Properties of Heisenberg ladders; large-scale SSE results

Magnetic susceptibility Low-T theoretical forms:

Odd L_y: from nonlinear -sigma model

Eggert, Affleck, Takahashi, PRL 73, 332 (1994)

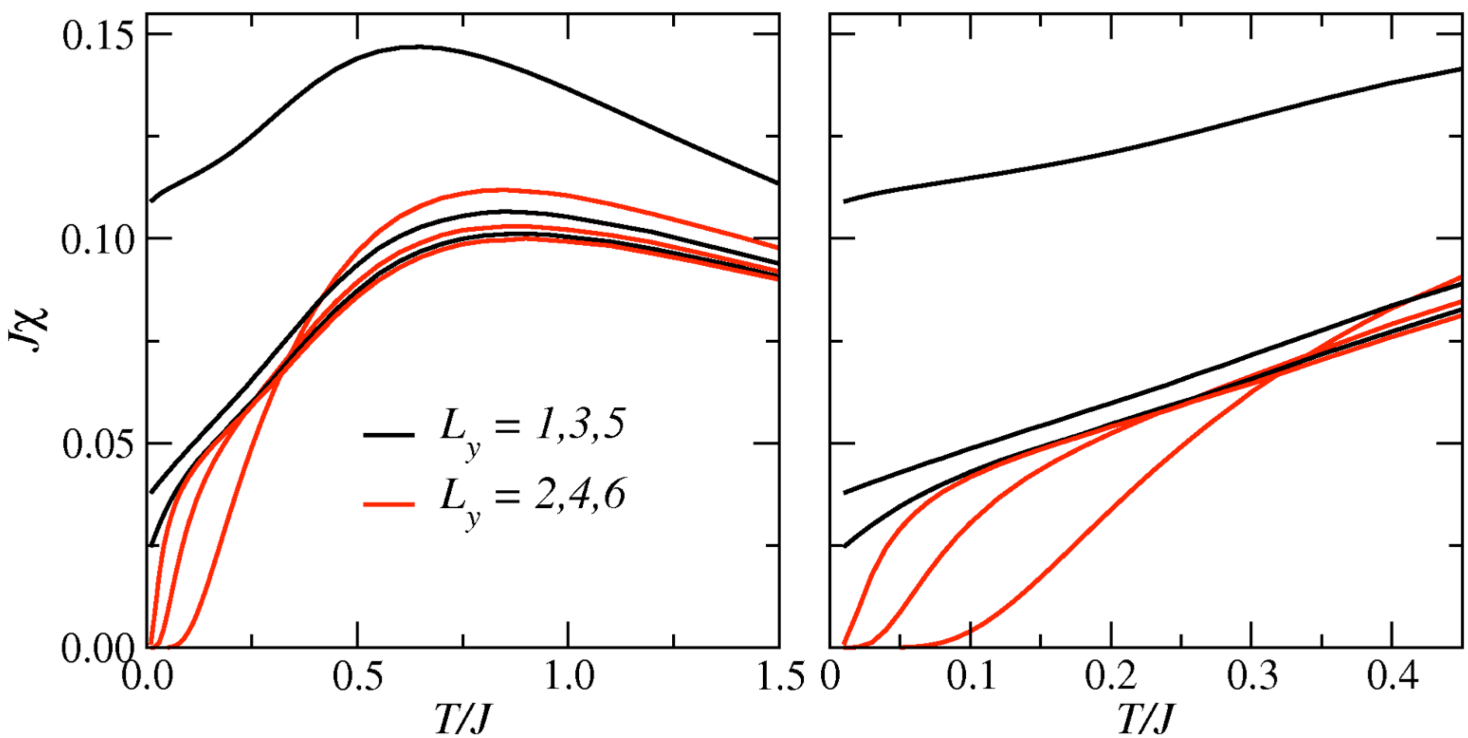
$$\chi(T) = \frac{1}{2\pi c} + \frac{1}{4\pi c \ln(T_0/T)}$$

