Art of Computation

--- How to deal with quantum systems
without quantum computers? ---

Naoki Kawashima

Path Integral Formulation

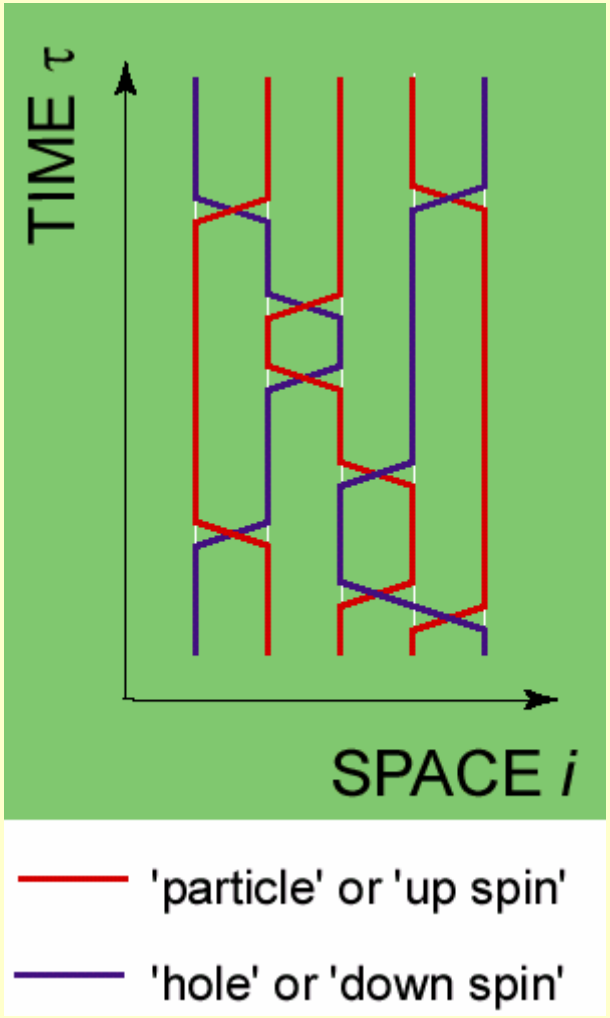
$$Z = \int D\psi \exp\left(- \int_0^\beta d\tau L(\psi, \dot{\psi}) \right)$$

$$= \sum_{\{\psi_\kappa\}} \exp\left(- \sum_{k=1}^{m} \Delta\tau \, L(\psi_{\kappa-1}, \psi_\kappa) \right)$$

$$= \sum_{\{\psi_\kappa\}} \prod_{\mathrm{k}=1}^{\mathrm{m}} \prod_{(i,j)} \exp\left(- \Delta\tau \, L_{(i,j)}(\psi_{\kappa-1}, \psi_\kappa) \right)$$

$$= \sum_S \prod_p w(S_p)$$

$$= \sum_S W(S)$$



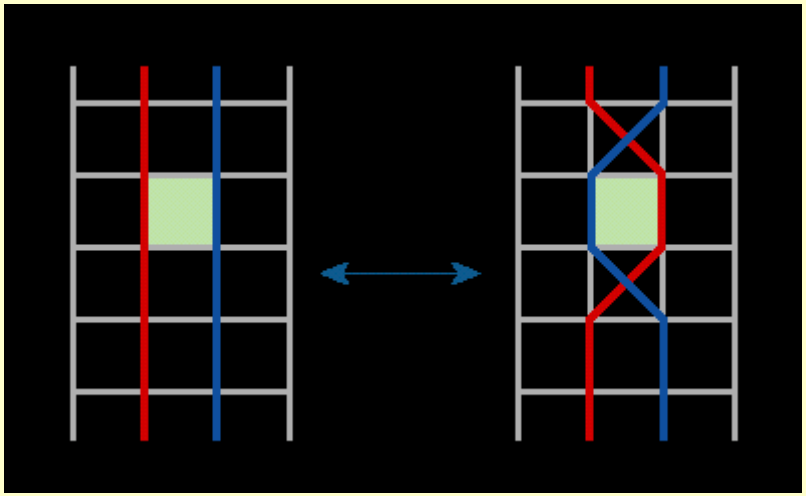
The way we use to do it --- Local Update

① Choose one square

② Propose a new state

③ Generate a random number

④ Accept the proposed state if the random number is smaller than a certain value



Shortcomings of local update

- Local (conventional) algorithms are slow.
  --- Critical slowing down,
  slowing down due to small $\Delta\tau$, etc.

- Local algorithms are sometimes non-ergodic
  --- The total magnetization never changes

- Off diagonal quantities cannot be measured efficiently

Cluster Algorithms for Quantum Spin Systems

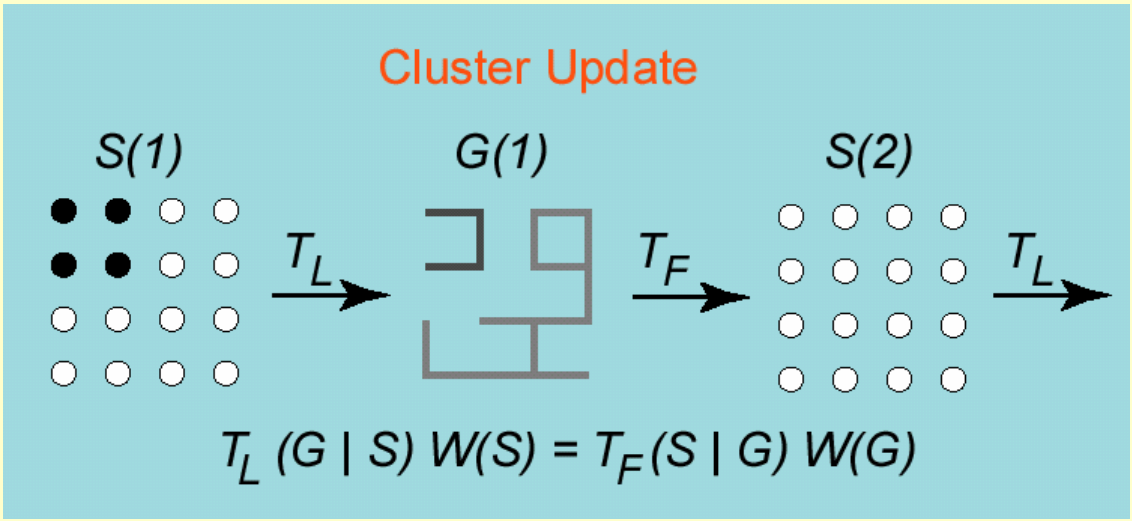
- Monte Carlo methods with graphical variables
  ---- Swendsen & Wang
- Path-integral representation of the partition function
  ---- Feynman, Suzuki
- Loop algorithm for quantum Monte Carlo
  ---- Evertz, Lana & Marcu
- Generalization to larger (S>1/2) spins
  ---- N.K. & Gubernatis
- Continuous Imaginary time limit
  ---- Beard & Wiese
- Improved estimators for off diagonal quantities
  ---- Brower, Chandrasekharan & Wiese
- Solution to negative sign problems in some cases
  ---- Chandrasekharan & Wiese

Monte Carlo methods with auxiliary graphical variables

$$Z = \sum_S W(S) = \sum_{S,G} W(S,G) = \sum_{S,G} V(G)\Delta(S,G)$$

(Generalized Fortuin-Kastelyn formula)

$$\Delta(S,G) = \begin{cases} 1 & \text{(spin are aligned in each cluster)} \\ 0 & \text{(otherwise)} \end{cases}$$



