Quantum Critical Behavior in Geometrically-Frustrated Systems

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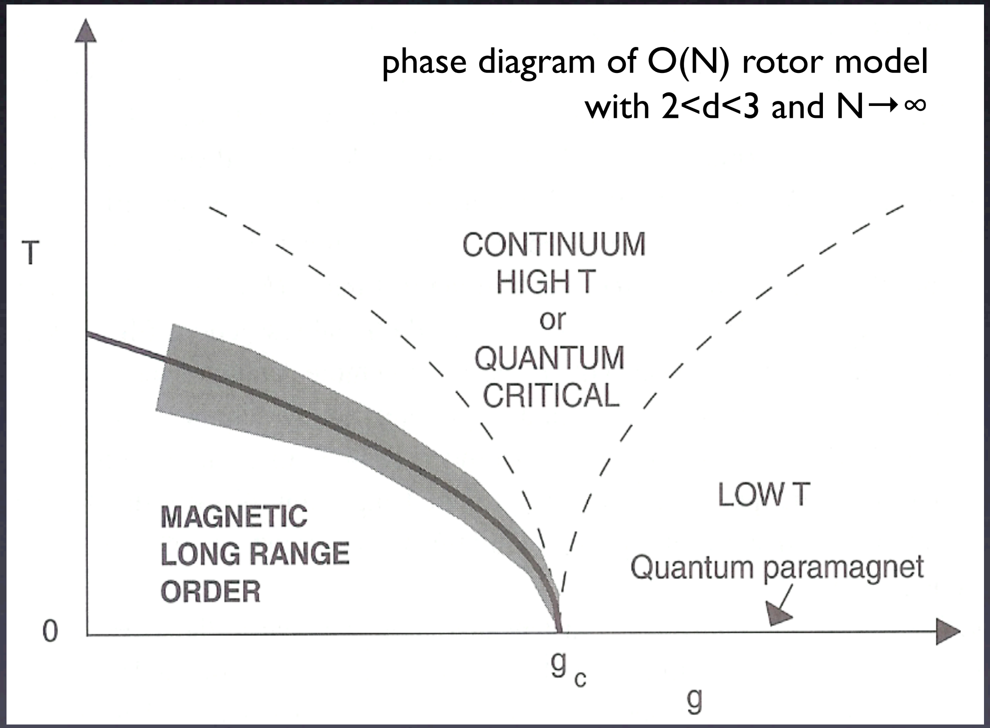
Outline

- scope of this study
- localized spin systems
  - antiferromagnetic Heisenberg model on pyrochlore lattice
- itinerant electron systems
  - Hubbard model on triangular lattice
  - electron systems coupled with classical degrees of freedom

Quantum Critical Point and Related Phenomena

- long-range order is suppressed by tuning parameters, leading to quantum critical point
  - classical scaling regime shrinks as $T_c \rightarrow 0$
  - para phase above is governed by the nature of quantum critical point
- novel states? novel universality class?
- how to control? - frustration and competing interactions



S. Sachdev, *'Quantum Phase Transition'*

Scope of This Study...

- microscopic theory of the quantum critical behavior
  - specific microscopic model - c.f. field theory
  - for both localized spin systems and itinerant electron systems
  - tuning frustration and competing interactions
  - unbiased numerical simulation beyond perturbation, mean-field approximation, ...

Localized Spin Systems

- fingerprint of quantum critical behavior in classical-spin Heisenberg model on pyrochlore lattice

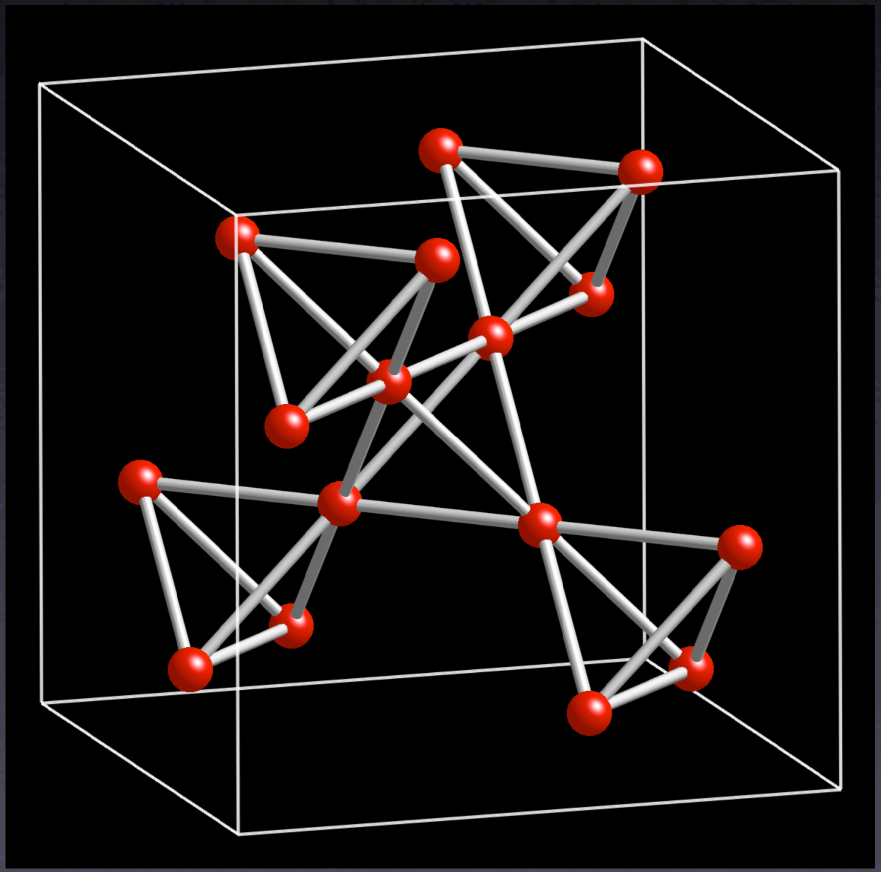
in collaboration with Karlo Penc and Nic Shannon

Pyrochlore Antiferromagnets

- classical Heisenberg model with nearest-neighbor couplings only

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

- severe frustration: no long-range ordering down to T=0
- macroscopic degeneracy in the ground state: classical spin liquid (Moessner and Chalker, 1998)
- power-law spin correlation ~ $1/r^3$ (Henley, 2005)



