The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2253-5

Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

24 - 29 July 2011

Random-singlet phases beyond one spatial dimension

K. Beach

University of Alberta
Edmonton, Alberta
Canada

RANDOM SINGLET PHASES BEYOND ONE SPATIAL DIMENSION

Kevin Beach, University of Alberta

Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

ICTP, July 2011

UNIVERSITY OF ALBERTA

THINKING ABOUT DISORDER

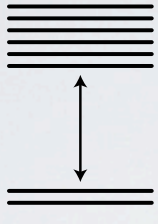
- Depending on your point of view, disorder is either
  - a lamentable reality in material systems; to be eliminated in the pursuit of ever more pure samples
  - yet another interesting knob to turn (in the same vein as competing interactions, external fields, etc.)
- Taking the more optimistic perspective, we ask:
  - can disorder stabilize interesting quantum phases?
  - can it drive nontrivial zero-temperature transitions?

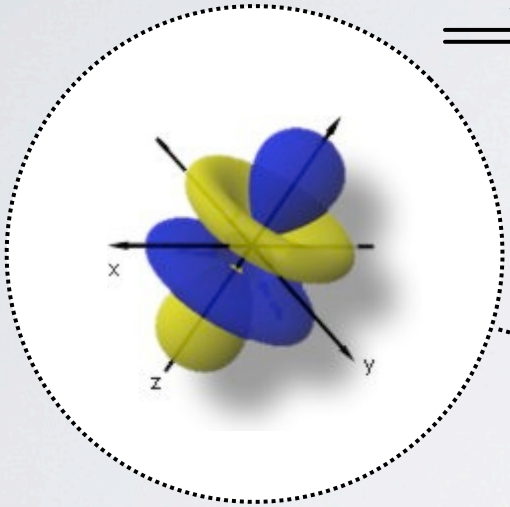
TALK OUTLINE

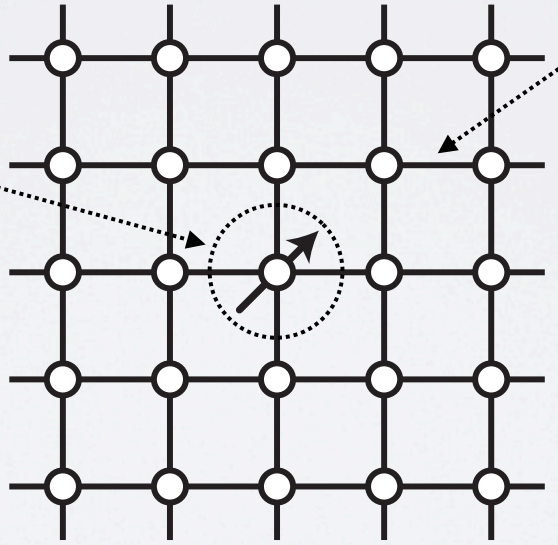
- What happens when we disorder an antiferromagnet?
- Focus here on *non-frustrated* systems

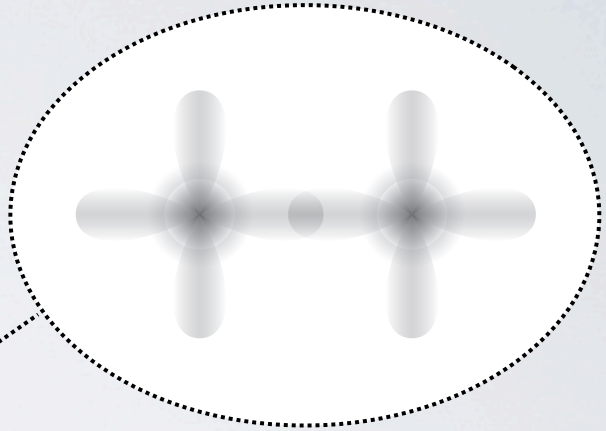
- Spin models with site dilution or disordered nearest-neighbour exchange couplings; large-scale, unbiased simulations possible
- Random singlet (RS) phase in the linear chain + RG picture
- Generalization to higher dimensions (large N construction)
- Test stability of RS states with quantum Monte Carlo

LATTICE MODELS





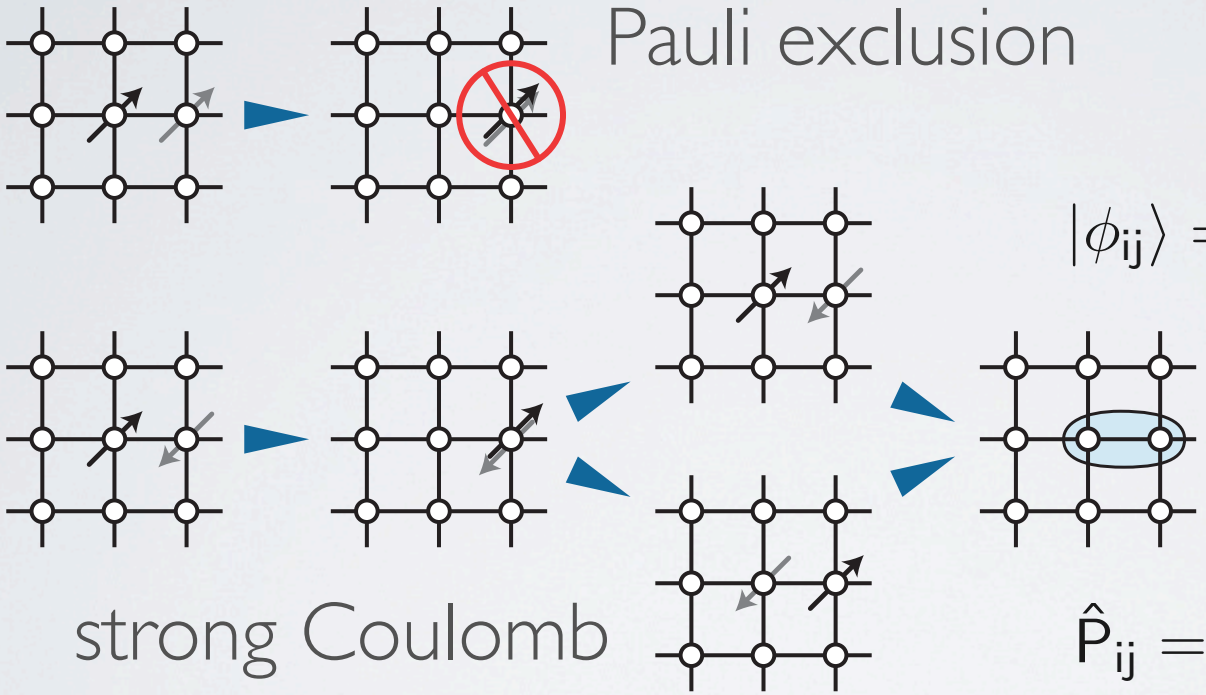




tight-binding picture
of orbital overlaps

two-state basis for
localized S=1/2 spins

EXCHANGE INTERACTION



Pauli exclusion

strong Coulomb repulsion

$$|\phi_{ij}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle\right)$$

$$\hat{P}_{ij} = |\phi_{ij}\rangle\langle\phi_{ij}| = \tfrac{1}{4} - S_i \cdot S_j$$

effective coupling $J_{ij} > 0$

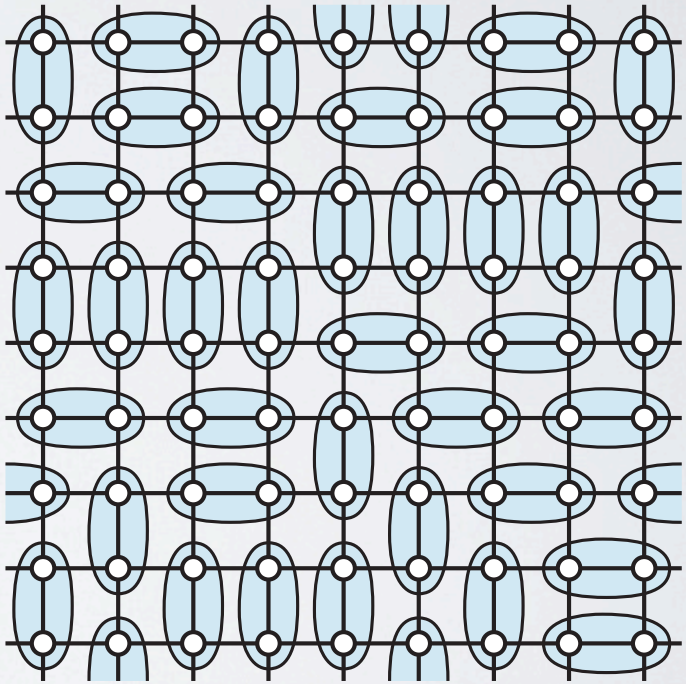
SINGLET PRODUCT STATES

- for each static singlet tiling,

$$E = \frac{1}{z} \times \frac{zN}{2} \times \left(-\frac{3J}{4}\right) = -\frac{3JN}{8}$$

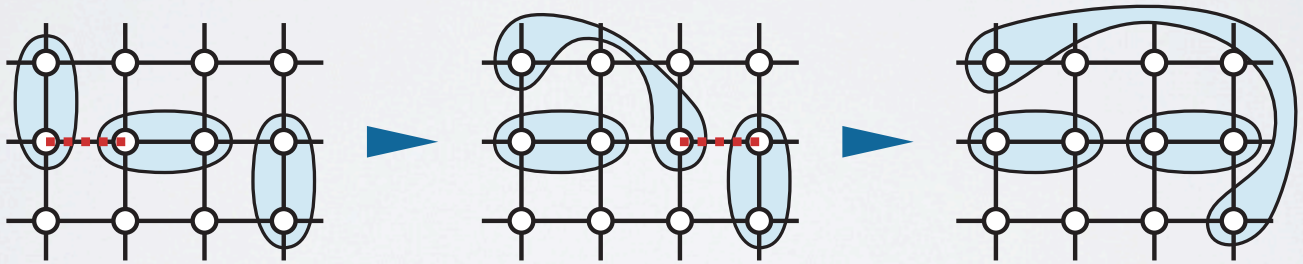
- only 1/z of the n.n couplings can be satisfied at a time

- degeneracy lifted by quantum fluctuations



SINGLET FLUCTUATIONS

- "off-diagonal" processes induce singlet rearrangements
- generate bonds of all odd Manhattan lengths (connecting sites in the A and B sublattices)

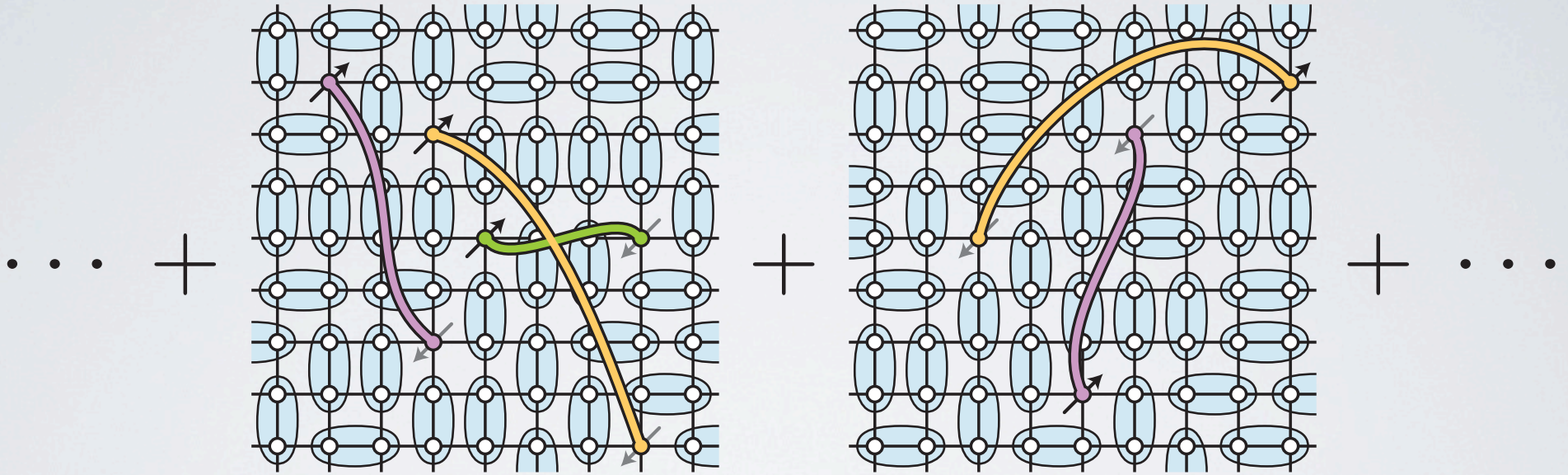


e.g., on the square lattice: $E/N = -0.375J$

$\downarrow$

$-0.669J$

NÉEL ORDER



- system-spanning bonds proliferate (communicating spin-spin correlations over long distances)
- many relevant configurations contribute to the ground state

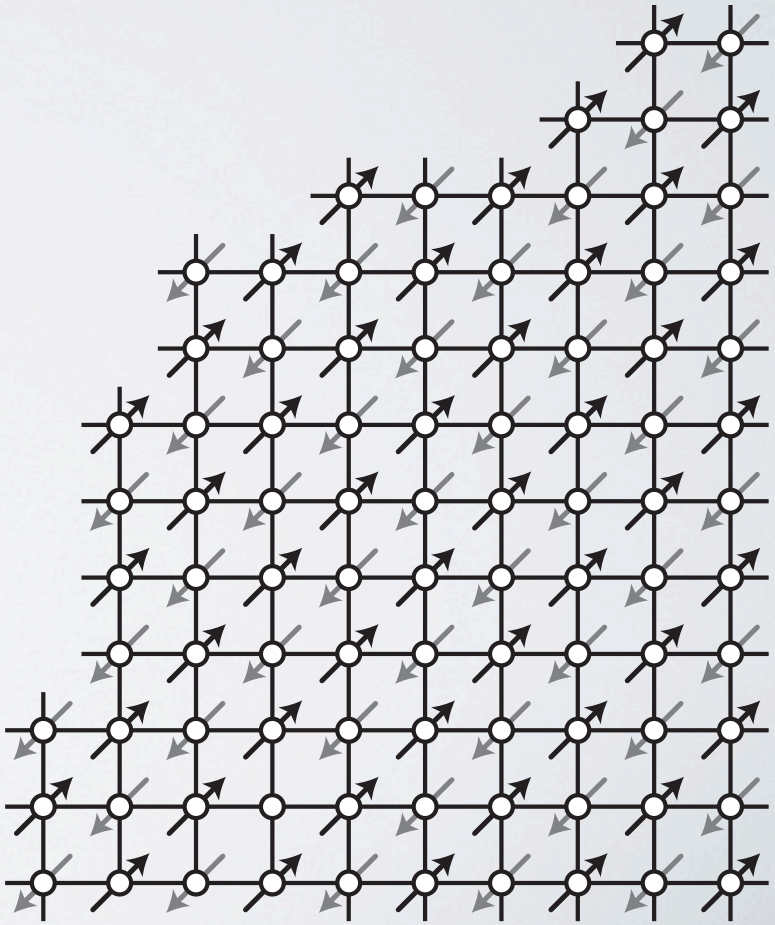
NÉEL ORDER

- Continuously connected to the large S limit:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{P}_{ij} = J \sum_{\langle i,j \rangle} S_i \cdot S_j + \text{const.}$$

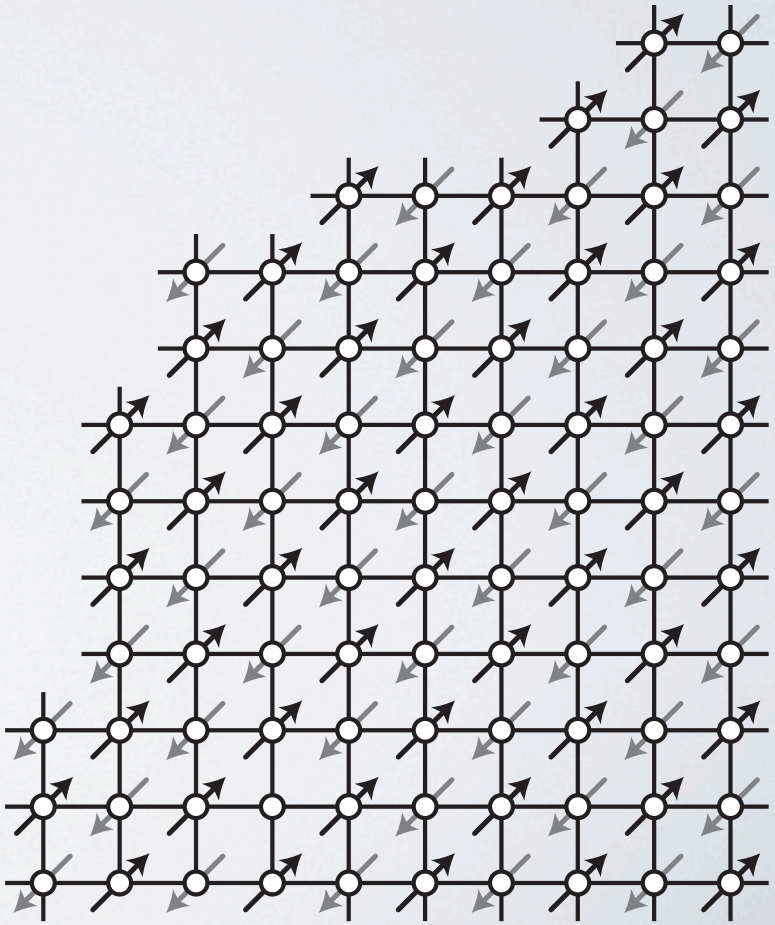
$$n_i = \lim_{S \to \infty} \frac{S_i}{\sqrt{S(S+1)}}$$

$$E = J \sum_{\langle i,j \rangle} n_i \cdot n_j$$

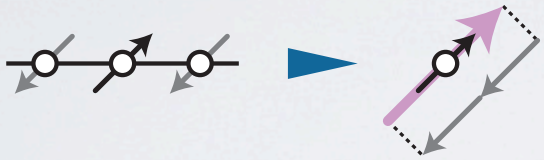


NÉEL ORDER

- Non-frustrated S=1/2 spin models
- Nearest-neighbour exchange interactions on a bipartite lattice
- Néel order is a generic feature when the coordination is greater than 2

