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2253-10

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

24 - 29 July 2011

Monte Carlo Simulations on Deconfined Critical Phenomena

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ICTP Workshop

MONTE CARLO SIMULATIONS ON DECONFINED CRITICAL PHENOMENA

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ISSP

July 25, 2011 ICTP, Trieste

Collaborators

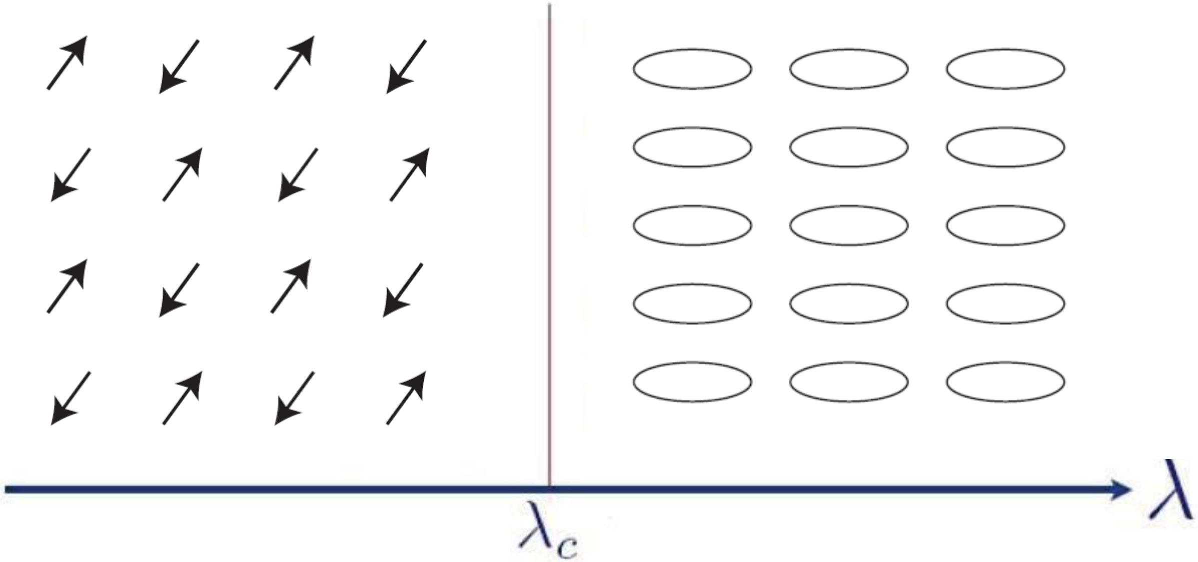
Kanji HARADA (Kyoto)
Jie LOU (ISSP)
Anders SANDVIK (BU)

京 ("Kei") collaboration:

ISSP: Lou, Watanabe, Masaki, Kawashima,
Tokyo: Todo, Matsuo,
Hyogo: Suzuki
Kyoto: Harada

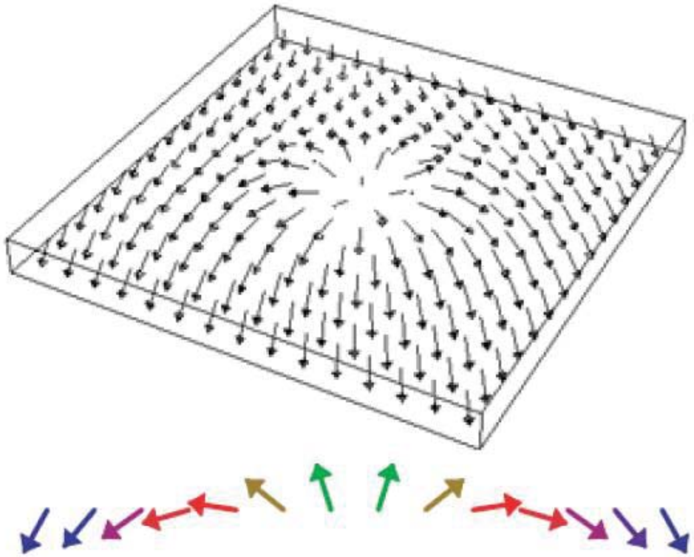
Magnetic/Non-Magnetic Transition

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



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

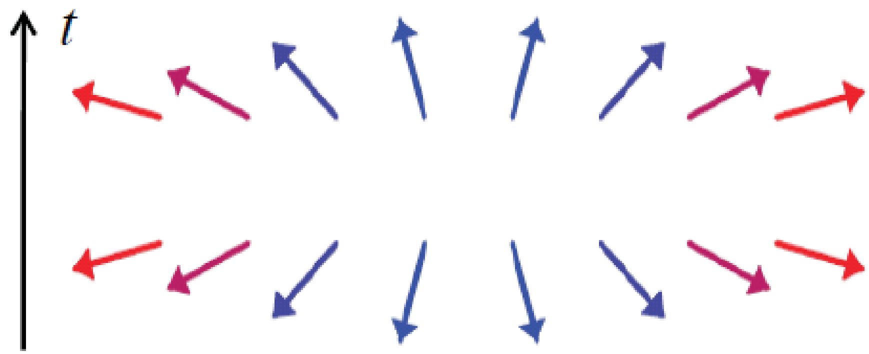
Conventional Transition



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...

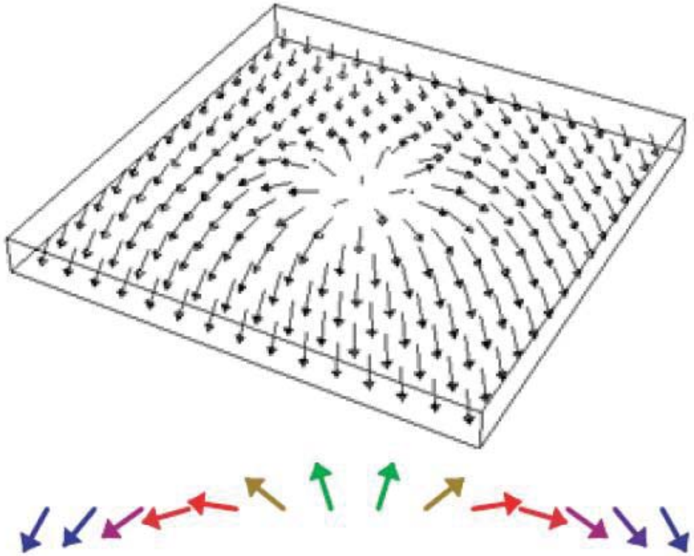


... there must be a singular point in space-time.

Skyrmion number:

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

Deconfined Critical Phenomena

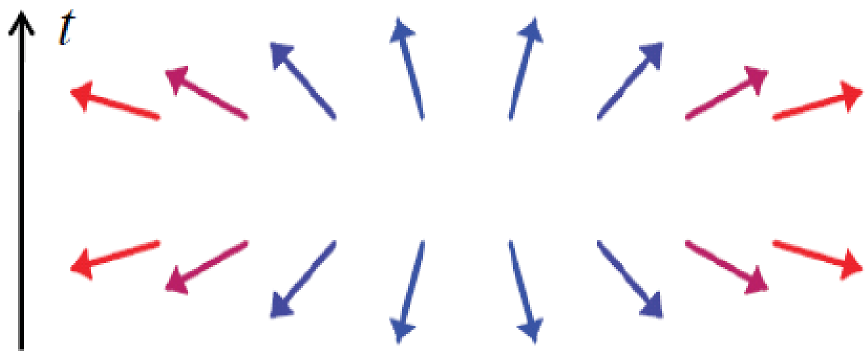


T. Senthil, et al, Science 303, 1490 (2004)

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.

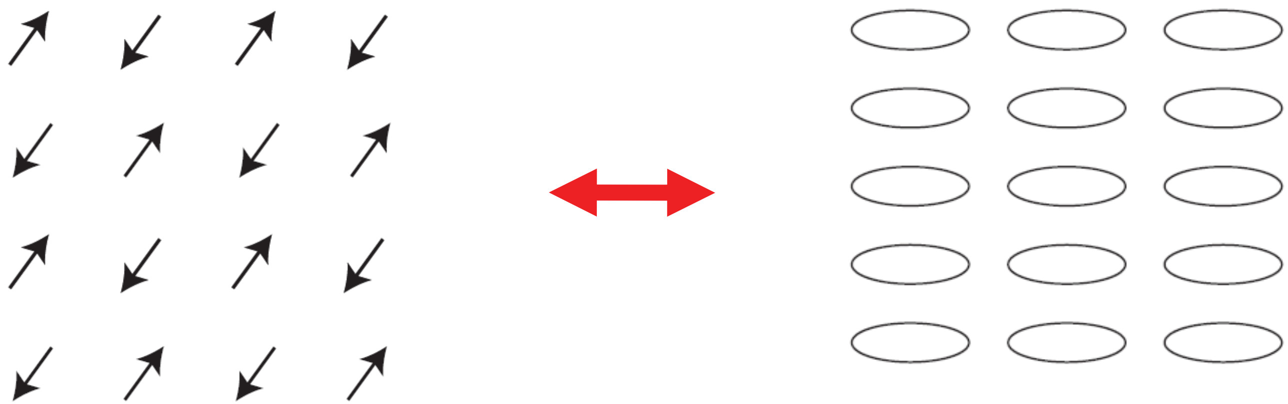
Skyrmion number:

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

Symmetries Around DCP

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

Neel | **VBS**



Neel		VBS
broken	Spin rotation symmetry	not broken
not broken	Lattice symmetry	broken

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

SU(N) Heisenberg Model

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

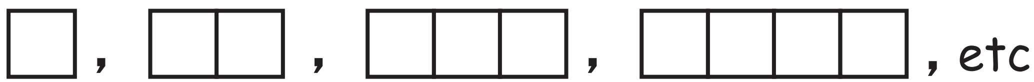
$$H = \frac{J}{N} \sum_{(r,r')} S_\beta^\alpha(r) \bar{S}_\alpha^\beta(r')$$

$S_\beta^\alpha(r) \cdots$ 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:

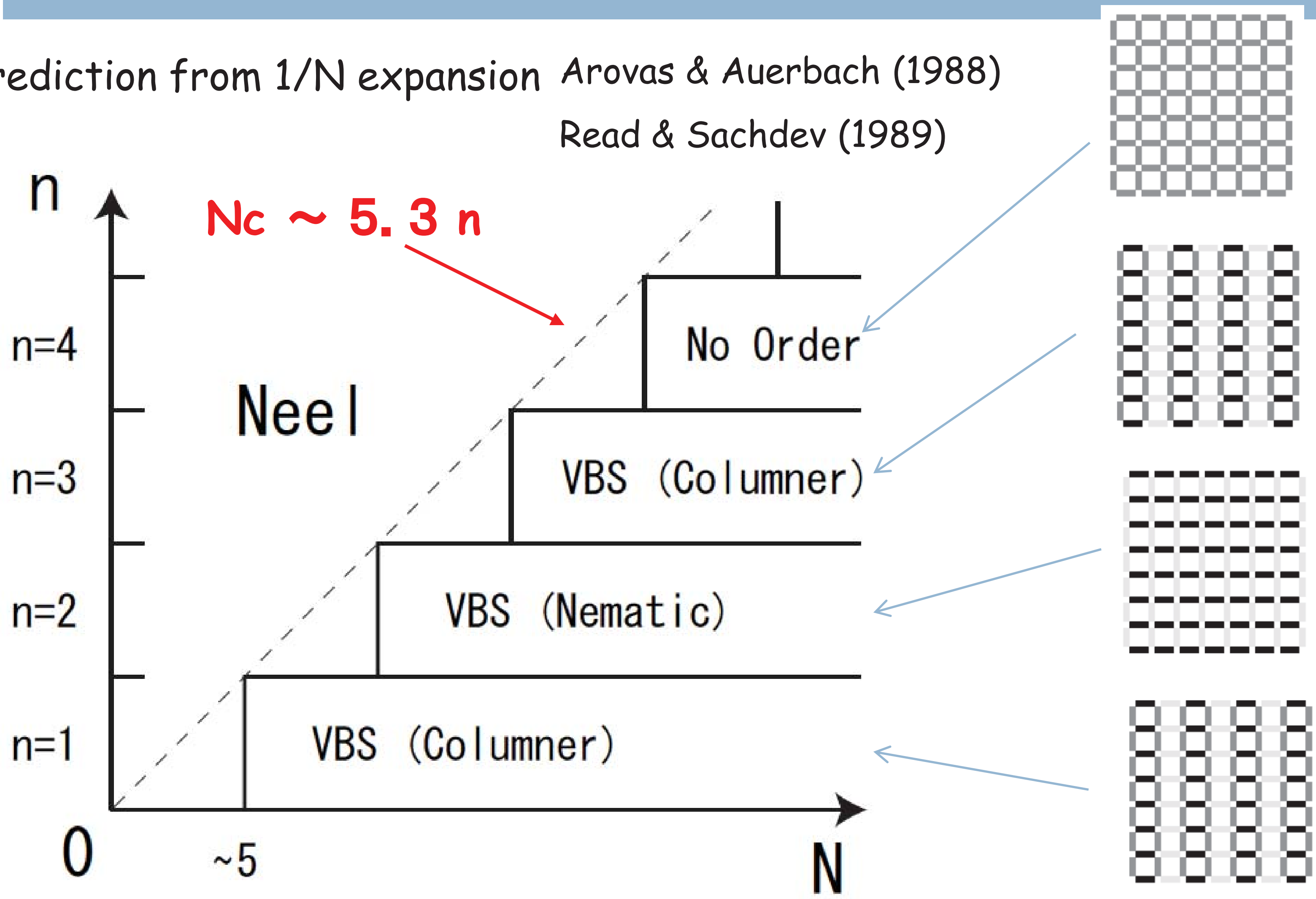


n=1 (fundamental representation.)   n=2   n=3   n=4

2D Analogue of "Haldane" States

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

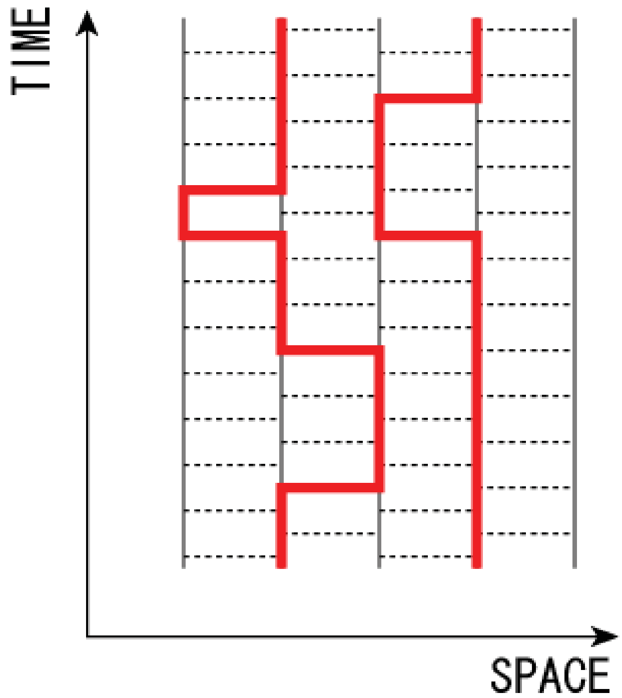
Read & Sachdev (1989)



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

Path-Integral Monte Carlo Method

Suzuki 1976



$$Z = \sum_{S} W(S)$$

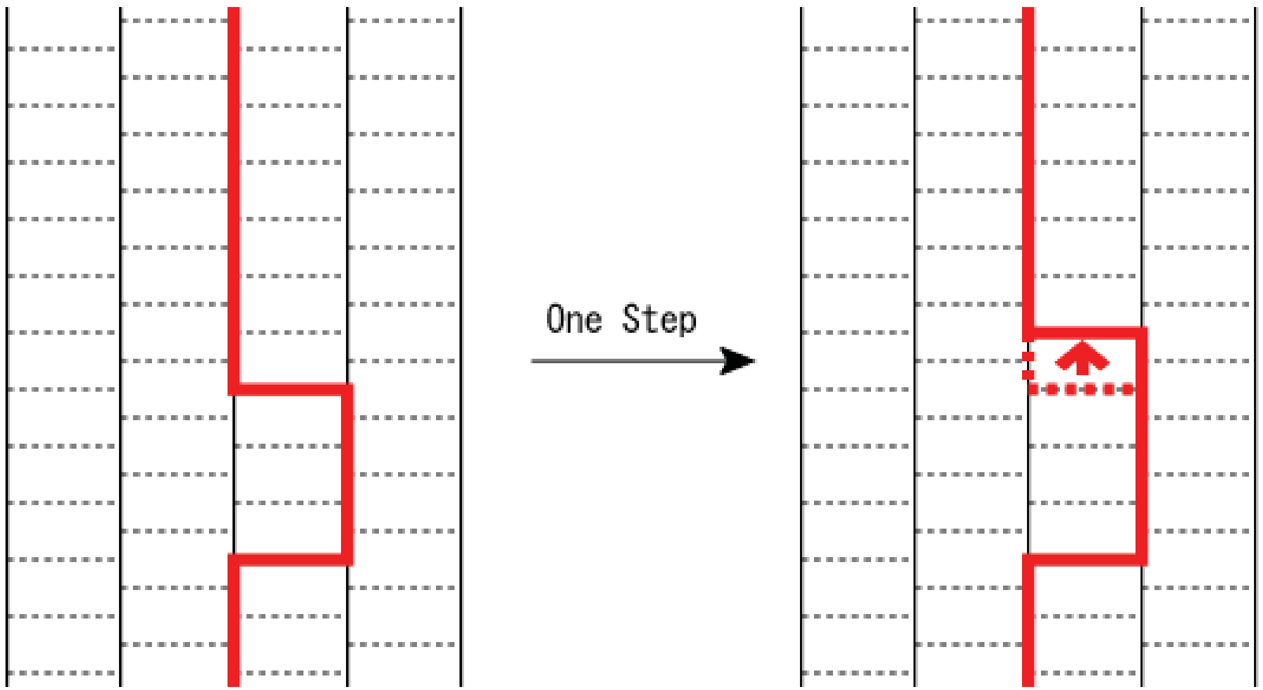
S: The whole pattern of world-lines

┈┈┈ Interaction Vertex("shaded plaquettes")

━━ World Line

Method Used before 1993

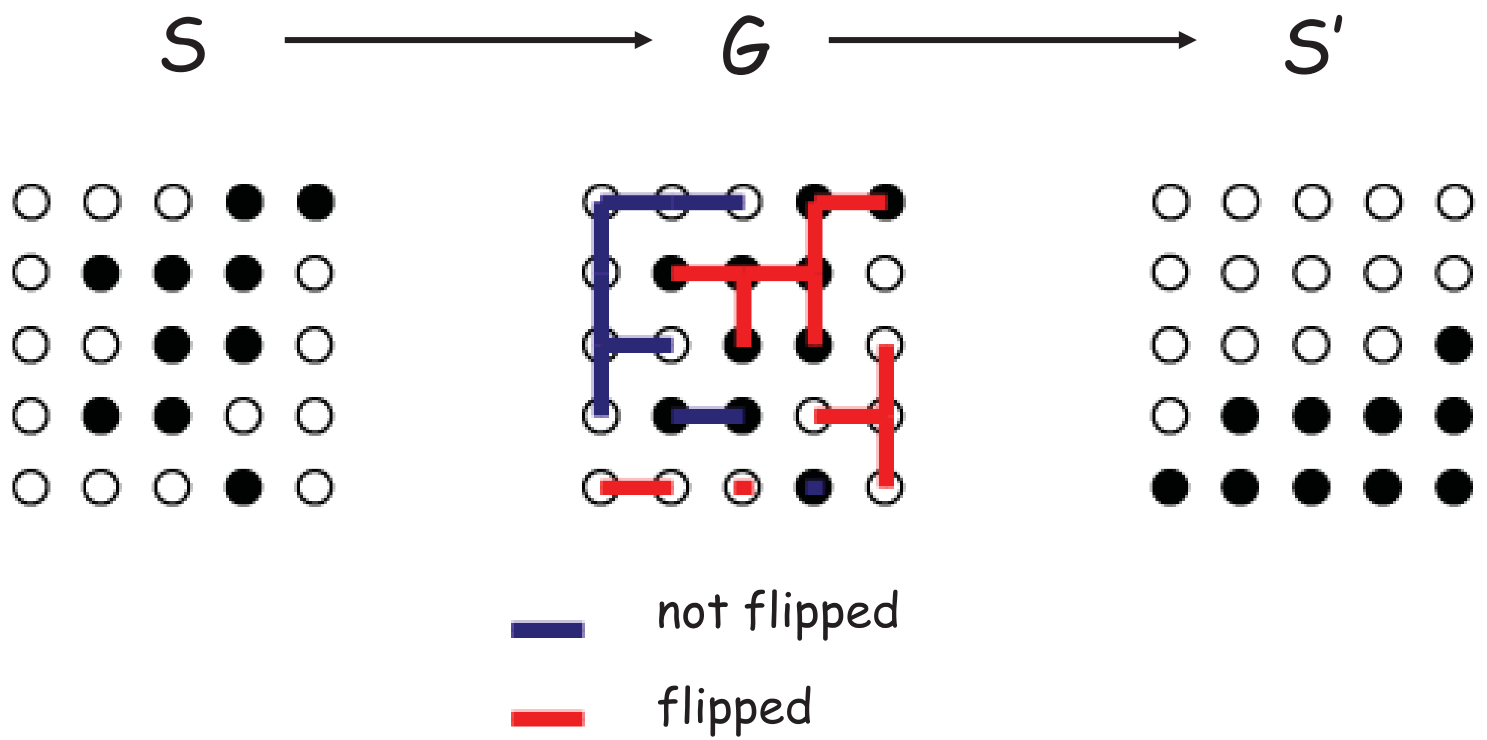
The patterns are updated only locally.



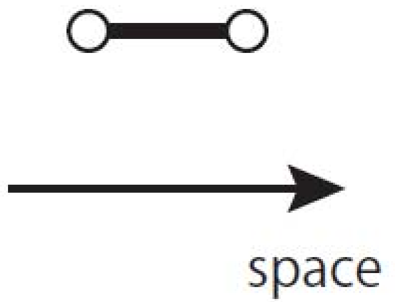
Many Problems --- No change in topological numbers, critical slowing down, high-precision slowing down, etc.