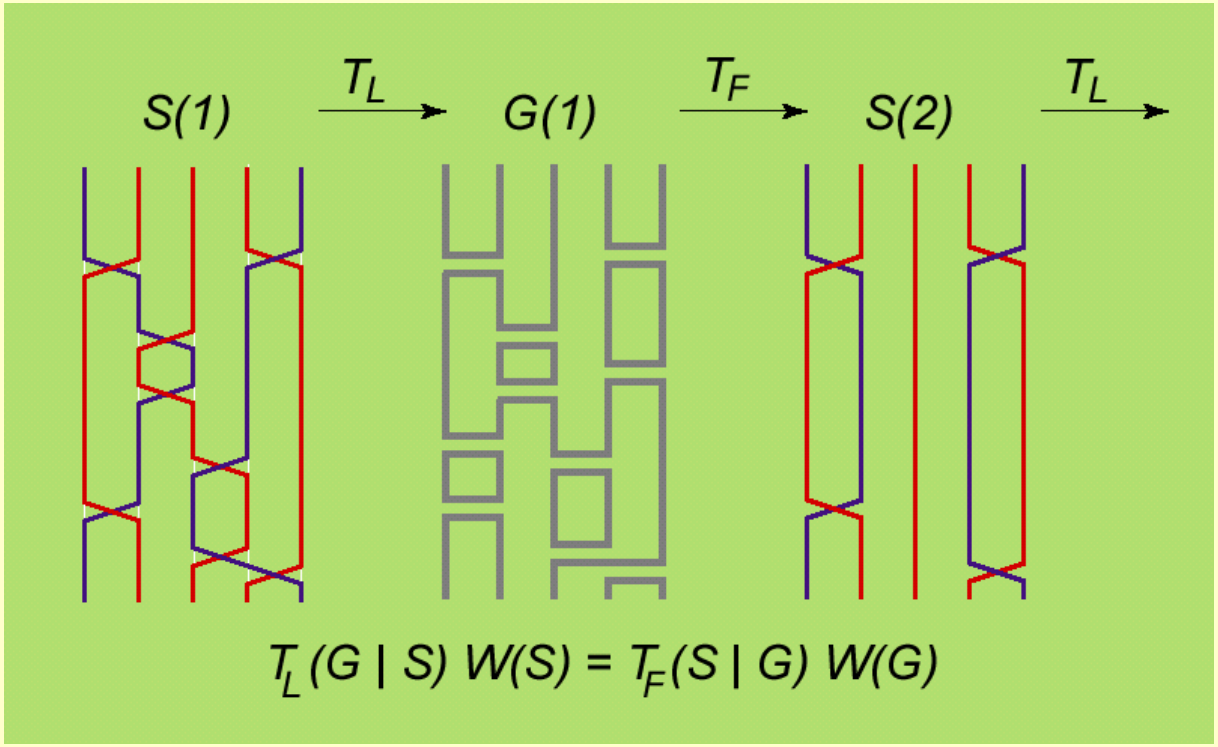
Loop Algorithm

=

Generalized Fortuin-Kasteleyn Representation

+

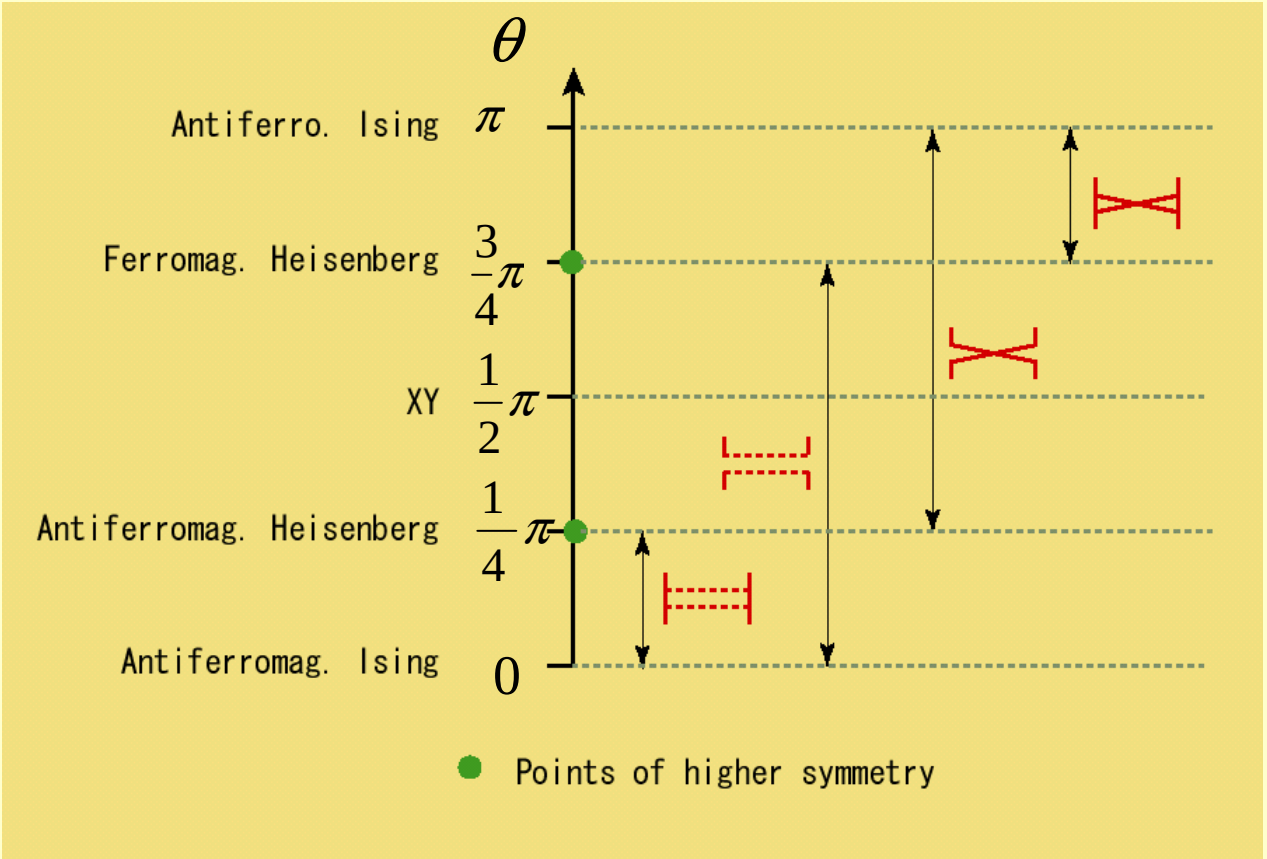
Path Integral Formulation



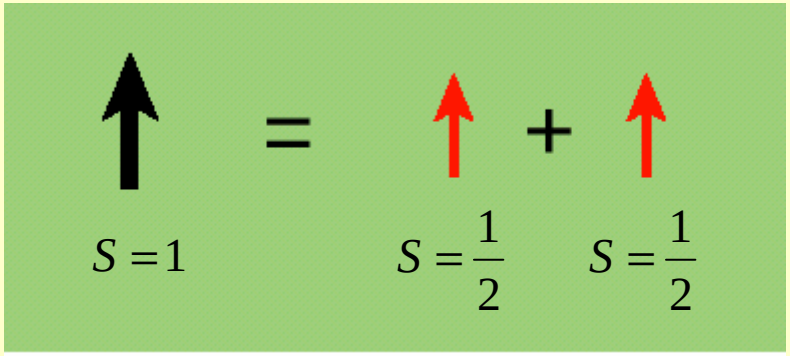
Types of graphs

$$H = \sum_{(i,j)} H_{ij} \quad H_{ij} \equiv \left(J_x \hat{S}_i^x \hat{S}_j^x + J_y \hat{S}_i^y \hat{S}_j^y + J_z \hat{S}_i^z \hat{S}_j^z \right) = -\sum_{G_{ij}} a(G_{ij}) \Delta(G_{ij})$$

$$J_x = J_y = J \sin\theta, \; J_z = J\cos\theta$$



Generalization to larger spins



$$\hat{\mathbf{S}}_i \Rightarrow \frac{\mathbf{1}}{2} \sum_{\mu=1}^{2S} \hat{\boldsymbol{\sigma}}_{i,\mu} \qquad \underset{\mathrm{S}}{\mathrm{Tr}}(\cdots) = \underset{\sigma}{\mathrm{Tr}}(\hat{P}\cdots)$$

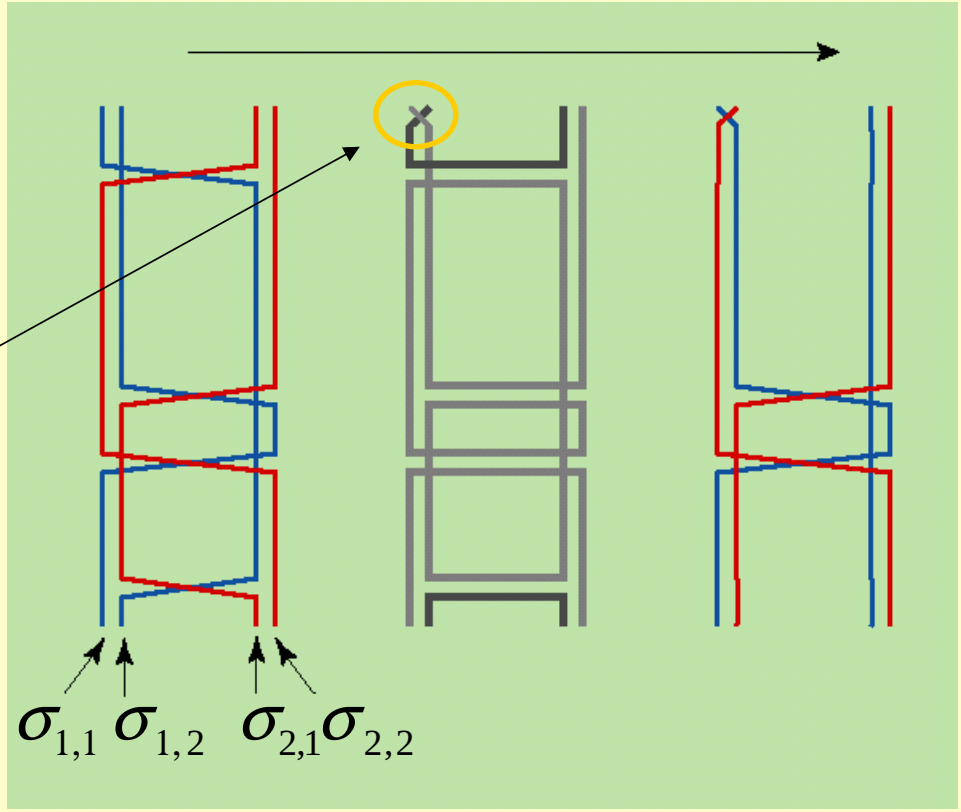
$$\hat{\mathbf{S}}_i = \text{(Original Spin)}$$

