NTU Colloquium

QUANTUM MONTE CARLO AND NON-GINZBURG-LANDAU TYPE PHASE TRANSITION

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NEC	Kota Sakakura … K

K … Parallelization on "K"
SUN... SU(N) Heisenberg model
BIQ ... Biquadratic Heisenberg model
PWU ... Paralllelization of worm update
JQ ... SU(N) J-Q model
OPT ... Optical lattice

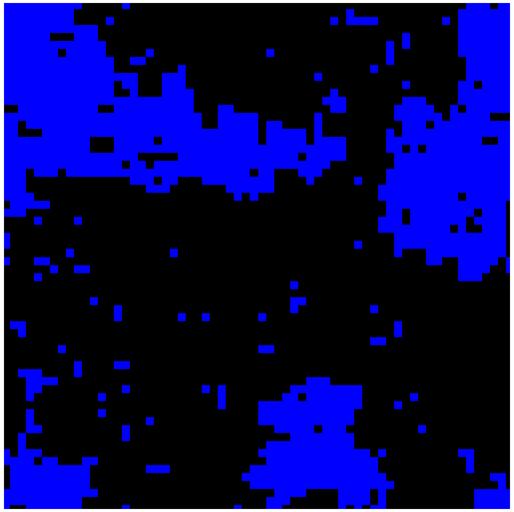
Ising Model

Critical Slowing Down in Monte Carlo …

The typical size of magnetic domains: $\xi \sim a \times (T/Tc - 1)^{\nu}$
The size of the updating unit: (a single site) $\sim a$
The effect of spin flip at a point propagates by some diffusion-like process which makes $z \sim 2$.
So, it takes

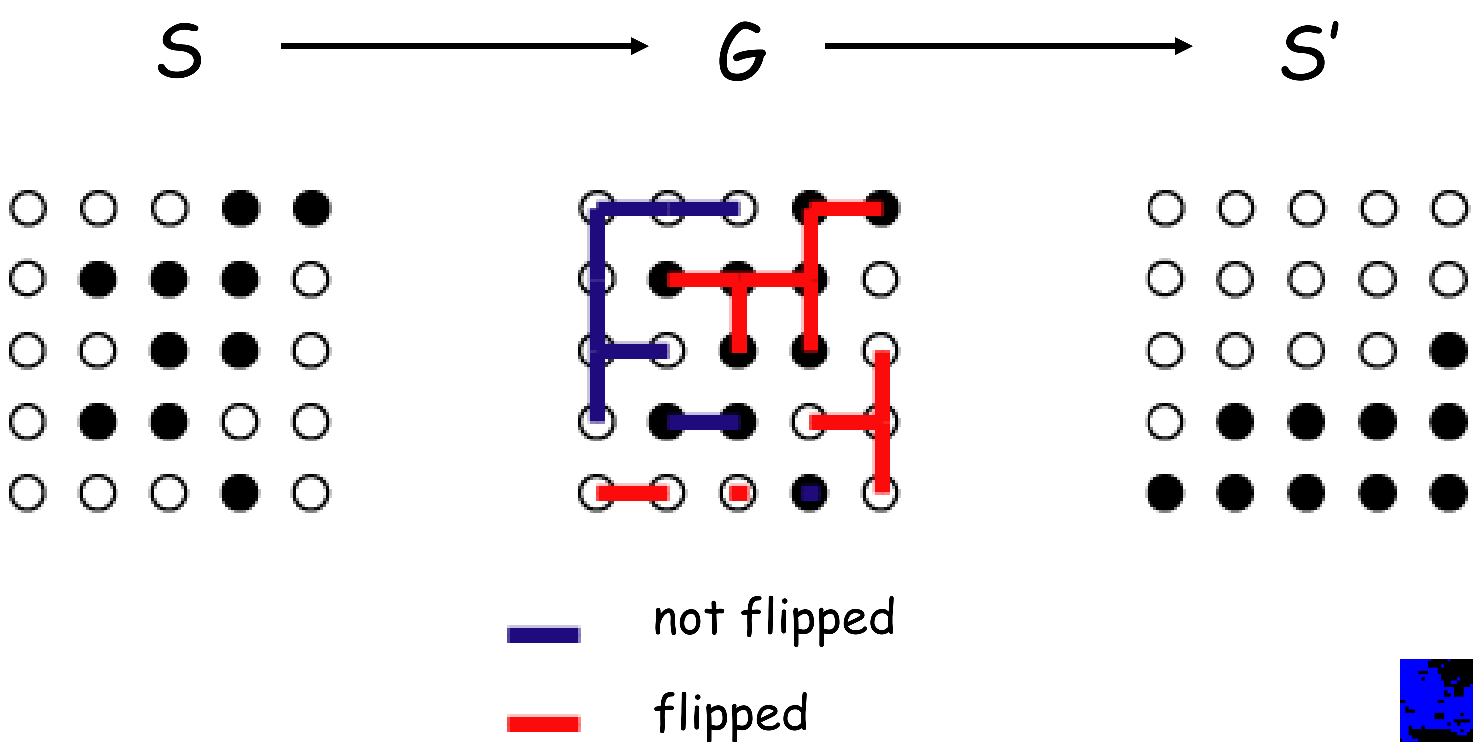
$$\tau \sim (T-Tc)^{\nu z}$$

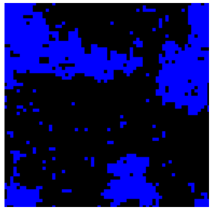
Monte Carlo steps for a magnetic domain undertake a substantial change (annihilation, creation, relocation, etc).



Swendsen-Wang Algorithm

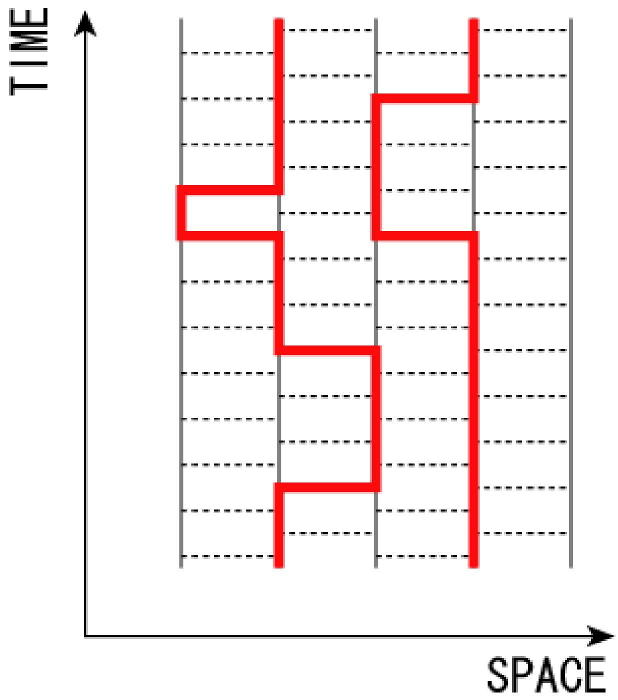
Swendsen-Wang 1987 ... Binding spins together to form a cluster.





Path-Integral Monte Carlo Method

Suzuki 1976



$$Z = \sum_S W(S)$$

$$W(S) = \prod_{p:\ \text{plaquette}} w(S_p)$$

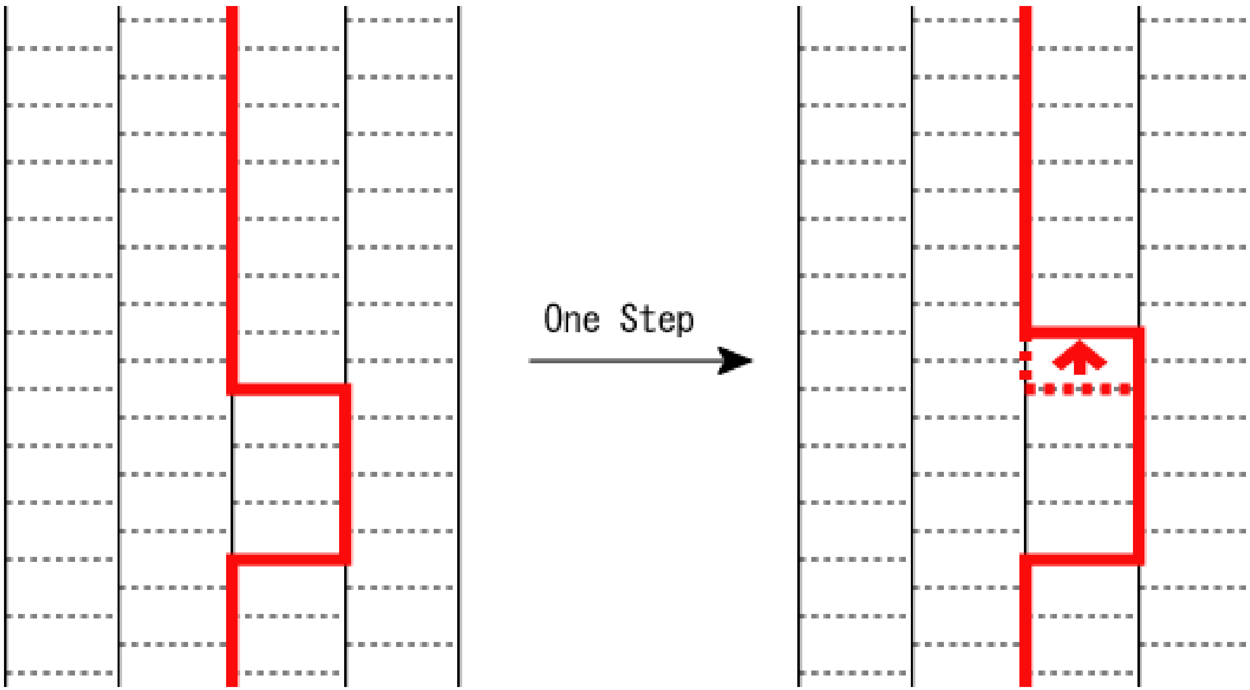
S: The whole pattern of world-lines

Interaction Vertex(“shaded plaquettes”)

World Line

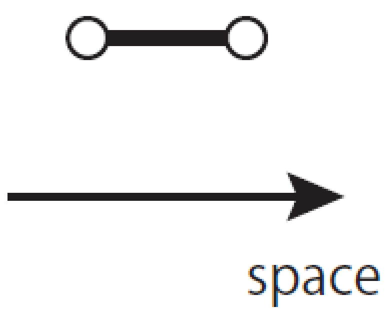
Method Used before 1993

The patterns are updated only locally.

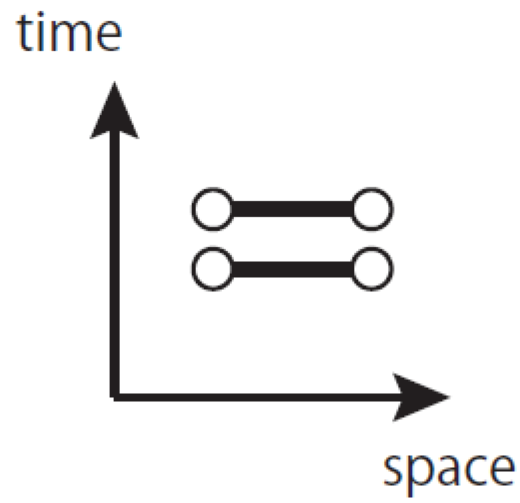


Many Problems --- No change in topological numbers, critical slowing down, high-precision slowing down, etc.

