

Title: Condensed Matter Seminar

Date: Oct 16, 2012 03:00 PM

URL: <http://pirsa.org/12100078>

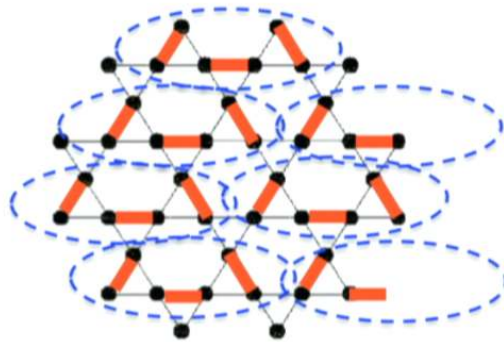
Abstract:

# Valence Bonds Crystal Ground states

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Columnar dimer state

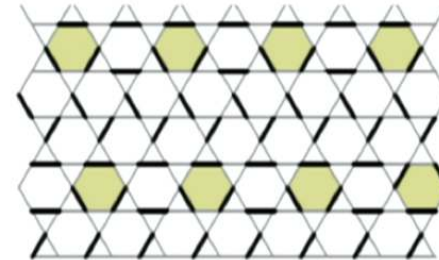
Budnik AA, 2004



soft to local rotations

Striped hexagons

Nikolic, Senthil

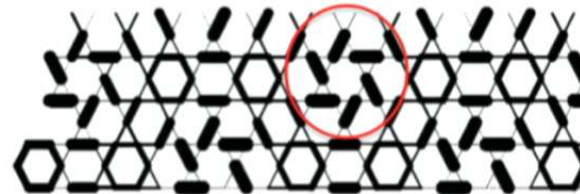


“Honeycomb VBC”

36 site cell

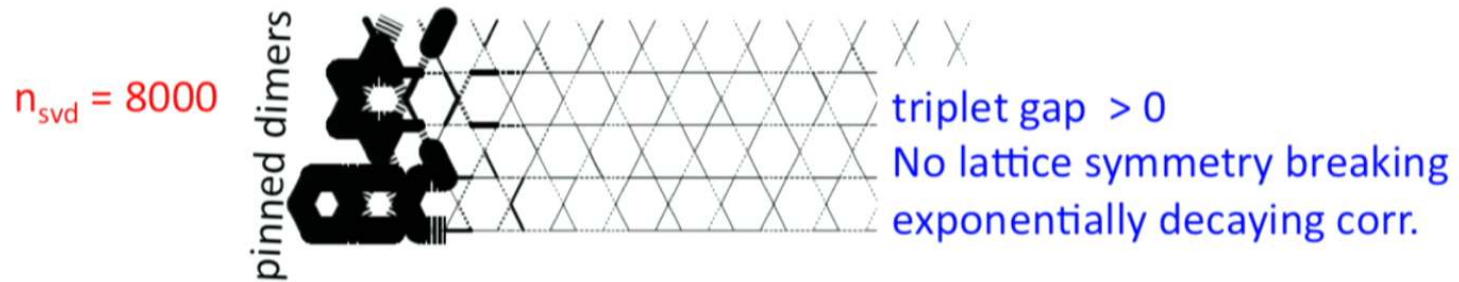
Marston,Zeng  
Singh,Huse  
Evenbly,Vidal

“pinwheel” p6



# Spin liquid states

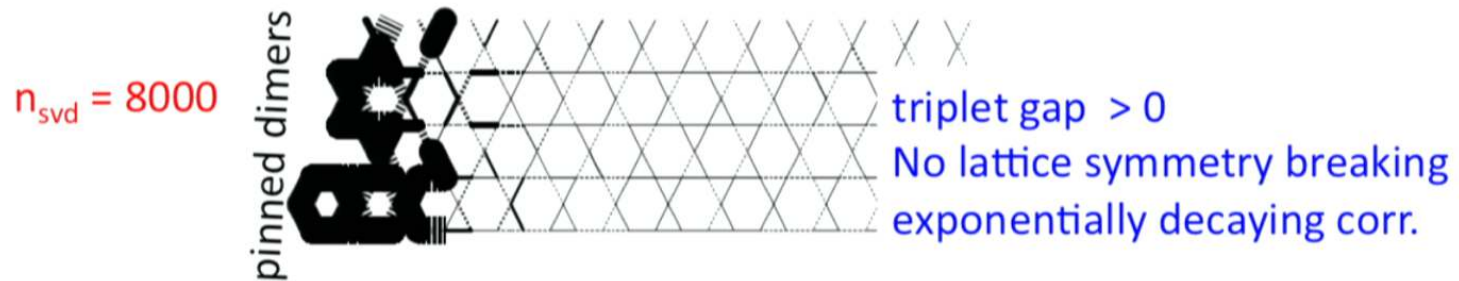
DMRG: Yan, Huse, White **Gapped Spin Liquid**



$$e_0^{GSL} = -0.4385$$

# Spin liquid states

DMRG: Yan, Huse, White    Gapped Spin Liquid



$$e_0^{GSL} = -0.4385 \quad \text{Z2 entanglement entropy (Jiang, Wang, Balents)}$$



# Spin liquid states

DMRG: Yan, Huse, White **Gapped Spin Liquid**

$n_{\text{svd}} = 8000$

pinned dimers

triplet gap  $> 0$   
No lattice symmetry breaking  
exponentially decaying corr.

$$e_0^{GSL} = -0.4385 \quad \text{Z2 entanglement entropy (Jiang, Wang, Balents)}$$

