Sign Problem Free Monte Carlo Simulation of Itinerant Ferromagnetism

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Mean Field Argument

$$H = -t \sum_{<i,j>} c^\dagger_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

Stoner Criterion: $U \rho_F^{-1} > 1$

Non Perturbative result

- Lieb-Mattis (1962): No 1D FM
- Nagaoka FM(1966): Single hole+Infinite U
- Mielke 1991: Flat-band FM Divergent DOS

Open question on Itinerant FM

- Non-perturbative treatment on finite temperature is lacking

  Stoner mean field + RPA calculation does not lead to Curie-Weiss behavior of spin susceptibility

$$\chi_{Paul}(T) = \chi_0(1 - c(\frac{T}{T_F})^2)$$

$$\chi_{RPA} = \frac{\chi_{Pauli}(T)}{1 - U\chi_{Pauli}(T)} \approx \frac{A}{1-(T/T_c)^2}$$

$$\neq \frac{A}{1 - T/T_c}$$

Exact Results for Itinerant Ferromagnetism in Multi-orbital Systems on Square and Cubic Lattices

Y. Li, E. Lieb, C. Wu Phys. Rev. Lett. 112, 217201 2014

- Fully polarized ground state at strong coupling limit
- Generic filling (0<n<2)
- Itinerant system
- No-node ground state

Model: P orbital Hubbard model

$$H_{hopping} = -t \sum_{<i,j>_x} p^\dagger_{x,i,\uparrow} p_{x,j,\uparrow} + \sum_{<i,j>_y} p^\dagger_{y,i,\uparrow} p_{y,j,\uparrow} + h.c.$$

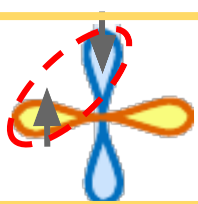
Directional Hopping

$$H_{int} = \sum_{\mu} \frac{U}{2} n_{\mu,\uparrow} n_{\mu,\downarrow} + \frac{V}{2} \sum_{\mu \neq \nu} n_\mu n_\nu - \frac{J}{2} \sum_{\mu \neq \nu} (\vec{S}_\mu \vec{S}_\nu - \frac{1}{4} n_\mu n_\nu)$$

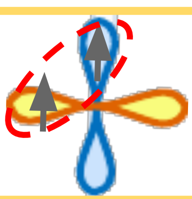
$U \to \infty$

$$+\Delta \sum_{\mu \neq \nu} c^\dagger_{\mu,\uparrow} c^\dagger_{\mu,\downarrow} c_{\nu,\downarrow} c_{\nu,\uparrow}$$