Even L_y: from large J_y/J_x expansion

Troyer, Tsunetsugu, Wurz, PRB 50, 13515 (1994)

$$\chi(T) = \frac{a}{\sqrt{T}} \mathrm{e}^{-\Delta/T}$$

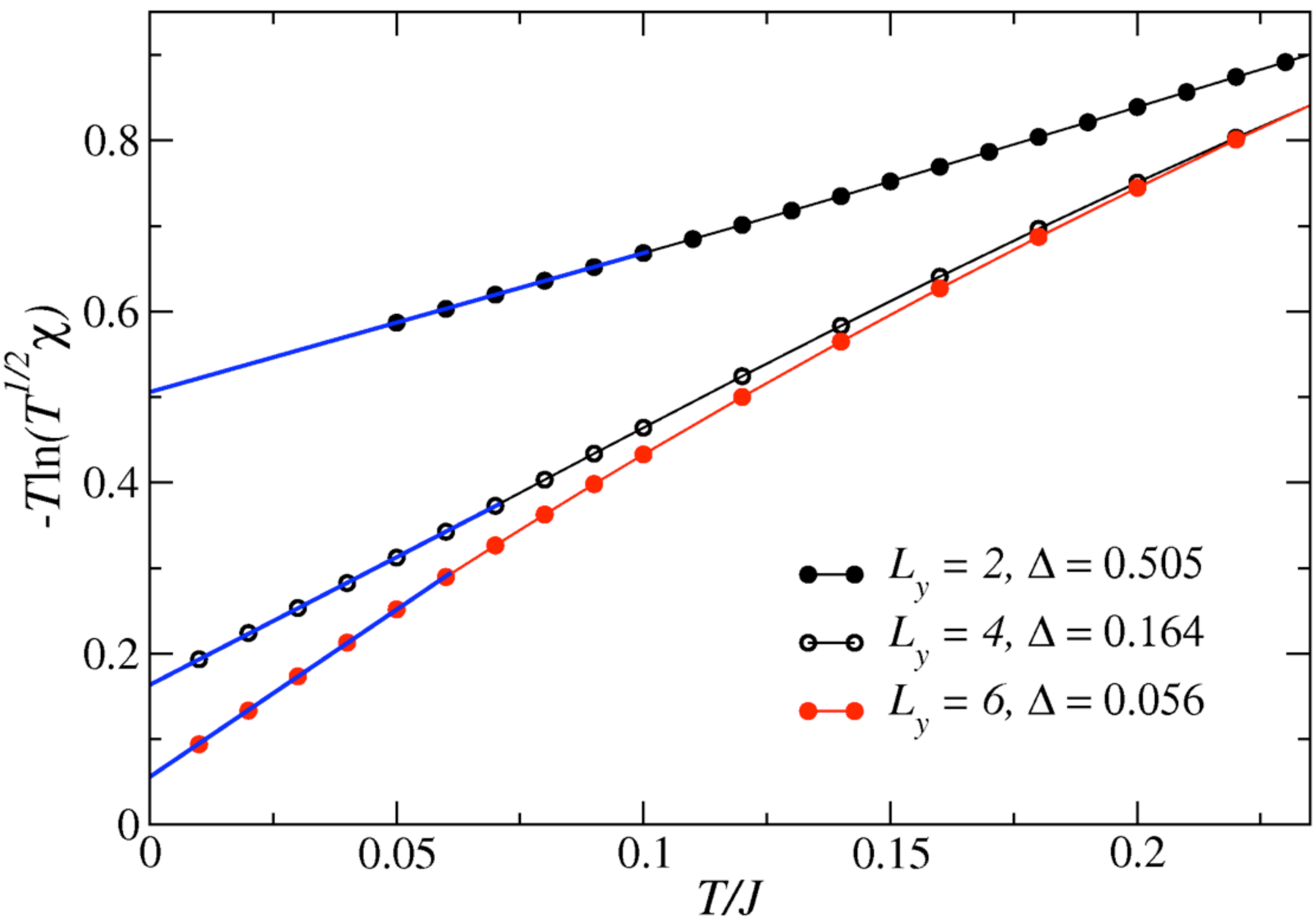
SSE results for large L_x (up to 4096, giving $L_x \to \infty$ limit for T shown);



Extracting the gap for evel-L_y systems

From the low-T susceptibility form:

$$\chi(T) = \frac{a}{\sqrt{T}} e^{-\Delta/T} \;\Rightarrow\; -T\ln(\sqrt{T}\chi) = \Delta - T\ln(a)$$

