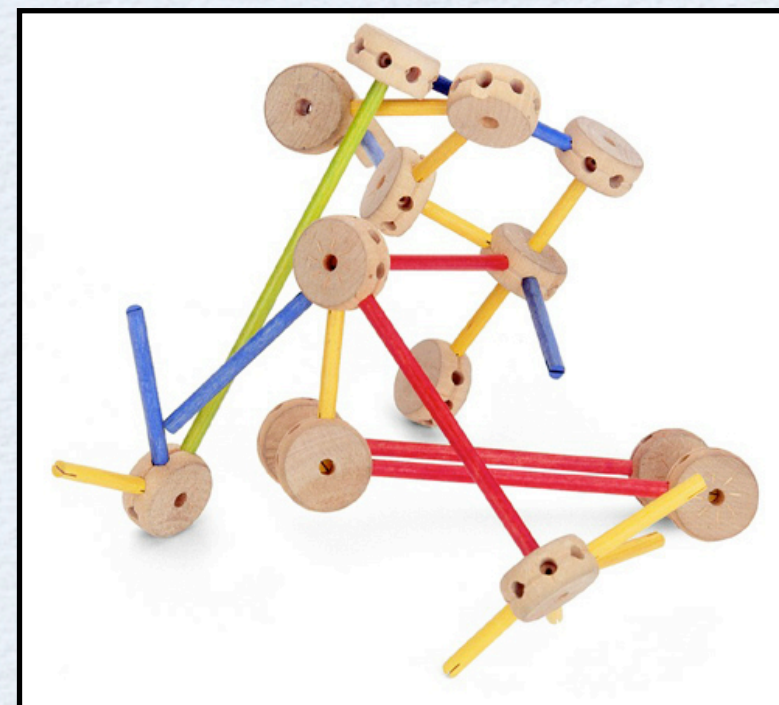


# New Directions in Valence Bond Solid Antiferromagnets or Quantum Magnetism with Tinker Toys

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# Local interactions prefer local singlets

Heisenberg antiferromagnet :  $\mathcal{H} = \mathbf{S}_i \cdot \mathbf{S}_j$

$$E = \frac{1}{2}J(J+1) - S(S+1)$$

where  $J \in \{0, 1, \dots, 2S\}$ . Singlet ( $J=0$ ) has lowest energy.

Lattice Heisenberg antiferromagnet :  $\mathcal{H} = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$

Ground state (Bethe Ansatz) energy per bond (d=1 chain):

$$E_0 = \frac{1}{4} - \ln 2 = -0.443147\dots$$

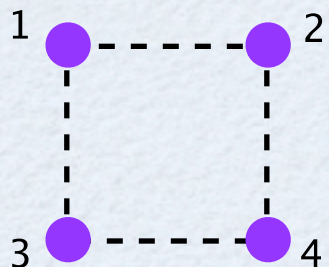
$$E_{\text{singlet}} = -\frac{3}{4} = -0.75$$

Not every bond can be a singlet!



# Small antiferromagnetic clusters

Two spins  $S = 1/2$ : singlet ground state  $|\Psi\rangle = 2^{-1/2} \{ |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \}$

Four spins  $S = 1/2$ :   $\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 0 \oplus 1 \oplus 1 \oplus 1 \oplus 2$

Solution: two independent singlets,  $|\text{vertical}\rangle$  and  $|\text{horizontal}\rangle$

(linear dependence:  $|\text{diagonal}\rangle = |\text{vertical}\rangle - |\text{horizontal}\rangle$ )

phase convention:  $\sqrt{2} |\text{bond } i < j\rangle = |\uparrow_i \downarrow_j\rangle - |\downarrow_i \uparrow_j\rangle$

ground state:  $\sqrt{3} |\Psi\rangle = |\text{horizontal}\rangle + |\text{vertical}\rangle$

“resonating valence bonds” (RVB)



# The quantum Néel state

Classical Néel state:  $|\text{CN}\rangle = \left| \begin{array}{cccc} \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \end{array} \right\rangle$   $m = S$

selected by  $S_i^z S_j^z$   
(A/B sublattice)

Quantum Néel state:

$$|\text{QN}\rangle = \left| \begin{array}{cccc} \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \end{array} \right\rangle - \frac{1}{4(z-1)S} \left| \begin{array}{cccc} \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \end{array} \right\rangle + \dots$$

$m = S - 1$   
reduced due to  $S_i^+ S_j^-$

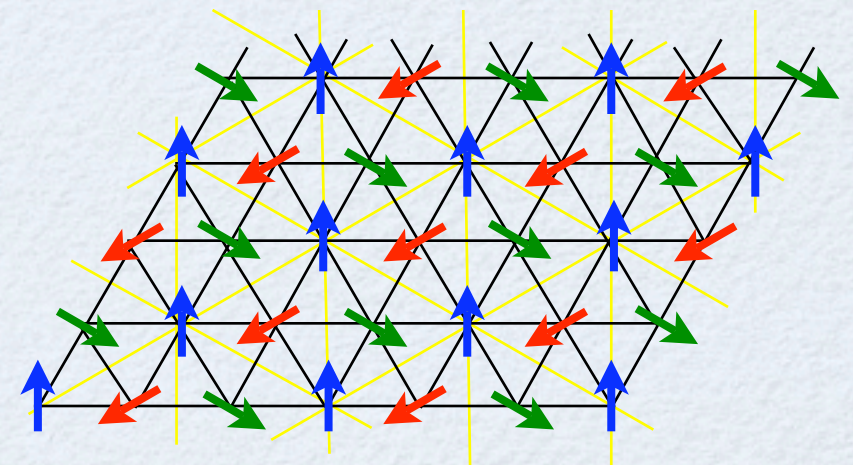
Classical order is reduced due to quantum fluctuations.

E.g. square lattice:  $M \simeq 0.31$  for  $S = \frac{1}{2}$  (Reger and Young, 1988)

Triangular lattice: three-sublattice

$\sqrt{3} \times \sqrt{3}$  Néel state has  $M \simeq 0.20$

(Bernu et al., 1994)





# Majumdar-Ghosh model (1969)

(Majumdar and Ghosh, 1969)

$$|\Psi_A\rangle = \left| \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \quad \boxed{\bullet\text{---}\bullet\text{---}\bullet} \bullet \right\rangle$$

$2n \quad 2n+1$

total spin  $\frac{1}{2}$

Generally we have  $\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}$  missing quadruplet!

Form projection operator :  $(\mathbf{S}_i + \mathbf{S}_j + \mathbf{S}_k)^2 = \begin{cases} 3/4 \\ 15/4 \end{cases}$

$$\implies P_{3/2}(i, j, k) = \frac{1}{3} \left[ (\mathbf{S}_i + \mathbf{S}_j + \mathbf{S}_k)^2 - \frac{3}{4} \right]$$

$$\mathcal{H} = \sum_n P_{3/2}(n-1, n, n+1) = \frac{4}{3} \sum_n \left[ \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \frac{1}{2} \mathbf{S}_n \cdot \mathbf{S}_{n+2} \right] + E_0$$

elementary excitations

$$|k, \text{magnon}\rangle = \sum_n e^{2nik} \left| \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \quad \cdots \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \right\rangle$$

$2n$

$$|k, \text{soliton}\rangle = \sum_n e^{2nik} \left| \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \quad \uparrow \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \quad \bullet\text{---}\bullet \right\rangle$$

$2n$

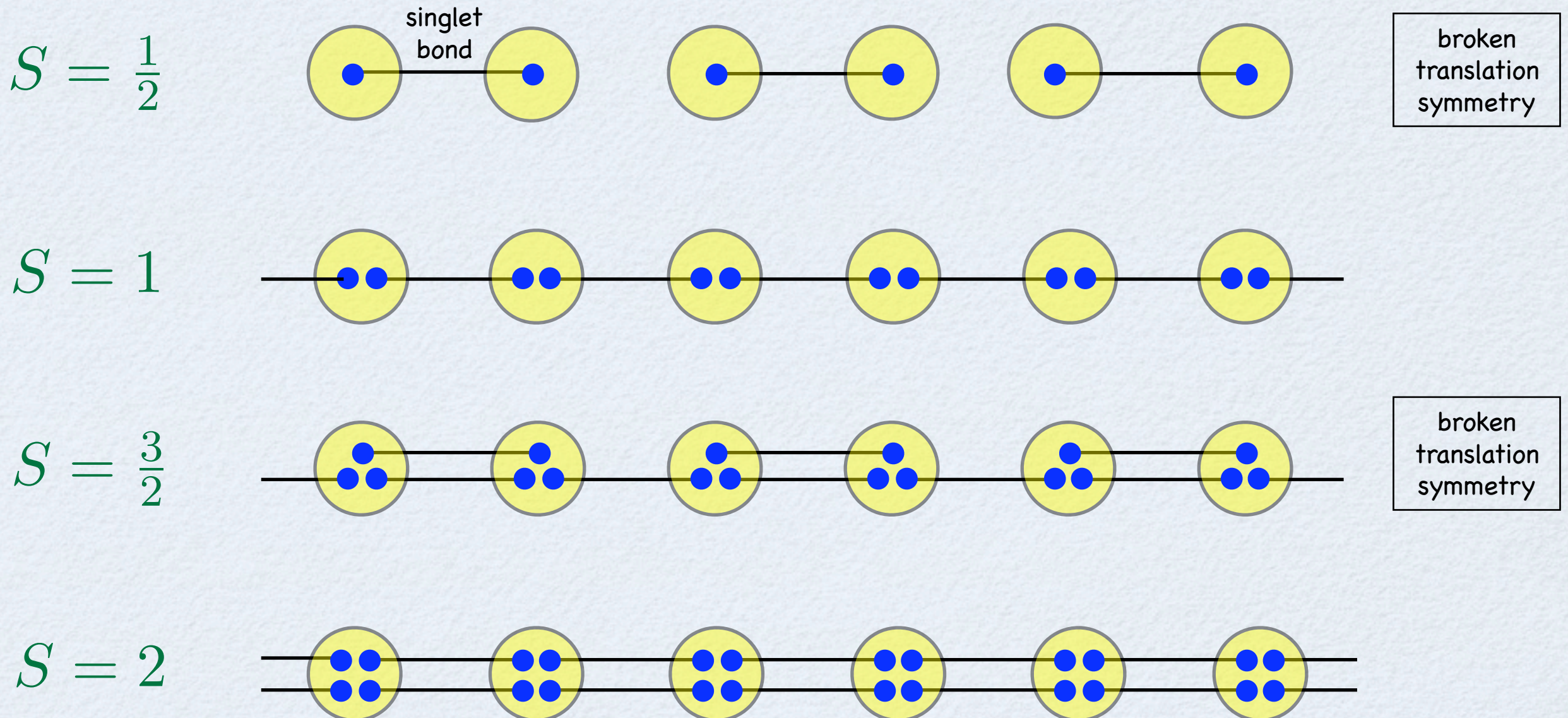


# Valence bond solid states

(Affleck, Kennedy, Lieb, and Tasaki, 1987)

Spin  $S$  from symmetrized product of  $2S$  spin- $\frac{1}{2}$  :

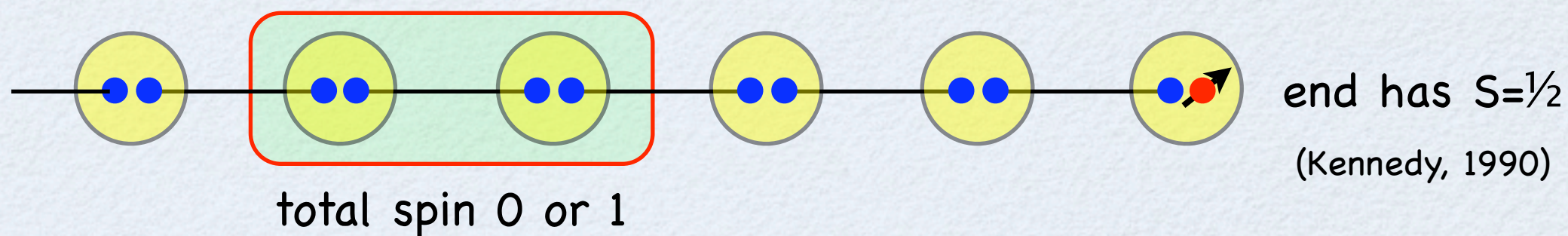
$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1, \quad \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}, \quad \text{etc.}$$





# Projection operators

S=1 AKLT chain :



projector onto total  
bond spin  $|\mathbf{S}_i + \mathbf{S}_j| = J$  :

$$P_J^{[S]}(ij) = \prod_{\substack{k=0 \\ (k \neq J)}}^{2S} \frac{(\mathbf{S}_i + \mathbf{S}_j)^2 - k(k+1)}{J(J+1) - k(k+1)}$$

this is a polynomial of order  $2S$  in  $(\mathbf{S}_i \cdot \mathbf{S}_j)$

projector onto  $J=2$  :

$$P_{J=2}^{[S=1]} = \frac{1}{6} + \frac{1}{2} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_j)^2$$

AKLT Hamiltonian :

$$\mathcal{H} = \sum_n \left[ \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \frac{1}{3} (\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2 \right]$$

bilinear

biquadratic



# Antiferromagnetic S=1 Heisenberg chain

exchange interaction      anisotropy: prefers  $S_n^z = 0$

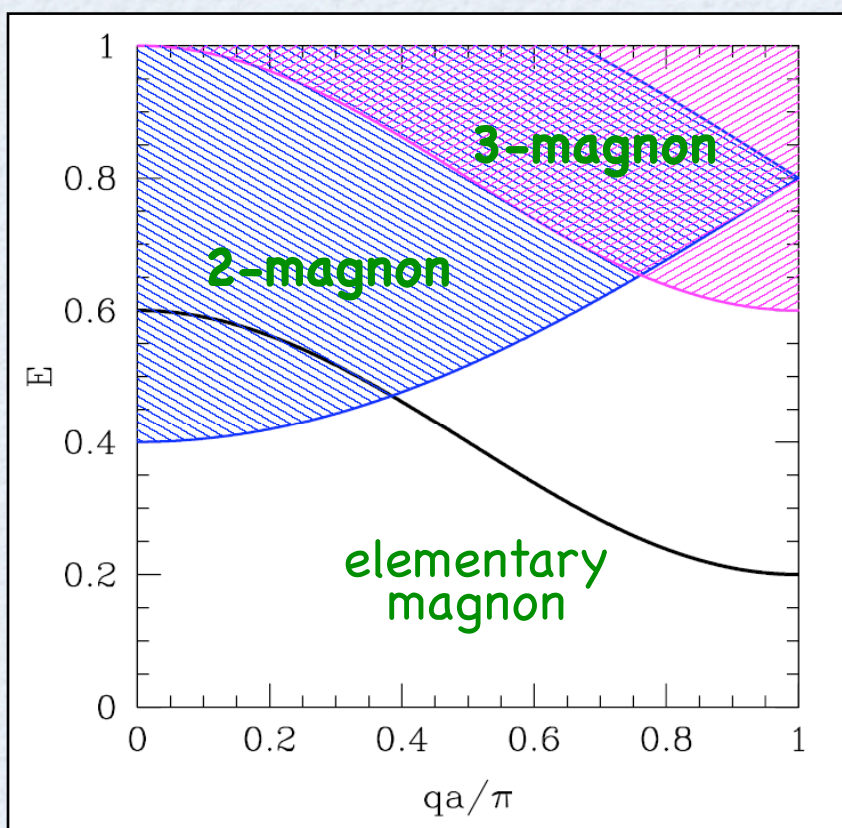
$$\mathcal{H} = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + D \sum_n (S_n^z)^2$$

The elementary excitation is a triplet (S=1) with dispersion  $\omega(\mathbf{q})$ , with an excitation gap at  $\mathbf{q}=\pi$ . matrix elements. This is the **Haldane gap**.