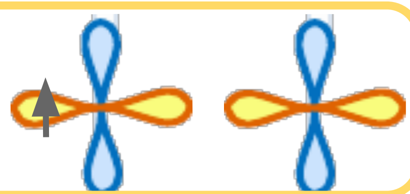
$E = V + J$

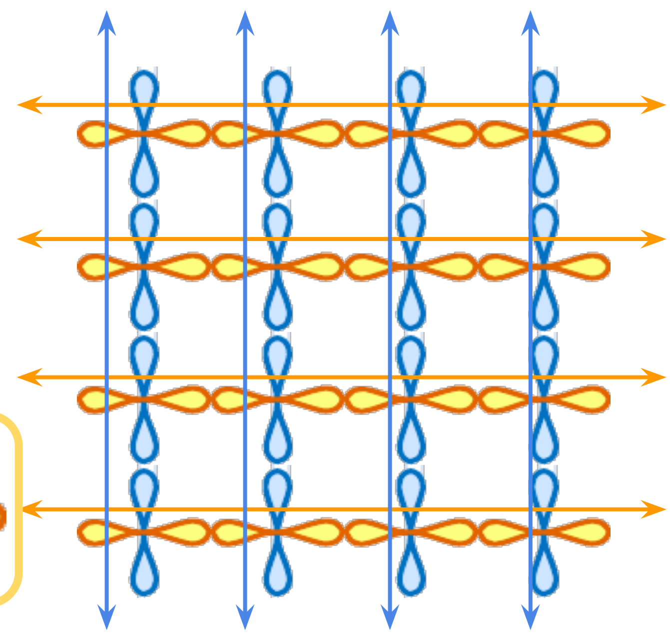


$E = V$



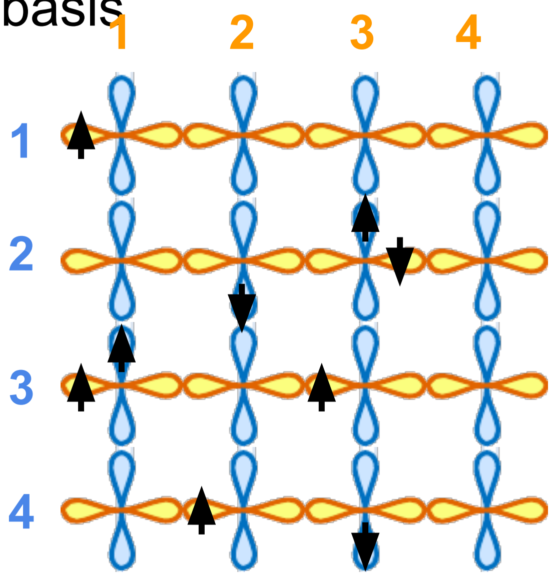
$E = 0$





Sign Problem Free Monte Carlo

The off diagonal elements of the Hamiltonian is negative/zero in a suitable basis



$$p^{\dagger}_{x,\{1,1\},\uparrow}p^{\dagger}_{x,\{3,2\},\downarrow}p^{\dagger}_{x,\{1,3\},\uparrow}p^{\dagger}_{x,\{3,3\},\uparrow}p^{\dagger}_{x,\{2,4\},\uparrow}$$

$$p^{\dagger}_{y,\{1,3\},\uparrow}p^{\dagger}_{y,\{2,2\},\downarrow}p^{\dagger}_{y,\{3,2\},\uparrow}p^{\dagger}_{y,\{3,4\},\downarrow}|0\rangle$$

- Hopping: $-p^{\dagger}_{x,i,\uparrow}p_{x,j,\uparrow}$
- Hund's Coupling: $-S^{-}_{y,i}S^{+}_{x,i} = -p^{\dagger}_{y,i,\downarrow}p_{y,i,\uparrow}p^{\dagger}_{x,i,\uparrow}p_{x,i,\downarrow}$

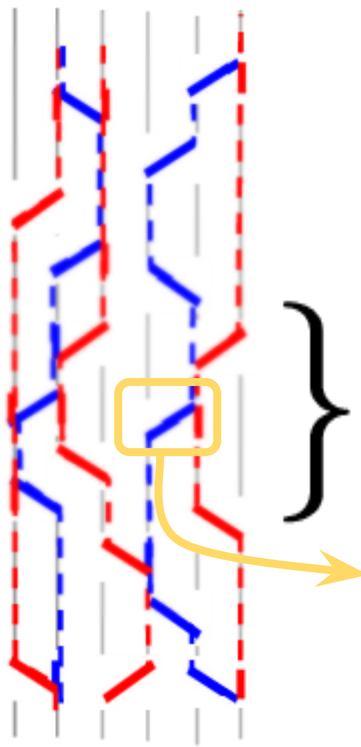
Stochastic Series Expansion + Directed loop