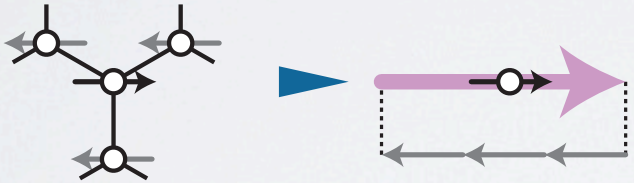


MEAN-FIELD PICTURE



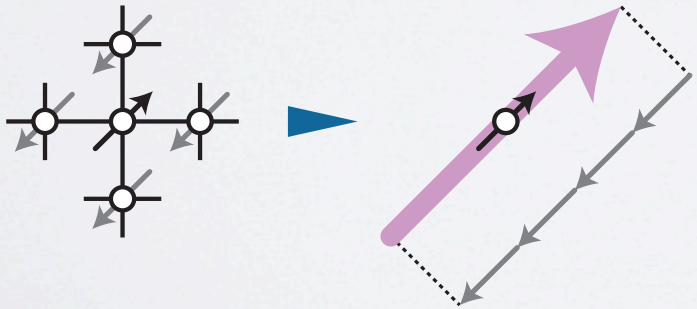
$$C(r) = \frac{(\log r)^{1/2}}{r}$$

low coordination



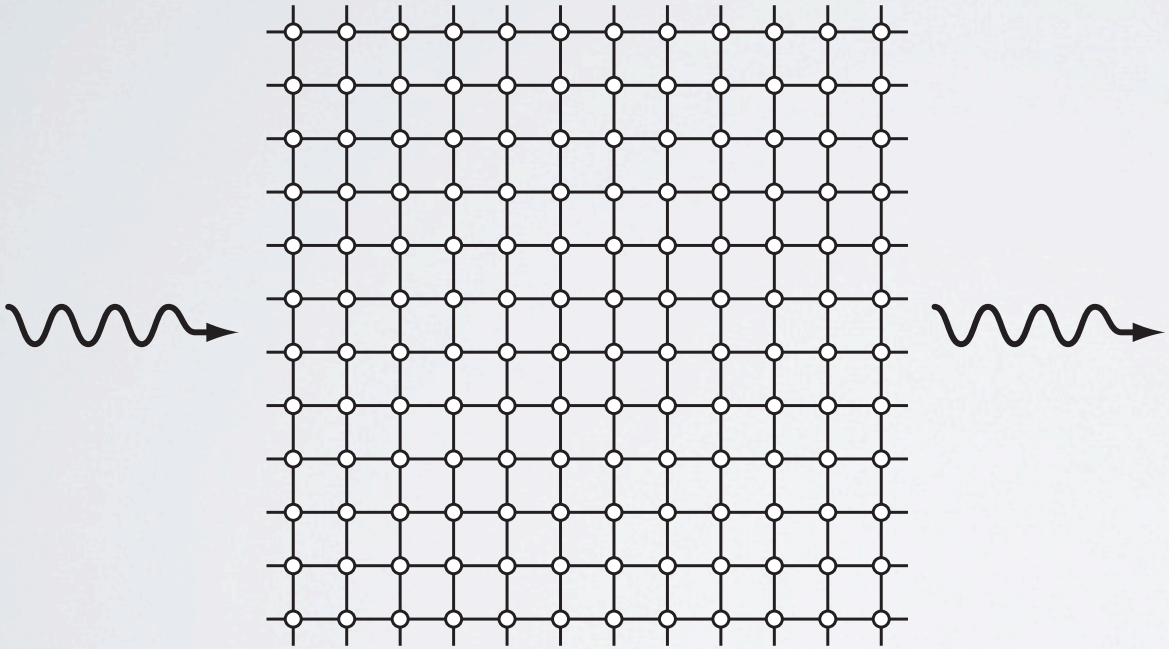
$$C(r) = \text{const.} + \frac{1}{r}$$

high coordination



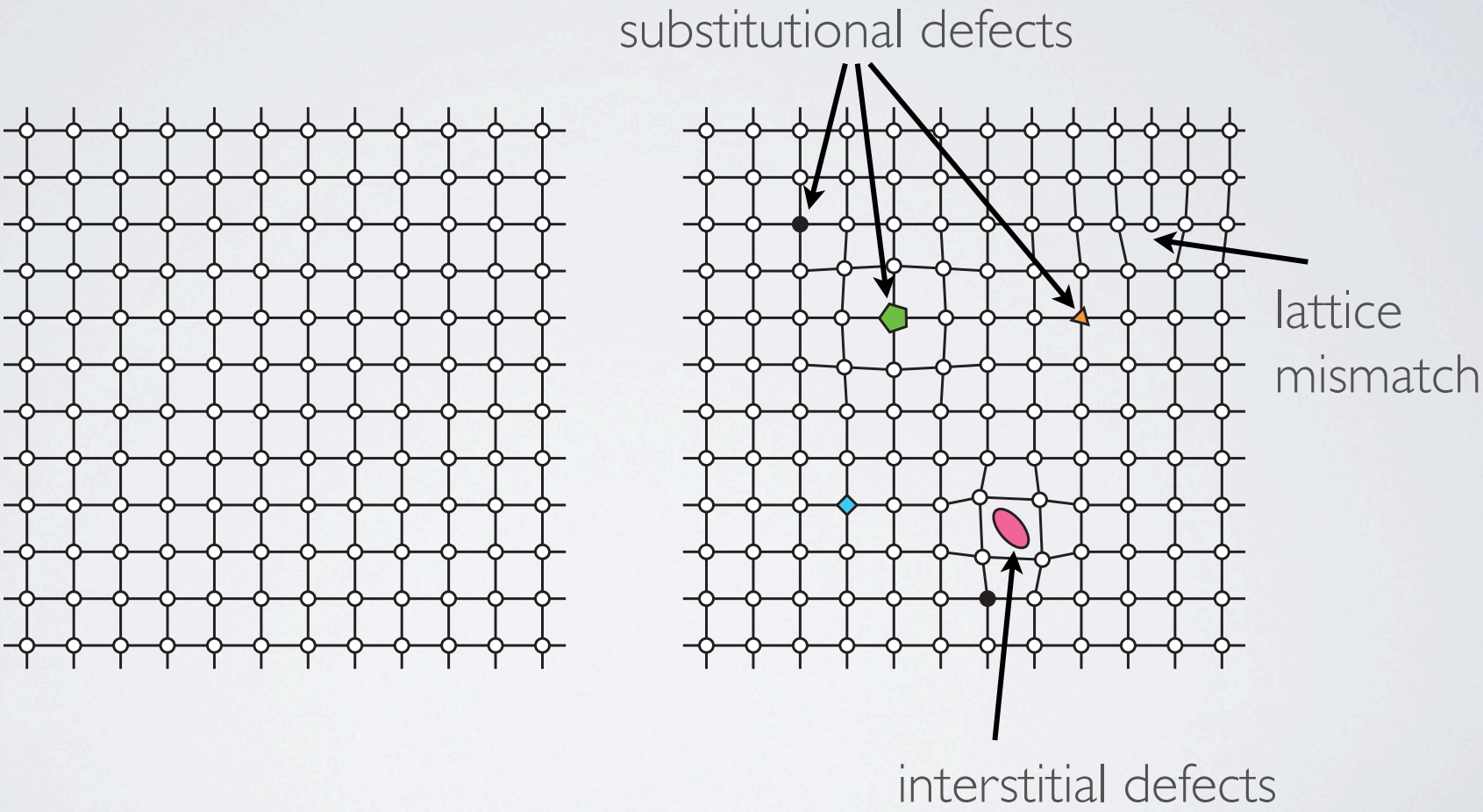
conventional AFM order is favoured

CRYSTALLINE ENVIRONMENT

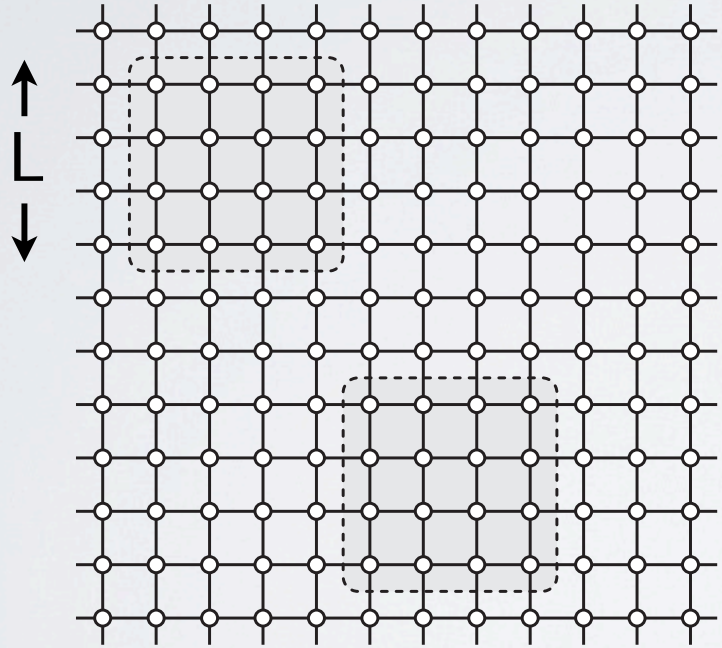


- (discrete) translational invariance implies that (crystal) momentum is a good quantum number
- existence of well-defined wavevectors is crucial to most analytical approaches

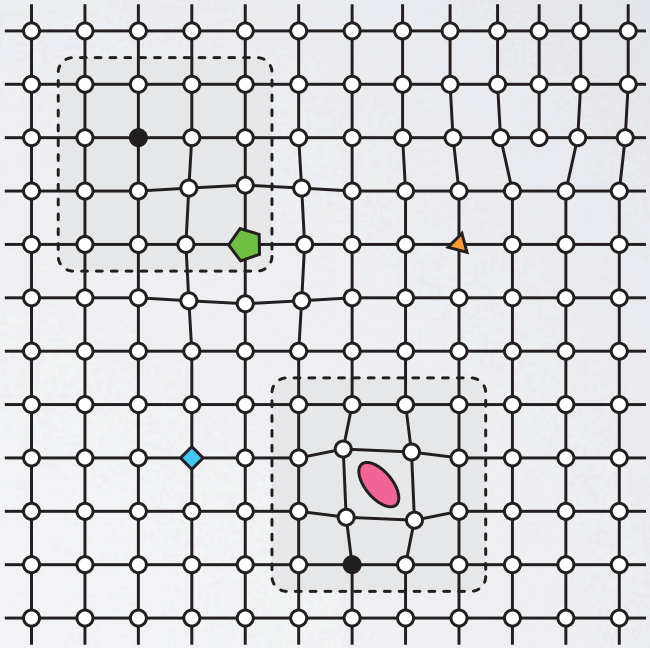
QUENCHED DISORDER



QUENCHED DISORDER



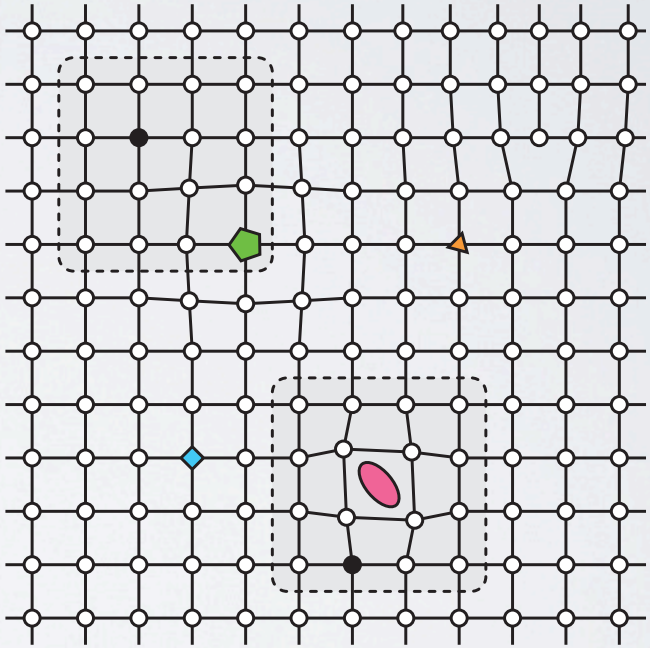
all patches are equivalent



all patches are unique

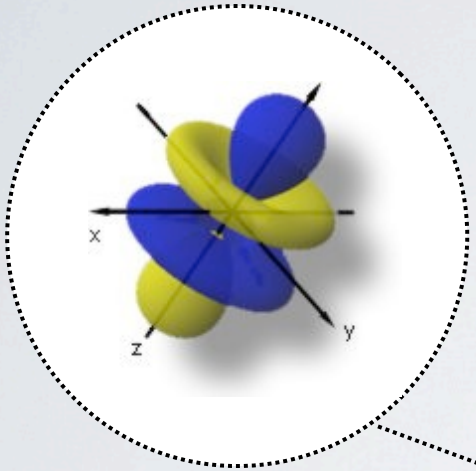
QUENCHED DISORDER

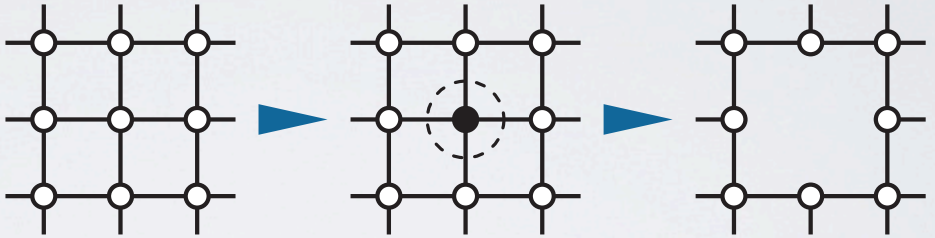
- requires brute-force averaging
- limit is doubly infinite: patch size and number of realizations

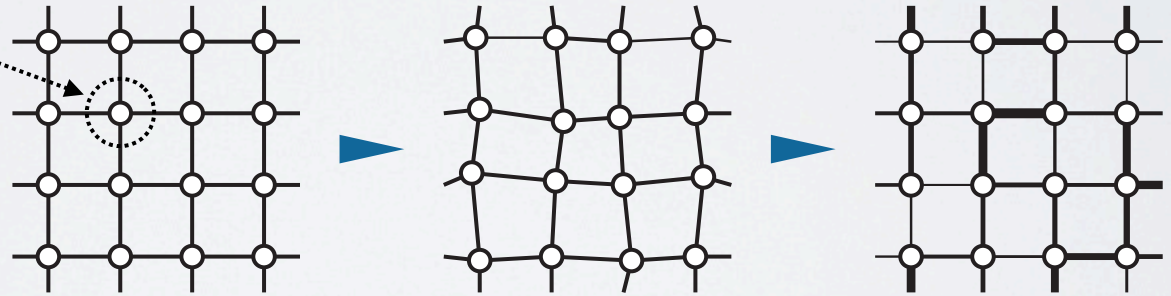


DISORDERED SPIN MODELS

Site dilution





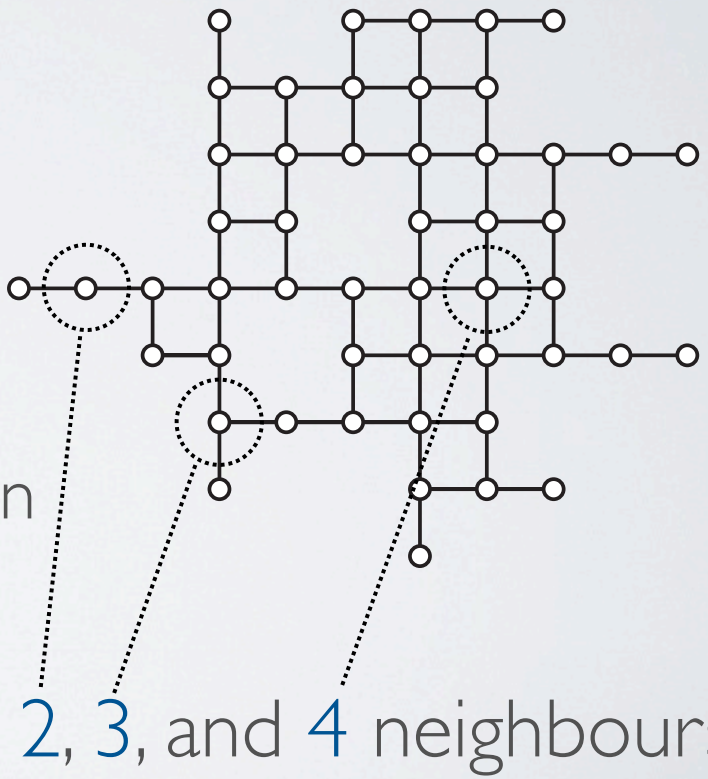


S=1/2 degrees of freedom

Random exchange

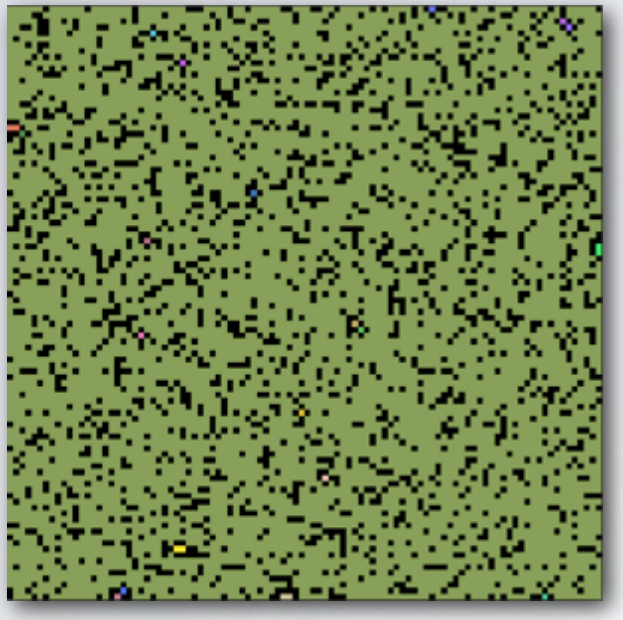
SITE DILUTION EFFECTS

- Creation of orphan clusters (finite in size and disconnected from the spanning cluster or "backbone")
- Fluctuations in local coordination
- Increasingly disruptive in low dimension (cuts the linear chain entirely)



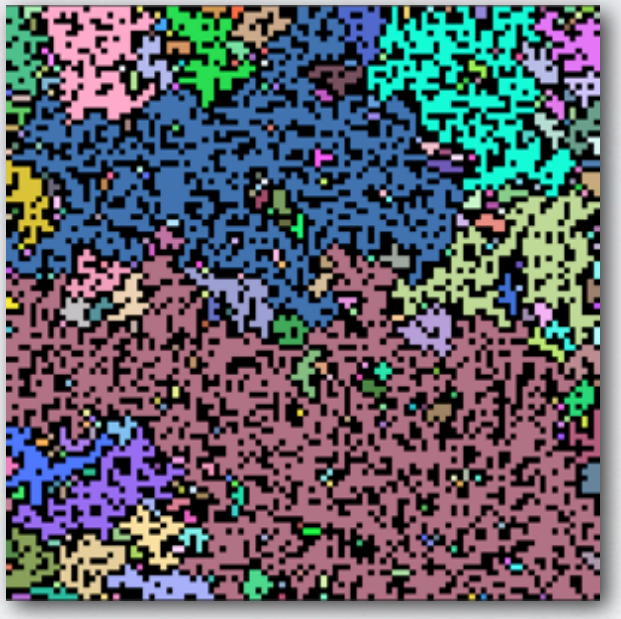
CLASSICAL PERCOLATION

few orphans



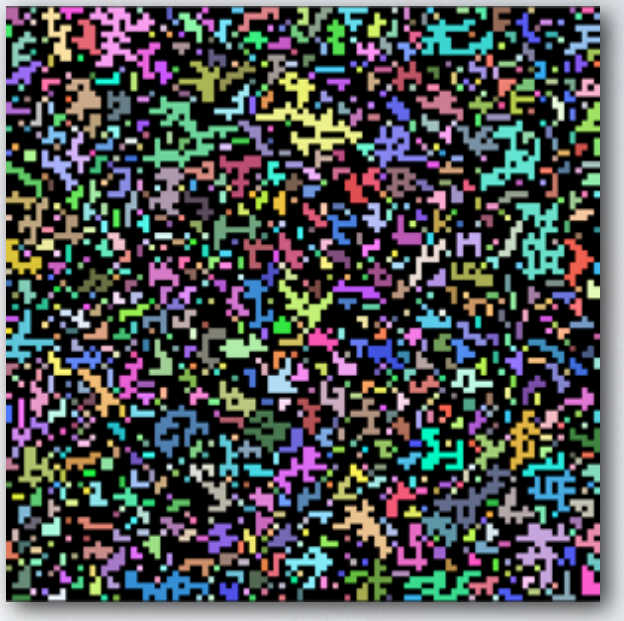
$p = 0.2$

mostly orphans



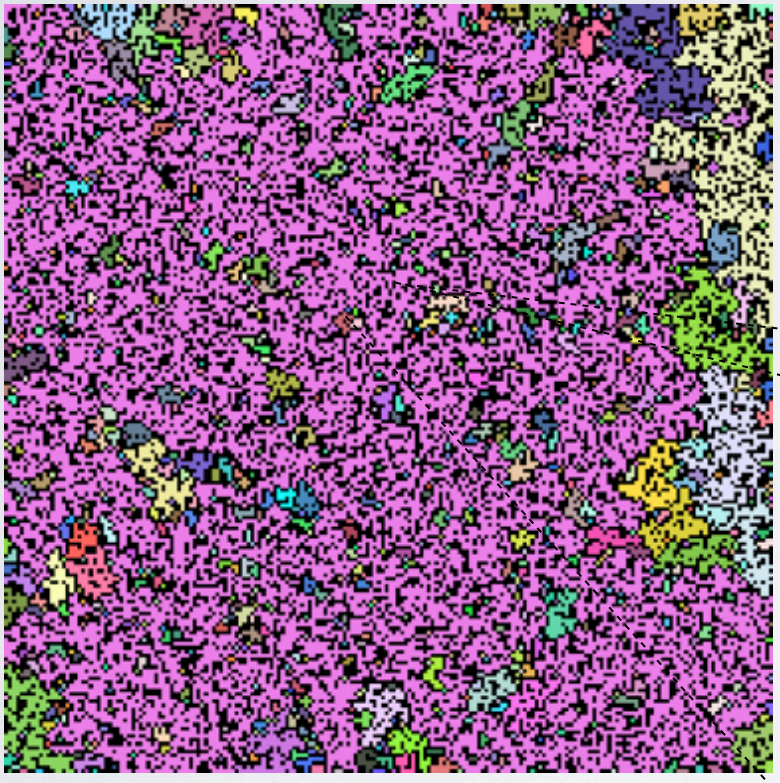
$p = p_c \doteq 0.407$

all orphans

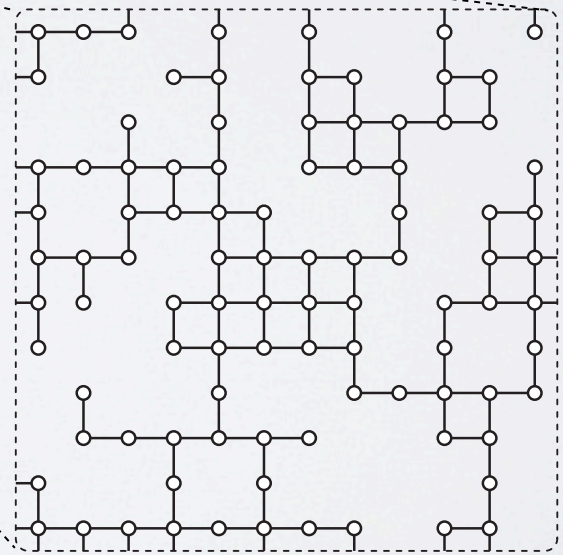


$p = 0.6$

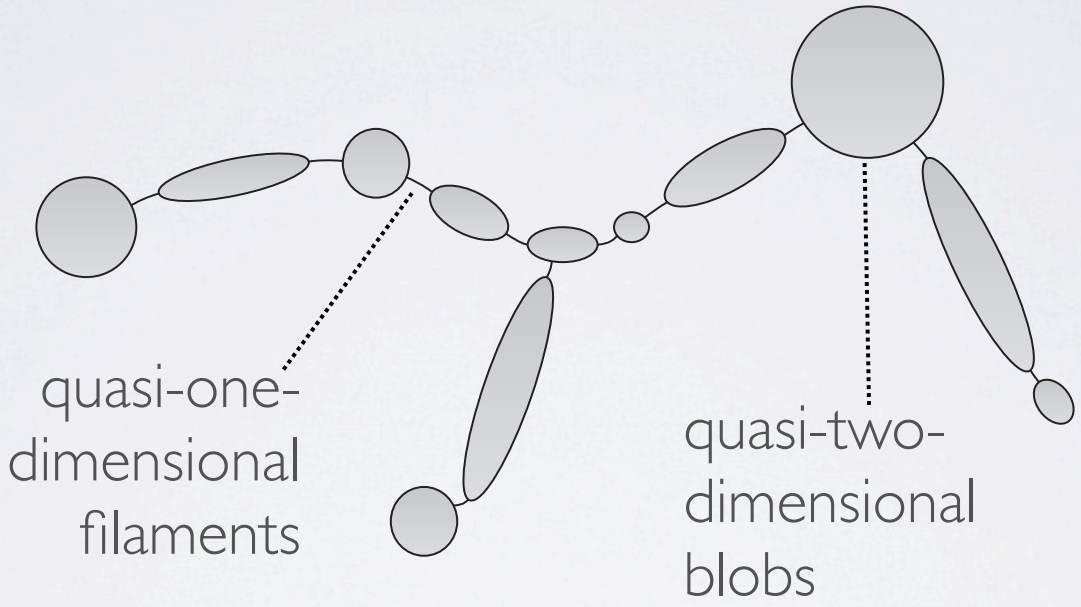
PERCOLATION



- percolating cluster has fractal dimension 91/48
- average coordinate is 2.5 (<3)