Generalizing SW algorithm to QMC

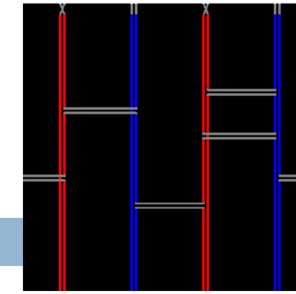


A "bond" in the Swendsen-Wang algorithm



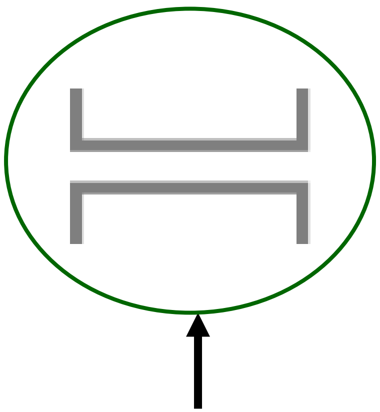
Loop elements in the loop algorithm for QMC

Loop Algorithm for QMC

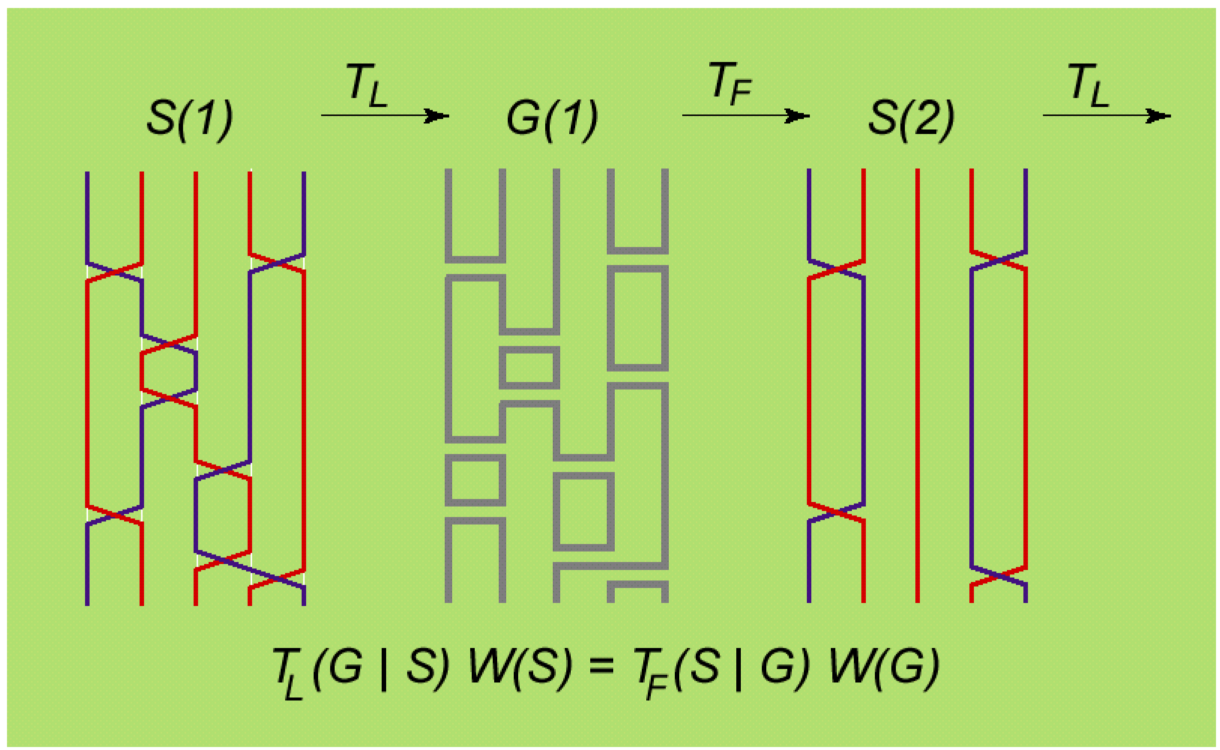


Evertz-Lana-Marcu 1993

Cluster Algorithm on Path-Integral Representation:

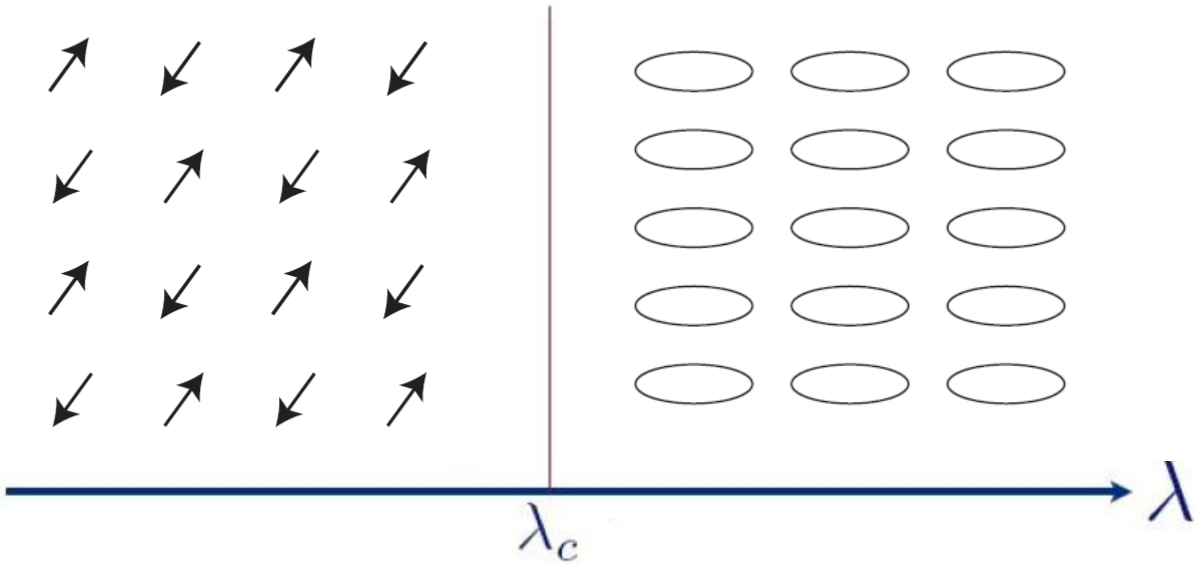


A graph element (for S=1/2 anti-ferromagnetic Heisenberg model)



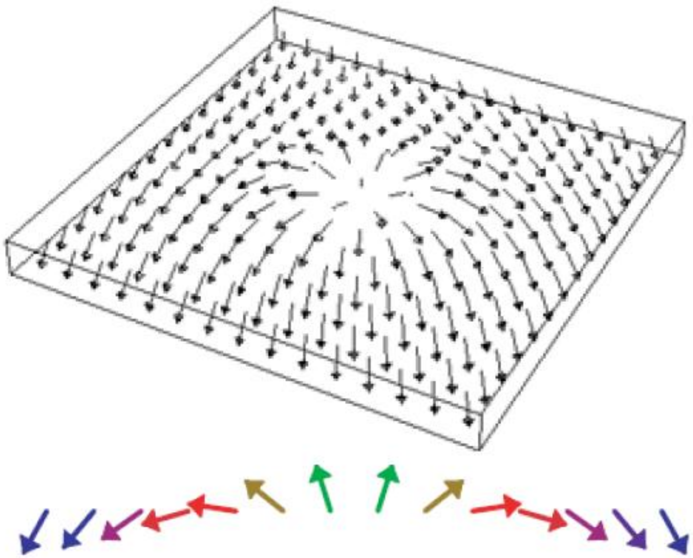
Magnetic/Non-Magnetic Transition

"Bond-alternation" enforces the transition to the VBS state.



$$H = J \sum_{\mathbf{x}=(x,y),\mu=x,y} S_{\mathbf{x}} \cdot S_{\mathbf{x}+e_\mu} + \lambda J \sum_{\mathbf{x}=(x,y),x:\text{odd}} \left(1+(-1)^x\right) S_{\mathbf{x}} \cdot S_{\mathbf{x}+e_x}$$

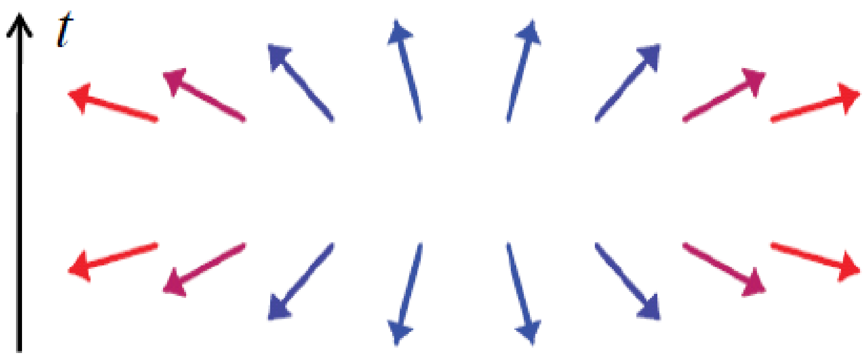
Conventional Transition



At the transition point, the Skyrmion number is not conserved.
Monopole ("hedgehog")
= The skyrmion-number-changing event .

Example: 2+1 D O(3) Wilson-Fisher f.p.

If the skyrmion number changes at some point of time...

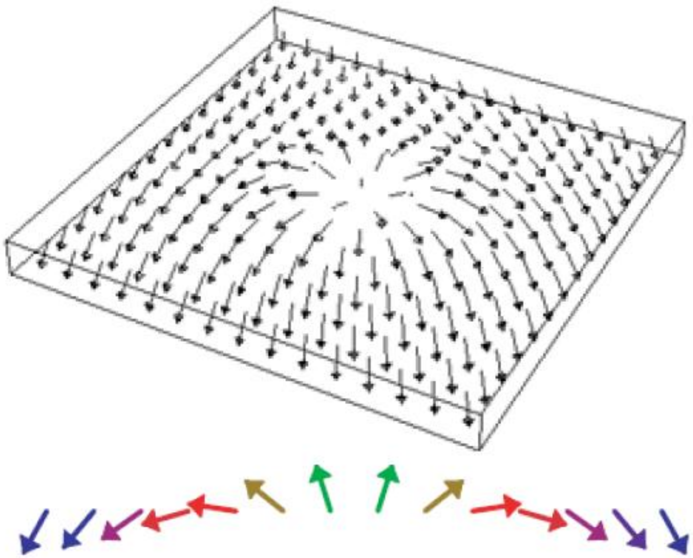


Skyrmion number:

$$Q = \frac{1}{4\pi} \int d^2\mathbf{x}\, \mathbf{n} \cdot \left(\partial_x \mathbf{n} \times \partial_y \mathbf{n} \right)$$

... there must be a singular point in space-time.

Deconfined Critical Phenomena

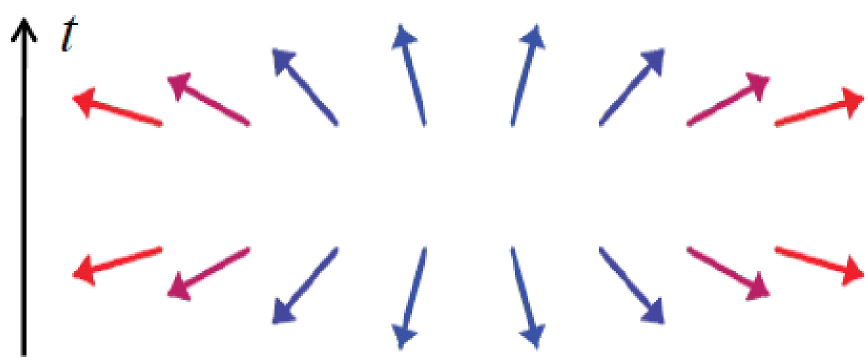


T. Senthil, et al, Science 303, 1490 (2004)

At the deconfined critical point, the skyrmion number is asymptotically conserved, and monopoles are prohibited.

Example: non-compact CP(1) model ?

If the skyrmion number changes at some point of time...



... there must be a singular point in space-time.

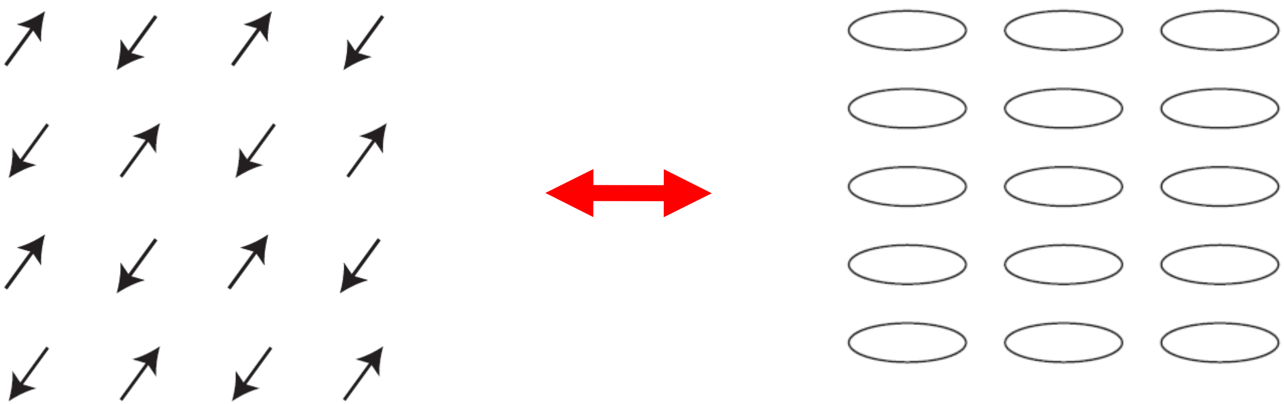
Skyrmion number:

$$Q = \frac{1}{4\pi} \int d^2\mathbf{x}\, \mathbf{n} \cdot \left(\partial_x \mathbf{n} \times \partial_y \mathbf{n} \right)$$

Symmetries Around DCP

We cannot say one phase has higher symmetry than the other.