$$Z = Tr(e^{-\beta H}) = \sum W$$

OF Syljuåsen, AW Sandvik Physical Review E, 2002

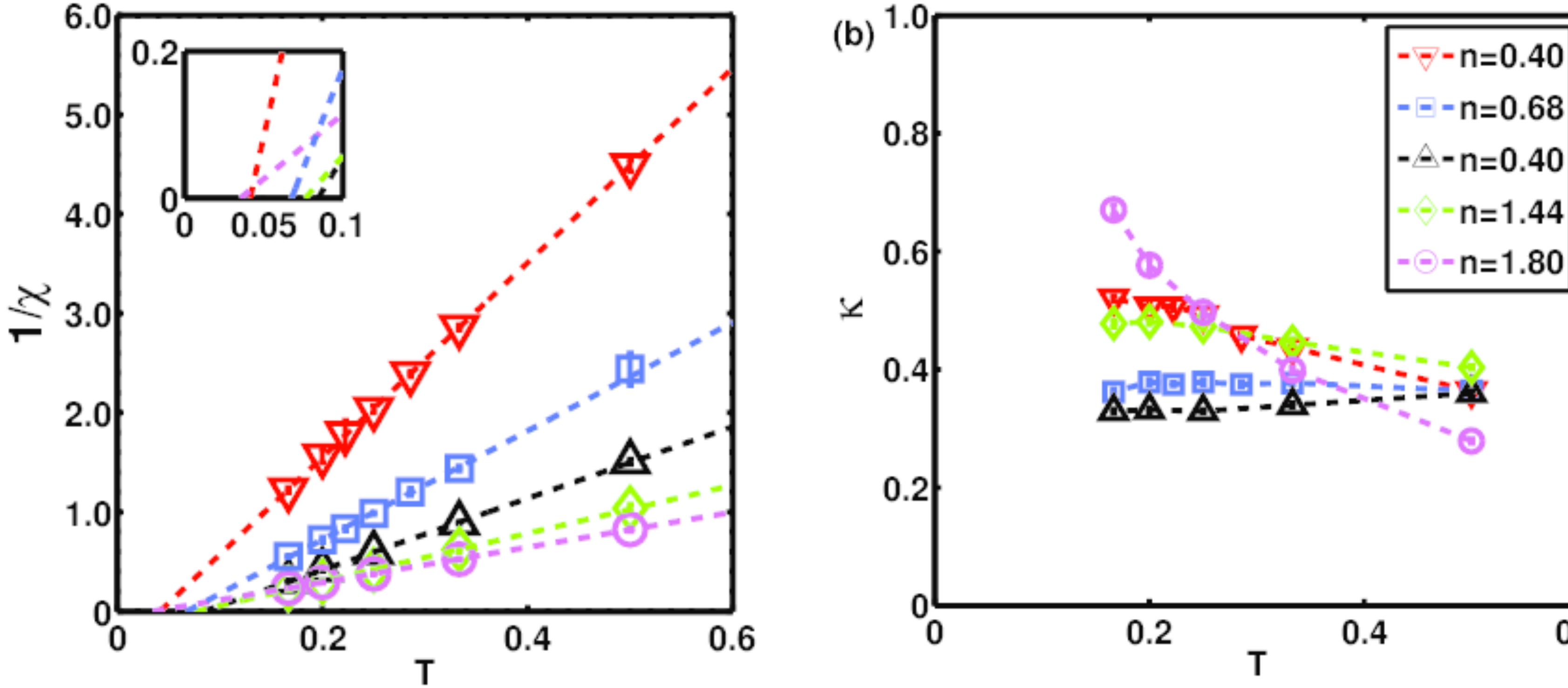
$$W = C\{g\} \langle \phi | (-H)^n | \phi \rangle$$

$$= \sum \Bigg\{ \quad \Bigg\}$$



$$\langle \phi_\alpha | -H | \phi_\beta \rangle$$

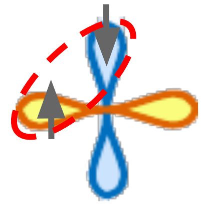
Result: V=0, t=1, J=2



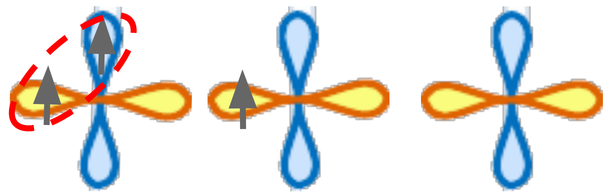
$$\chi = \frac{C}{T - T_0}$$

Compressibility satures to a finite value when T approaches 0, indicating metallic phases

