Title: Quantum Spin Simulations (PHYS 7380) - Lecture 4

Date: Apr 08, 2010 11:00 AM

URL: http://pirsa.org/10040046

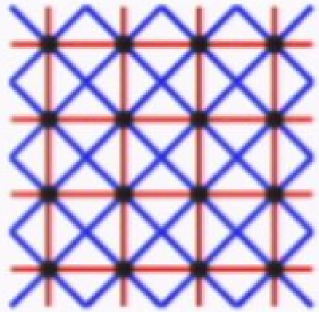
Abstract:

Frustration due to longer-range antiferromagnetic interactions in 2D

Quantum phase transitions as some coupling (ratio) is varied

J$_1$-J$_2$ Heisenberg model is the prototypical example

$$H = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



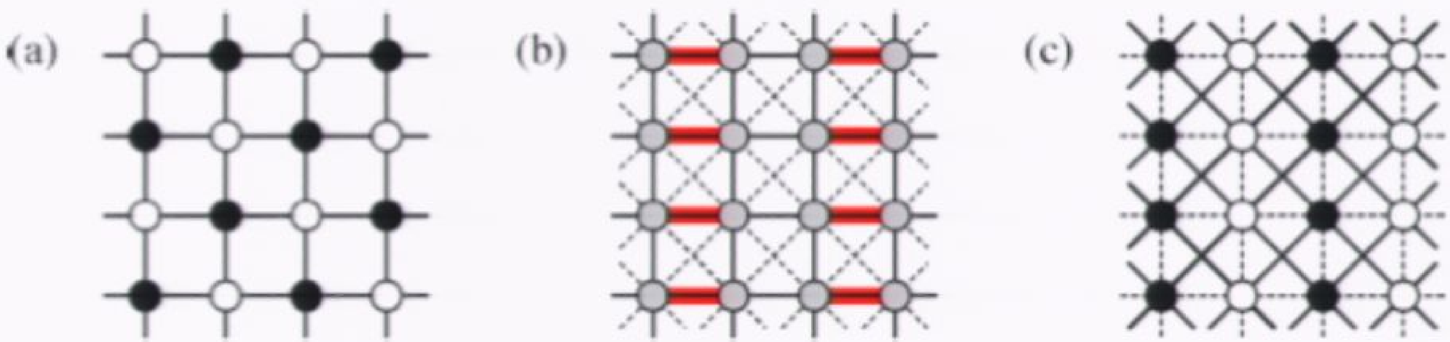
$— = J_1$

$— = J_2$

$$g = J_2/J_1$$

Ground states for small and large g are well understood

- Standard Néel order up to g≈0.45
- collinear magnetic order for g>0.6



$0 \le g < 0.45$ $\quad$ $0.45 \le g < 0.6$ $\quad$ 0 6

A non-magnetic state exists between the magnetic phases

- Most likely a VBS (what kind? Columnar or “plaquette?)
- Some calculations (interpretations) suggest spin liquid

Deconfined quantum criticality

[Senthil et al., Science 303, 1490 (2004)]

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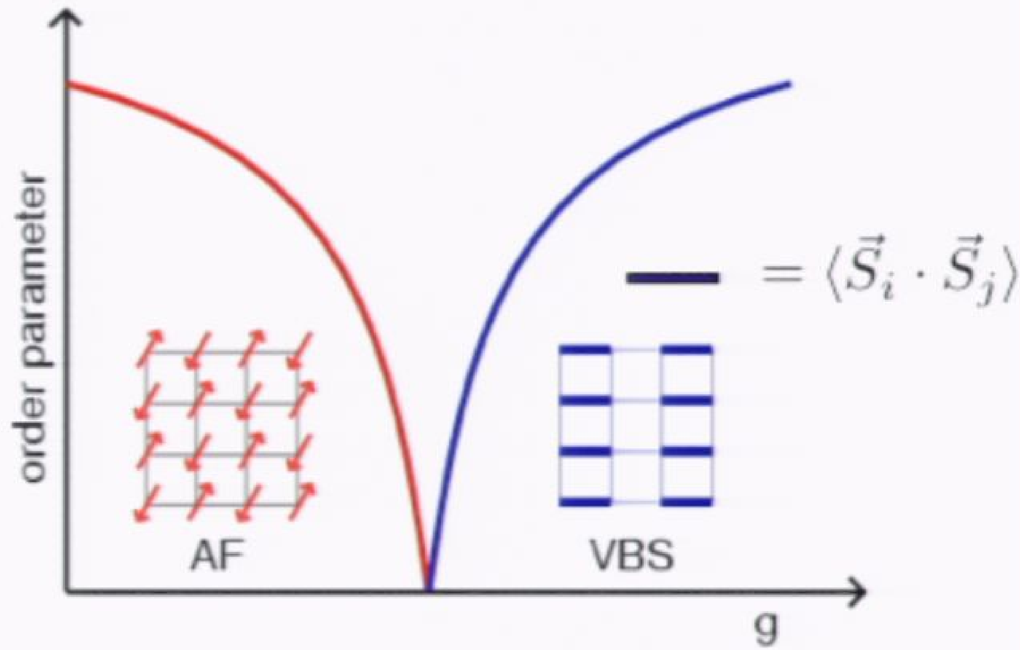

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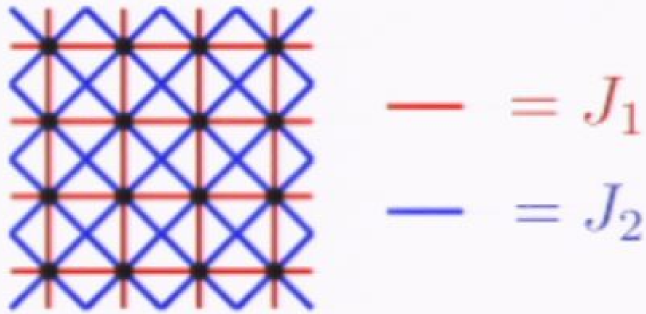

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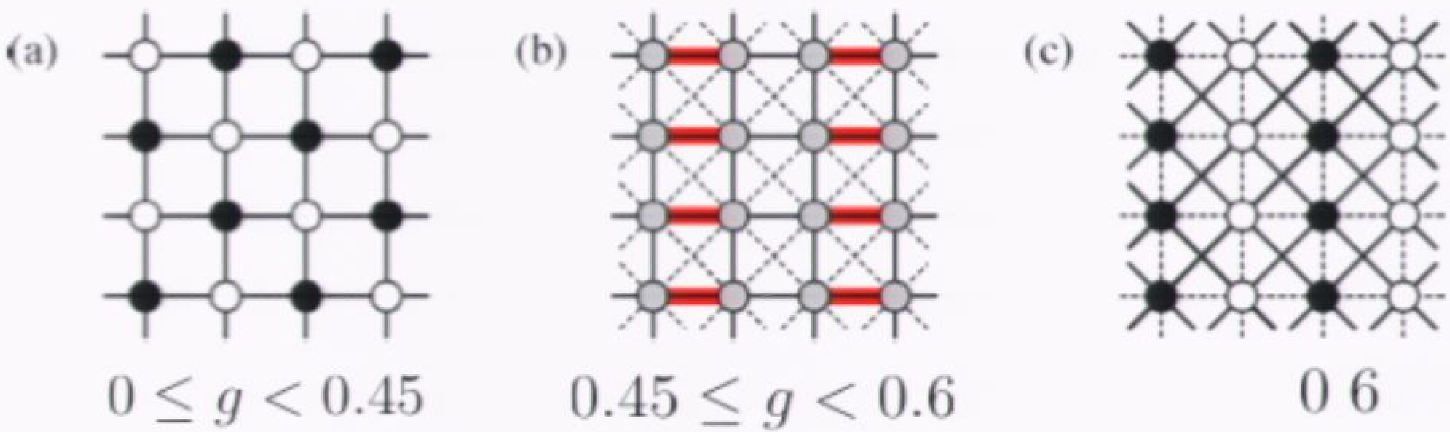

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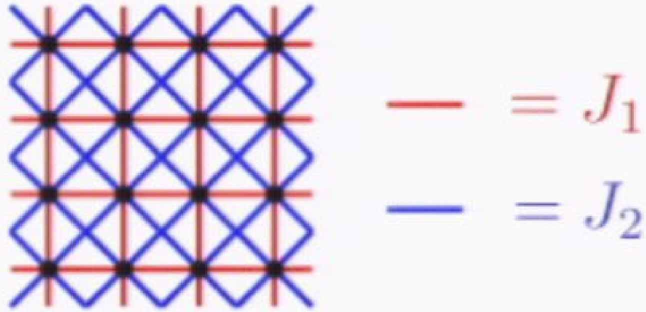

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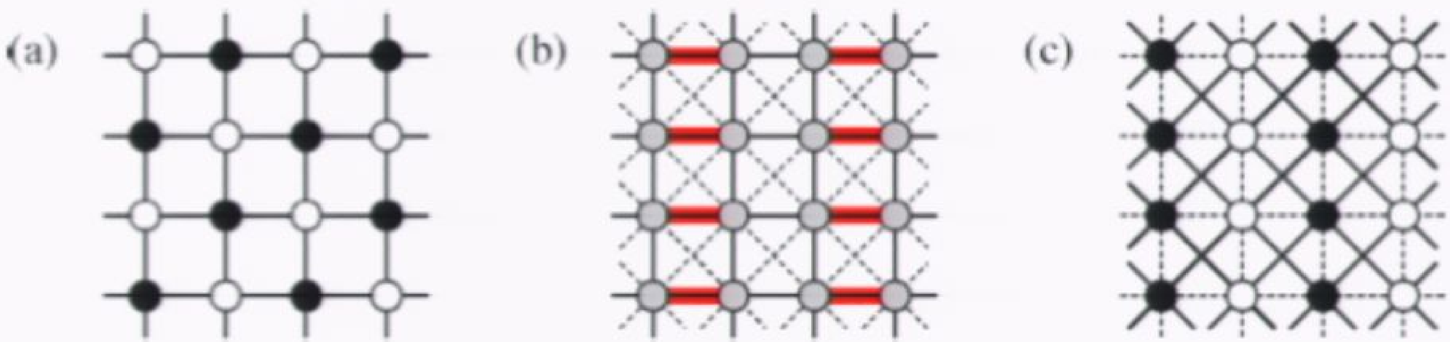

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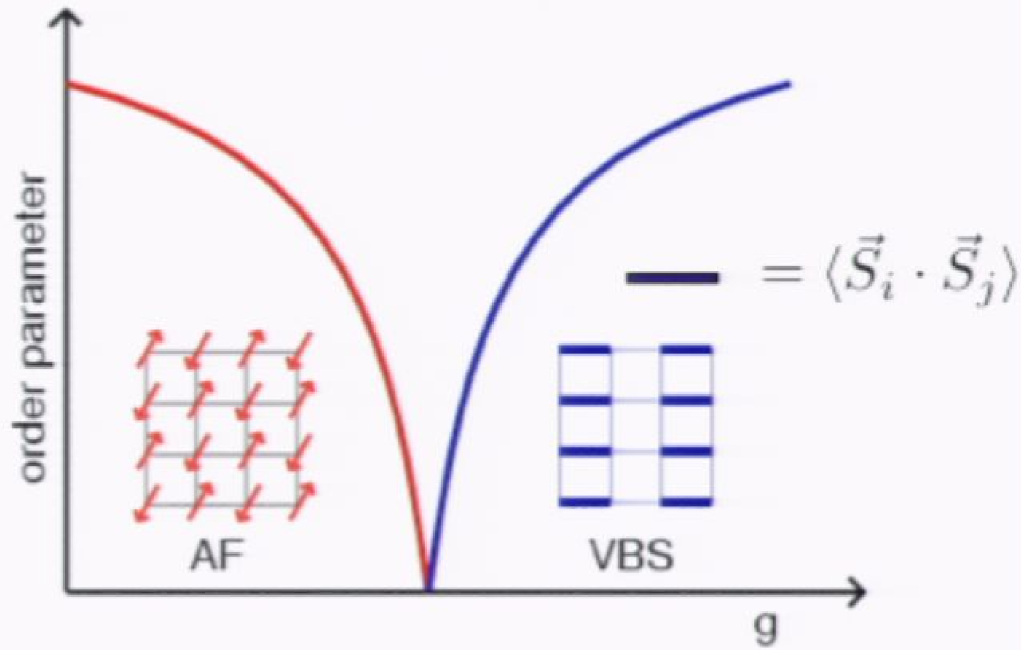
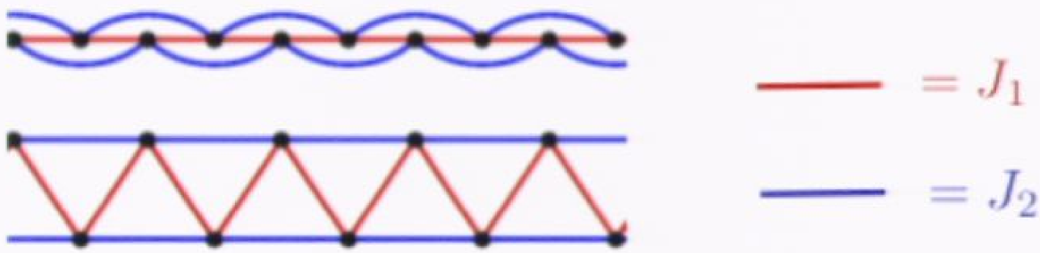


S=1/2 Heisenberg chain with frustrated interactions



Different types of ground states, depending on the ratio **$g=J_2/J_1$** (both >0)

Conditions on magnetic order: The Mermin-Wagner theorem

A continuous symmetry cannot be broken for

- a 2D system (classical or quantum-mechanical) at T>0
- a 1D system at T=0,T>0
  - quantum to classical mapping gives 2D T>0 system (path integral)

The Heisenberg model has a continuous symmetry

- spin-rotation invariance [global SU(2) rotation invariance]
- so cannot have Néel order at T>0 in 2D and not at all in 1D

2D Heisenberg model (e.g., square lattice)

- spin correlation length diverges exponentially fast as T→0

$$C(r_{ij}) = \langle \vec{S}_i \cdot \vec{S}_j \rangle \sim (-1)^{x_{ij}+y_{ij}} \mathrm{e}^{-r_{ij}/\xi}, \quad \xi \to \infty \text{ as } T \to 0$$

1D Heisenberg chain (S = 1/2, 3/2, ...)