Perturbations to Classical Spin Liquid State

- further-neighbor exchanges $J_{\mathrm{further}} \sum_{ij} \vec{S}_i \cdot \vec{S}_j$

  → magnetic (dipole) long-range order

- biquadratic interaction $-b \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j)^2$

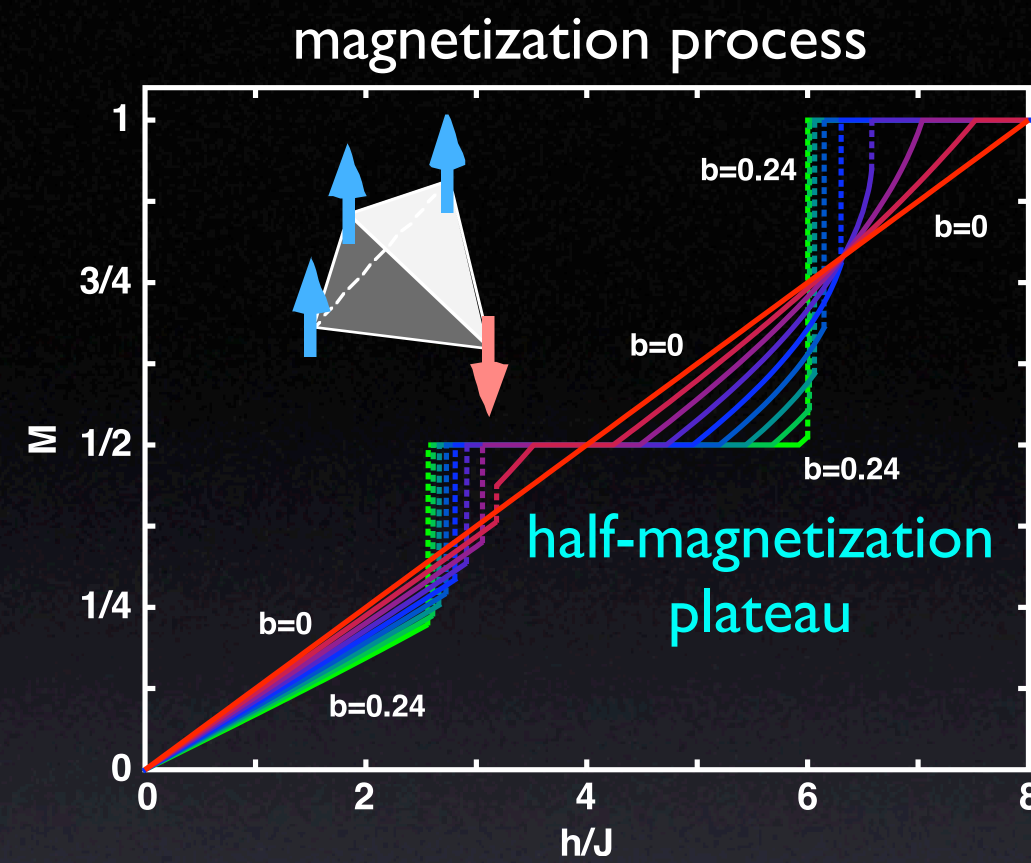
  → spin nematic (quadrupole) order

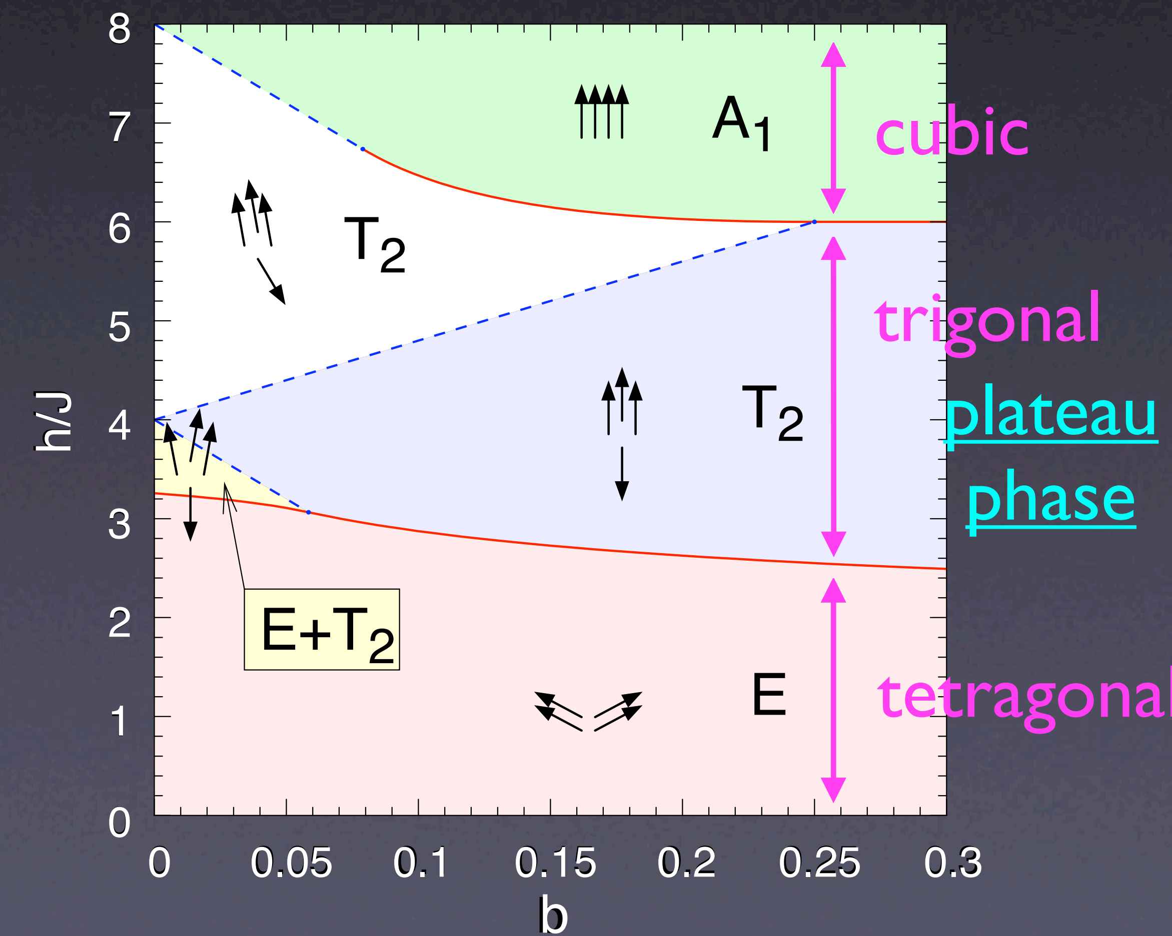
- external magnetic field $-\sum_i \vec{h} \cdot \vec{S}_i$