$$\hat{\boldsymbol{\sigma}}_{i,\mu} = \text{(Pauli Spin)}$$

One MC step for larger spins

$$\hat{\mathbf{S}}_i \Rightarrow \frac{\mathbf{1}}{2} \sum_{\mu=1}^{2S} \hat{\boldsymbol{\sigma}}_{i,\mu}$$

$$\mathrm{Tr}_{\mathrm{S}}(\cdots) = \mathrm{Tr}_{\sigma}(\hat{P}\cdots)$$



Related method (1)
--- Stochastic Series Expansion (SSE) ---

$$H = -\sum_{G_i} \hat{O}_{G_i}$$

$$\left(\text{cf} : H = \sum_{G_{ij}} \hat{\Delta}(G_{ij}) \right)$$

$$S \equiv (\psi_1, \psi_2, \cdots, \psi_L)$$

$$G \equiv (G_1, G_2, \cdots, G_L)$$

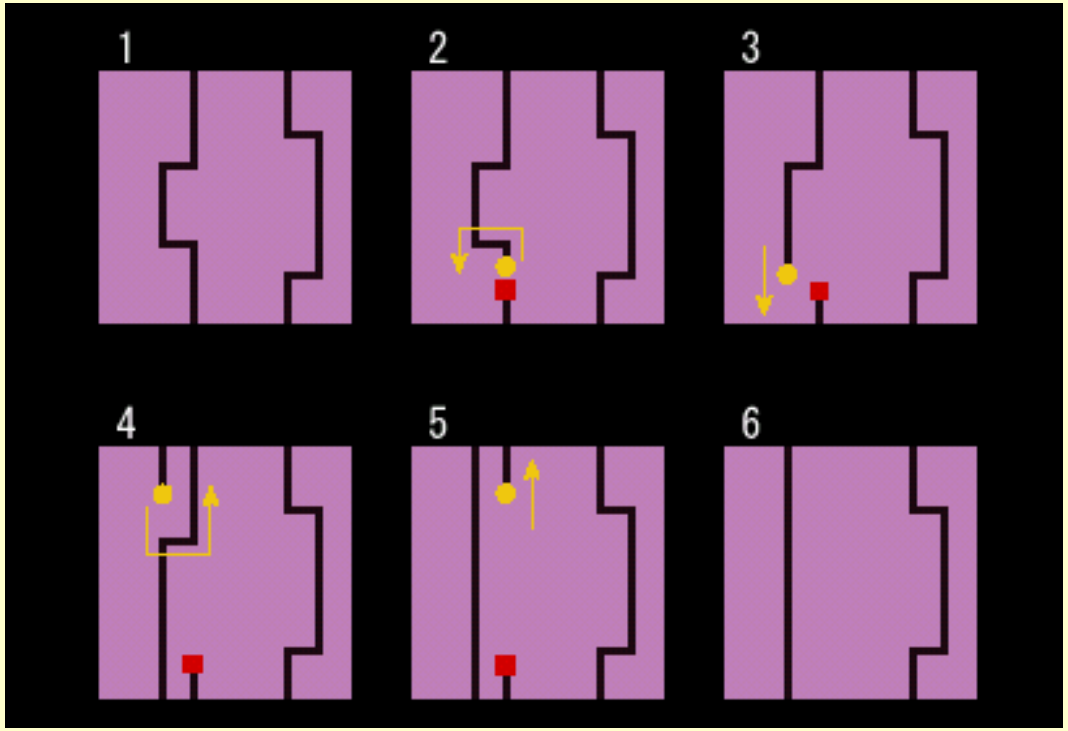
$$\begin{aligned}
Z &= Tr(e^{-\beta H}) \\
&\approx \sum_{\psi} \sum_{n=0}^{L} \frac{\beta^n}{n!} \left\langle \psi \middle| (-H)^n \middle| \psi \right\rangle \\
&= \sum_{\psi} \sum_{G} \beta^n \frac{(L-n)!}{L!} \left\langle \psi \middle| \hat{O}_{G_L} \hat{O}_{G_{L-1}} \cdots \hat{O}_{G_1} \middle| \psi \right\rangle \\
&= \sum_{S} \sum_{G} \beta^n \frac{(L-n)!}{L!} \left\langle \psi_1 \middle| \hat{O}_{G_L} \middle| \psi_L \right\rangle \cdots \left\langle \psi_2 \middle| \hat{O}_{G_L} \middle| \psi_1 \right\rangle \\
&= \sum_{S} \sum_{G} W(S,G)
\end{aligned}$$

SSE is also a Markov process in the space of (S,G) just like the loop algorithm with path-integral scheme.

SSE is simpler because of the absence of τ. Apart from it, it's essentially the same as the path-integral scheme.

Related method (2)
--- Worm Algorithm ---

State space is extended by including paricle number non-conserving states.



With this extension we can overcome the difficulty due to strong external field.

Related Methods

- Representations:
  - Path integral representation (Suzuki)
  - Series expansion (Handscomb, Sandvik)

- Updating methods:
  - Local updates
  - Loop updates (Everts et al)
  - Worm updates (Prokofev et al)

… All 2 x 3 = 6 combinations are possible. (Troyer)

Classical Picture for Quadrupolar Phase

Ferromagnetic  $\sum \mathbf{S_i} \neq \mathbf{0}$

Antiferromagnetic  $\sum (-1)^i \mathbf{S}_i \neq \mathbf{0}$

Spin Nematic
(or Quadrupolar)  $\sum \left(\left(S_i^z\right)^2 - \frac{\mathbf{S}^2}{3} \right) \neq 0$

Paramagnetic 

CF: CeB_6 , TmTe

High-Order Interaction and Quadrupole Order

Quadrupole (or higher) order

$$Q^{xx} = \sum_i \left(\left(S_i^x\right)^2 - \frac{S(S+1)}{3} \right), \quad Q^{xy} = \frac{1}{2} \sum_i \left(S_i^x S_i^y + S_i^y S_i^x \right), \quad etc.$$

… never exists in S=1/2 spin systems

$$\left(S_i^\mu\right)^2 = \frac{1}{4}$$

High-Order Interaction and Quadrupole Order

Quadrupole order may appear in

- Bilinear-Biquadratic Spin Model for S≧1

$$H = -\sum_{(i,j)} \left(J_L \mathbf{S}_i \cdot \mathbf{S}_j + J_Q \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 \right)$$

- Heisenberg model (S≧2) with strong cubic anisotropy

$$H = -J \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j - D \sum_i \left(\left(S_i^x \right)^4 + \left(S_i^y \right)^4 + \left(S_i^z \right)^4 \right)$$

- XY model with strong tetragonal anisotropy

$$H = -\sum_{(i,j)} \left[J \left(S_i^x S_j^x + S_i^y S_j^y \right) + D \left(\left(S_i^x \right)^2 \left(S_j^x \right)^2 + \left(S_i^y \right)^2 \left(S_j^y \right)^2 \right) \right]$$