Swendsen-Wang Algorithm

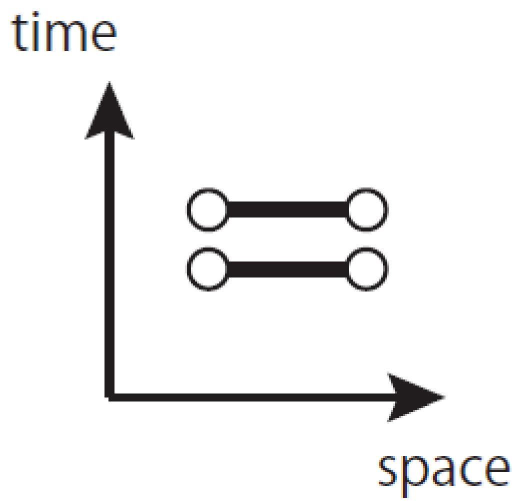
Swendsen-Wang 1987 ... Binding a cluster of spins together.



Generalizing SW algorithm to QMC



A "bond" in the Swendsen-Wang algorithm

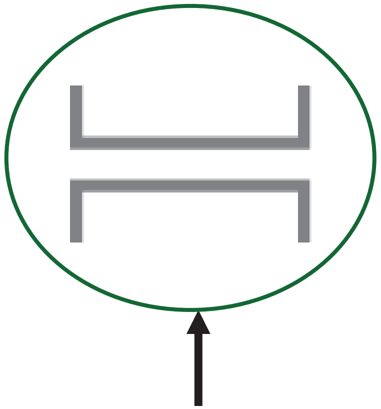


Loop elements in the loop algorithm for QMC

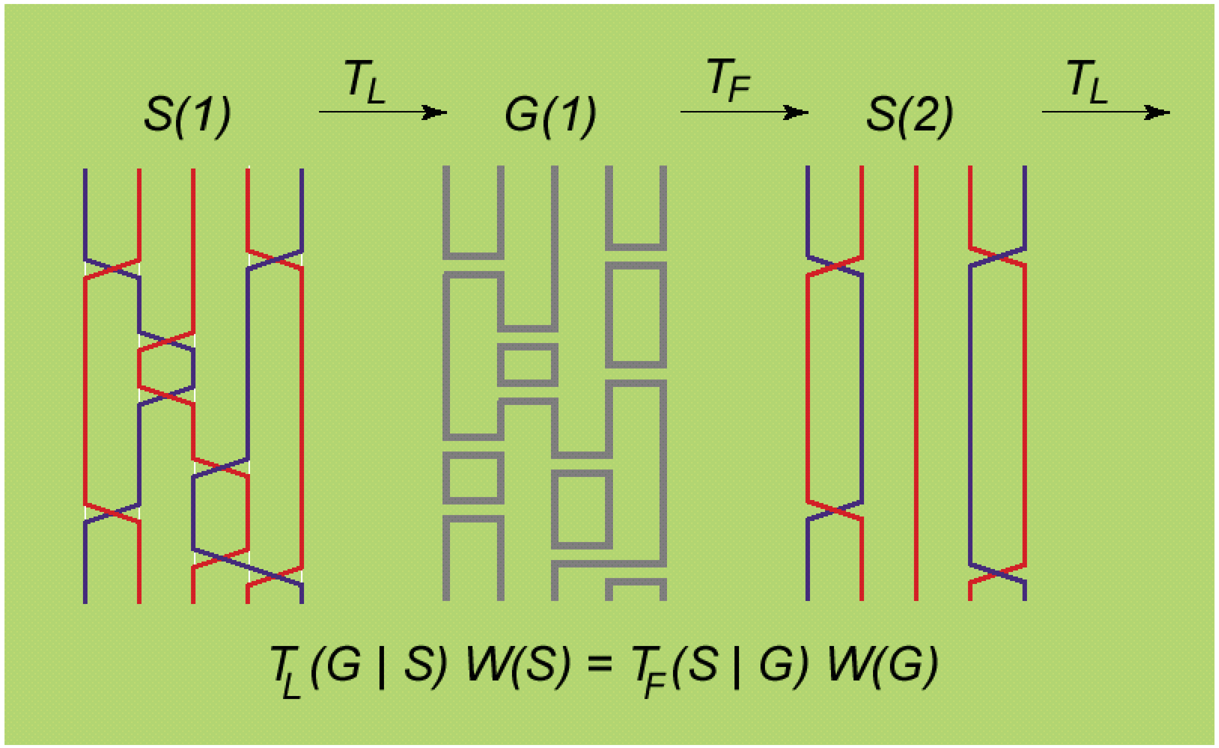
Loop Algorithm for QMC

Evertz-Lana-Marcu 1993

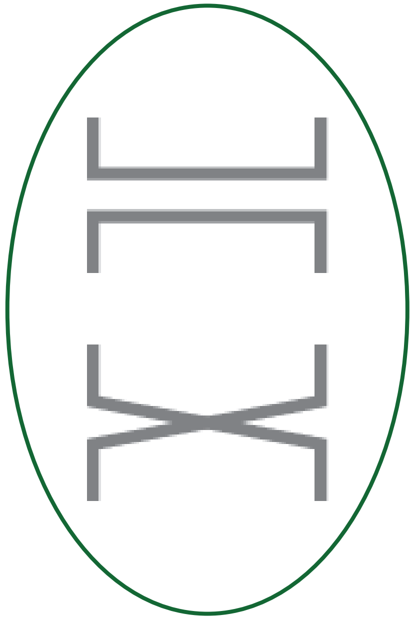
Cluster Algorithm on Path-Integral Representation:



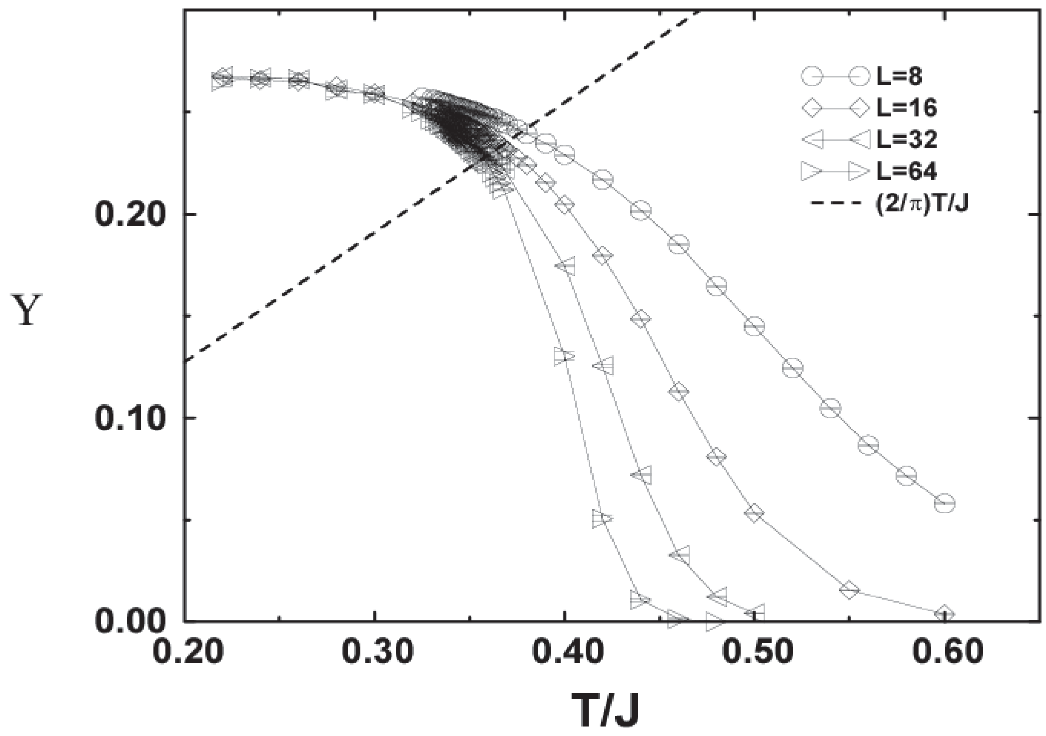
A graph element (for S=1/2 anti-ferromagnetic Heisenberg model)



S=1/2 XY Model



Harada-Kawashima 1998



Tc = 0.34271(5)J

New kind of pressure --- 「京」

京 = 10^{16}


TOP500 SUPERCOMPUTER SITES

ISC events cloud computing

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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

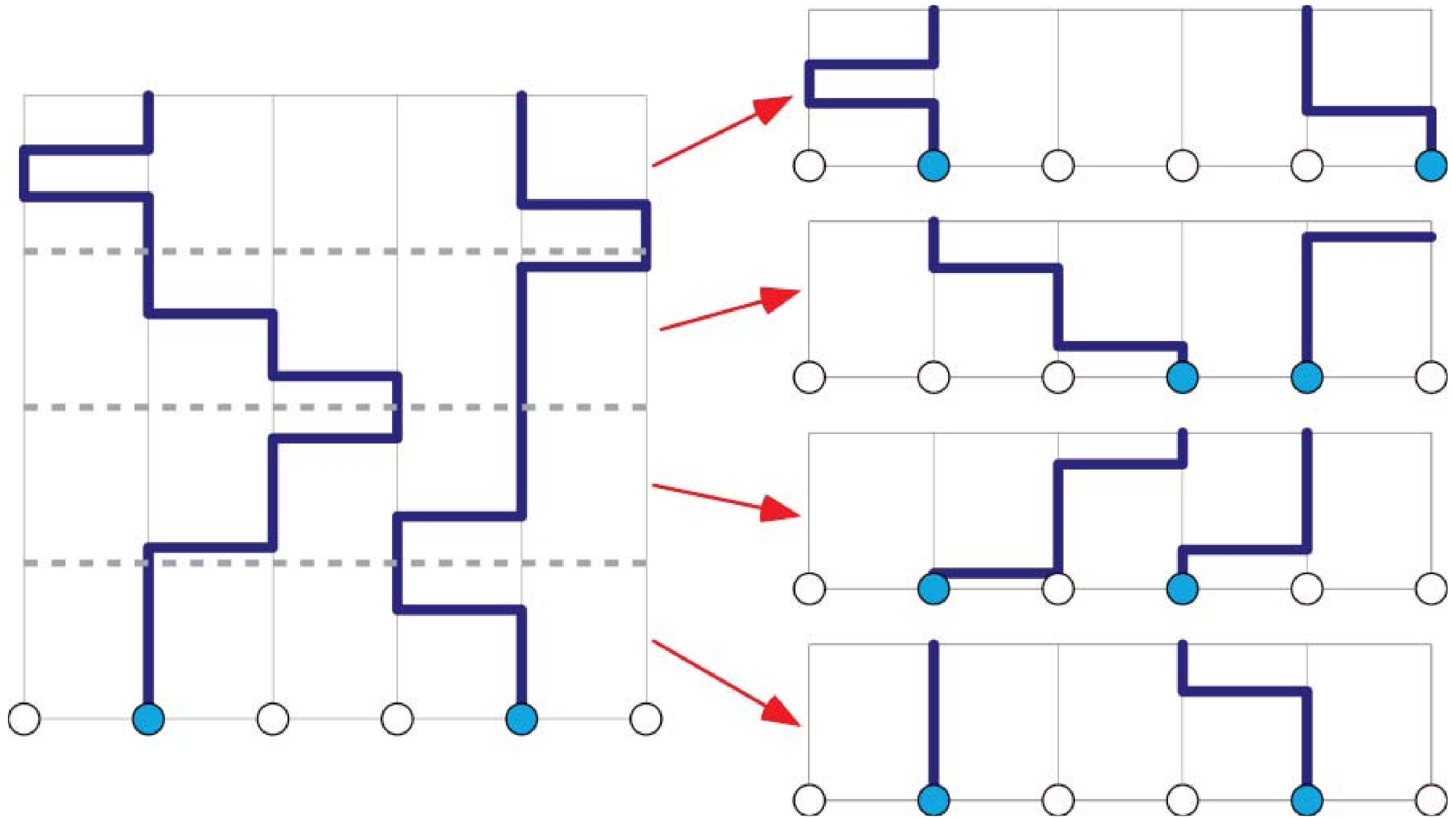
Japan Reclaims Top Ranking on Latest TOP500 List of World's Supercomputers

