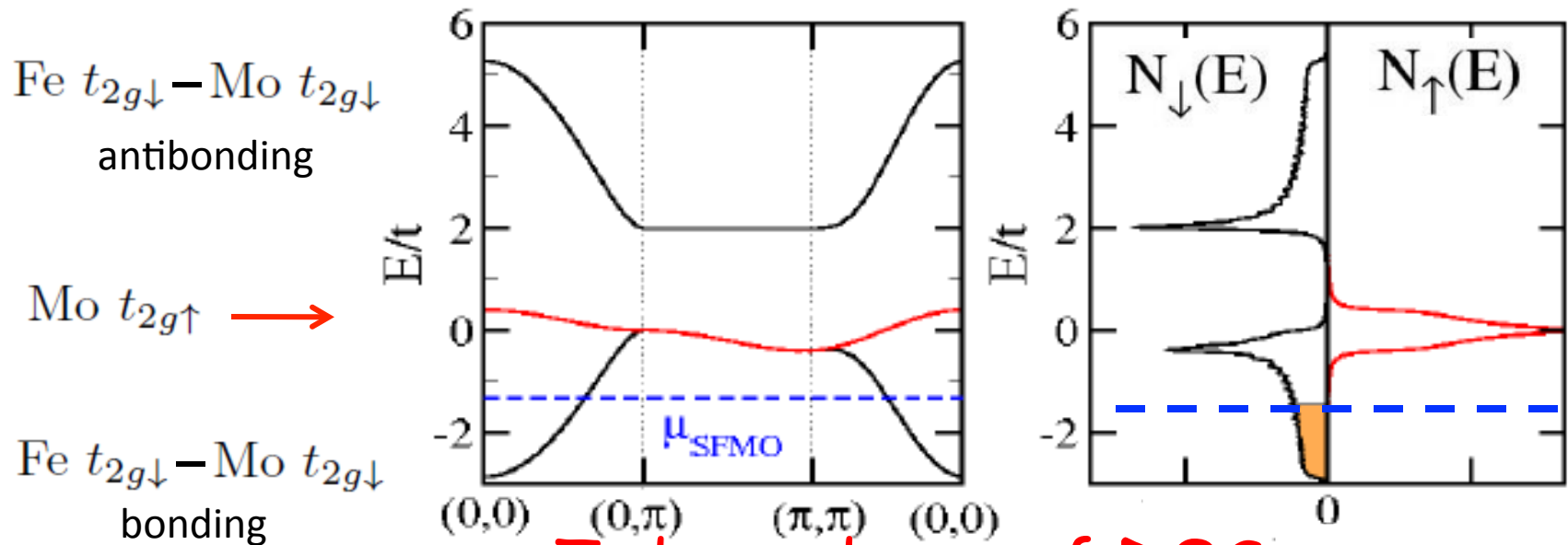
$t = 0.27$  eV;