$$E = J_h$$

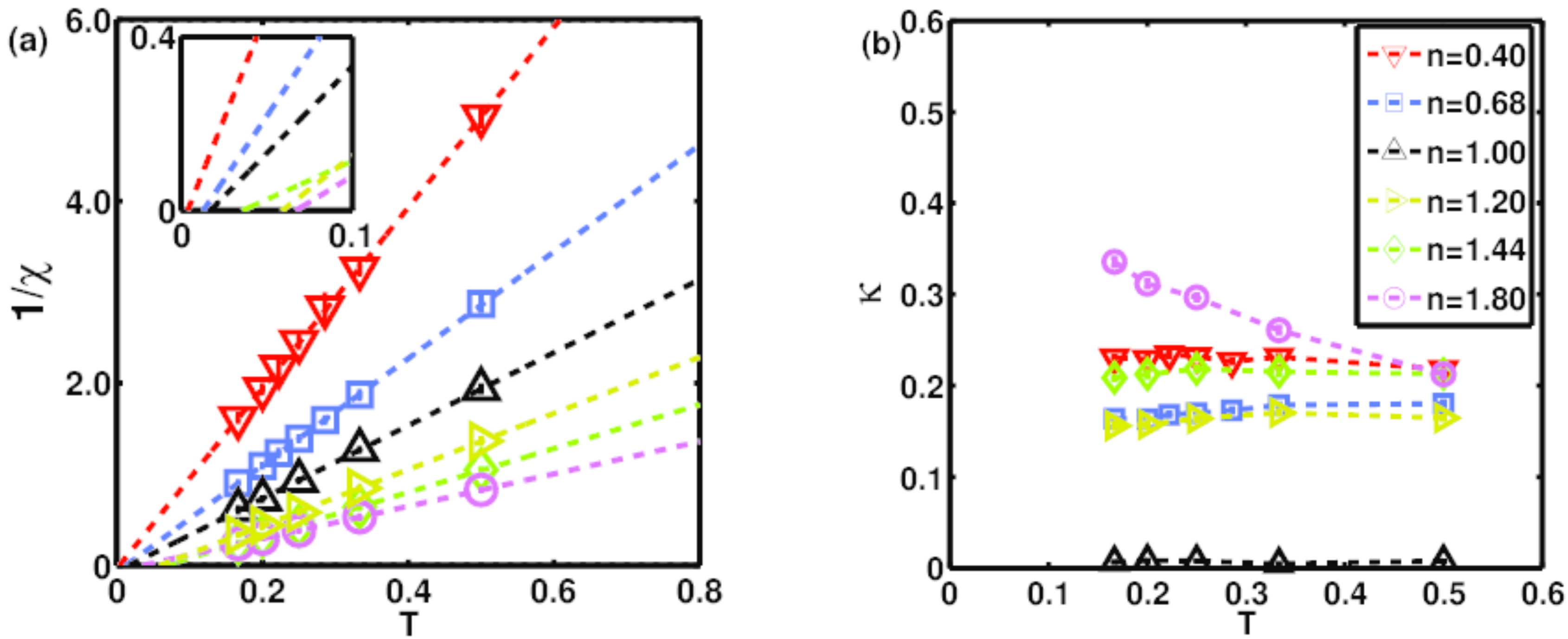


$$E = 0$$



The ground state is