Bilinear-Biquadratic Model with S=1

$$H = -\sum_{(i,j)} \left(J_L \mathbf{S}_i \cdot \mathbf{S}_j + J_Q \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 \right)$$

$$J_L = -J \cos\theta, \quad J_Q = -J \sin\theta$$

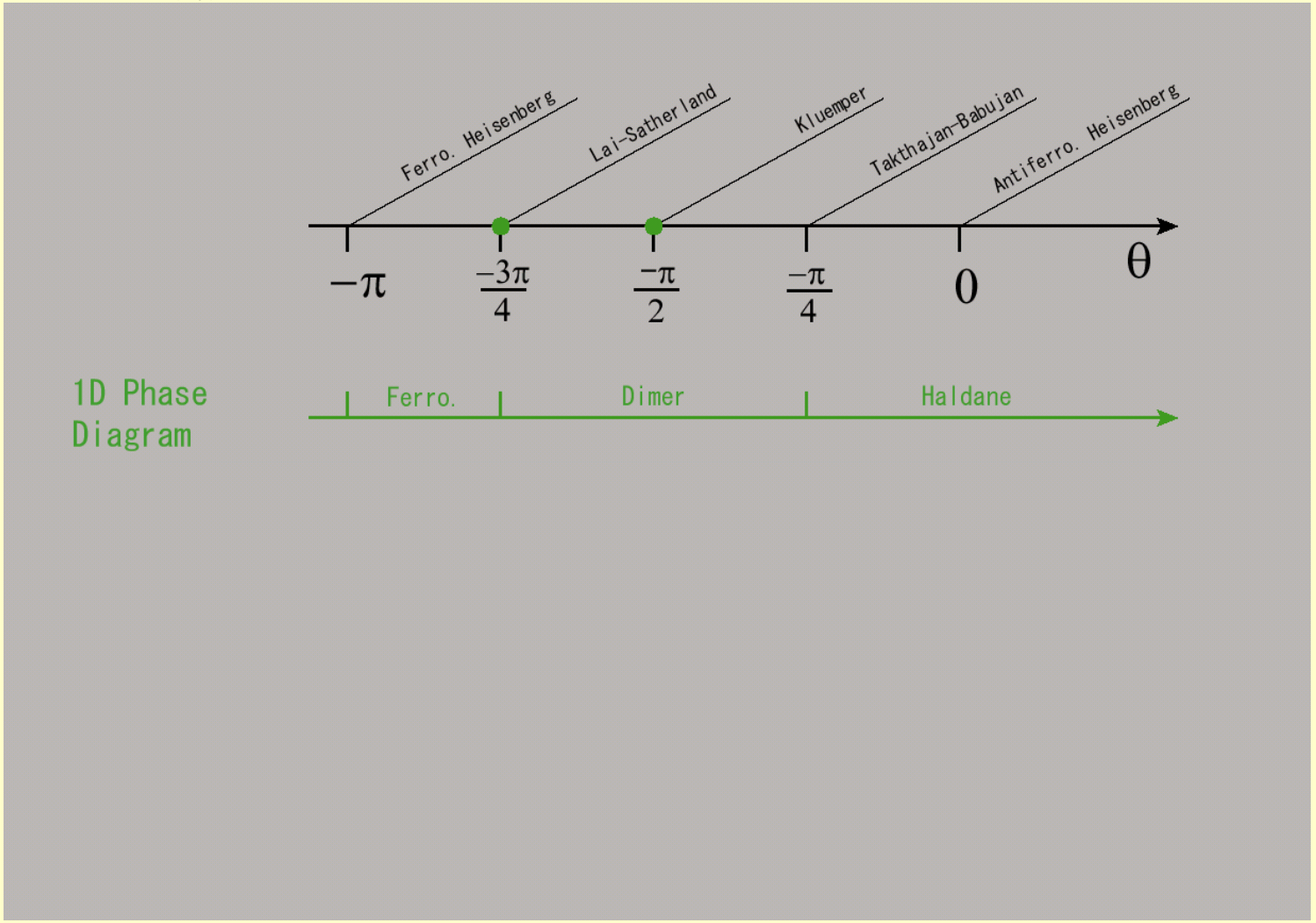
$$\mathbf{S}^2 = 2 \quad (S = 1)$$

Invariant under SU(2) spin rotation

Invariant under SU(3) spin rotation at θ/π=-3/4,-1/2,1/4,1/2

1D Phase Diagram

$$H = -\sum_{(i,j)} \left(J_L \mathbf{S}_i \cdot \mathbf{S}_j + J_Q \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 \right) \qquad J_L = -J\cos\theta, \;\; J_Q = -J\sin\theta$$



Chubukov Phase in 1D

$$H = -\sum_{(i,j)} \left(J_L \mathbf{S}_i \cdot \mathbf{S}_j + J_Q \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 \right)$$

$$J_L = -J \cos\theta, \quad J_Q = -J \sin\theta$$

Chubukov 1991 :

Negative energy spin wave mode in dimer phase

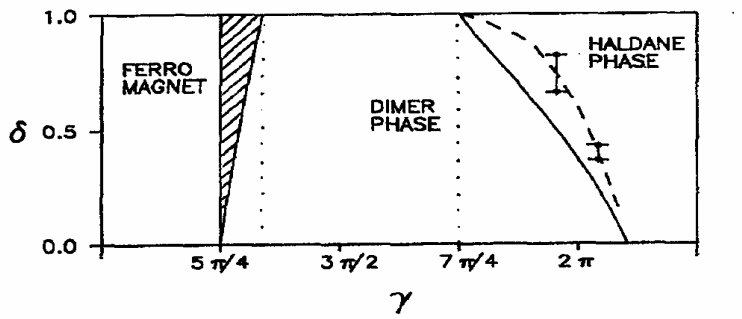


FIG. 2. $T=0$ quantum phase diagram in the γ,δ plane of the modified $S=1$ model (7). Two different disordered phases, 1D versions of antiferromagnetic and spin nematic states, are separated by the dimer phase with broken translational symmetry. The phase boundaries are calculated in the "spin-wave" approximation. The anharmonic corrections are believed not to shift the boundary line ending at the Bethe ansatz solvable point $\gamma=7\pi/4$. The dashed line is a result of numerical calculations of Ref. 30.

Disordered phase with a finite gap exists between ferromagnetic phase and dimer phase

The intermediate phase (Chubukov Phase)

= " Disordered version of spin nematic phase "

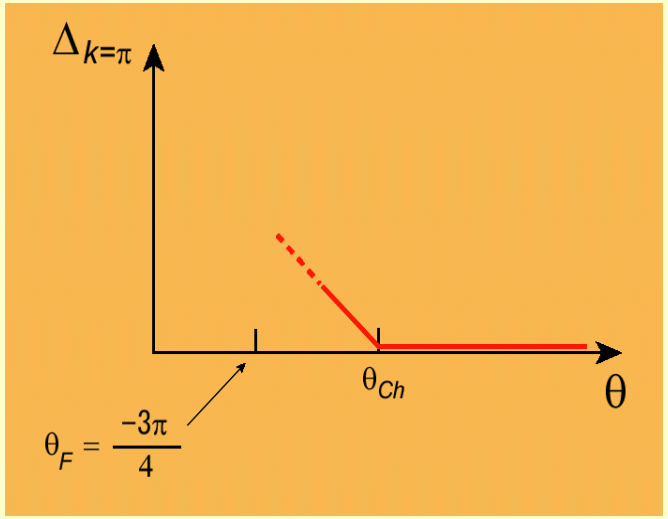
(cf: Haldane phase = " Disordered version of antiferromagnetic phase ")

Gap at k=π

Fath & Solyom 1995:

$$\Delta_{k=\pi} \equiv \langle \psi_- | H | \psi_- \rangle - \langle \psi_+ | H | \psi_+ \rangle$$

$$\Delta_{k=\pi} = \begin{cases} \text{finite} & \text{(Chubukov phase)} \\ O(L^{-1}) & \text{(Critical)} \\ O(e^{-aL}) & \text{(Dimer phase)} \end{cases}$$



$$\psi_\pm \approx |\cdots\rangle \pm |\cdots\rangle$$

Calculation of the k=π gap

Fath & Solyom 1995:

Exact diagonalization for $\Delta_{k=\pi}$

Crossing point of $L \times \Delta$ curves approaches $\theta = -3\pi/4$

… no gapped phase

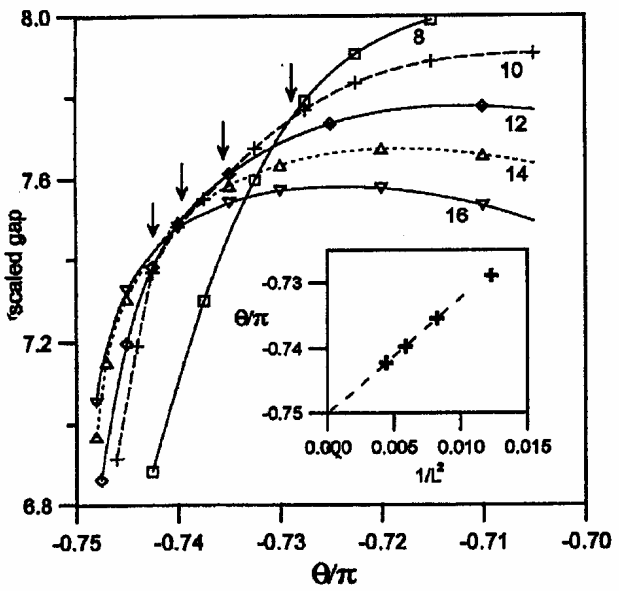


FIG. 2. Scaled gap $L(E_\pi - E_{GS})$ between the lowest $k = \pi$ level, and the ground state having momentum $k = 0$, as a function of θ for chains with $L = 8, 10, \ldots, 16$ sites. Arrows indicate the crossing point of curves belonging to chain lengths L and $L + 2$. Inset shows the L^{-2} scaling behavior of the crossing points.