$t'/t = 0.1$ ;  $\Delta/t = 2.5$

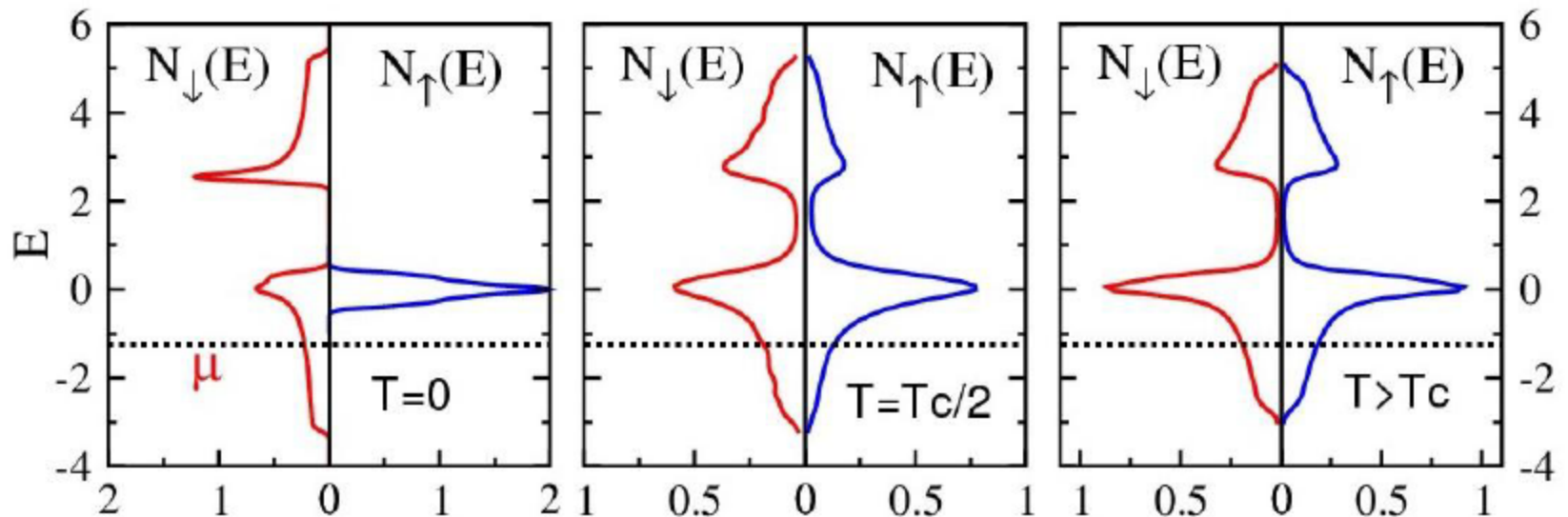
Input parameters  
consistent with DFT

- \* D. D. Sarma et al, PRL **85**, 2549 (2000);
- \* R. Mishra, O. Restrepo, W. Windl, P. Woodward, Chem. Mater. **22**, 6092 (2011).