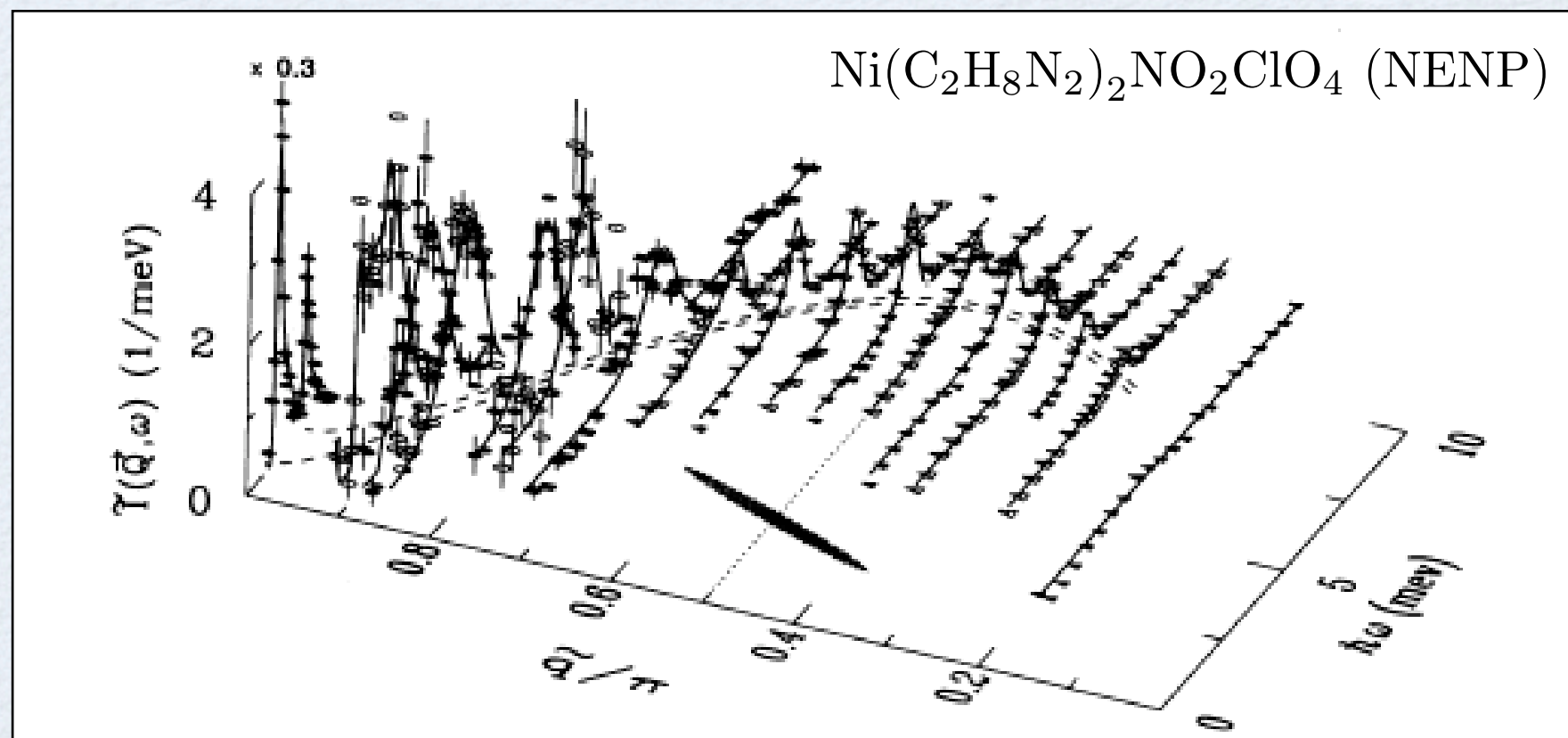
$$\langle \mathbf{S}_l \cdot \mathbf{S}_{l+n} \rangle \sim (-1)^n |n|^{-1/2} \exp(-|n|a/\xi)$$

F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983)

magnon / multimagnon continua for AKLT chain



S. Ma et al., PRL **69**, 3571 (1992)





# Schwinger bosons

DPA and Auerbach, 1988  
Read and Sachdev, 1990

Schwinger representation of SU(2):

$$S^+ = a^\dagger b \quad S^z = \frac{1}{2}(n_a - n_b)$$

$$S^- = a b^\dagger \quad 2S = n_a + n_b$$

Heisenberg interaction:

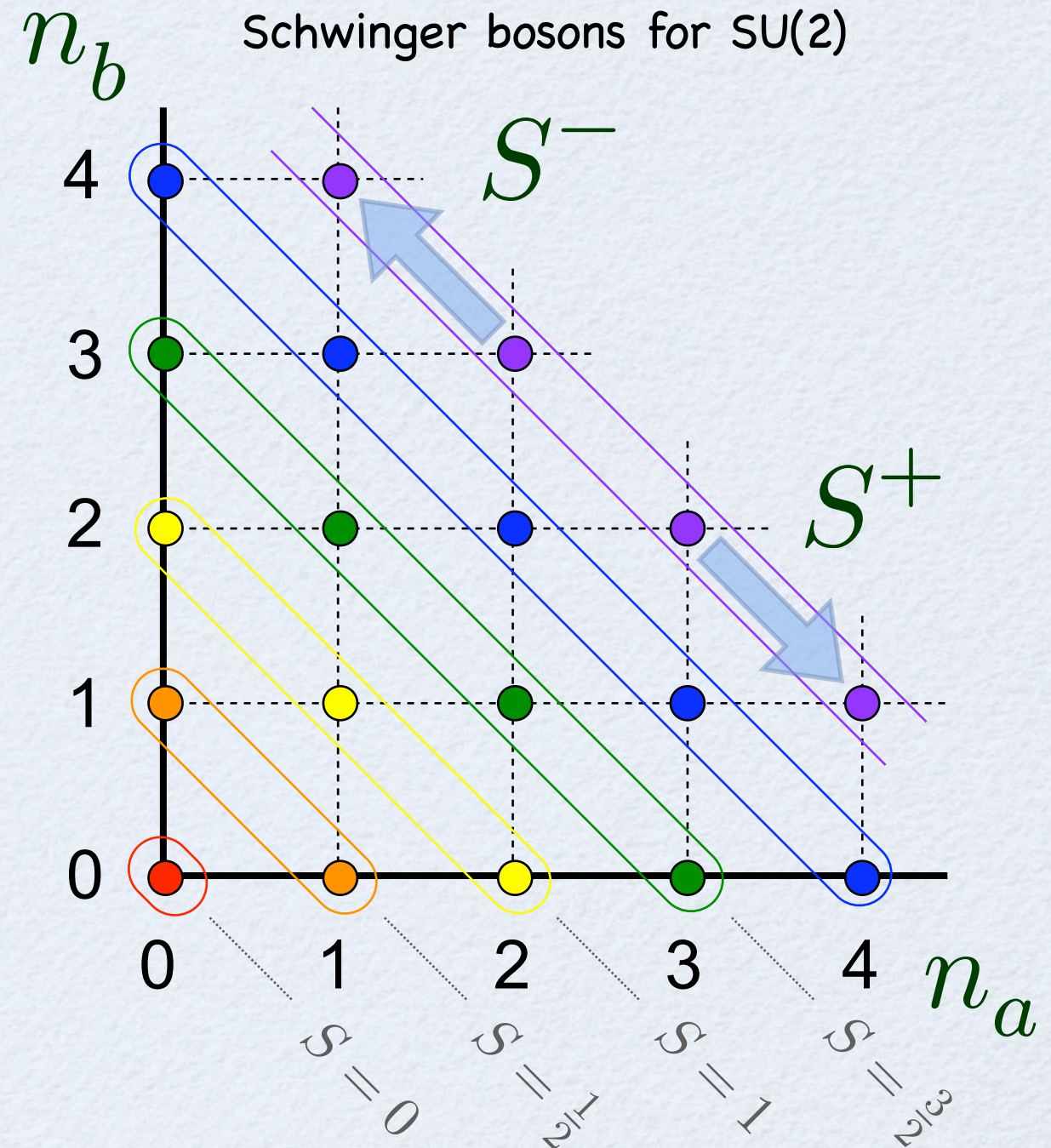
$$S_i \cdot S_j = S^2 - \frac{1}{2} A_{ij}^\dagger A_{ij}$$

$$A_{ij} = a_i b_j - b_i a_j$$

$N$  copies

$$A_{ij} = \sum_{m=1}^N (a_{im} b_{jm} - b_{im} a_{jm})$$

$$n_c = \sum_{m=1}^N (a_{im}^\dagger a_{im} + b_{im}^\dagger b_{im}) \equiv \kappa N$$



which is the Sp(N) extension

$$SU(2) \cong Sp(1) \Rightarrow \kappa = S$$

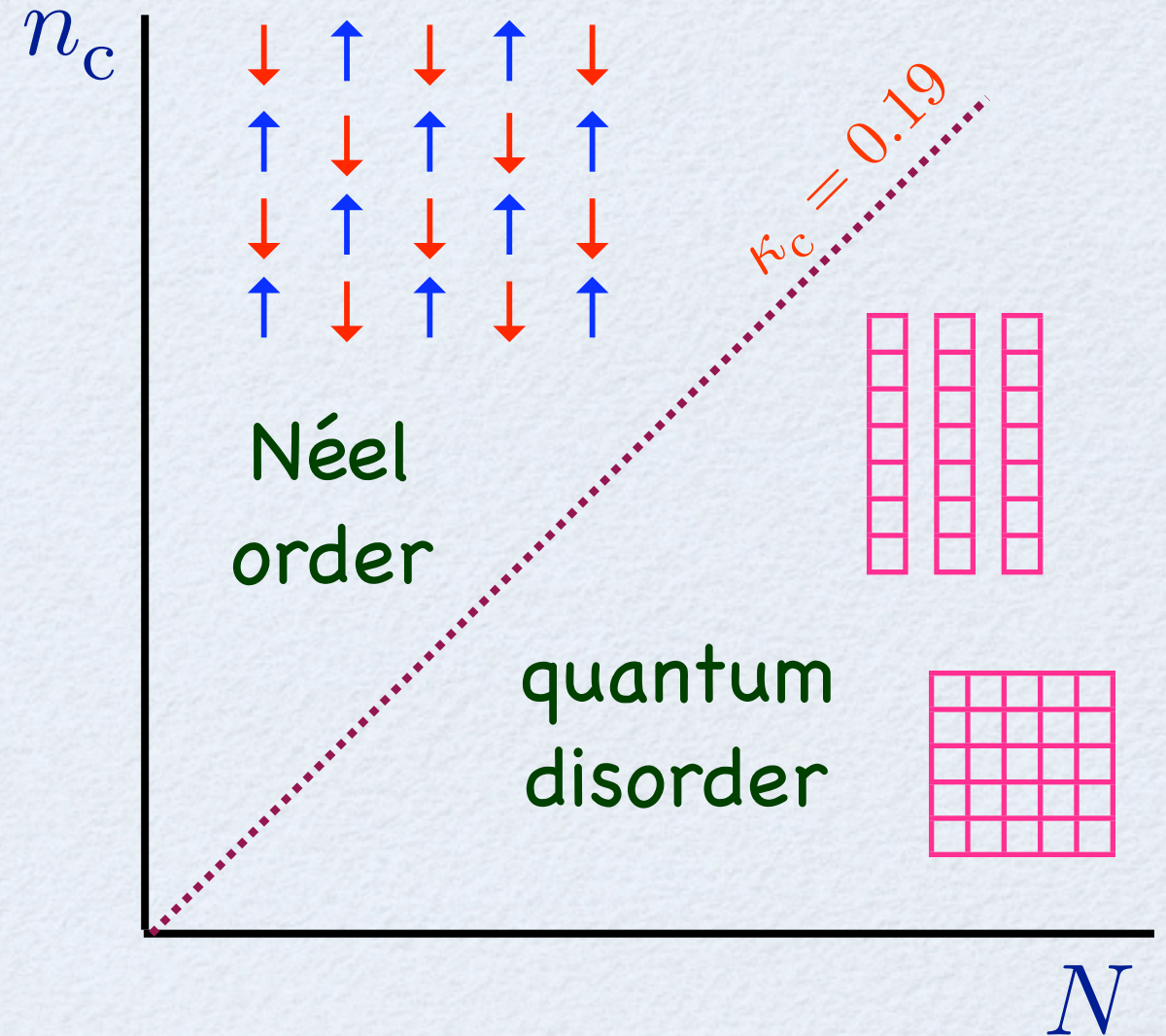


# The model: Sp(N) quantum antiferromagnet

$$A_{ij} = \sum_{m=1}^N (a_{im} b_{jm} - b_{im} a_{jm})$$

$$n_c = \sum_{m=1}^N (a_{im}^\dagger a_{im} + b_{im}^\dagger b_{im}) \equiv \kappa N$$

$$\mathcal{H} = -\frac{1}{2N} \sum_{i<j} J_{ij} A_{ij}^\dagger A_{ij}$$

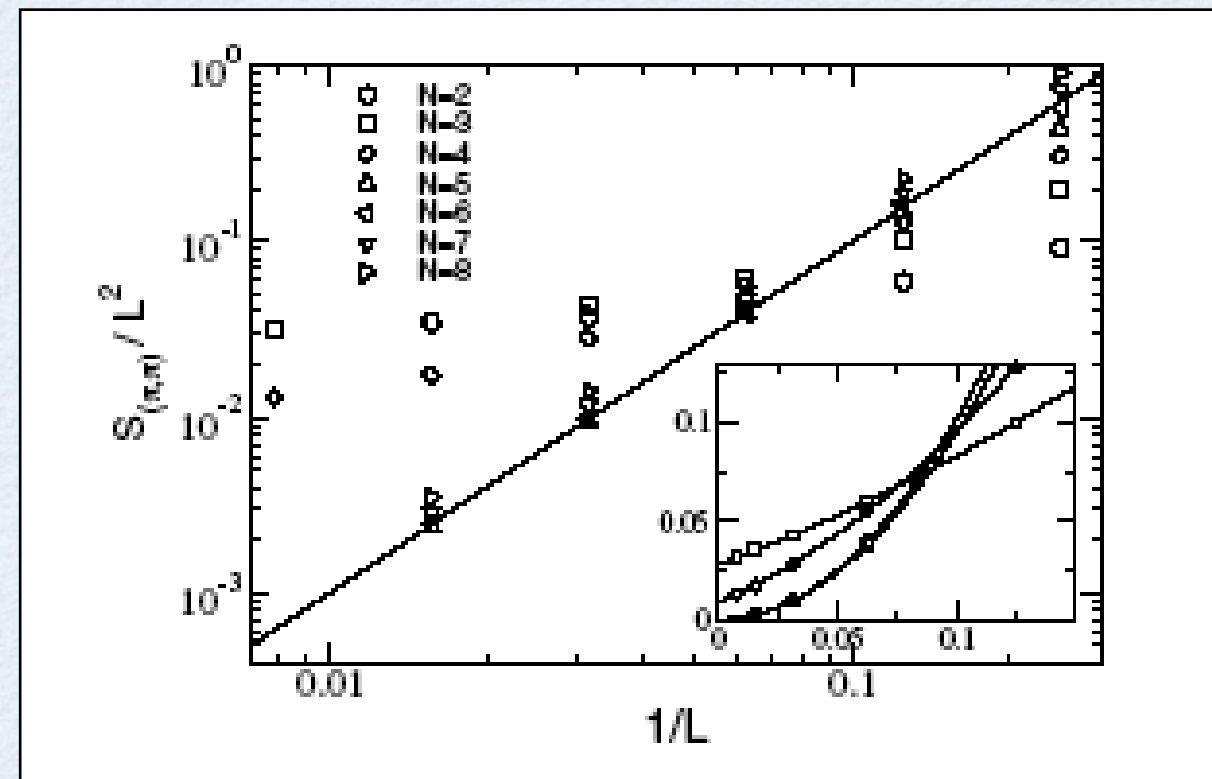


K. Harada, N. Nawashima, and M. Troyer (2003):

SU(N) antiferromagnet with  $n_c=1$  (square lattice) via quantum Monte Carlo method.

