# Worm Algorithms

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# Outline of the Talk

1. Introducing Prokofev-Svistunov worm algorithm
2. A worm algorithm for 2D spin-glass
3. Heat capacity, domain wall free energy, and worm cluster fractional dimension

# Worm Algorithms

- Worm algorithms were first proposed for quantum systems and classical ferromagnetic systems:
  - Prokof'ev and Svistunov, PRL **87** (2001) 160601
  - Alet and Sørensen, PRE **67** (2003) 015701

# High-Temperature Expansion of the Ising Model

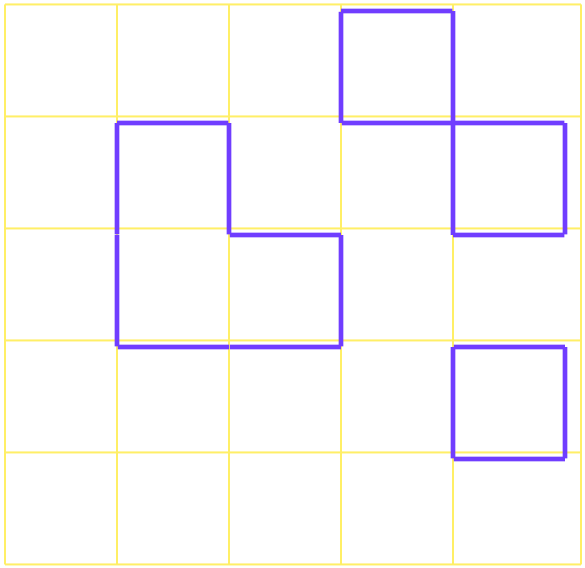
$$Z = \sum_{\sigma} e^{K\sum_{<ij>}\sigma_i\sigma_j} \propto \sum_{\sigma}\prod_{<ij>}(1+\sigma_i\sigma_j \tanh K)$$

$$= 1 + N \tanh^4 K + \ldots \qquad K = J/(k_B T)$$

$$= \sum_{b} \tanh^{\Sigma b_{ij}} K, \quad b_{ij} = 0,1, \quad \sum_j b_{ij} = \text{even}$$

The set of new variables $b_{ij}$ on each bond are not independent, but constrained to form closed polygons by those of $b_{ij}$=1.

# A High-Temperature Expansion Configuration



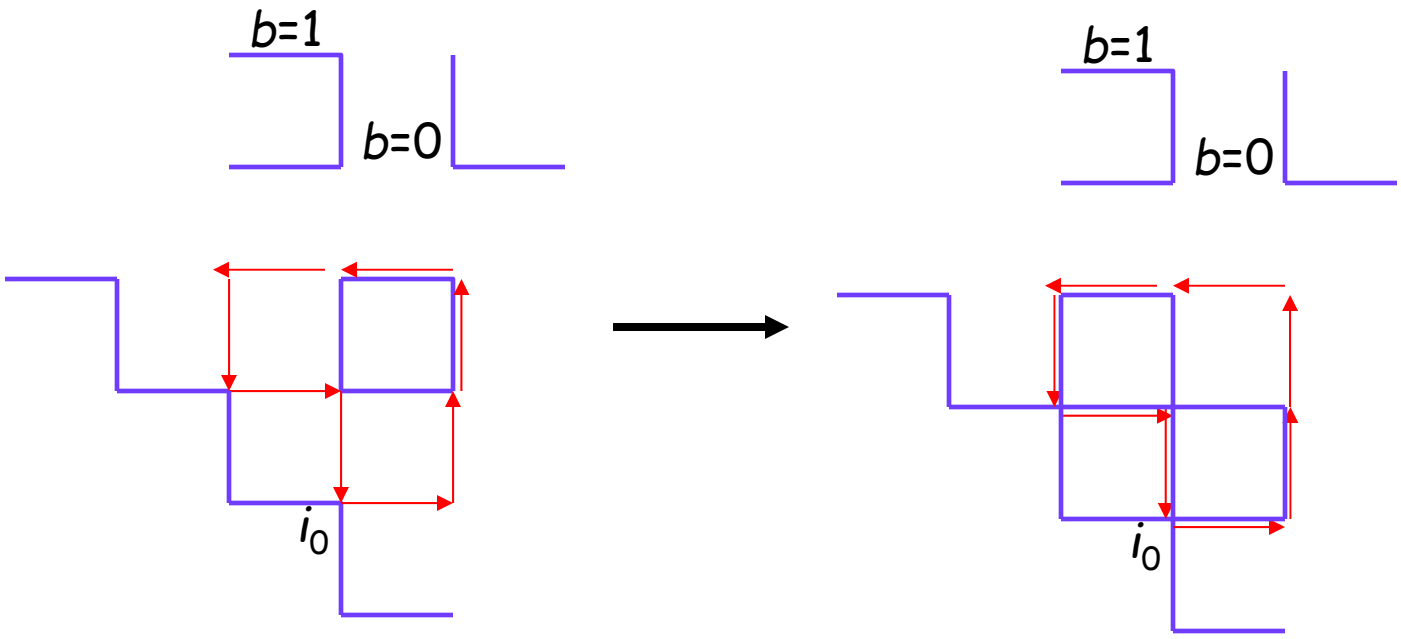
$$\sum_{j \in nn \text{ of } i} b_{ij} = 0, 2, 4$$

The bonds in 2D Ising model high-temperature expansion. The weight of each bond is tanh$K$. Only an even number of bonds can meet at the site of the lattice.