- spin correlations decay algebraically (almost) at T=0

$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \frac{\ln^{1/2}(r/r_0)}{r}, \qquad (T=0)$$

1D Heisenberg chain (S = 1, 2, ...)

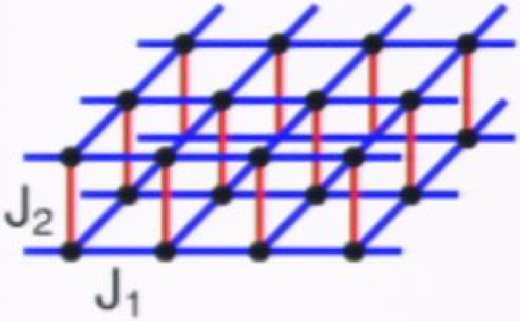
- spin correlations decay exponentially at T=0 (the “Haldane conjecture”)

$$C(r) = \langle \vec{S}_i \cdot \vec{S}_{i+r} \rangle \sim (-1)^r \mathrm{e}^{-r/\xi_S} \qquad \xi_S \to \infty \text{ as } S \to \infty$$

Quantum phase transitions (T=0; change in ground-state)

Example: Dimerized S=1/2 Heisenberg models

- every spin belongs to a dimer (strongly-coupled pair)
- many possibilities, e.g., bilayer, dimerized single layer



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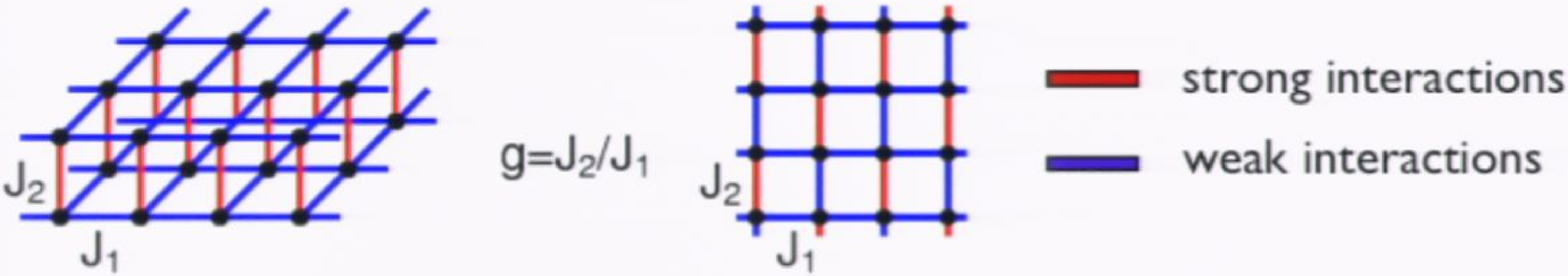
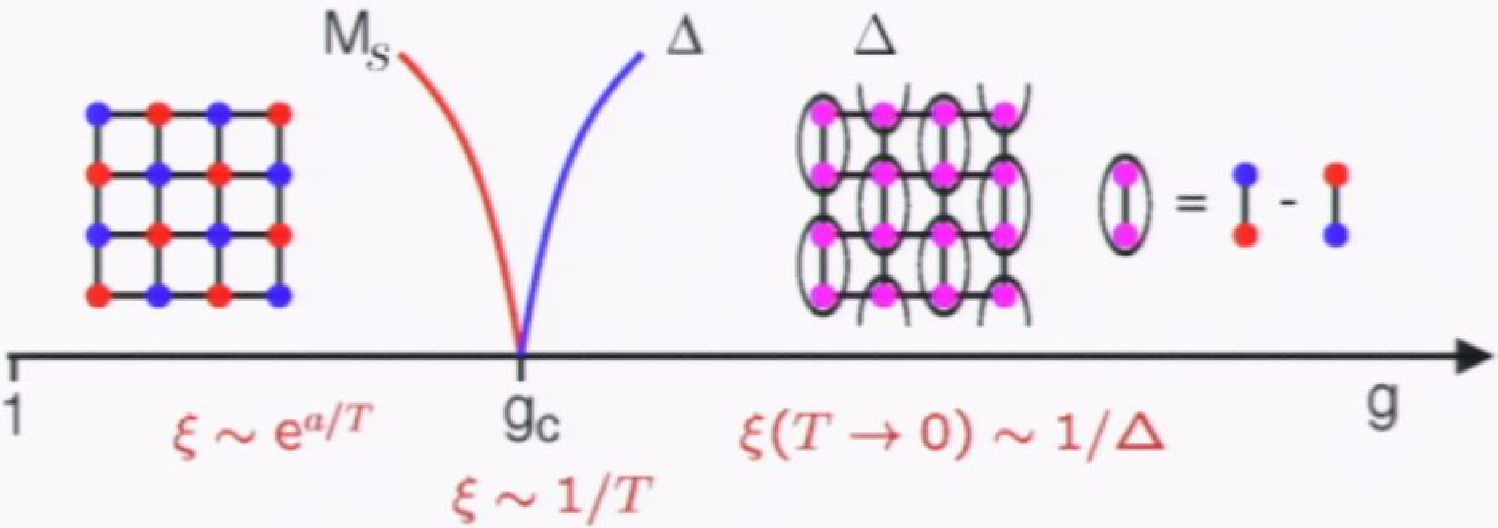


Singlet formation on strong bonds → Neel - disordered transition

Ground state (T=0) phases



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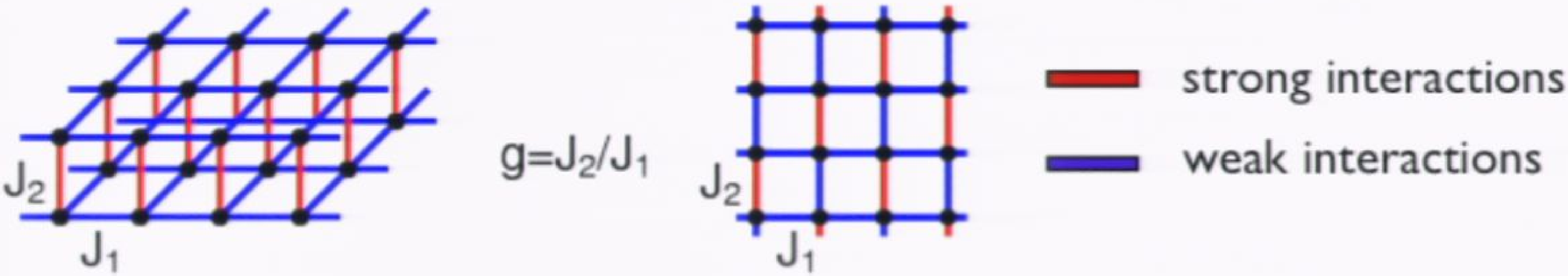

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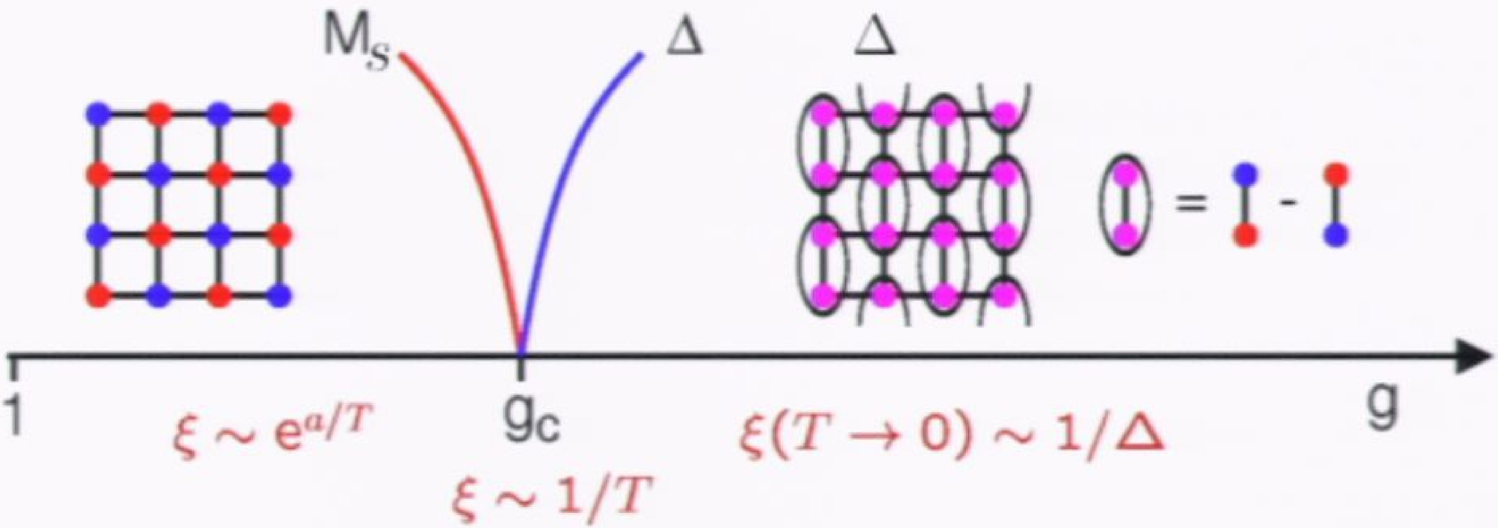
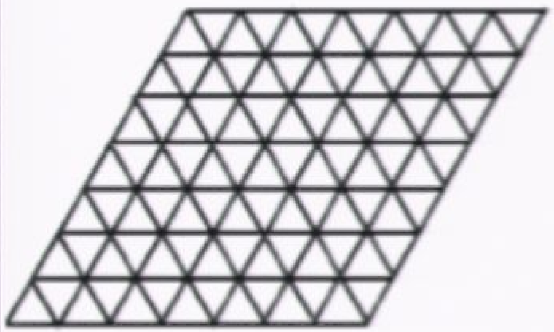


2D quantum spins map onto (2+1)D classical spins (Haldane)

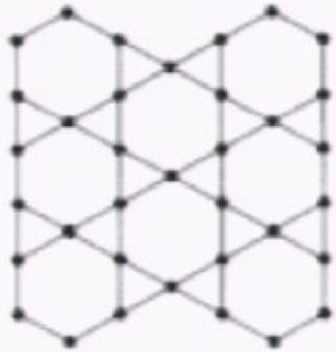
Frustration in higher dimensions

There are many (quasi-)2D and 3D materials with **geometric spin frustration**

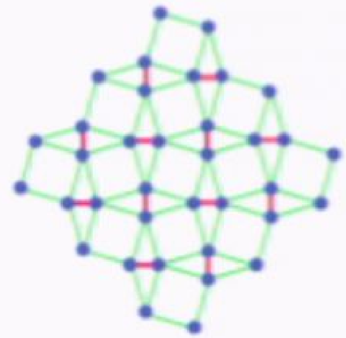
- no classical spin configuration can minimize all bond energies



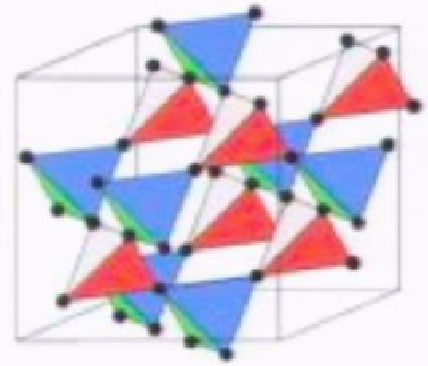
triangular (hexagonal)



Kagome



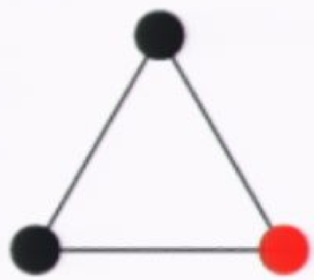
$SrCu_2(BO_3)_2$ (Shastry-Sutherland)

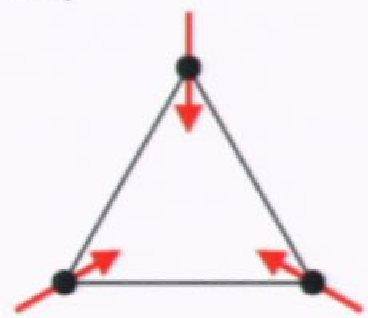


Pyroclore

A single triangular cell:

- 6-fold degenerate Ising model
- "120° Néel" order for vectors





Infinite triangular lattice

- highly degenerate Ising model (no order)
- "120° Néel" (3-sublattice) order for vectors

S=1/2 quantum triangular Heisenberg model

- the classical 3-sublattice order most likely survives [White and Chernyshev, PRL 2007]

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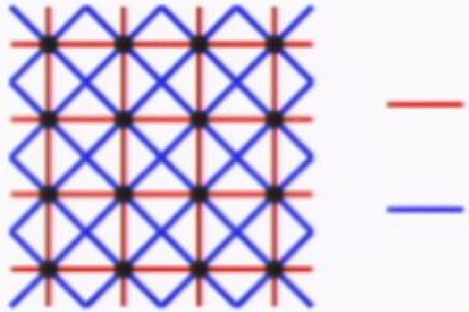