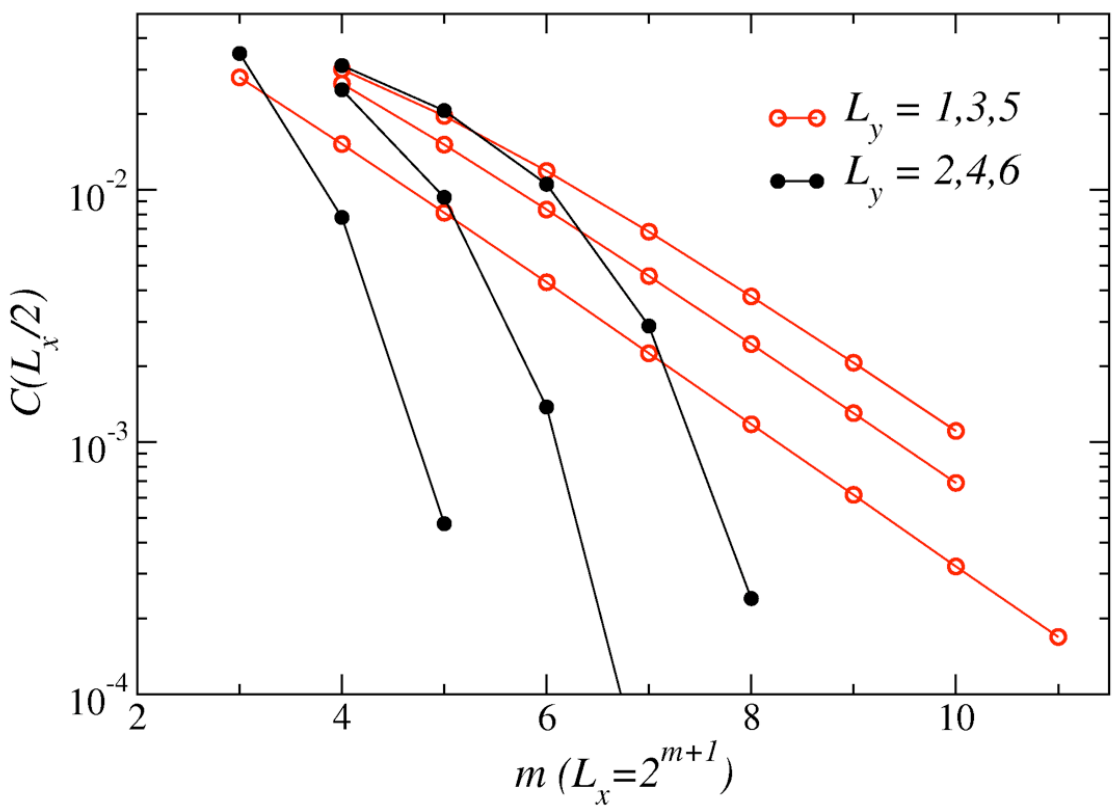


T=0 spin correlations of ladders

Expected **asymptotic** behaviors

$$C(r) = A\frac{(-1)^r}{r}\ln\left(\frac{r}{r_0}\right)^{1/2}$$ (odd L_y) $$C(r) = Ae^{-r/\xi}$$ (even L_y)

We also expect short-distance behavior reflecting 2D order for large L_y



short-long distance cross-over behavior starts to become visible, but larger L_y needed to see signs of 2D order for $r<L_y$