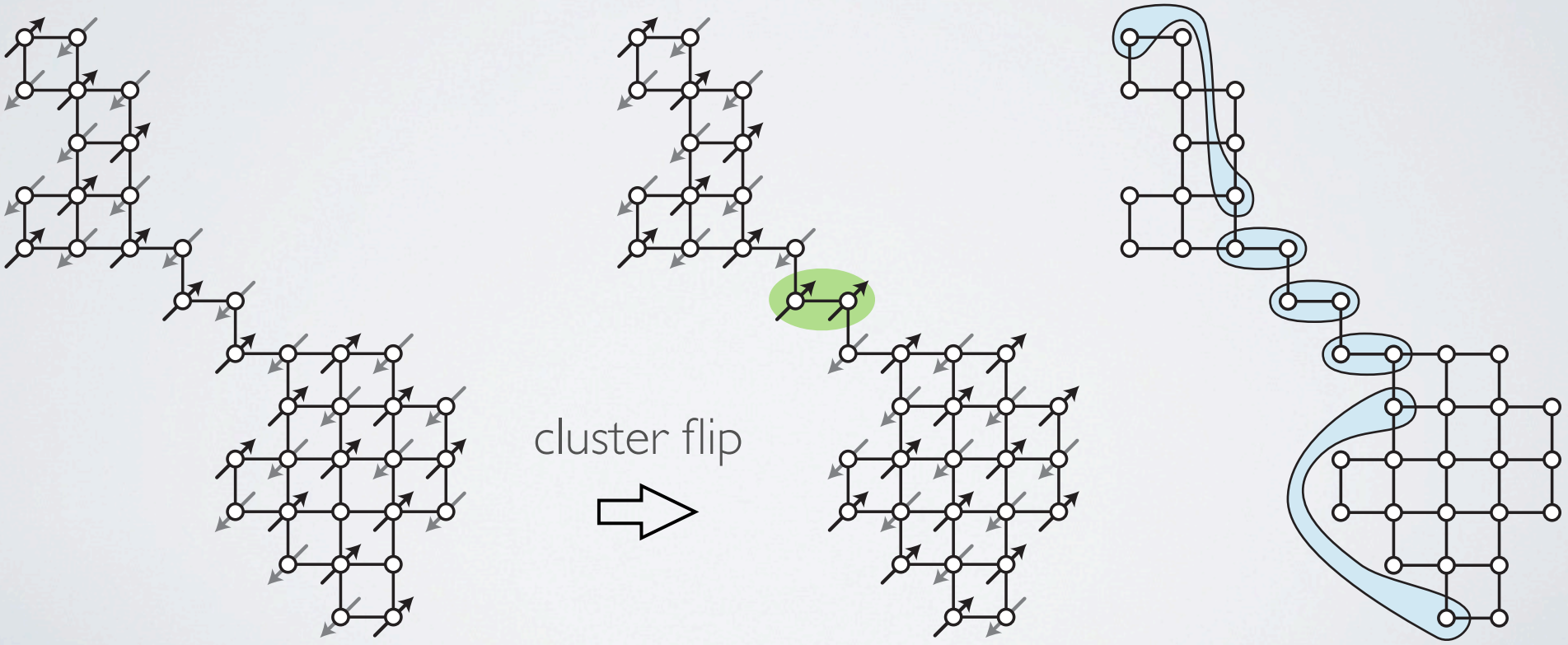


BLOBS AND FILAMENTS

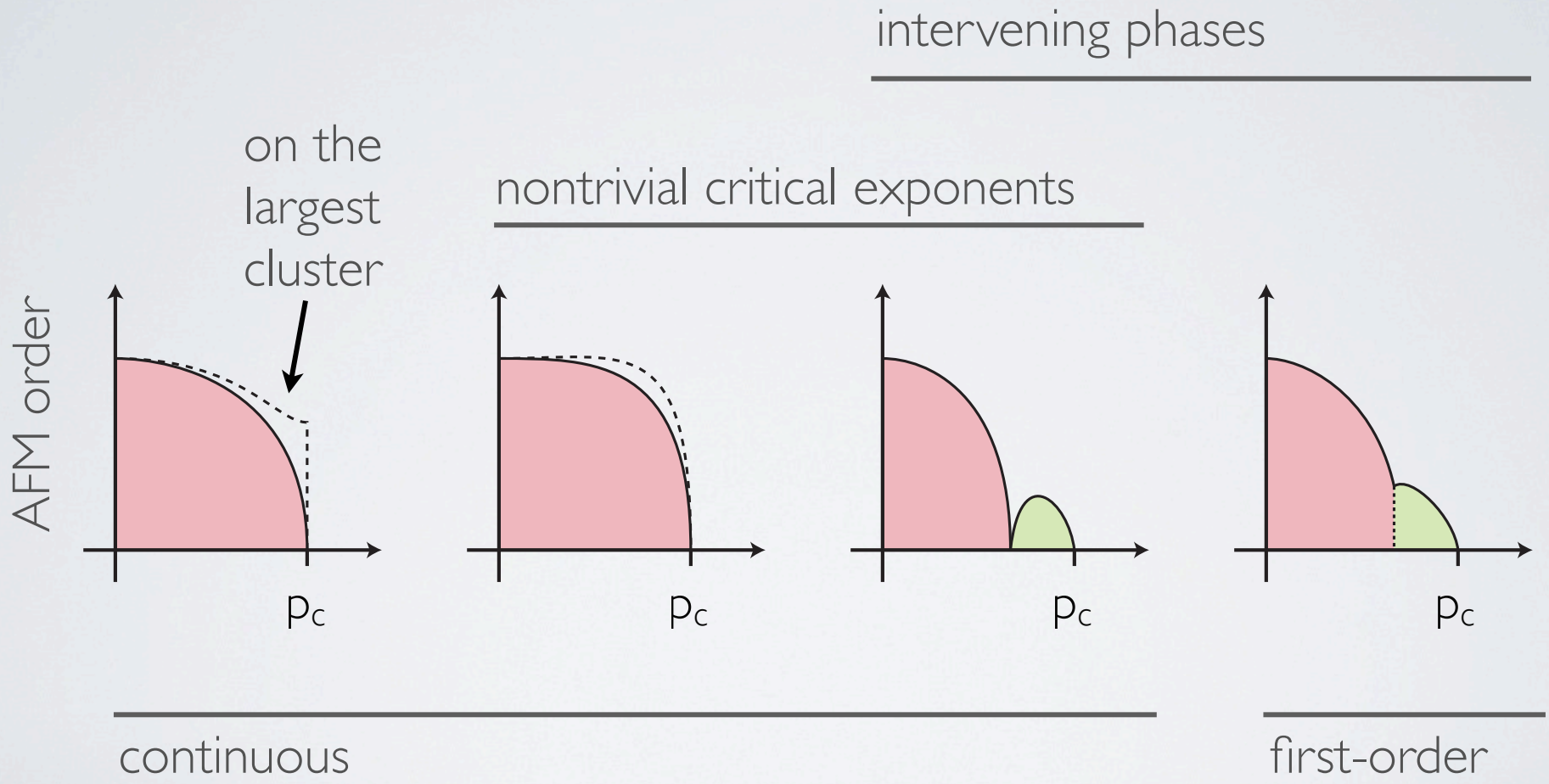


BLOBS AND FILAMENTS

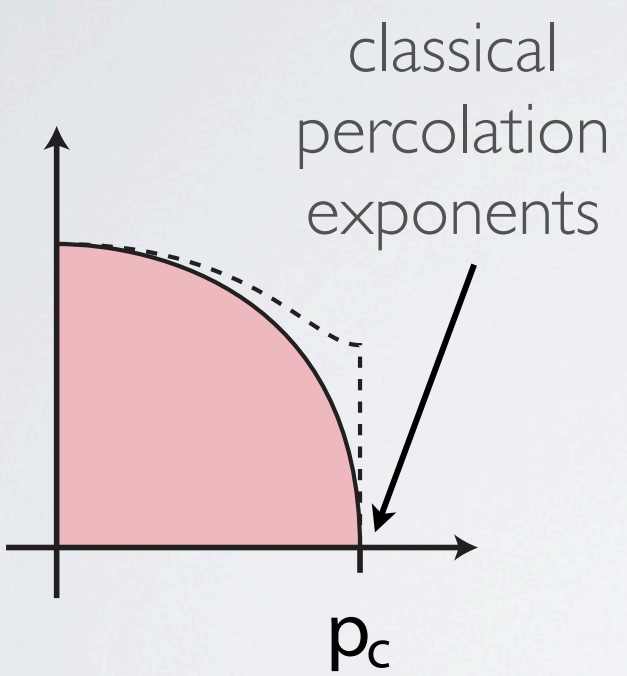
- does the percolating cluster support magnetic order?

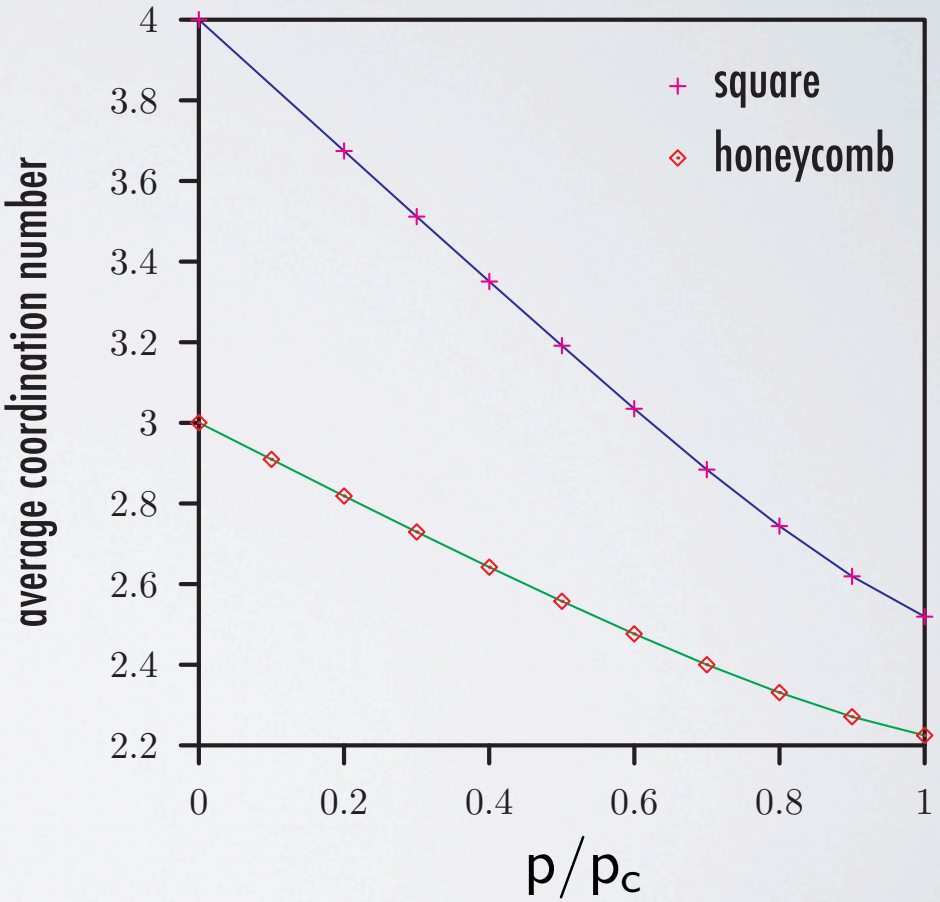


PHASE DIAGRAM?



TRIVIAL RESULT





Sandvik, PRB 66, 024418 (2002)
Castro et al., PRB 73, 054422 (2006)

TOO BLUNT AN INSTRUMENT

- Random site dilution is not disruptive enough:
  - it's not able to kill magnetic long-range order
  - AFM is too robust on regular lattices in dimension ≥ 2
- At the same time, it is far too disruptive:
  - quickly breaks the system into disjoint pieces (esp. 1D)
  - classical percolation dominates at transitions

RANDOM SINGLET PHASE

- S=1/2 quantum Heisenberg model on the linear chain is unstable to even infinitesimal exchange disorder
- The existence and nature of the resulting random singlet phase is established by real-space RG analysis (decimation)
- Not applicable to lattices with coordination $z > 2$
- Numerical simulations indicate that AFM order is robust with respect to exchange disorder

REAL-SPACE DECIMATION

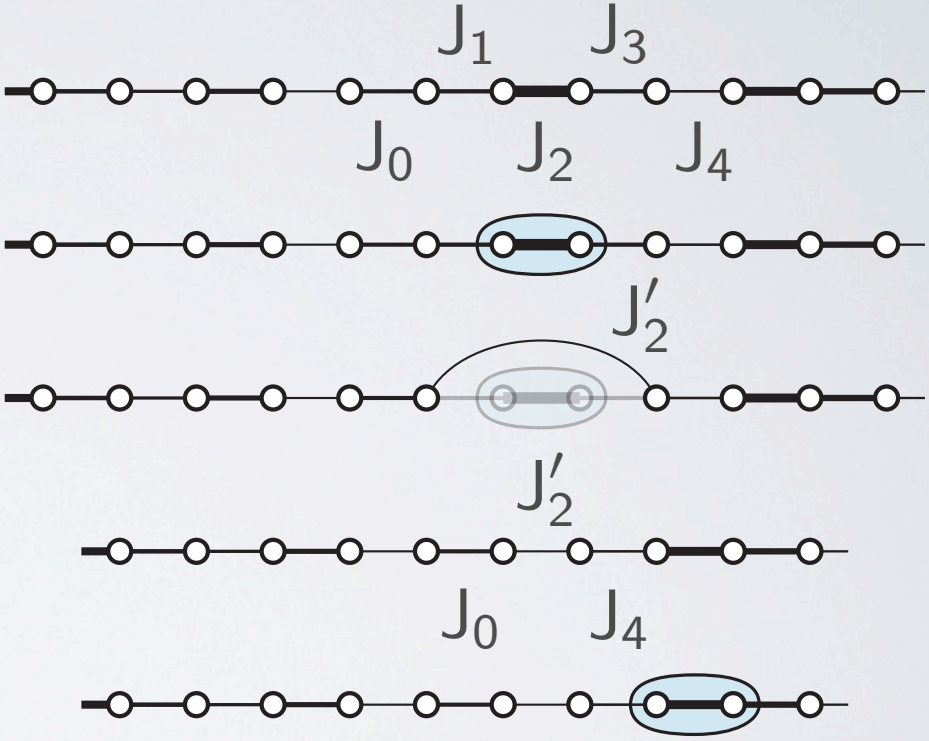
- at each stage, form a singlet across the strongest bond

$$H[L, \{J_{ij}\}] \rightarrow H[L-2, \{J'_{ij}\}]$$

- new effective coupling via perturbation theory

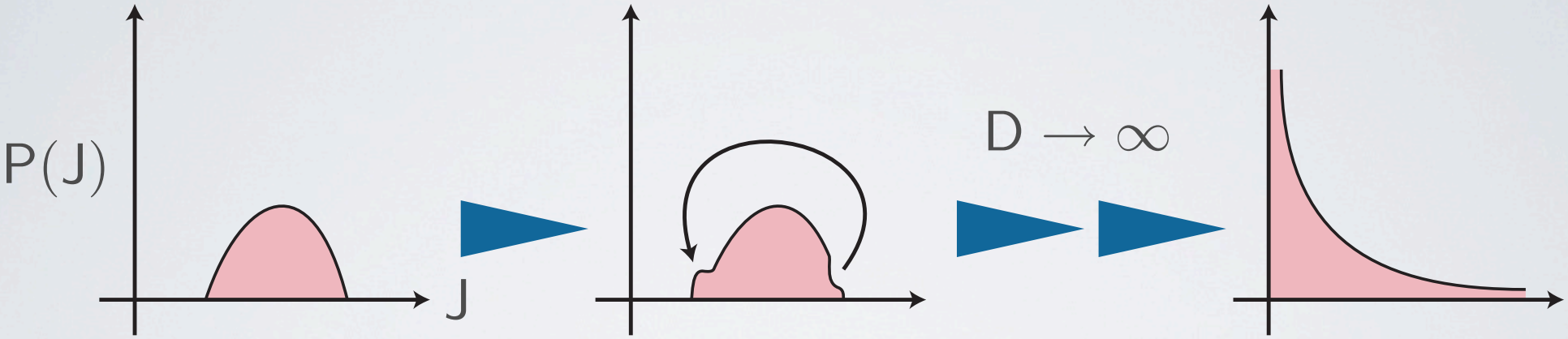
$$J'_2 := \frac{J_1 J_3}{J_2}$$

- unique pattern of singlet bonds $|RS\rangle$ at infinite-randomness fixed point



Dasgupta and Ma, PRB **22**, 1305 (1980)
Fisher, PRB **50**, 3799 (1994)
Rafael and Moore, PRL **93**, 260602 (2004)

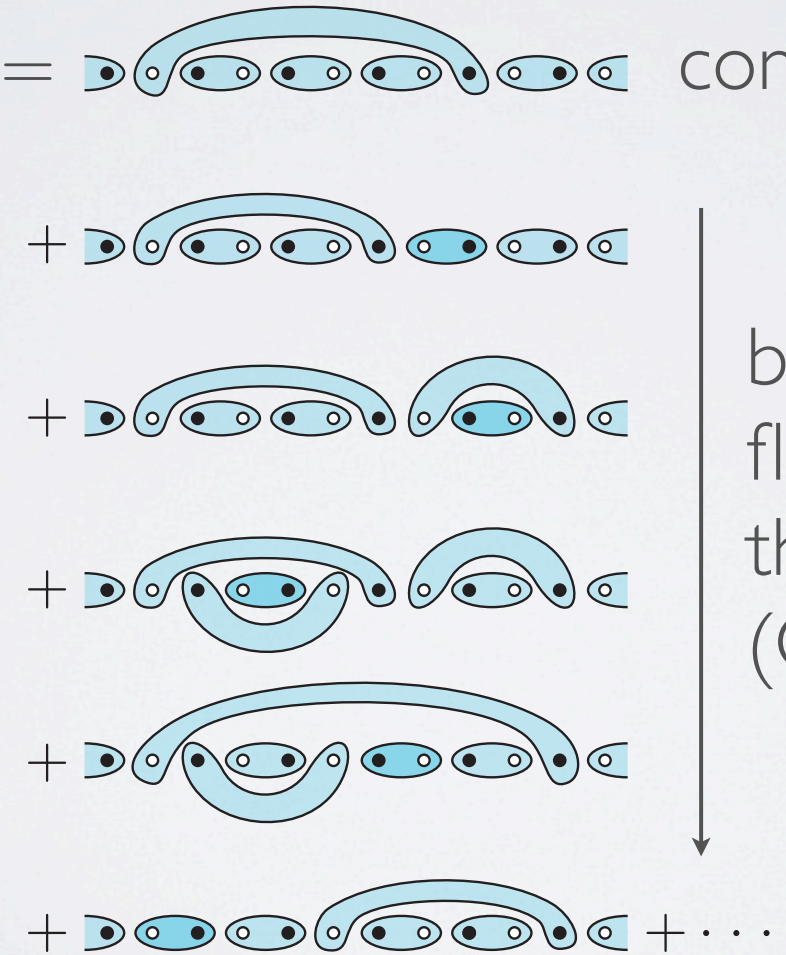
RESULTING RG FLOW



- All initial distributions flow to a singular $P(J) \sim J^{-1+1/D}$
  $\rightarrow 1/J$
- Strong-disorder properties are universal $C(r) \sim \frac{1}{r^2}$

TRUE GROUND STATE

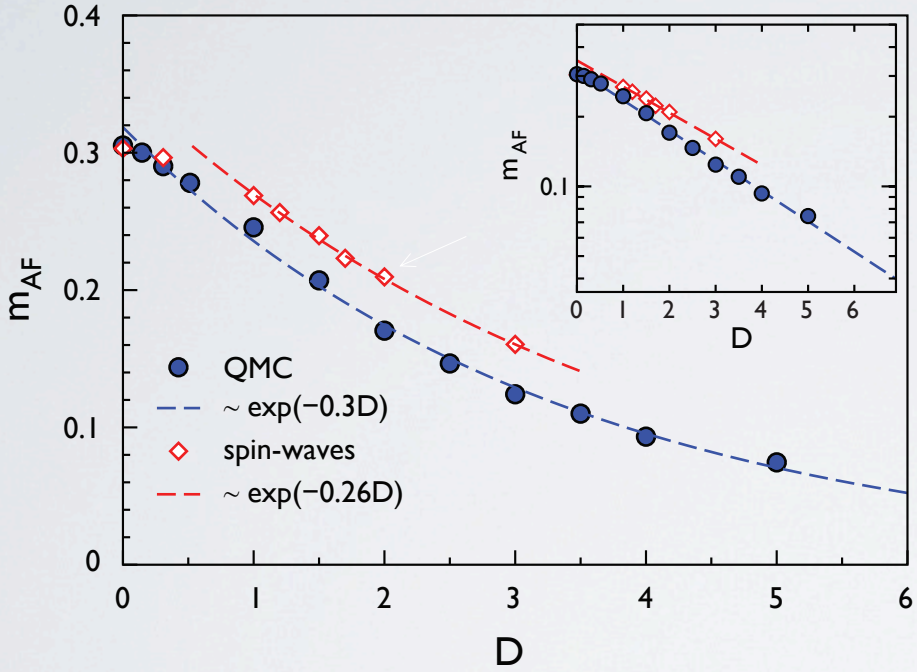
$e^{-\tau \hat{H}}|RS\rangle =$

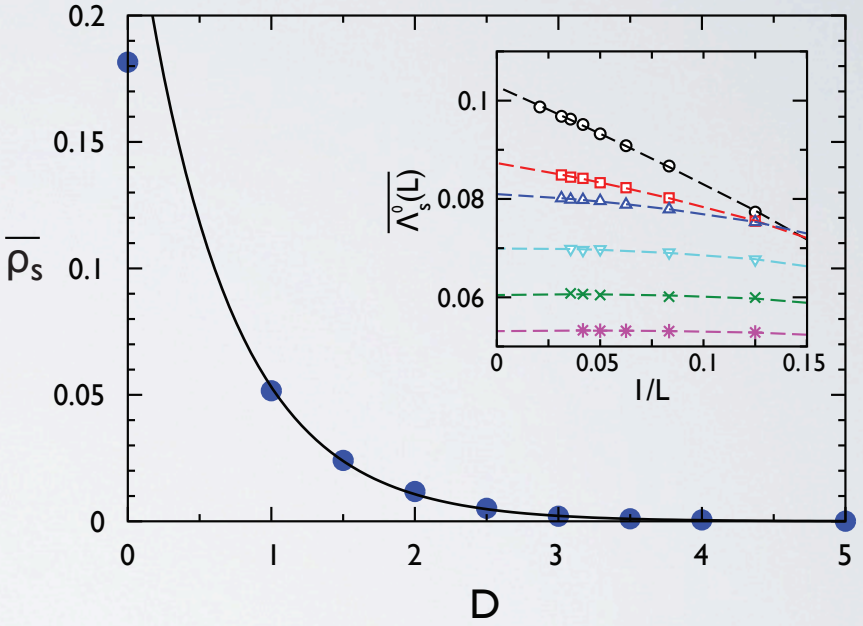


random singlet configuration

bond fluctuations that are *negligible* (QMC)

SQUARE-LATTICE QMC



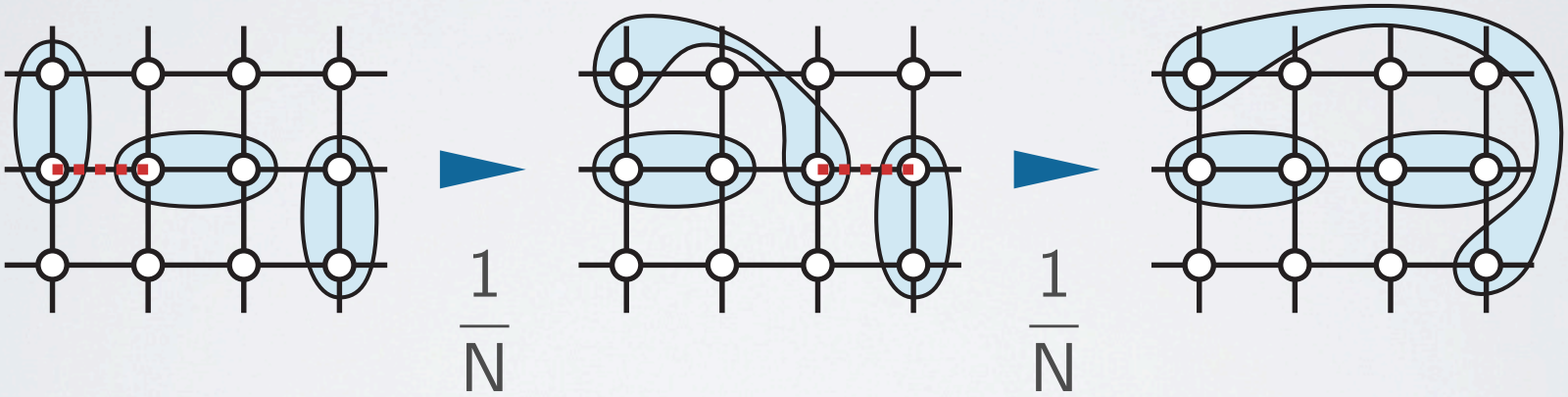


- simulations reveal no critical value of D

Laflorencie *et al.*, PRB **73**, 060403(R) (2006)