# Worm Algorithm (Prokof'ev & Svistunov, 2001)

1. Pick a site $i_0$ at random. Set $i = i_0$
2. Pick a nearest neighbor $j$ with equal probability, move it there with probability $(\tanh K)^{1-b_{ij}}$. If accepted, flip the bond variable $b_{ij}$ (1 to 0, 0 to 1). $i = j$.
3. Increment: $++G(i-i_0)$
4. If $i = i_0$ , exit loop, else go to step 2.
5. The ratio $G(i-i_0)/G(0)$ gives the two-point correlation function

# The Loop

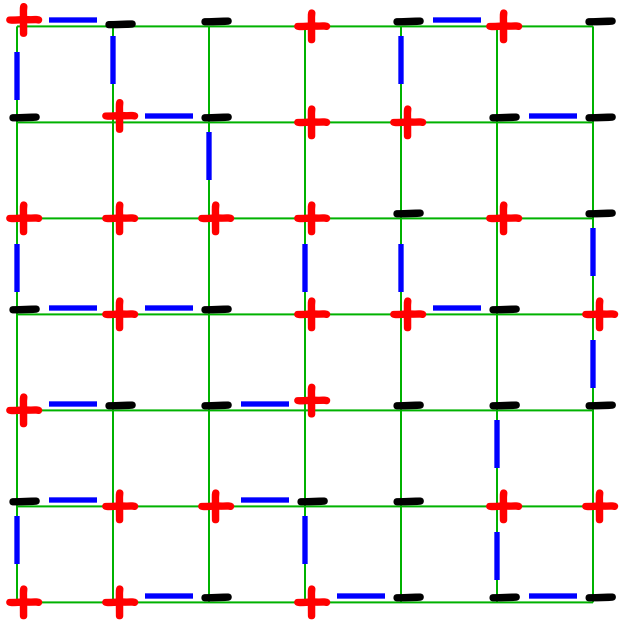



Erase a bond with probability 1, create a bond with probability $\tanh[J/(kT)]$. The worm with $i \neq i_0$ has the weight of the two-point correlation function $g(i_0, i)$.

# Statistics, Critical Slowing Down

- Direct sampling of the two-point correlation function $\langle \sigma_i \sigma_j \rangle$ in every step
- The total number of bonds and its fluctuations (when a closed loop form) are related to average energy and specific heat.
- Much reduced critical slowing down ($\tau \approx \log L$) for a number of models, such as 2D, 3D Ising, and XY models

# Spin Glass Model



blue $J_{ij}$=-J, green $J_{ij}$=+J

$$E(\sigma) = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j\,, \qquad \sigma_i = \pm 1$$

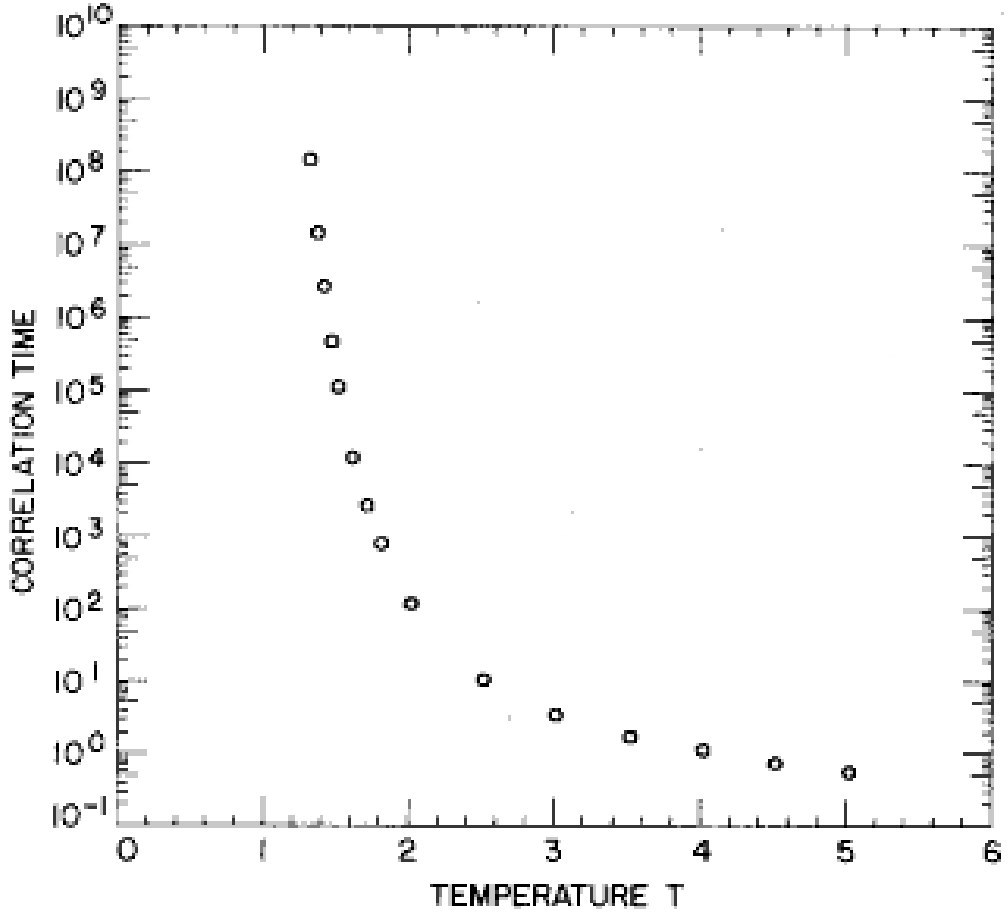
A random interacting Ising model - two types of random, but fixed coupling constants (ferro $J_{ij} > 0$, anti-ferro $J_{ij} < 0$). The model was proposed in 1975 by Edwards and Anderson.