# Half-metallic Ground State

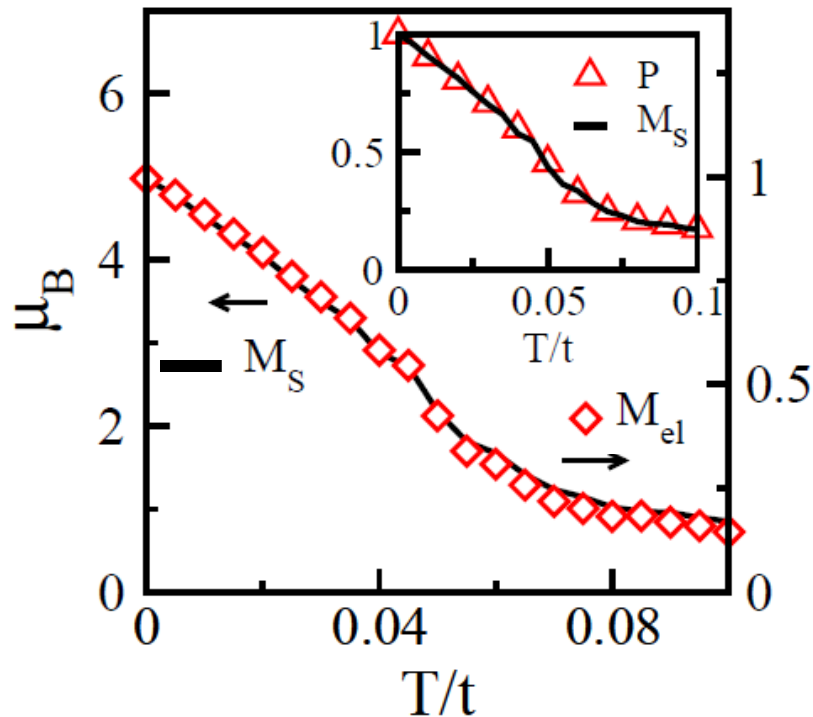


## T-dependence of DOS





# Conduction Electron Magnetism tied to Fe-Spin Magnetism



## Magnetization

Ferri-  
magnetism

$$M = M_s - M_{el}$$

$$M_{el} = \frac{n_{\uparrow} - n_{\downarrow}}{n_{\uparrow} + n_{\downarrow}}$$

- $M_{el} \propto M(T)$

- $P(T) \propto M(T)$

## Polarization (at $E_f$ )

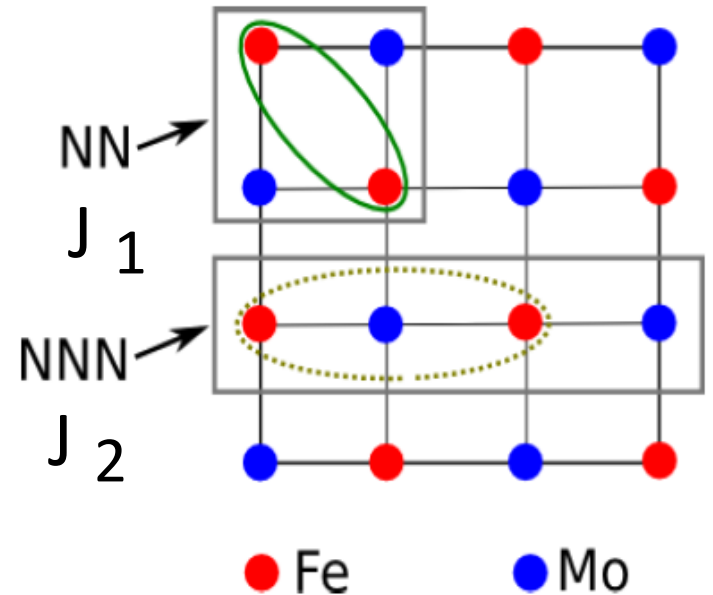
$$P = \frac{N_{\uparrow}(0) - N_{\downarrow}(0)}{N_{\uparrow}(0) + N_{\downarrow}(0)}$$

Conduction Electron Magnetism  
proportional to Fe-Spin Magnetism

→ Effective Hamiltonian for  
classical Fe-spins  
must describe all magnetic properties

- computationally &
- conceptually simpler

Generalize the 2-site  
Anderson-Hasegawa (1955)  
analysis for manganites to  
**Double Perovskites**



Exact solution for 2-unit cells

→ **Low-energy effective Hamiltonian for DP's**

$$H_{eff} = -J_1 \sum_{\langle i,j \rangle} f_1 (\mathbf{S}_i \cdot \mathbf{S}_j) - J_2 \sum_{\langle\langle i,j \rangle\rangle} f_2 (\mathbf{S}_i \cdot \mathbf{S}_j)$$