Dimer order parameter (D) in 1D

$$D \equiv \sum_i (-1)^i \, \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

Singh & Gelfand 1988:

Series expansion …

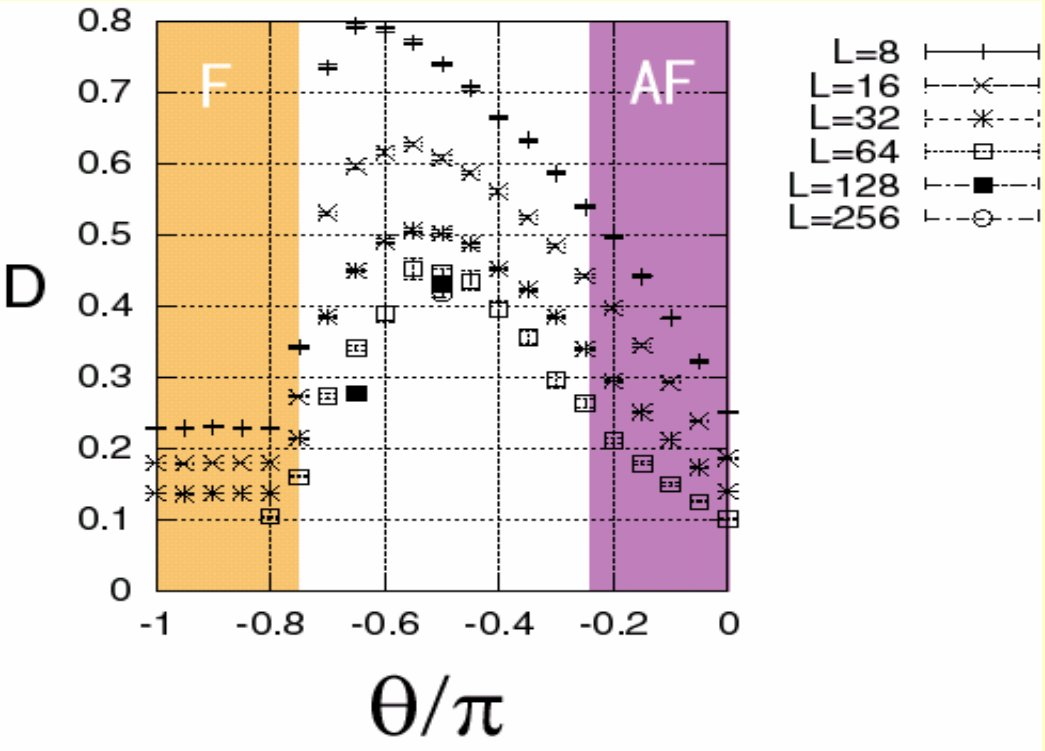
$$\langle D \rangle = 0.375(5) \quad \text{at} \quad \theta = -\frac{\pi}{2}$$

D vs θ at T = 0

Roughly consistent with the standard picture (i.e. no intermediate region)

But not conclusive for Chubukov phase

Quantum Monte Carlo



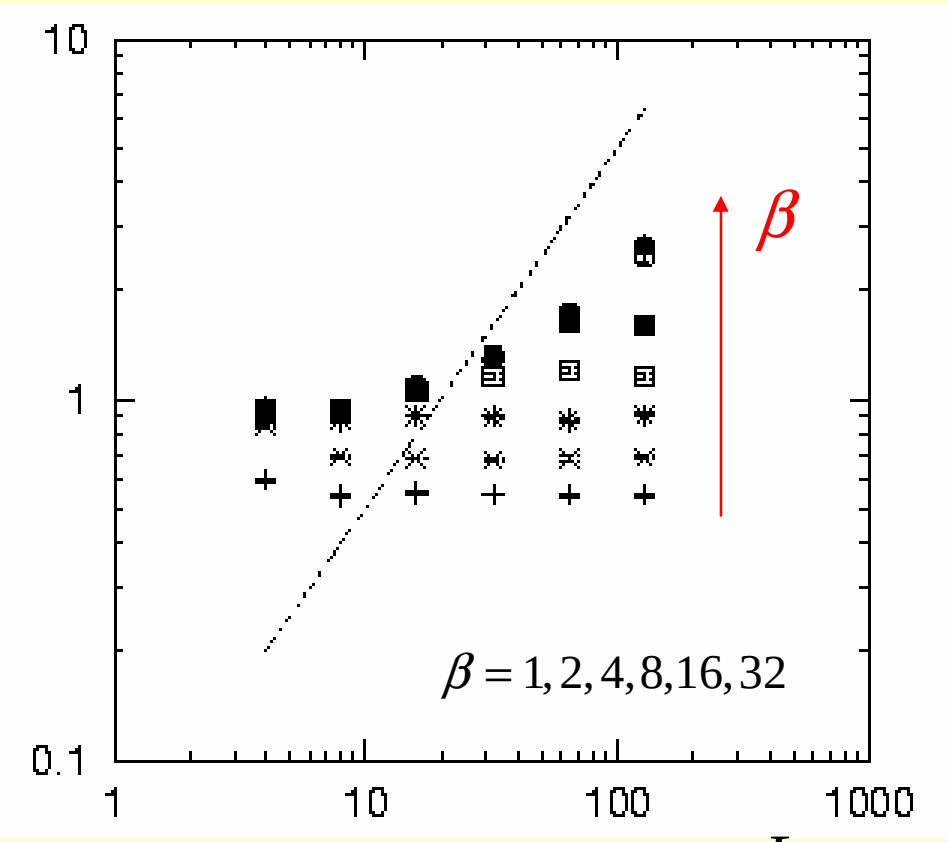
Harada, Kawashima, Batista & Gubernatis (2001)

Dimerization Order Parameter

$\theta/\pi = -0.6$

D^2/L diverges

… Probably this is in the dimer regime



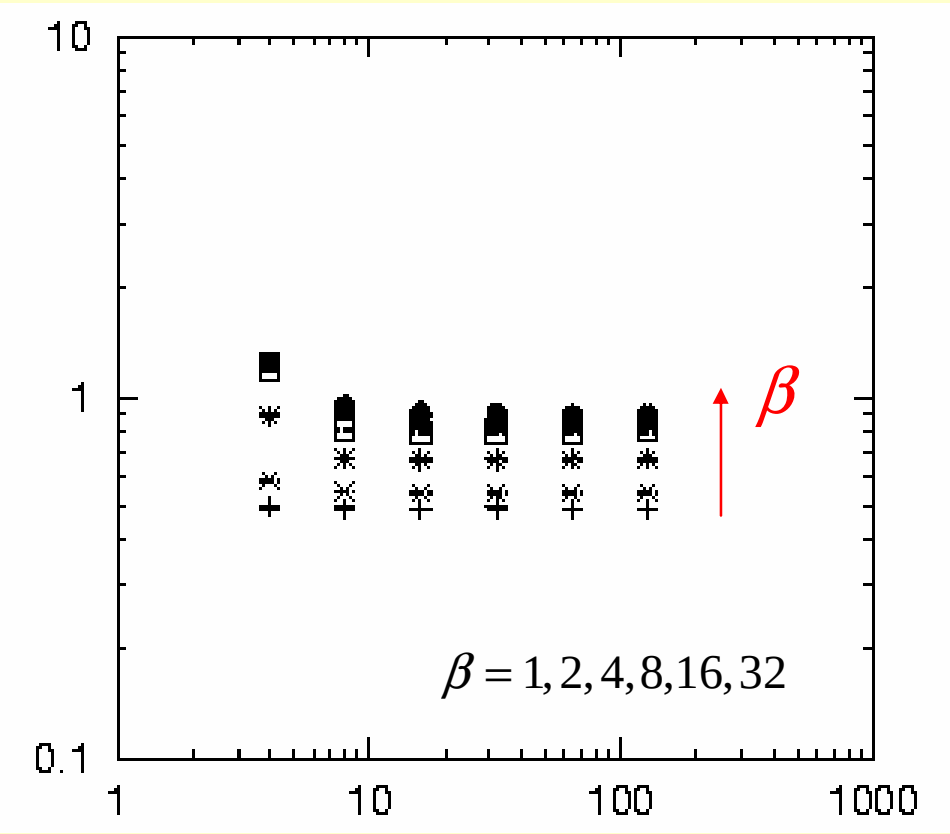
Harada, Kawashima, Batista & Gubernatis (2001)