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

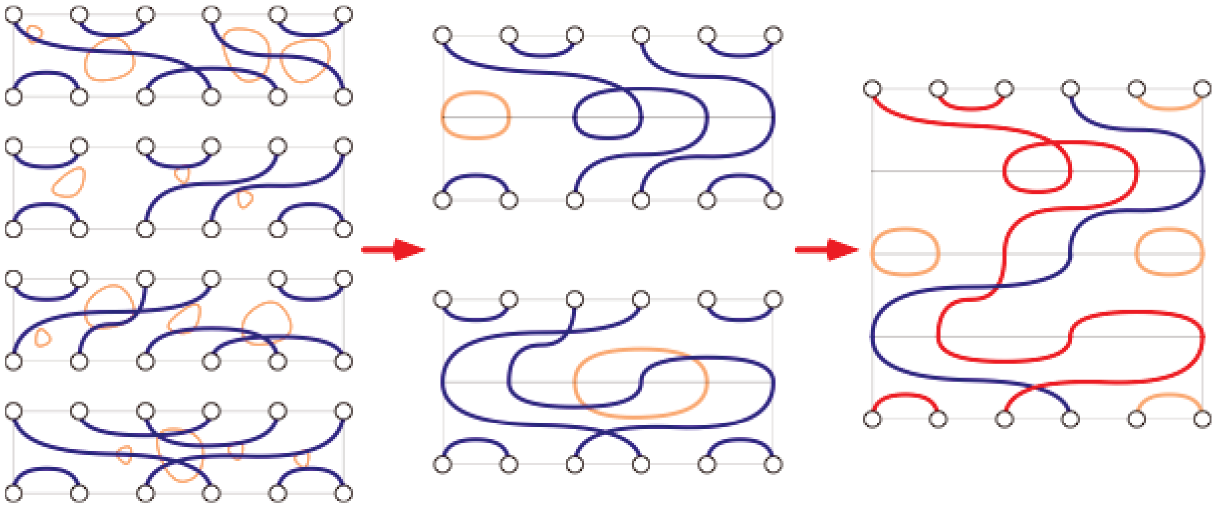
S. Todo & H. Matsuo



Parallelization of loop algorithm

S. Todo & H. Matsuo

Binary-tree algorithm for cluster identification

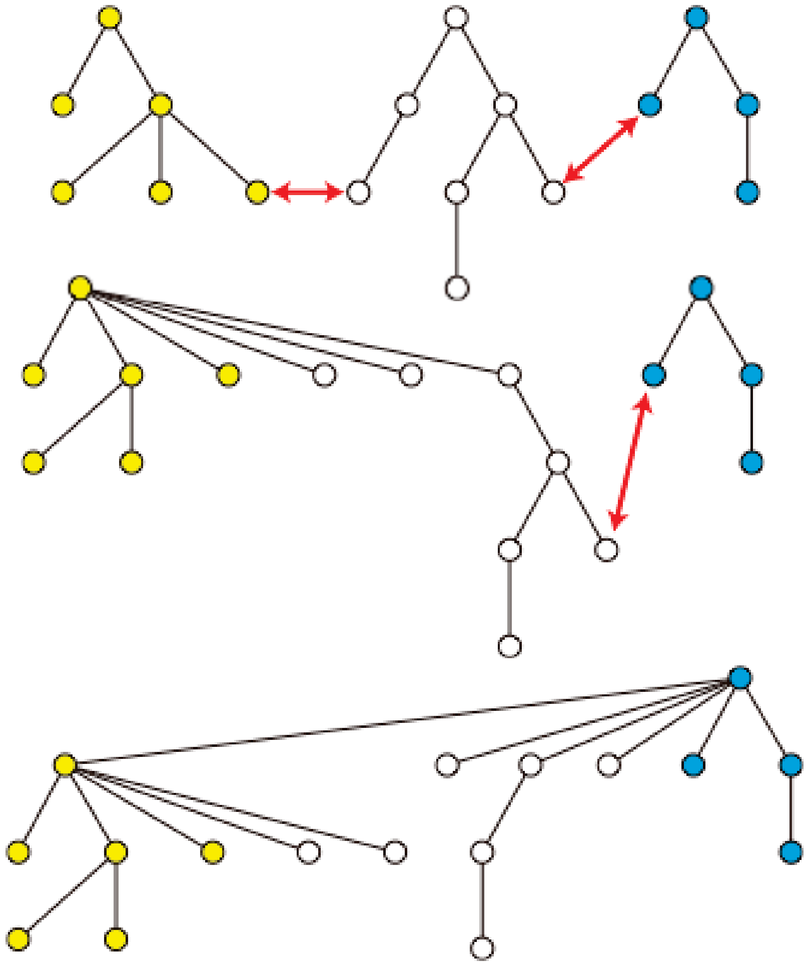


$$(N \log N_{\mathrm{p}})/(\frac{N\beta}{N_{\mathrm{p}}}) = N_{\mathrm{p}} \log N_{\mathrm{p}}/\beta$$

... 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)

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

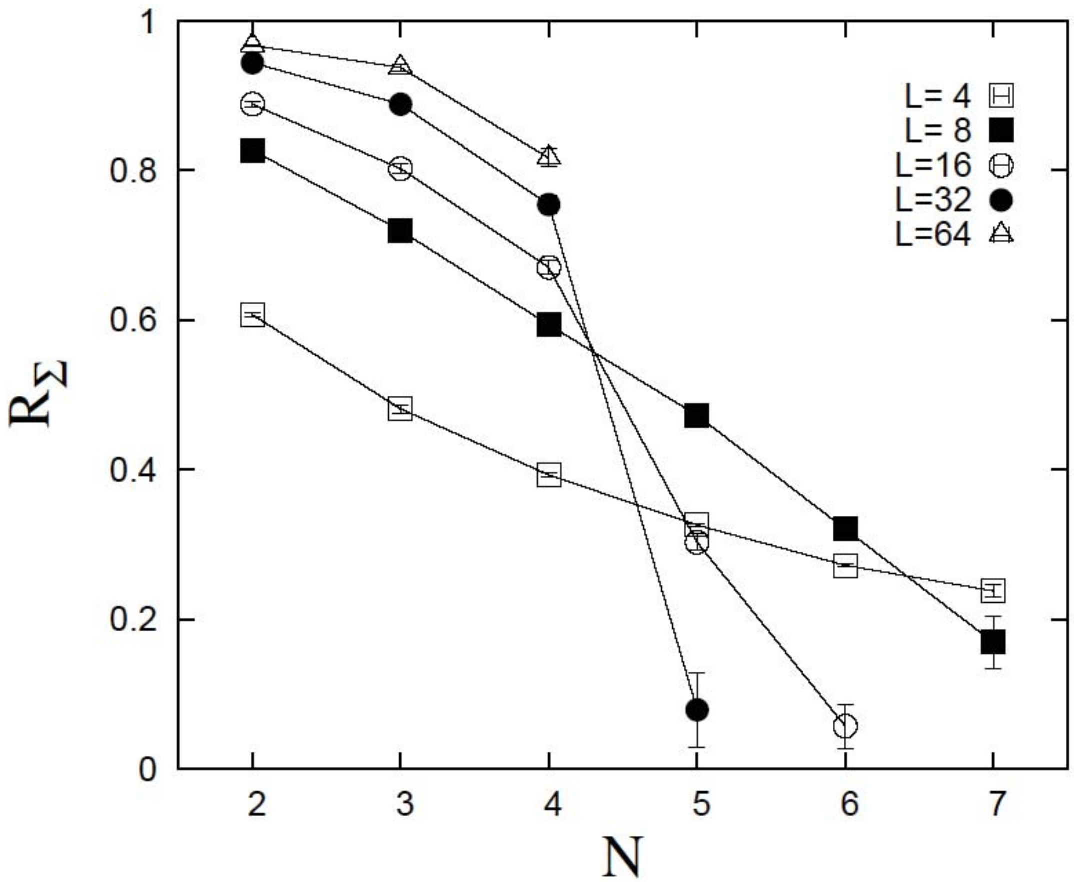
$$R_M(L) \equiv \frac{C_M(L/2)}{C_M(L/4)}$$