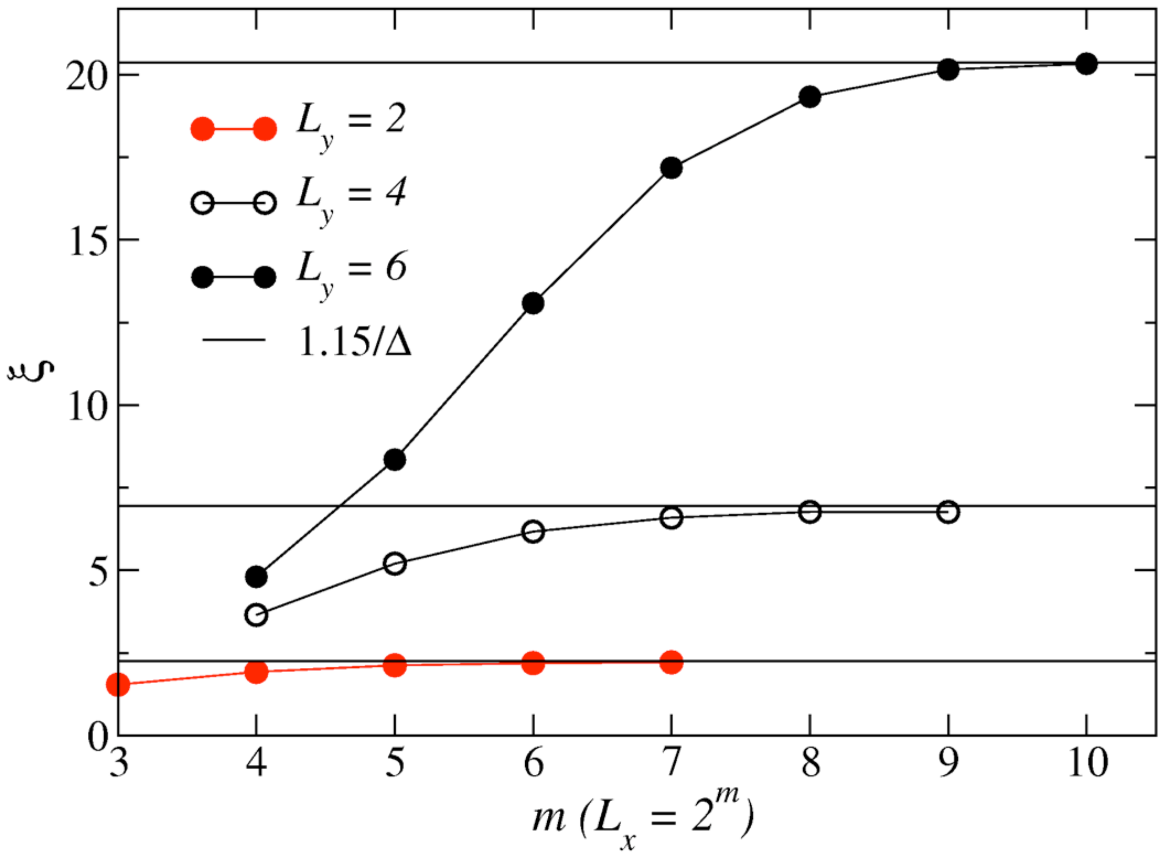
- L×L lattices used to study 2D case

Correlation length for even-L_y

$$C(r) \propto \mathrm{e}^{-r/\xi}, \qquad \xi \propto \frac{1}{\Delta}$$

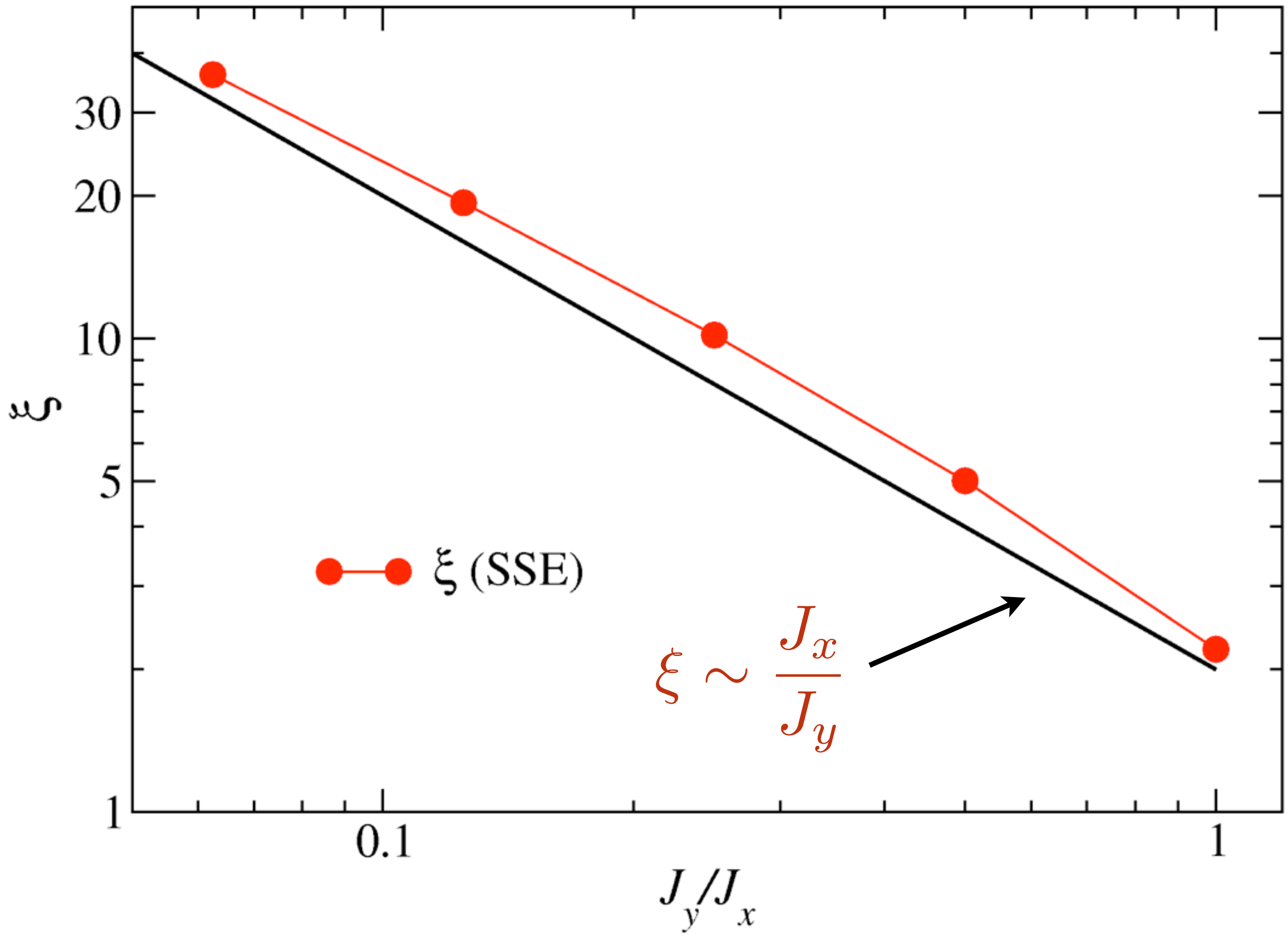
We need system lengths $L_x >> \xi$ to compute ξ reliably. Use:

$$\xi^2 = \frac{1}{q^2}\left(\frac{S(\pi,\pi)}{S(\pi-q,\pi)} - 1\right) \qquad S(\mathbf{q}) = \sum_{\mathbf{r}} \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}} C(\mathbf{r})$$



Correlation length versus J_y/J_x for L_y=2

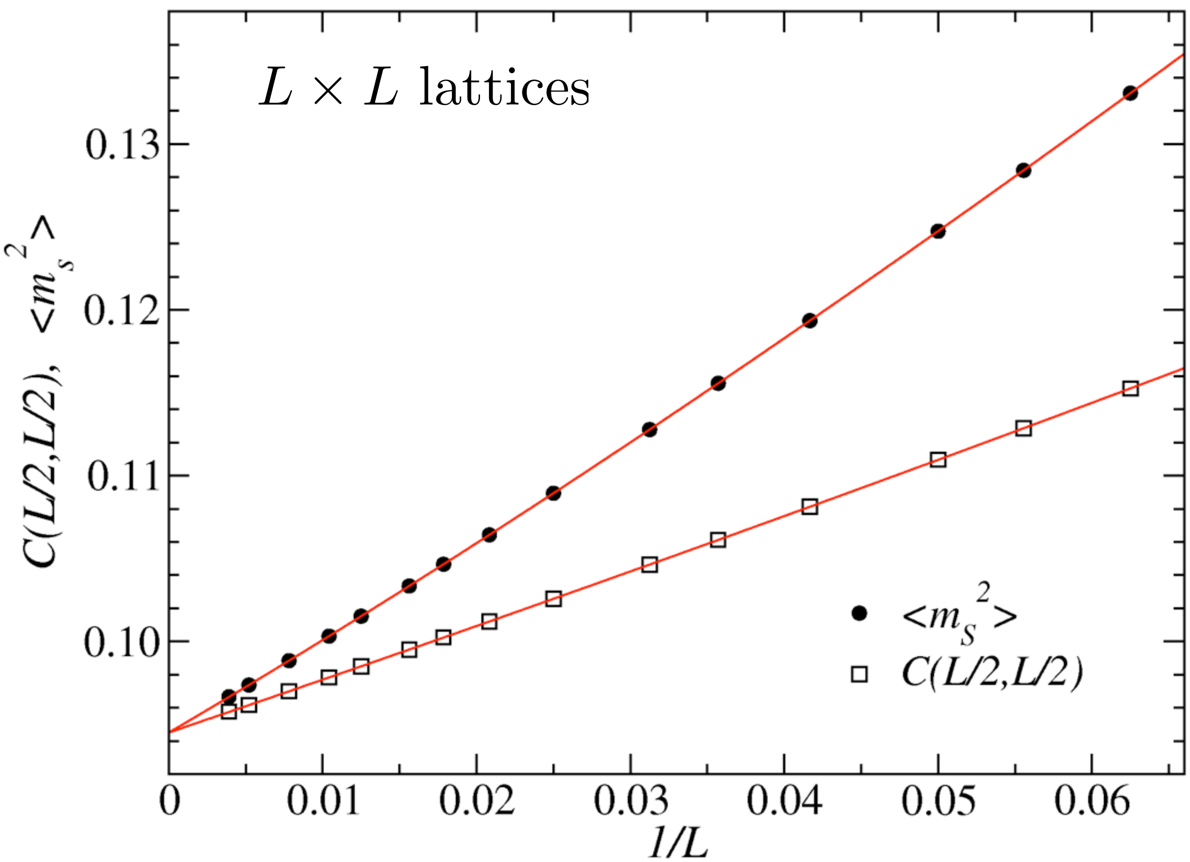
the single chain is critical (1/r correlations) → ξ diverges as J_y/J_x → 0