Dimerization Order Parameter

$\theta/\pi = -0.7$

D^2/L stays constant

… Probably this is NOT in the dimer regime



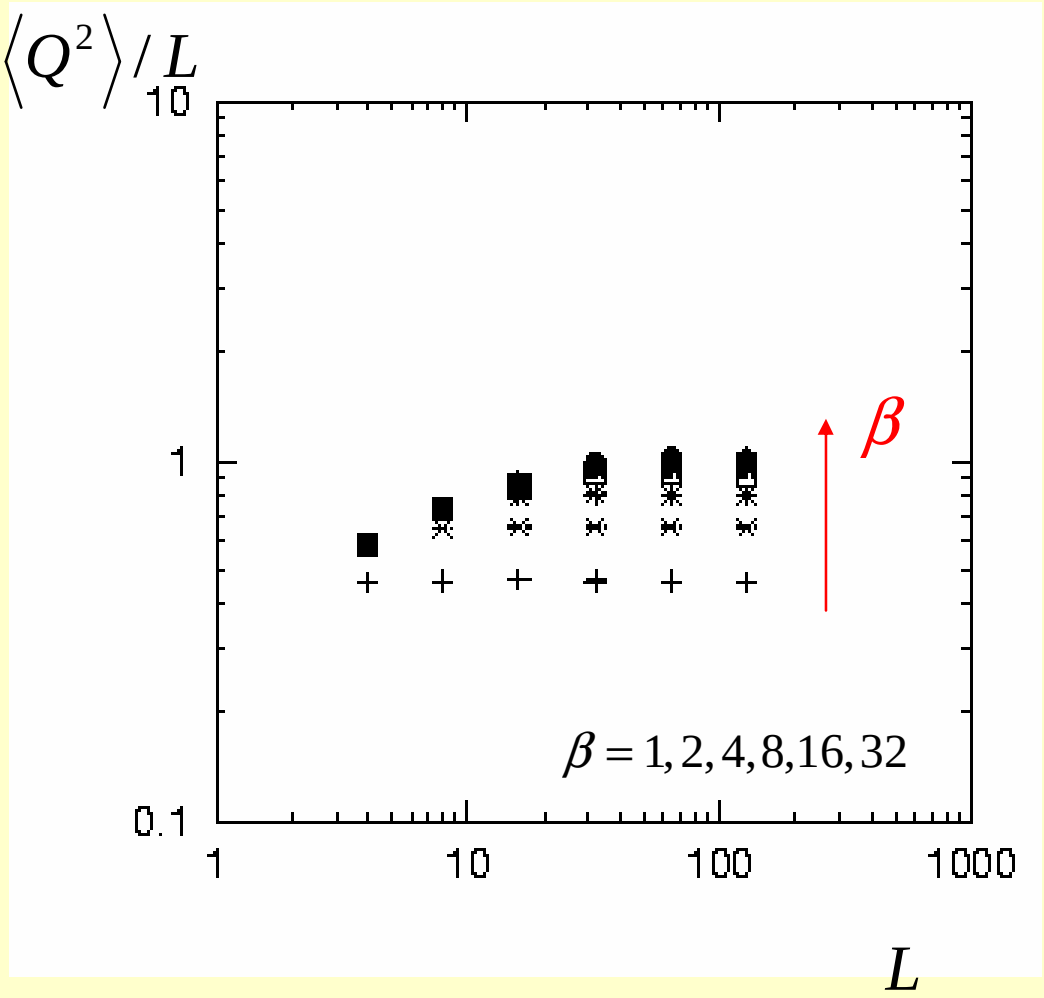
Harada, Kawashima, Batista & Gubernatis (2001)

Quadrupole Moment

$\theta/\pi = -0.6$

Q^2/L stays constant

… Probably this is in the dimer regime



Harada, Kawashima, Batista & Gubernatis (2001)

Quadrupole Moment

$\theta/\pi = -0.7$

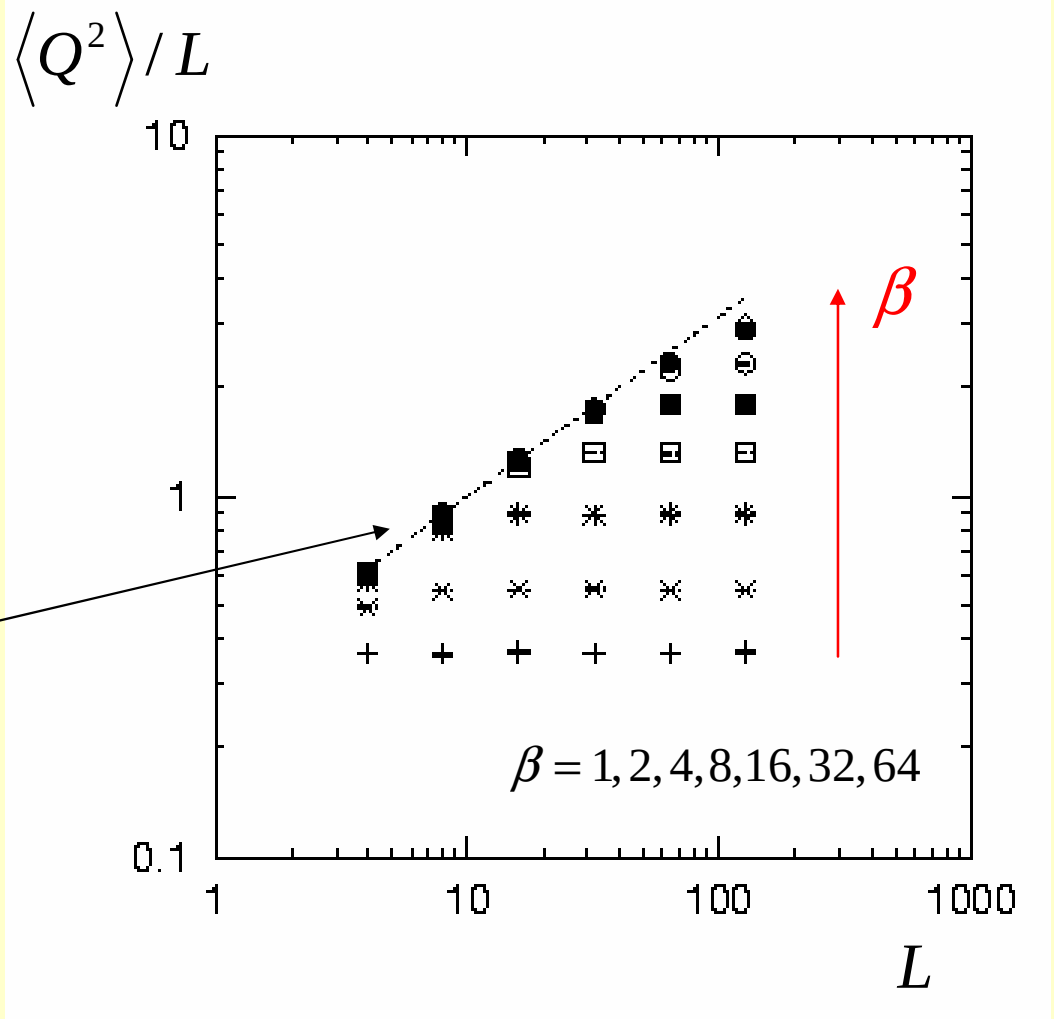
Q^2/L seems to diverge

… Probably this is in some semi-ordered or gapless regime

The straight line corresponds to

$$\langle Q^2 \rangle / L \propto L^{0.5}$$

i.e. $2 - \eta \approx 0.5$



Harada, Kawashima, Batista & Gubernatis (2001)

Summary

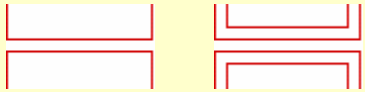
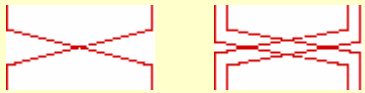
--- Weakly ordered spin nematic phase ---

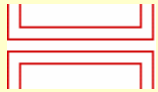
- We have found evidences for the presence of an intermediate phase.
- The intermediate phase is characterized by the divergence of quadrupolar structure factor.
- However, the phase is gapless as Fath and Solyom claimed, in contrast to Chubukov's prediction.