Neel		VBS

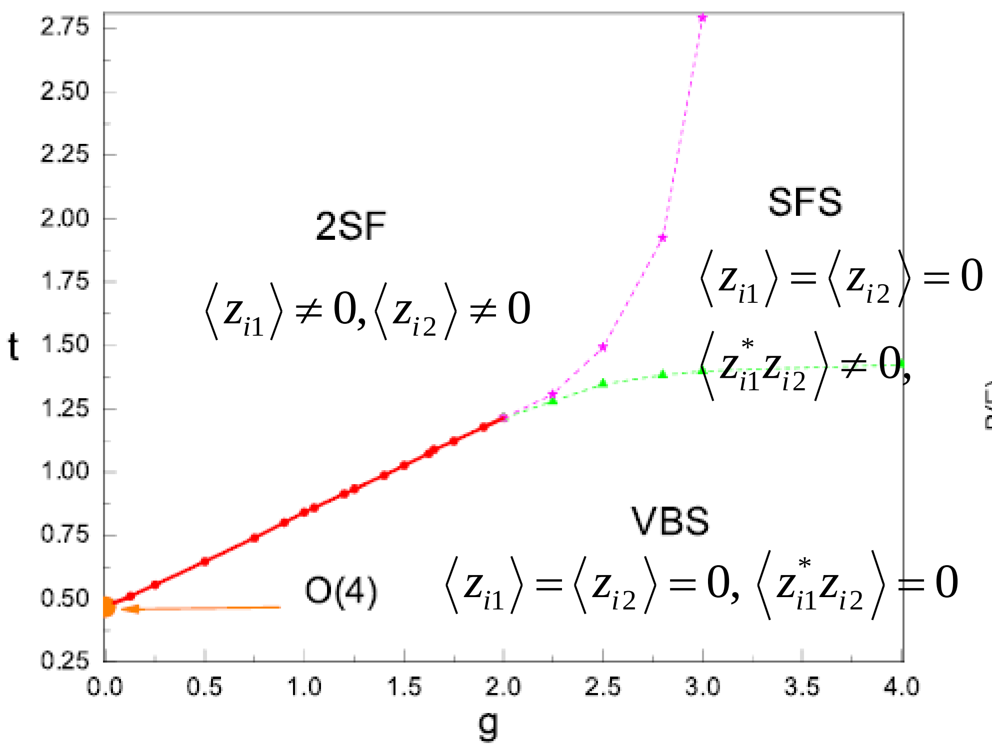


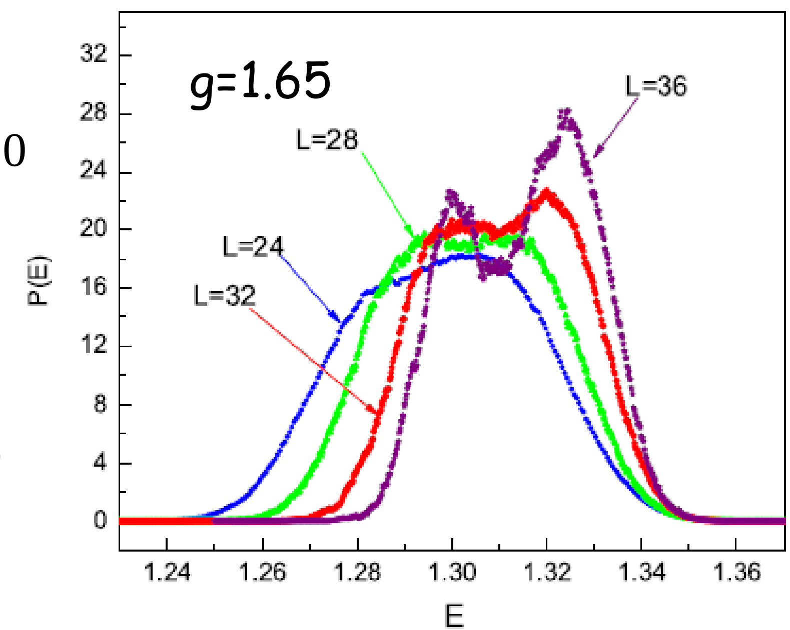
broken	Spin rotation symmetry	not broken
not broken	Lattice symmetry	broken

T. Senthil, et al., Science 303, 1490 (2004)

SU(2) Symmetric NCCP^1 Model

$$S = -t\sum_{(ij)}\sum_{\alpha=1,2}\left(z_{i\alpha}^{*} z_{j\alpha} e^{iA_{ij}} + \text{c.c.}\right) + \frac{1}{8g}\sum_{\square}(\nabla\times A)^2 \qquad \left(\sum_{\alpha=1,2}\left|z_{j\alpha}\right|^2 = 1\right)$$





Kuklov, Matsumoto, et al, PRL 101, 050405 (2008)

SU(N) Heisenberg Model

A general extension of the SU(2) anti-ferromagnetic Heisenberg model

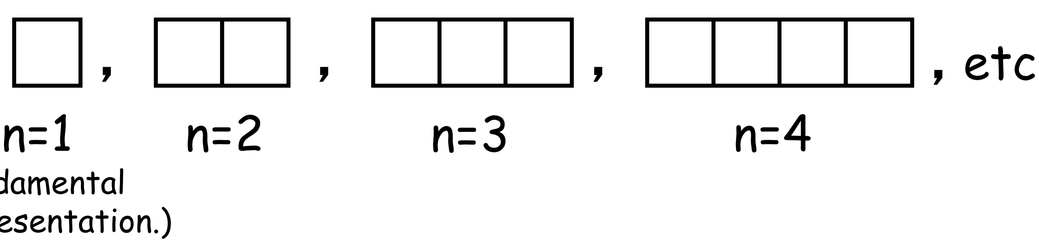
$$H = \frac{J}{N} \sum_{(r,r')} S_{\beta}^{\alpha}(r) \bar{S}_{\alpha}^{\beta}(r')$$

$S_{\beta}^{\alpha}(r) \cdots$ generators of SU(N) rotation represented by some representation R

$\bar{S}_{\beta}^{\alpha}(r) \cdots$ the same with the conjugate representation

$$\left[S_{\beta}^{\alpha}, S_{\delta}^{\gamma} \right] = \delta_{\delta}^{\alpha} S_{\beta}^{\gamma} - \delta_{\beta}^{\gamma} S_{\delta}^{\alpha} \qquad \alpha, \beta, \gamma, \delta = 1, 2, \cdots, N$$

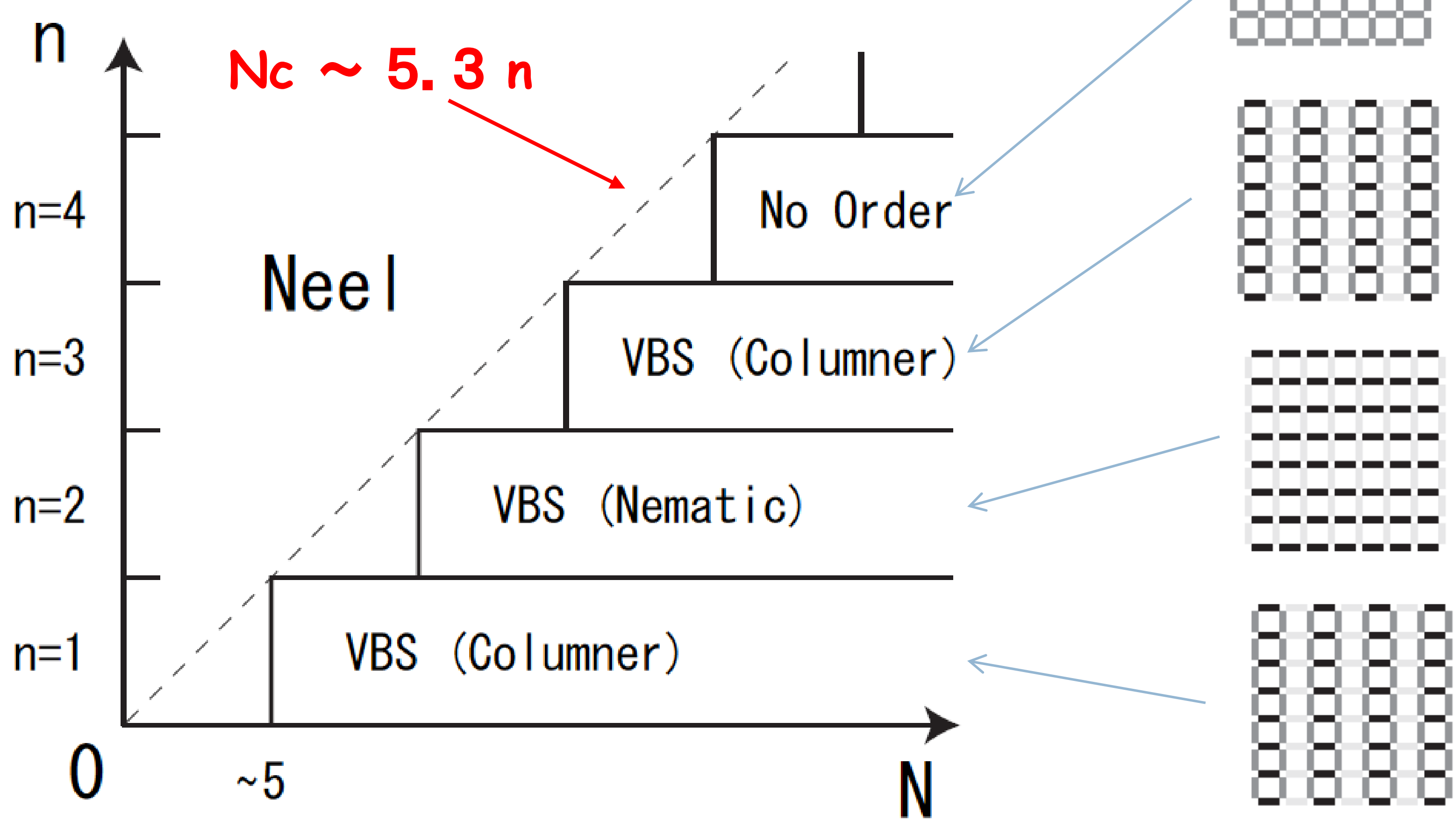
Representation:



2D Analogue of "Haldane" States

Prediction from 1/N expansion Arovas & Auerbach (1988)

Read & Sachdev (1989)



2D Isotropic Case (Tanabe, N.K.)