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

Neel order dissapears at N

4<Nc<5

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



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

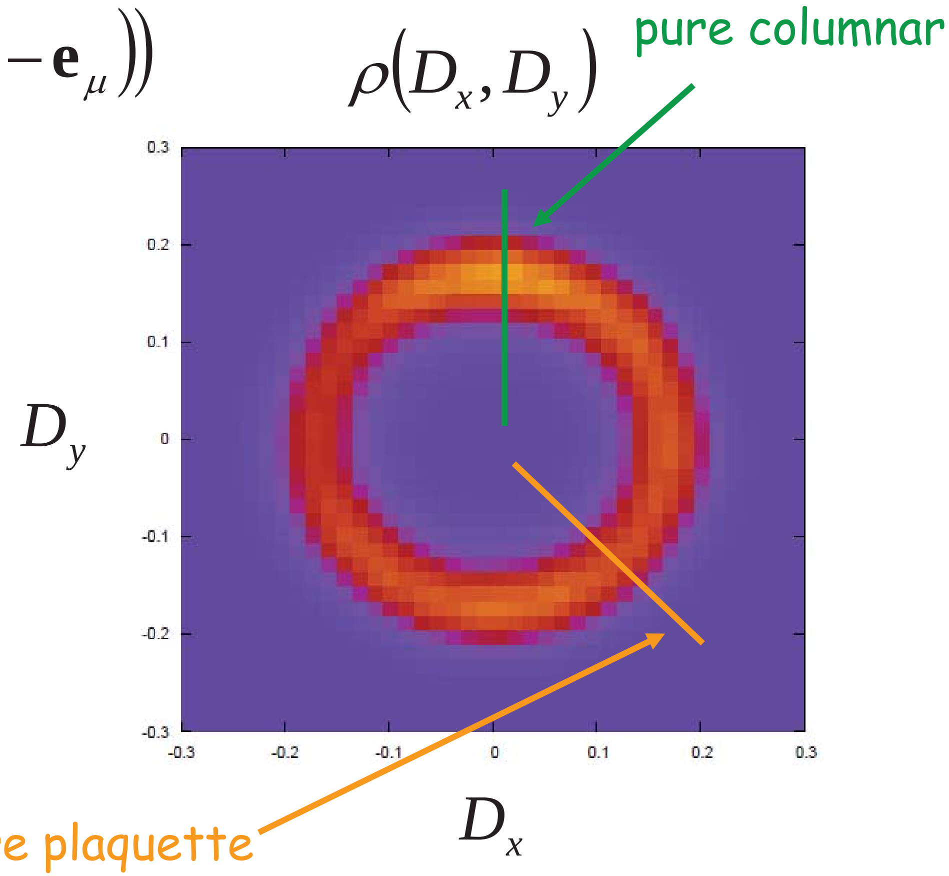
Ground-State Manifold is U(1) Symmetric

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

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

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

$\rho(D_x, D_y)$

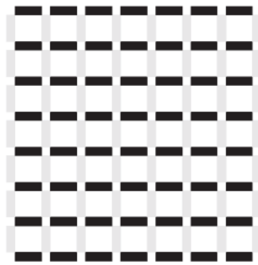


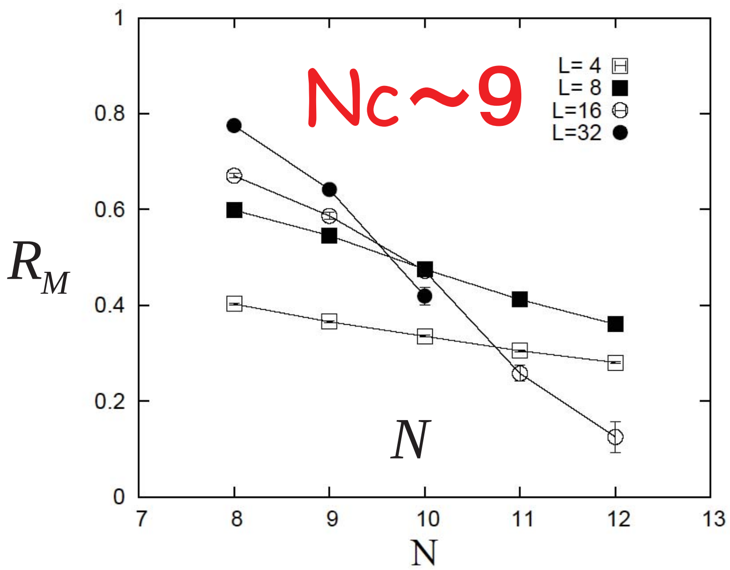
N=10, n=1, L=32, β=20

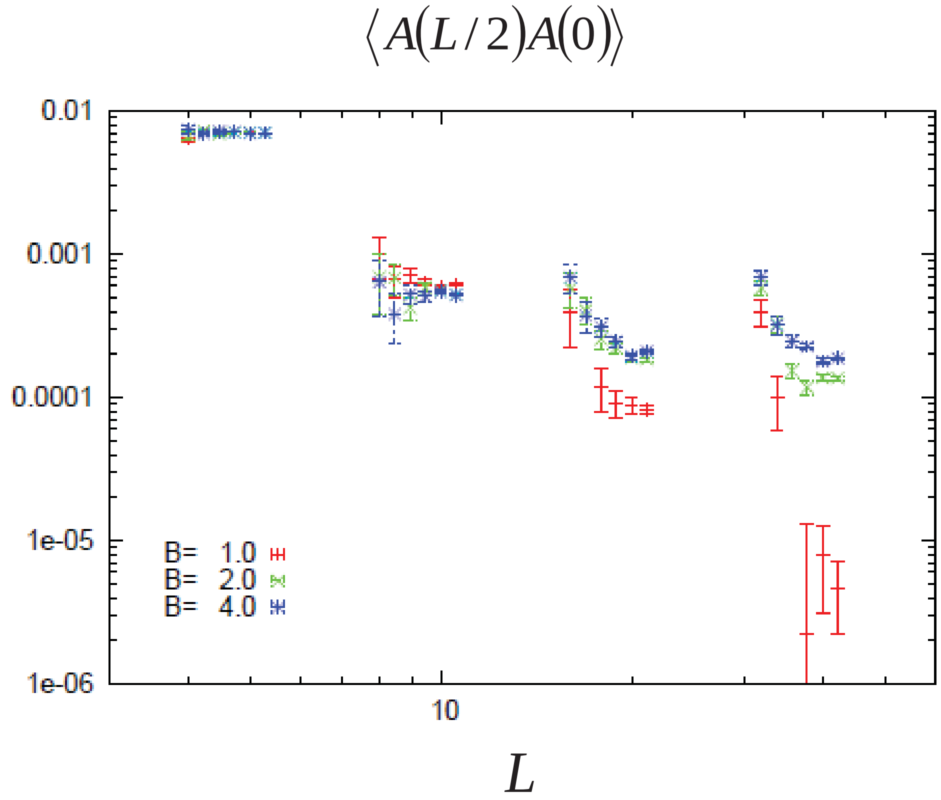
The system is asymptotically U(1) symmetric though the original microscopic model does not possess this symmetry.

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

SU(N) Model (n=2)





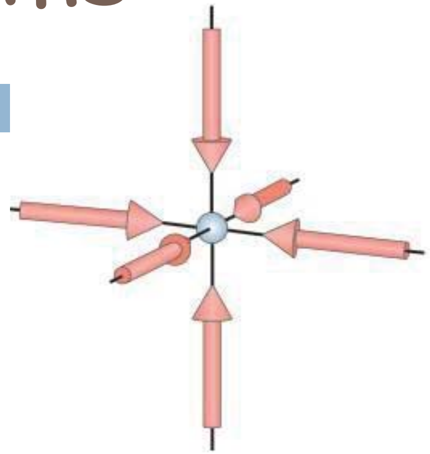


$$\begin{pmatrix} A(\mathbf{R}) = V_x(\mathbf{R}) - V_y(\mathbf{R}); \\ V_\mu(\mathbf{R}) \equiv \frac{1}{n_B^2} \sum_{\alpha=1}^{N} n_\alpha(\mathbf{R}) n_\alpha(\mathbf{R} + \mathbf{e}_\mu) \end{pmatrix}$$

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

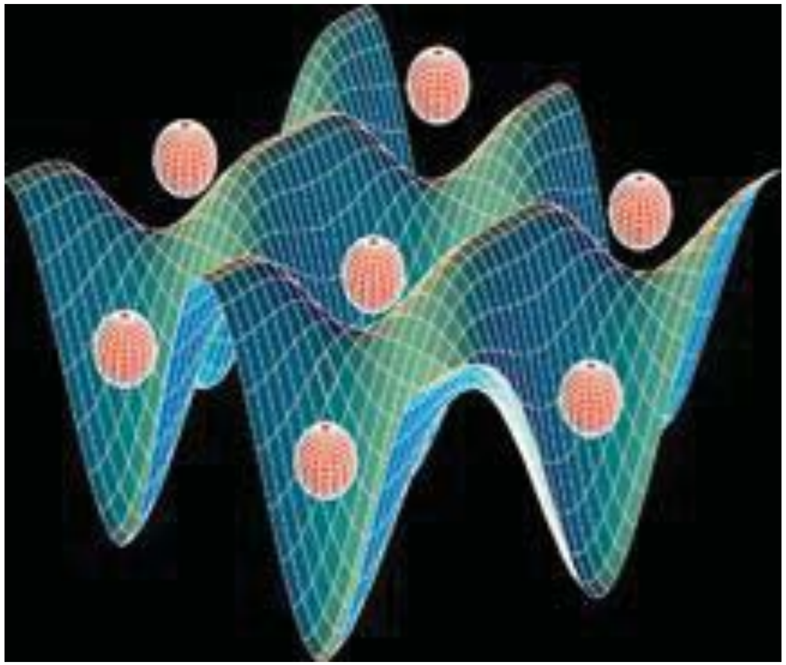
2D Isotropic Case (Tanabe, N.K.)

Laser-Trapped Cold Atoms



Three orthogonal laser beams form a periodic lattice potential for atoms.

^{87}Rb ($S_{total}=1$)



M. Greiner et al,
Nature 415 (2002) 39.

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

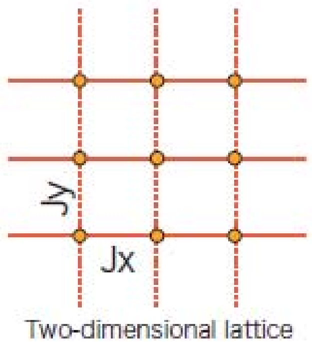
$$H = \sum_{(ij)} \left\{ J_L \left(\mathbf{S}_i \cdot \mathbf{S}_j \right) + J_Q \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 \right\} + \text{const}$$

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

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

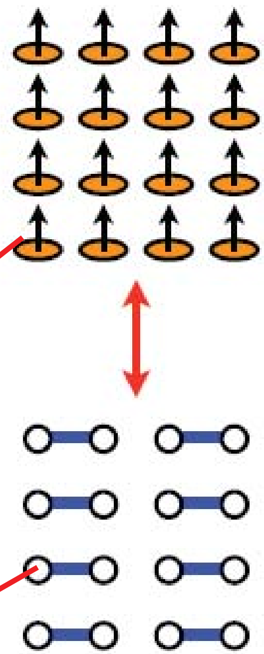
^{23}Na: $0 < U_0 < U_2$ $(J_Q < J_L < 0)$