2D Heisenberg model; long-range order at T=0

Spin-wave theory shows large sublattice magnetization; m_s=0.3034

- including up to $1/S^2$ corrections gives m_s=0.3070
- large-scale QMC (SSE, valence-bond projector) gives m_s=0.3074

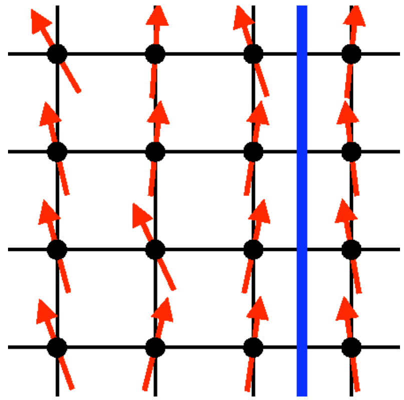


comparing results of

- m_s averaged over all sites (then squared)
- the spin correlation function C(L/2,L/2) at the longest distance

Linear size correction predicted from spin wave theory (and also more general symmetry arguments)

The spin stiffness (helicity modulus)



Corresponds to an Young's modulus of an elastic medium
- an important ground-state parameter of a spin system
- finite for an ordered state
- equivalent to the superfluid stiffness in boson language

Sensitivity of the ground-state energy (free energy at T>0) to "twisting" the spins along a boundary column

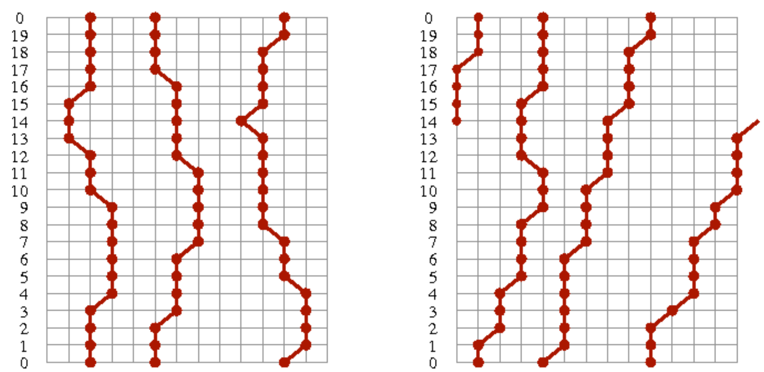
$$\rho_s^\gamma = \frac{1}{L}\frac{d^2\langle H(\phi)\rangle}{d\phi^2}, \qquad \phi = \text{"twist" at boundary in } \gamma \text{ direction}$$

Twist imposed by changing the Heisenberg interaction at the boundary

$$\mathbf{S}_i \cdot \mathbf{S}_j \to \mathbf{S}_i \cdot R\mathbf{S}_j, \qquad R = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