SU(N) GENERALIZATION

- bond rearrangements (off-diagonal elements of H) suppressed

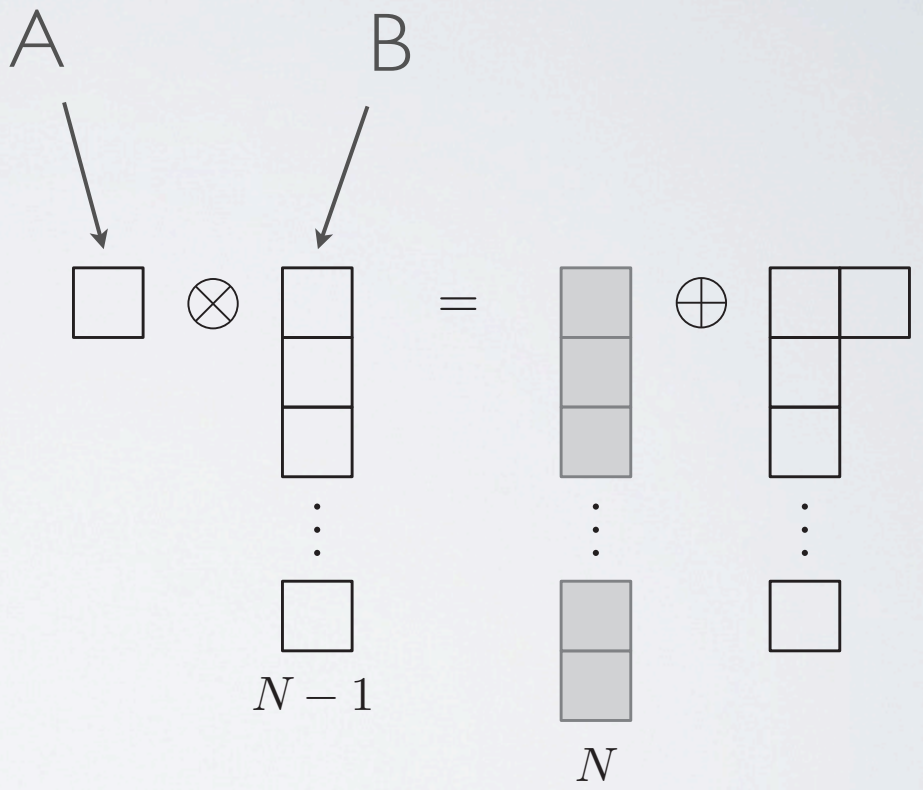


tune this to small values

Kawashima and Tanabe, PRL **98**, 057202 (2007)
Beach *et al.*, PRB **80**, 184401 (2009)

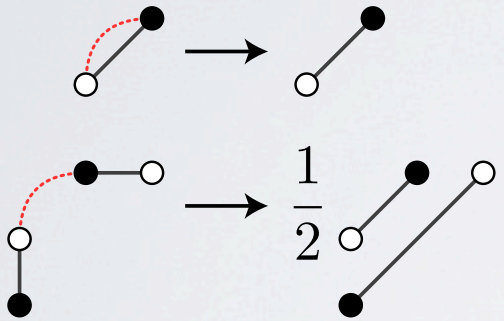
SU(N) GENERALIZATION

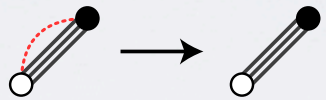
- enlarge group symmetry
- place the fundamental rep on one sublattice and its conjugate on the other

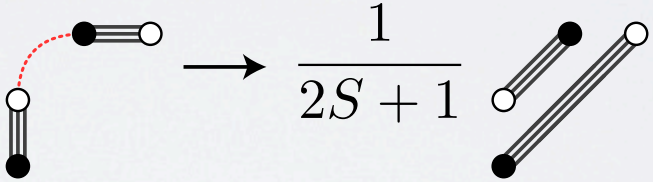


SU(N) GENERALIZATION

$$P_{ij} = \frac{\prod_t (\mathbf{S}_i \cdot \mathbf{S}_j - E_t)}{\prod_t (E_s - E_t)} = \prod_{j=1}^{2S} \left[1 - 2 \left(\frac{S(S+1) + \mathbf{S}_i \cdot \mathbf{S}_j}{j(j+1)} \right) \right]$$







$$N = 2S + 1$$

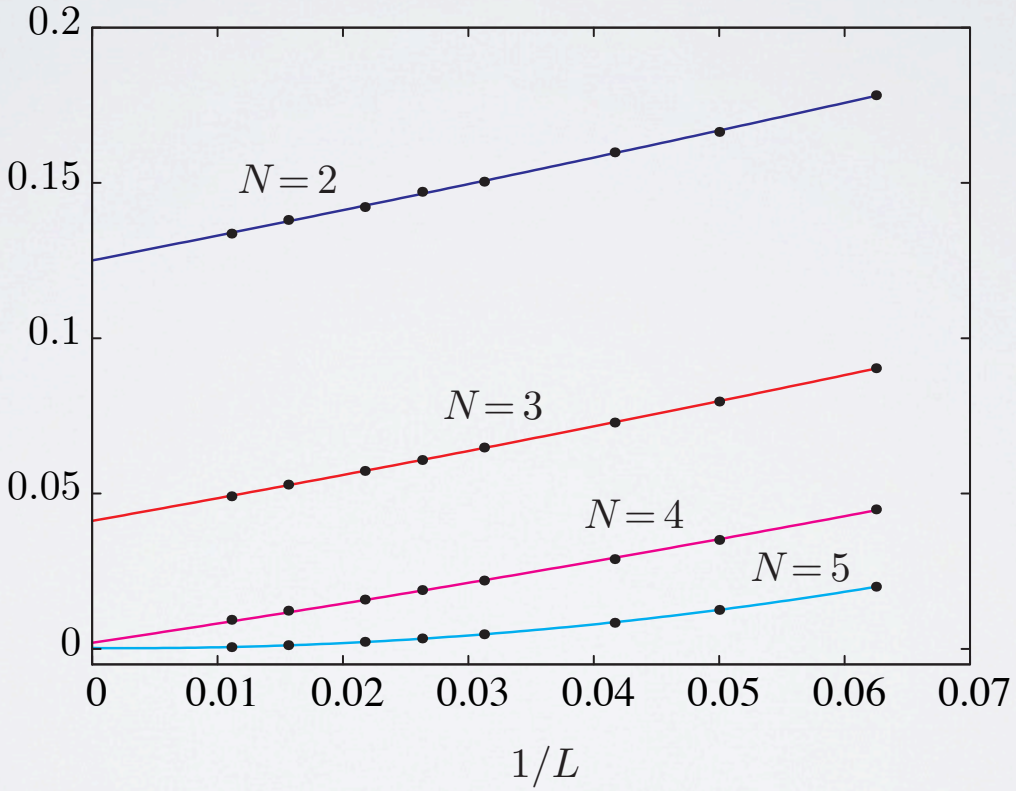
$$P_{ij} = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j \qquad (S = \tfrac{1}{2})$$

$$P_{ij} = \frac{1}{3} \left[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 1 \right] \qquad (S = 1)$$

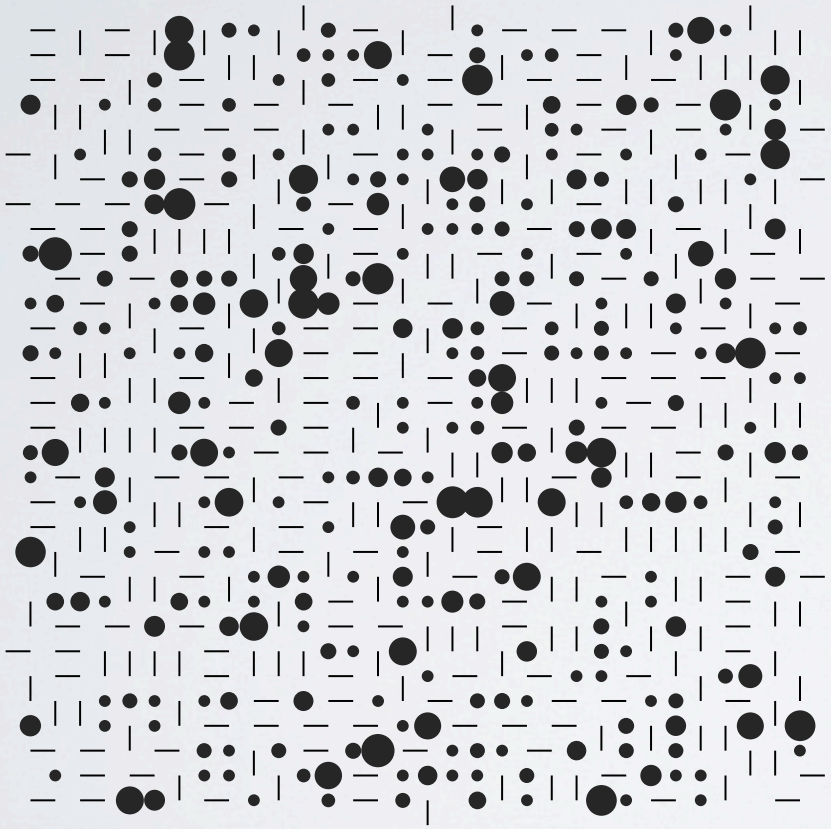
$$\vdots$$

SUPPRESSING AFM ORDER

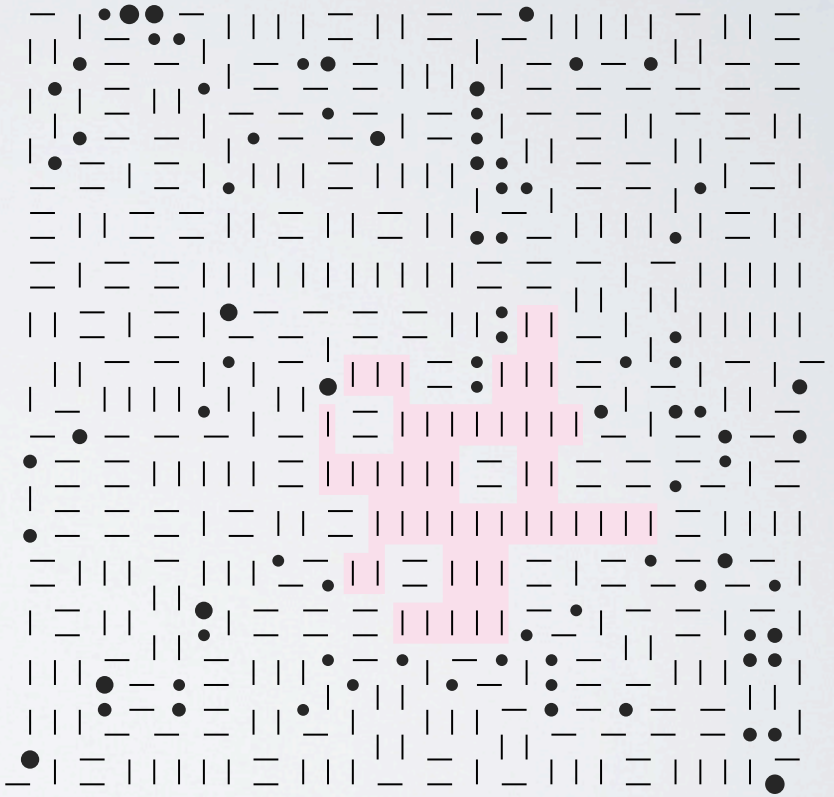
second loop moment (AFM)



BOND SNAPSHOT



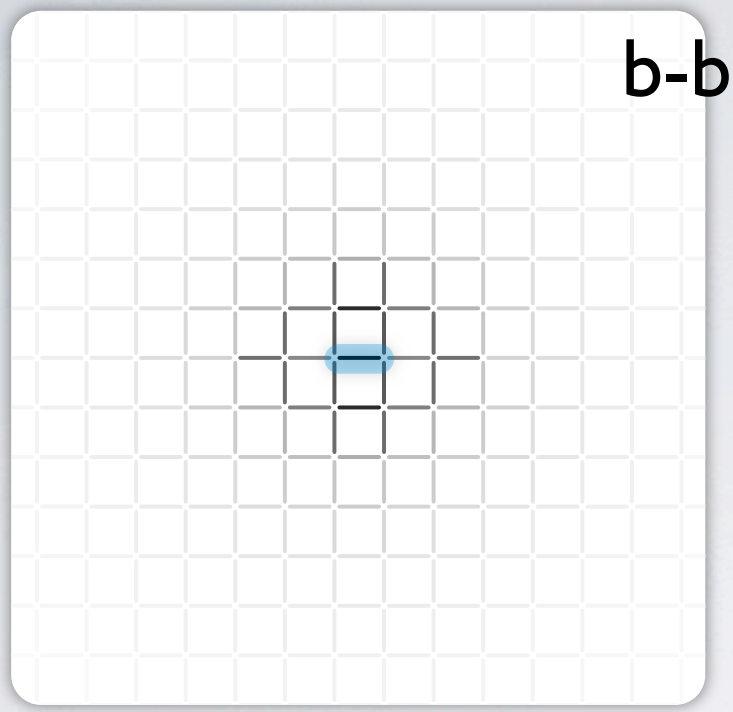
$N = 2$

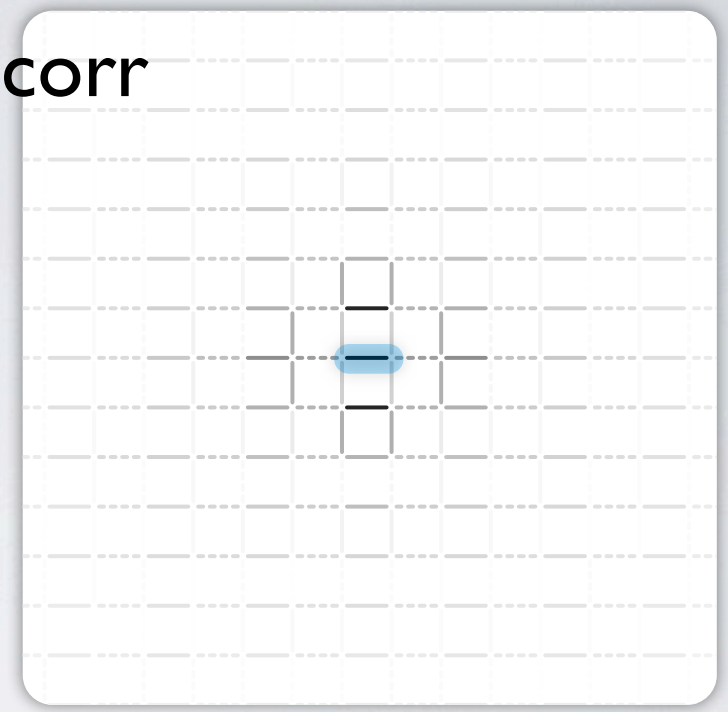


$N = 7$

b-b corr

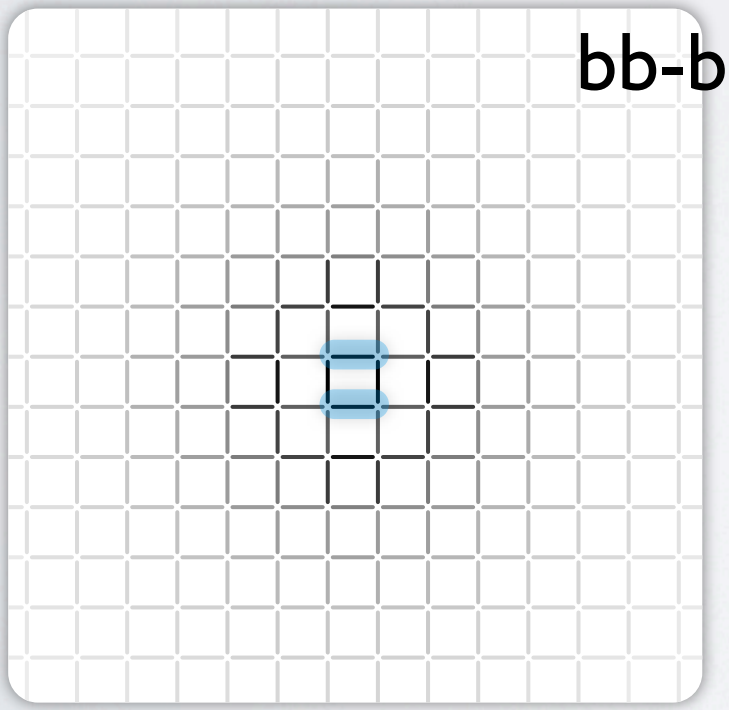
$N = 2$

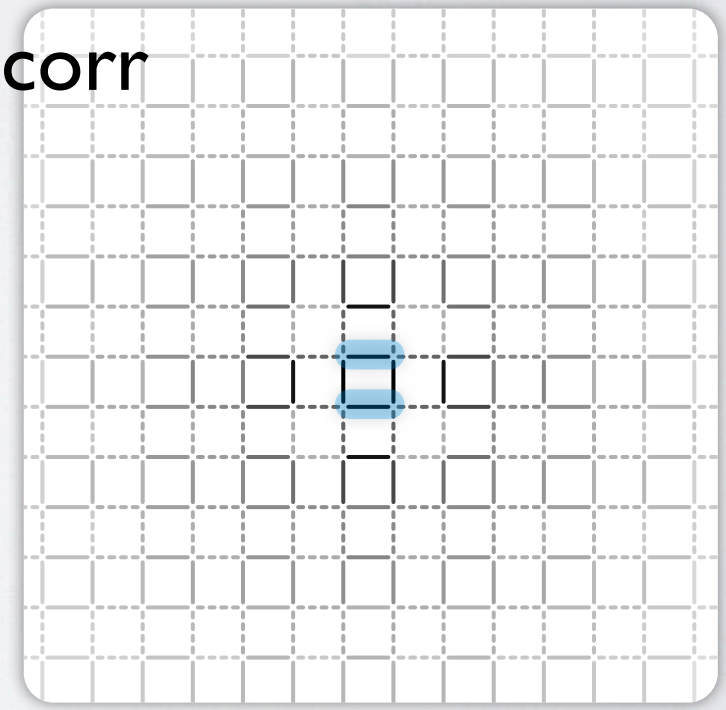




$N = 7$

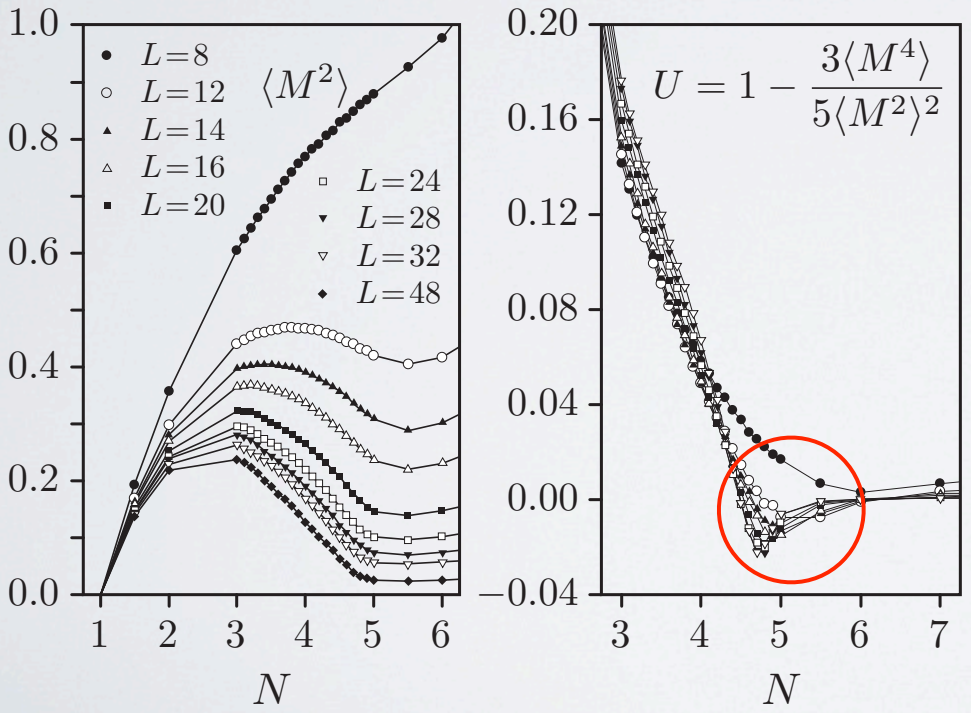
bb-b corr



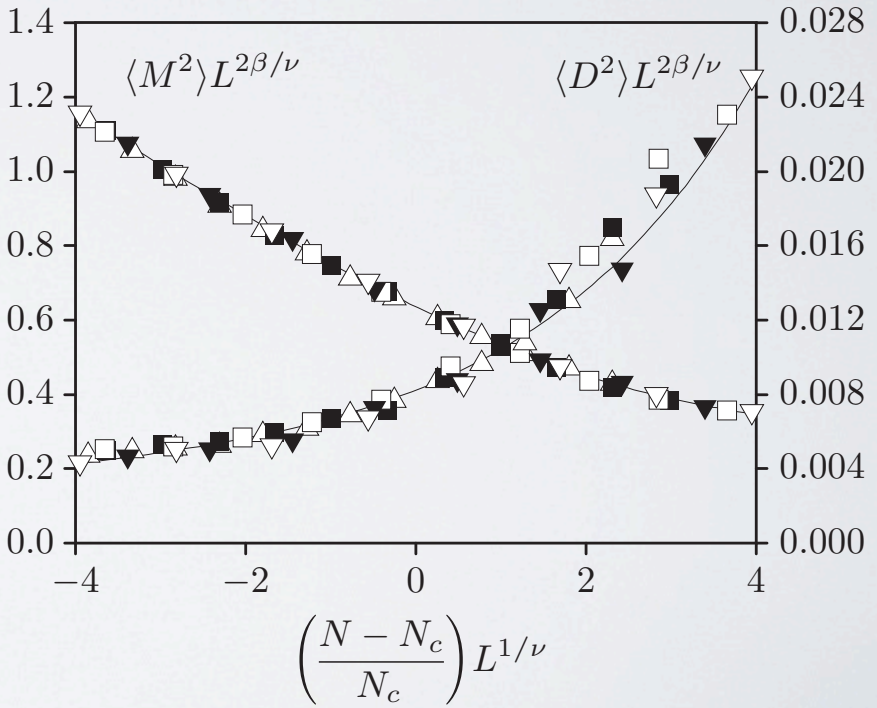


"CONTINUOUS N"

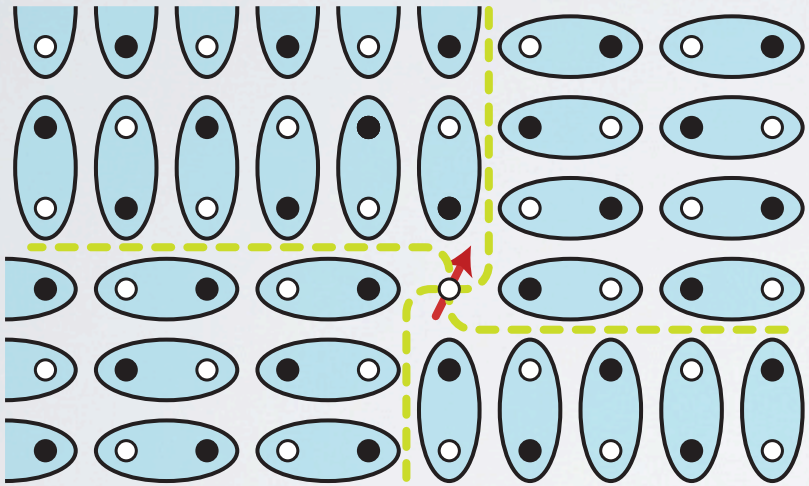
positive kurtosis occurs because the distribution is sub-Gaussian