$= J_1$

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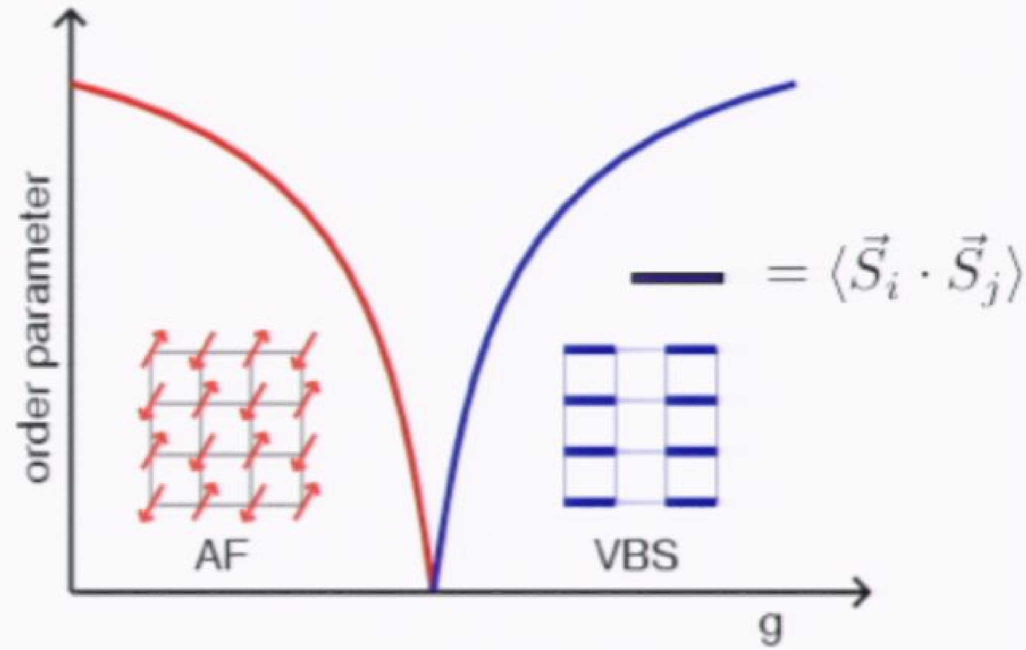

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  - theory of deconfined quantum critical points has continuous transition
- nature of the VBS fluctuations?
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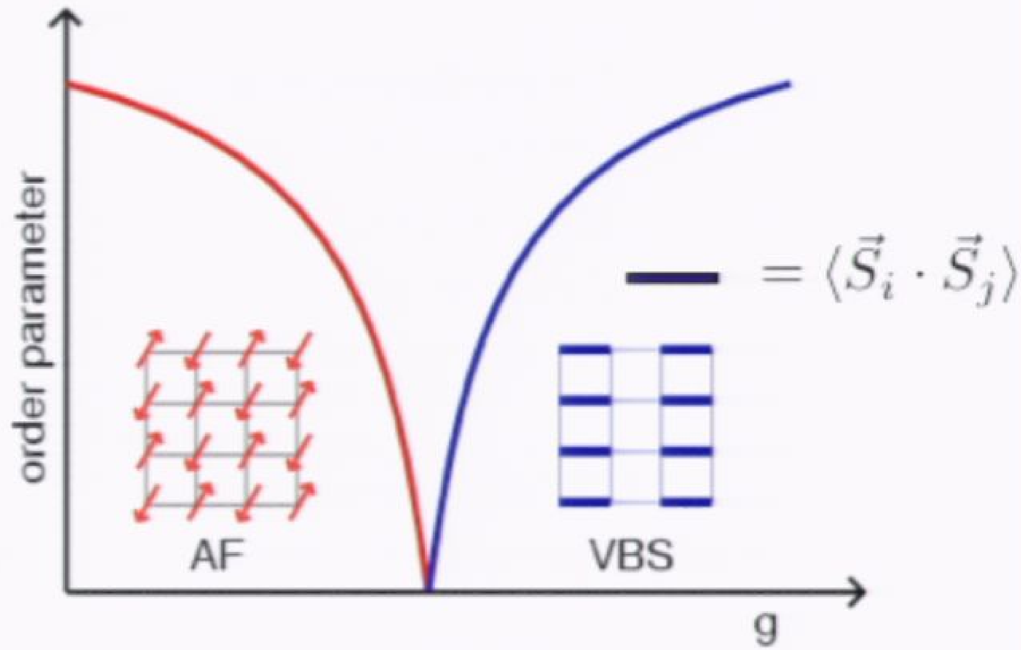

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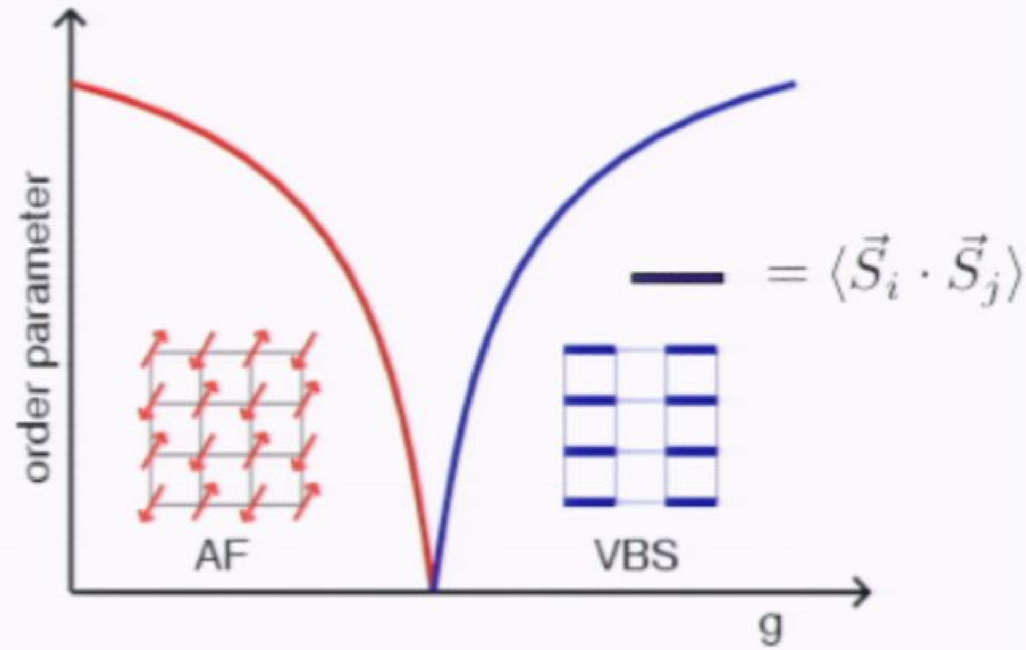
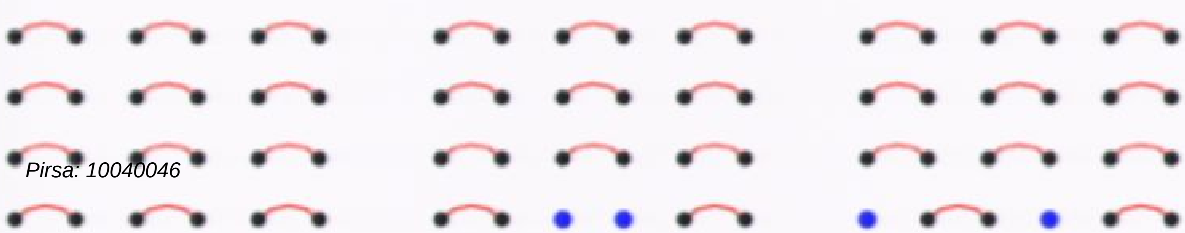


Spinon deconfinement upon approaching the critical point



Confinement inside VBS phase associated with new length scale and emergent

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- the theory is based on continuum field-theory (Lagrangian)
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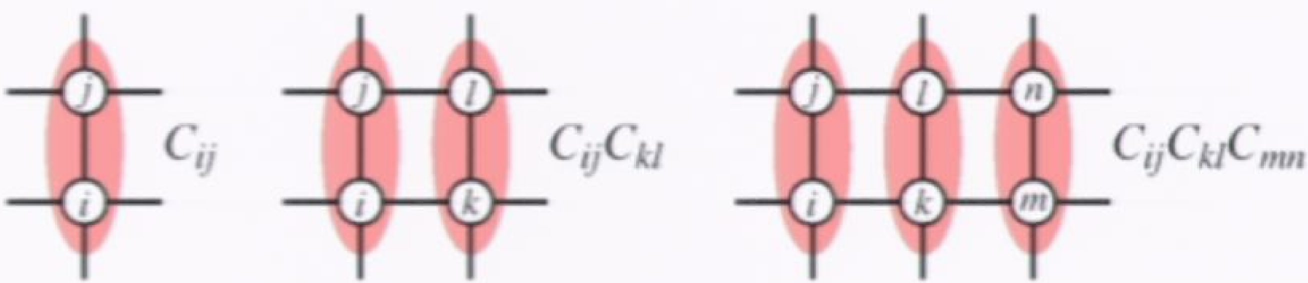

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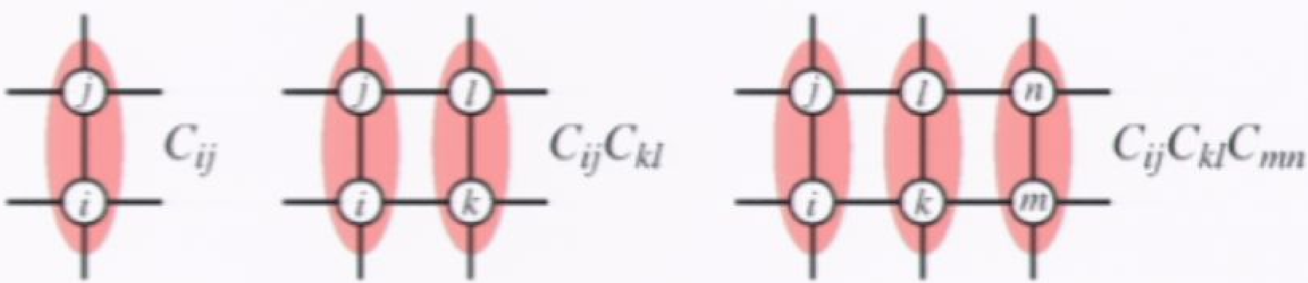

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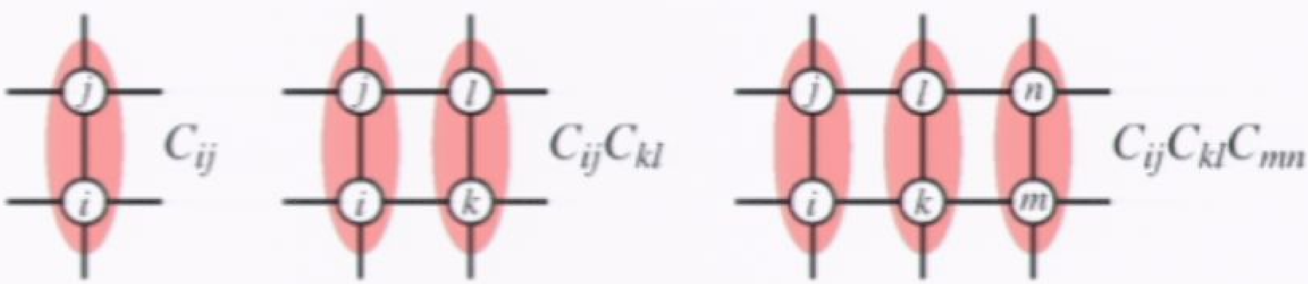

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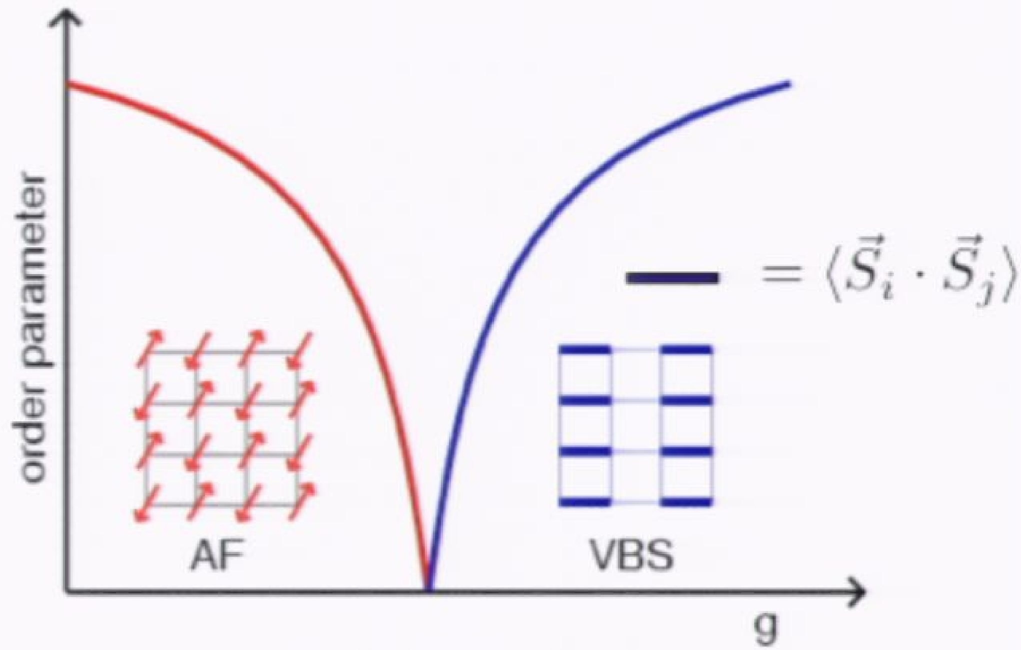