New challenge ---「京」

京 = 10^{16}

0.64 M cores

TOP500 SUPERCOMPUTER SITES

ISC events cloud computing

PROJECT | LISTS | STATISTICS | RESOURCES | NEWS

TOP 10 Systems - 06/2011

1	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect
2	Tianhe-1A - NUDT TH MPP, X5670 2.93Ghz 6C, NVIDIA GPU, FT-1000 8C
3	Jaguar - Cray XT5-HE Opteron 6-core 2.6 GHz
4	Nebulae - Dawning TC3600 Blade, Intel X5650, NVidia Tesla C2050 GPU
5	TSUBAME 2.0 - HP ProLiant SL390s G7 Xeon 6C X5670, Nvidia GPU, Linux/Windows
6	Cielo - Cray XE6 8-core 2.4 GHz

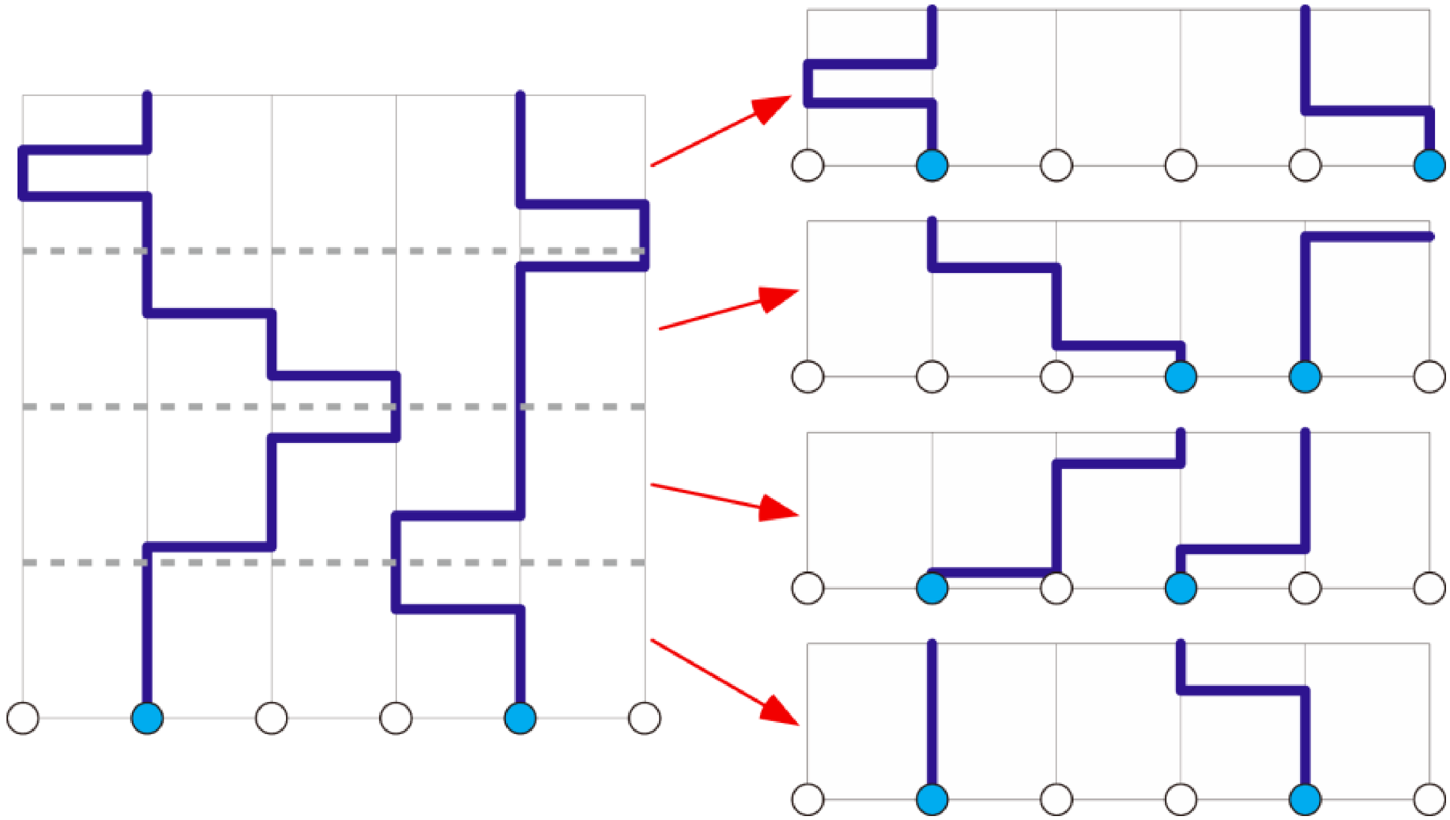
Japan Reclaims Top Ranking on Latest TOP500 List of World's Supercomputers

Thu, 2011-06-16 19:24

HAMBURG, Germany—A Japanese supercomputer capable of performing more than 8 quadrillion calculations per second (petaflop/s) is the new number one system in the world, putting Japan back in the top spot for the first time since the Earth Simulator was dethroned in November 2004, according the latest edition of the TOP500 List of the world's top supercomputers. The system, called the K Computer, is at the RIKEN Advanced Institute for Computational Science (AICS) in Kobe.

Parallelization of loop algorithm

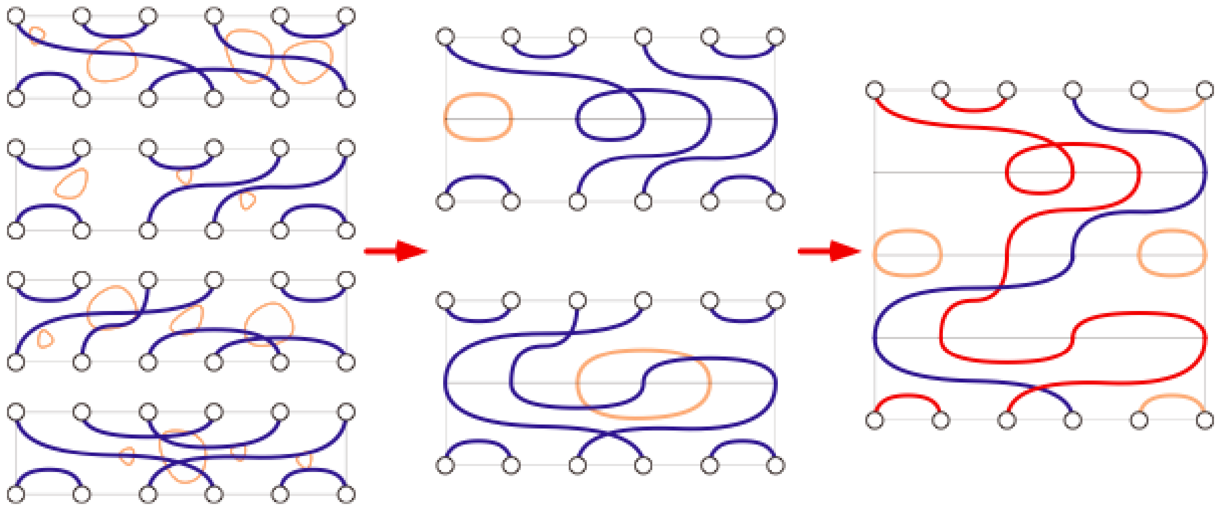
S. Todo & H. Matsuo



Parallelization of loop algorithm

S. Todo & H. Matsuo

Binary-tree algorithm for cluster identification

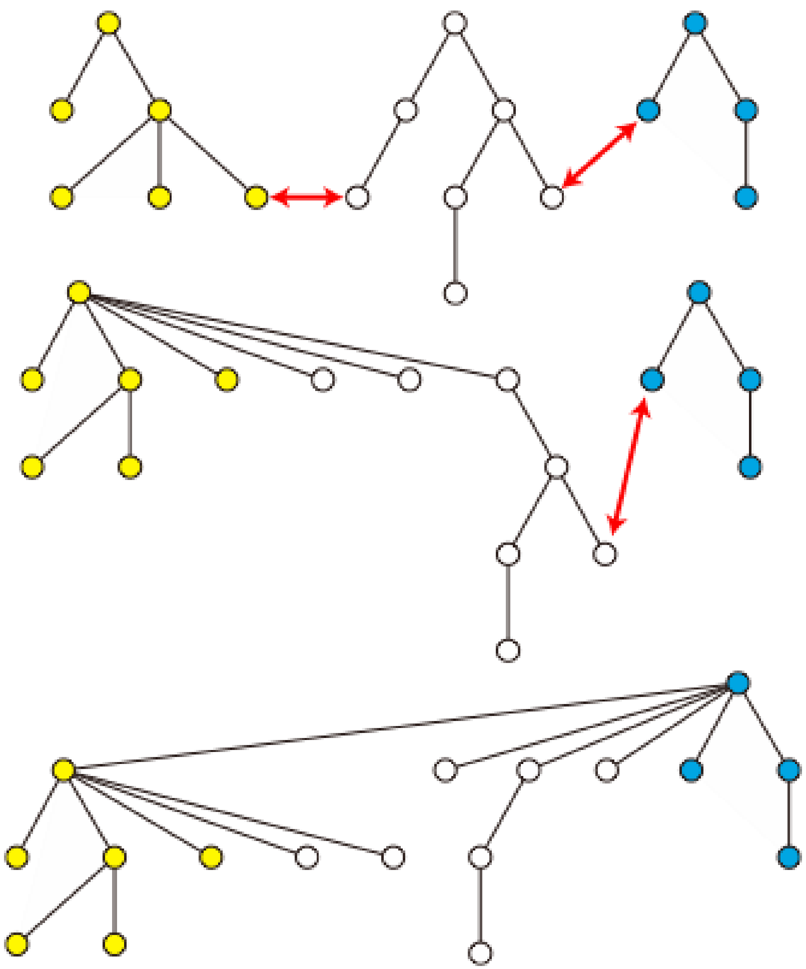


$$(N \log N_{\mathrm{p}})/(\frac{N\beta}{N_{\mathrm{p}}}) = N_{\mathrm{p}} \log N_{\mathrm{p}}/\beta$$

... Relative overhead is negligible at very low temperatures

Asynchronous lock-free union-find algorithm

S. Todo & H. Matsuo



(1) find root of each cluster/tree
(2) unify two clusters
(3) compress path to the new root

Locking whole clusters is no good.
(reduces parallelization efficiency)

Finding root and path compression are "thread-safe"

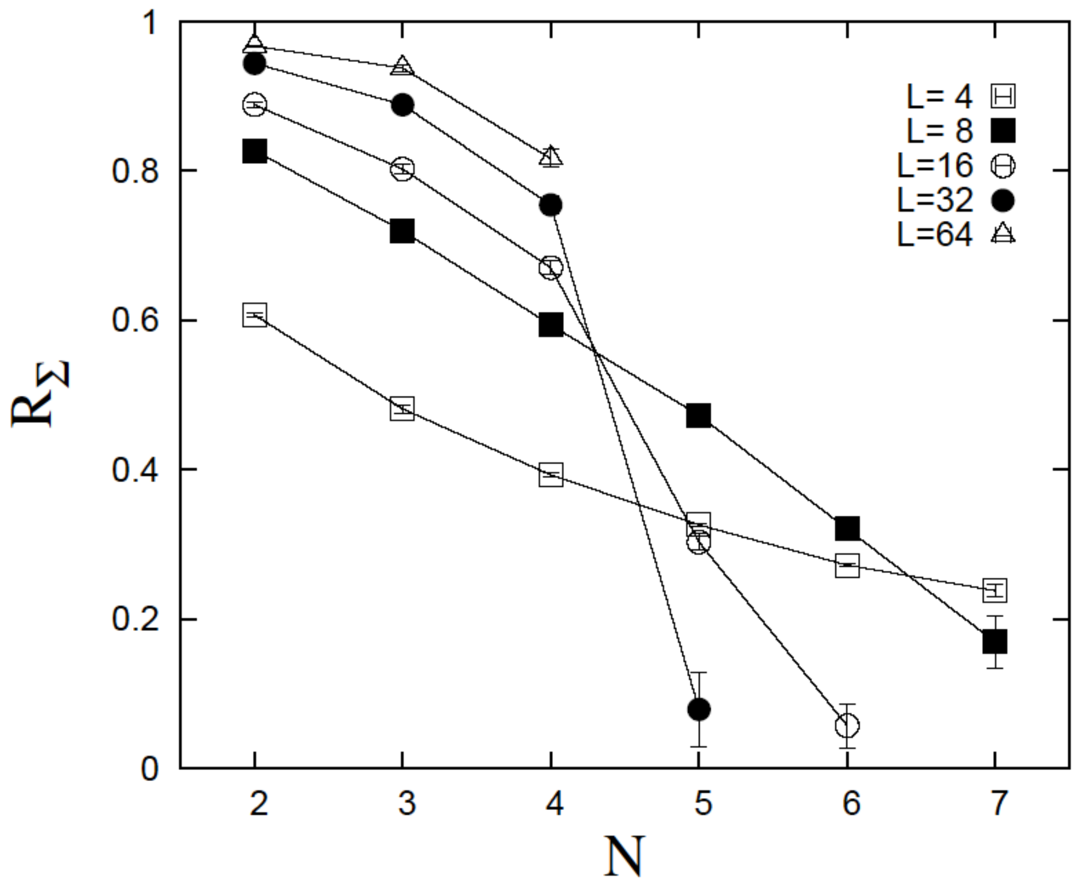
Lock-free unification can be achieved by using CAS (compare-and-swap) atomic operation

Fundamental Representation (n=1)