$$f_1(x) = 8\sqrt{2 + \sqrt{2 + 2x}}$$

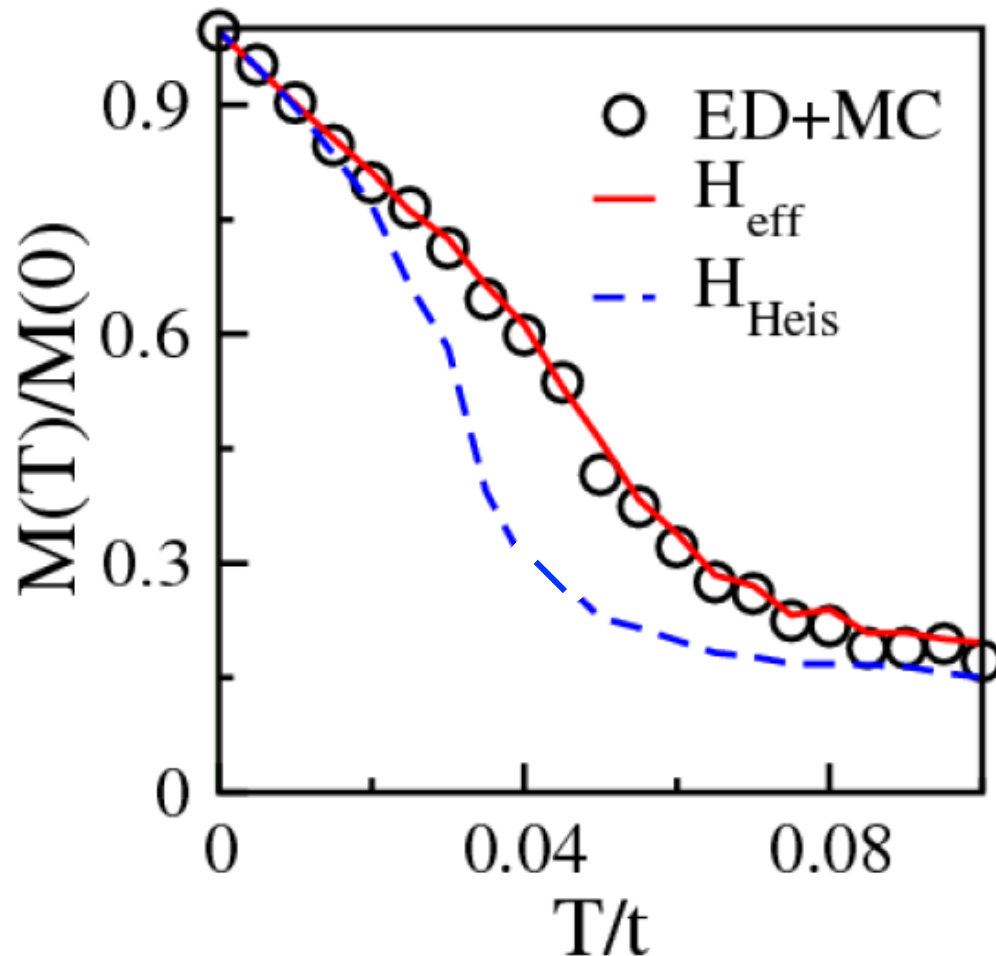
$$f_2(x) = (5 + \sqrt{5})\sqrt{6 + 2\sqrt{3 + 2x}}$$

\* Different from both Heisenberg and A-H Hamiltonians

\* KE sets the scale of ferromagnetic exchange  $J_1$  and  $J_2$

## Validating the Effective Spin Model:

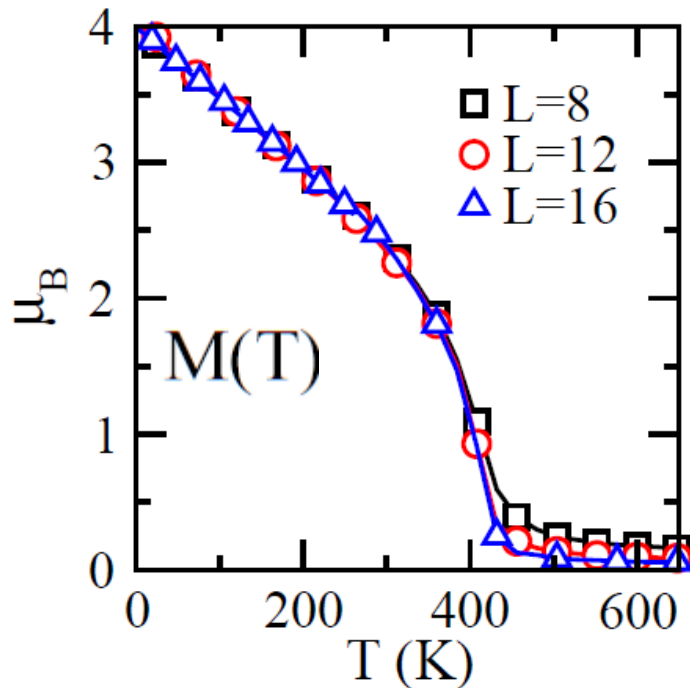
Compare  $M(T)$  with that of the Full Model



- $H_{\text{eff}}$  works
  - NN + NNN Heisenberg model does not
- FM exchange  $J_1$  and  $J_2$  are T-independent