Results at T=0

Penc *et al.*, 2004

- solutions for 4-sublattice ordering with wave vector $\boldsymbol{q}$=0 ($J_{further}$ are implicitly taken into account)
- for finite biquadratic coupling b>0: half-magnetization plateau (blue area in the phase diagram)
- 3-up 1-down collinear state in each tetrahedron unit



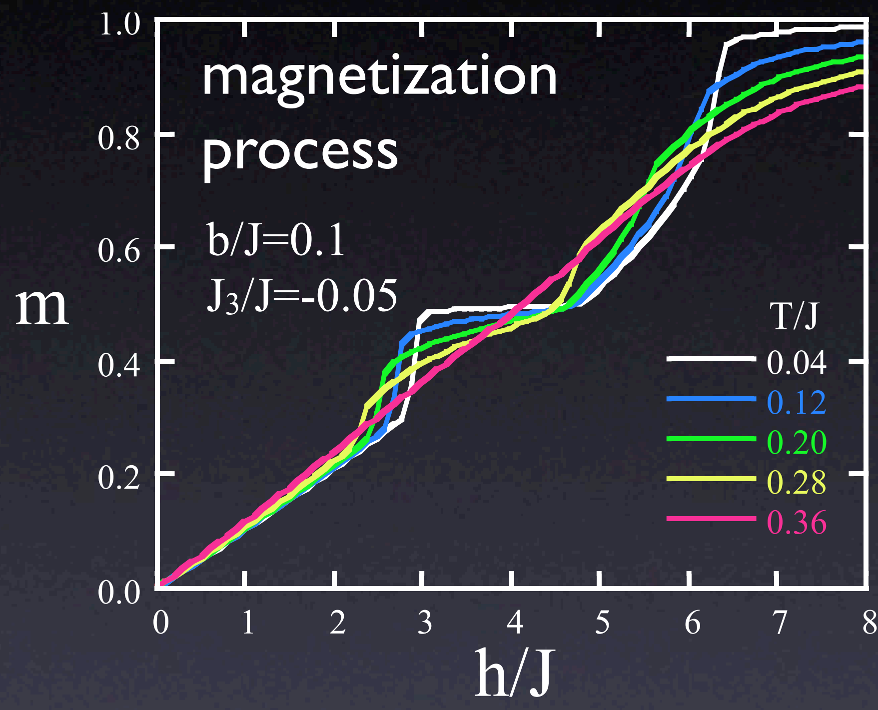


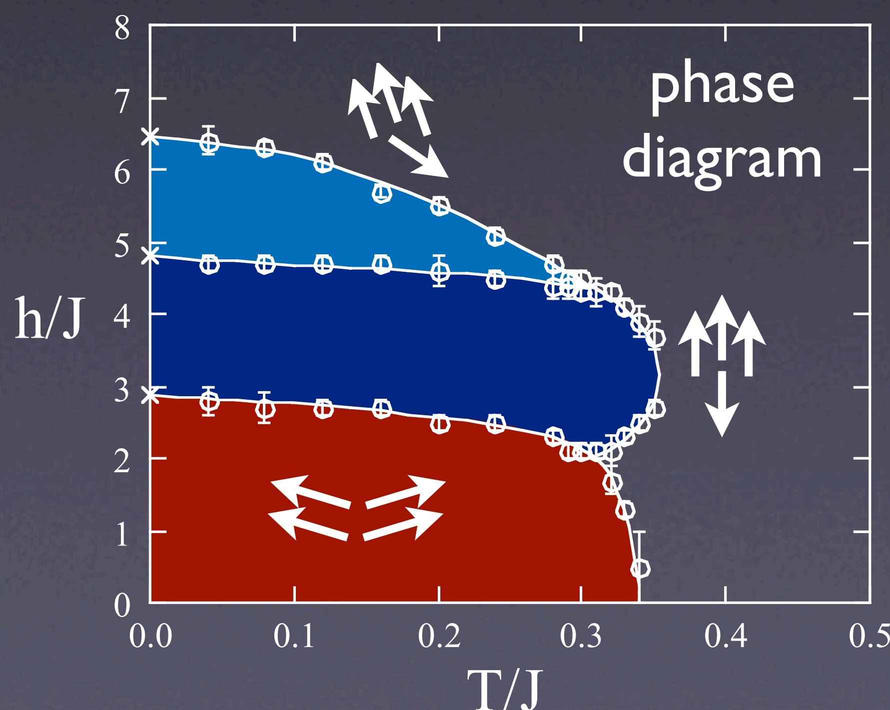
Monte Carlo Results at Finite Temperatures

- plateau remains robust at finite temperatures
- all the phases show magnetic (dipole) ordering, stabilized by $J_{further}$

  $T_c \sim O(zJ_{further})$

- good agreement with experiments in Cr spinels, $HgCr_2O_4$ and $CdCr_2O_4$
  (H. Ueda *et al.*, 2005, unpublished)