fully polarized state

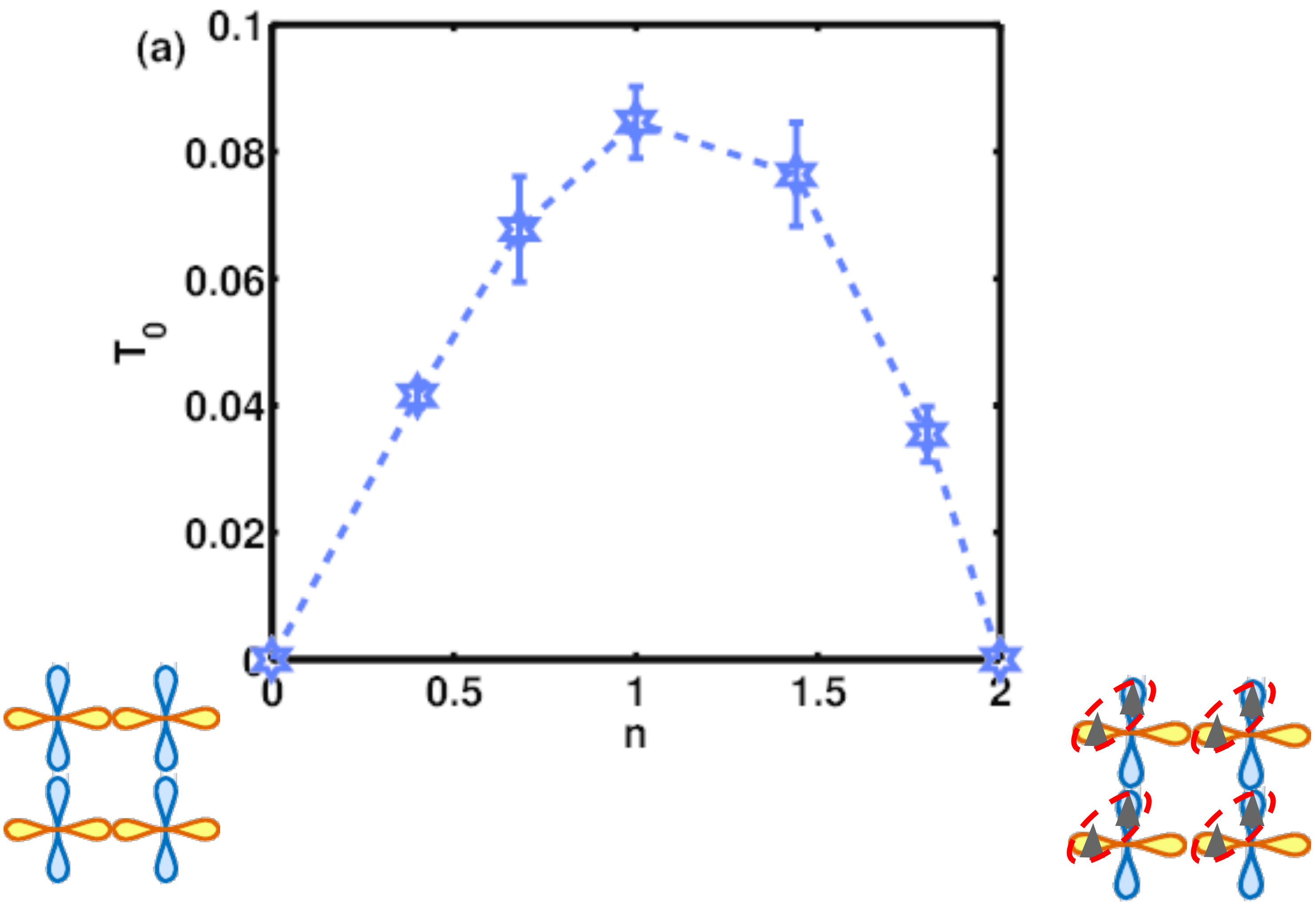
Result: Large V (V=8)