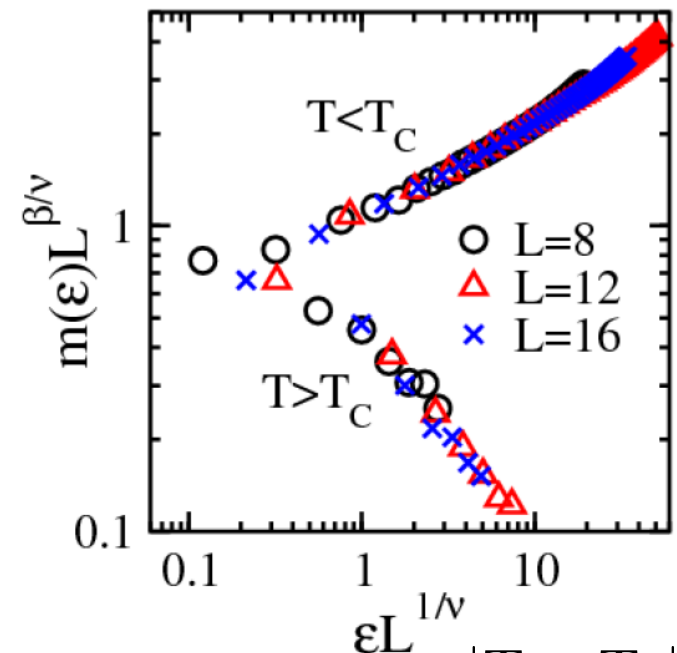
# Magnetization $M(T)$ and $T_c$

MC Calculations using  $H_{\text{eff}}$   
on  $L \times L \times L$  systems



→ State-of-the-art calculation  
of  $T_c$  that includes critical  
thermal fluctuations

Finite Size Scaling



$$d=3 \text{ O}(3) \quad \epsilon = \frac{|T - T_c|}{T_c}$$

universality class

$$\beta=0.362 \quad \nu=0.704$$

$$\rightarrow T_c = 0.14t$$

# Outline:

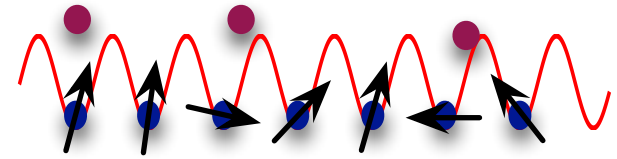
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General Theme: Searching for minimal models  
Bringing together atomic gases and condensed matter systems

## System:

$^{40}\text{K}$  (two species, up and down)

Mott insulator in a deep optical lattice

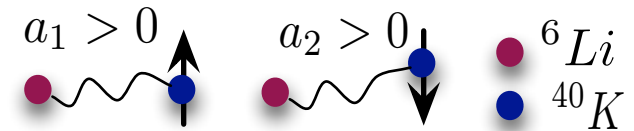


$^6\text{Li}$  (single species) do \*not\* see optical lattice

but will interact with  $^{40}\text{K}$  up and  $^{40}\text{K}$  down

with different scattering lengths

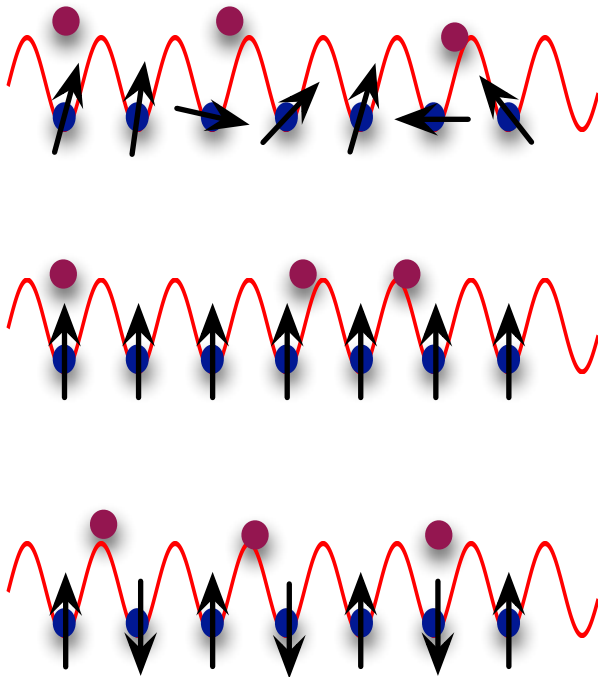
$a_1$  ( $\text{Li}-^{40}\text{K}$  up) and  $a_2$  ( $\text{Li}-^{40}\text{K}$  down).