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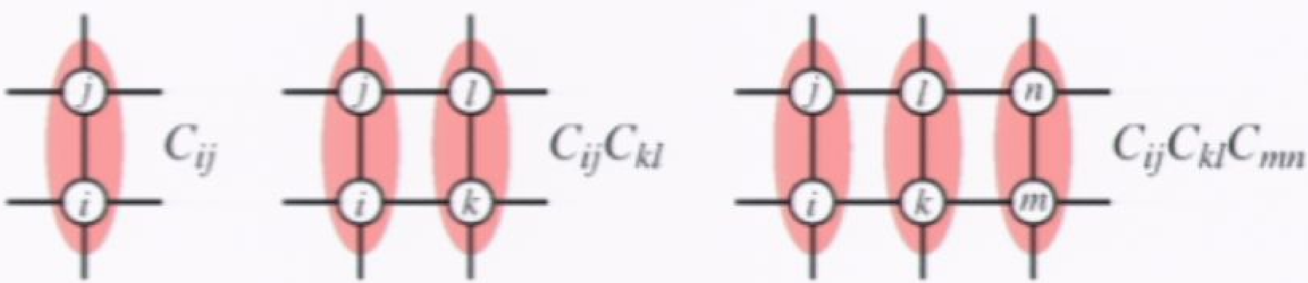

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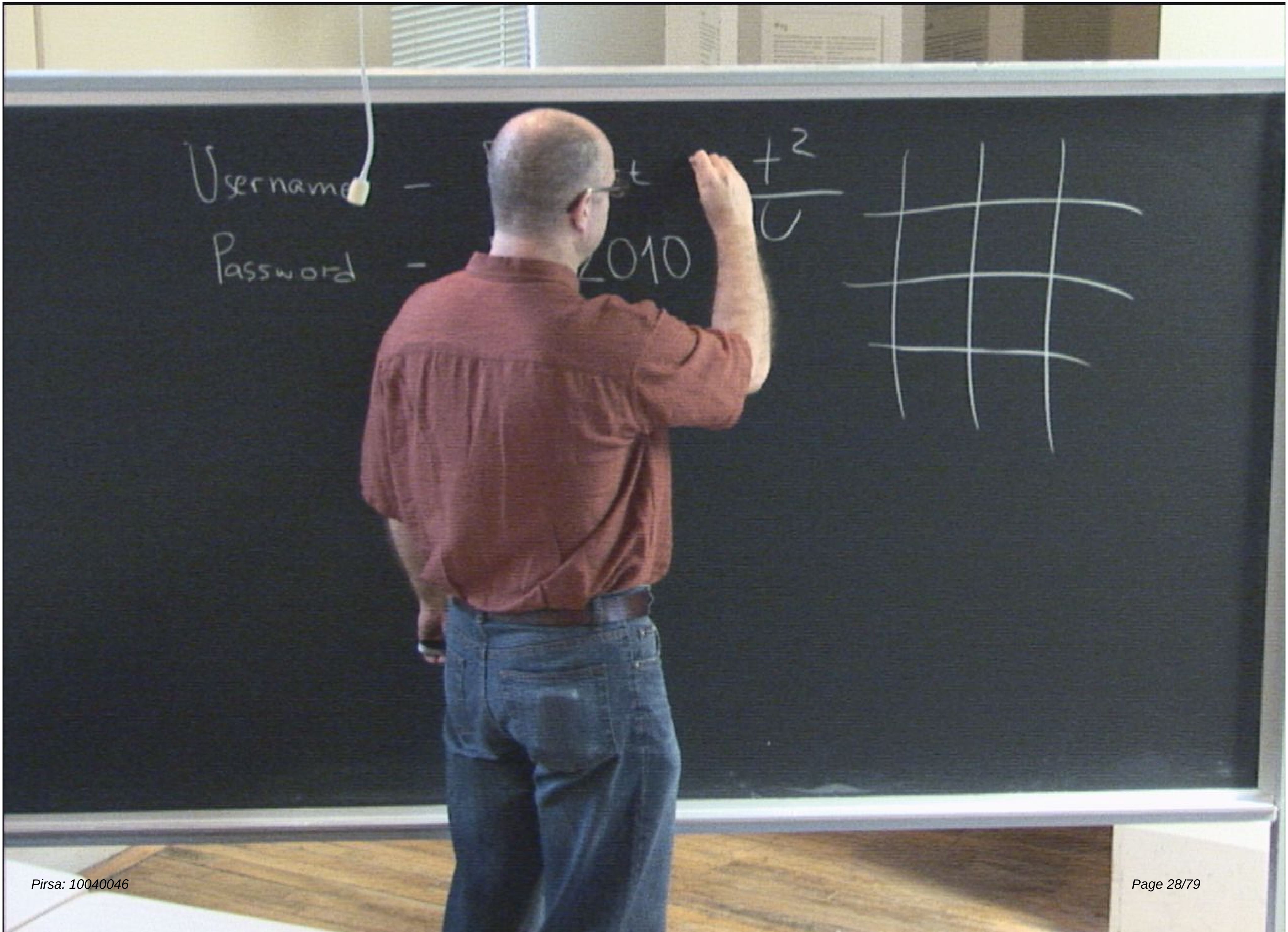

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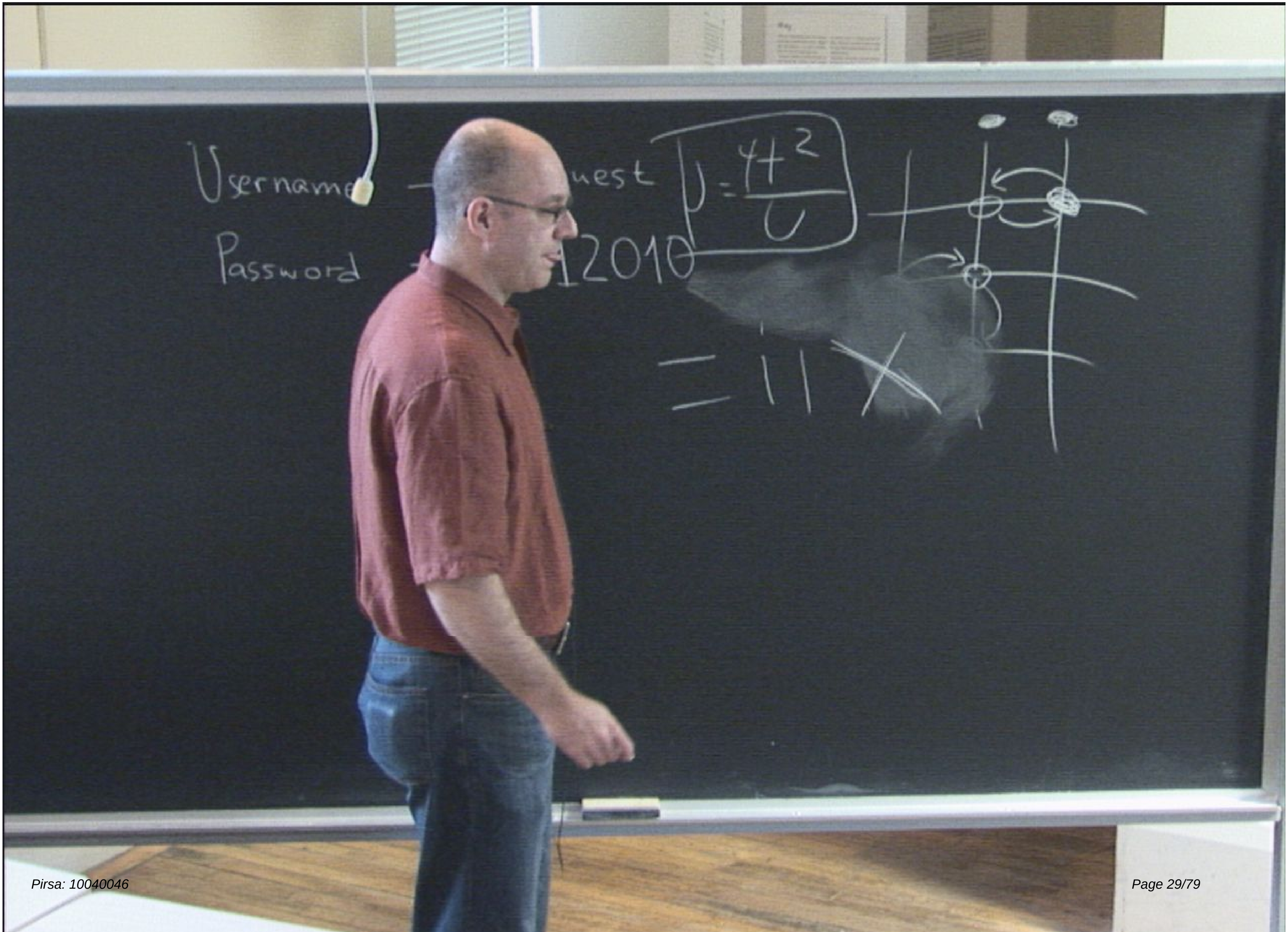
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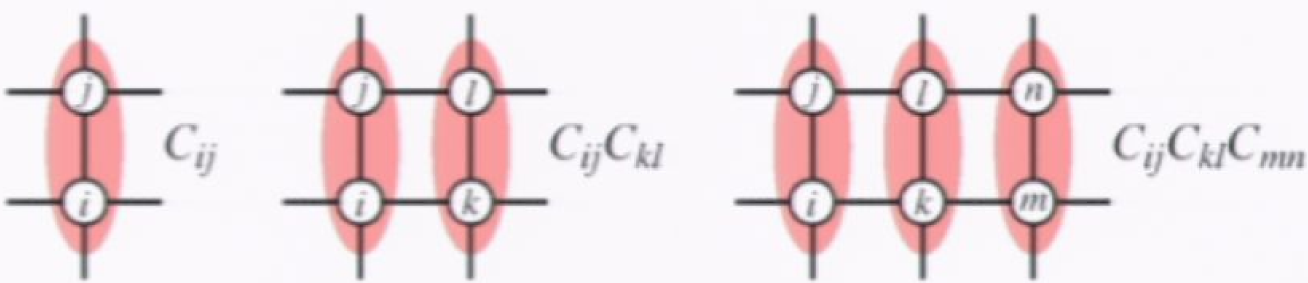

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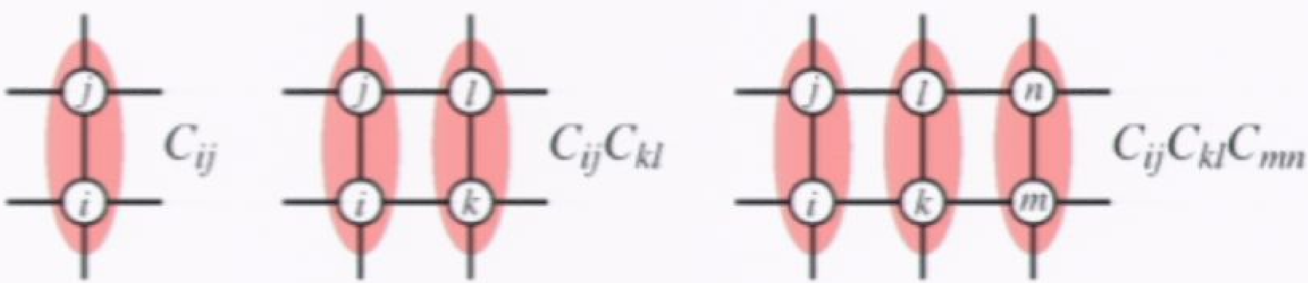


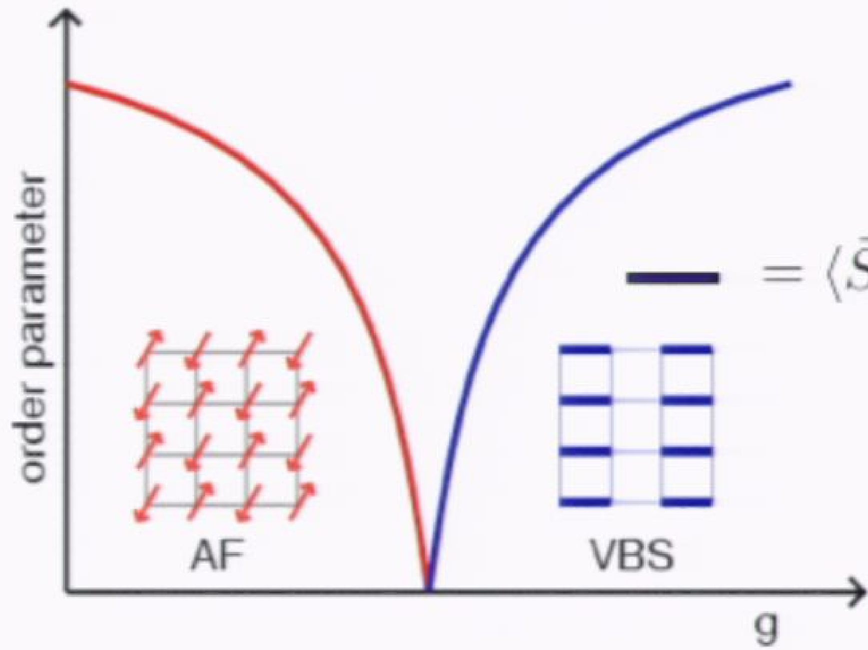
Deconfined quantum criticality

$$H = J\sum_{\langle i,j\rangle} S_i \cdot S_j + g \times \cdots$$

[Senthil et al., Science 303, 1490 (2004)]