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



Anisotropy parameter

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

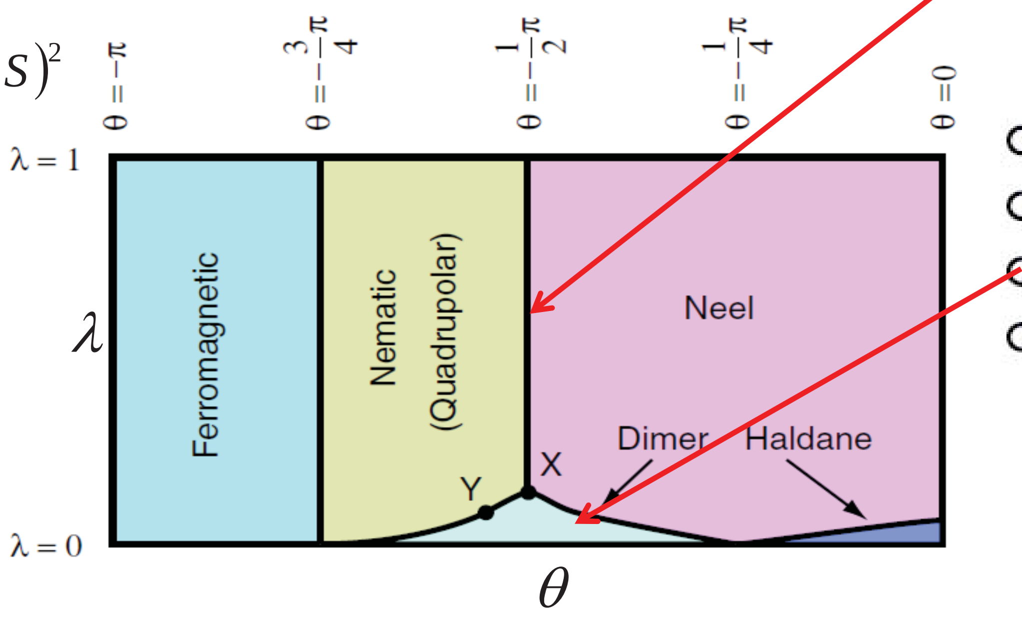


$$H = J_{\mathrm{L}}^{\mu}(S \cdot S) + J_{\mathrm{Q}}^{\mu}(S \cdot S)^2$$

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

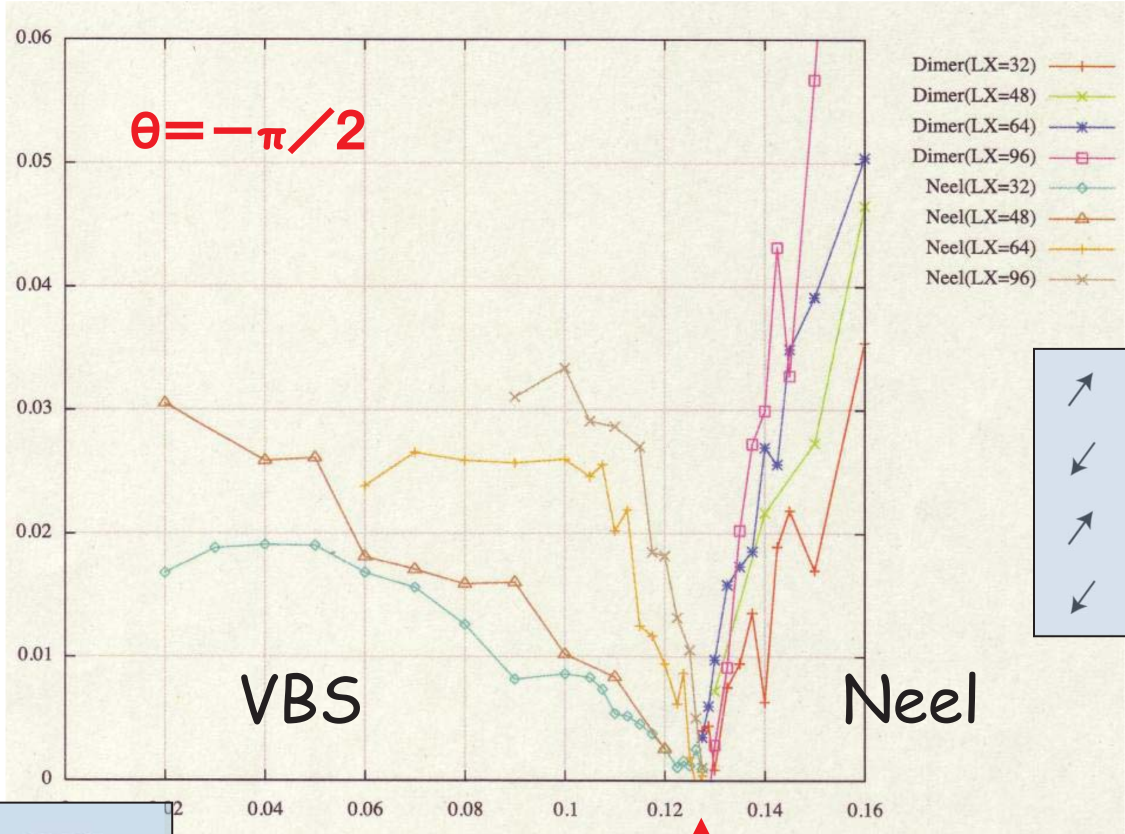
$$J_{\mathrm{L}}^{\mu} = -J^{\mu} \cos\theta$$

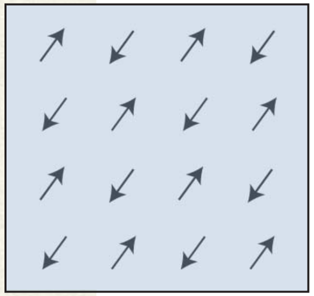
$$J_{\mathrm{Q}}^{\mu} = -J^{\mu} \sin\theta$$

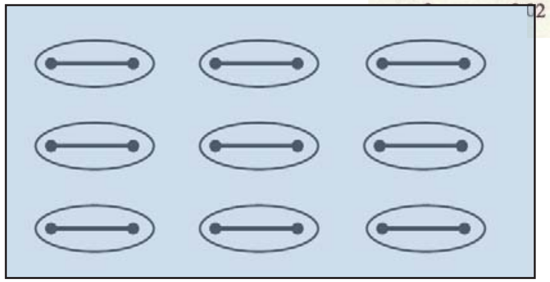


Diversing Correlation Lengths

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



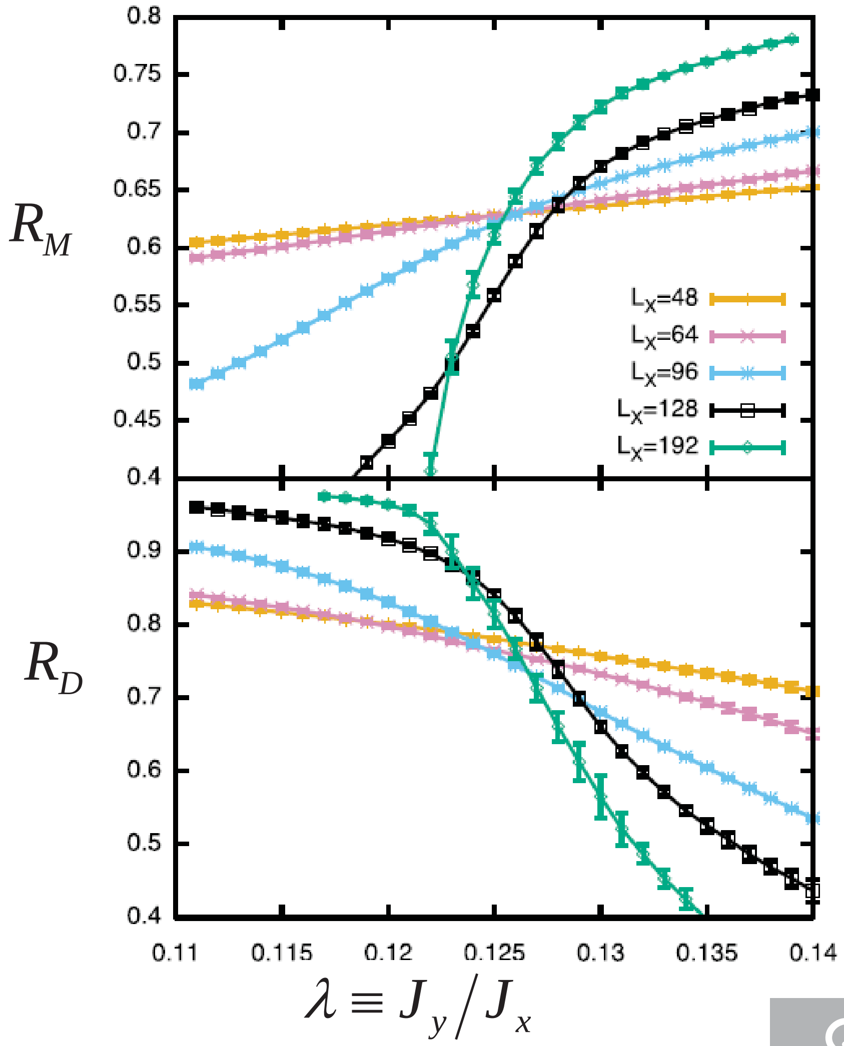




$$J_y / J_x$$

2 correlation length diverges at the same point.

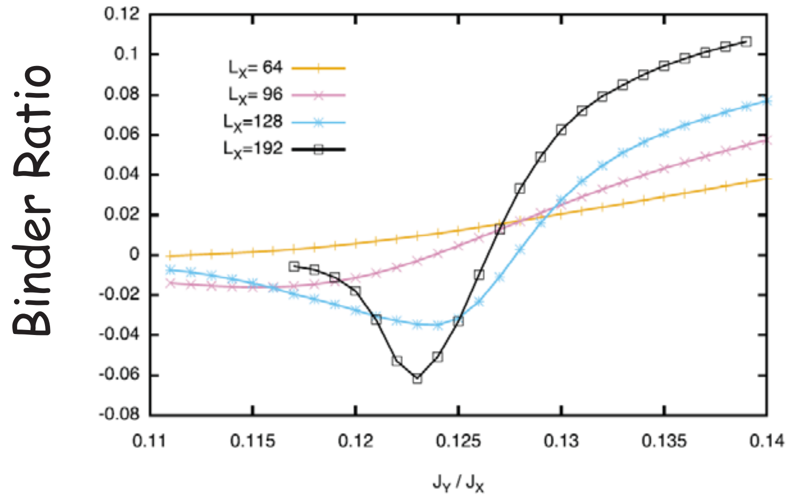
θ=−0. 5π (SU(3) symmetric)



A single transition is likely...

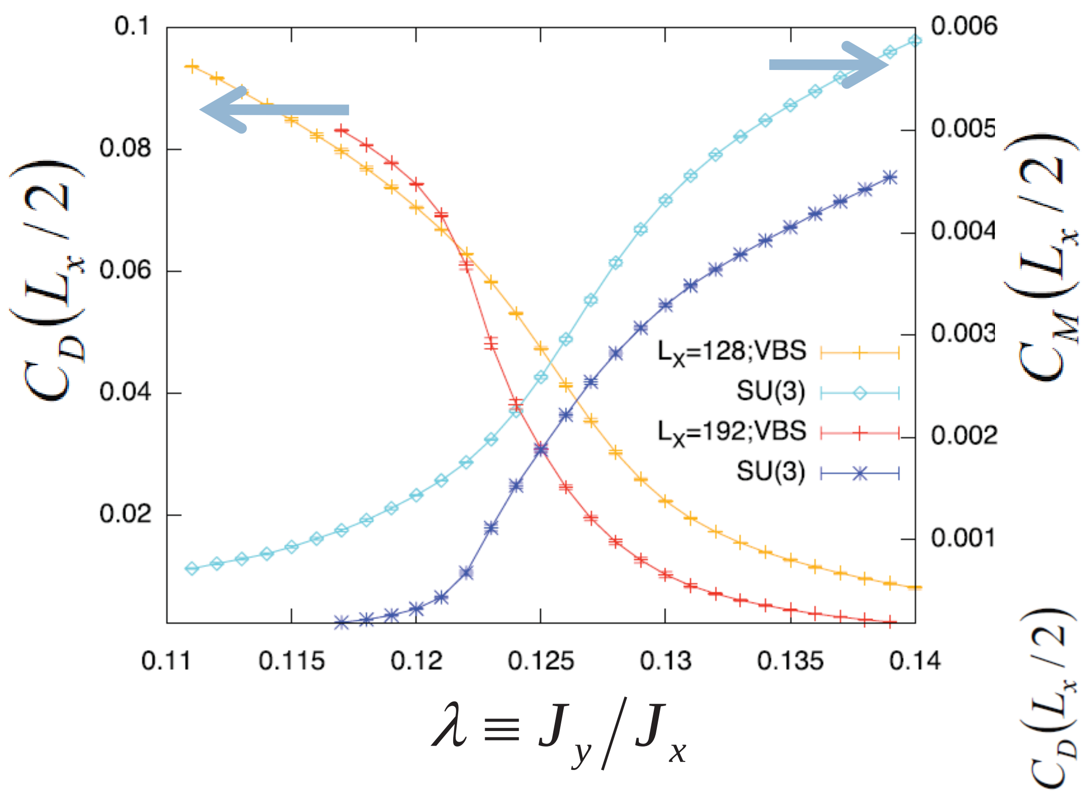
$$\lambda_c = 0.125(5)$$

Cannot obtain a reliable finite-size scaling plot.