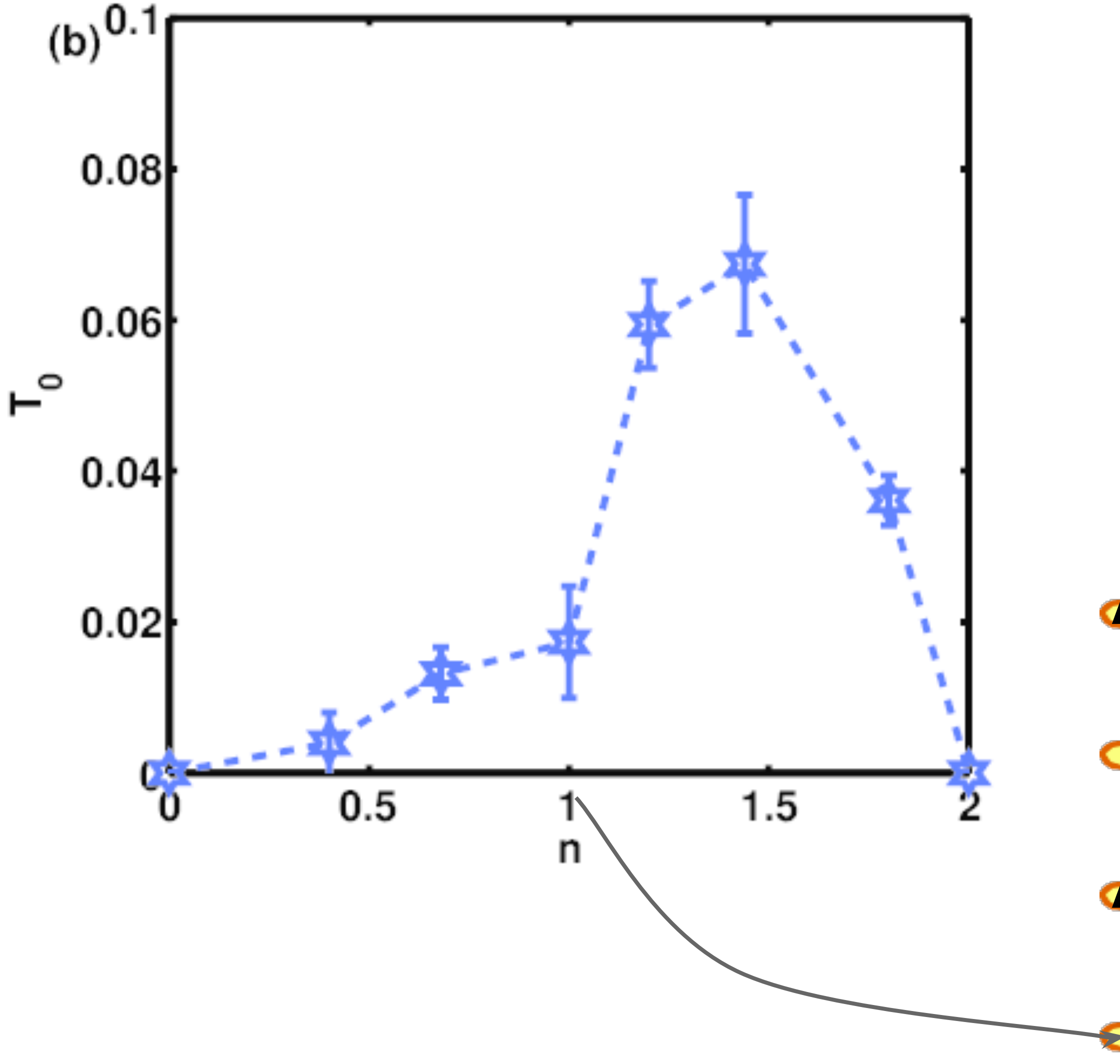
$$E = V$$

Gapped excitation at quarter filling

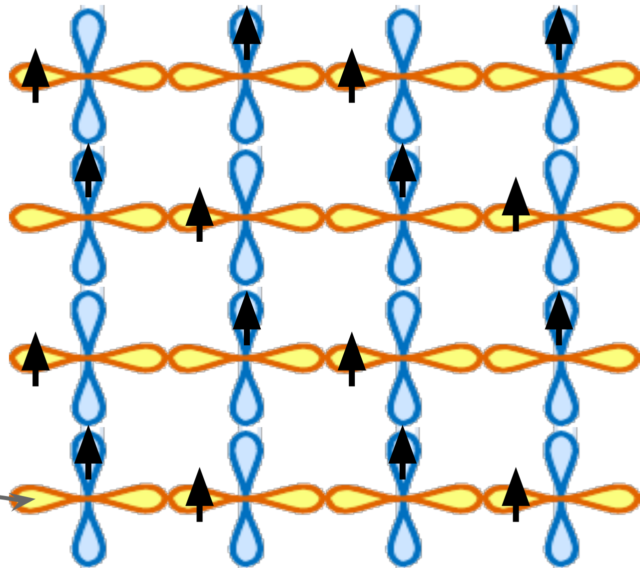
FM energy scale: T_0 (V=0)



FM energy scale: T_0 (V=8)