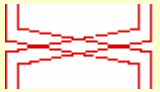
Cluster Algorithm for biquadratic model

Harada and Kawashima (2001)

- Negative sign difficulty in the positive θ region
- "Double" graphs
- No freezing

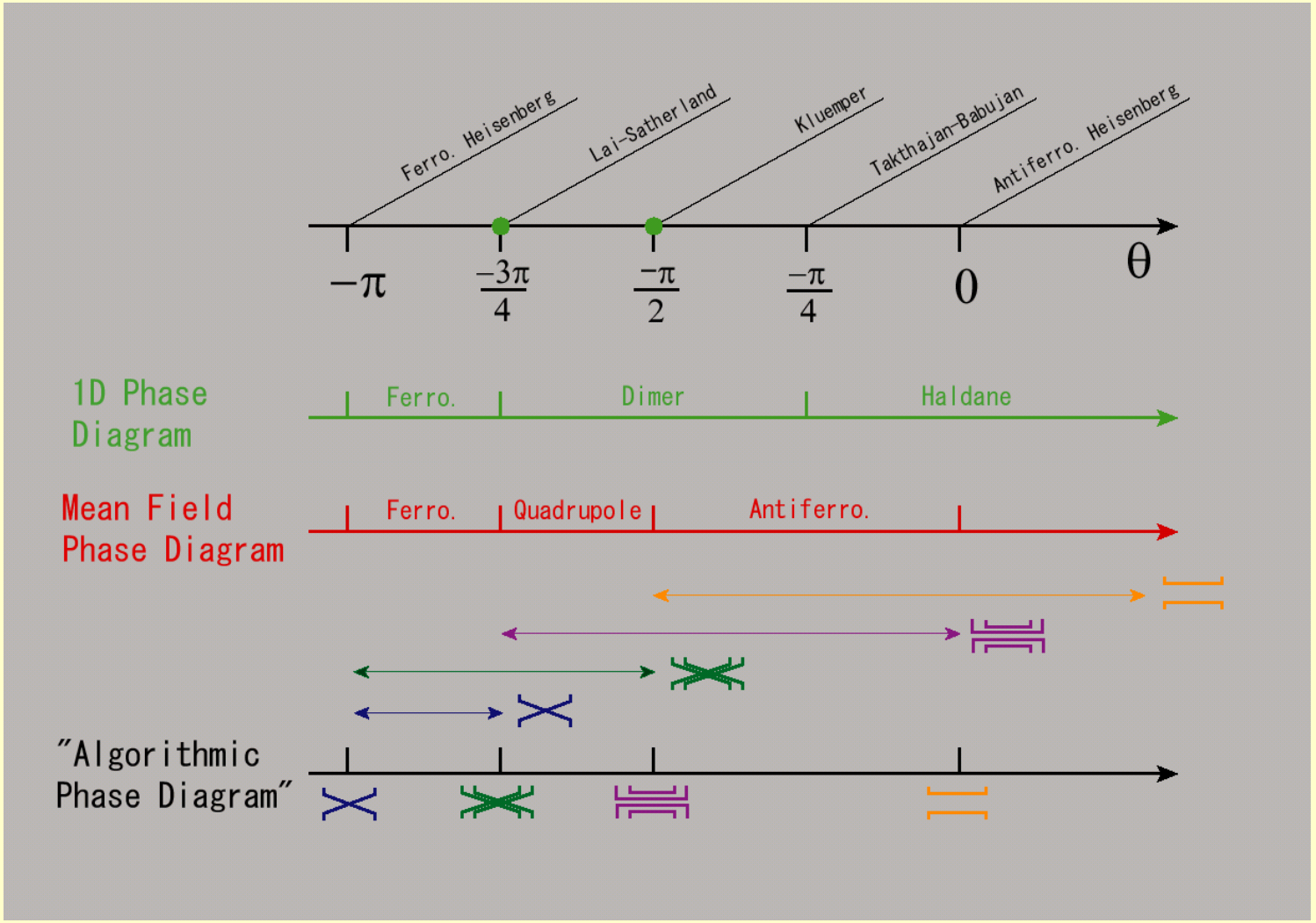
1. Antiferromagnetic regime
   … single horizontal and double horizontal 
2. Ferromagnetic regime
   … single cross and double cross graphs 
3. Spin-nematic regime
   … double horizontal and double cross graphs
4. SU(3) points are represented by a single kind of double graphs

$$H = -\sum_{(i,j)} \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^2 = -\sum_{(i,j)} \hat{\Delta}_{ij} \left(\quad \right)$$ 

$$H = -\sum_{(i,j)} \left(\mathbf{S}_i \cdot \mathbf{S}_j + \left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^2\right) = -\sum_{(i,j)} \hat{\Delta}_{ij} \left(\quad \right)$$ 

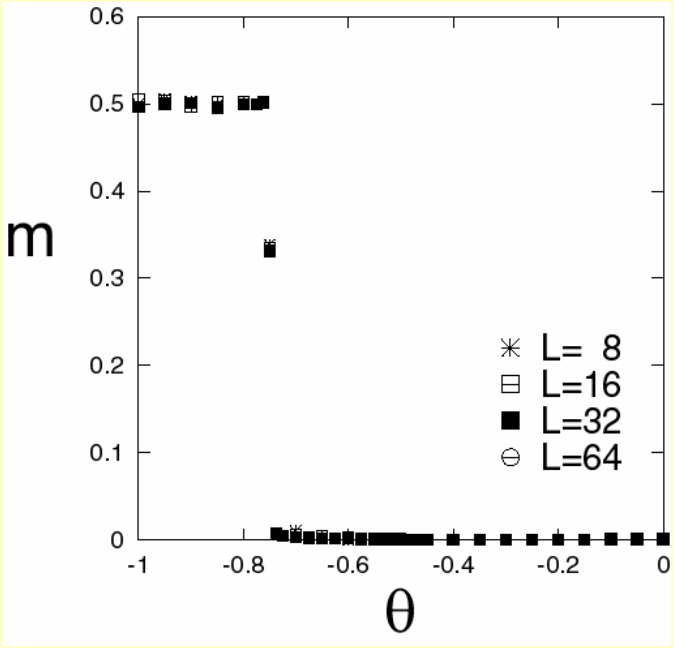
"Algorithmic Phase Diagram"

$$H = -\sum_{(i,j)} \left(J_L \mathbf{S}_i \cdot \mathbf{S}_j + J_Q \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 \right) \qquad J_L = -J \cos\theta, \;\; J_Q = -J \sin\theta$$

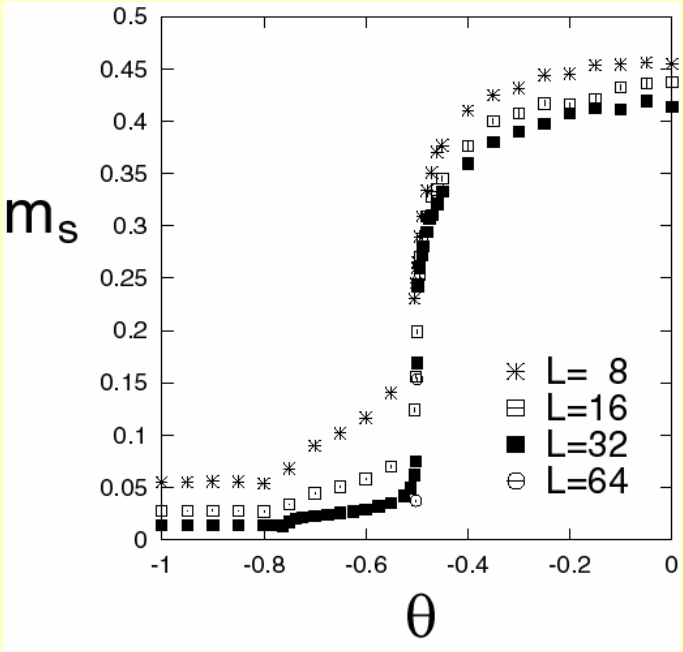


Magnetic Moment in 2D

Uniform Magnetization



Staggered Magnetization



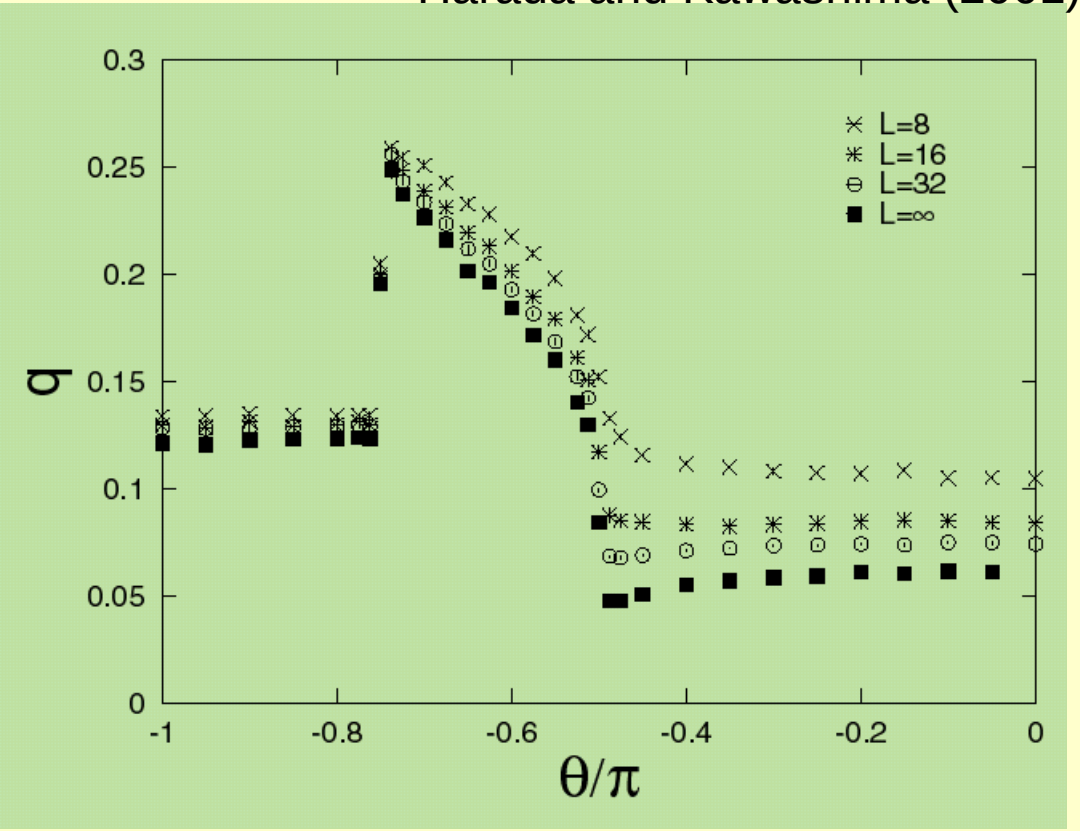
Harada and Kawashima (2001)