$N \leq 4$  : Néel order

$N \geq 5$  : quantum disorder  
(columnar valence bond crystal)



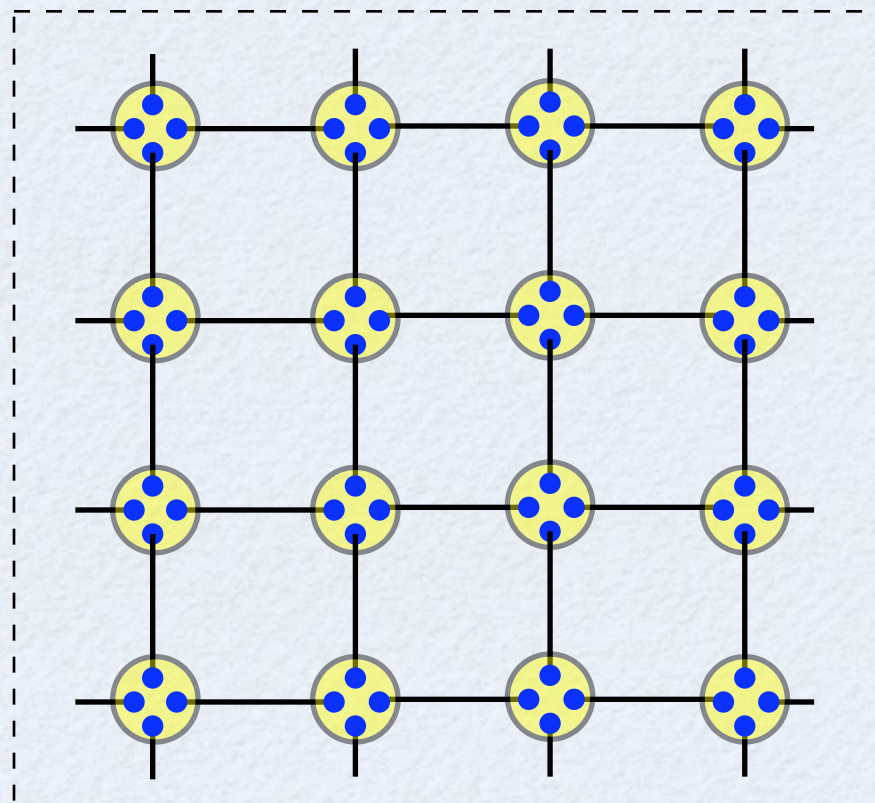


# General VBS states

(AKLT, 1987; DPA, Auerbach, Haldane, 1988)

$$|\Psi\rangle = \prod_{\langle ij\rangle} (a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger)^{m_{ij}} |0\rangle$$

Schwinger boson representation  
(local symmetrization is automatic)



$$S = 2$$

Local spin quantum number :  $S_i = \frac{1}{2} \sum_j' m_{ij}$

With  $m$  bond singlet operators per link,  
the maximum bond spin is  $J_{\max} = 2S - m$

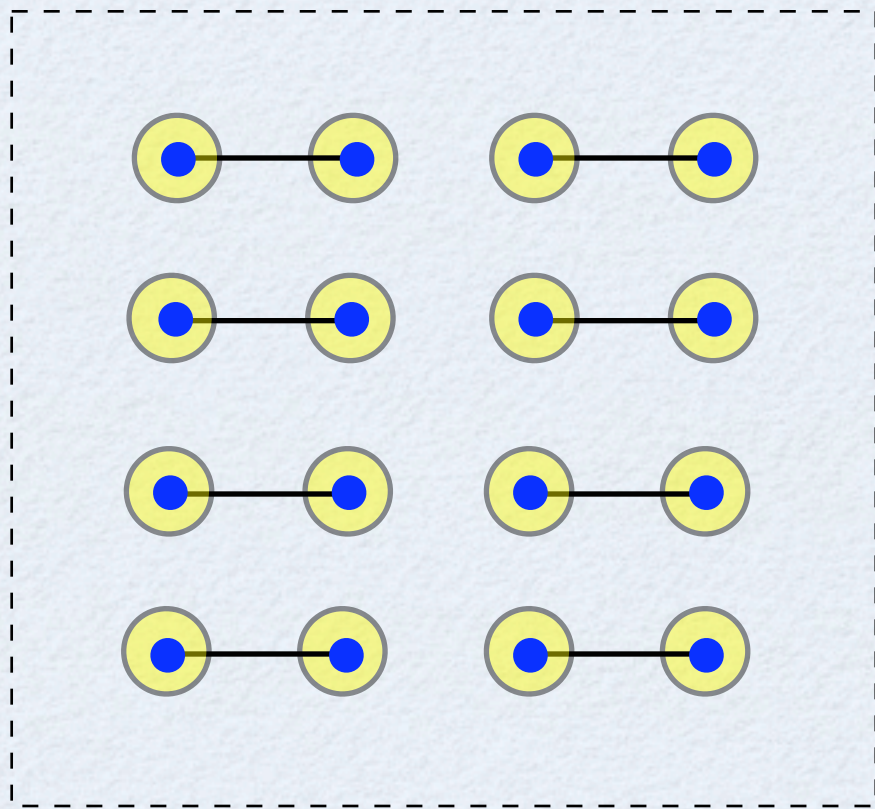
Then with  $H = \sum_{\langle ij\rangle} \sum_{J_{\max}+1}^{2S} V_J P_J^{[S]}(ij)$ ,

we have  $H |\Psi(\mathcal{L}, m)\rangle = 0$ .

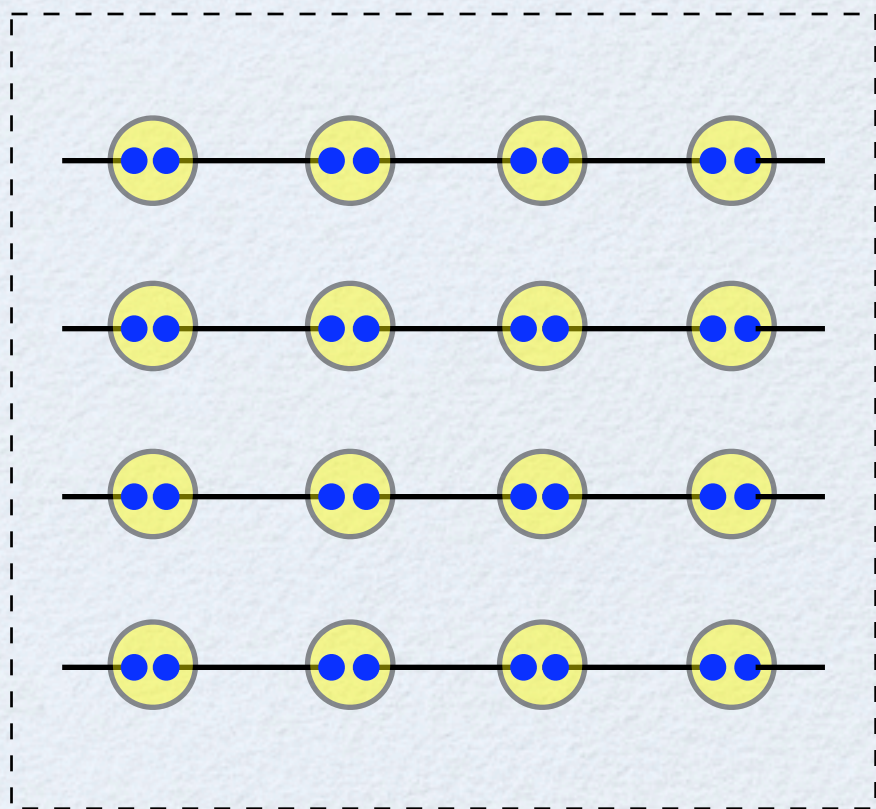
VBS states are zero energy eigenstates.

Haldane predicted ground state degeneracies in quantum disordered phases depending on  $2S \bmod 4$ . These are realized with VBC states.