Question

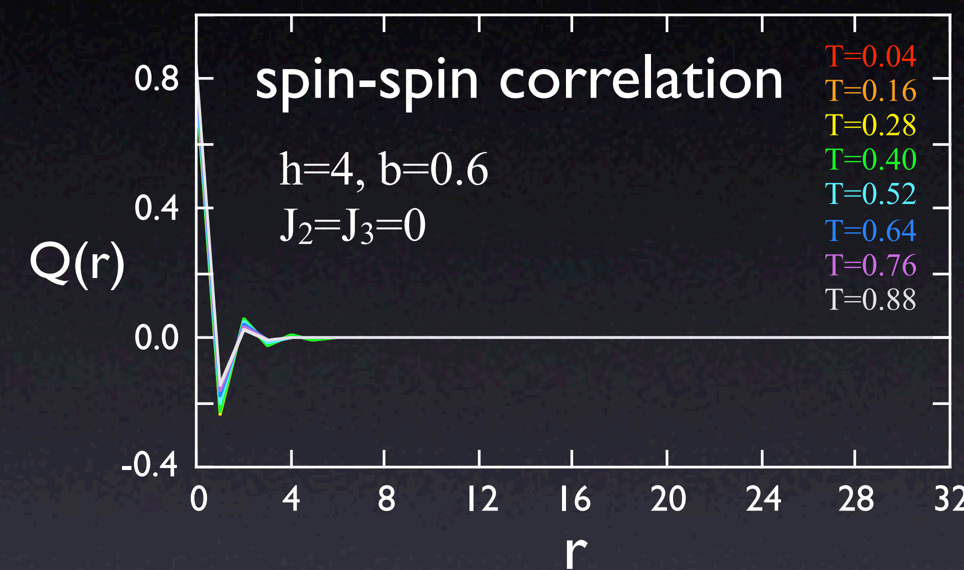
- ✓ energy scale of magnetic (dipole) ordering is set by $J_{further}$: T_c goes to zero as $J_{further} \rightarrow 0$

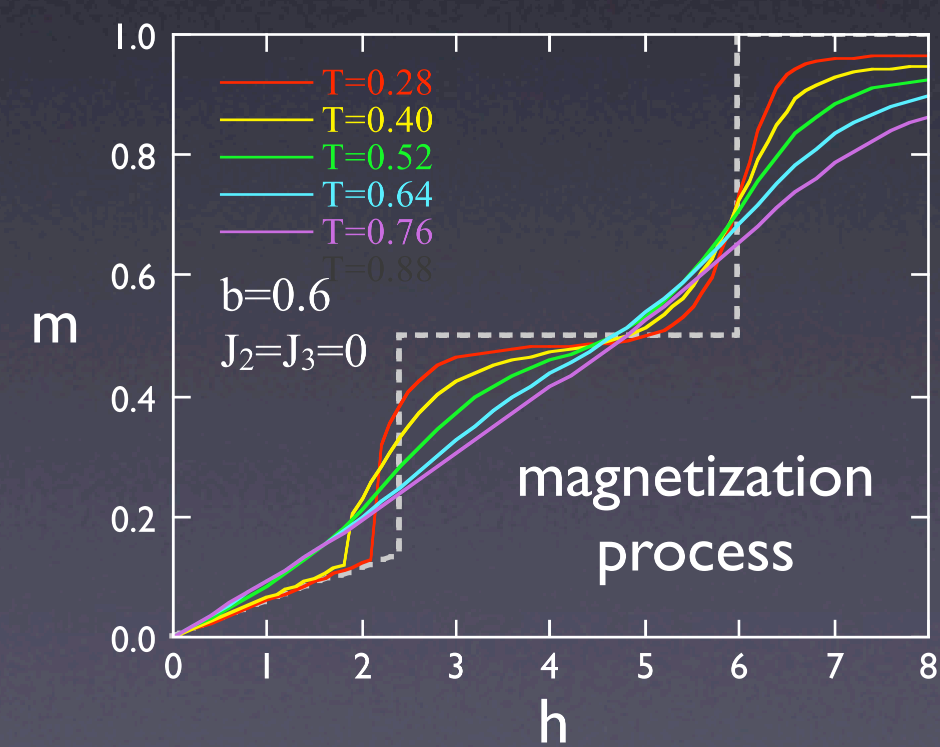
- What happens when $J_{further} \rightarrow 0$, i.e. $T_c \rightarrow 0$? Does the plateau disappear? Degeneracy? Fingerprint of quantum critical behavior?

‘Spin-liquid’ Plateau

- $J_{further} \rightarrow 0$, but a finite b
- nearest-neighbor coupling only: no magnetic order down to the lowest temperature
- *But* the plateau survives as the case with dipole ordering.

…Why? How?





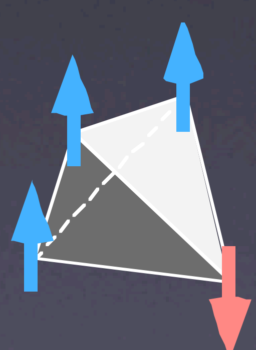
Spin Collinearity grows...

- spin collinearity rapidly grows at T* and becomes long range at low T

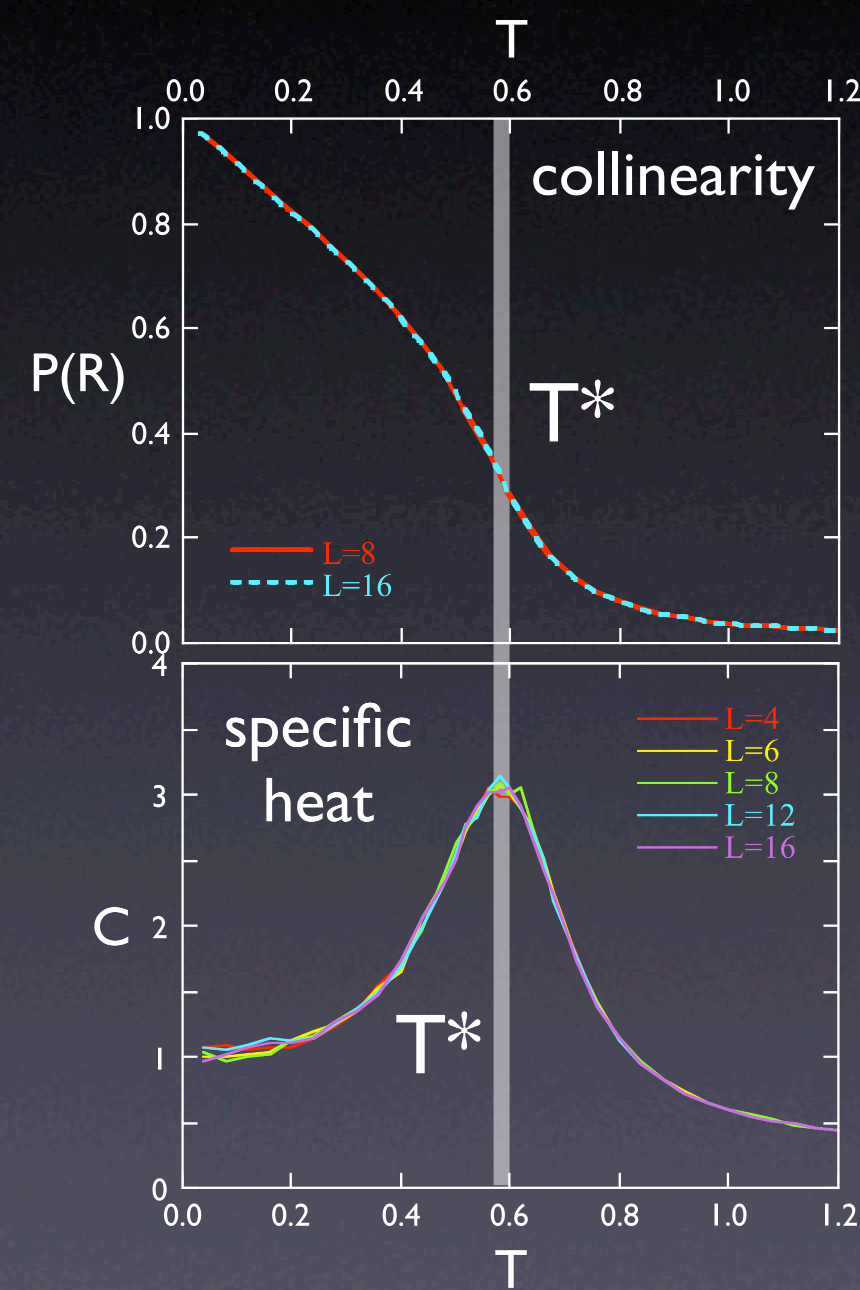
$$P(\vec{r}_{ij}) = \frac{3}{2}\left[\langle(\vec{S}_i \cdot \vec{S}_j)^2\rangle - \frac{1}{3}\right]$$