High-temperature worm algorithm does not work as the weight $\tanh(J_{ij}K)$ change signs.

# Spin-Glass, Still a Problem?

- 2D Ising spin-glass $T_c = 0$
- 3D Ising spin-glass $T_c > 0$
- Low$T$ phase, droplet picture vs replica symmetry breaking picture, still controversial
- Relevant to biology, neutral network, optimization, etc

# Slow Dynamics in Spin Glass




Correlation time in single spin flip dynamics for 3D spin glass. $\tau \propto |T-T_c|^6$.

From Ogielski, Phys Rev B **32** (1985) 7384.

# Advanced Algorithms for Spin-Glasses (3D)

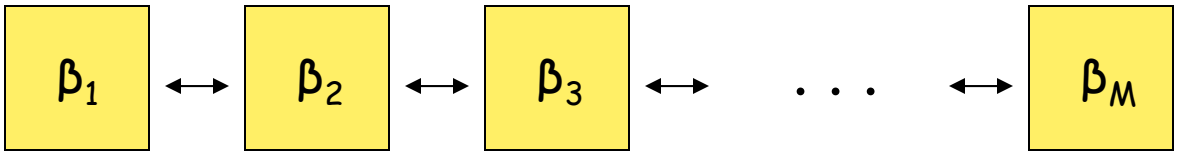
- Simulated Tempering (Marinari & Parisi, 1992)
- Parallel Tempering, also known as replica exchange Monte Carlo (Hukushima & Nemoto, 1996)

# Special 2D Algorithms

- Replica Monte Carlo, Swendsen & Wang 1986
- Cluster algorithm, Liang 1992
- Houdayer, 2001

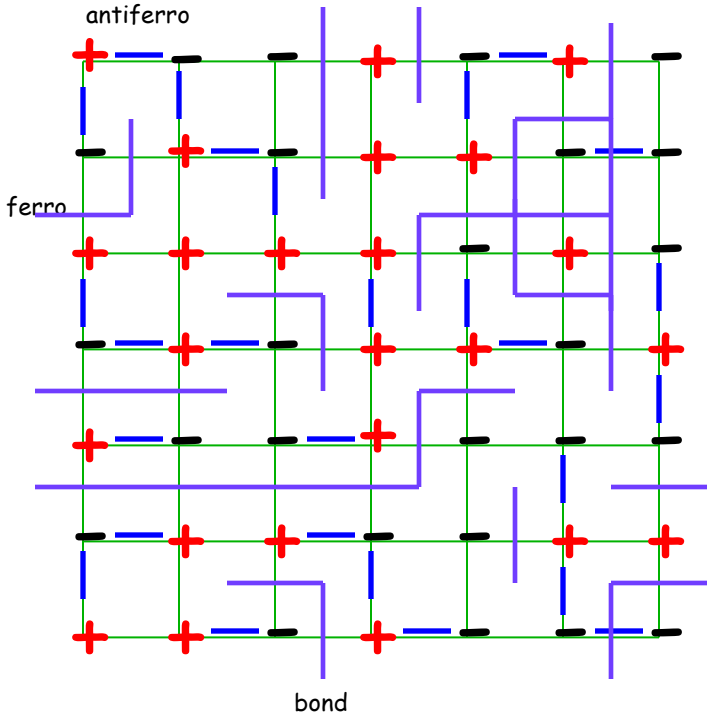
# Replica Monte Carlo

- A collection of $M$ systems at different temperatures is simulated in parallel, allowing exchange of information among the systems.




Parallel Tempering: exchange configurations

# Strings/Domain Walls in 2D Spin-Glass




*b*=0 no bond for satisfied interaction, *b*=1 have bond

The bonds, or strings, or domain walls on the dual lattice uniquely specify the energy of the system, as well as the spin configurations modulo a global sign change.

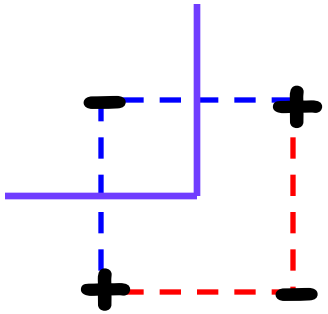
The weight of the bond configuration is

$$\prod_{<ij>} w^{b_{ij}}, \qquad w = \exp[-2J/(kT)]$$

[a low temperature expansion]

# Constraints on Bonds

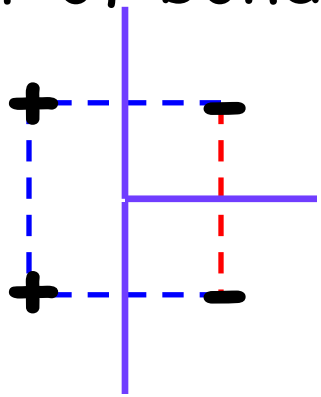
- An even number of bonds on unfrustrated plaquette