Quantum phase transition in a 2D system with one spin per unit cell

- antiferromagnetic for small g
- valence-bond solid (VBS) for large g (spontaneously broken symmetry)



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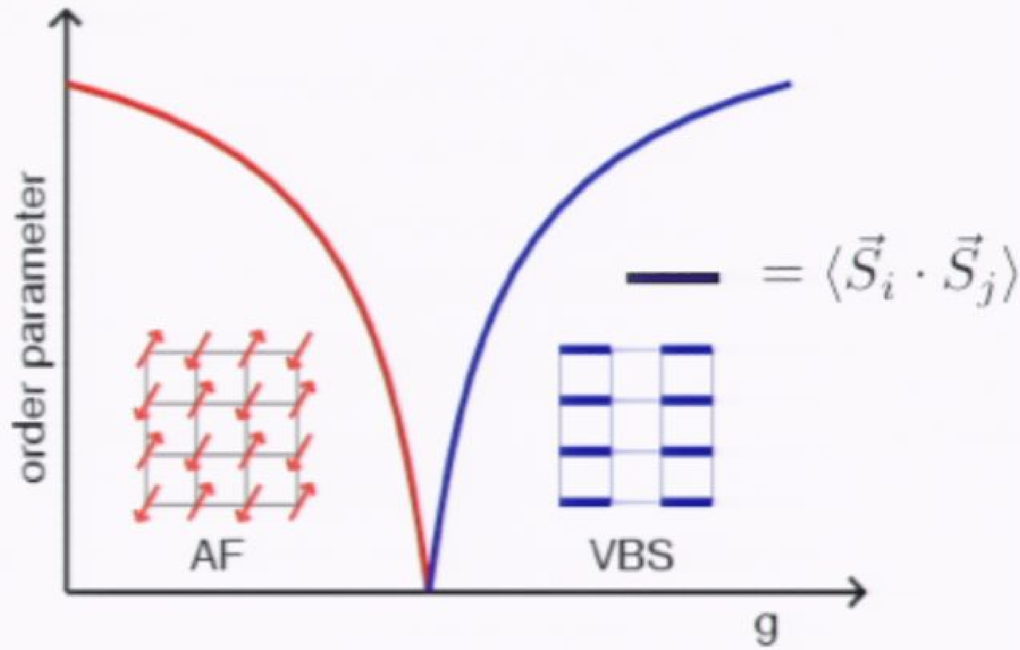
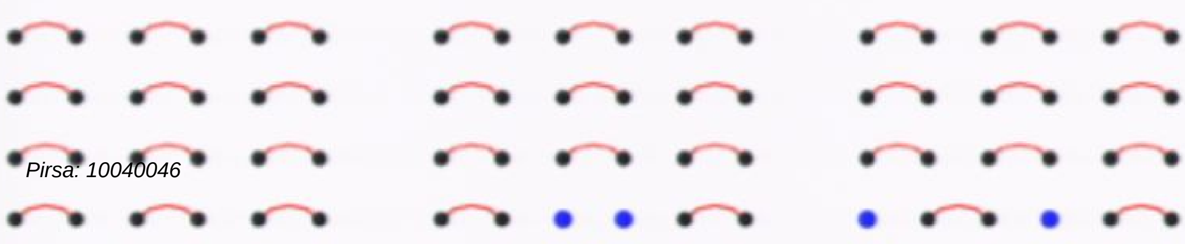
Questions
- is the transition continuous?
  - normally order-order transitions are first order (Landau-Ginzburg)
  - theory of deconfined quantum critical points has continuous transition
- nature of the VBS fluctuations?
  - emergent U(1) symmetry predicted



Spinon deconfinement upon approaching the critical point



Confinement inside VBS phase associated with new length scale and emergent

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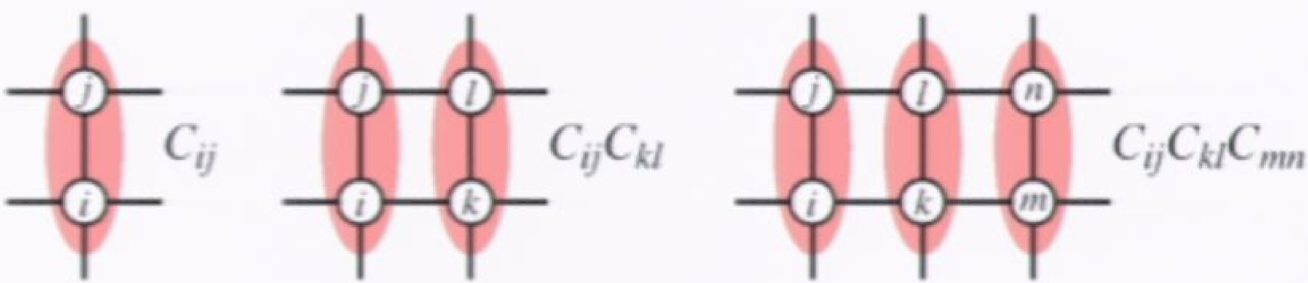

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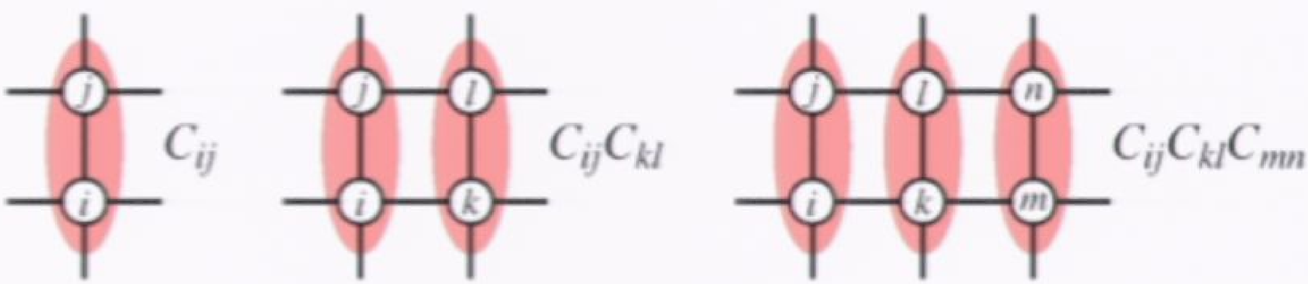

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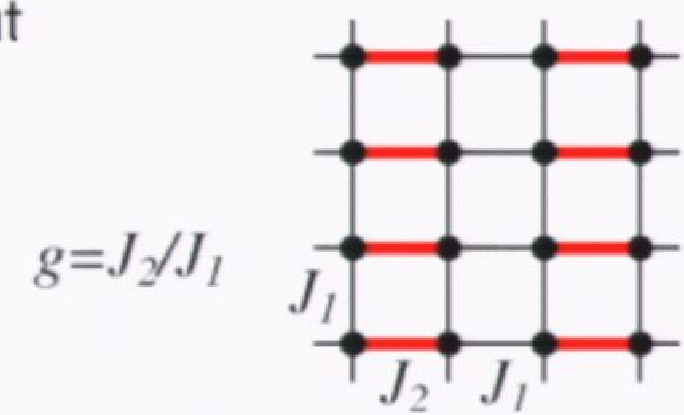
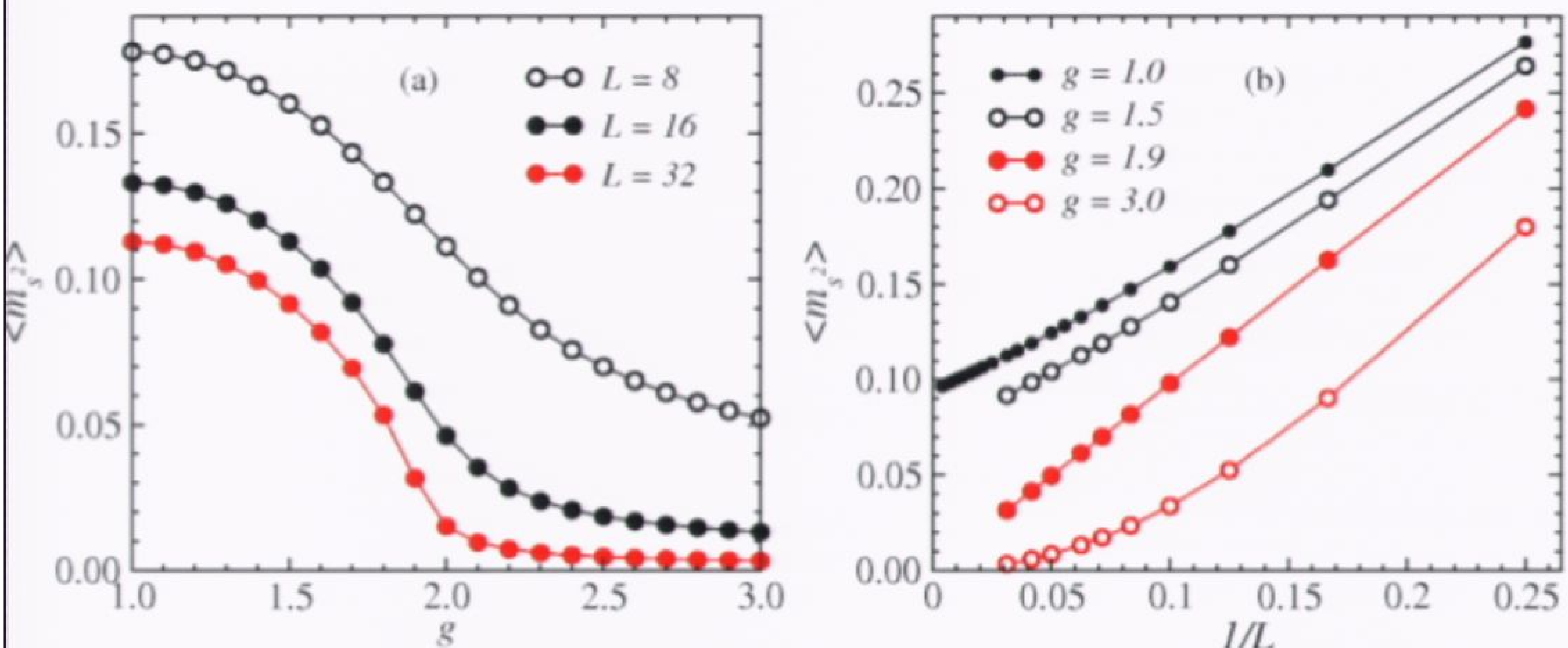


Example: Dimerized Heisenberg model

- QMC results for L×L lattices



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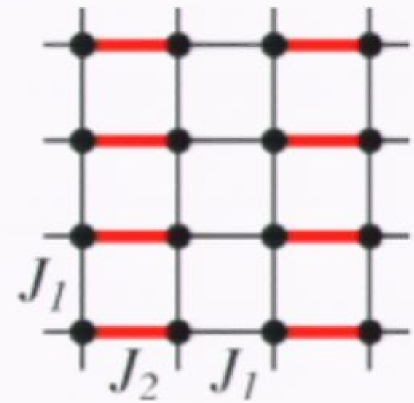

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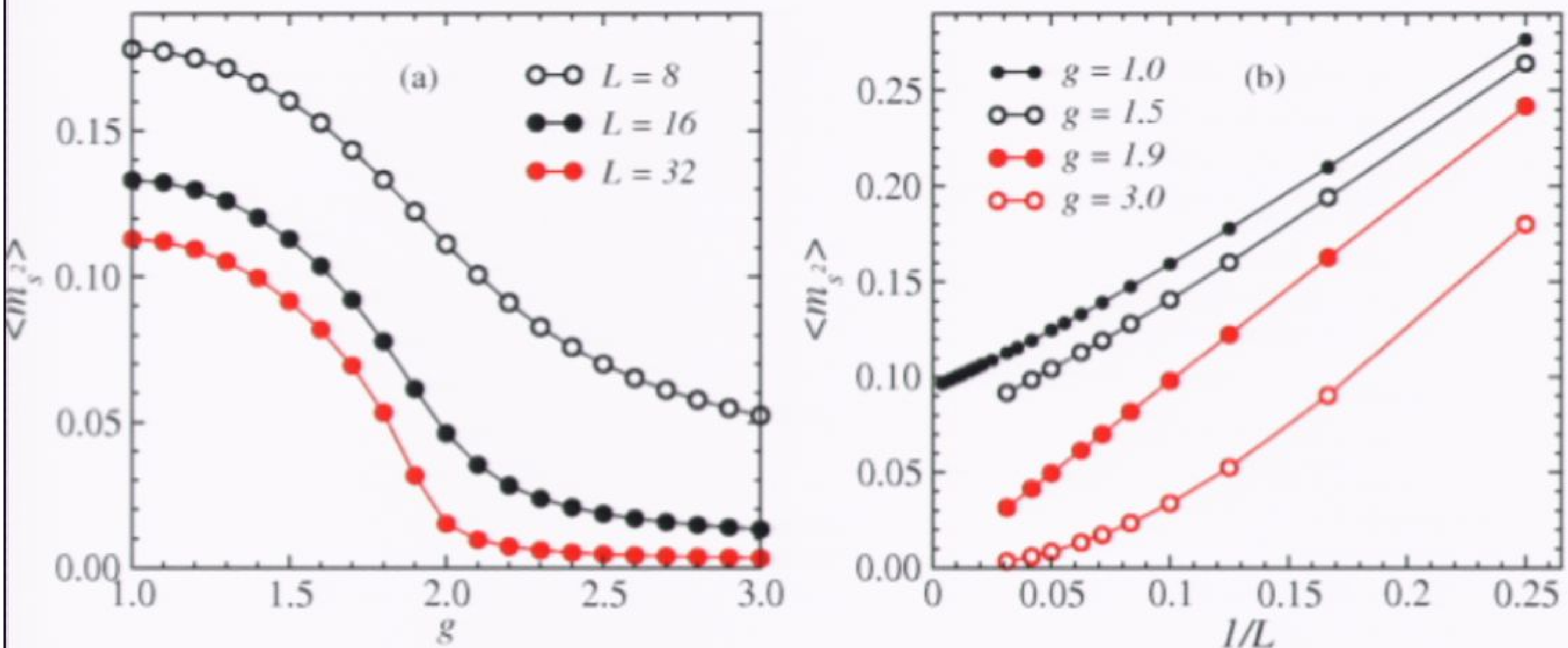