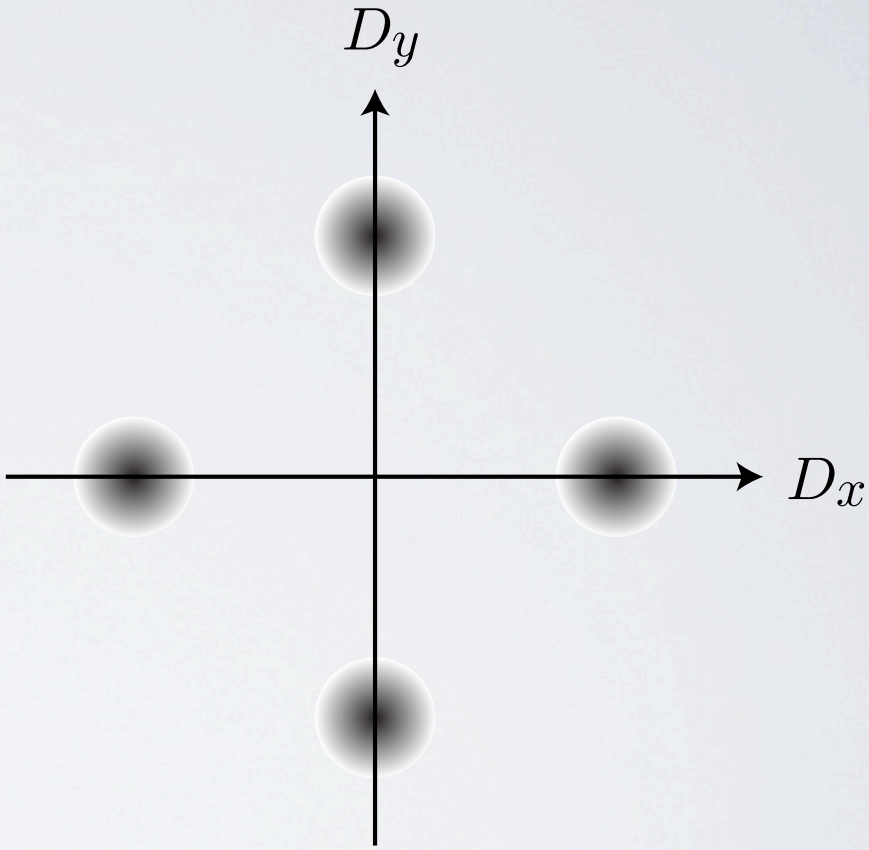


$N_c = 4.6$



EMERGENT U(1) SYMMETRY

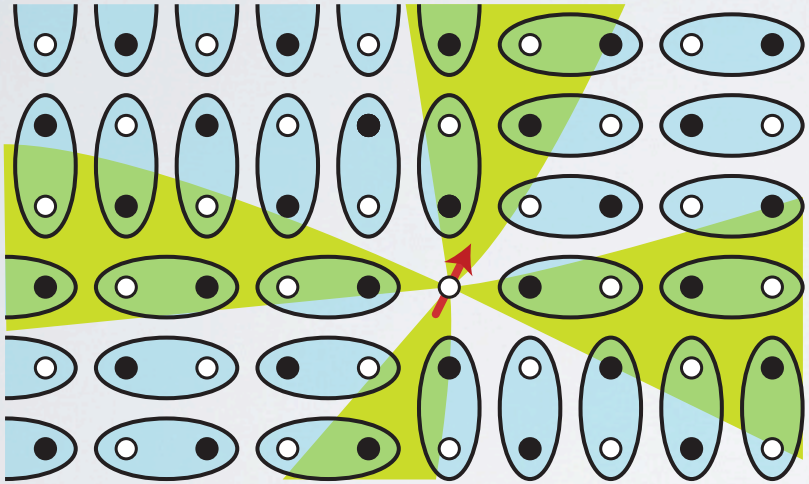


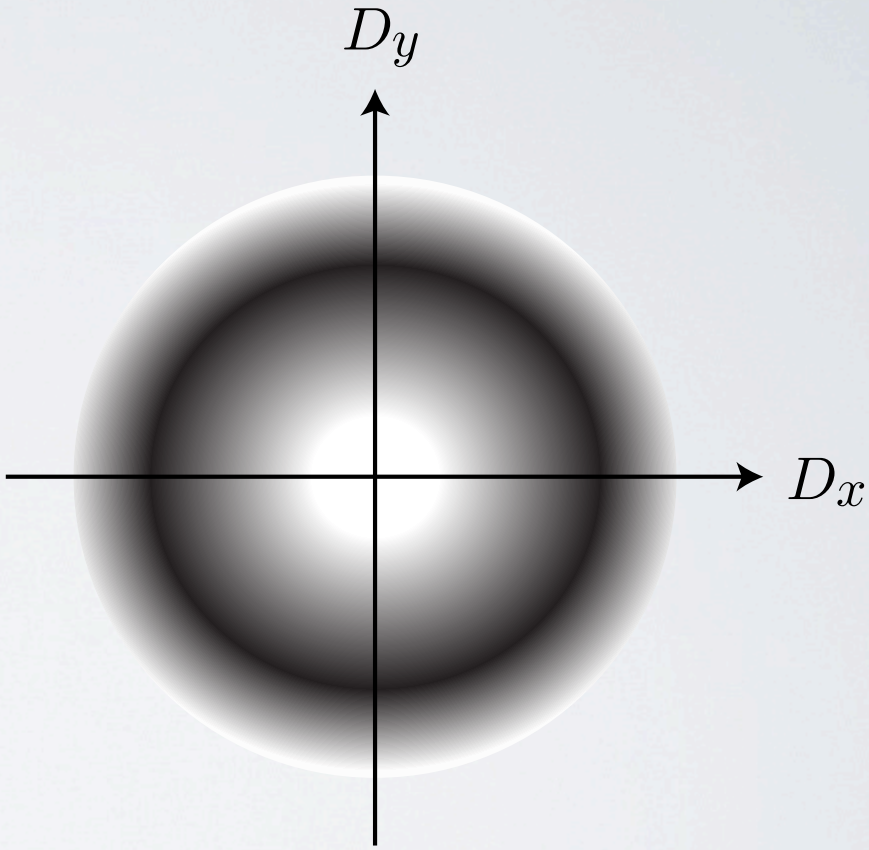


$$D_a = \sum_{\mathbf{r}} (-1)^{\mathbf{r}\cdot\hat{a}} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{a}} \quad (a = x, y)$$

EMERGENT U(1) SYMMETRY

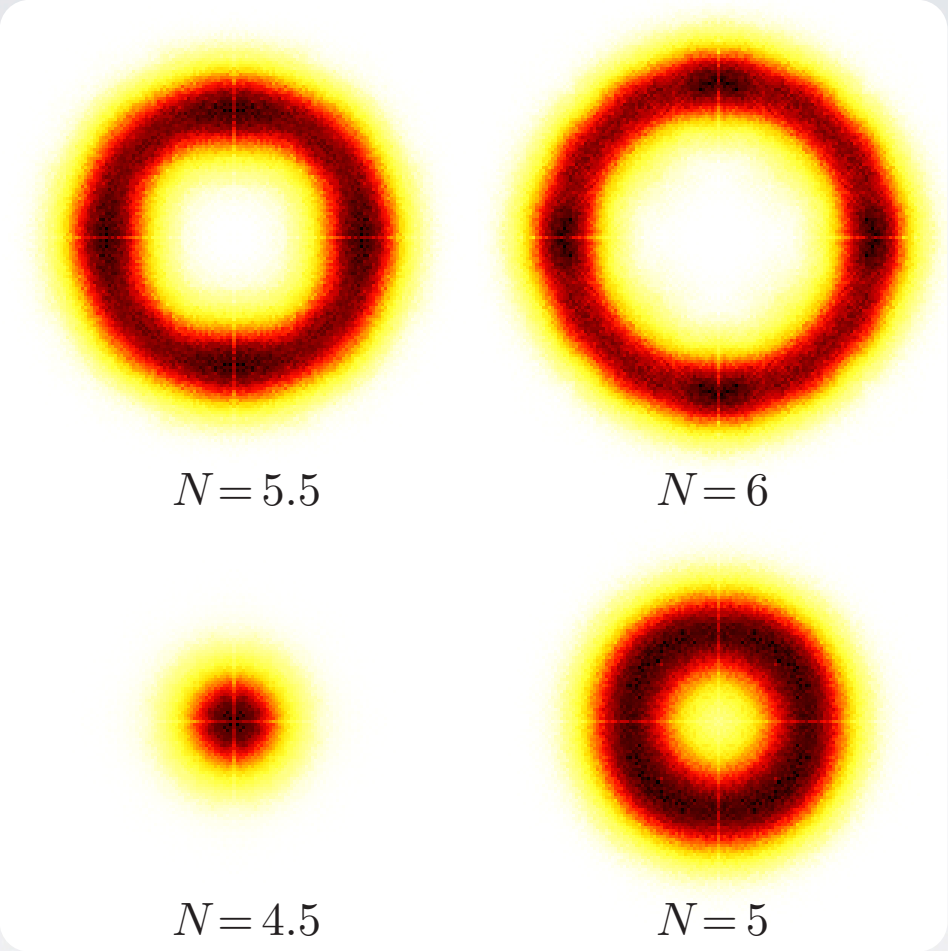
$\mathbb{Z}_4 \to U(1)$





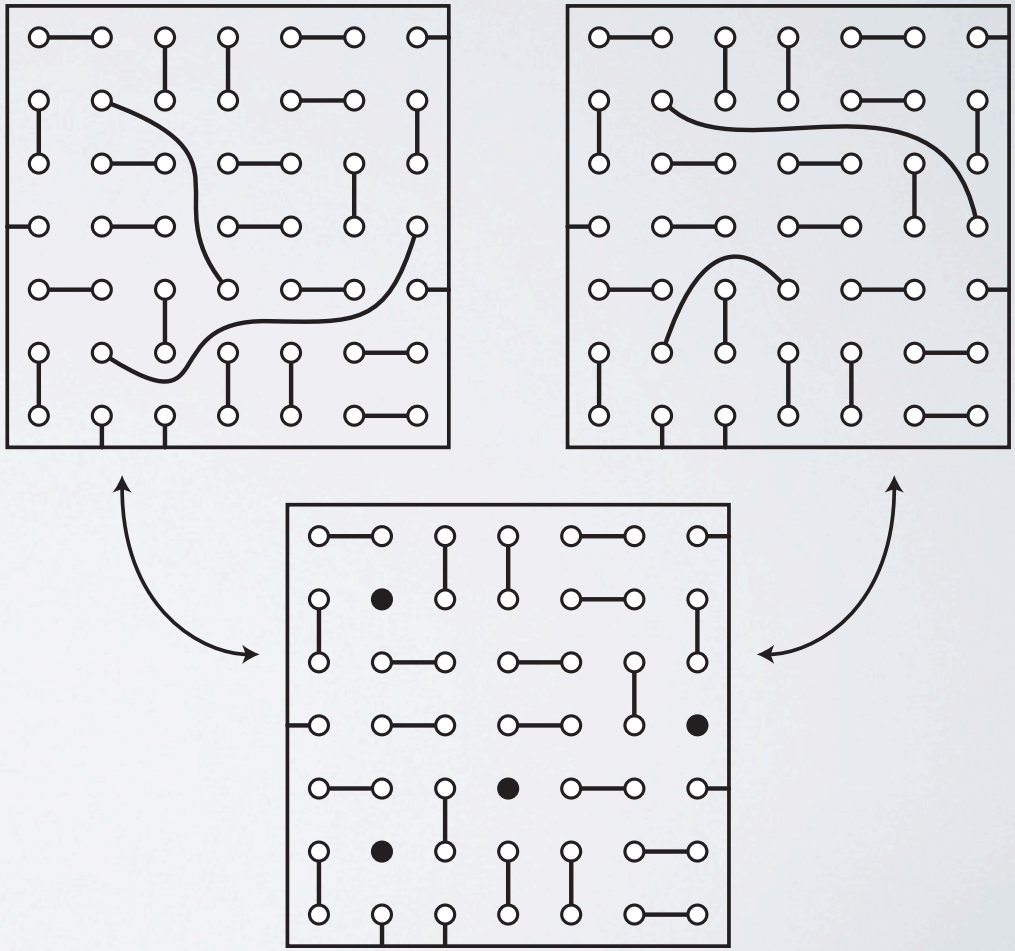
$$D_a = \sum_{\mathbf{r}} (-1)^{\mathbf{r}\cdot\hat{a}} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{a}} \quad (a = x, y)$$

DIMER ORDER HISTOGRAMS



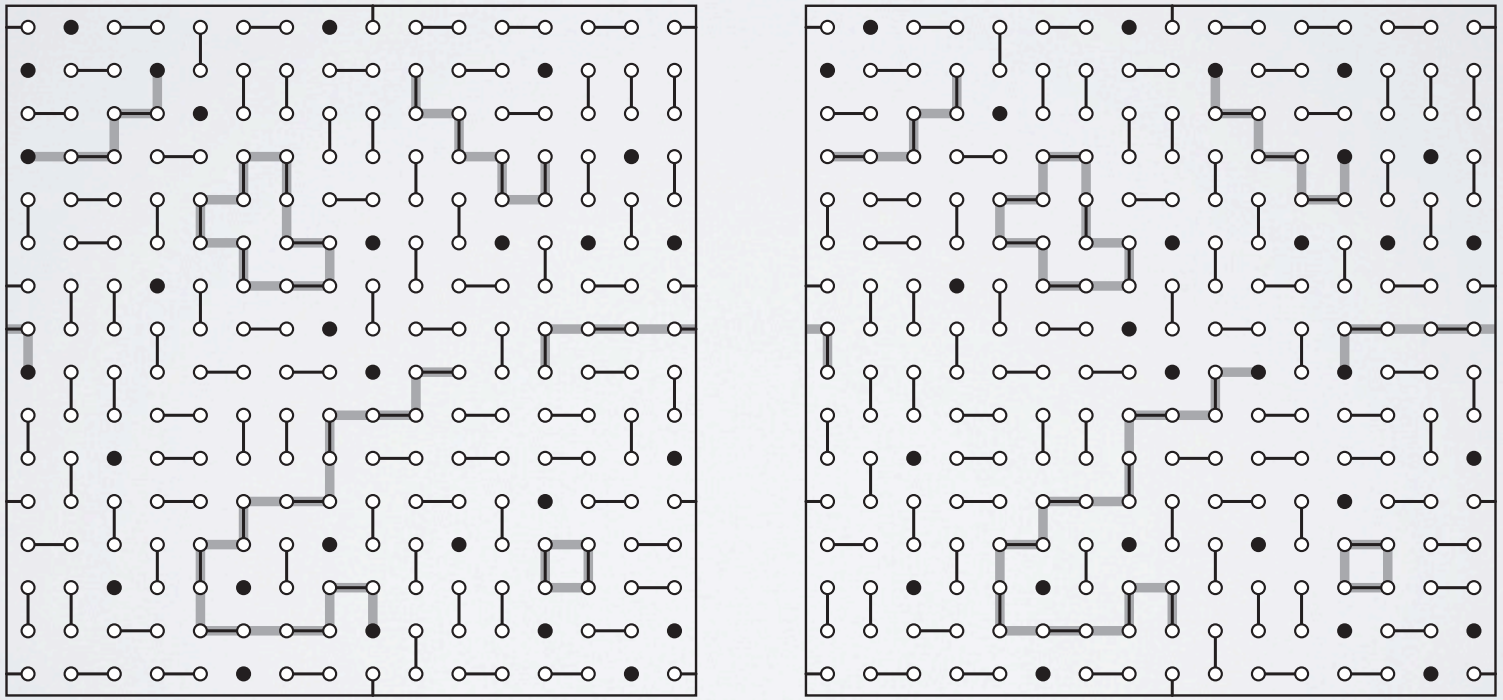
DIMERS AND MONOMERS

- in the 1/N=0 limit, long bonds have no meaning
- resulting classical system of short-ranged dimers and monomers



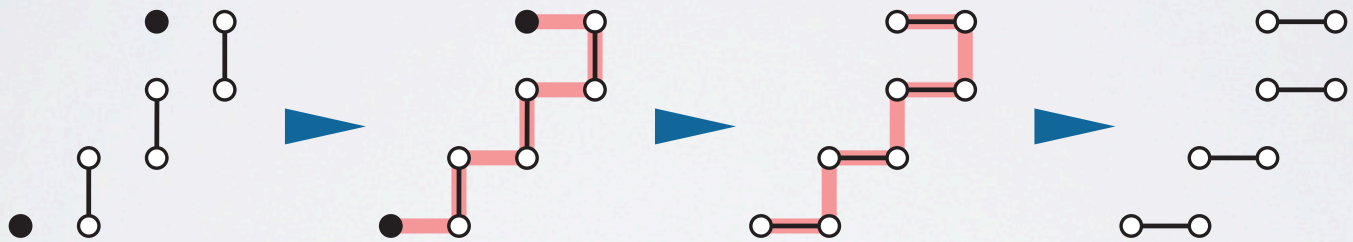
CLASSICAL ENERGY MINIMIZATION

- simulated annealing using worm-like moves

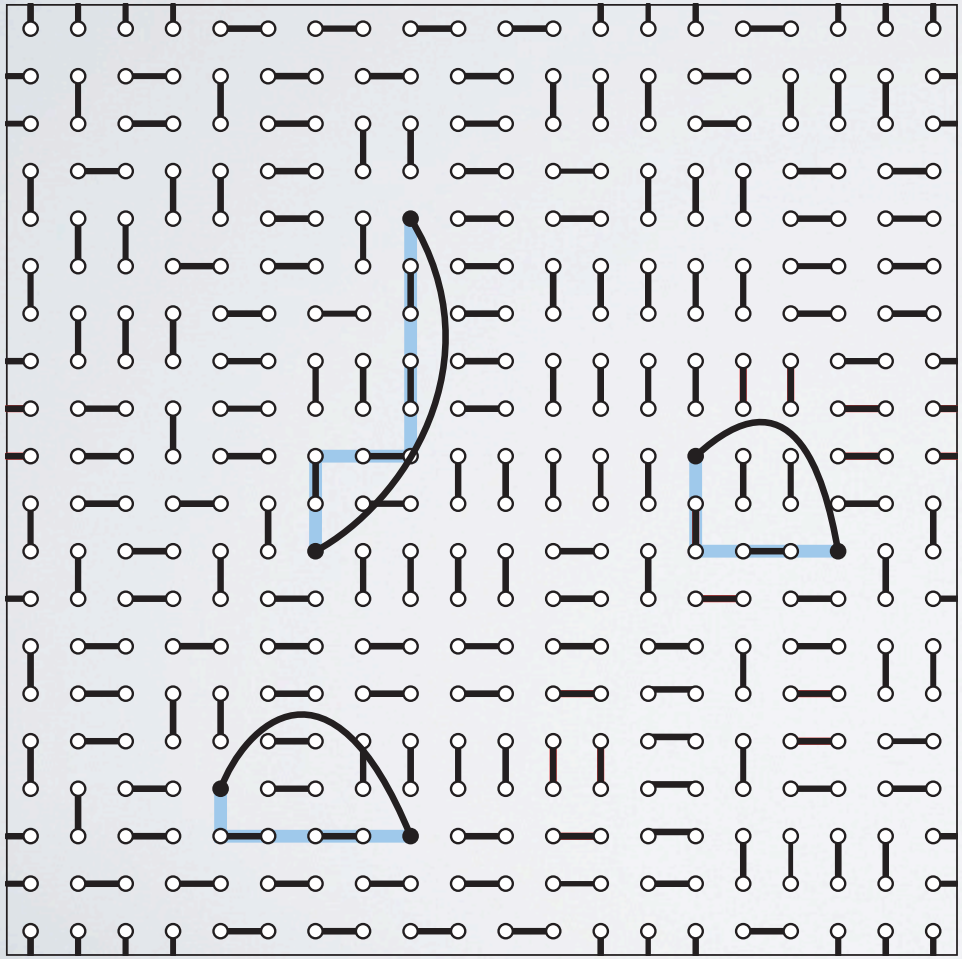


ELIMINATION OF MONOMERS

- low-energy configurations contain few monomers
- the remaining ones are largely uncorrelated