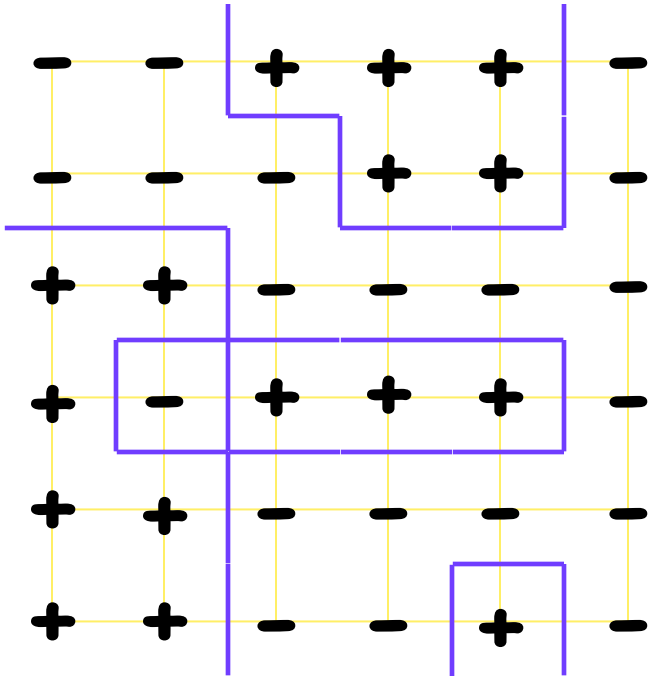
Blue: ferro

Red: antiferro

- An odd number of bonds on frustrated plaquette



# Peierls' Contour



The bonds in ferromagnetic Ising model is nothing but the Peierls' contours separating + spin domains from – spin domains.

The bonds live on dual lattice.

# Worm Algorithm for 2D Spin-Glass

1. Pick a site $i_0$ at random. Set $i = i_0$
2. Pick a nearest neighbor $j$ with equal probability, move it there with probability $w^{1-b_{ij}}$. If accepted, flip the bond variable $b_{ij}$ (1 to 0, 0 to 1). $i = j$.
3. If $i = i_0$ and winding numbers are even, exit, else go to step 2.

$$w = \exp(-2K)$$

See J-S Wang, PRE **72** (2005) 036706.

# N-fold Way Acceleration

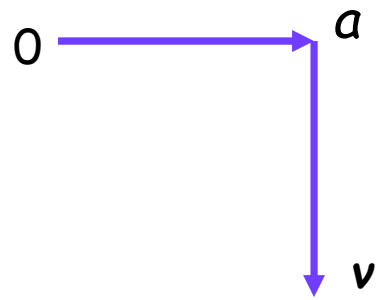
- Sample an *n*-step move with exit probability:

$$P(\nu \mid \mu) = \left[ (I - W^{AA})^{-1} W^{AA'} \right]_{\mu\nu}$$

where *A* is a set of states reachable in *n*-1 steps of move. *A'* is complement of *A*. *W* is associated transition matrix.

# Two-Step Probabilities

$$P(0 \to a \to \nu) = d_0 \frac{W_{0a} W_{a\nu}}{1 - W_{aa}},$$




$$W_{ij} = W(i \to j) = \begin{cases} 1/4, & b_{ij} = 1 \\ \exp(-2K)/4, & b_{ij} = 0 \\ 1 - \sum_{j=1}^{4} W_{ij}, & i = j \end{cases}$$