No magnetic order in the intermediate region

Quadrupole Moment in 2D

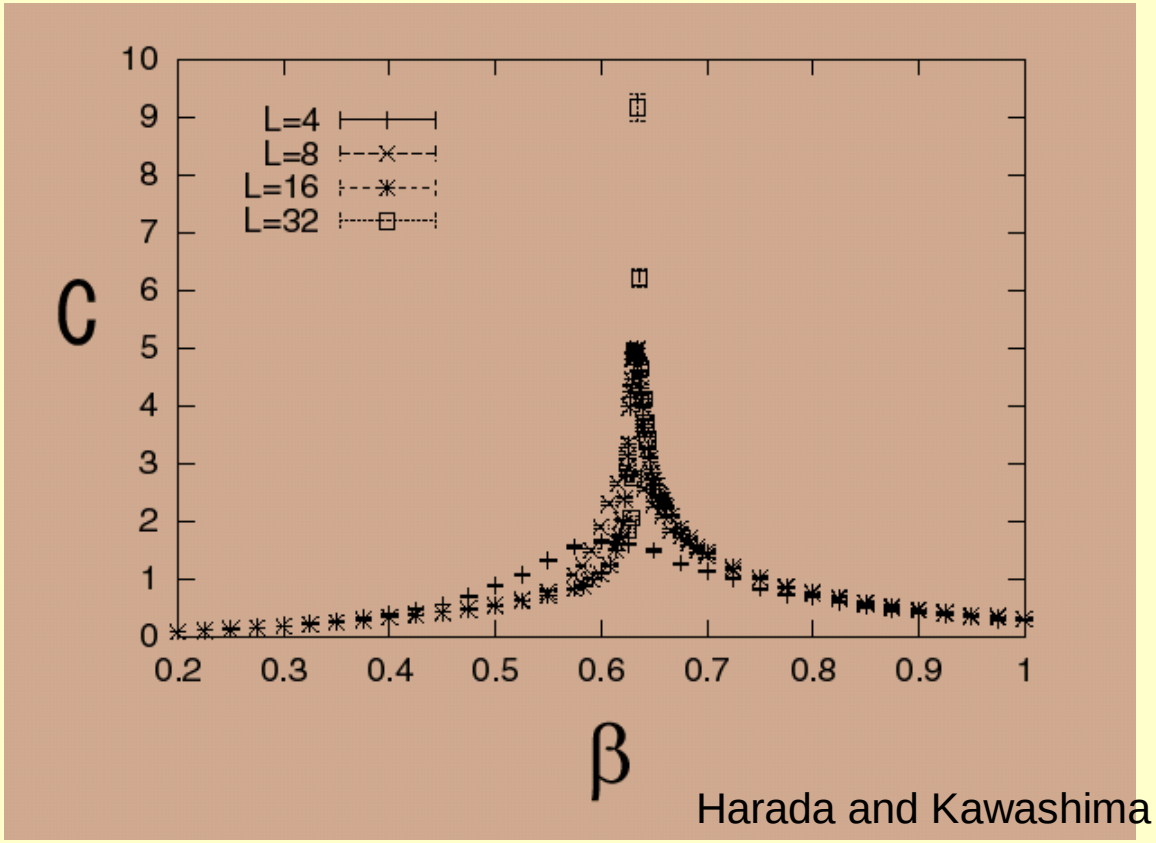
T=0
L=8,16,32

Harada and Kawashima (2001)



The intermediate phase is a quadrupolar phase.

Specific Heat in 3D



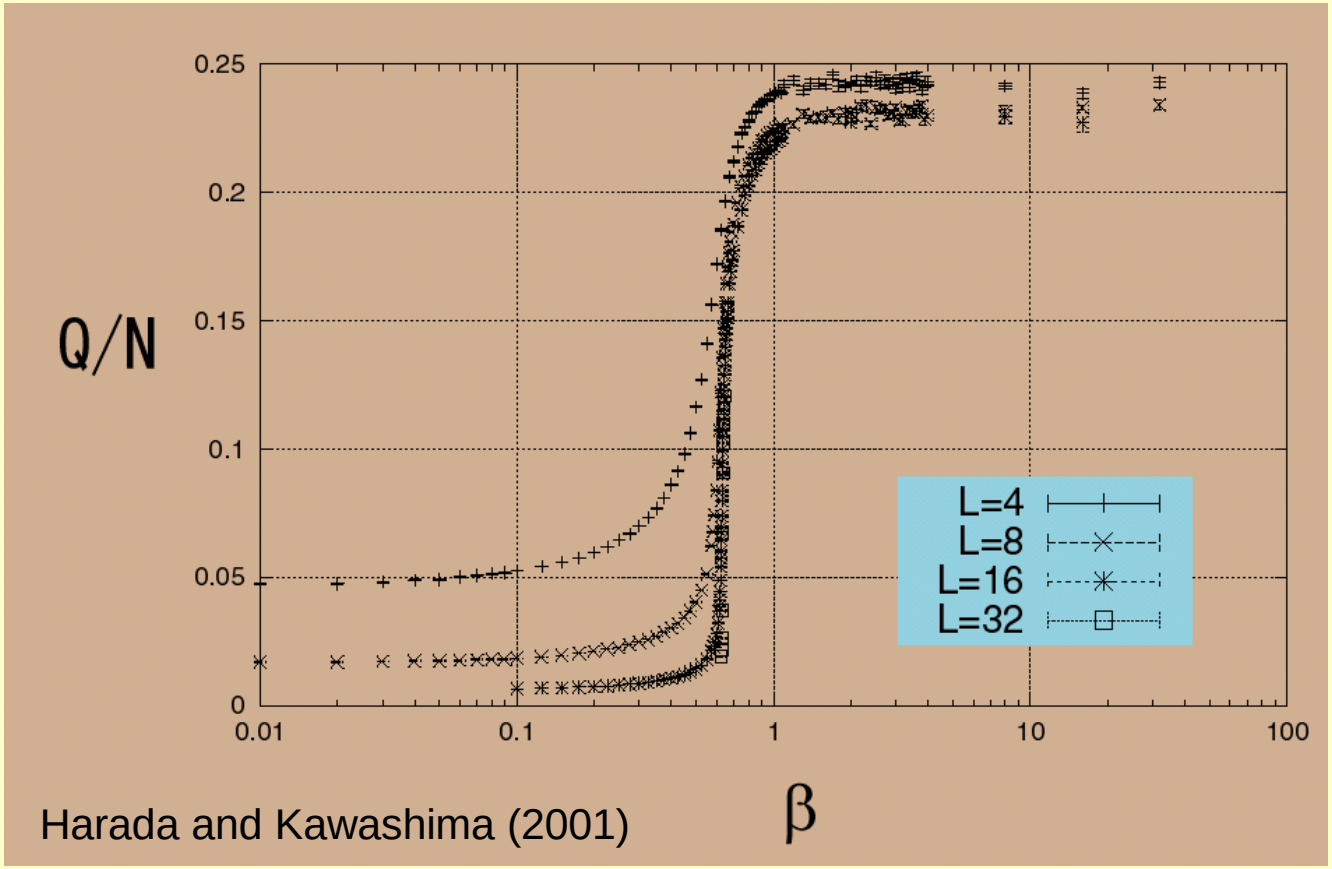
Harada and Kawashima (2001)

Sharp peak with clear size dependence

… 2nd order phase transition with $\alpha>0$, or 1st order

(cf: For dipolar transitions, $\alpha<0$)

Quadrupole Moment vs Temperature



Harada and Kawashima (2001)

Very sharp, like a first order phase transition

Summary

Monte Carlo method:

- Robust
- Dimensionality does not matter much
- Enhanced by various different updating methods.
- Graphical decomposition reflects the symmetry properties of the model.
  1) Types of graphs change at points of higher symmetry
  2) Hamiltonians with higher symmetry are represented by a fewer types of graphs.