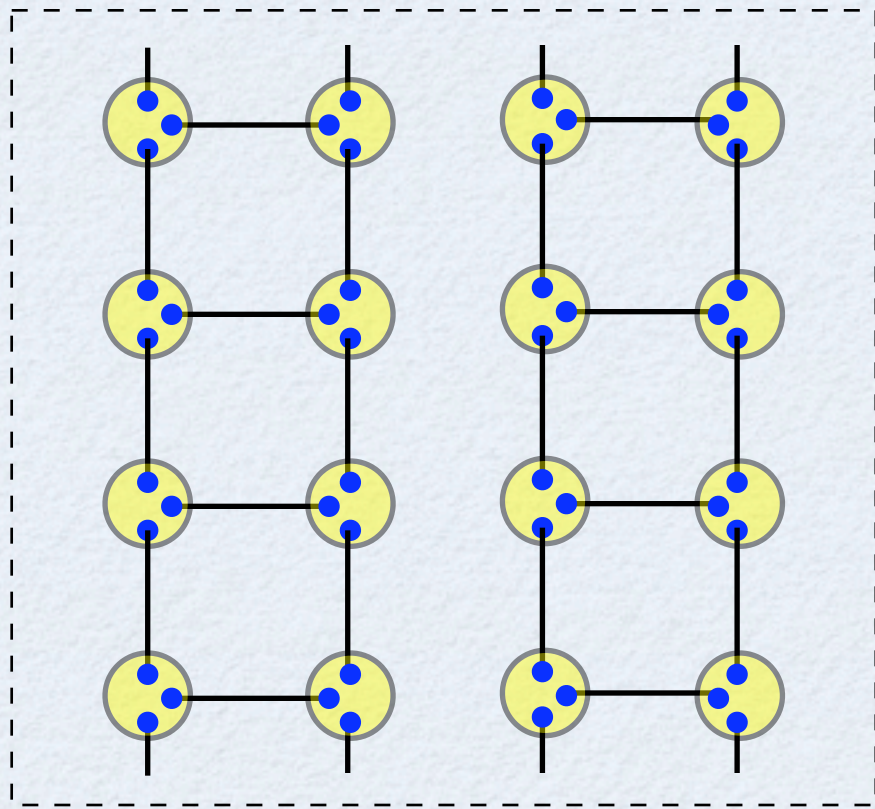




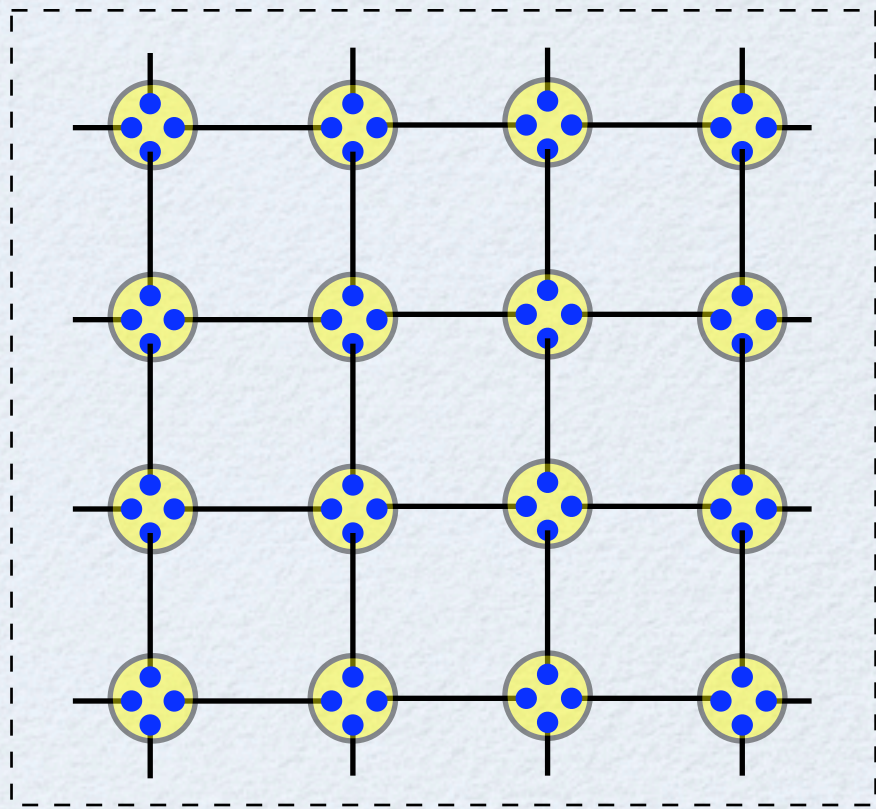
$$S = \frac{1}{2}$$



$$S = 1$$

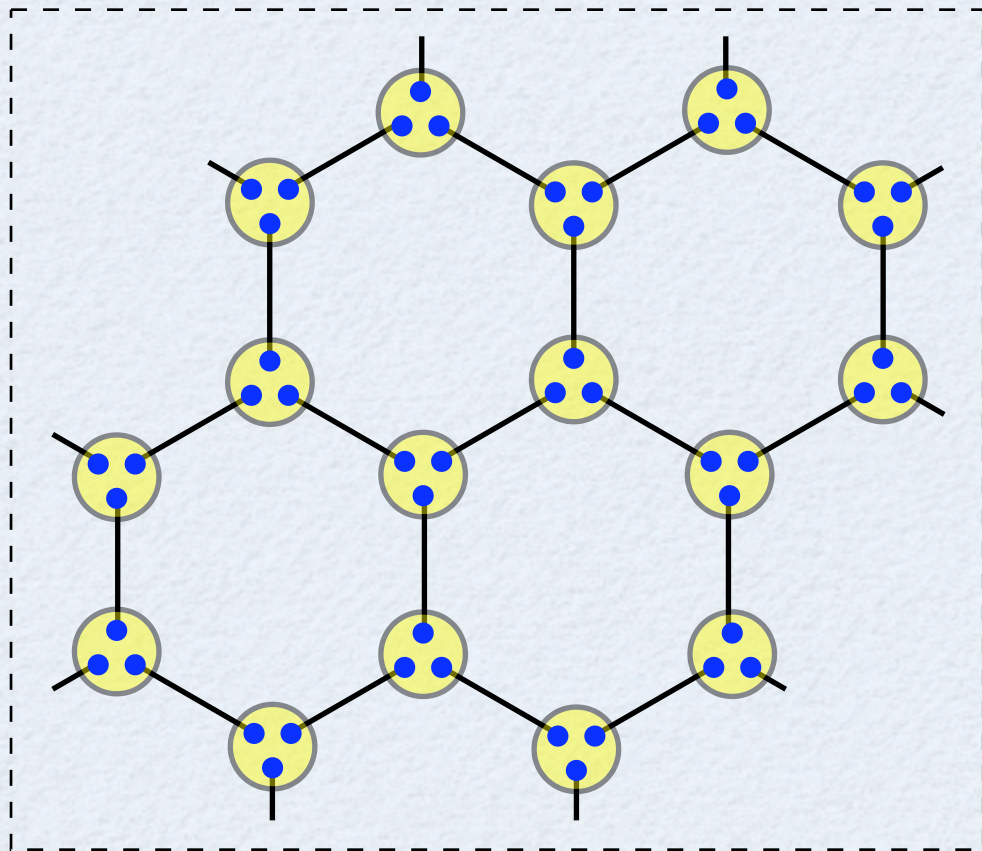


$$S = \frac{3}{2}$$

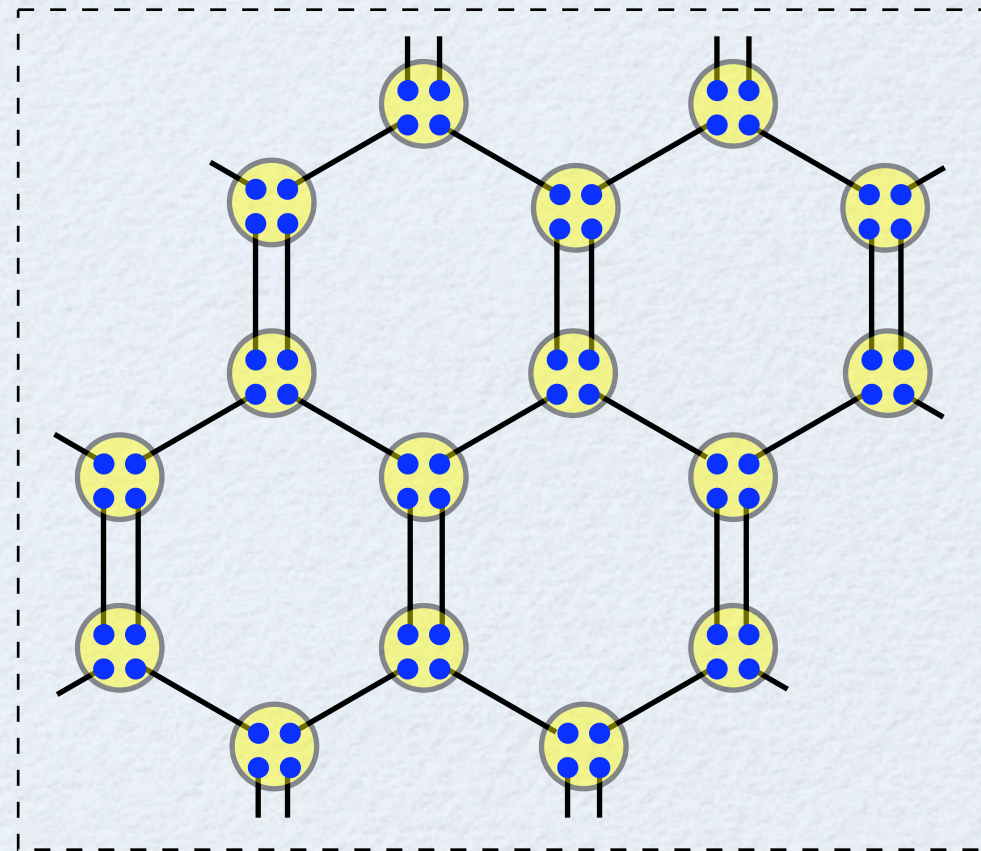


$$S = 2$$

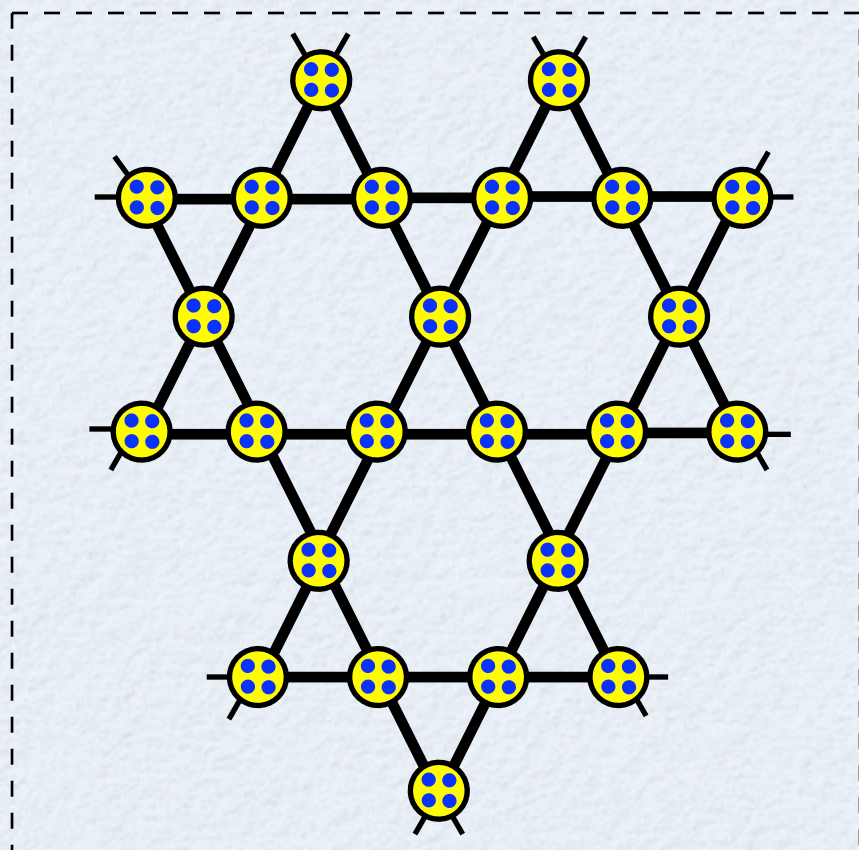




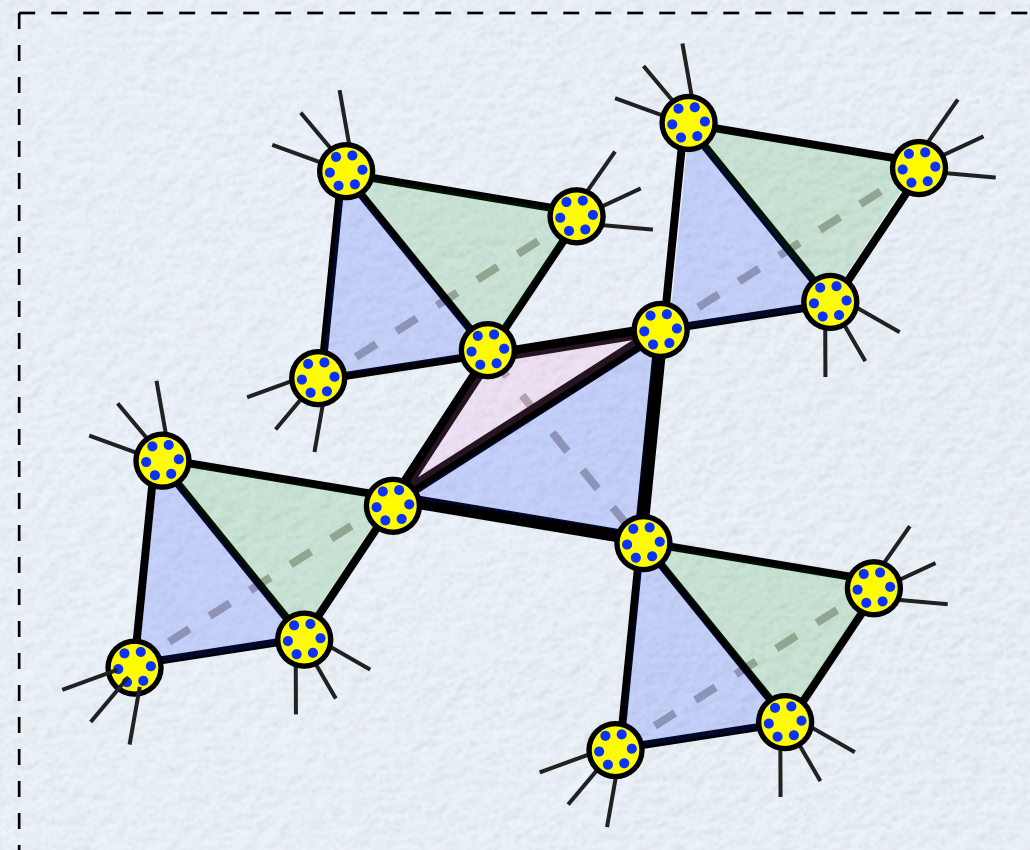
$S = 3/2$  honeycomb



$S = 2$  honeycomb



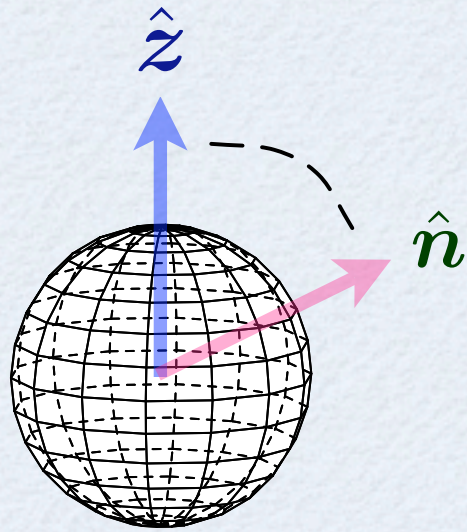
$S = 2$  Kagomé



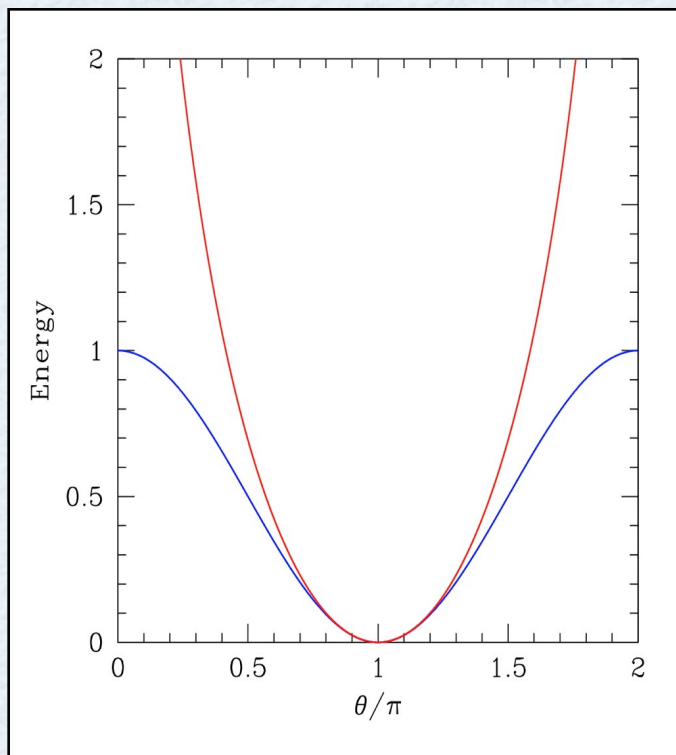
$S = 3$  pyrochlore



# Spin coherent states



$$(\hat{n} \cdot \mathbf{S}) |\hat{n}\rangle = S |\hat{n}\rangle$$



$$|\hat{n}\rangle = (2S!)^{-1} (ua^\dagger + vb^\dagger)^{2S} |0\rangle$$

$$u = \cos\left(\frac{1}{2}\theta\right)$$

$$v = \sin\left(\frac{1}{2}\theta\right) e^{i\phi}$$

matrix elements :  $\langle \Phi | \hat{T} | \Psi \rangle = \int \frac{d\hat{n}}{4\pi} \Phi^*(\hat{n}) T(\hat{n}) \Psi(\hat{n})$

$$\Psi_{\text{AKLT}}[\hat{n}] = \prod_{\langle ij \rangle} (u_i v_j - v_i u_j)^m$$

$$|\Psi_{\text{AKLT}}|^2 = \prod_{\langle ij \rangle} \left( \frac{1 - \hat{n}_i \cdot \hat{n}_j}{2} \right)^m \equiv e^{-H_{\text{cl}}/T}$$

classical model :  $H_{\text{cl}} = - \sum_{\langle ij \rangle} \ln \sin^2\left(\frac{1}{2}\vartheta_{ij}\right)$

temperature :  $T = \frac{1}{m}$

All equal time quantum correlations in the AKLT states may be computed as the **finite temperature** ( $T=m^{-1}$ ) correlations of a related **classical** model  $H_{\text{cl}}$  on the **same lattice**



# VBS as a Matrix Product State

Matrix product states (d=1) :

Klümper, Schadschneider, Zittarz, 1991  
Fannes, Nachtergaele, Werner, 1992  
Rommer and Ostlund, 1995  
Verstraete, Porras, Cirac 2004

$$|\Psi\rangle = \sum_{\{\sigma_n\}} \text{Tr} (A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_N}) |\sigma_1 \sigma_2 \cdots \sigma_N\rangle$$

Local Hilbert space :  $|\sigma\rangle$  ,  $\sigma \in \{1, \dots, d_L\}$  ,  $A \in \text{GL}(n, \mathbb{C})$