- crossover temperature T* corresponds to a broad peak of the specific heat

  entropy release from ‘↑↑↑↓’ formation



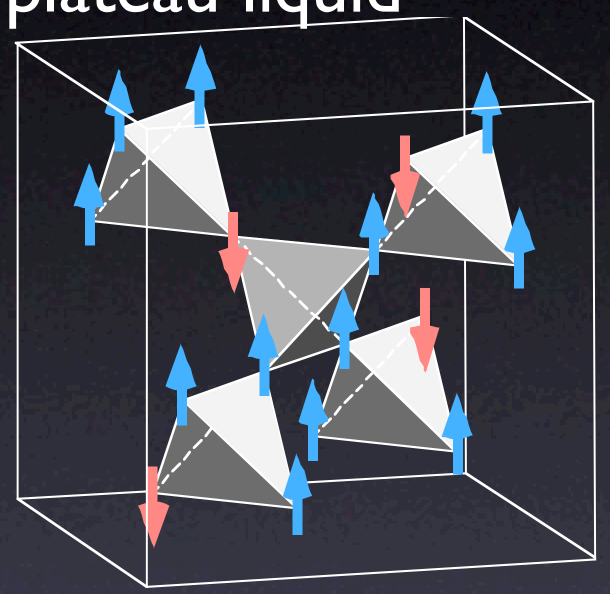
- T* scales to b



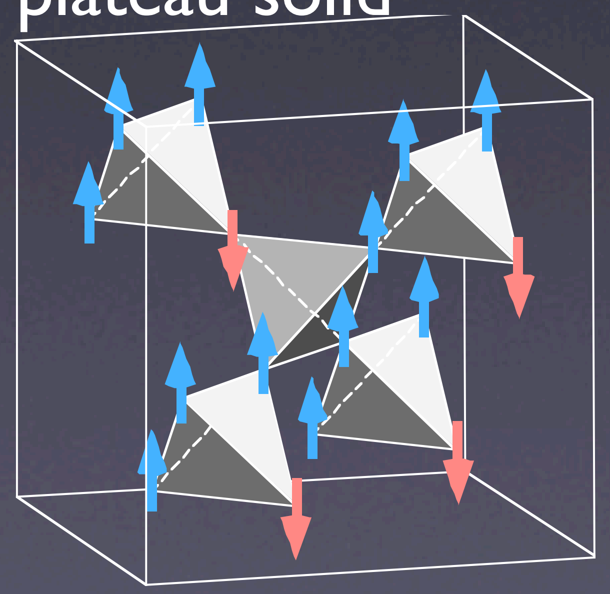
Spin 'Pseudogap' State with Macroscopic Degeneracy

- pyrochlore is corner-sharing network of tetrahedra - loose connection
- b term selects ↑↑↑↓ state in each tetrahedron, but the position of ↓ may be incoherent: collinear state without any magnetic order
- macroscopic degeneracy ~1.3^N
- spin gap persists - 'pseudogap'