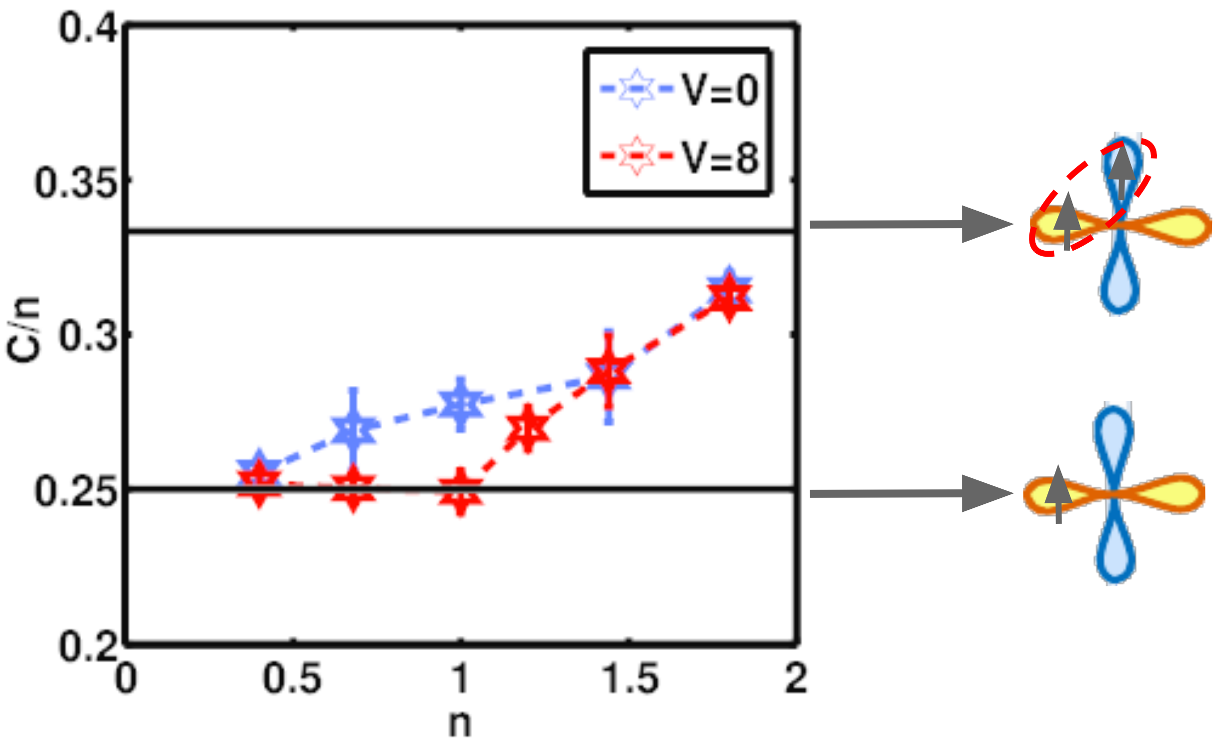


Antiferromagnetic orbital order at quarter filling



The effective moment

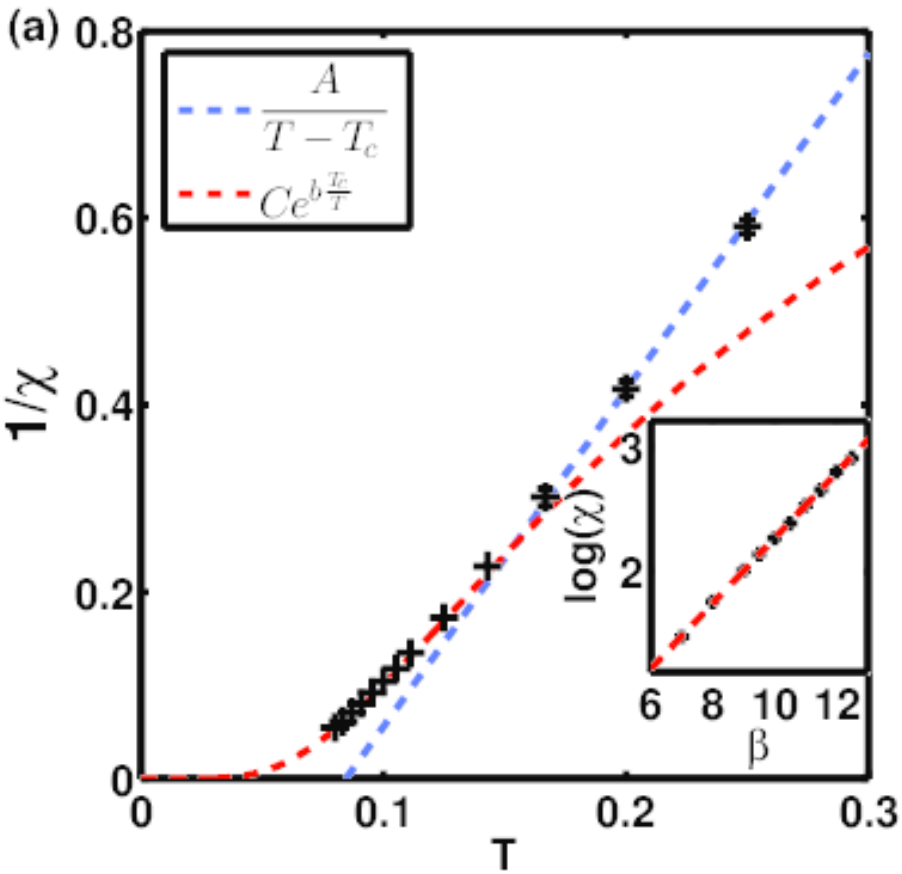
$$c = \frac{1}{3} n_m s(s+1)$$



Spin 1 local moment

Spin ½ local moment

Low temperature



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

D. P. Arovas and A. Auerbach, Phys. Rev. B 38, 316 (1988)

Summary

- Hamiltonian with fully polarized ground state
- Local moment like spin susceptibility
- Metallic compressibility (V=0)
  Antiferromagnetic orbital mott insulator (quarter filling and strong V)
- Spin susceptibility crosses over to exponential growth at low temperature