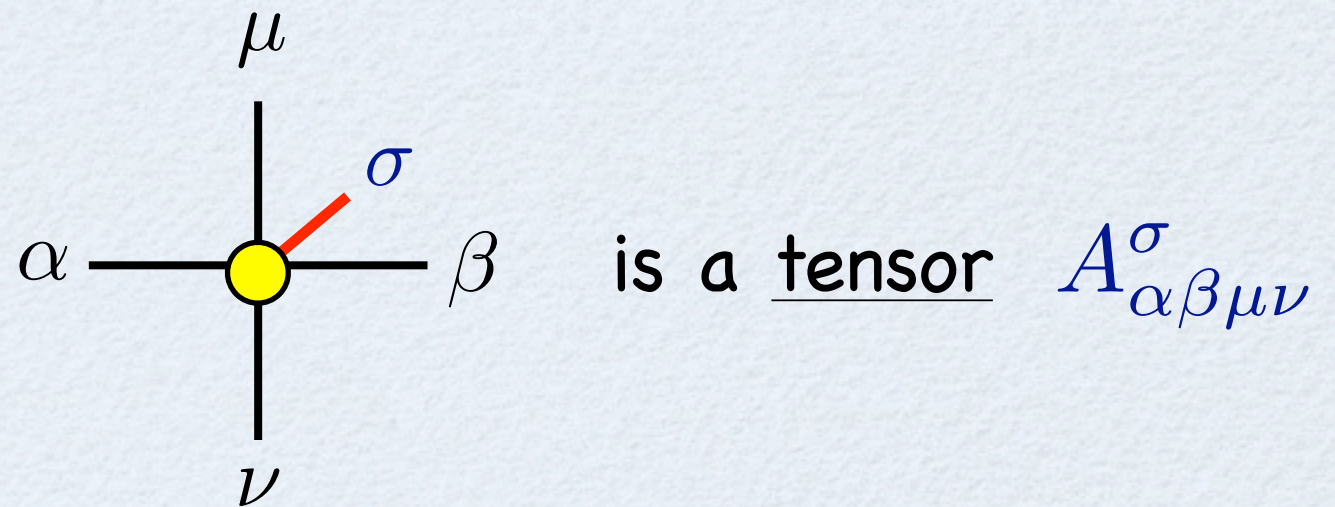
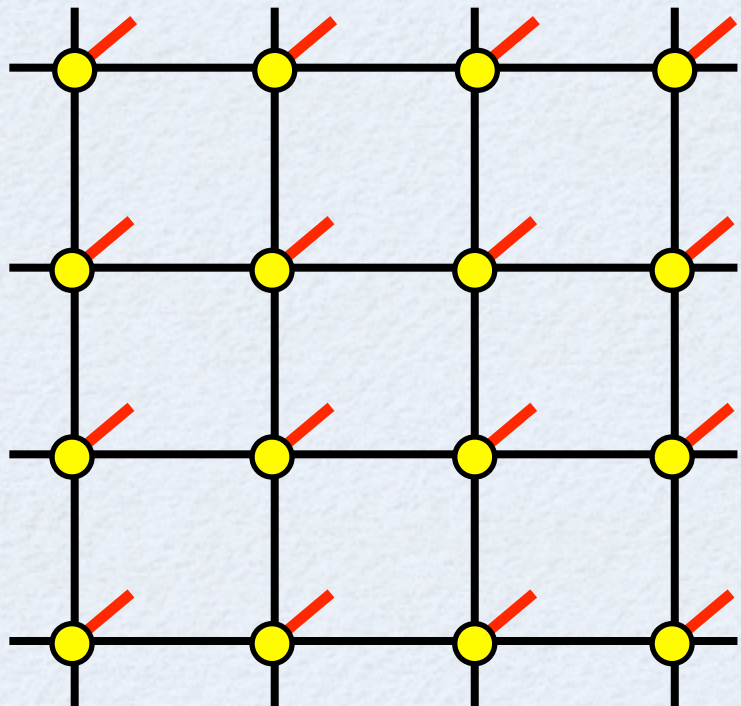
$$\begin{aligned} \text{S=1 VBS chain : } \Psi[Z] &= \prod_n \epsilon^{\mu\nu} z_{n,\mu} z_{n+1,\nu} \\ &= \cdots (z_{n-1,\rho} \epsilon^{\mu\nu} z_{n-1,\mu}) (z_{n,\nu} \epsilon^{\alpha\beta} z_{n,\alpha}) (z_{n+1,\beta} \epsilon^{\sigma\tau} z_{n+1,\sigma}) \cdots \\ &= \text{Tr} [M(z_1)M(z_2) \cdots M(z_N)] \end{aligned}$$

with  $M_{\mu\nu}(z) = z_\mu \tilde{z}_\nu$  , where  $z = \begin{pmatrix} u \\ v \end{pmatrix}$  ,  $\tilde{z} = \begin{pmatrix} -v \\ u \end{pmatrix}$

In the discrete basis,  $A_{\mu\nu}^\sigma = L_\mu^\sigma R_\nu^\sigma$  , a restricted class of MPS



# General VBS as a Tensor Product State



$$|\Psi_{\text{TPS}}\rangle = \sum_{\{\sigma_i\}} \mathcal{C} \left( \prod_i A^{\sigma_i} \right) |\sigma_1, \dots, \sigma_N\rangle$$

contract tensor indices on links

For the general VBS state,  $A_{\alpha\beta\mu\nu}^{\sigma} = N_{\mu}^{\sigma} S_{\nu}^{\sigma} W_{\alpha}^{\sigma} E_{\beta}^{\sigma}$

The contractions are now trivial, e.g.  $N_{\mu}^{\sigma_{m,n}} S_{\mu}^{\sigma_{m,n+1}} \equiv e^{-\phi(\sigma_{m,n}, \sigma_{m,n+1})}$

Correlations are those of an associated classical model :

$$|\Psi_{\sigma_1, \dots, \sigma_N}\rangle^2 = \exp \left( - \sum_{\langle ij \rangle} V(\sigma_i, \sigma_j) \right)$$



# VBS phase transition

Parameswaran, Sondhi, DPA  
arXiv cond-mat/0807.3189

Recall  $H_{\text{cl}} = - \sum_{\langle ij \rangle} \ln \left( \frac{1 - \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j}{2} \right)$  with  $T = \frac{1}{m}$

Mean field theory :  $\hat{\mathbf{n}}_i = \mathbf{m}_i + \delta \hat{\mathbf{n}}_i$  ,  $\langle \hat{\mathbf{n}}_i \rangle = \mathbf{m}_i$  ,  $\hat{h}_i = - \sum_j' \frac{\mathbf{m}_j}{1 - \mathbf{m}_i \cdot \mathbf{m}_j}$

MF Hamiltonian :  $H_{\text{cl}}^{\text{MF}} = - \sum_i \mathbf{h}_i \cdot \hat{\mathbf{n}}_i$  , self-consistency :  $\mathbf{m}_i = \coth \left( \frac{h_i}{T} \right) - \frac{T}{h_i}$

Assuming a uniform solution on a bipartite lattice,  $h = zm / (1 + m^2)$  , and

$$T_c^{\text{MF}} = \frac{z}{3} \Leftrightarrow m_c^{\text{MF}} = \frac{3}{z}$$

**VBS states with  $m > m_c$  will have Néel order, hence if  $m_c < 1$  ( $T_c > 1$ )  
on a given lattice, all VBS states on that lattice will be ordered**

Since all lattices in  $d > 2$  dimensions have  $z > 3$ , MFT predicts no quantum disorder  
However, MFT overestimates  $T_c$ , hence underestimates  $m_c$  - there may be hope!

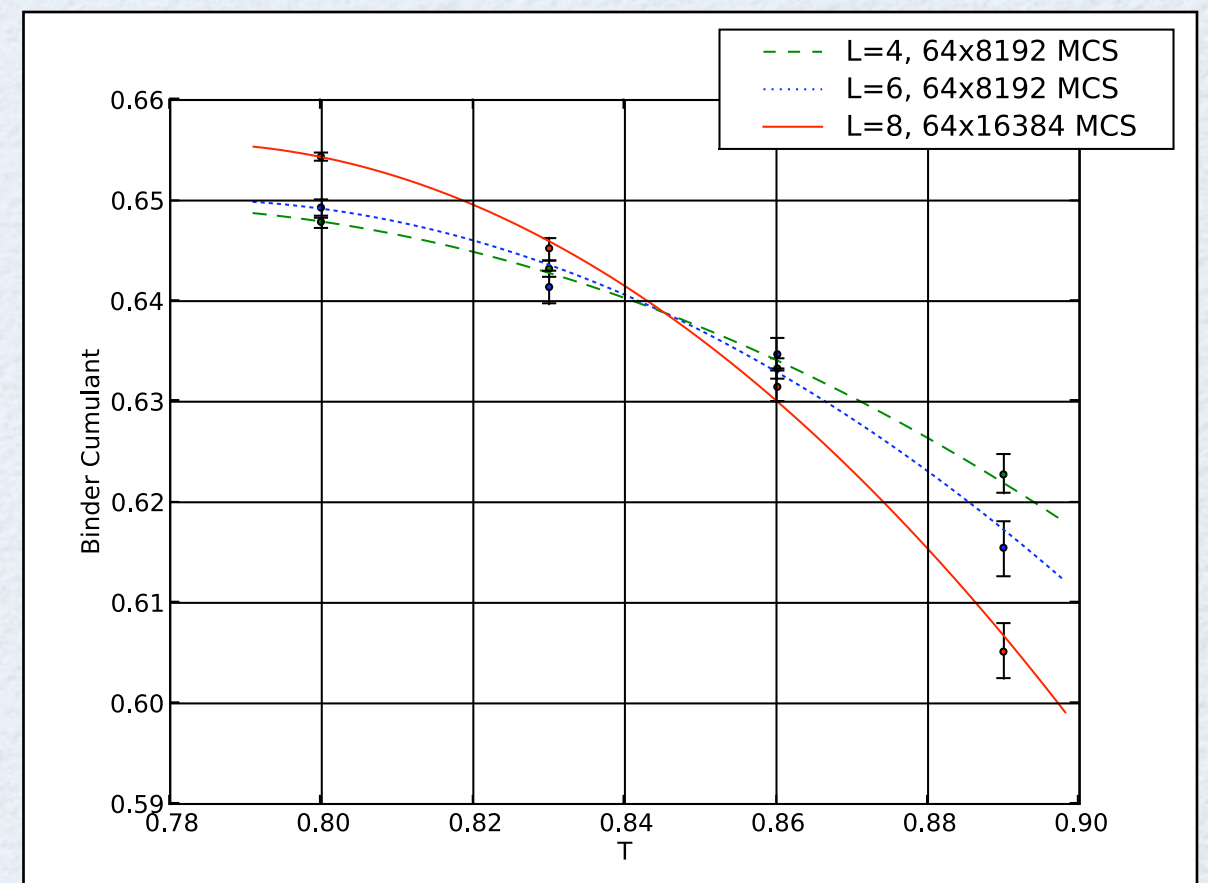
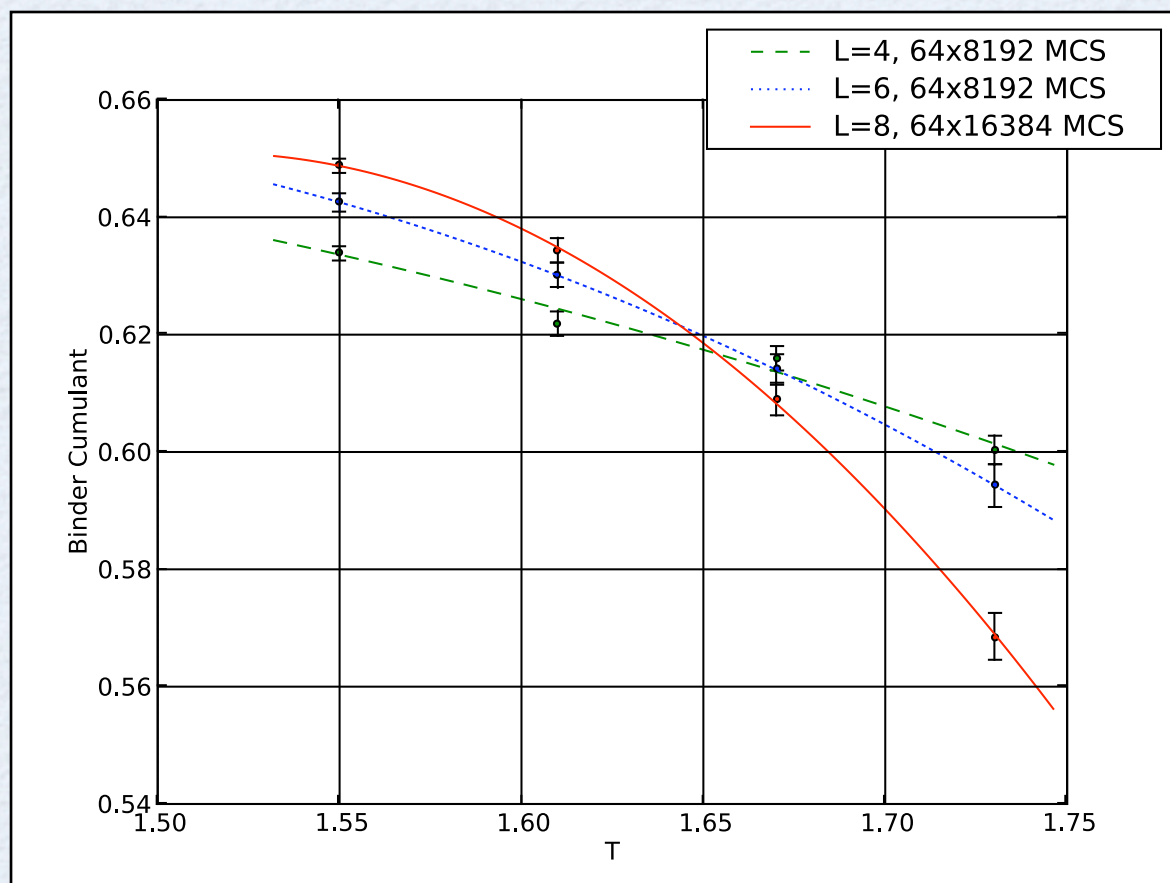


# The phase transition can be investigated using classical Monte Carlo

- Simple single-spin Metropolis algorithm
- 'Multithreaded' Monte Carlo: run  $M$  Markov chains with  $N$  sites each; reject first  $N/2$  sites and use the rest to average
- Unbiased error estimate from standard deviation of the  $M$  independent averages
- Test using high temperature expansion,  $T_c$  for known models; MFT gives  $T_c^{MF} = z/3$
- Estimate  $T_c$  using Binder cumulant crossing  $B = 1 - \frac{\langle (M^2)^2 \rangle}{3\langle M^2 \rangle^2}$  ,  $M = \sum_i \eta_i \hat{n}_i$

simple cubic lattice :  $T_c=1.64$  ( $T_c^{MF}=2$ )

diamond lattice :  $T_c=0.834$  ( $T_c^{MF}=1.33$ )