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

Correlation Function SU(3), Lx<=192

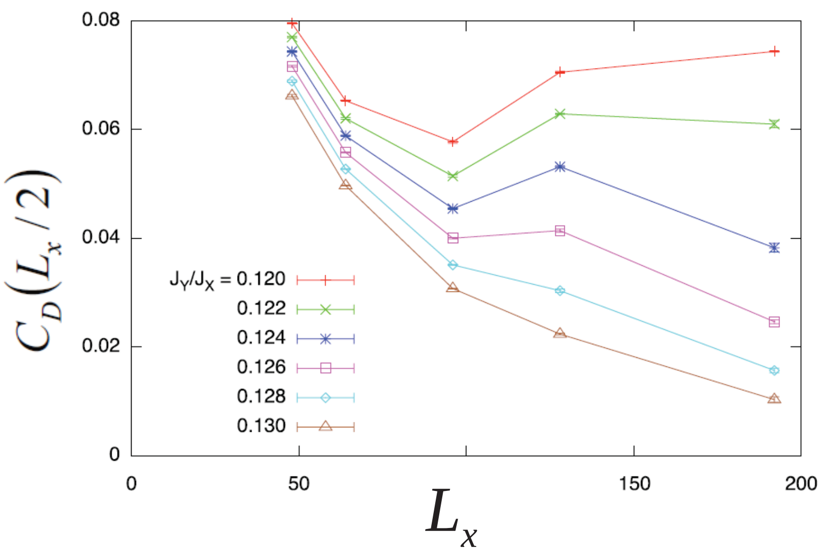


$$C_Q(R) \equiv \langle Q(0) Q(R) \rangle$$

$$(Q = M, D)$$

$$R = L_x / 2$$

Still non-monotonic at L=192



$$\lambda_C \approx 0.125$$

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

CP^2 Theory

T. Grover and T. Senthil, PRL98 247202 (2007):

Double-instanton events are irrelevant at CP^2 critical point. So, a DCP-like continuous phase transition is plausible in the quasi-1D case as well.

Multi-spin Interactions

A. W. Sandvik, Phys. Rev. Lett. 98, 227202 (2007)

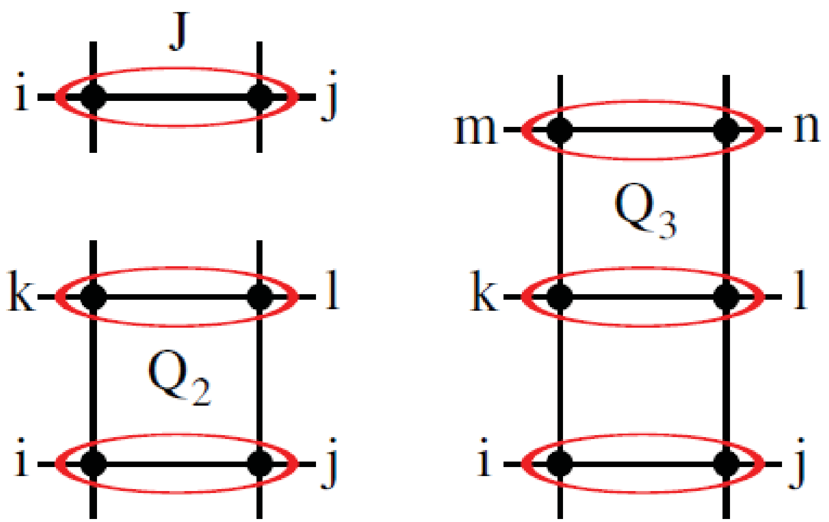
J. Lou, A. Sandvik, N.K.: PRB 80, 180414R (2009)

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

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

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

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



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

SU(2) J-Q Model

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

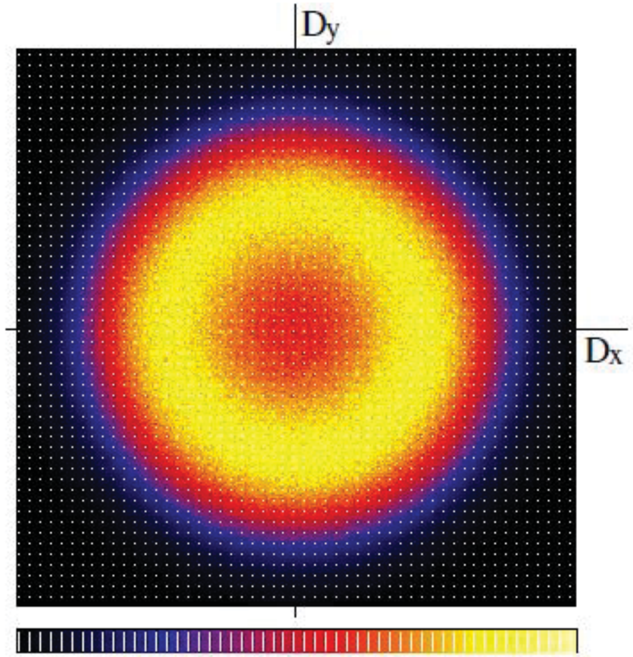


FIG. 5 (color online). Histogram of the dimer order parameter for an $L = 32$ system at $J/Q = 0$. The ring shape demonstrates an emergent $U(1)$ symmetry, i.e., irrelevance of the Z_4 anisotropy of the VBS order parameter.

U(1) Nature is confirmed at the critical point.

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

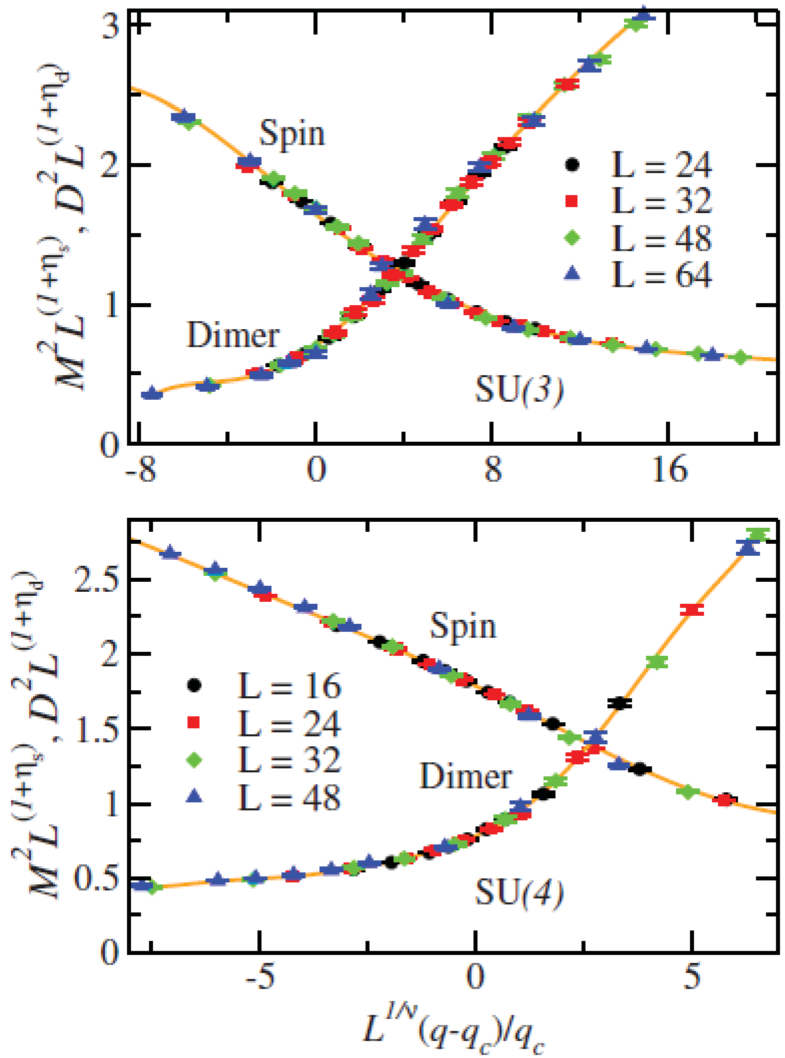
J. Lou, A. Sandvik, N.K (2009)

SU(3) J-Q2

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

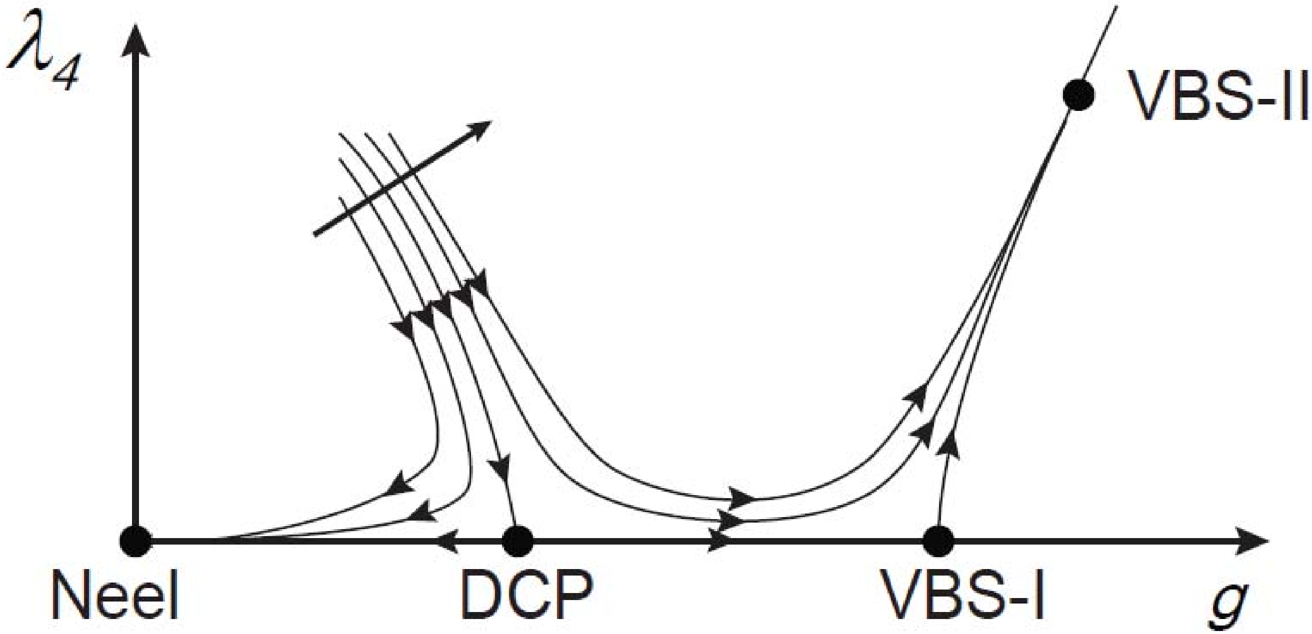
SU(4) J-Q2

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



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

Recovery of Discreteness



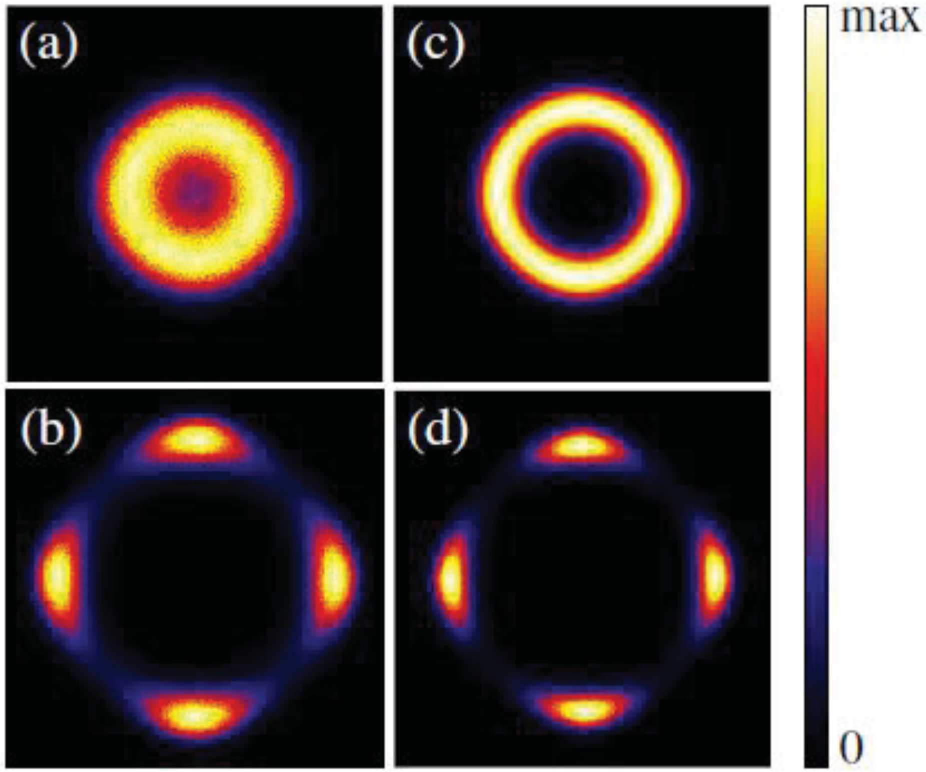
The exponent nu on the VBS side may be affected by the additional fixed point and can be differ from the Neel side.