One can show that the stiffness is related to the winding number fluctuations

$$\rho_s^\gamma = \frac{3}{2}\frac{1}{\beta}\langle W_\gamma^2\rangle, \qquad \gamma = x, y$$

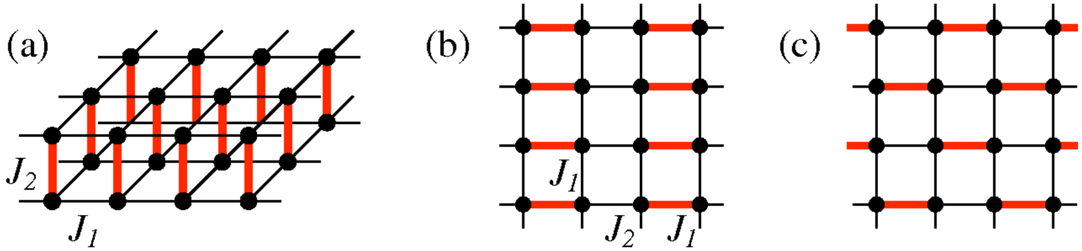


In SSE we have to count spin flip "events"

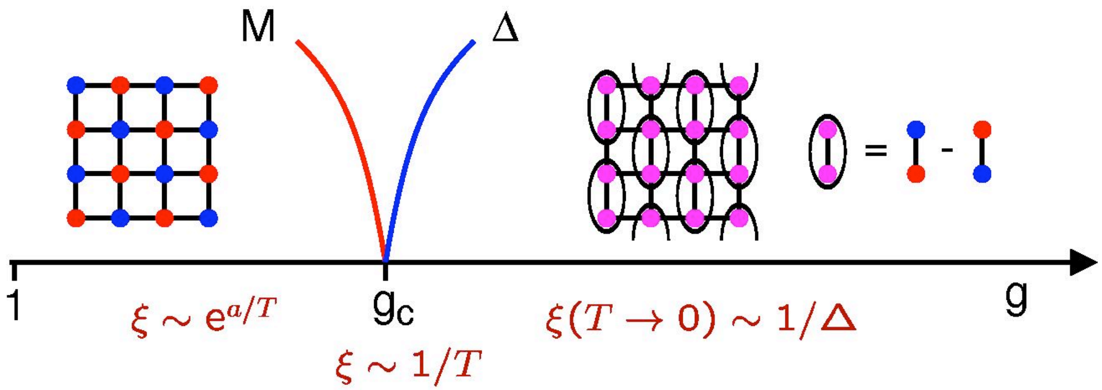
$$W_\gamma = \frac{1}{L}\sum_{p=0}^{n-1} J_\gamma, \quad J_\gamma = \pm 1 \quad \text{(currents)}$$

2D quantum-criticality (T=0 transition)

Examples: bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Neel - disordered transition



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

• Continuum field theory: nonlinear σ-model (Chakravarty, Halperin, Nelson)

⇒3D classical Heisenberg (O3) universality class expected

Dynamic Exponent z

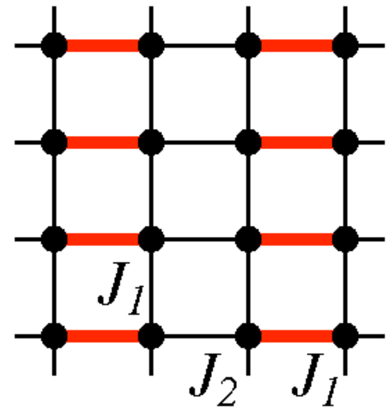
- relates space and time directions
- finite-size gap Δ scales as L^{-z}
- replace classical dimensionality d by d+z in scaling expressions

$$\xi_\tau \sim \xi_r^z, \qquad \Delta \sim L^{-z}$$

Analysis of the transition of dimerized (columnar) Heisenberg system

Two options of choosing the temperature in finite-lattice calculations

- get the ground state as T→0 limit
    - in practice **T<<Δ** (finite-size gap)
- use **1/T=β = aL^z** to analyze the transition
    - if z is known (or to test proposal)
    - the results should not depend on aspect ratio **a**



Use the Binder ratio

$$R_2 = \frac{\langle m_{sz}^4 \rangle}{\langle m_{sz}^2 \rangle^2}$$

to locate the critical coupling ratio g_c

Significant drifts in the crossing points, large lattices needed

$$g_c \approx 1.91$$