RECONNECTING LONG BONDS



- effective coupling derived from perturbation theory

$$\frac{J_1 J_3 J_5 \cdots J_{2k+1}}{J_2 J_4 \cdots J_{2k} N^k}$$

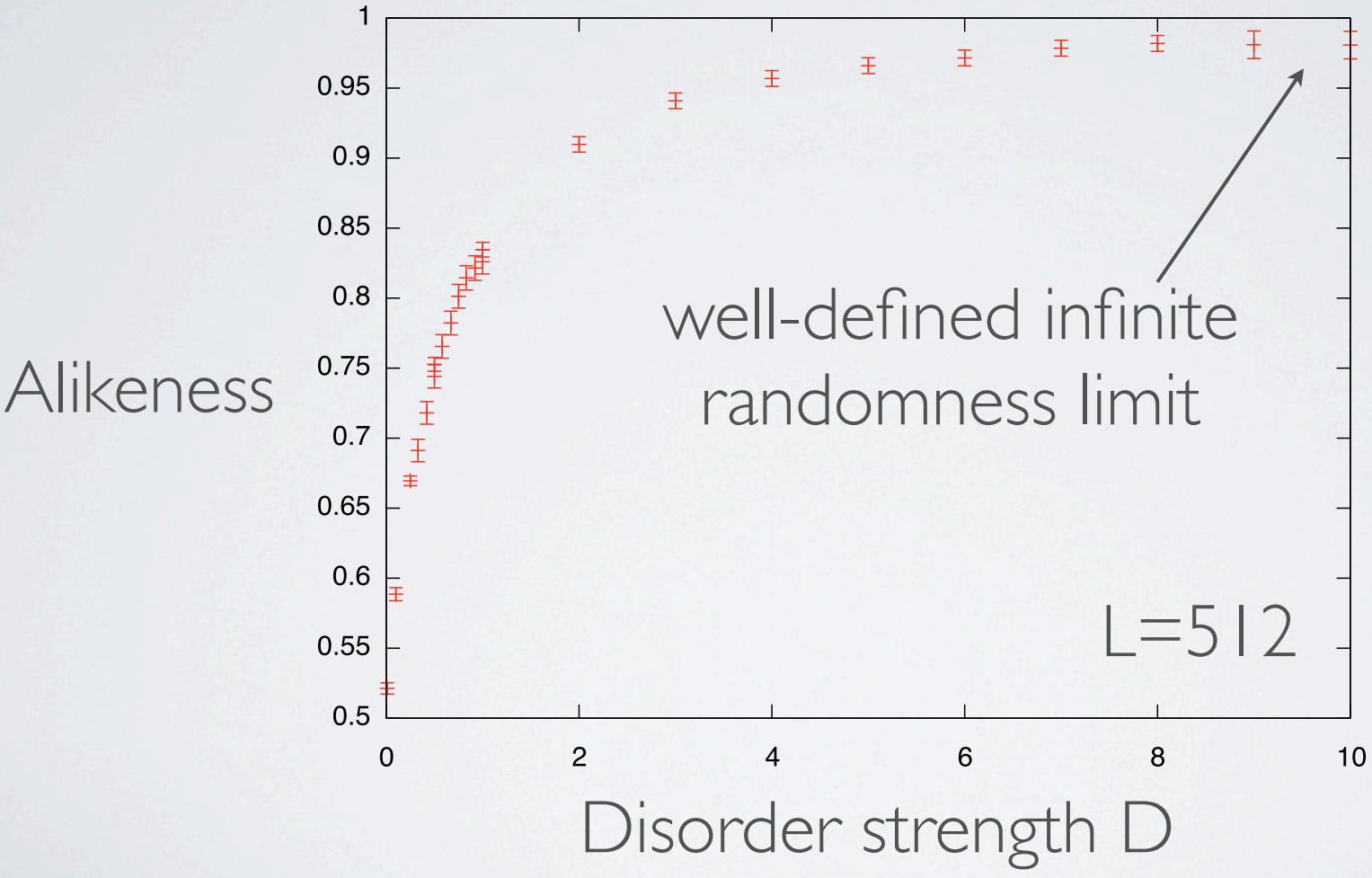
- decays exponentially in the Manhattan length

$$J_{ij}^{\text{eff}} \sim \left(\frac{1}{\sqrt{N}}\right)^{L_{ij}-1}$$

$1/N=0^{+}$ CONSTRUCTION

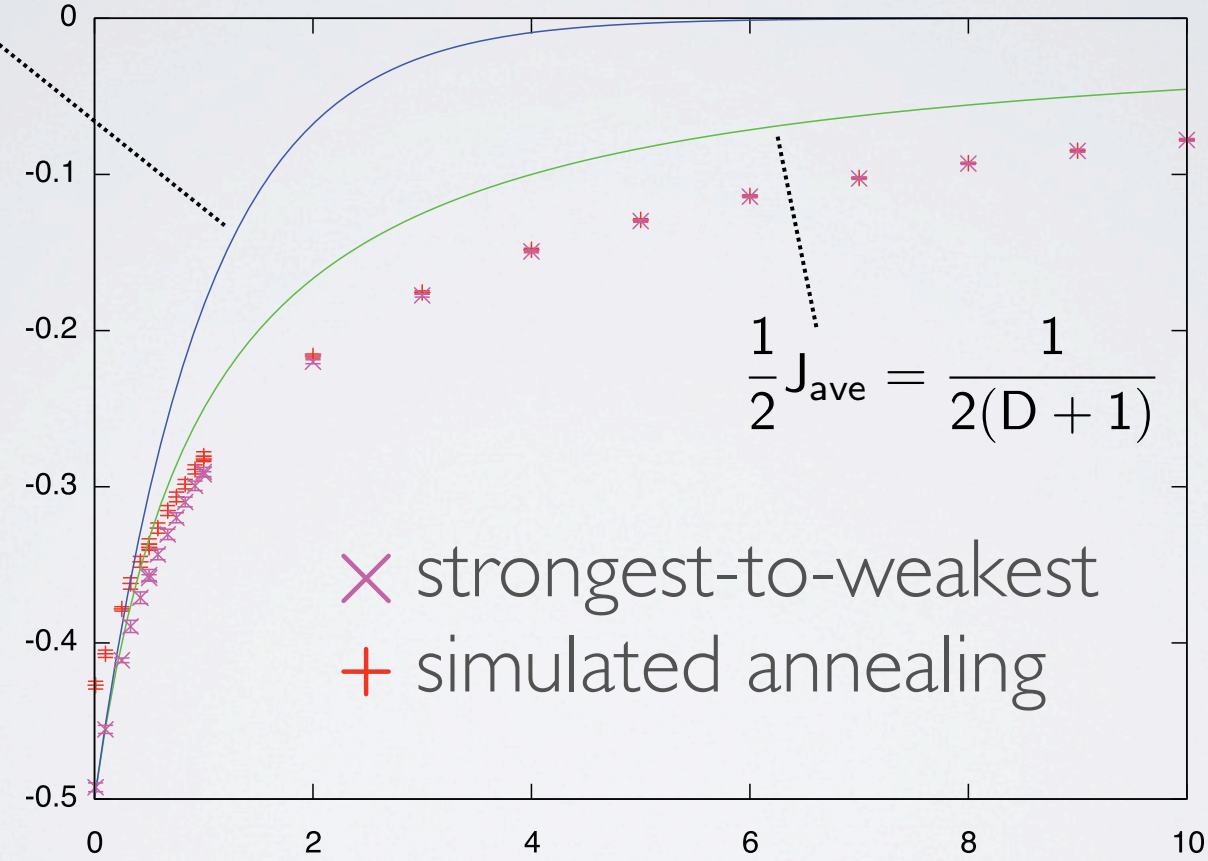
- Well-defined infinite randomness limit
- $D < \infty$ configurations easily obtained via classical energy optimization (highly reproducible)
- Long bonds: reconnect monomers closest to farthest
- Correlation functions ($1/r^{2d}$ powerlaw) determined by geometric considerations alone

$1/N=0^{+}$ LINEAR CHAIN

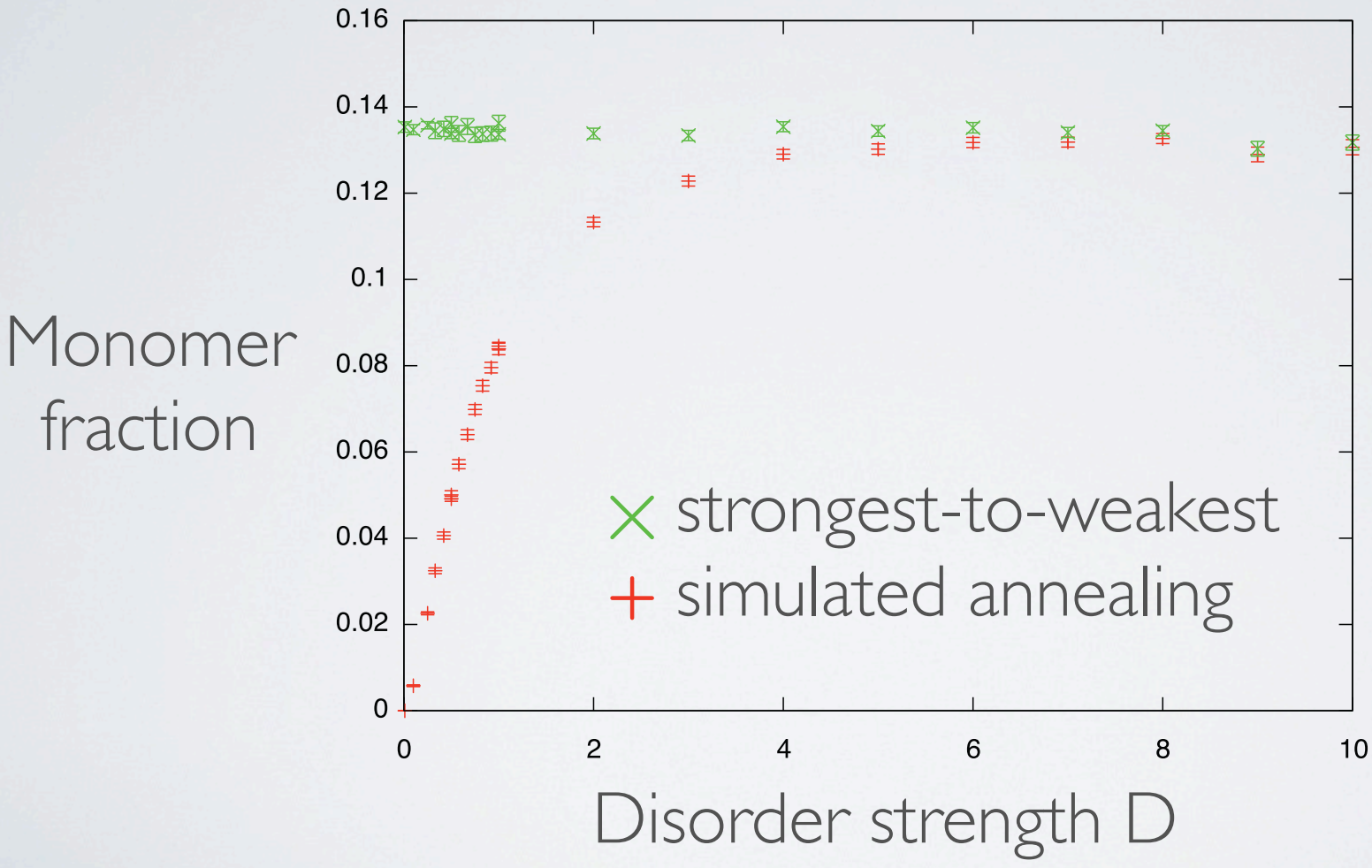


1/N=0$^+$ LINEAR CHAIN

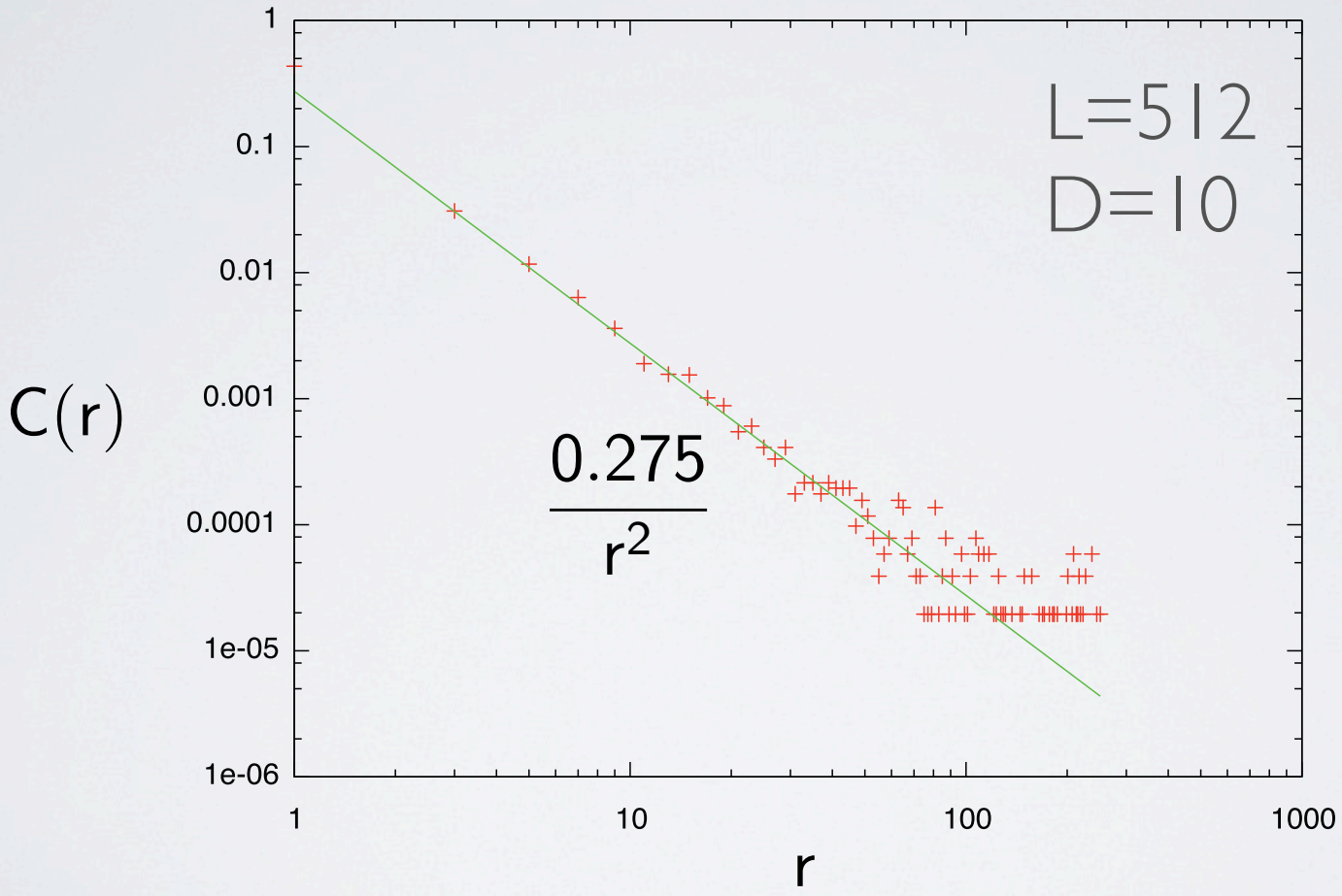
$$\frac{1}{2}J_{typ} = \frac{1}{2}e^{-D}$$