It is often known how various quantities should depend on L

Finite-size scaling and critical points

Phase transitions can be continuous or first-order (discontinuous)

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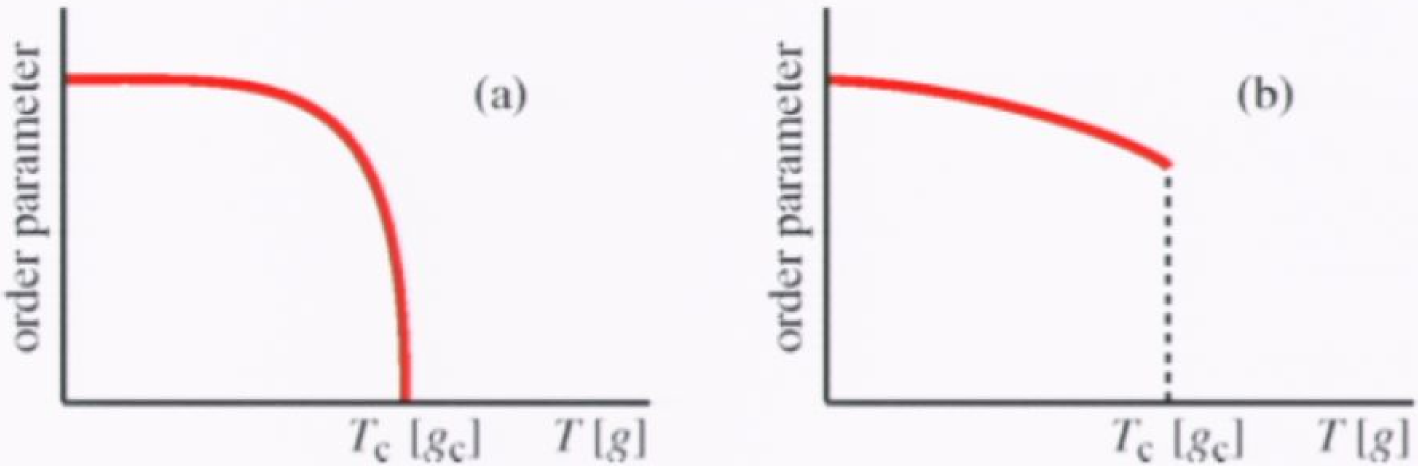

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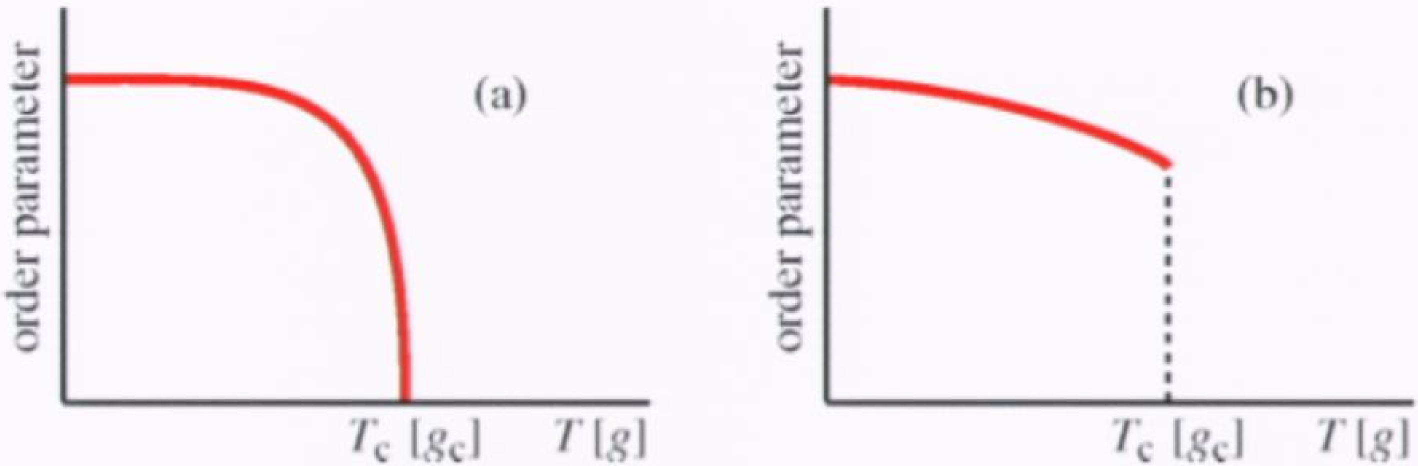

Prototypical classical model with a critical point: 2D Ising model

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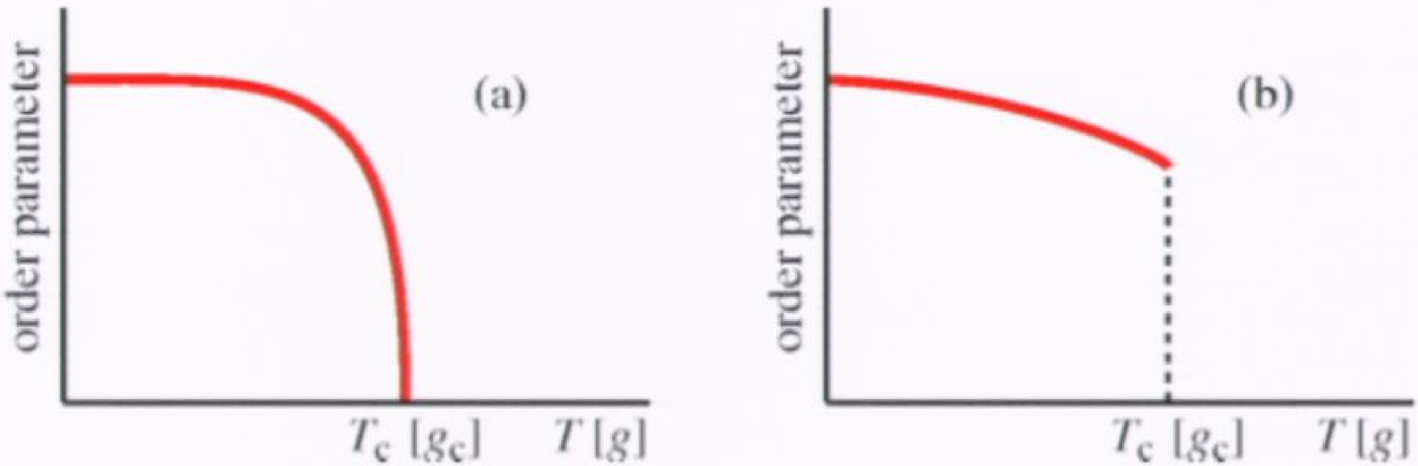

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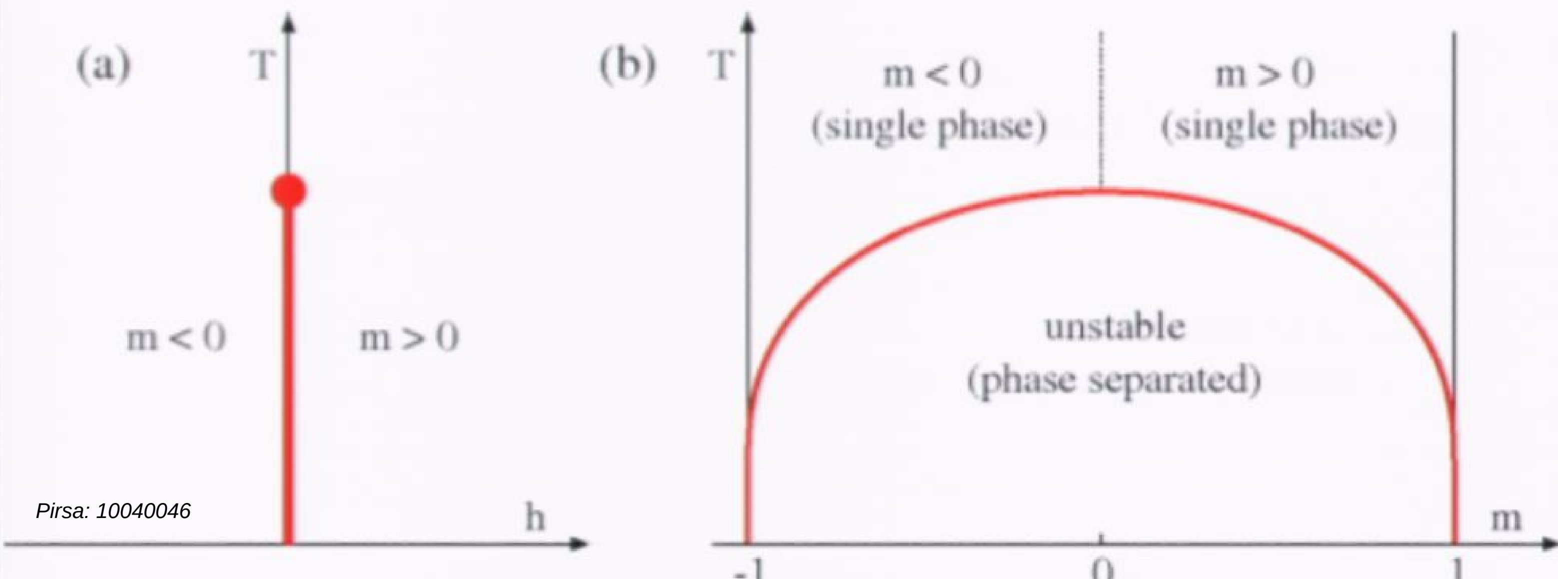
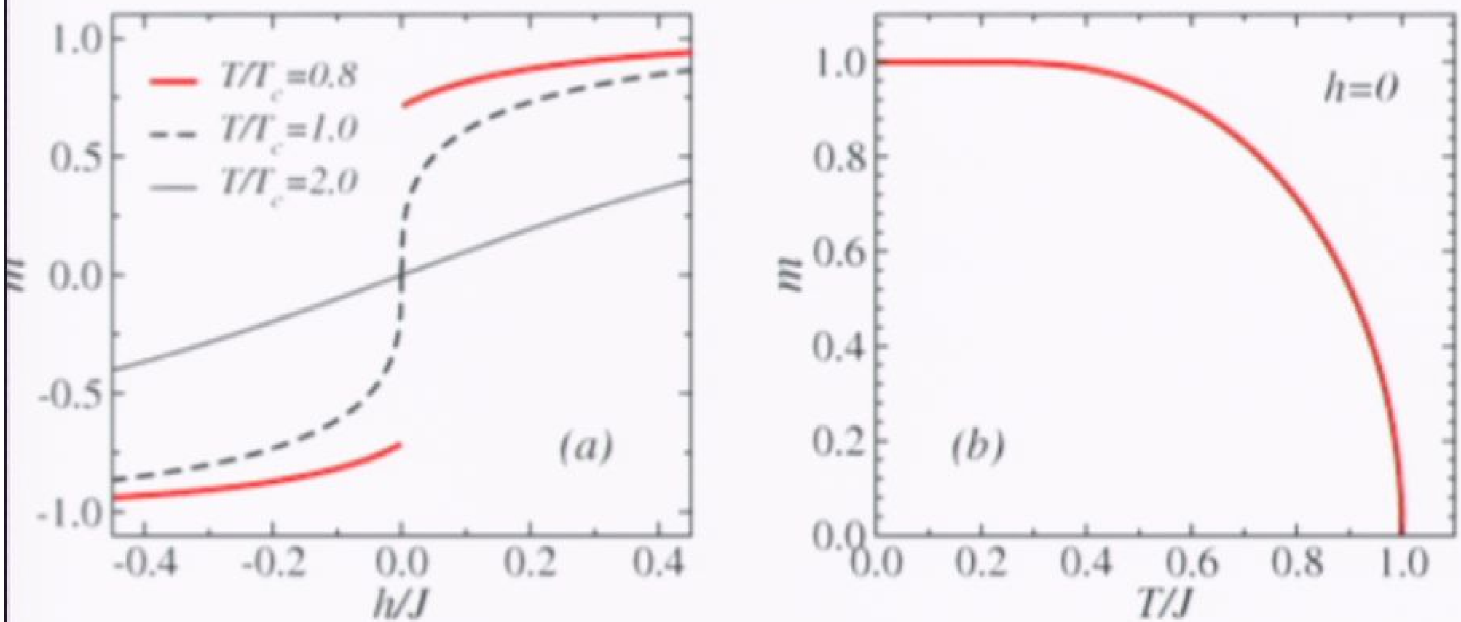


$$\frac{T_c}{J} = \frac{2}{\ln(1+\sqrt{2})}$$

$$\approx 2.269$$

Mean-field solution: $J = J_i = \sum_j J_{ij} \qquad m = \tanh[(Jm+h)/T], \qquad (m = \langle \sigma_i \rangle)$