plateau liquid

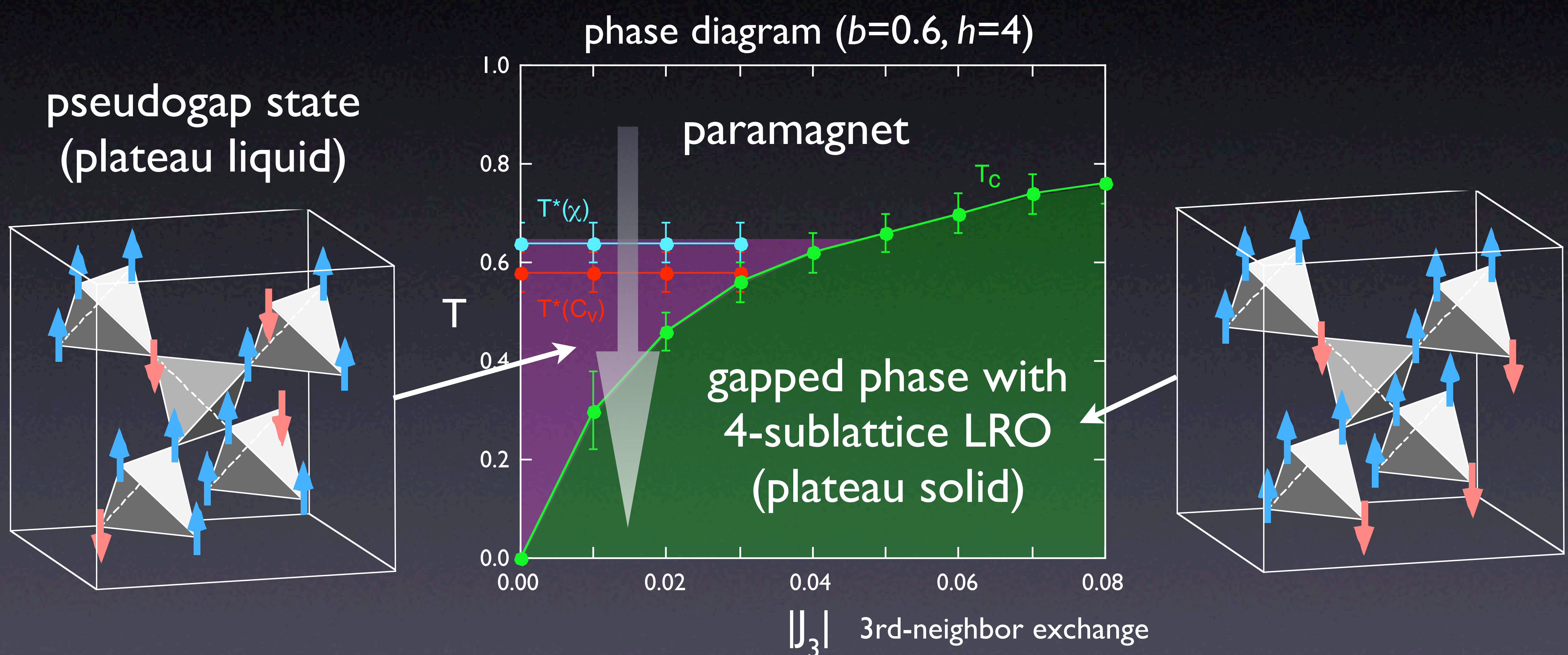


plateau solid



Pseudogap vs Gapped LRO

Plateau 'Liquid-Solid' Transition



para → preformed local order with pseudo gap
→ gapped long-range ordered phase

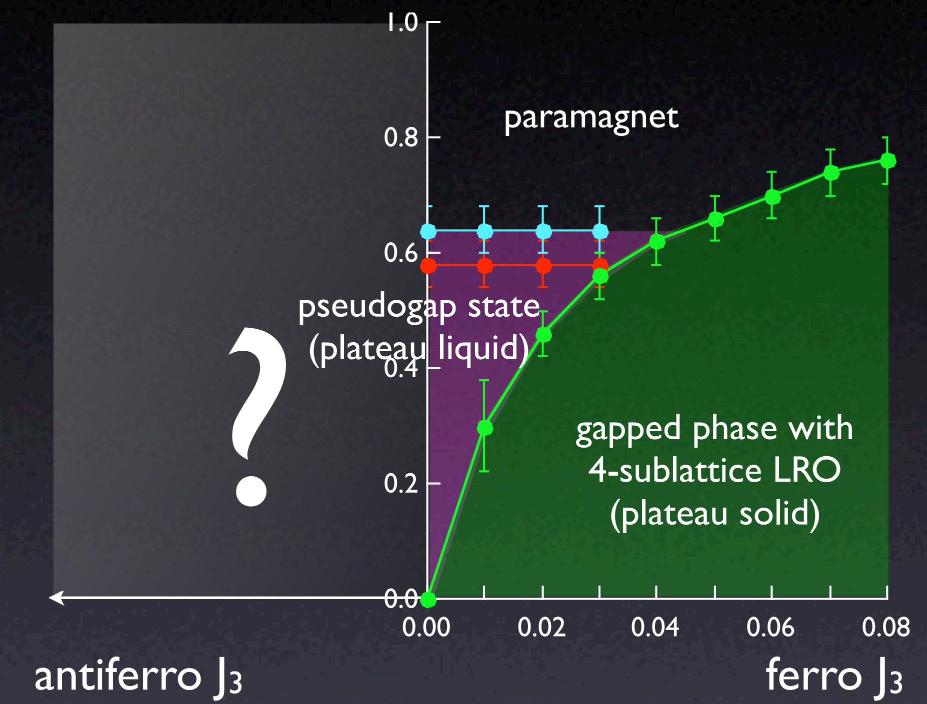
Perspectives...

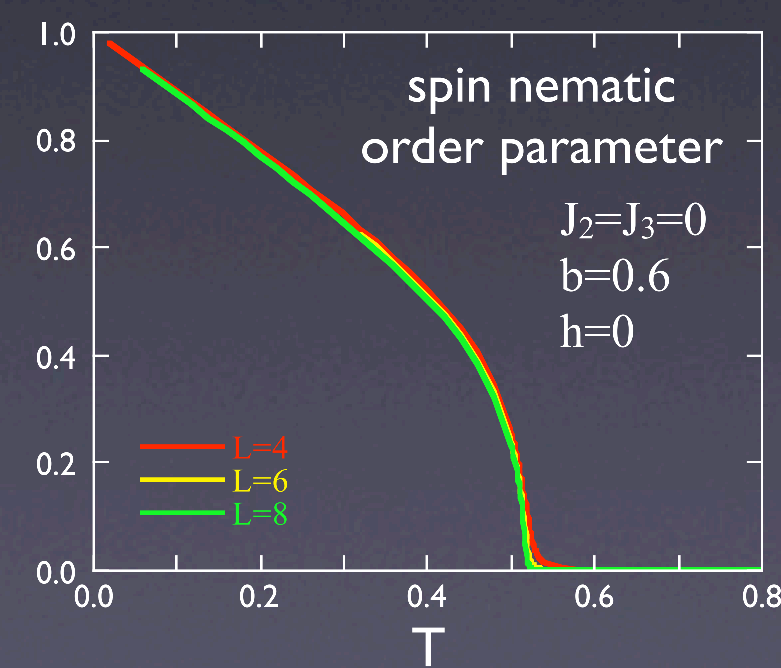
- systematic study of the (h-b-$J_{further}$-T) phase diagram

  competing phases at the critical point? order from disorder?

- critical phenomena of the spin nematic (quadrupole) transition

- effects of quantum fluctuations





Itinerant Electron Systems
(ongoing projects...)