$d_0$ is fixed by normalization

# Time-Dependent Correlation Function and Spin-Glass Order Parameter

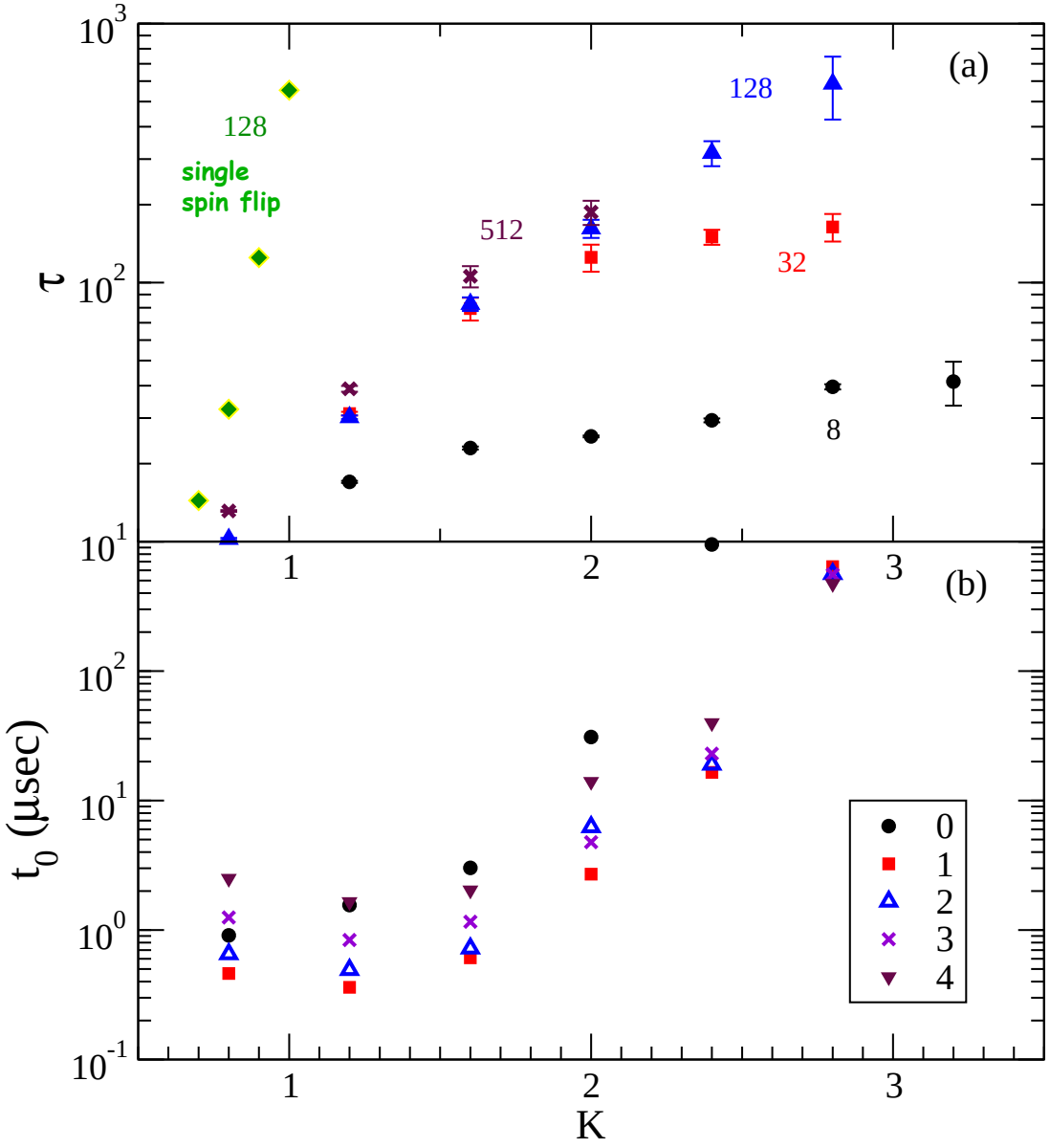
- We define

$$f(t) = \left[ \frac{\langle Q_s Q_{s+t} \rangle - \langle Q_s \rangle \langle Q_{s+t} \rangle}{\langle Q_s^2 \rangle - \langle Q_s \rangle^2} \right]_J \approx A \exp\left( -\frac{t}{\tau} \right)$$

where

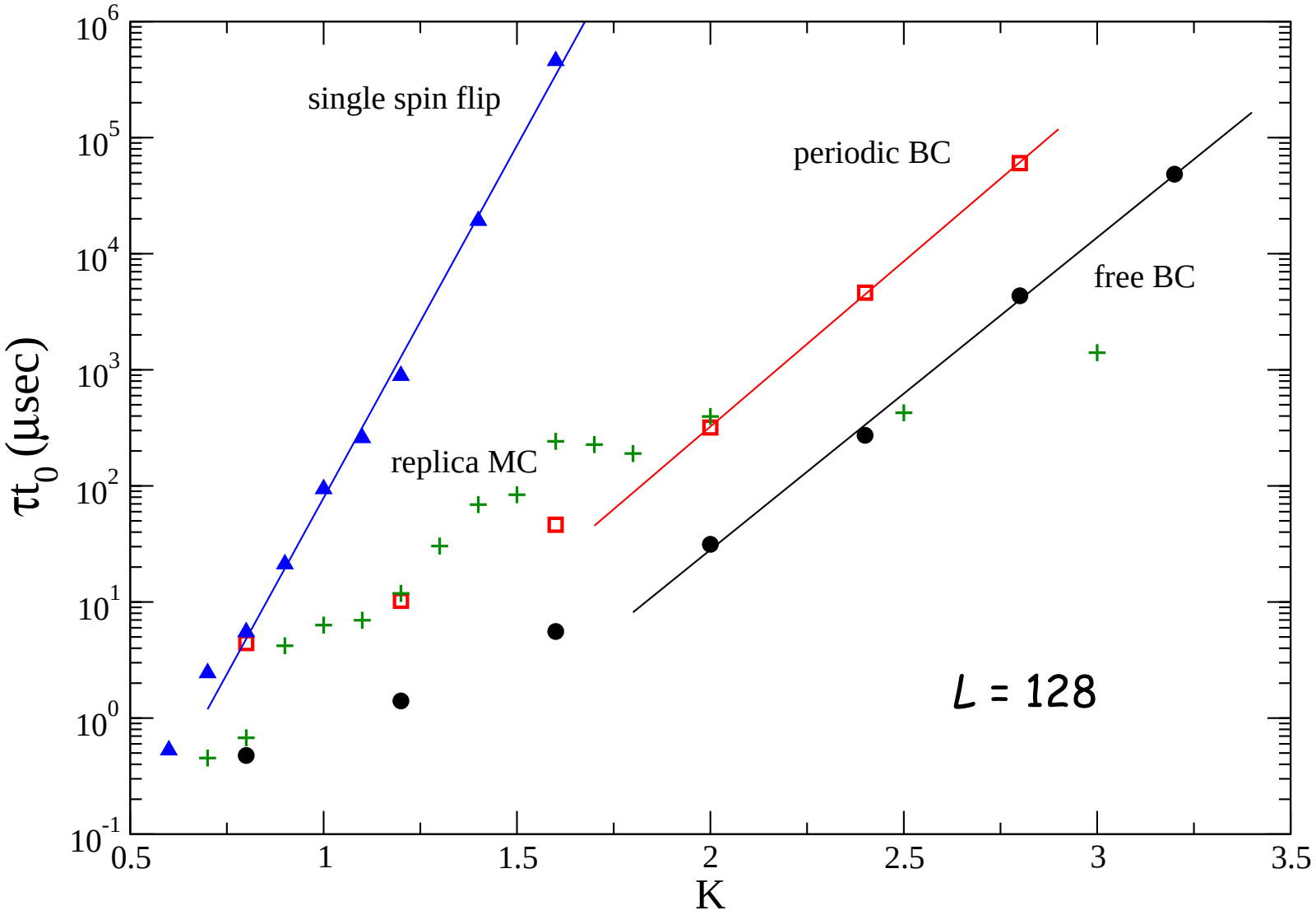
$$Q = \left| \sum_i \sigma_i^1 \sigma_i^2 \right|$$