Tanabe & N.K.: PRL 98 057202 (2007)

$$M(\mathbf{R}) \equiv S_1^1(\mathbf{R}) - S_2^2(\mathbf{R})$$

$$R_M(L) \equiv \frac{C_M(L/2)}{C_M(L/4)} = \frac{\langle M(L/2)M(0)\rangle}{\langle M(L/4)M(0)\rangle}$$

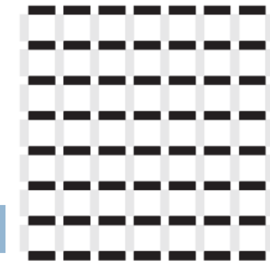


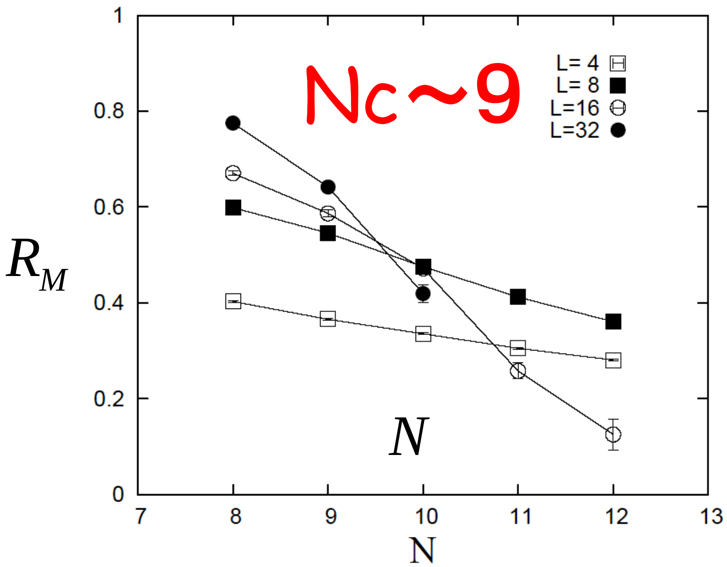
Neel order dissapears at N

4<Nc<5

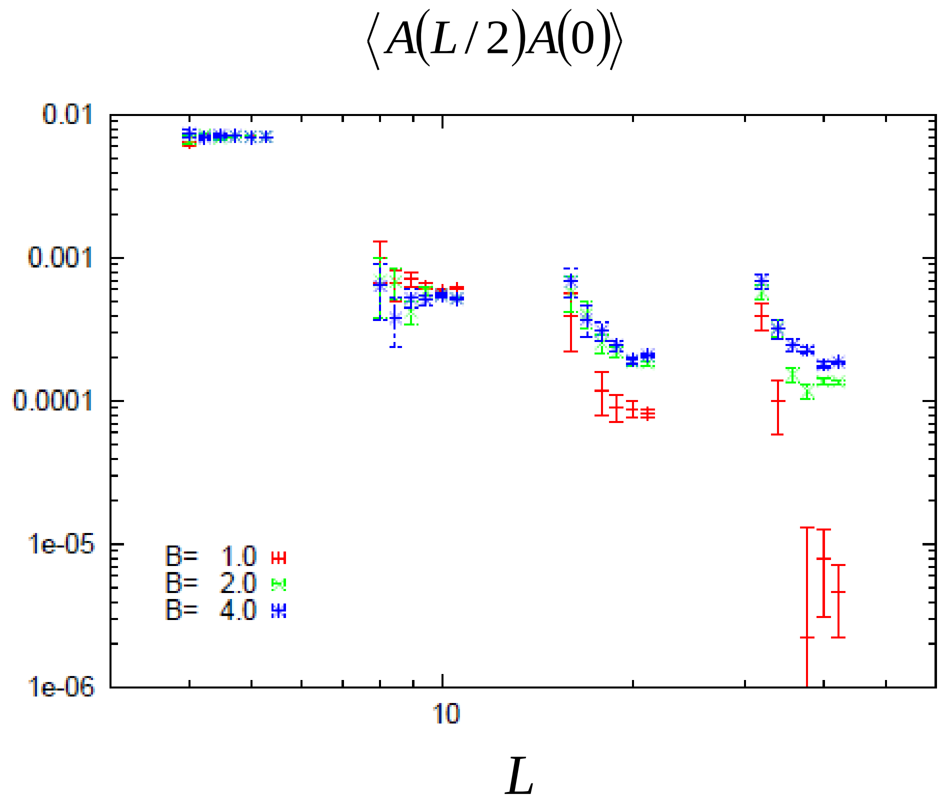
2D Isotropic Case (Tanabe, N.K.)

SU(N) Model (n=2)





$$\left(\begin{aligned} &A(\mathbf{R}) = V_x(\mathbf{R}) - V_y(\mathbf{R}); \\ &V_\mu(\mathbf{R}) \equiv \frac{1}{n_B^2} \sum_{\alpha=1}^{N} n_\alpha(\mathbf{R}) n_\alpha(\mathbf{R} + \mathbf{e}_\mu) \end{aligned}\right)$$



Very small but finite LRO is present.
Lattice rotation symmetry is broken.

2D Isotropic Case (Tanabe, N.K.)

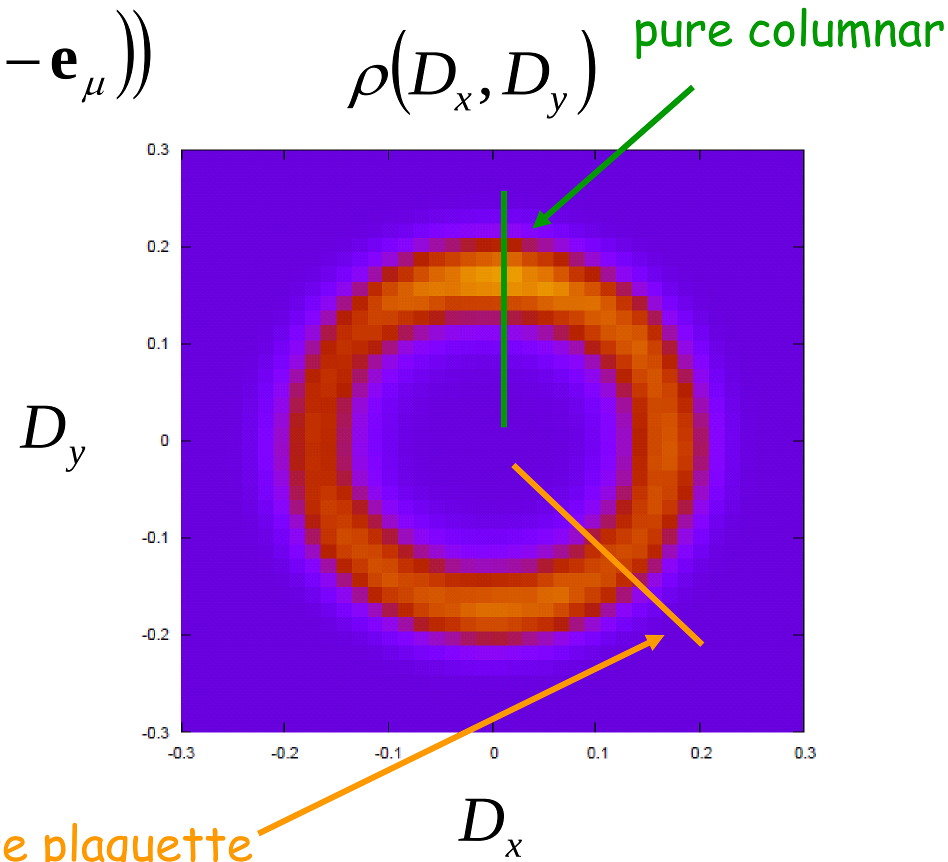
Ground-State Manifold is U(1) Symmetric

Tanabe & N.K.: PRL 98 057202 (2007)

$$D_\mu \equiv \frac{1}{V}\sum_{\mathbf{R}}\left(P\left(\mathbf{R},\mathbf{R}+\mathbf{e}_\mu\right)-P\left(\mathbf{R},\mathbf{R}-\mathbf{e}_\mu\right)\right)$$

$$\left(P\left(\mathbf{R},\mathbf{R}'\right)\equiv\sum_{\alpha=1}^{N}S_\alpha^\alpha\left(\mathbf{R}\right)S_\alpha^\alpha\left(\mathbf{R}'\right)\right)$$

$\rho\left(D_x, D_y\right)$



N=10, n=1, L=32, β=20

The system is asymptotically U(1) symmetric though the original microscopic model does not possess this symmetry.

... Reflection of the U(1) symmetry at DCP

Multi-spin Interactions

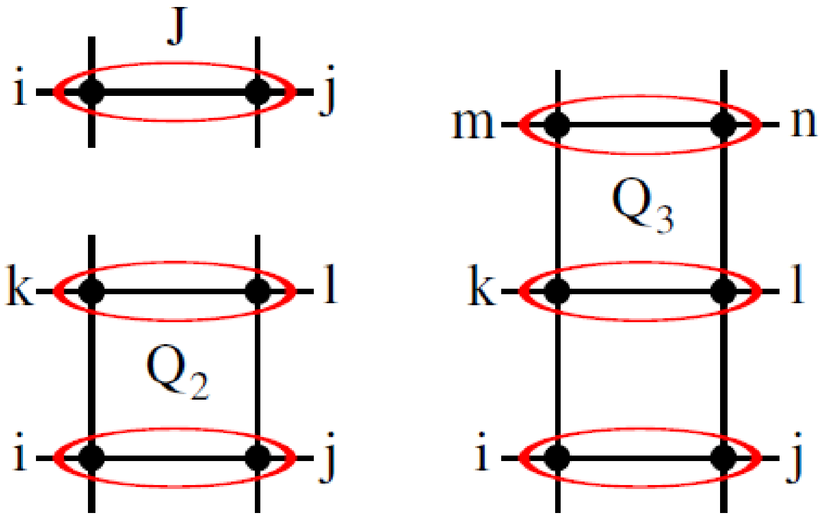
A. W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007)
J. Lou, A. Sandvik, N.K.: PRB 80, 180414R (2009)

$$H_1 = J\sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J\sum_{\langle ij \rangle} C_{ij} + \frac{L^2 J}{2}$$

$$C_{ij} = \frac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j$$

$$H_2 = -Q_2 \sum_{\langle ijkl \rangle} C_{kl} C_{ij}$$

$$H_3 = -Q_3 \sum_{\langle ijklmn \rangle} C_{mn} C_{kl} C_{ij}$$



2D JQ-Model (Lou, Sandvik, N.K.)

SU(2) J-Q Model

A. W. Sandvik, PRL98, 227202 (2007)

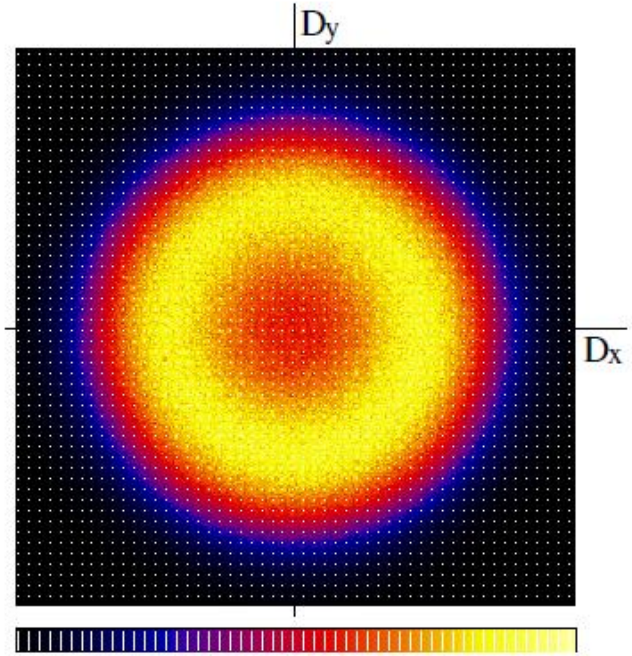


FIG. 5 (color online). Histogram of the dimer order parameter for an $L = 32$ system at $J/Q = 0$. The ring shape demonstrates an emergent $U(1)$ symmetry, i.e., irrelevance of the Z_4 anisotropy of the VBS order parameter.