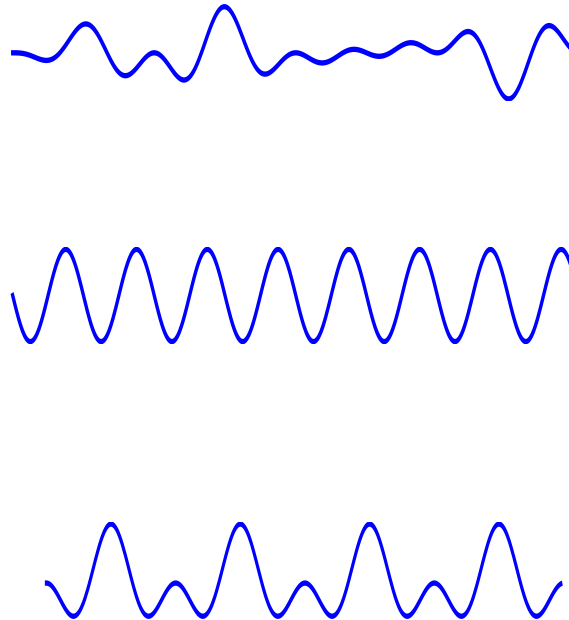
Consider the case when interaction  
Between  $^6\text{Li}$  and  $^{40}\text{K}$  are repulsive,  
depending on spins

Li sees an external potential which \*depends\*  
on the magnetic structure of the  $^{40}\text{K}$  atoms.

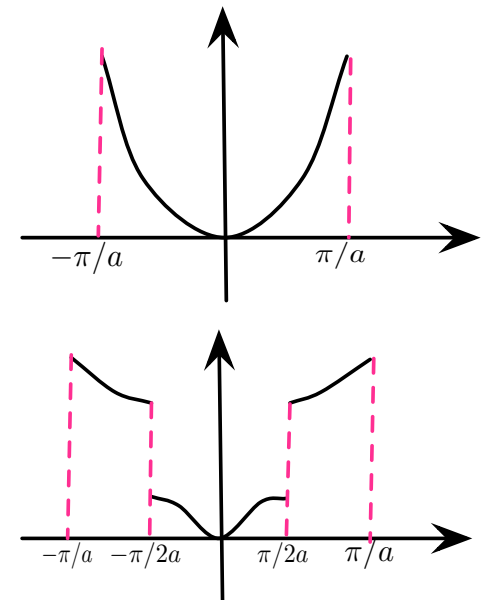
Schematic diagrams



External potential seen by  $^6\text{Li}$



Maybe localized





Is it possible to tune the filling of  ${}^6\text{Li}$ , the scattering length  $a_1$  and  $a_2$ , to realize either F or AF ordering of  ${}^{40}\text{K}$ ?

Total energy of system:

$$E_p(n, a_1, a_2)$$

(paramagnetic background of spins)

$$E_f(n, a_1, a_2)$$

(ferromagnetic background)

$n=1$ , first band filled

Use band width dependence on  $a_1$  and  $a_2$  to make ferromagnetic state favorable (double exchange mechanism)

$$E_{af}(n, a_1, a_2)$$

(antiferro background)

$n=0.5$ , first band is half filled,  
Use gap opening at  $\pi/2a$  to favor AF

Advantage:  $T_c$  scale set by delocalized Li primarily

# Future....

- Itinerant FM: double exchange mechanism in atomic gases; scale for  $T_c$  set by Fermi energy
- Multiorbital Mott insulators
- Doped multiorbital Mott insulators;  
novel states



Soon Yong Chang



Mohit Randeria



Onur Erten



O. Nganba Meetei



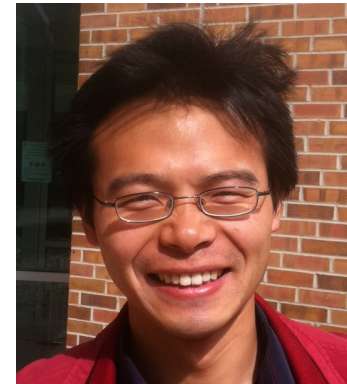
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Patrick Woodward



William Cole



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