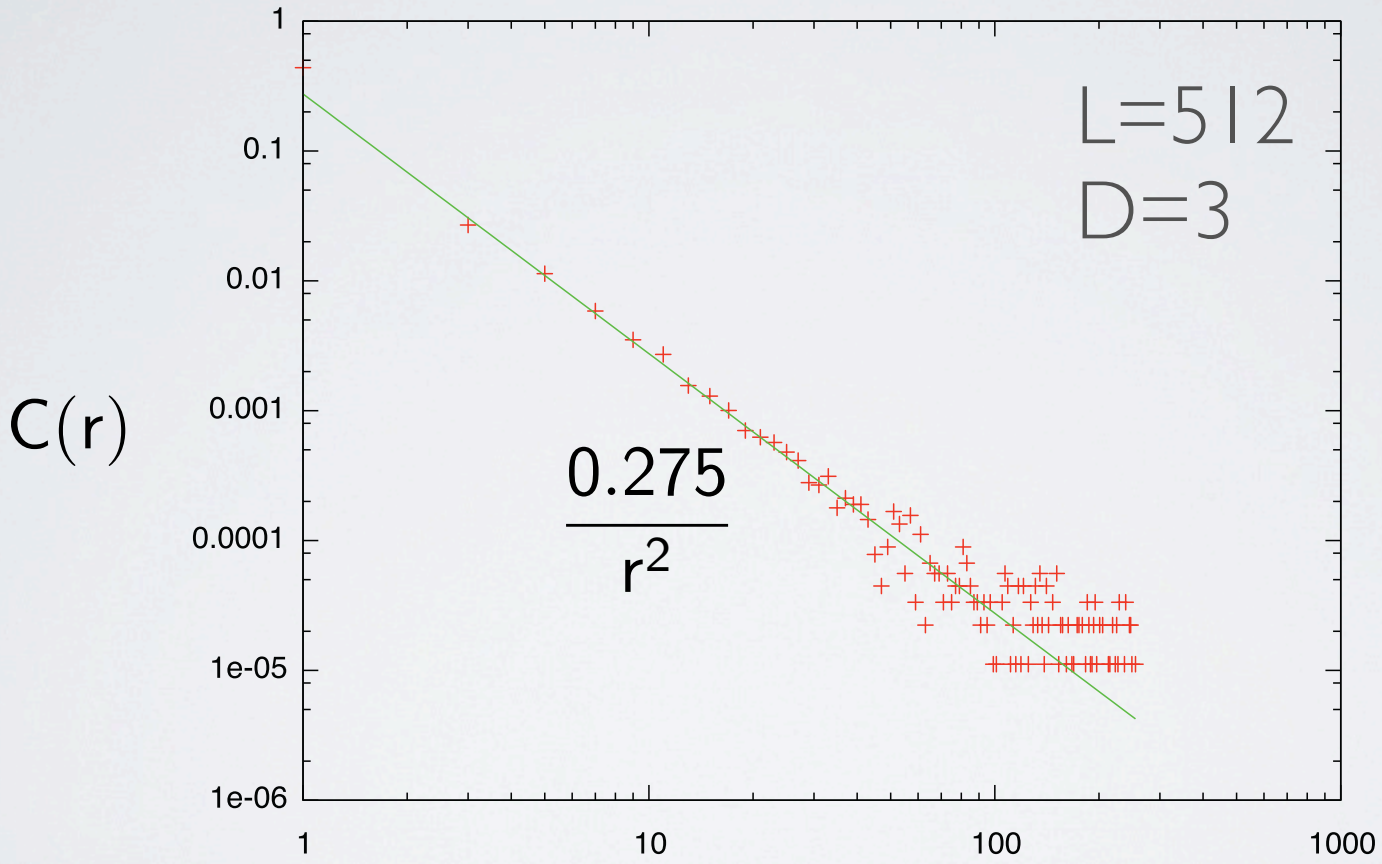
$1/N=0^{+}$ LINEAR CHAIN



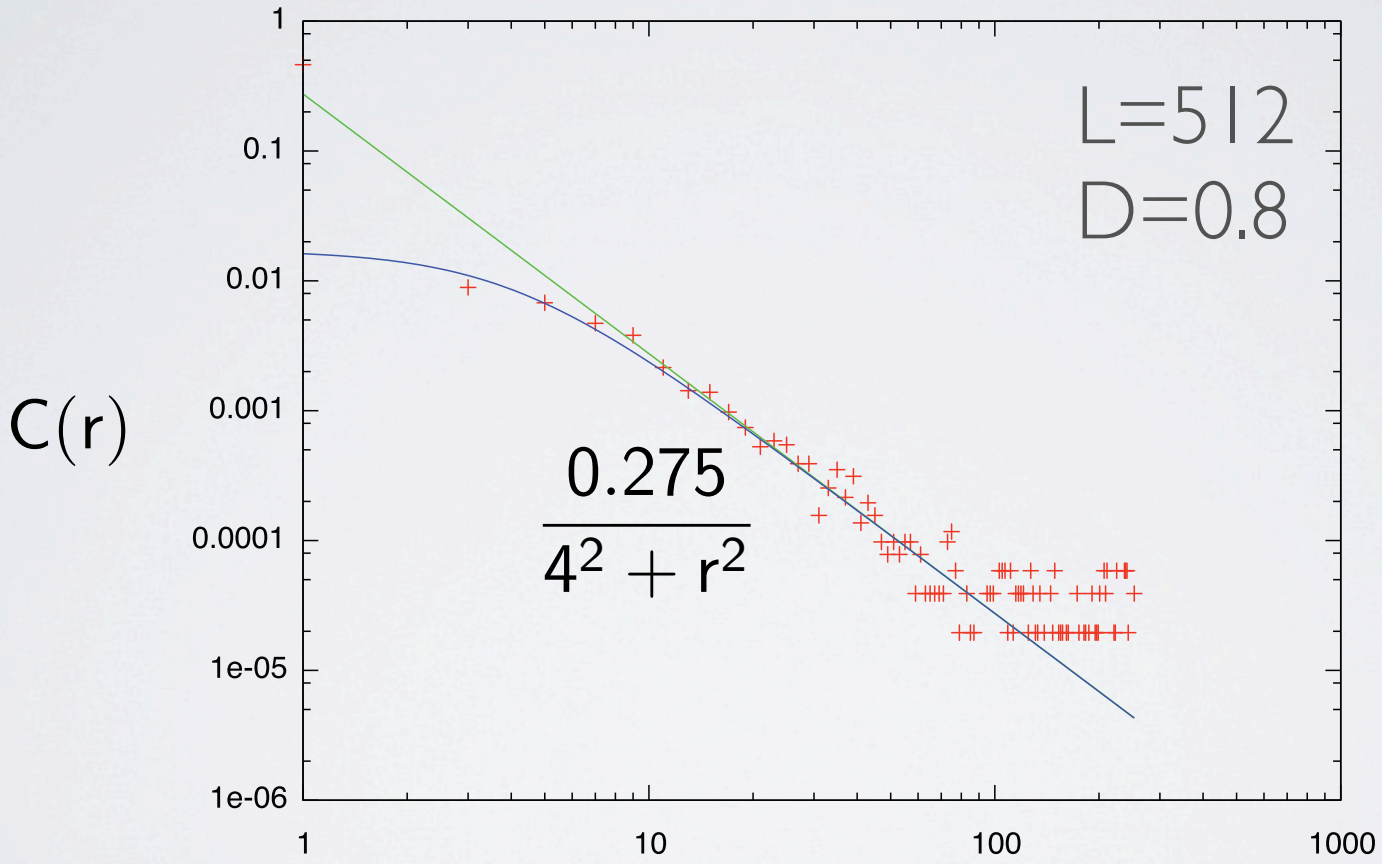
$1/N=0^{+}$ LINEAR CHAIN



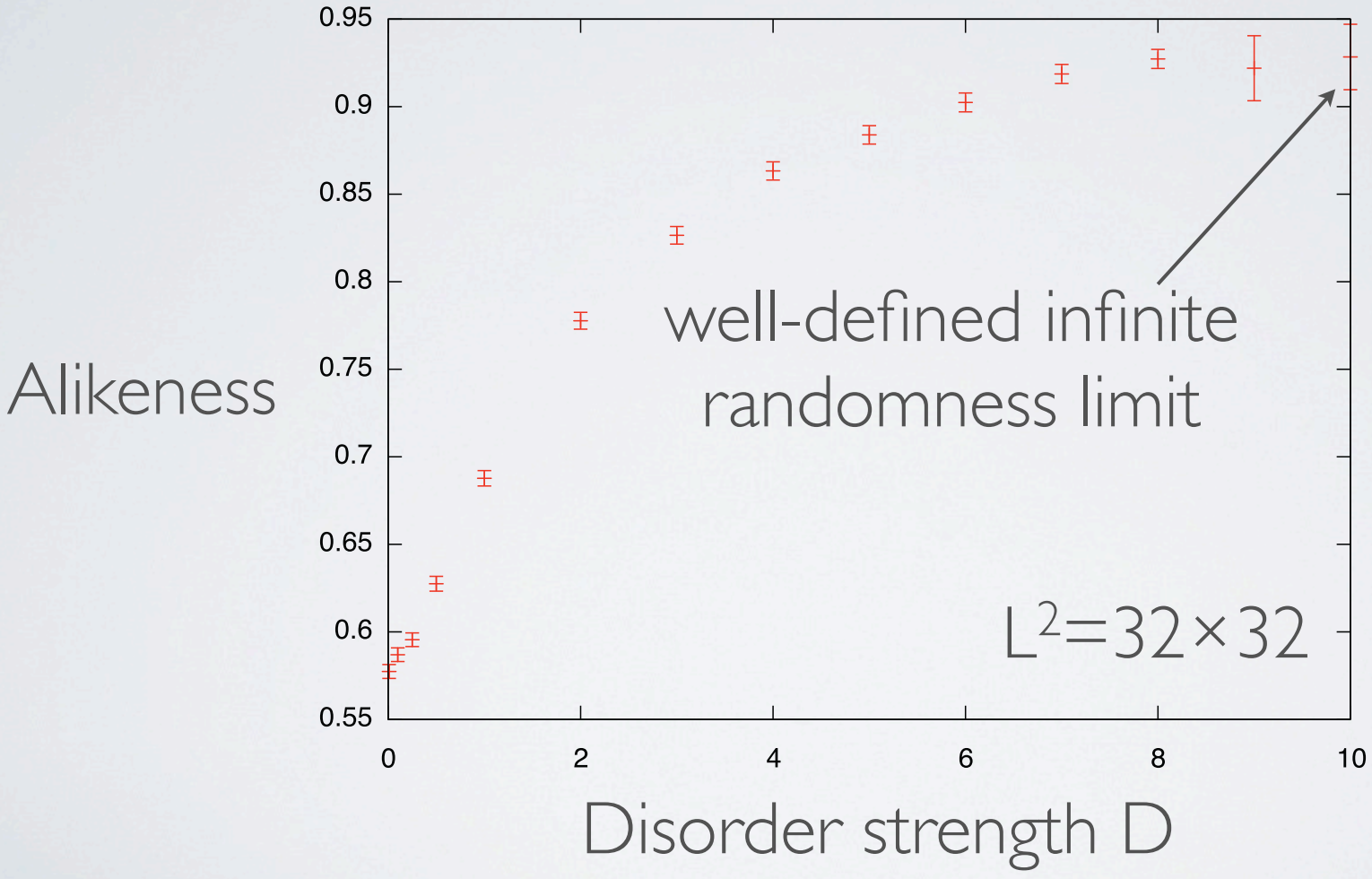
$1/N=0^{+}$ LINEAR CHAIN



$1/N=0^{+}$ LINEAR CHAIN

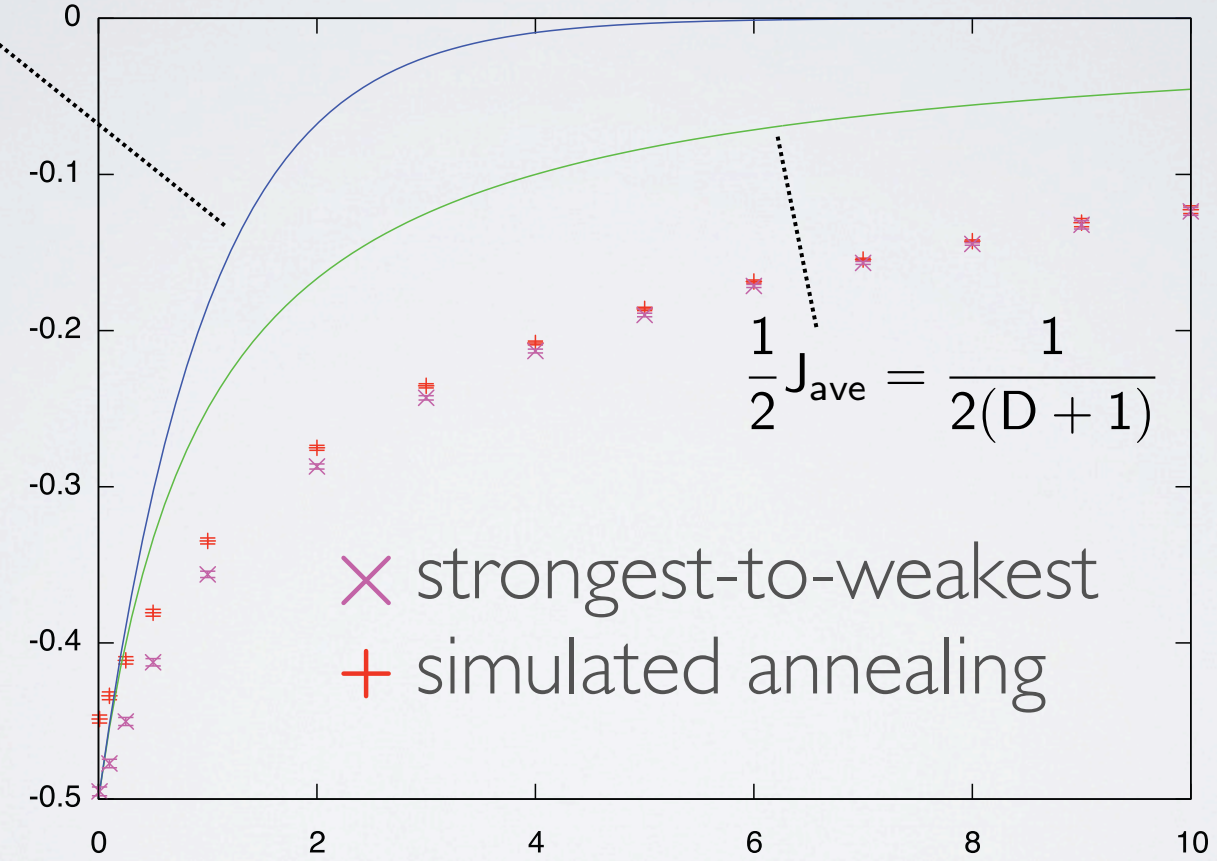


$1/N=0^+$ SQUARE LATTICE

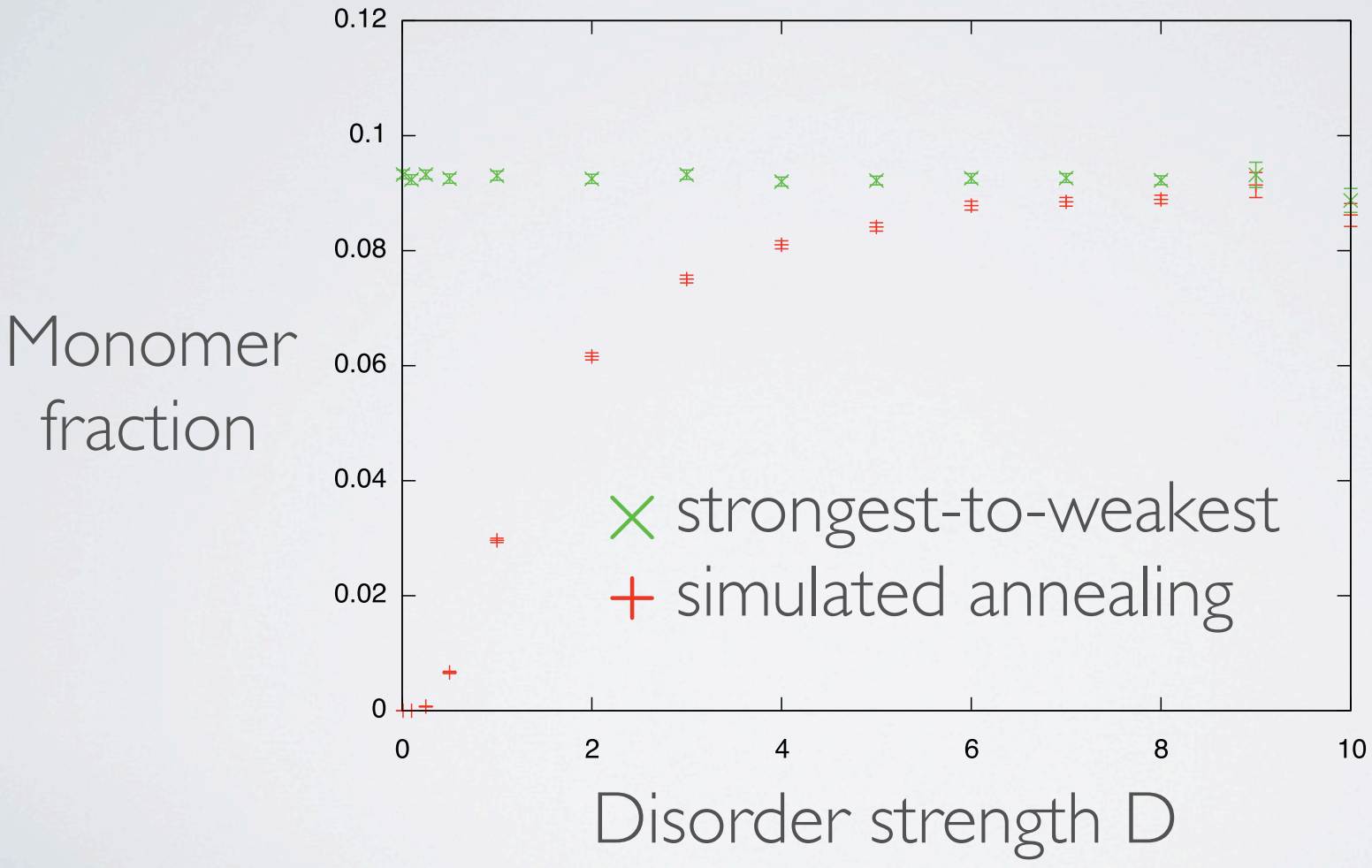


1/N=0$^+$ SQUARE LATTICE

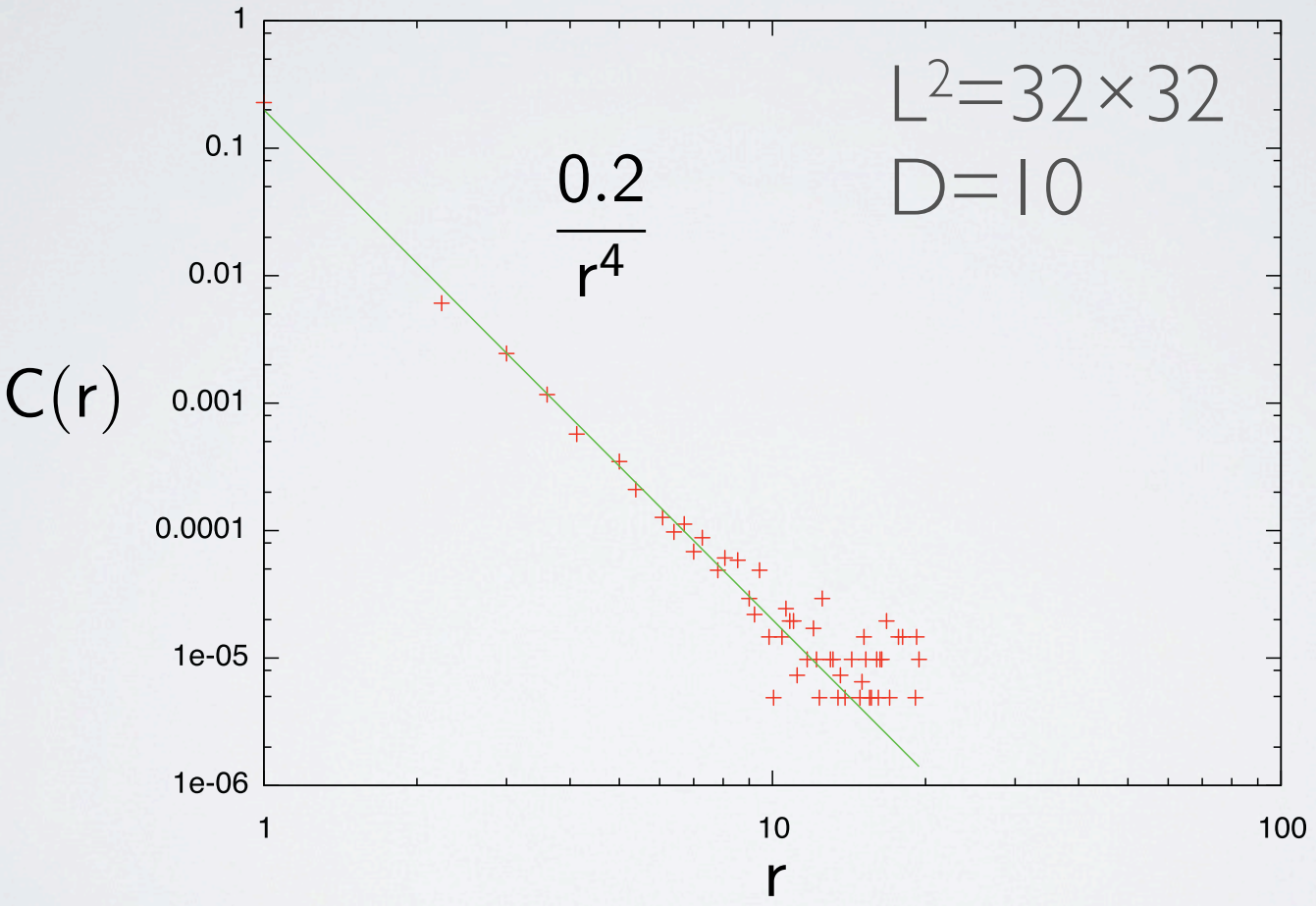
$$\frac{1}{2}J_{typ} = \frac{1}{2}e^{-D}$$