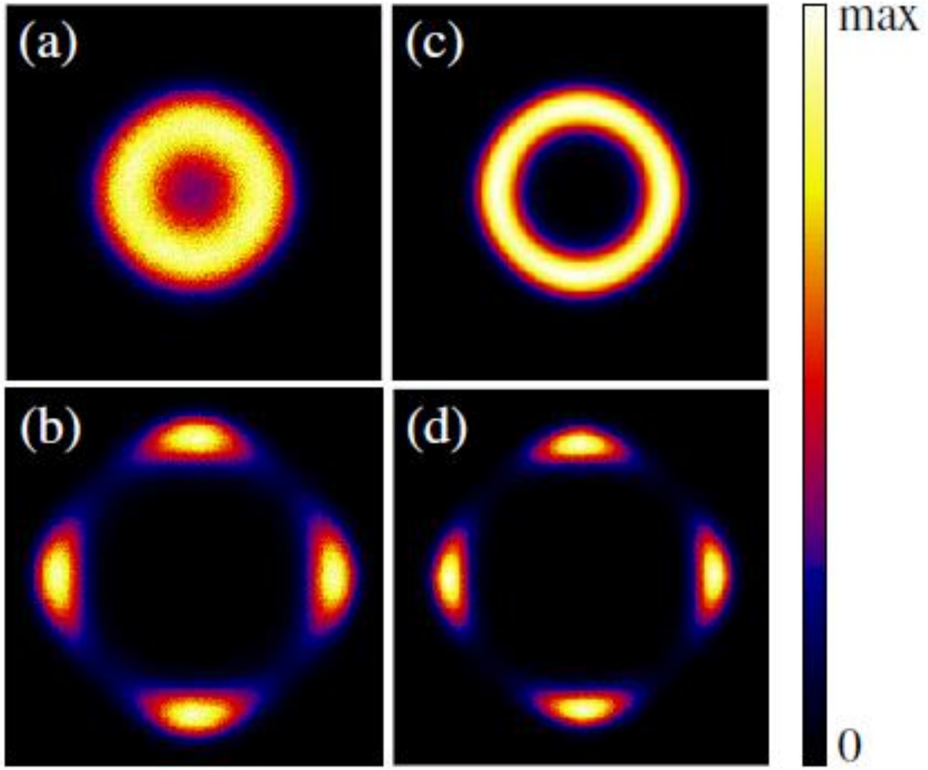
U(1) Nature is confirmed near the critical point. (Slightly on the dimer order side.)

VBS - VBS Crossover

SU(2) J-Q3 SU(3) J-Q2

Small Q

Large Q



J. Lou, A. Sandvik, N.K (2009)

Scaling Properties of Anisotropy

J. Lou, A. Sandvik, N.K. (2009)

$$D_4^2 \equiv \int dD_x dD_y \; P(D_x, D_y) \times (D_x^2 + D_y^2) \cos(4\theta)$$

$$D_4^2 = L^{-(1+\eta_d)} F_4(q L^{1/a_4 \nu})$$

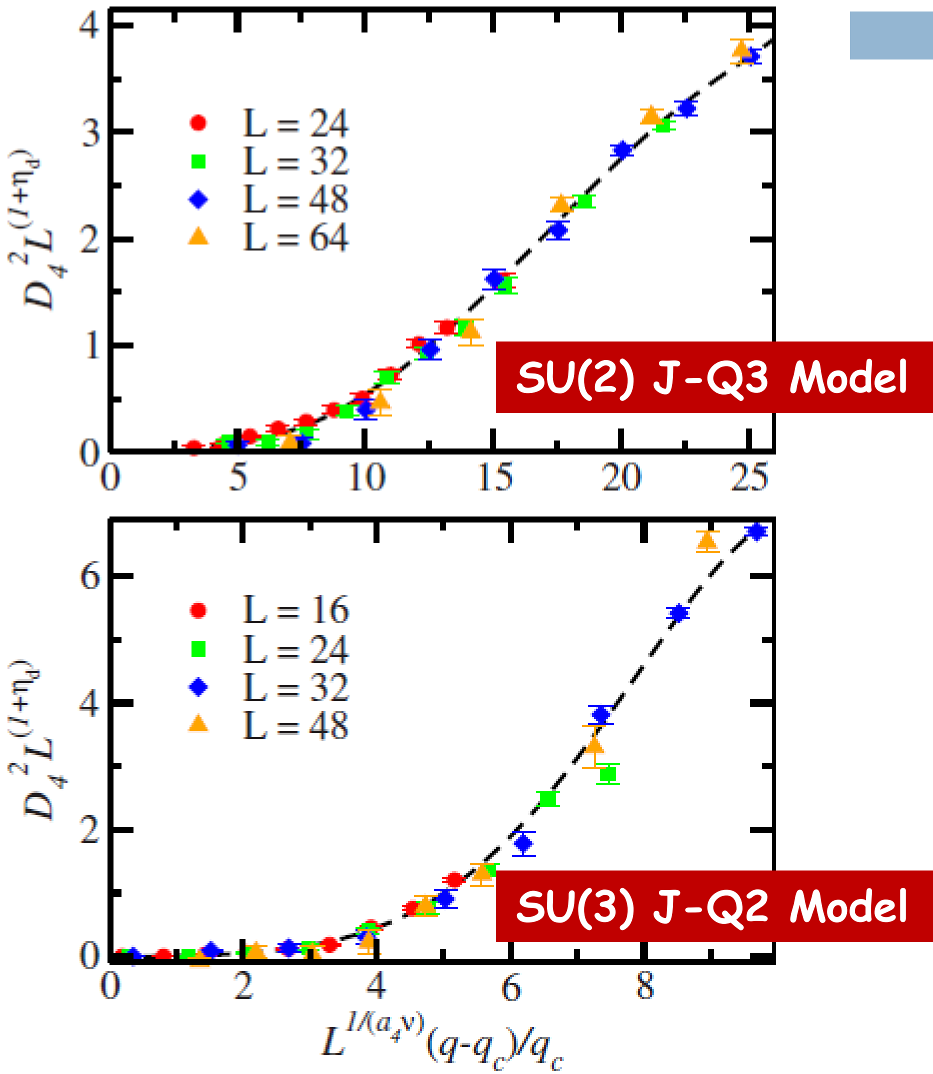
CF: J. Lou, A. W. Sandvik, and L. Balents, PRL (2007).

SU(2) J-Q3

$$\eta_d = 0.20(2), \;\; \nu = 0.69(2), \;\; a_4 = 1.20(5)$$

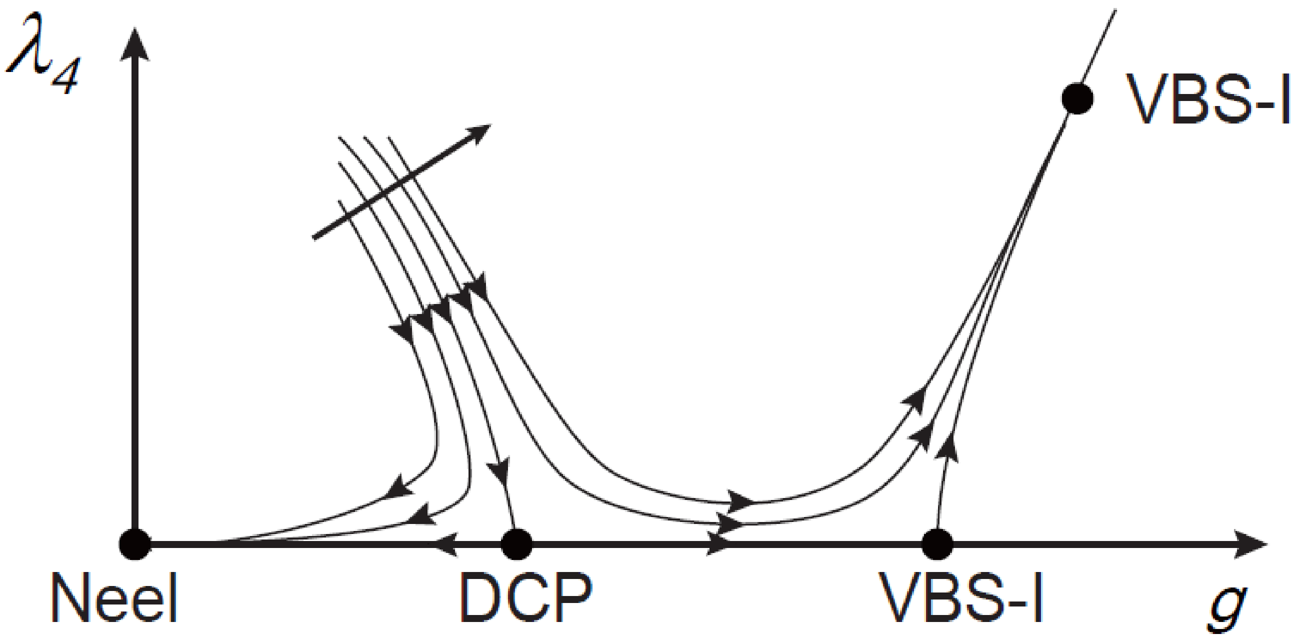
SU(3) J-Q2

$$\eta_d = 0.42(3), \;\; \nu = 0.65(3), \;\; a_4 = 1.6(2)$$



2D JQ-Model (Lou, Sandvik, N.K.)

Recovery of Discreteness



The exponent nu on the VBS side may be affected by the additional fixed point and can be differ from the Neel side.

J—Q Model

Jie Lou, A. Sandvik and N.K.:
Phys. Rev. B **80**, 180414 (2009)

$$H = H_1 + H_2 + H_3$$

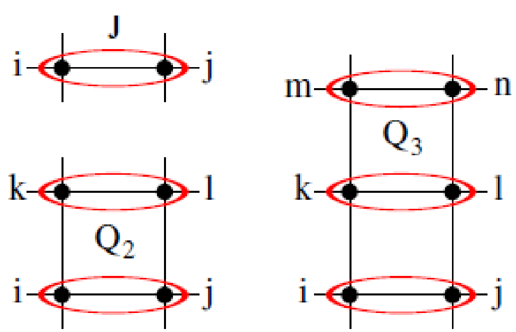
$$H_1 = -J \sum_{(ij)} C_{ij},$$

$$H_2 = -Q_2 \sum_{(ijkl)} C_{ij} C_{kl},$$

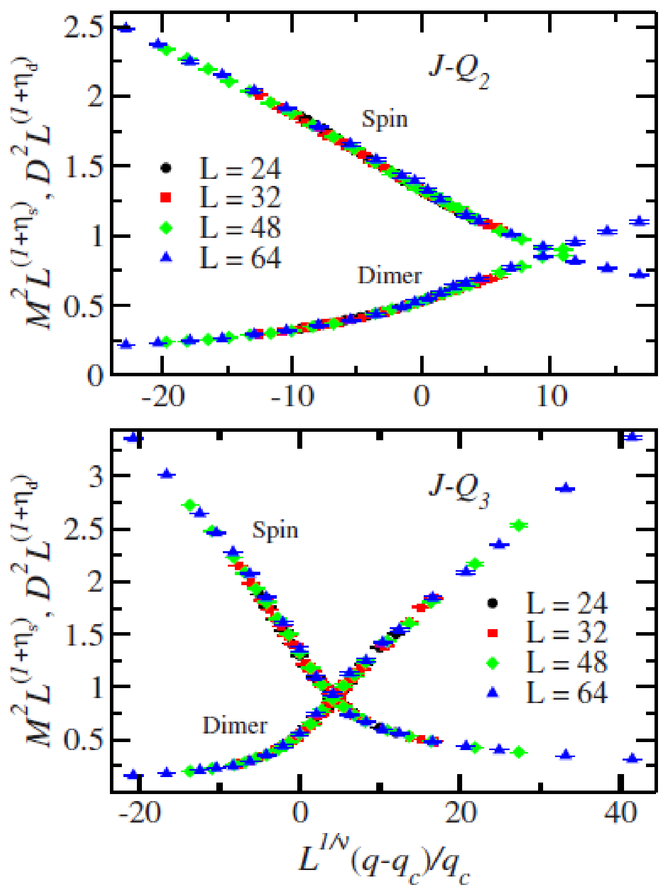
$$H_3 = -Q_3 \sum_{(ijklmn)} C_{ij} C_{kl} C_{mn}$$

$$C_{ij} = -\sum_{\alpha,\beta} \mathcal{J}_i^{\alpha\beta} \mathcal{J}_j^{\beta\alpha}$$

$$\left(= \frac{1}{4} - \boldsymbol{S}_i \cdot \boldsymbol{S}_j \quad (\text{for } N = 2, n = 1) \right)$$



SU(2) J-Q Model



Continuous Transition is suggested.