VBS - VBS Crossover

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

Small Q

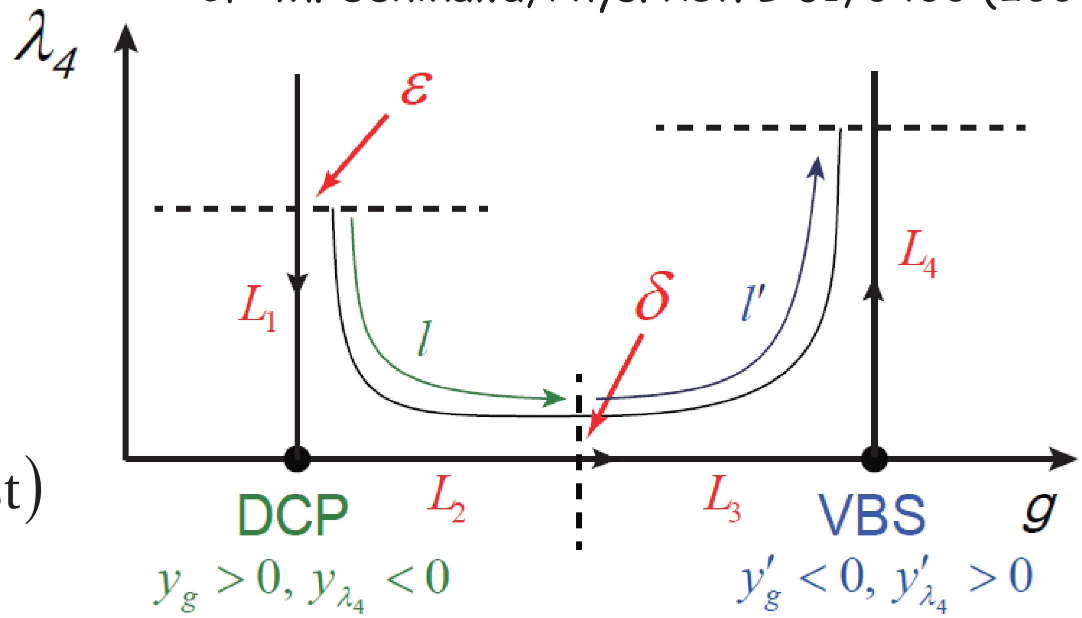
Large Q



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

Two Length Scales

CF: M. Oshikawa, Phys. Rev. B 61, 3430 (2000).



$$L_2 = \varepsilon e^{y_g l} \Rightarrow l = \frac{1}{y_g}\log\frac{L_2}{\varepsilon}$$

$$L_4 = \delta e^{y'_{\lambda_4} l'} \Rightarrow l' = \frac{1}{y'_{\lambda_4}}\log\frac{L_4}{\delta}$$

$$\delta = L_1 e^{y_{\lambda_4} l} \Rightarrow l' = \left|\frac{y_{\lambda_4}}{y'_{\lambda_4}}\right| l + (\mathrm{const})$$

$$\xi = e^{l} \propto \varepsilon^{-y_g^{-1}}$$

For quantities arising from Λ4:

$$\xi' = e^{l+l'} \propto \varepsilon^{-y_g^{-1}\left(1+\left|\frac{y_{\lambda_4}}{y'_{\lambda_4}}\right|\right)}$$

$$\nu' = a\nu$$

$$\left(a = 1 + \left|\frac{y_{\lambda_4}}{y'_{\lambda_4}}\right|\right)$$

$$\mathrm{CF:}\quad a = \left|\frac{y_{\lambda_4}}{2}\right| \quad (\mathrm{Oshikawa})$$

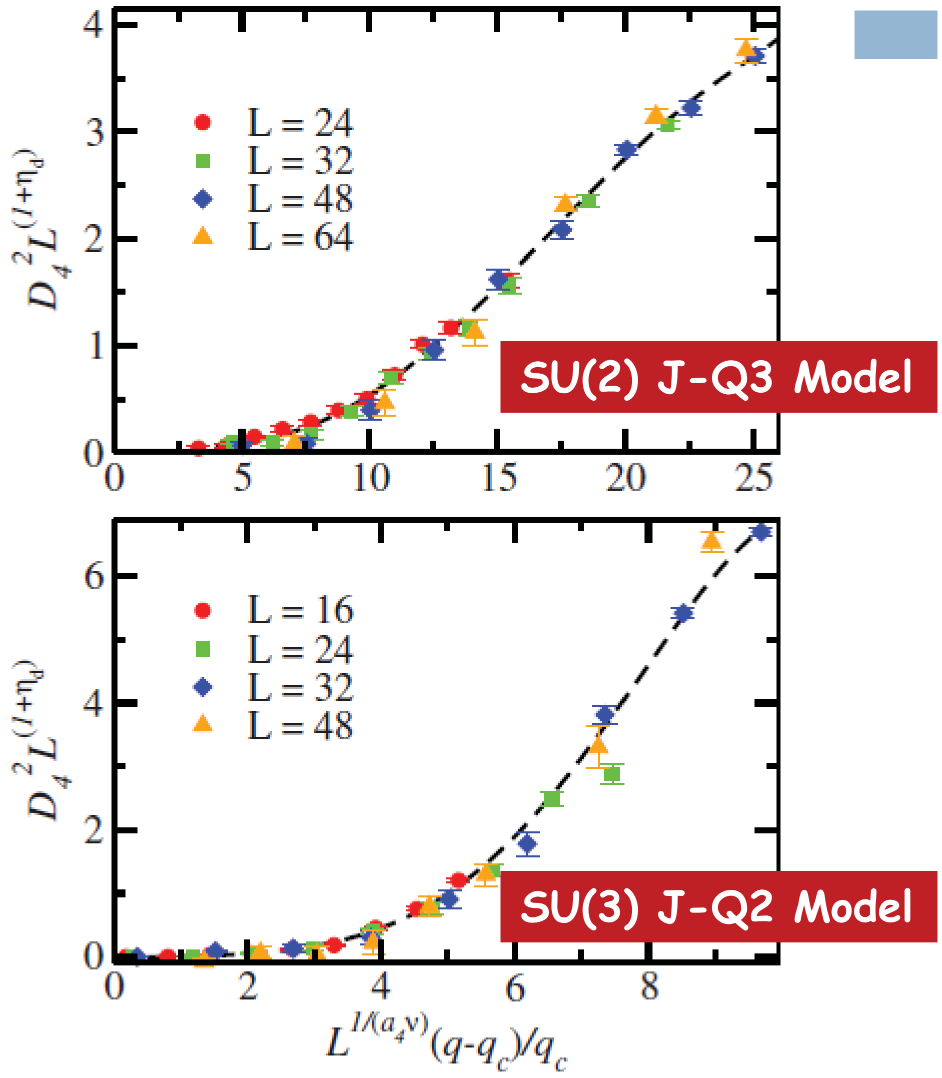
Scaling Properties of Anisotropy

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

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

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

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.)

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)

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

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

A_μ : $U(1)$ gauge field

A_μ is non-compact

$\leftrightarrow$ conservation of the gauge current

$$J^G_\mu = \varepsilon_{\mu\nu\lambda}\partial_\mu A_\lambda$$

$\leftrightarrow$ absense of monopoles

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

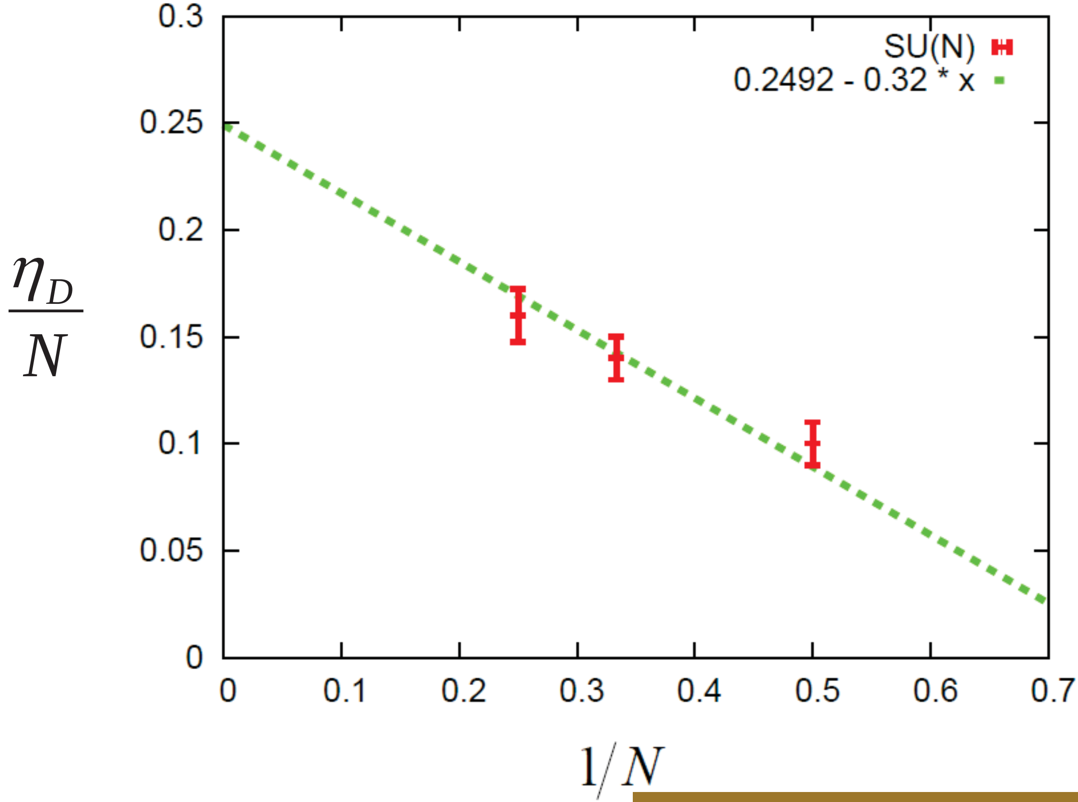
$$\langle D(R)D(0)\rangle = \langle \Psi_{\mathrm{VBS}}(R)\Psi_{\mathrm{VBS}}(0)\rangle = \langle v^+(R)v(0)\rangle \propto \frac{1}{R^{2\Delta_1}}$$

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

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

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

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



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

Conclusion

(1) Isotropic SU(N) Heisenberg Model
- ✔ VBS Ground State
- ✔ Proximity to DCP critical phenomena

(2) 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.)

(3) Multi-Spin Interactions (J-Q Models)
- ✔ Consistent with DCP
- ✔ η_d proportional to N (The correction term is estimated)

END