# es

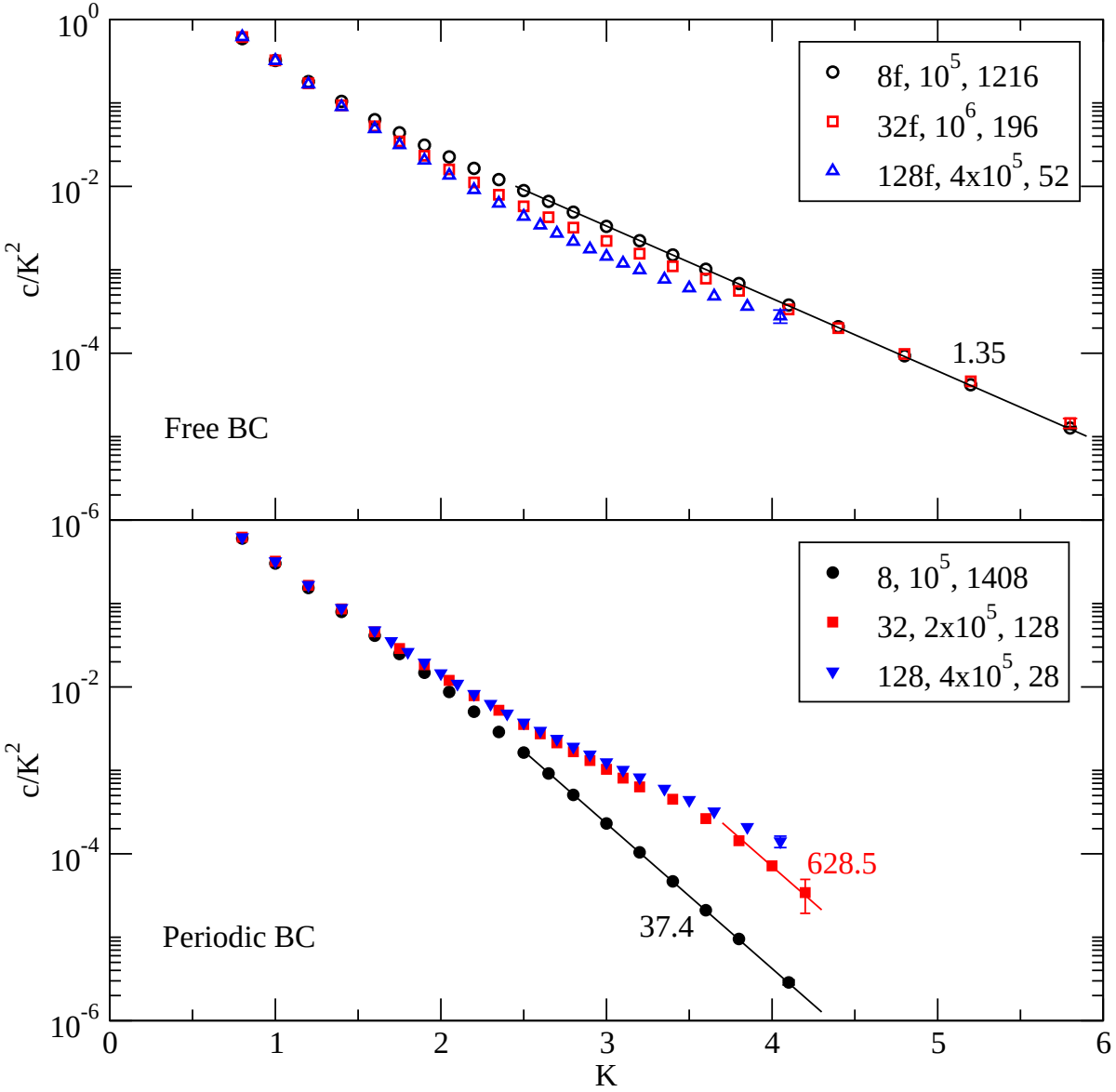



(a) Exponential relaxation times in units of loop trials of the worm algorithm.