# Pyrochlore VBS state

Parameswaran, Sondhi, DPA, Moessner

-  $z=6$    $S = 3m$

- highly frustrated lattice, with corner-sharing tetrahedra and kagomé planes

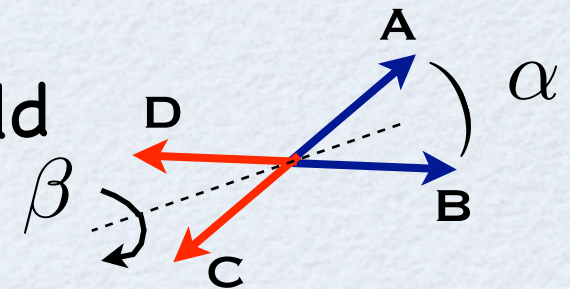
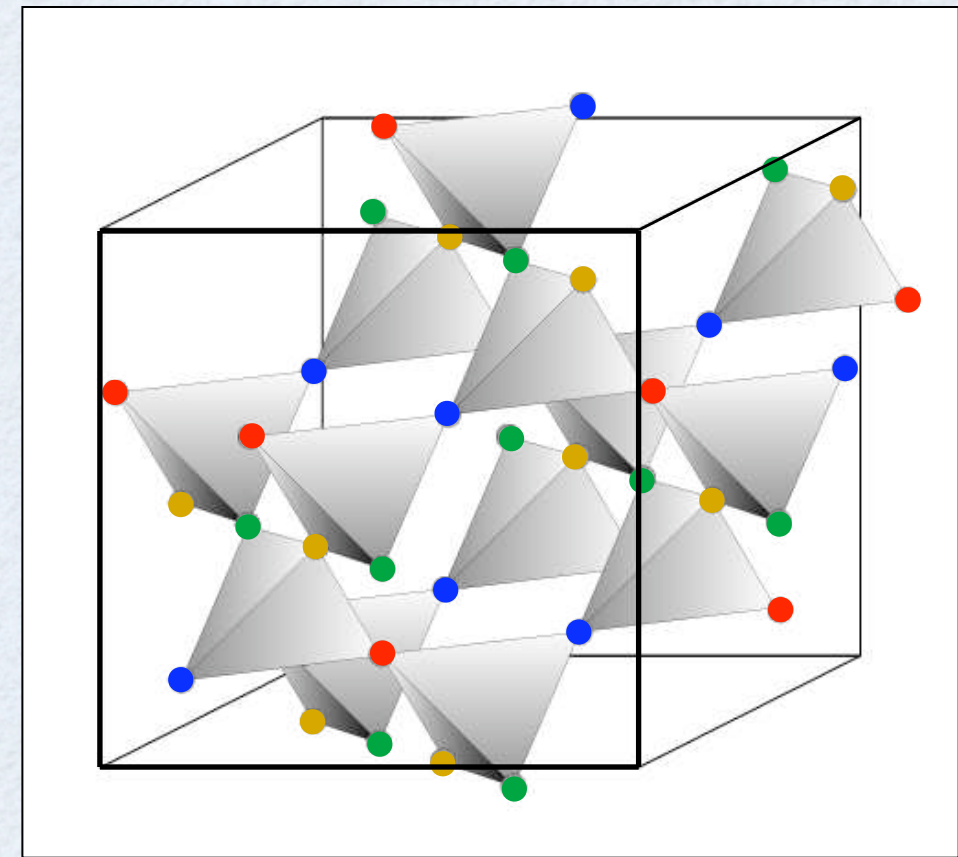
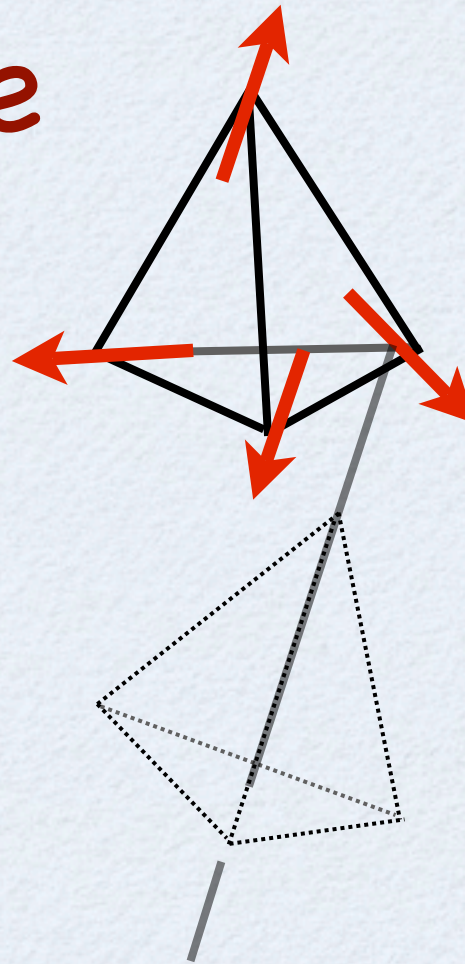
- Heisenberg AFM on tetrahedron

$(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2$  has **five**-dimensional ground state manifold (two DOF plus global  $O(3)$  rotations)

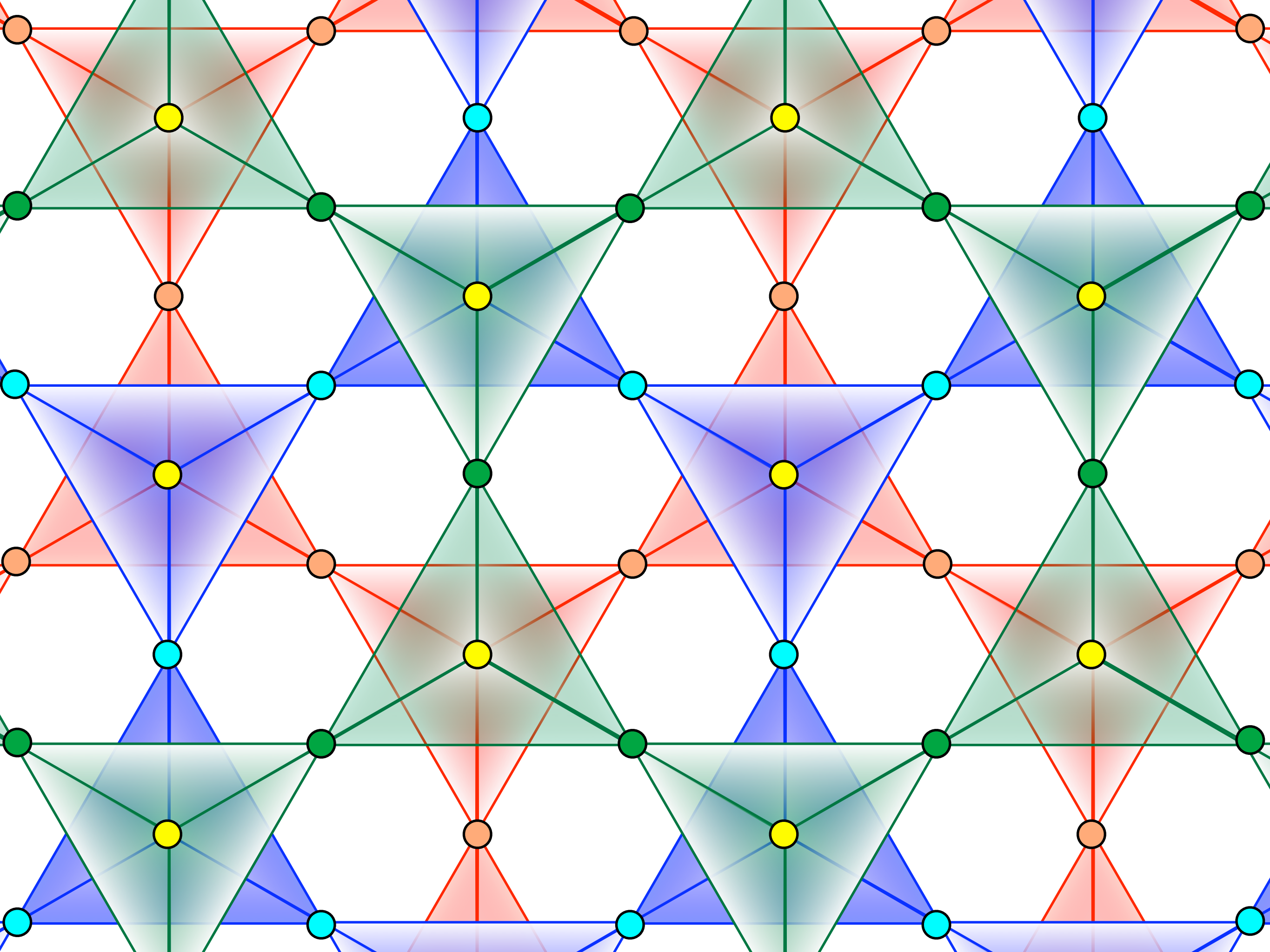
- Large- $N$  analysis of pyrochlore Heisenberg AFM (Isakov et al., 2004) finds system is paramagnetic down to  $T=0$

- AKLT  $H_{cl}$  has unique single tetrahedron ground state up to global  $O(3)$ , no local zero modes -- "order by disorder" at sufficiently low  $T$  ???

- Topology of ground state manifold not simply connected









# Simplex Solids

DPA, 2008

- generalization of VBS states to  $SU(N)$
- For  $SU(2)$ , we can always create a singlet with two spin- $S$  objects :

$$S \otimes S = 0 \oplus 1 \oplus 2 \oplus \dots \oplus 2S$$

This is no longer the case if  $SU(2)$  is replaced with  $SU(N)$ .

E.g. for  $SU(3)$ ,

$$\begin{array}{c} \square \\ \mathbf{3} \end{array} \otimes \begin{array}{c} \square \\ \mathbf{3} \end{array} = \begin{array}{c} \square \\ \square \\ \mathbf{\bar{3}} \end{array} \oplus \begin{array}{c} \square \quad \square \\ \mathbf{6} \end{array}$$

- Two ways to make singlets from  $SU(N)$  :

1. On bipartite lattices, use conjugate representation on B sublattice:

$$N \otimes \bar{N} = \bullet_1 \oplus \text{adj}_{N^2-1}$$

(this is the scheme originally used in the large- $N$  'Schwinger boson' MFT)

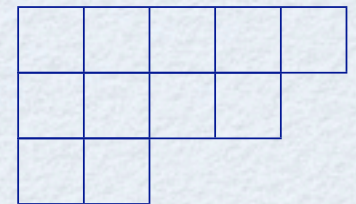


2. Retain same representation, but extend singlet over N lattice sites:

$$|\Gamma\rangle = \epsilon^{\alpha_1 \dots \alpha_N} b_{\alpha_1}^\dagger(i_1) \dots b_{\alpha_N}^\dagger(i_N) |0\rangle$$

For N=3, this is the color singlet from QCD.

Representations of SU(N) classified by Young tableaux :



We will assume each site in (p,0) representation



SU(N) spin operators:

$$S_{\beta}^{\alpha} = b_{\alpha}^{\dagger} b_{\beta} - \frac{p}{N} \delta_{\alpha\beta} \quad (\text{N flavors of Schwinger bosons})$$

$$\text{SU(N) algebra : } [S_{\beta}^{\alpha}, S_{\nu}^{\mu}] = \delta_{\beta\mu} S_{\nu}^{\alpha} - \delta_{\alpha\nu} S_{\mu}^{\beta}$$



Define the N-simplex singlet creation operator,

$$\mathcal{R}_\Gamma^\dagger = \epsilon^{\alpha_1 \dots \alpha_N} b_{\alpha_1}^\dagger(\Gamma_1) \dots b_{\alpha_N}^\dagger(\Gamma_N)$$

This is the generalization of  $a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger$  for SU(2)

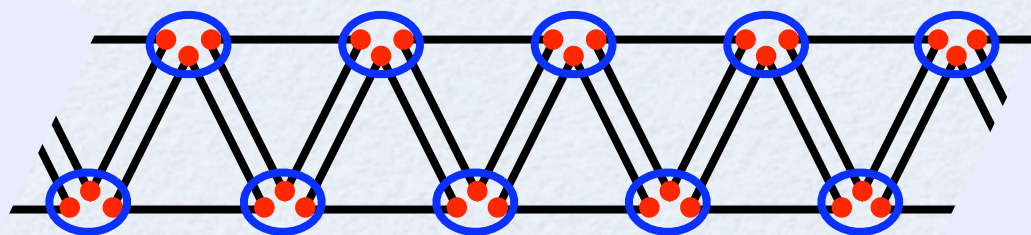
The general simplex solid wavefunction is then given by

$$|\Psi(\mathcal{L}; M)\rangle = \prod_\Gamma (\mathcal{R}_\Gamma^\dagger)^M |0\rangle \quad \text{with} \quad p = \zeta M$$

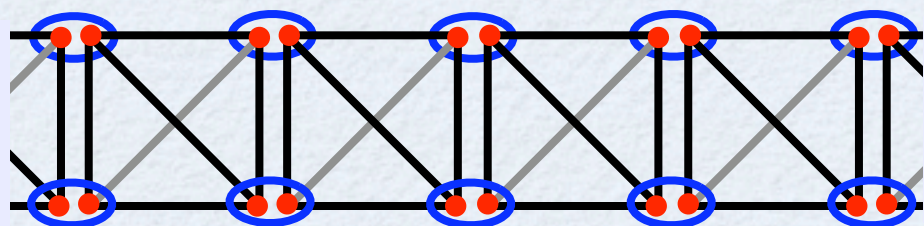
$\zeta =$  number of simplices associated with each site

Two examples in  $d=1$ :

SU(3)



SU(4)



$$\begin{array}{|c|c|c|} \hline & & \\ \hline \end{array} \otimes \begin{array}{|c|c|c|} \hline & & \\ \hline \end{array} =$$

10                      10

$$\begin{array}{|c|c|c|} \hline & & \\ \hline & & \\ \hline \end{array} \oplus \begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline \end{array} \oplus$$

10                      27

$$\begin{array}{|c|c|c|c|c|} \hline & & & & \\ \hline \end{array} \oplus \begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline \end{array}$$

28                      35

missing representations



SU(3) fits nicely on the kagomé :

$$|\Psi\rangle = \prod_{\triangle} \mathcal{R}_{\triangle}^{\dagger} \prod_{\nabla} \mathcal{R}_{\nabla}^{\dagger} |0\rangle$$

$$\begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array} \otimes \begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array} = \begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array} \oplus \begin{array}{|c|c|} \hline \square & \square & \square \\ \hline \end{array} \oplus \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \end{array}$$

6                      6                      6                      15                      15