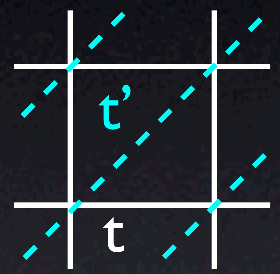
- Hubbard model on frustrated lattices

  in collaboration with Takashi Koretsune and Akira Furusaki

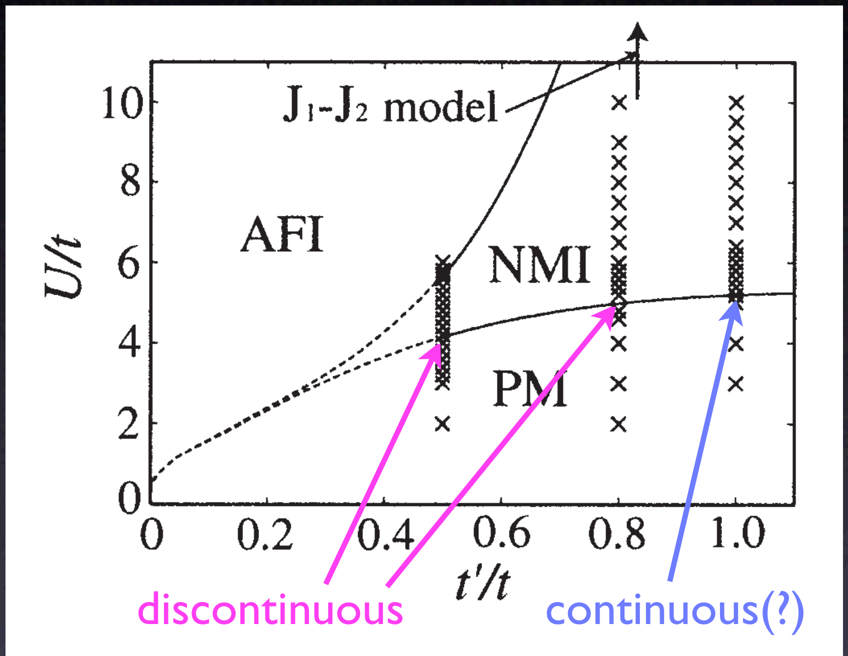
- electron systems coupled with classical degrees of freedom

Frustrated Hubbard Model at zero temperature

- Hubbard model on anisotropic triangular lattices

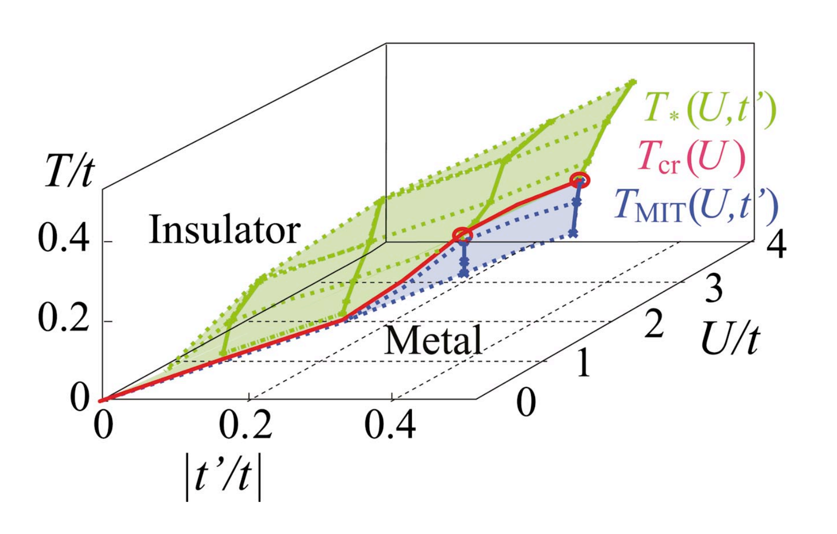


- PIRG results: phase transitions between para-metal and non-magnetic insulator
  - discontinuous at t'<t
  - (plausibly) continuous at t'~t



Morita, Watanabe and Imada, 2002

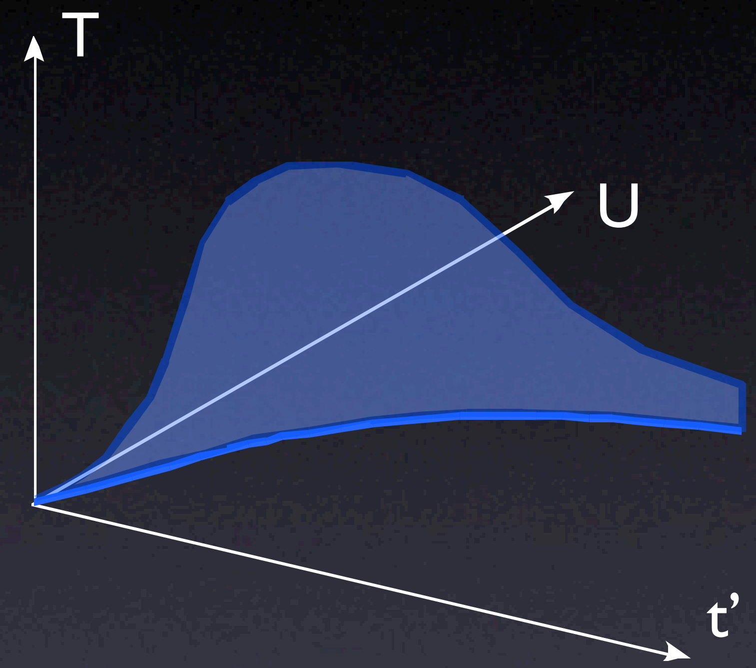
- correlator-projection results: 1st-order transition surface with a finite-T critical end curve for small t'/t