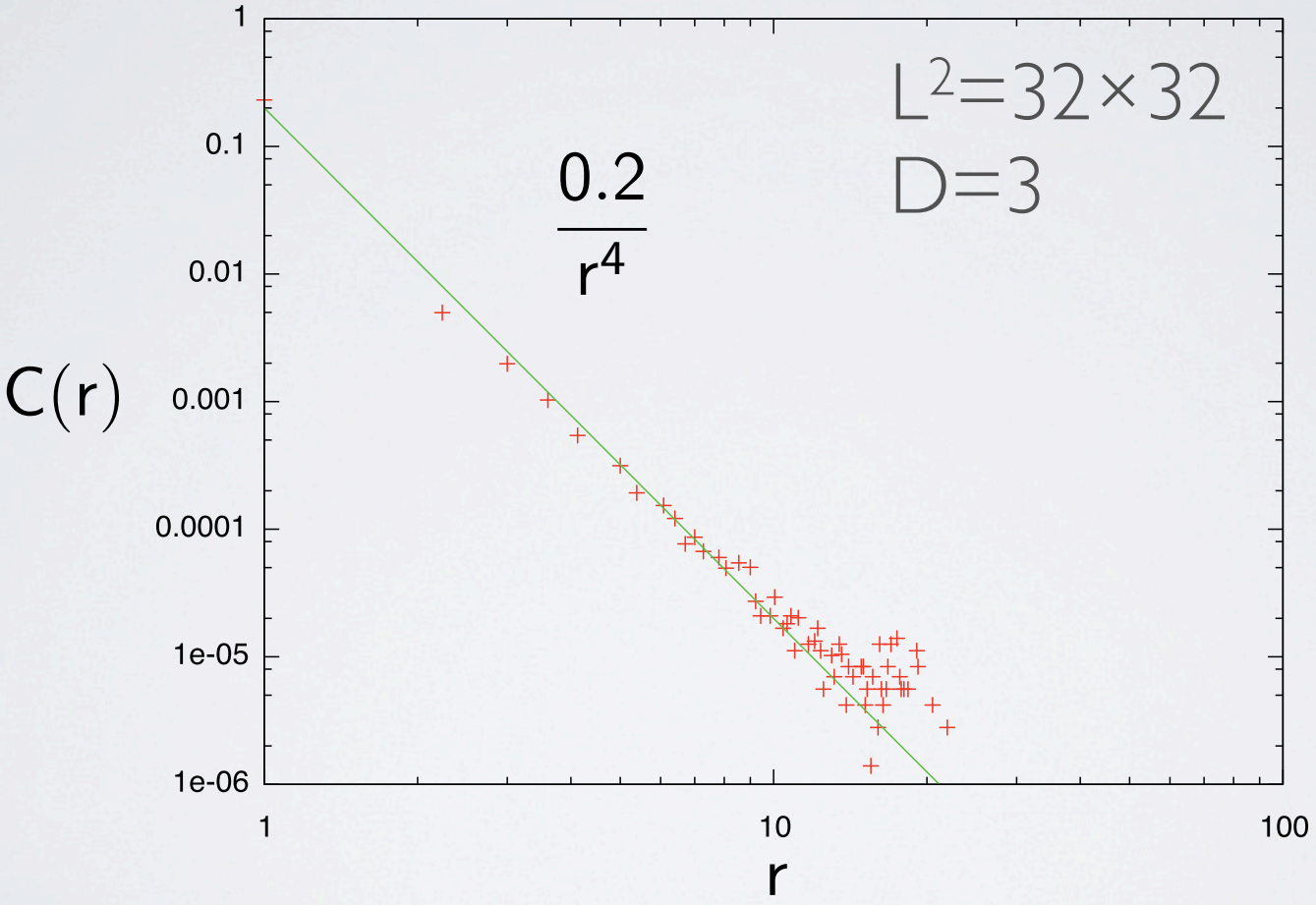
$1/N=0^+$ SQUARE LATTICE



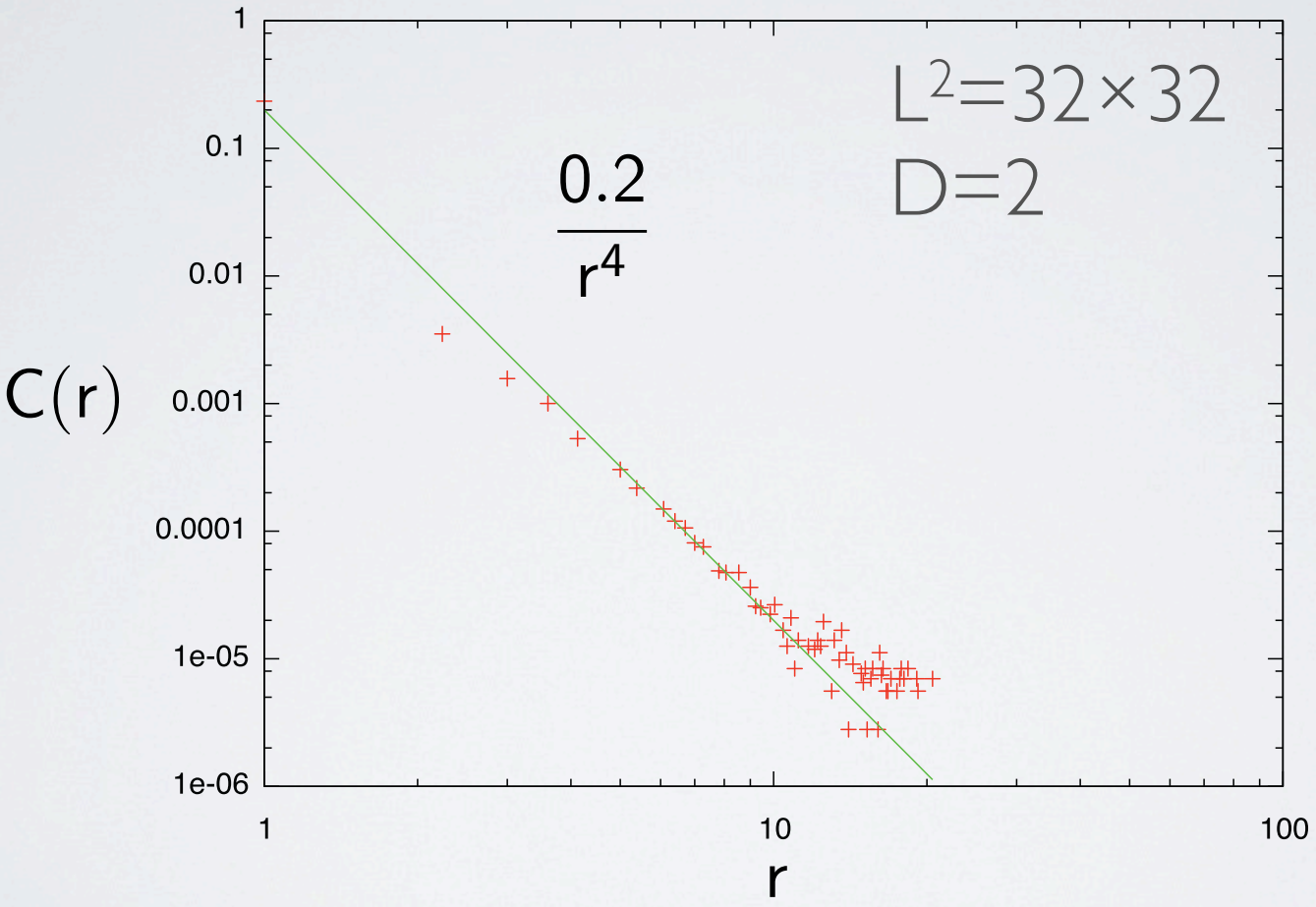
$1/N=0^+$ SQUARE LATTICE



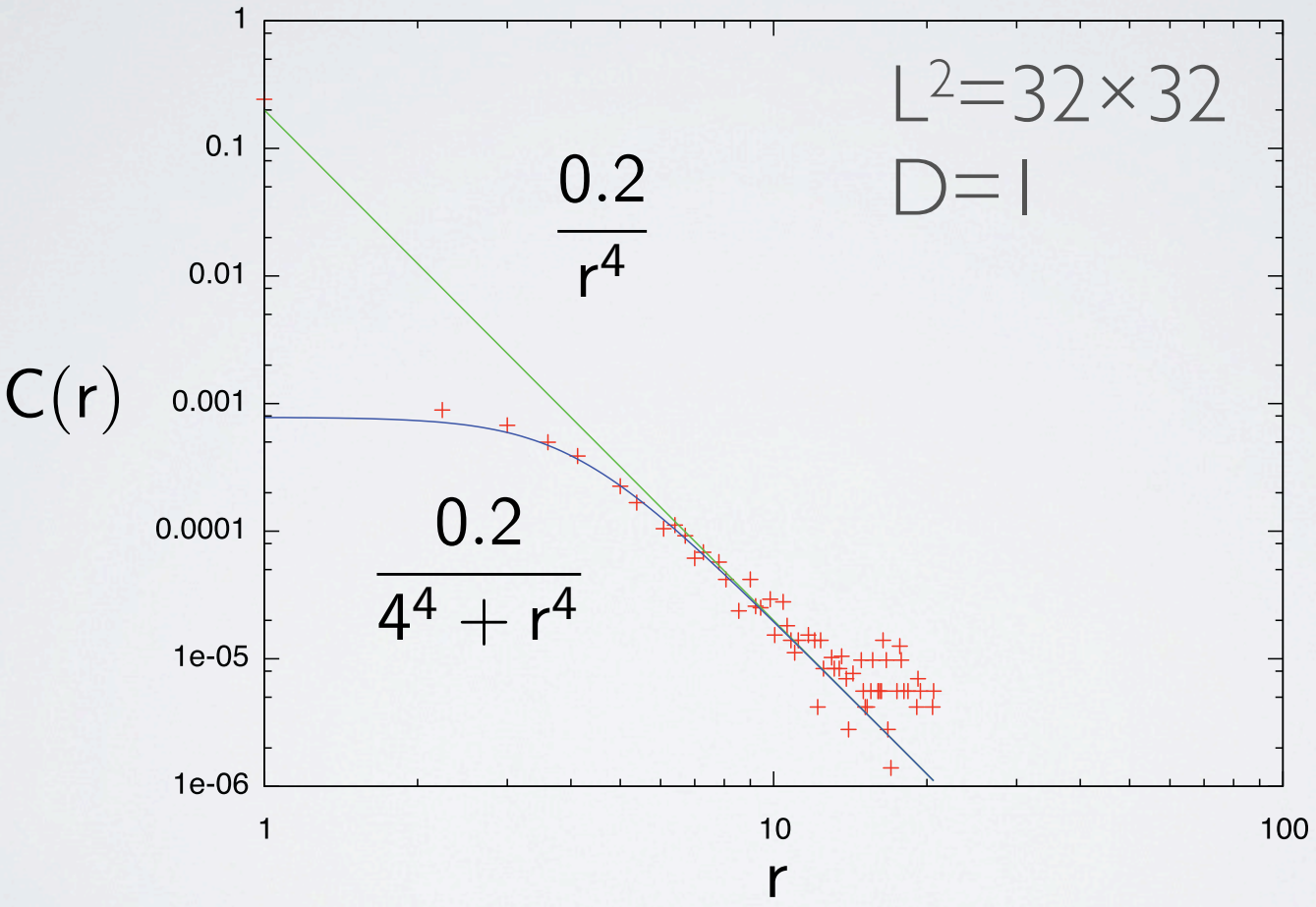
$1/N=0^{+}$ SQUARE LATTICE



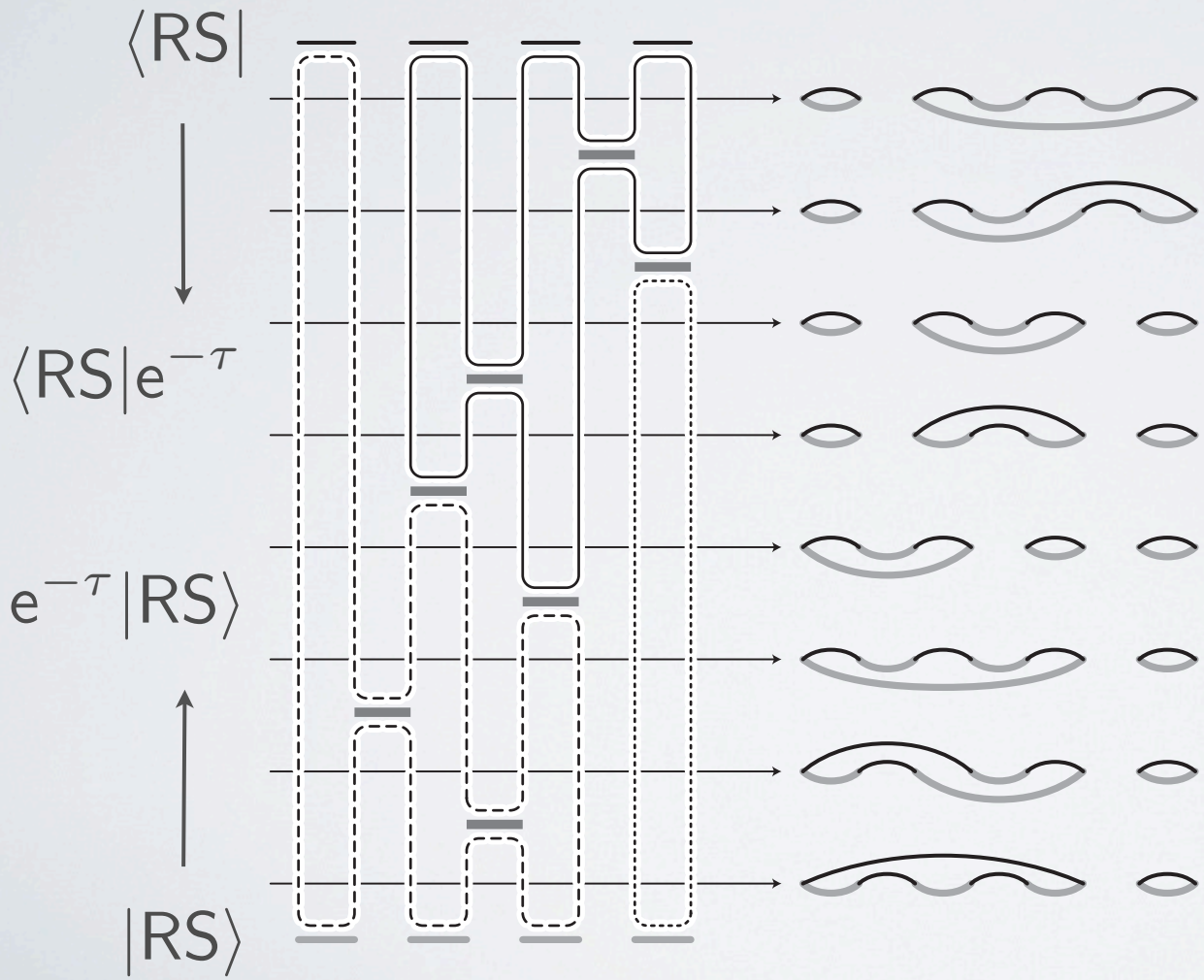
$1/N=0^{+}$ SQUARE LATTICE



$1/N=0^+$ SQUARE LATTICE

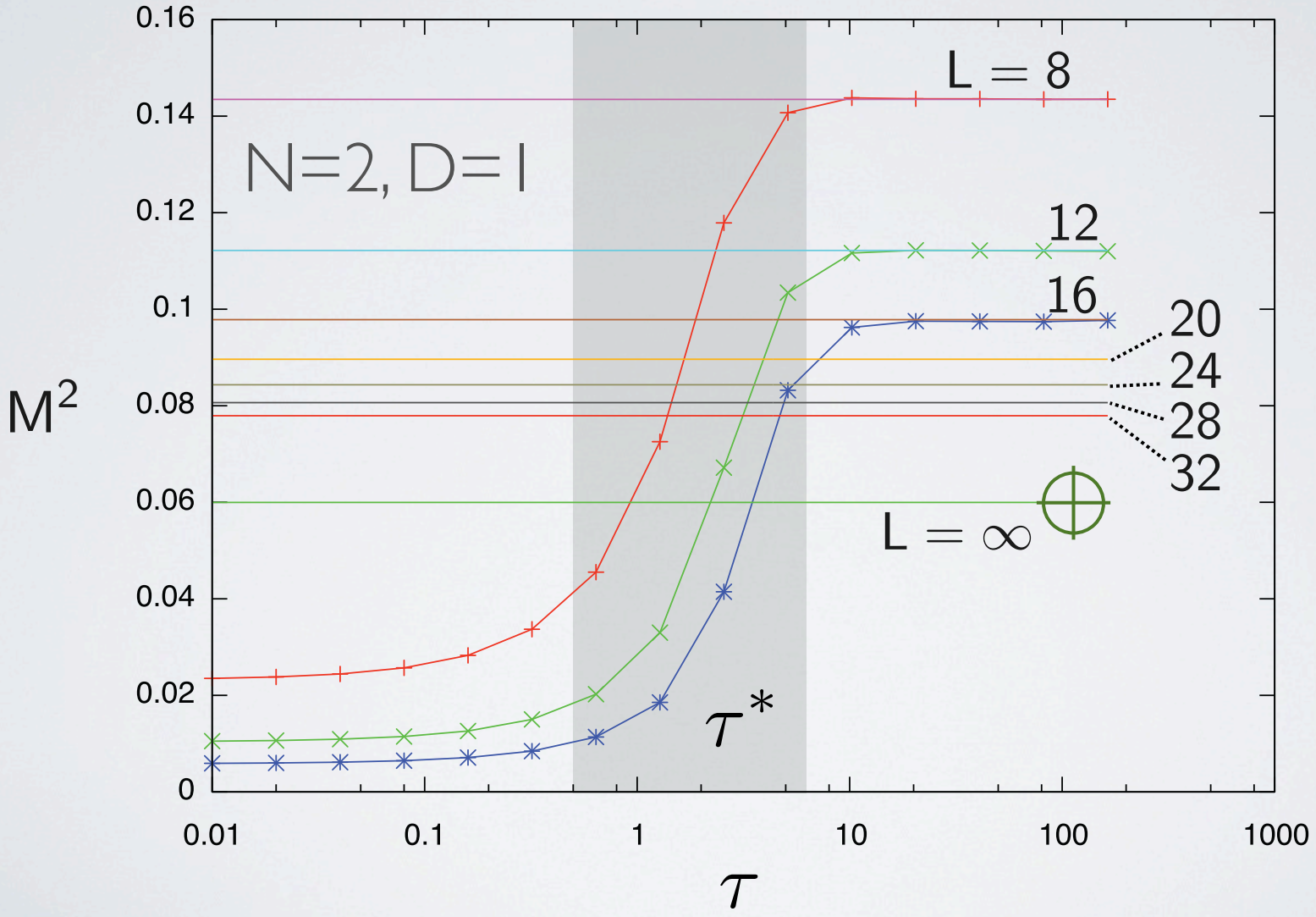


MONTE CARLO LOOPS

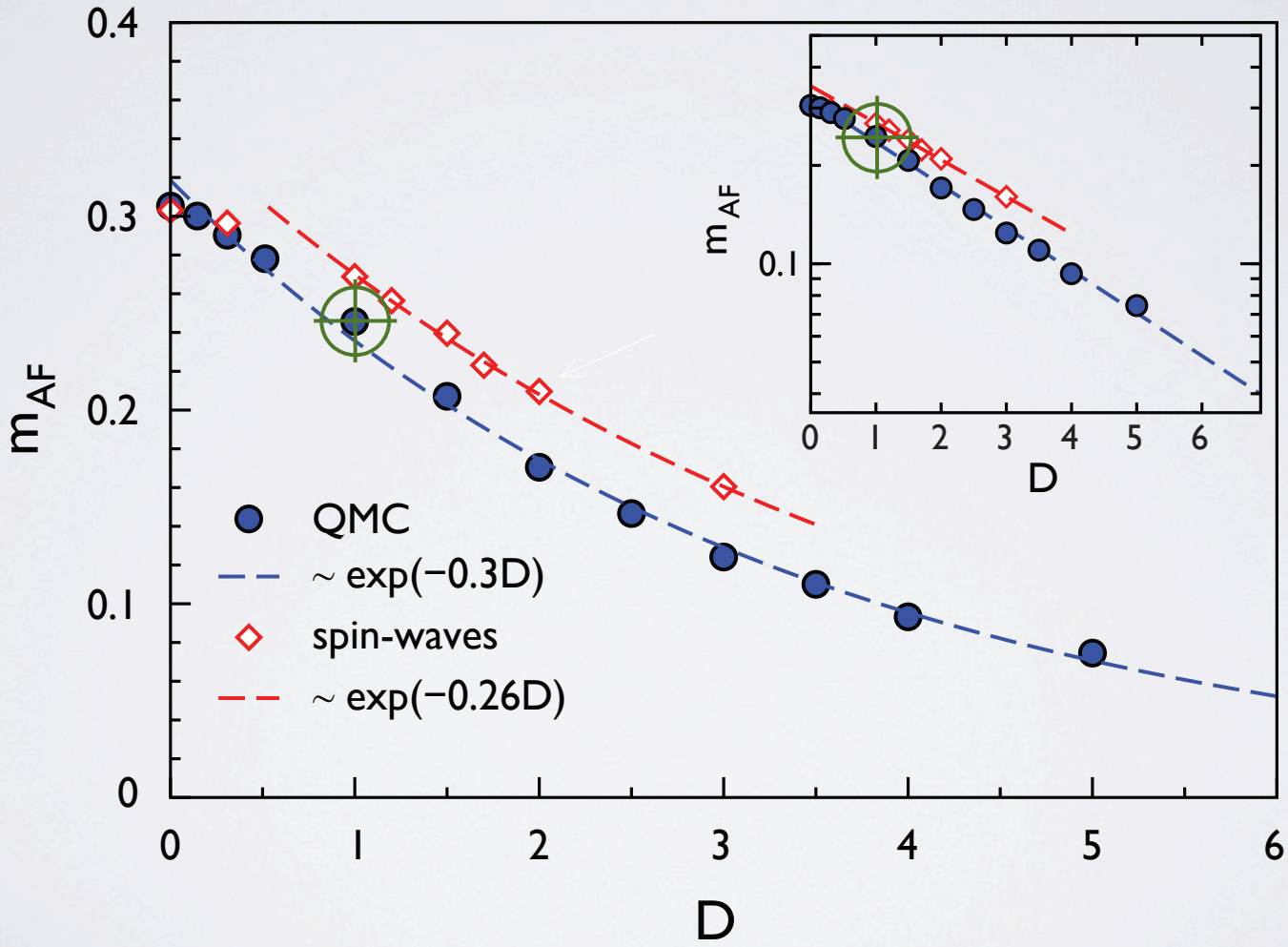


$$\frac{\langle RS|e^{-\tau H}Oe^{-\tau H}|RS\rangle}{\langle RS|e^{-2\tau H}|RS\rangle}$$

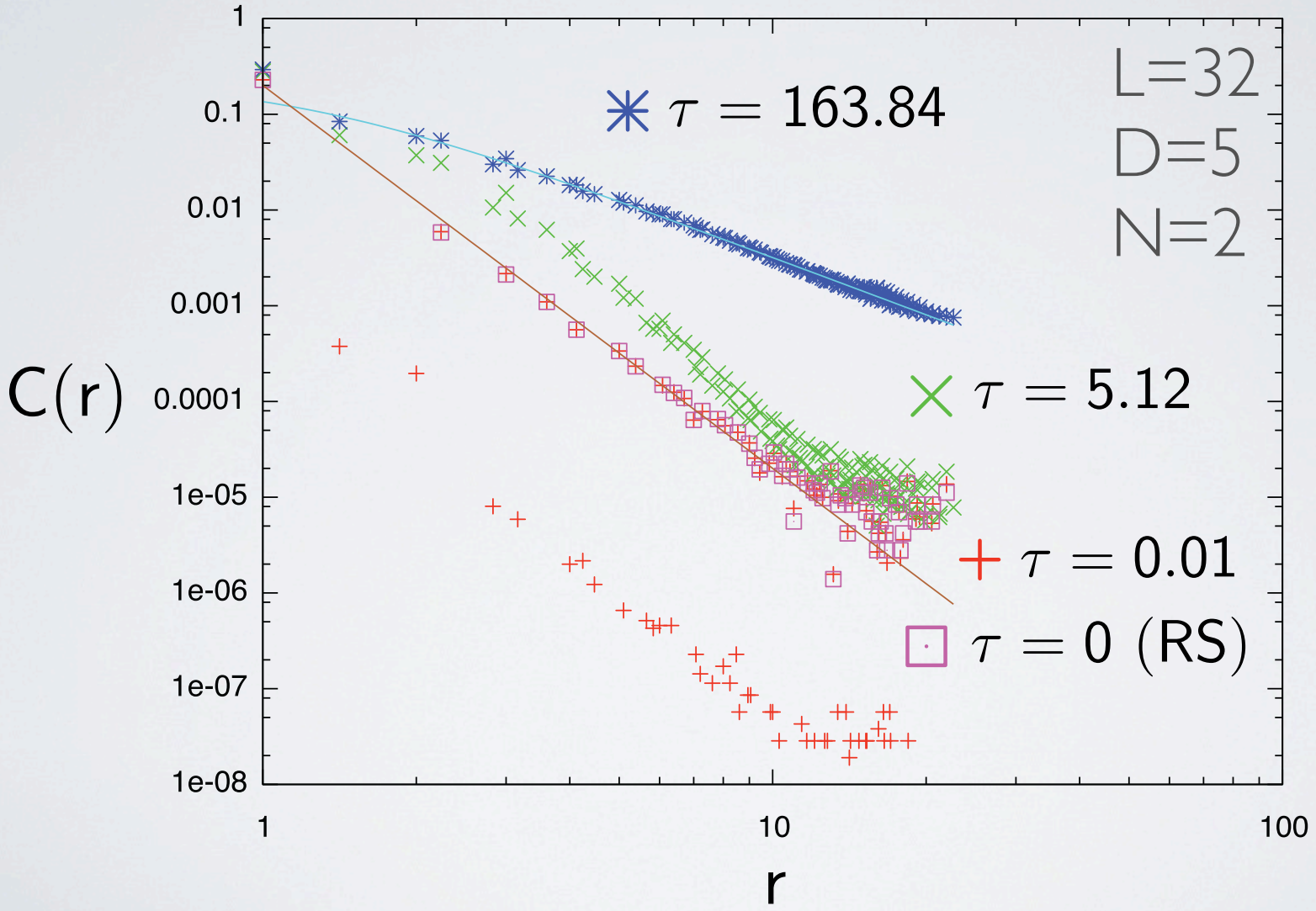
IMAG.TIME EVOLUTION



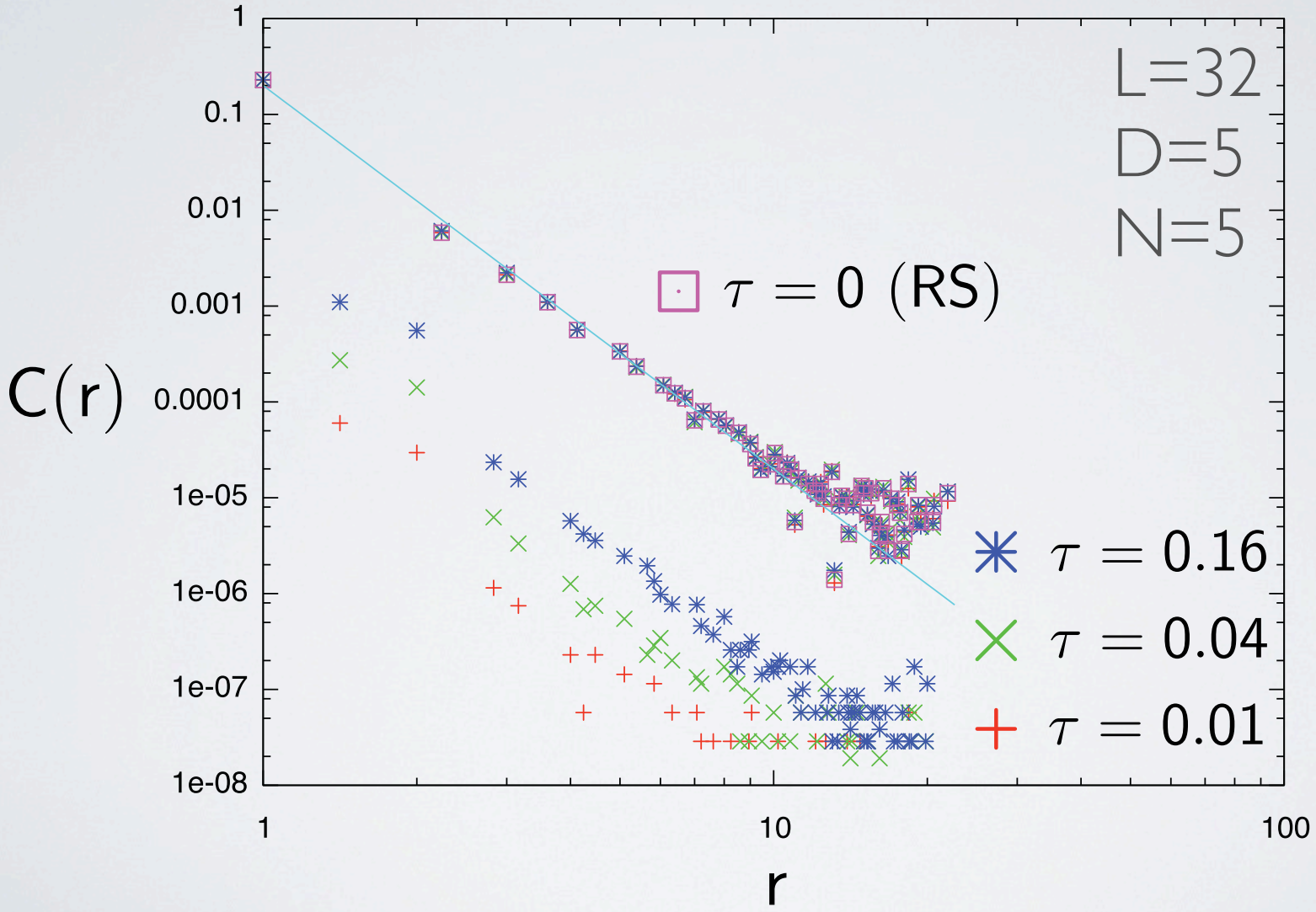
QMC COMPARISON



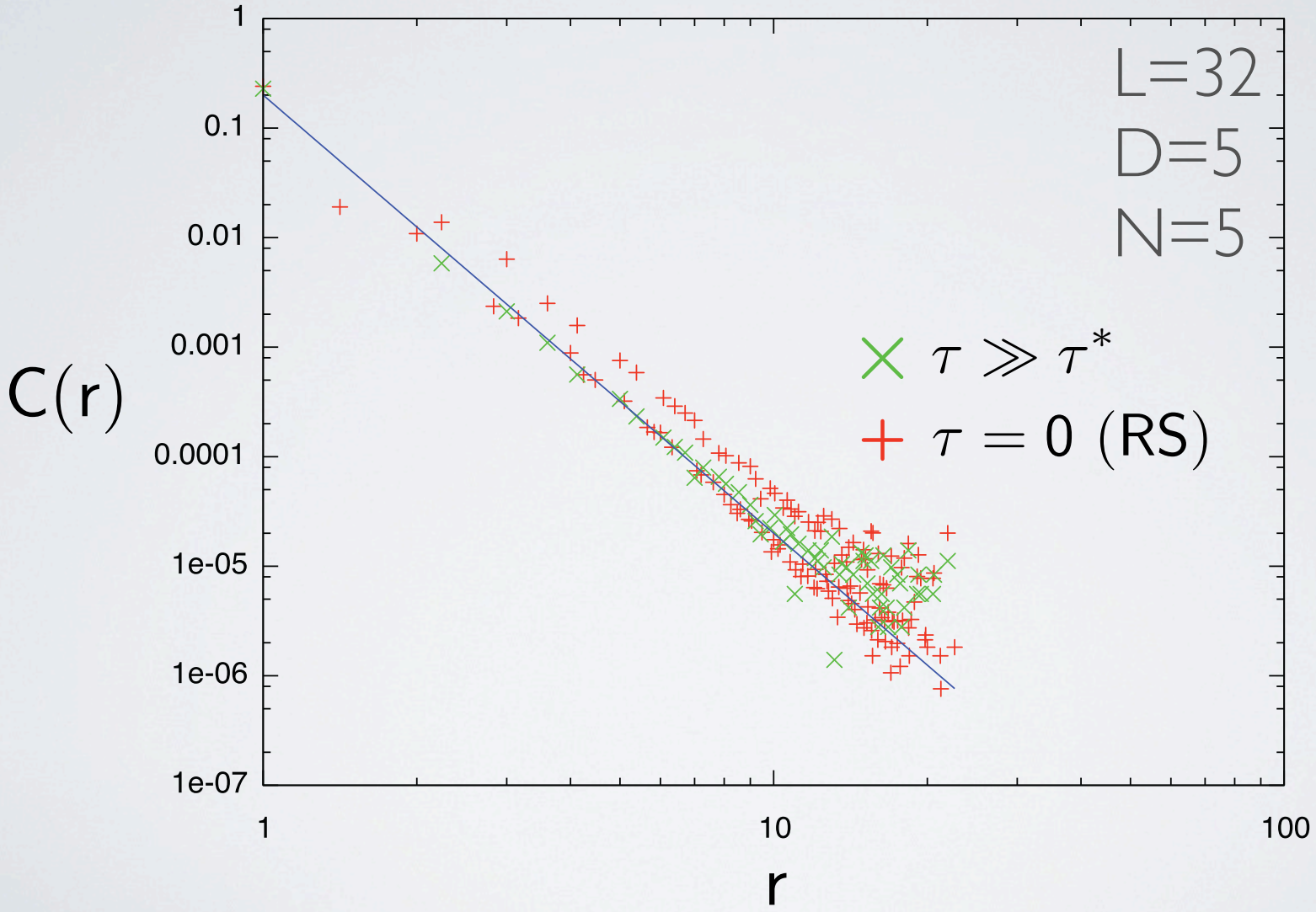
QMC COMPARISON



QMC COMPARISON



QMC COMPARISON



PHASE DIAGRAM

$C(r) = \text{const.} + \frac{1}{r}$

$C(r) \sim \frac{1}{r^4} = \frac{1}{r^{2d}}$