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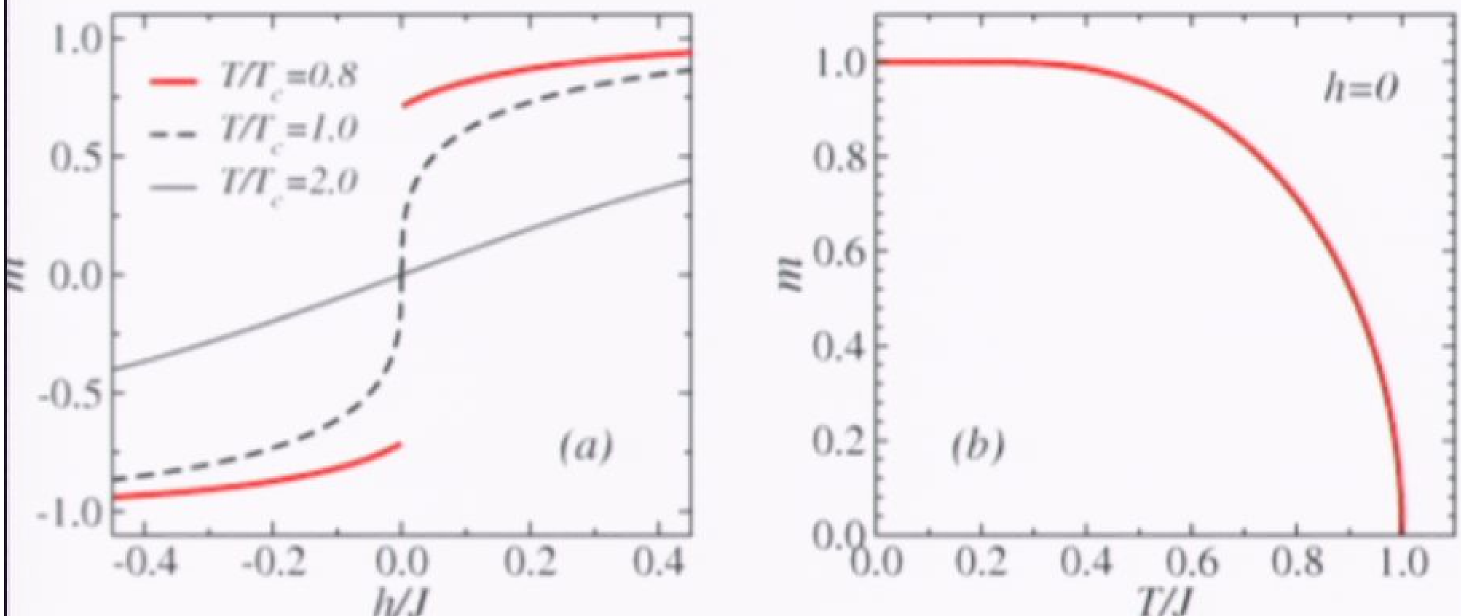
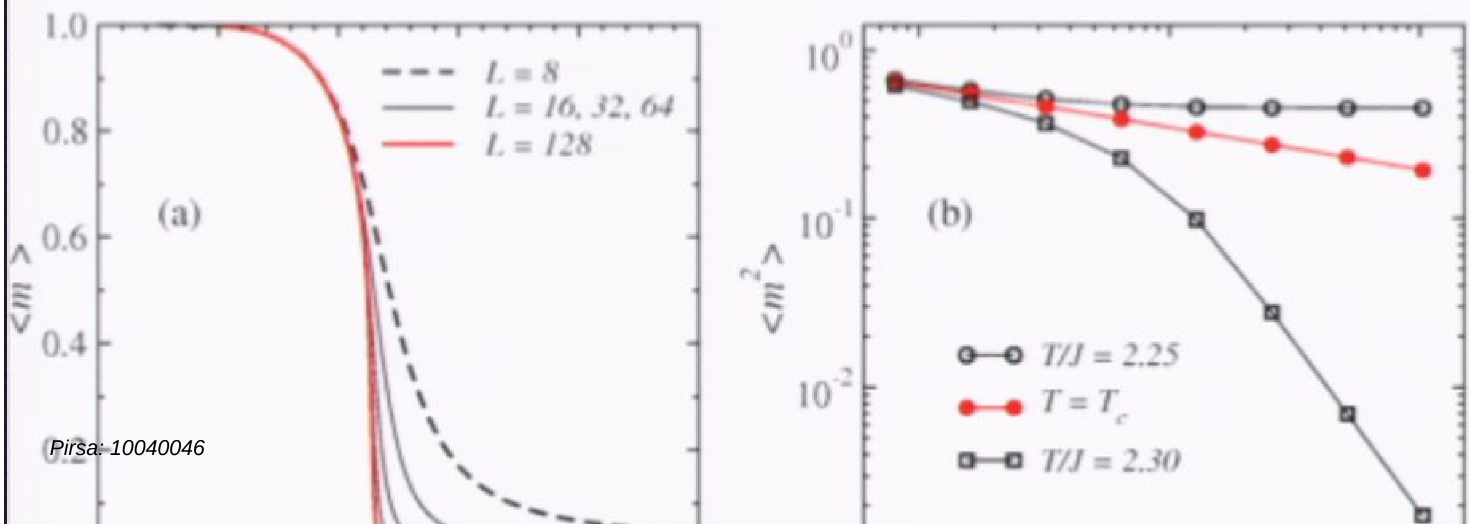


Monte Carlo results for L×L lattices (cluster algorithm, very small error bars)



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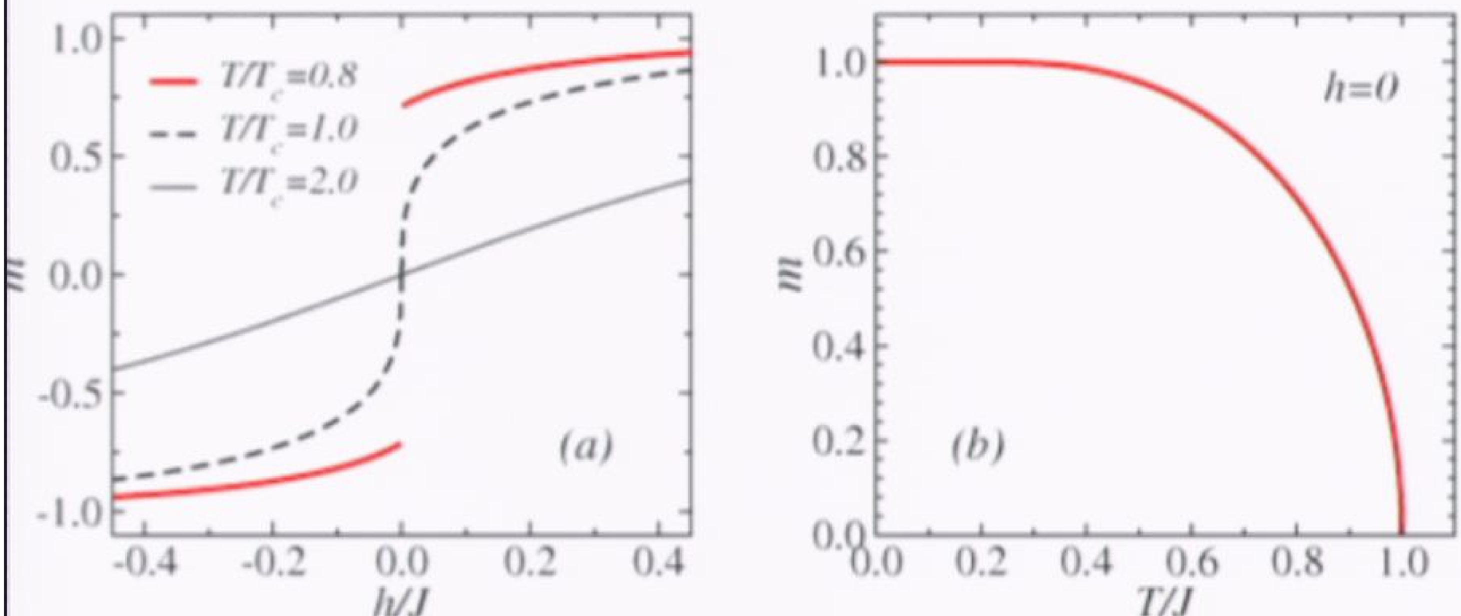

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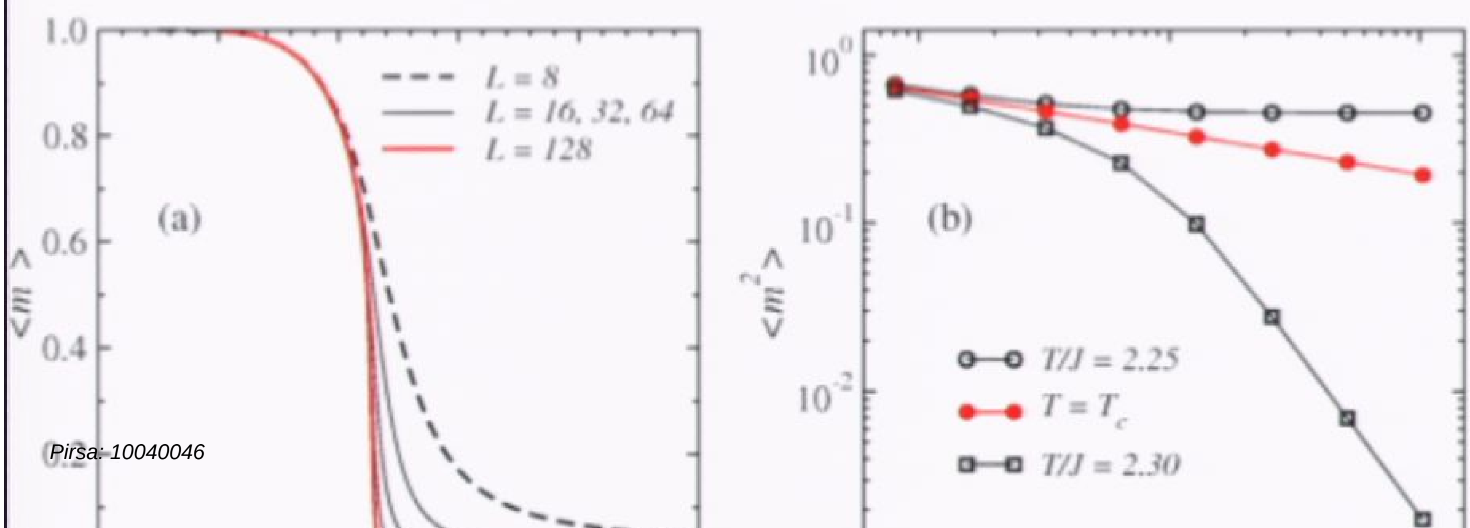