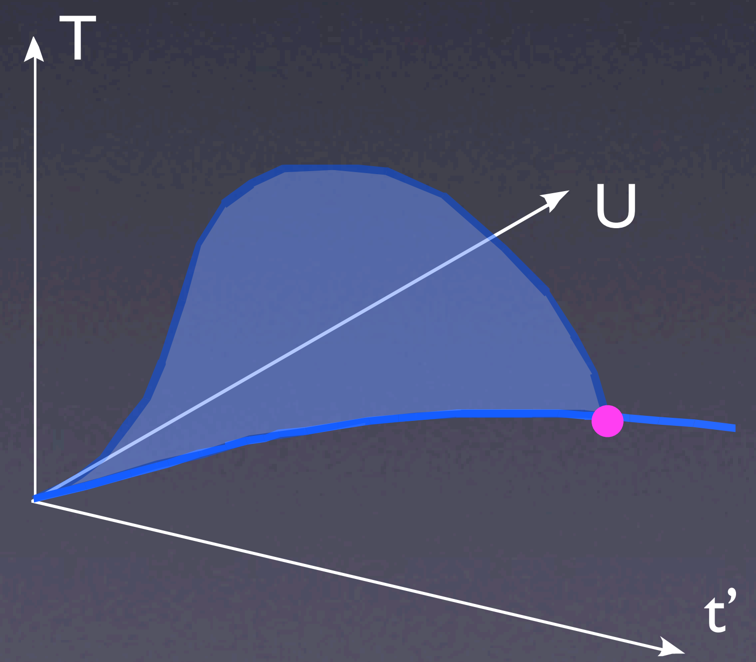


Onoda and Imada, 2003

Scope...

- quantum critical point ?
- If yes, what is the nature of quantum critical point ?
  - scaling arguments (Imada, 2005)
- Does dimensionality matter ?
  - cf. D=∞ result
- different approaches from PIRG
  - transcorrelated method, finite-T Lanczos method (Koretsune, P-07)





Electron Systems Coupled with Classical Degrees of Freedom

Holstein model $$H = -\sum_{ij} t_{ij} (c_i^\dagger c_j + \mathrm{H.c.}) - g \sum_i n_i x_i + \frac{k}{2} \sum_i x_i^2$$ electron-phonon

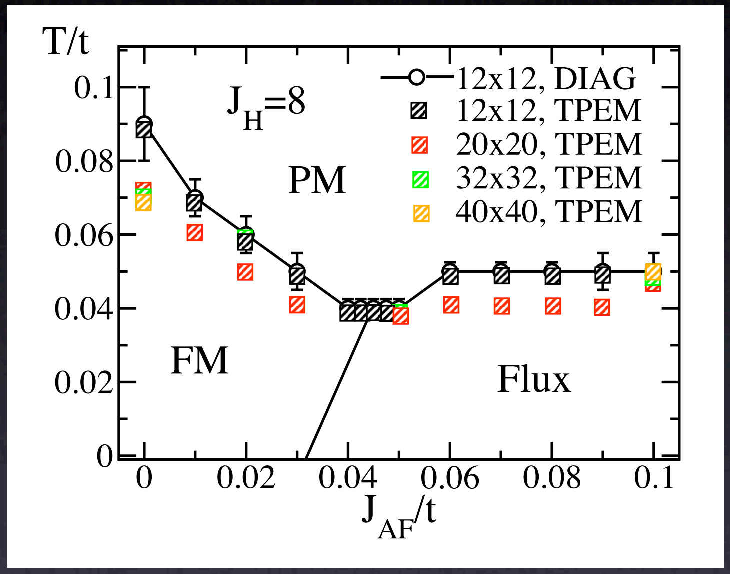
double-exchange model $$H = -\sum_{ij,\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.}) - J_{\mathrm{H}} \sum_i \vec{\sigma}_i \cdot \vec{S}_i$$ electron-spin

Falicov-Kimball model $$H = -\sum_{ij} t_{ij} (c_i^\dagger c_j + \mathrm{H.c.}) + U \sum_i c_i^\dagger c_i d_i^\dagger d_i$$ electron-charge

- rich physics: metal-insulator transition, magnetism, ...
- advantages:
  - no negative-sign problem in Monte Carlo simulation even in frustrated systems
  - order-*N* method (Furukawa and Motome, 1999, 2000, 2004)

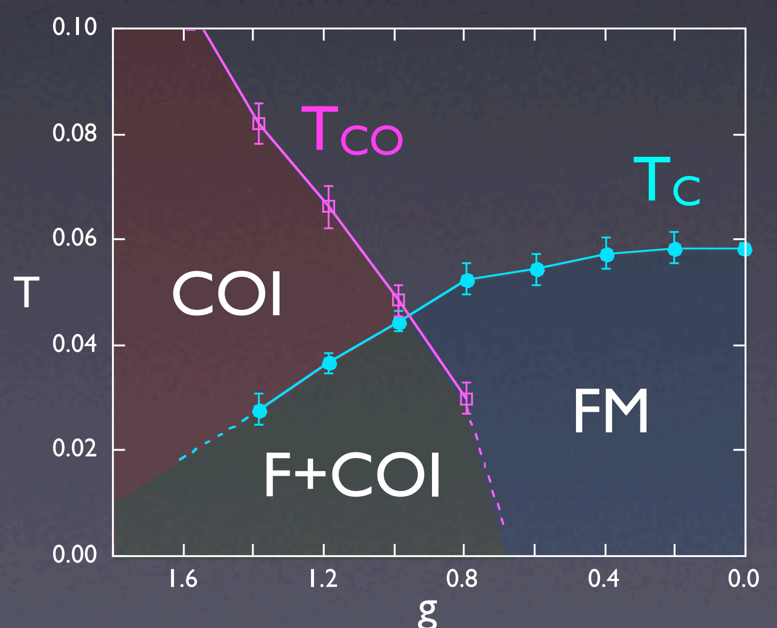
Example: Extended Double-Exchange Models

$$H = -\sum_{ij,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{H.c.}) - J_{\mathrm{H}}\sum_{i}\vec{\sigma}_i \cdot \vec{S}_i + \sum_{ij} J^{\mathrm{AF}}_{ij}\vec{S}_i \cdot \vec{S}_j - g\sum_{i} n_i x_i + \frac{k}{2}\sum_{i} x_i^2$$



Sen *et al.*, unpublished

- possible phase competitions at quarter filling in unfrustrated cases:
  - FM vs AFI (flux type)
  - FM vs COI (checkerboard type)



- frustration → collapse of the commensurate orderings

Is it possible to investigate quantum critical behavior ?

Blueprints...

- localized spin systems
  - further study of pyrochlore antiferromagnetic Heisenberg model
  - quantum vs. thermal fluctuations?
  - other systems?
- itinerant electron systems
  - Hubbard model on frustrated lattices
  - electron systems coupled with classical degrees of freedom