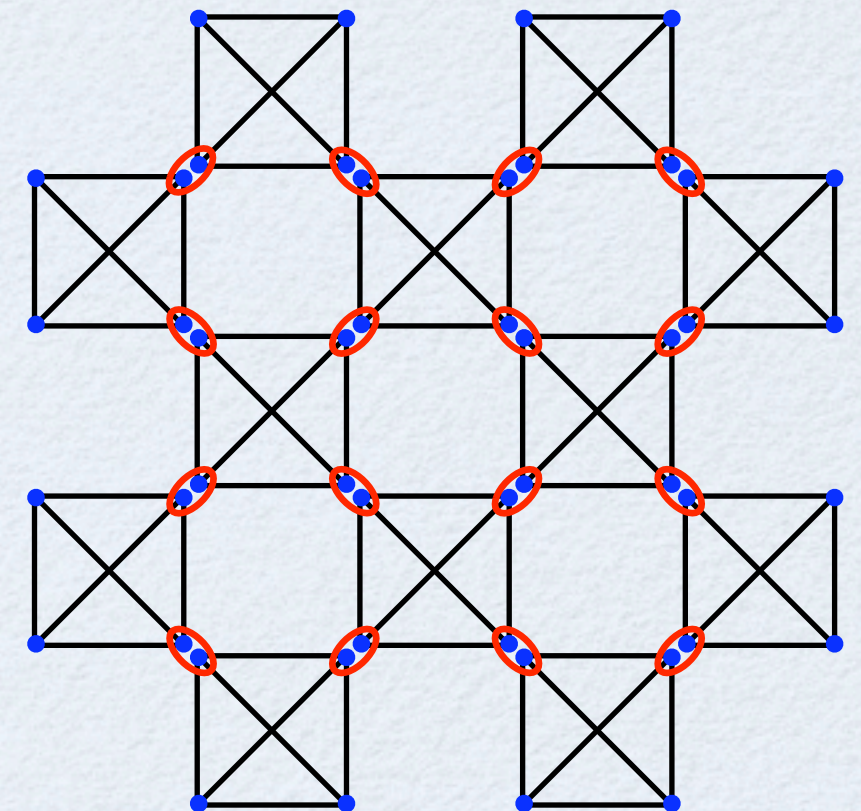
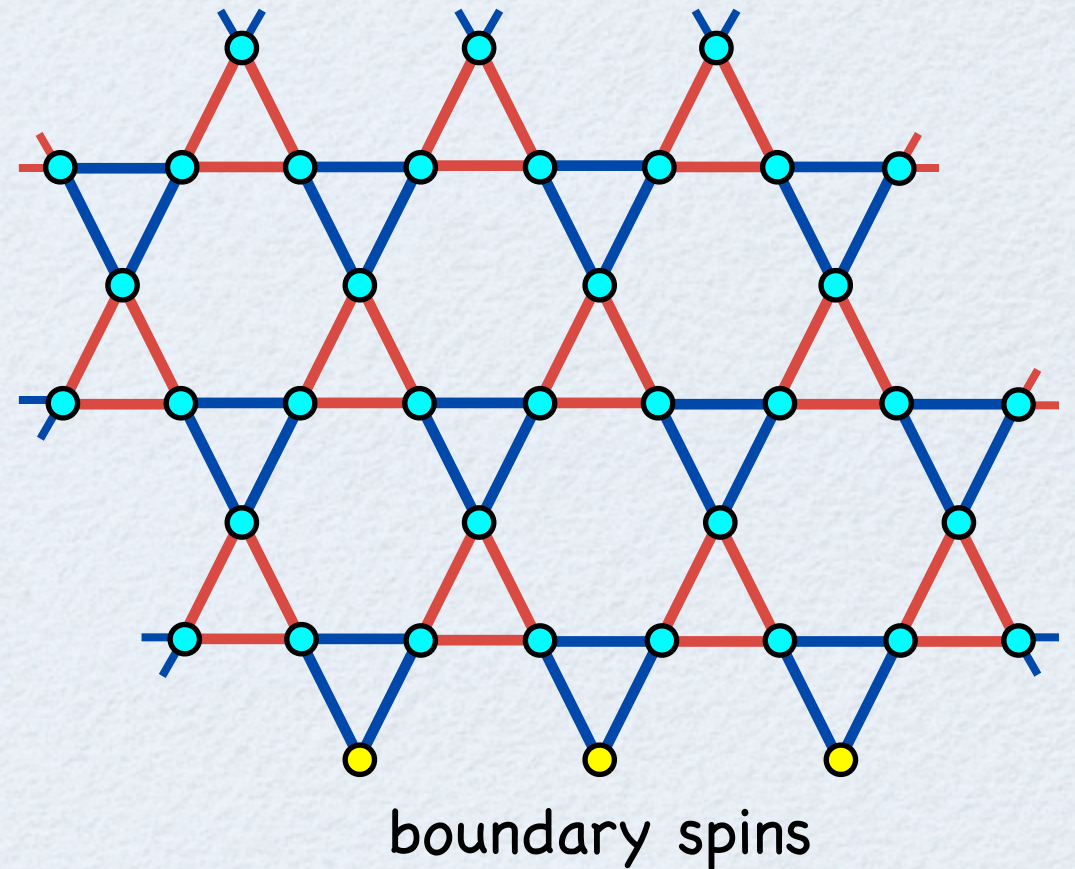
Hamiltonian :  $\mathcal{H} = \sum_{\langle ij \rangle} P_{\square\square\square}(ij)$

### Fractionalization at the edge

Bulk spins  $\bullet$  in  $\begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}$  representation  
6

while boundary spins  $\bullet$  in  $\begin{array}{|c|} \hline \square \\ \hline \end{array}$   
3

Recapitulates situation for AKLT states



$\begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}$  SU(4) state on checkerboard  
10



## Classical simplex Hamiltonian

SU(N) coherent states :  $|z; p\rangle = \frac{1}{\sqrt{p!}} \left( z_1 b_1^\dagger + \dots + z_N b_N^\dagger \right)^p |0\rangle$

Find  $|\Psi|^2 = \prod_{\Gamma} |R_{\Gamma}|^{2M} = e^{-H_{cl}/T}$  with  $H_{cl} = - \sum_{\Gamma} \ln |R_{\Gamma}|^2$

where  $|R_{\Gamma}|^2 = \epsilon^{\alpha_1 \dots \alpha_N} \epsilon^{\beta_1 \dots \beta_N} Q_{\alpha_1 \beta_1}(\Gamma_1) \dots Q_{\alpha_N \beta_N}(\Gamma_N)$  and  $Q_{\alpha\beta}(i) = \bar{z}_{\alpha}(i) z_{\beta}(i)$

Mean field ansatz:  $Q_{\alpha\beta}(i = \Gamma_{\sigma}) = \frac{1}{N} \delta_{\alpha\beta} + \underbrace{m}_{\text{order parameter}} \left( \underbrace{P_{\alpha\beta}^{\sigma}}_{\text{projector}} - \frac{1}{N} \delta_{\alpha\beta} \right) + \delta Q_{\alpha\beta}(i)$

Find  $M_c^{\text{MF}}(N, \zeta) = \frac{1}{T_c^{\text{MF}}(N, \zeta)} = \frac{N^2 - 1}{\zeta} = \frac{\text{\# directions Q can fluctuate}}{\text{simplex coordination number}}$

The simplex solids are more likely to form quantum disordered states.

E.g. for the SU(4) pyrochlore SS, find  $M_c^{\text{MF}} = \frac{15}{2}$ . The pyrochlore SS is unfrustrated, but should exhibit "order by disorder".



# Order by disorder

NOTA BENE: The kagomé simplex solid is an SU(3) quantum paramagnet and does not order for any  $m$ . The OBD calculation here should then reveal the preferred short range order. The SU(4) pyrochlore SS can exhibit true LRO.

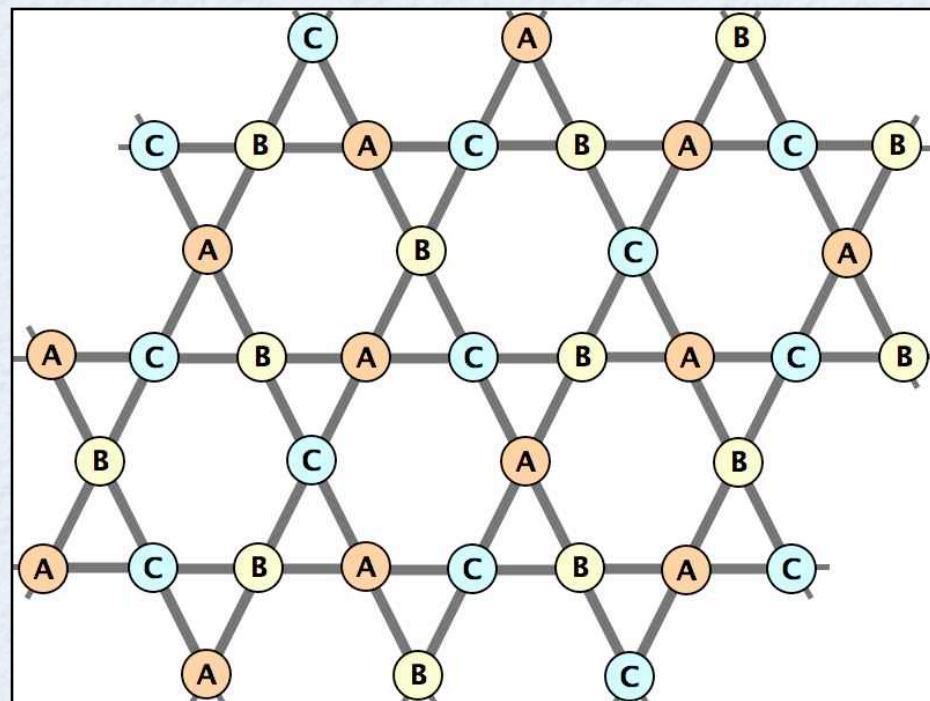
Derive a NL $\sigma$ M :  $z(i) = \omega_{\sigma(i)} (1 - \pi_i^\dagger \pi_i)^{1/2} + \pi_i$

Hamiltonian :  $H_{LT} = \sum_{\langle ij \rangle} |\pi_i^\dagger \omega_{\sigma(j)} + \omega_{\sigma(i)}^\dagger \pi_j|^2 + \lambda \left( \mathcal{N} |\chi|^2 + \sum_i \pi_i^\dagger \pi_i - \mathcal{N} \right)$

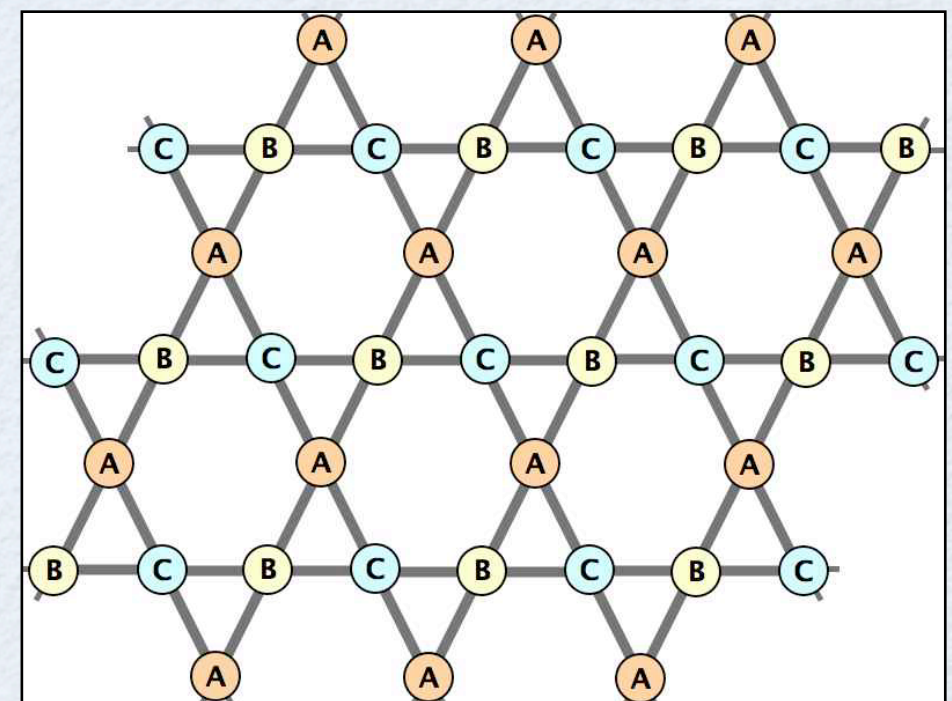
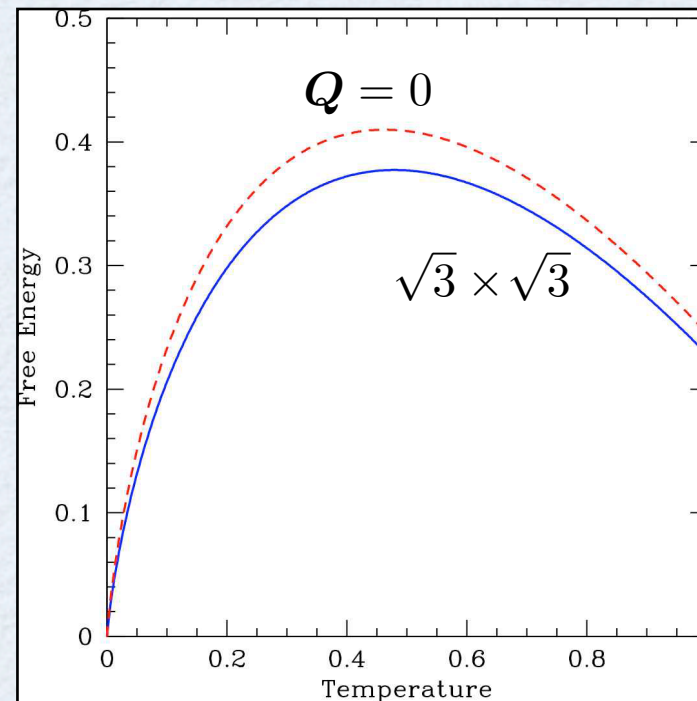
Free energy and mean field equation :

$$\frac{F}{\mathcal{N}} = -\lambda + \lambda |\chi|^2 + T \int_0^\infty d\varepsilon g(\varepsilon) \ln \left( \frac{\varepsilon + \lambda}{T} \right)$$

$$1 = |\chi|^2 + T \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{\varepsilon + \lambda}$$



$Q = 0$  state



$\sqrt{3} \times \sqrt{3}$  state



# Supersymmetric VBS states

DPA, Hasebe, Qi, Zhang (in preparation)

Parallels between VBS states and Laughlin-Haldane WF for FQHE :

$$\Psi_m^{\text{LH}} = \prod_{i < j} (u_i v_j - v_i u_j)^m$$

$$\Psi_m^{\text{AKLT}} = \prod_{\langle ij \rangle} (u_i v_j - v_i u_j)^m$$

$$H = \sum_{i < j} \sum_{L > m} V_L P_L(ij)$$

$$H = \sum_{\langle ij \rangle} \sum_{J > 2S - m} V_J P_J(ij)$$

Supersymmetric extension (K. Hasebe, 2005) :

$$\tilde{\Psi}_m = \prod_{i < j} (u_i v_j - v_i u_j + \theta_i \theta_j)^m$$

$$\{\theta_i, \theta_j\} = 0$$

Grassmann variables

Expand in powers of Grassmanns :

$$\tilde{\Psi}_m = \Psi_m^{\text{LH}} \cdot \left\{ 1 + m \sum_{i < j} \frac{\theta_i \theta_j}{u_i v_j - v_i u_j} + \dots + m^{N/2} \theta_1 \dots \theta_N \text{Pf} \left( \frac{1}{u_i v_j - v_i u_j} \right) \right\}$$



SUSY VBS state:

$$|\Psi(\mathcal{L}, M, r)\rangle = \prod_{\langle ij \rangle} \overbrace{(\epsilon_{\mu\nu} b_{i\mu}^\dagger b_{j\nu}^\dagger + r f_i^\dagger f_j^\dagger)}^{\chi_{ij}^\dagger}{}^M |0\rangle$$

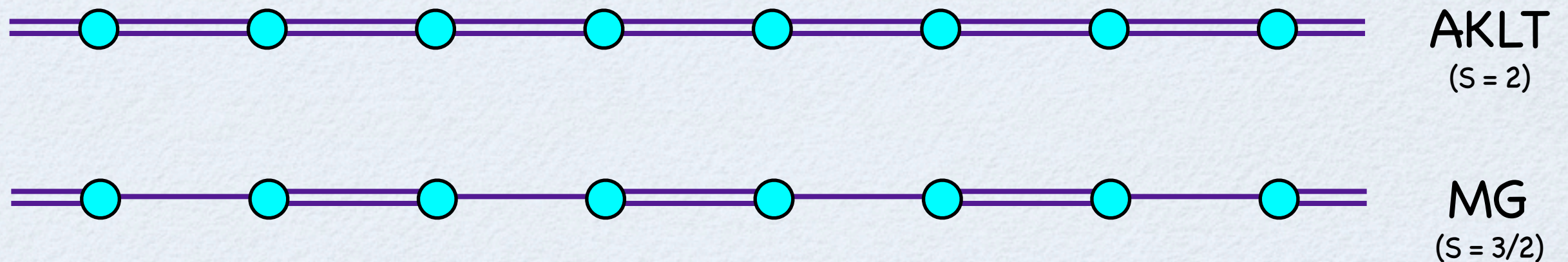
$\chi_{ij}^\dagger$  creates a linear combination of spin singlet and hole pair on link (ij).