SU(3) and SU(4) J-Q2 Models

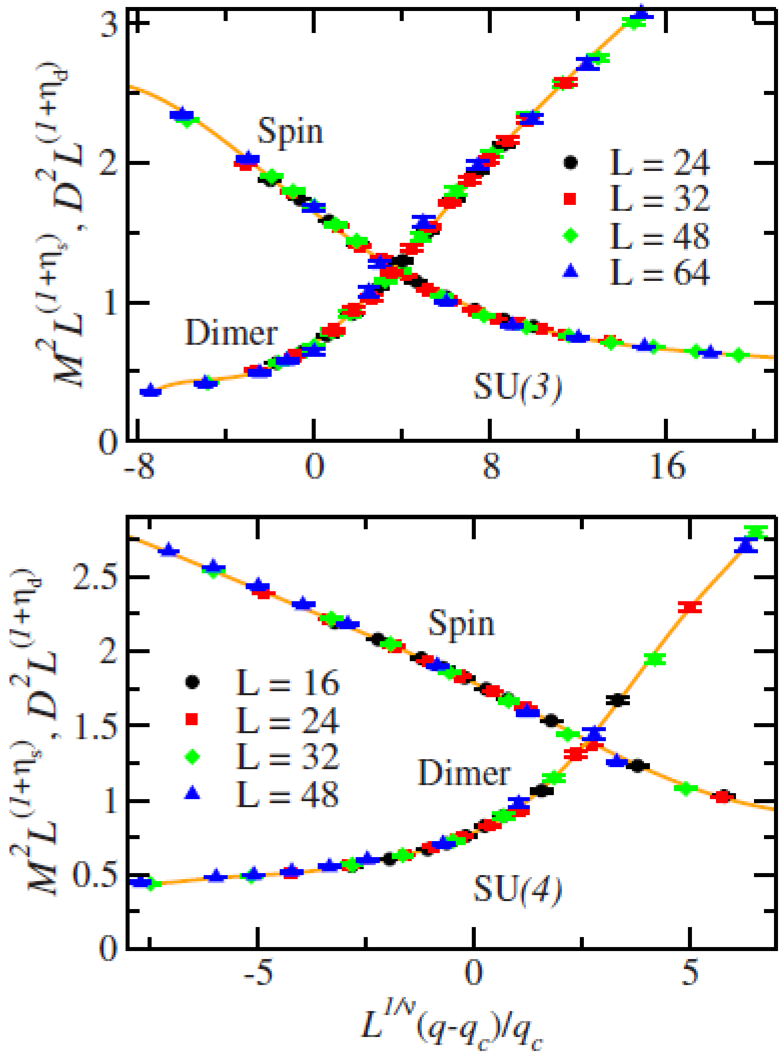
SU(3) J-Q2

$$\eta_s = 0.38(3), \quad \nu = 0.65(3)$$

SU(4) J-Q2

$$\eta_s = 0.42(5), \quad \nu = 0.70(2)$$

Jie Lou, A. Sandvik and N.K.:
Phys. Rev. B **80**, 180414 (2009)



Universality?

J. Lou, A. Sandvik, N.K.: PRB 80, 180414R (2009)

Model, symmetry	η_s	η_d	ν	a_4
J-Q_2, SU(2)	0.35(2)	0.20(2)	0.67(1)	
J-Q_3, SU(2)	0.33(2)	0.20(2)	0.69(2)	1.20(5)
J-Q_2, SU(3)	0.38(3)	0.42(3)	0.65(3)	1.6(2)
J-Q_2, SU(4)	0.42(5)	0.64(5)	0.70(2)	1.5(2)

For $N >> 1,\ \eta_s = 1.$

T. Senthil, et al, Science 303, 1490 (2004)
M. Levin and T. Senthil, Phys. Rev. B 70, 220403R (2004).

For $N >> 1,\ \eta_d \propto N.$

CP^{N-1} Field Theory:
M. A. Metlitski, et al, PRB 78, 214418 (2008);
G. Murthy and S. Sachdev, Nucl. Phys. B 344, 557 (1990).

2D JQ-Model (Lou, Sandvik, N.K.)

Scaling Dimension (CP^{N-1} Model)

Murthy and Sachdev, Nucl. Phys. B 344 557 (1990)
Metlitski, et al, PRB78 214418 (2008)

$$L = \left|D_\mu z\right|^2 + i\lambda\left(\left|z\right|^2 - \frac{1}{g}\right)$$

$$D_\mu \equiv \partial_\mu - iA_\mu$$

A_μ : $U(1)$ gauge field

$\Delta_q = (\text{monopole scaling dimension})$

A_μ is non-compact

$\leftrightarrow$ conservation of the gauge current

$$J_\mu^G = \varepsilon_{\mu\nu\lambda}\partial_\mu A_\lambda$$

$\leftrightarrow$ absense of monopoles

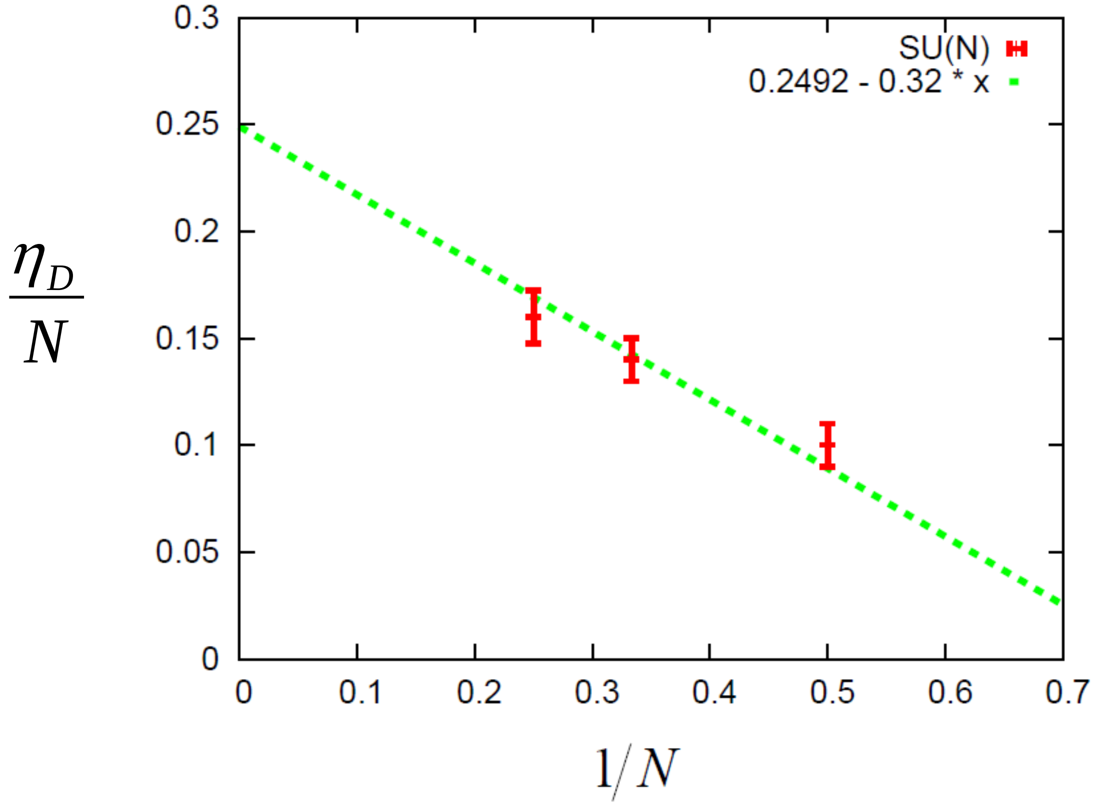
$$\left\langle D(R)D(0)\right\rangle = \left\langle \Psi_{\mathrm{VBS}}(R)\Psi_{\mathrm{VBS}}(0)\right\rangle = \left\langle v^+(R)v(0)\right\rangle \propto \frac{1}{R^{2\Delta_1}}$$

$$\lim_{N\to\infty}\frac{1+\eta_D}{N} = \frac{2\Delta_1}{N} \approx 0.2492 \quad \left(\rho_1 = \frac{\Delta_1}{2N} = 0.062296\cdots(\text{Murthy \& Sachdev})\right)$$

Monopole Scaling Dimension up to O(N^{-1})

$$\frac{\eta_D}{N} = \frac{2\Delta_1 - 1}{N} = 0.2492 - 0.32\frac{1}{N} + O\left(\frac{1}{N^2}\right)$$

Jie Lou, A. Sandvik and N.K.: Phys. Rev. B **80**, 180414 (2009)

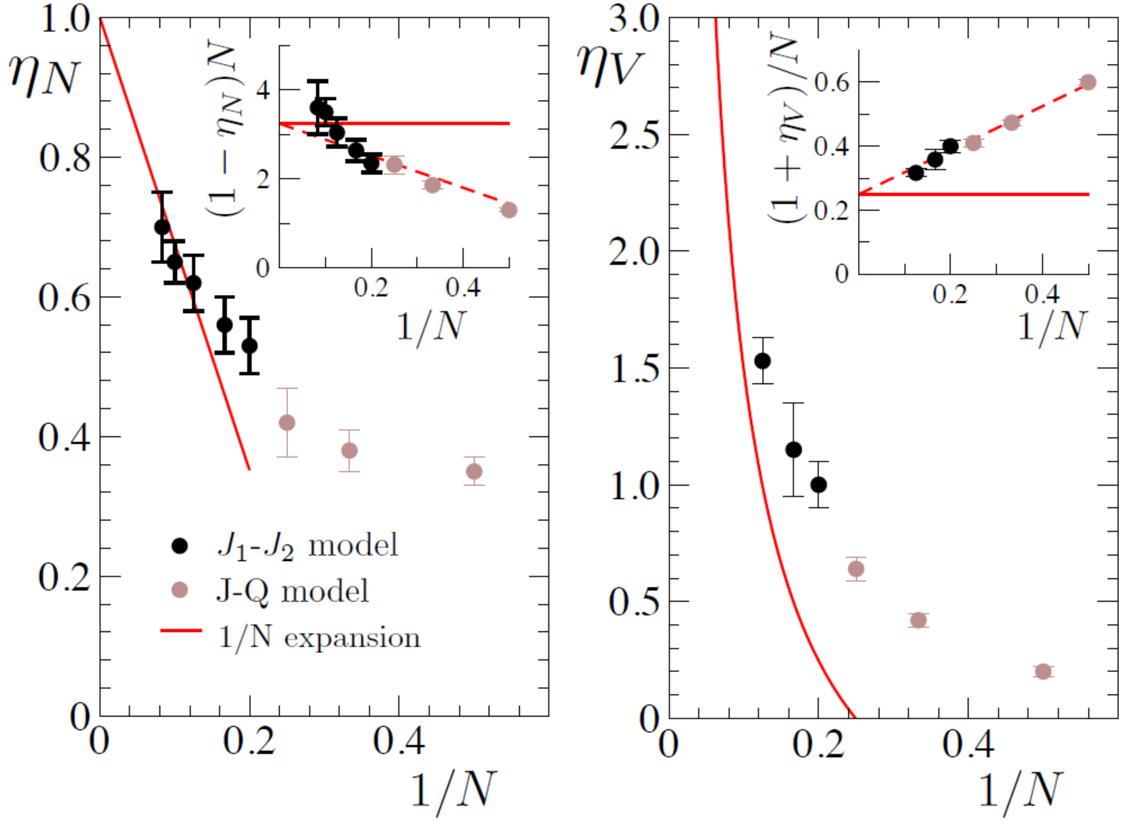


2D JQ-Model (Lou, Sandvik, N.K.)