(b) CPU times per loop trial per lattice site (32x32 system). Different symbols correspond to 0 to 4 step *N*-fold way acceleration.


single spin flip
periodic BC
free BC
replica MC
L = 128
τt0 (μsec)
K
10^6
10^5
10^4
10^3
10^2
10^1
10^0
10^-1
0.5
1
1.5
2
2.5
3
3.5

# Specific Heat when $T \to 0$

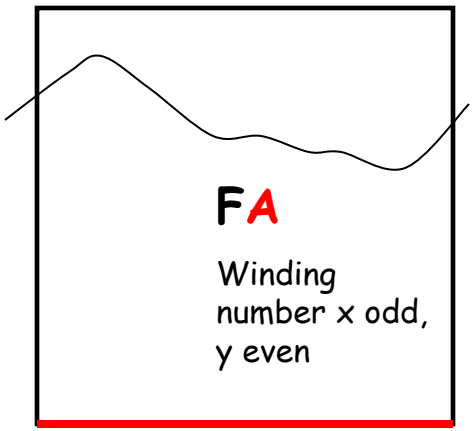


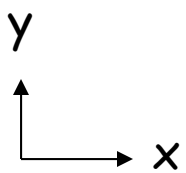

Free boundary condition: $c/K^2 \approx \exp(-2K)$.

Periodic BC: $c/K^2 \approx \exp(-2K)$ in thermodynamic limit ( $L \to \infty$ first). For finite system it is $\exp(-4K)$. $K = J/(kT)$

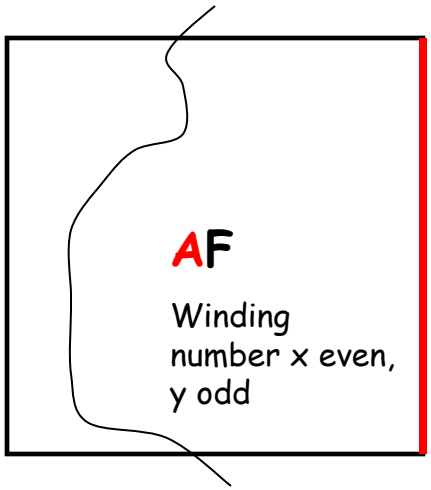
See also H G Katzgraber, *et al*, cond-mat/0510668.