It transforms as a singlet under the superalgebra  $OSp(1|2)$ . "SVBS" state.

The c-number  $r$  can interpolate between two limits :

$$|\Psi(\mathcal{L}, M, r)\rangle = \begin{cases} |\Psi_{\text{AKLT}}(\mathcal{L}, M)\rangle & \text{if } r=0 \\ |\Psi_{\text{RVB}}(\mathcal{L}, M-1)\rangle & \text{if } r=\infty \end{cases}$$

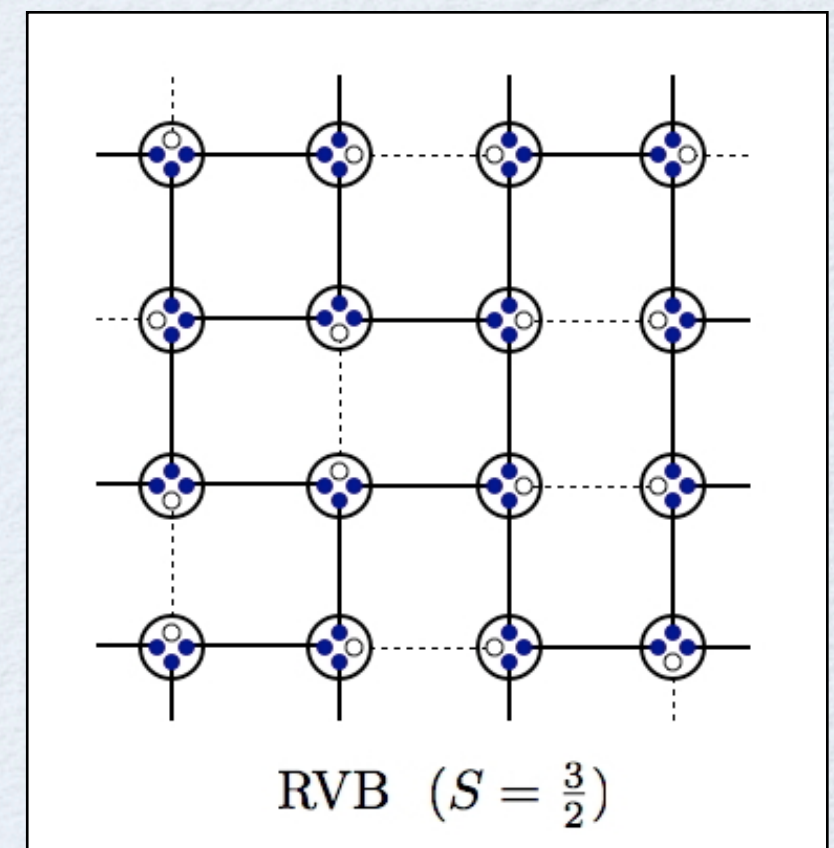
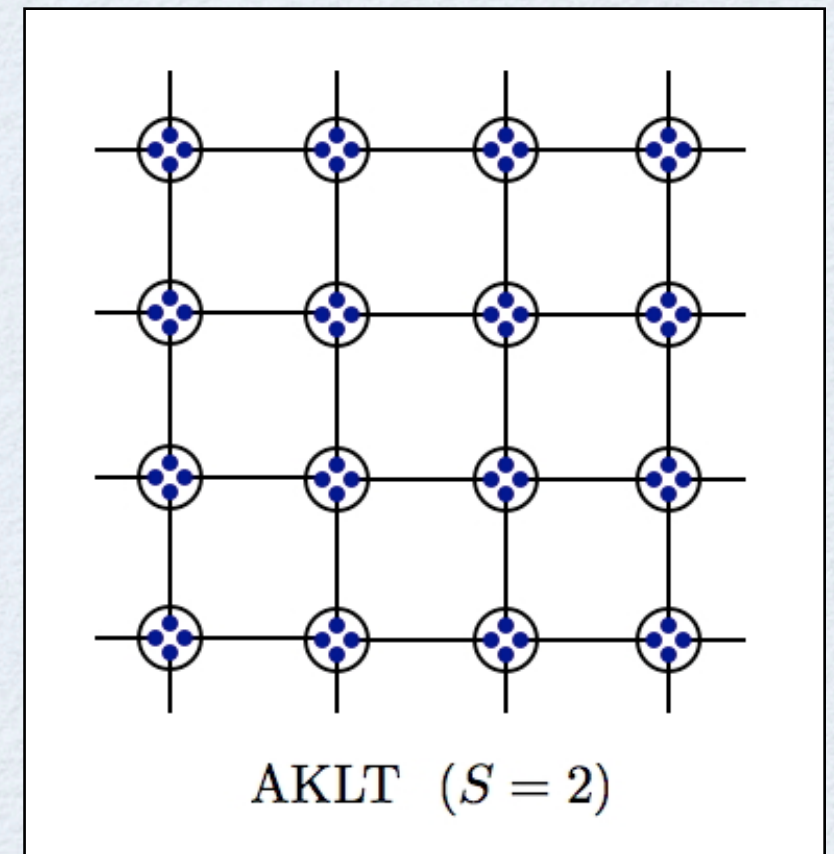
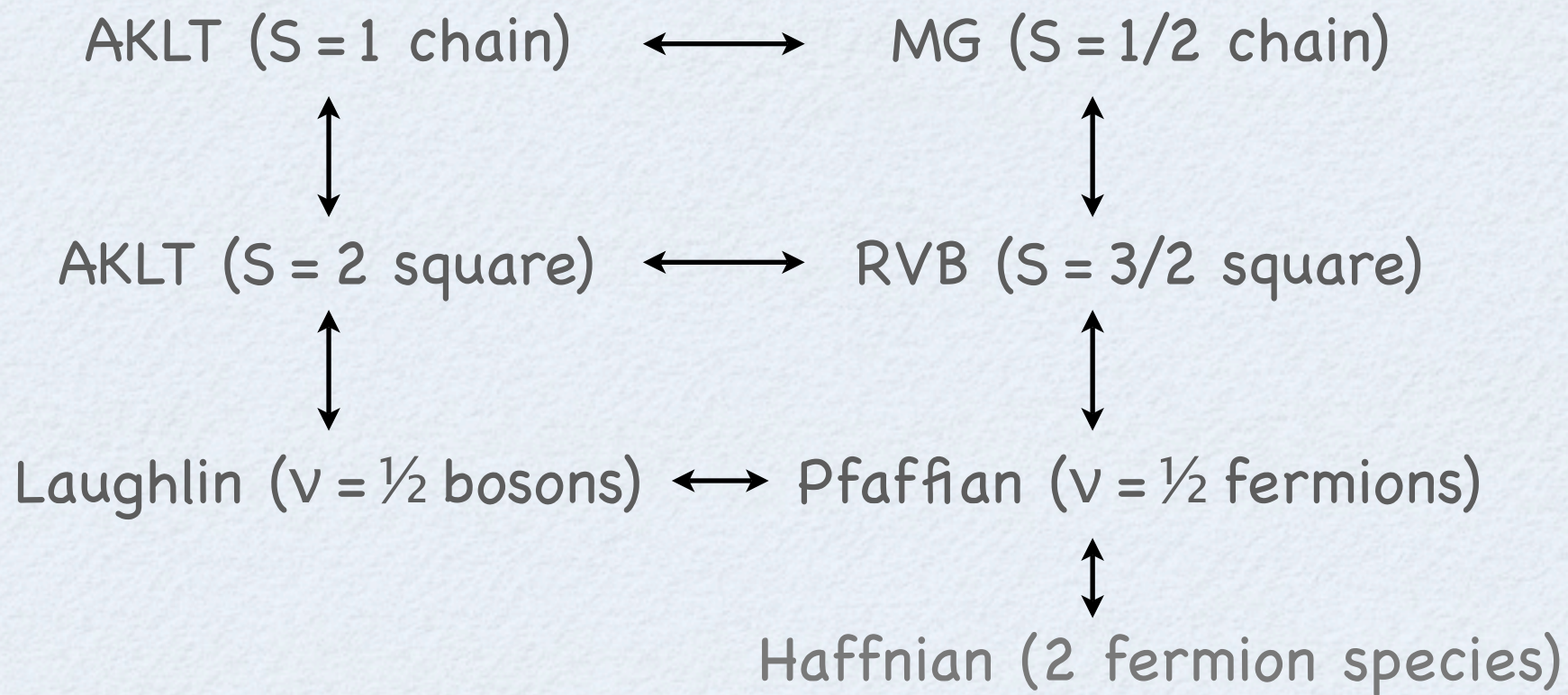
In  $d=1$ , the RVB state is the Majumdar-Ghosh state :





In  $d > 1$ , the  $r \rightarrow \infty$  limit is an RVB state.

Sketch of basic connections :



## $O\text{Sp}(1|2)$

$2p+1$  states in supermultiplet  $b_{\uparrow}^{\dagger}b_{\uparrow} + b_{\downarrow}^{\dagger}b_{\downarrow} + f^{\dagger}f = p$

Generators (5):

$$L_a = \frac{1}{2} b_{\mu}^{\dagger} \sigma_{\mu\nu}^a b_{\nu}$$

$$K_{\sigma} = \frac{1}{2} (x^{-1} f b_{\sigma}^{\dagger} + \sigma x f^{\dagger} b_{-\sigma})$$

Casimir:  $\mathcal{C} = \mathbf{L}^2 + \epsilon_{\mu\nu} K_{\mu} K_{\nu}$

Algebra:

$$\{K_{\mu}, K_{\nu}\} = \frac{1}{2} (i\sigma^y \sigma^a)_{\mu\nu} L_a$$

$$[L_a, K_{\mu}] = \frac{1}{2} \sigma_{\nu\mu}^a K_{\nu}$$

$$[L_a, L_b] = i\epsilon_{abc} L_c$$



## SVBS chains

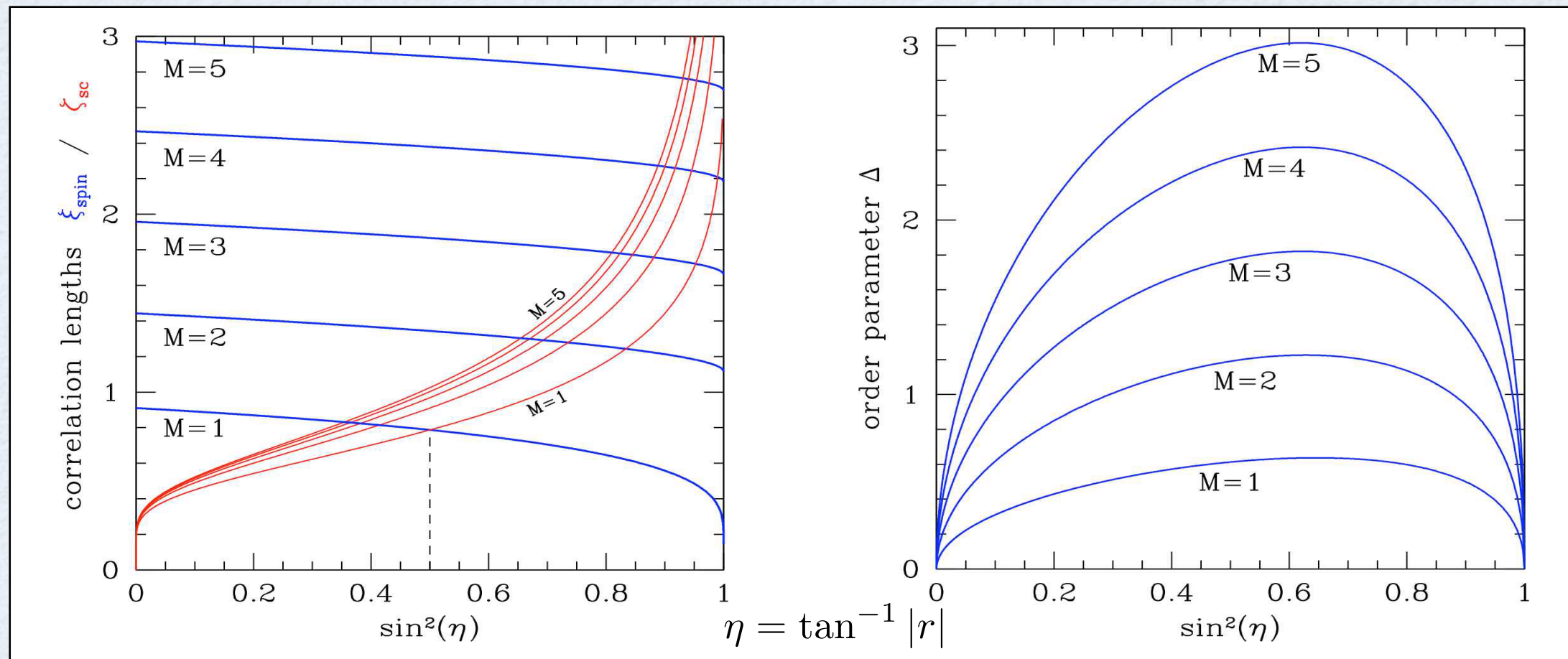
General wavefunction :  $|\Psi\rangle = \prod_i (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger + r f_i^\dagger f_{i+1}^\dagger)^M |0\rangle$

Correlations computed using spin-hole coherent states (Auerbach 1994):

$$|\hat{n}, \theta; p\rangle \equiv \frac{1}{\sqrt{p!}} (ua^\dagger + vb^\dagger - \theta f^\dagger)^p |0\rangle$$

Compute spin and superconducting correlators :

$$C_{\text{spin}}(n) = \langle \mathbf{L}(j) \cdot \mathbf{L}(j+n) \rangle, \quad C_{\text{SS}}(n) = \langle \epsilon^{\mu\nu} b_{j,\mu} b_{j+n,\nu} f_j^\dagger f_{j+n}^\dagger \rangle$$





# Conclusions

- VBS states a fertile playground for models of quantum magnetism
- VBS states are simplest example of matrix/tensor product states
- Equal time quantum correlations equivalent to finite temperature correlations of an associated classical model on the same lattice
- $S = 2$  VBS on diamond lattice is a quantum paramagnet, but  $S = 3$  VBS on cubic lattice already possesses Néel order

- Abundant generalizations exist:

C-breaking  $SU(2n)$  states Marston et al., 1991

$SO(n)$  VBS chains Tu et al., 2008

$SU(4)$  plaquette ladders Chen et al., 2005

- Fractionalization of representation at an edge

- Several analogies to FQHE physics