Recent Refinement by Kaul & Sandvik

R. Kaul and A. Sandvik, arXiv:1110.4130v1

$$\eta_N = 1 - 32/(\pi^2 N), \qquad 1 + \eta_V = 2\delta_1 N$$



Quantum Spin System

Yip (PRL 90 (2003) 250402):

$$H = -t \sum_{(ij)} \sum_{\sigma,\sigma'=-1,0,1} \left(b_{i\sigma}{}^{+} b_{j\sigma'} + b_{j\sigma'}{}^{+} b_{i\sigma} \right) + [\text{on-site Coulomb repulsion}]$$

Effective Hamiltonian to the 2nd order in t

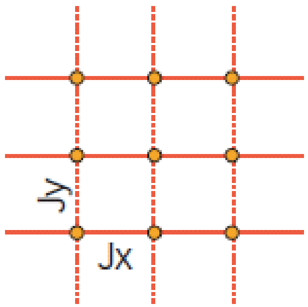
$$H = \sum_{(ij)} \left\{ J_L (\mathbf{S}_i \cdot \mathbf{S}_j) + J_Q (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \right\} + \text{const}$$

$$J_L = -\frac{2t^2}{U_2} \quad , \quad J_Q = -\frac{2}{3}\frac{t^2}{U_2} - \frac{4}{3}\frac{t^2}{U_0}$$

$$U_S = [\text{the on-site repulsion when the total spin is } S]$$

^{23}Na: $0 < U_0 < U_2$ $(J_Q < J_L < 0)$

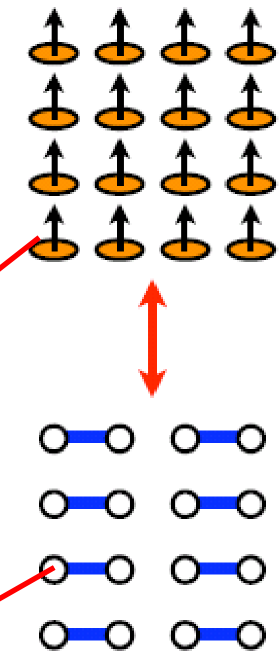
Bilinear-Biquadratic Model in 2D with strong spatial anisotropy (Phase Diagram)



Two-dimensional lattice

Anisotropy parameter

$$\lambda \equiv J_y / J_x \quad (J_y < J_x)$$

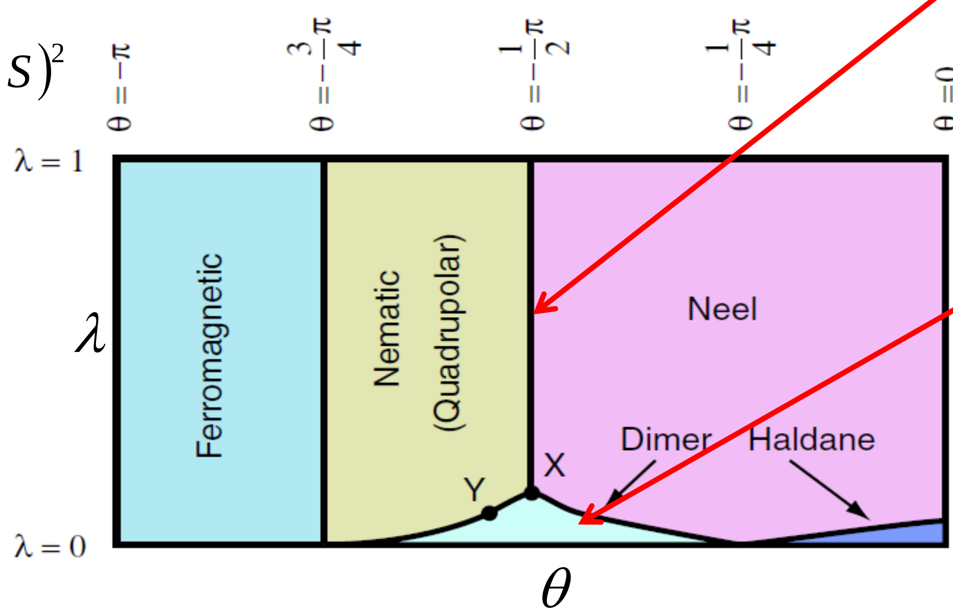


$$H = J_L^{\mu}(S \cdot S) + J_Q^{\mu}(S \cdot S)^2$$

$$(\mu = x, y)$$

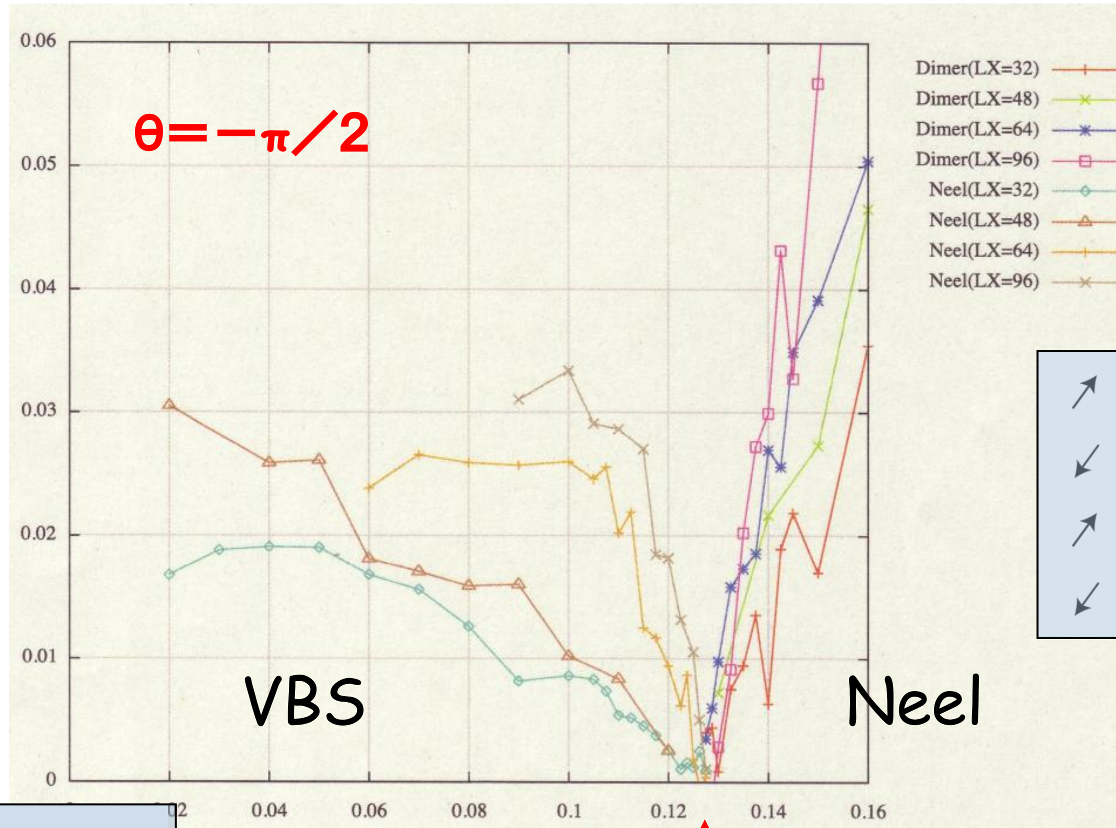
$$J_L^{\mu} = -J^{\mu} \cos\theta$$

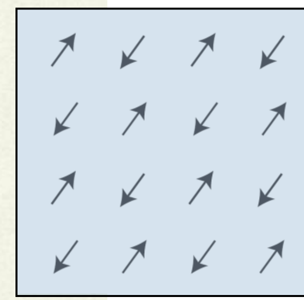
$$J_Q^{\mu} = -J^{\mu} \sin\theta$$

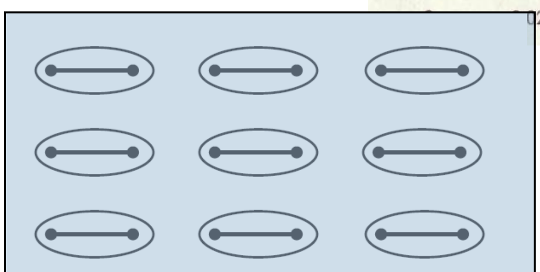


Diversing Correlation Lengths

$$\frac{1}{\xi_{spin}}, \frac{1}{\xi_{VBS}}$$



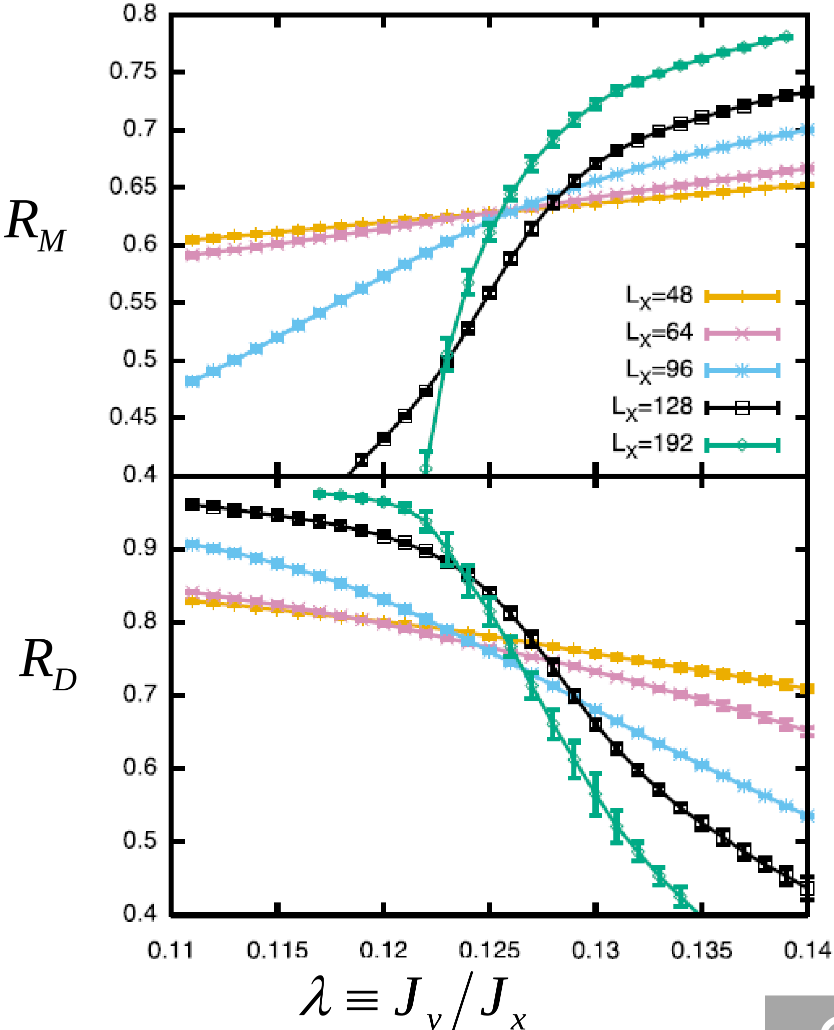




J_y / J_x

2 correlation length diverges at the same point.

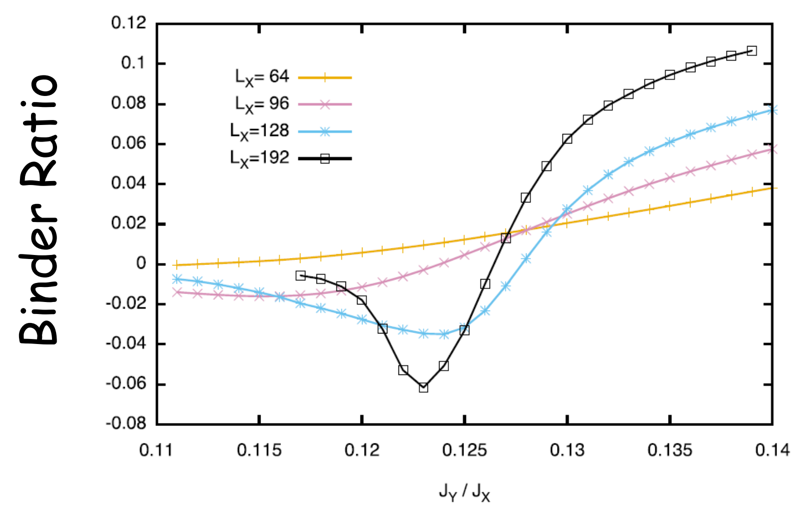
θ=−0. 5π (SU(3) symmetric)



A single transition is likely...

$$\lambda_c = 0.125(5)$$

Cannot obtain a reliable finite-size scaling plot.



Quasi-1D SU(N) (Harada, Troyer, N.K.)

Conclusion

(1) Isotropic SU(N) Heisenberg Model

- ✔ VBS Ground State
- ✔ Proximity to DCP critical phenomena

(2) Multi-Spin Interactions (J-Q Models)

- ✔ Consistent with DCP
- ✔ η_d proportional to N (The correction term is estimated)

(3) Quasi-1D SU(3) and SU(4) Models

- ✔ Direct transition is likely
- ✔ Still not clear if the transition is of the 2nd order

(We need bigger machines, and a better strategy.)