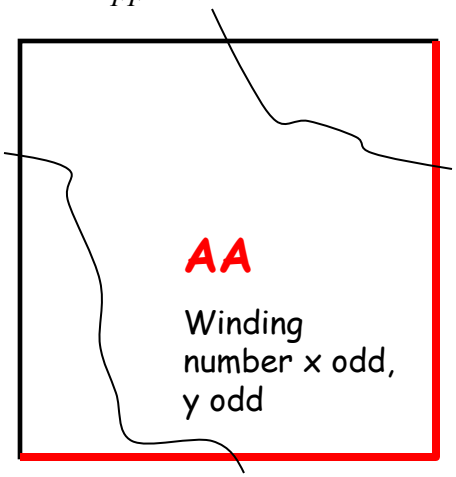
# Free Energy Difference

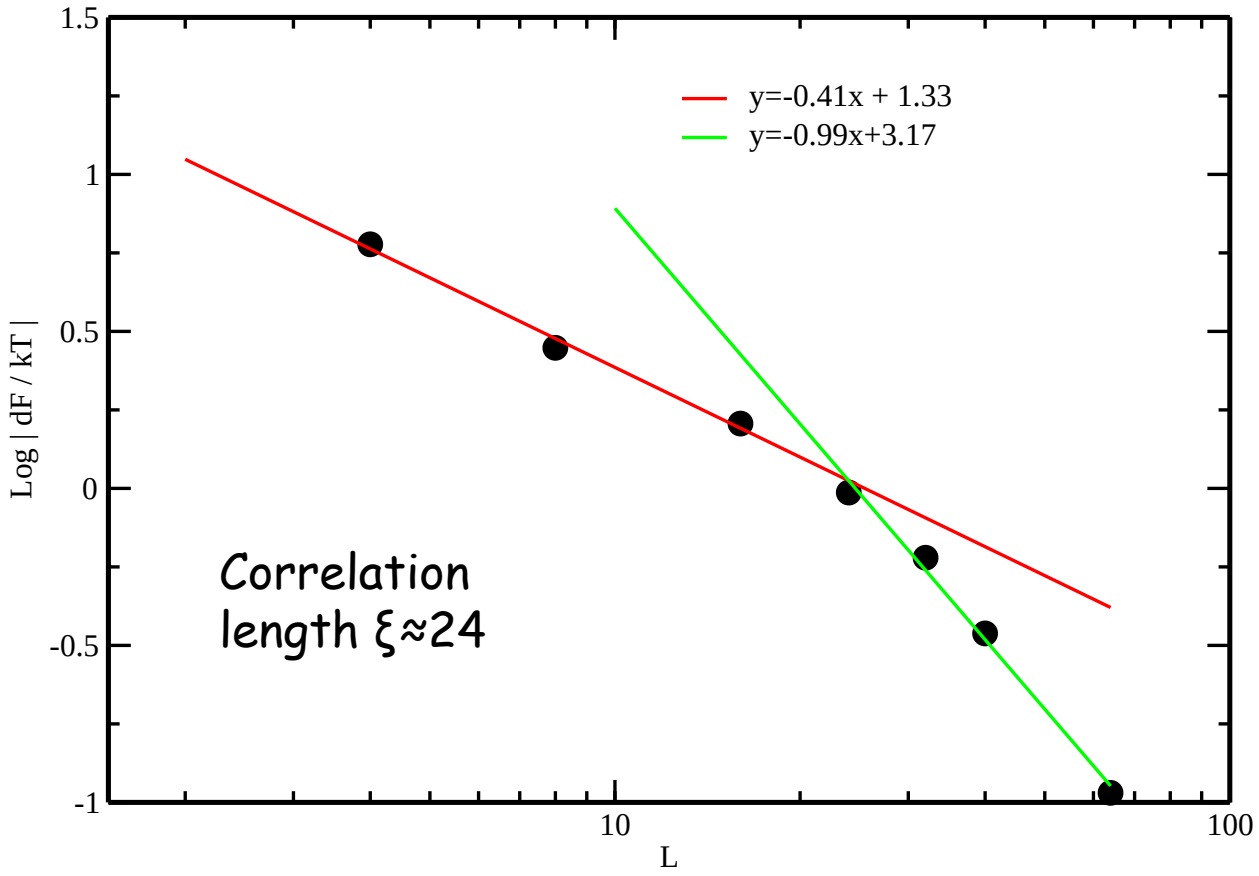

$$-\Delta F/(kT) = \log \frac{Z_{FA}}{Z_{FF}} = \log \frac{N_{FA}}{N_{FF}}$$




$N_{FF}$, $N_{FA}$, etc, number of times the system is in a specific winding number state, when the worm's head meets the tail. Red line denotes anti-periodic boundary condition.

# Free energy difference at T = 0.5

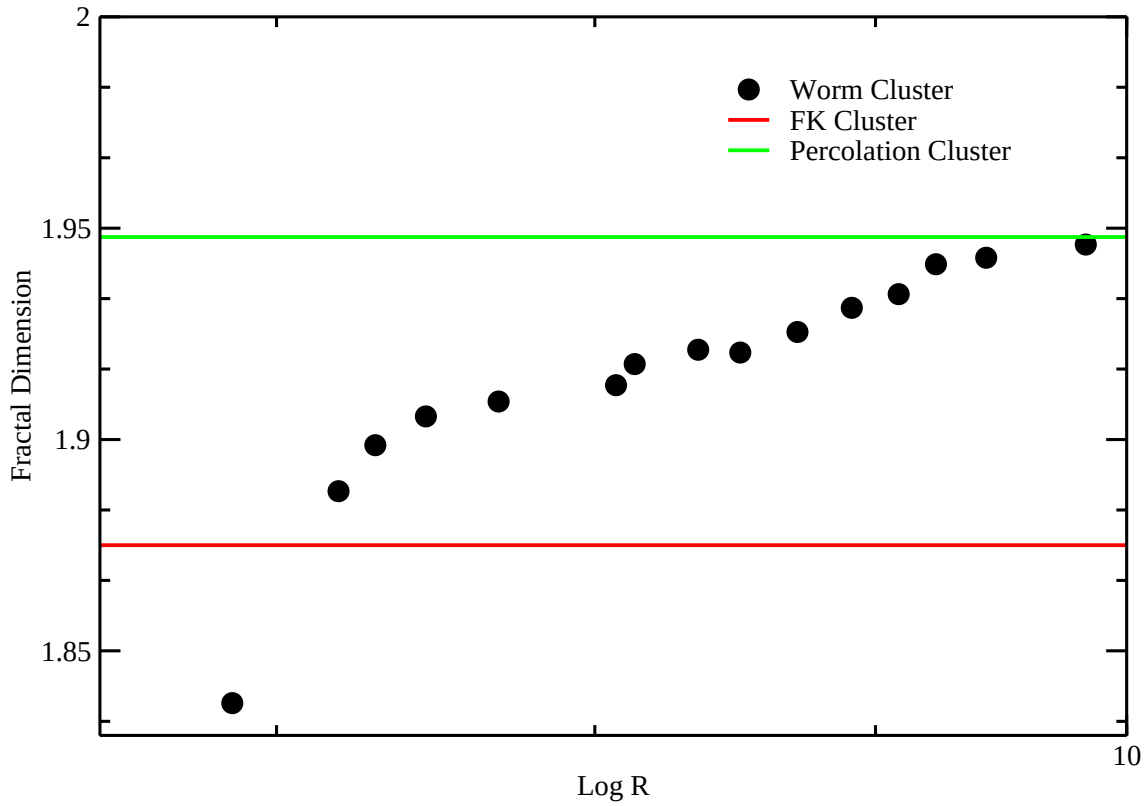



Difference of free energy between periodic BC (FF) and periodic/anti-periodic BC (FA), averaged over $10^3$ samples. $\Delta F \approx L^{\theta}$,

$\theta \approx -0.4$

J Luo & J-S Wang, unpublished

# Clusters in Ferromagnetic Tsing Model




Fractal dimension $D$ defined by $S=R^D$, where $R$ is radius of gyration. $S$ is the cluster size. Cluster is defined as the difference in the spins before and after the a loop move.

J Luo & J-S Wang, unpublished

# Summary Remarks

- Worm algorithm for 2D $\pm J$ spin-glass is efficient down to $T \approx 0.5$
- A single system is simulated
- Domain wall free energy difference can be calculated in a single run
- Slides available at http://web.cz3.nus.edu.sg/~wangjs under talks

# Postdoctorial Research Fellow Position Available

- Work with J-S Wang in areas of computational statistical physics, or nano-thermal transport.

- Send CV to wangjs@cz3.nus.edu.sg