Phase transition becomes apparent for large L

Critical exponent β can be extracted from L-scaling at Tc

$\langle m(\infty, T) \rangle \sim |T - T_c|^{\beta}$

Review of criticality and scaling

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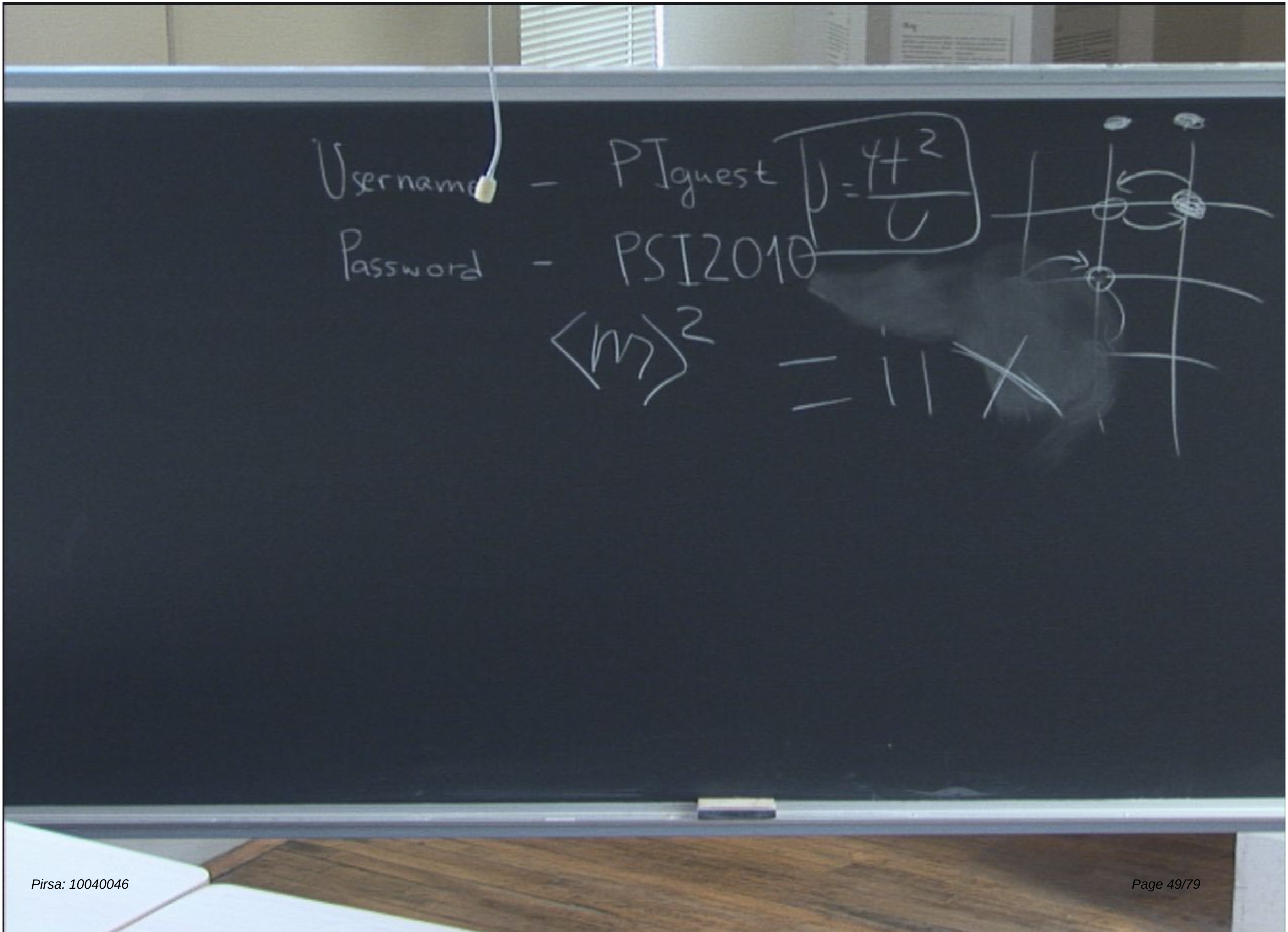
Username - PIguest
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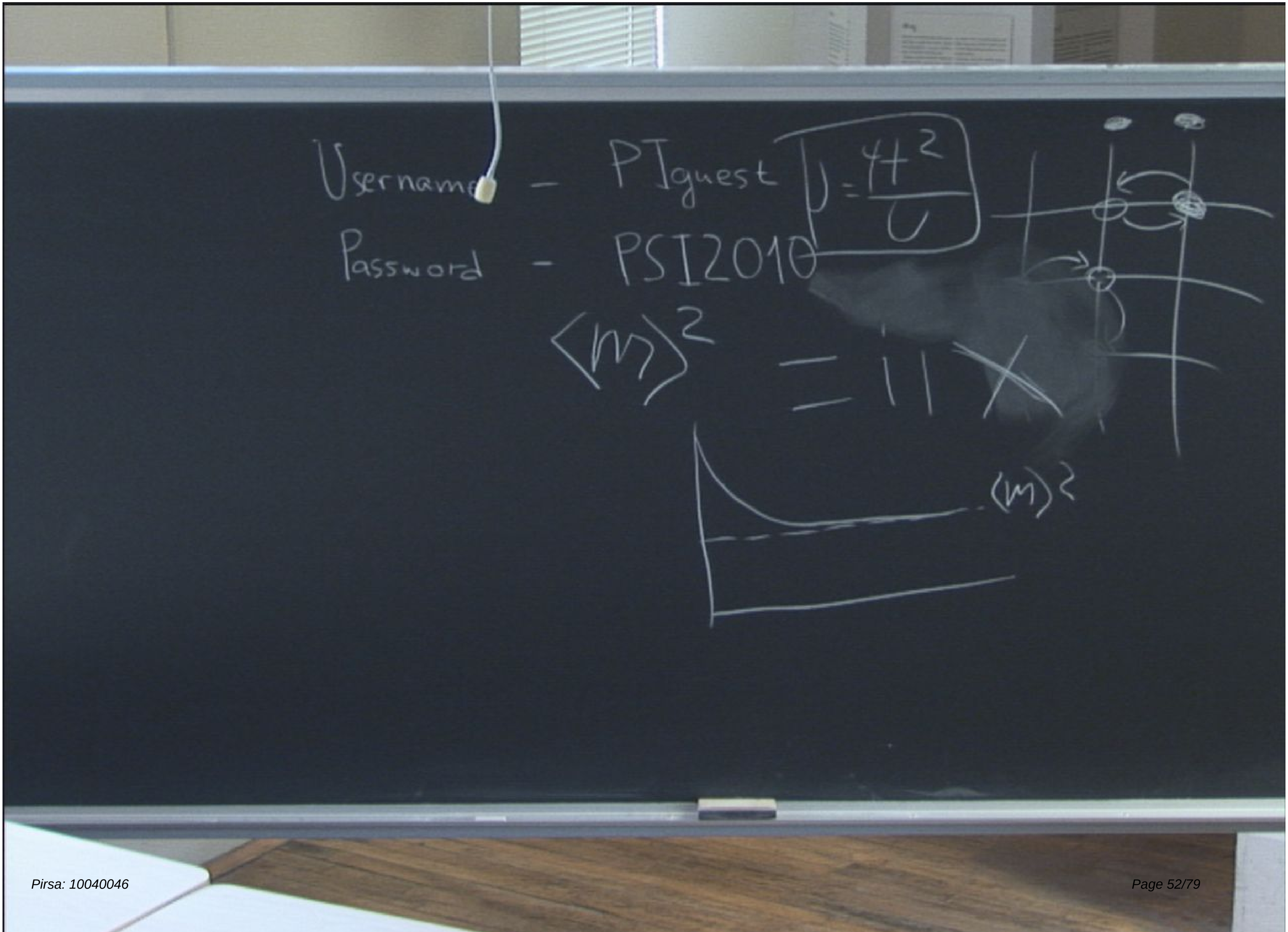
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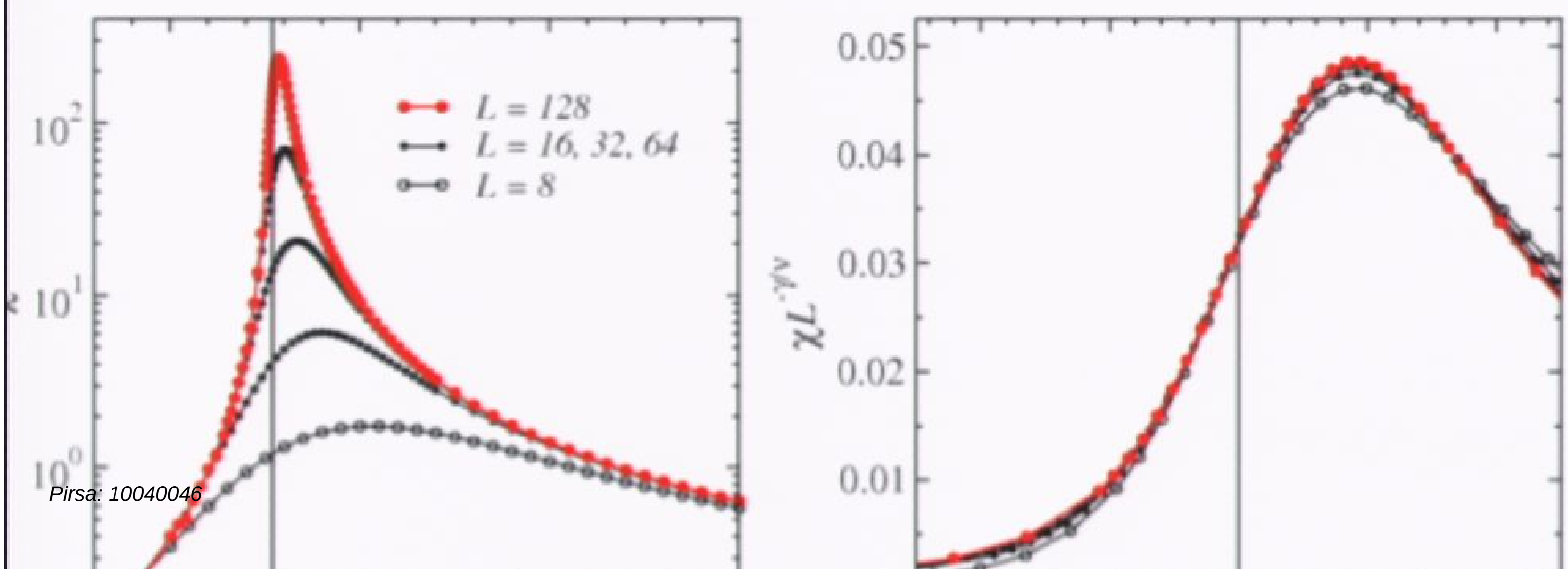

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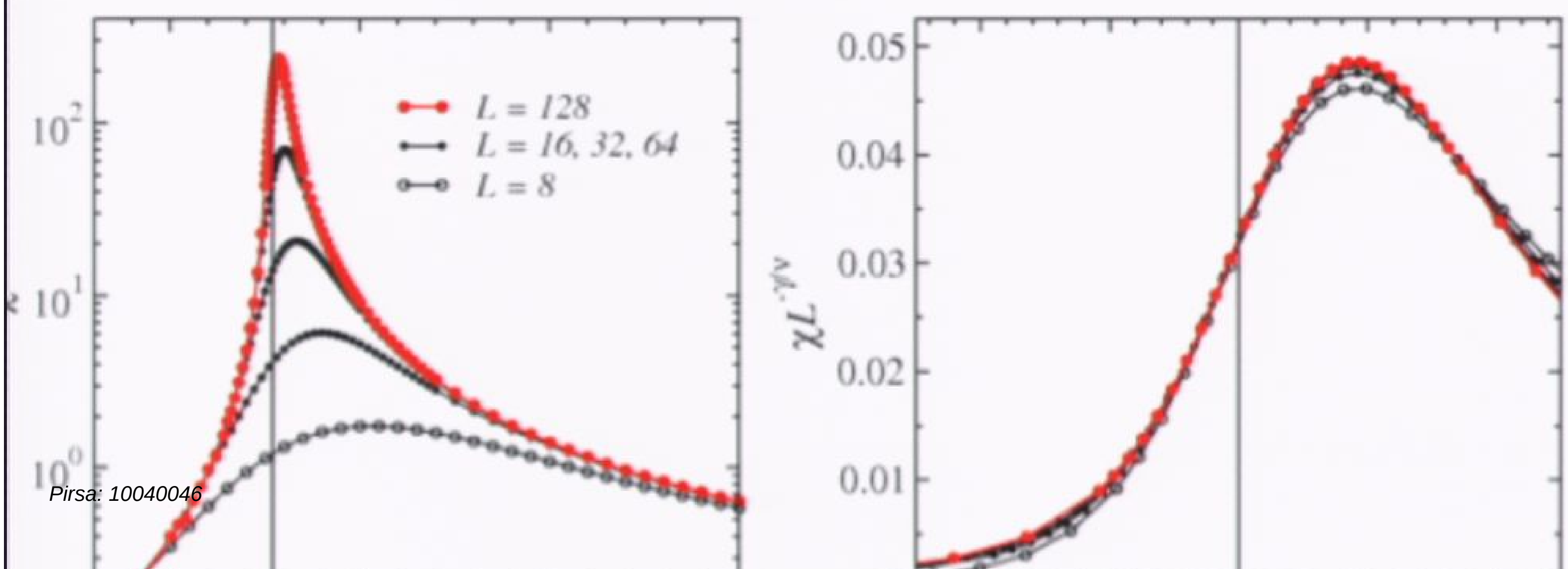

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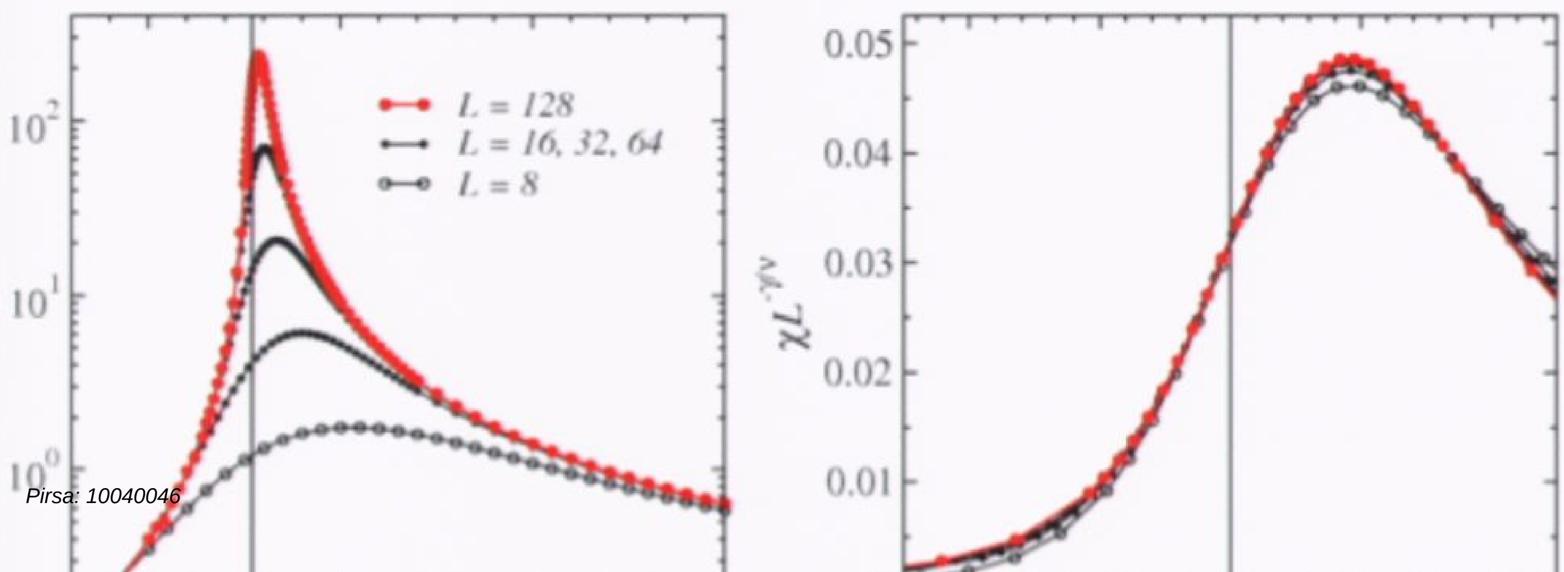

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