VMC: Iqbal, Becca, Sorella, Poilblanc **Algebraic Spin Liquid**

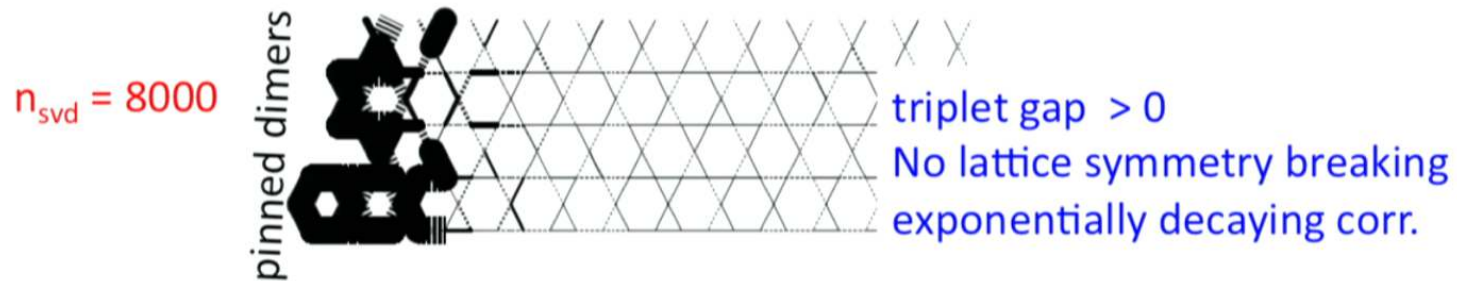
$$|\Psi_{p-LS}\rangle = \left( 1 + \sum_{k=1}^p \alpha_k \hat{\mathcal{H}}^k \right) |\Psi_{\text{VMC}}\rangle$$

Triplet gap = 0  
power law spin correlations

$$e_0^{ASL} = -0.4365$$

# Spin liquid states

DMRG: Yan, Huse, White **Gapped Spin Liquid**



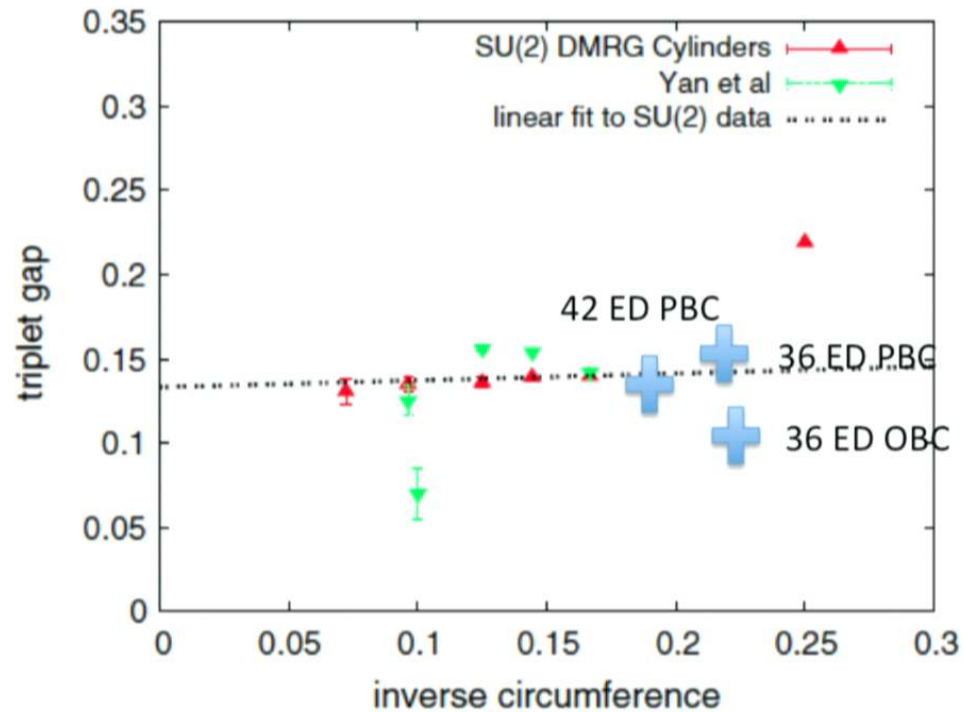
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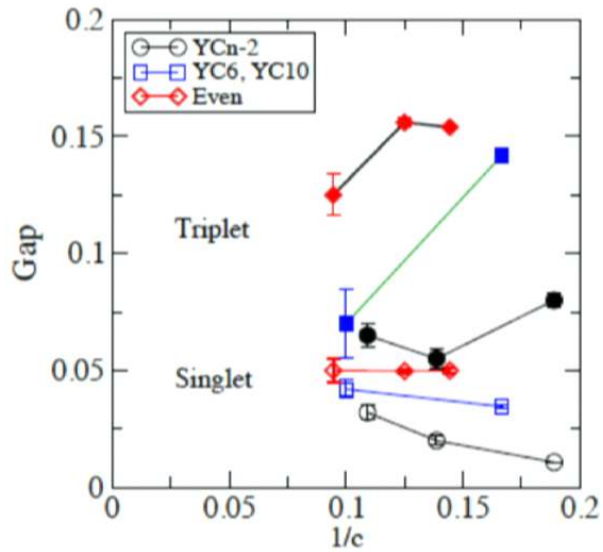
$$e_0^{ASL} = -0.4365 \quad \begin{array}{l} \text{Only 0.46\% difference in energy --} \\ \text{qualitative difference in long range correlations} \end{array}$$

# Triplet gap

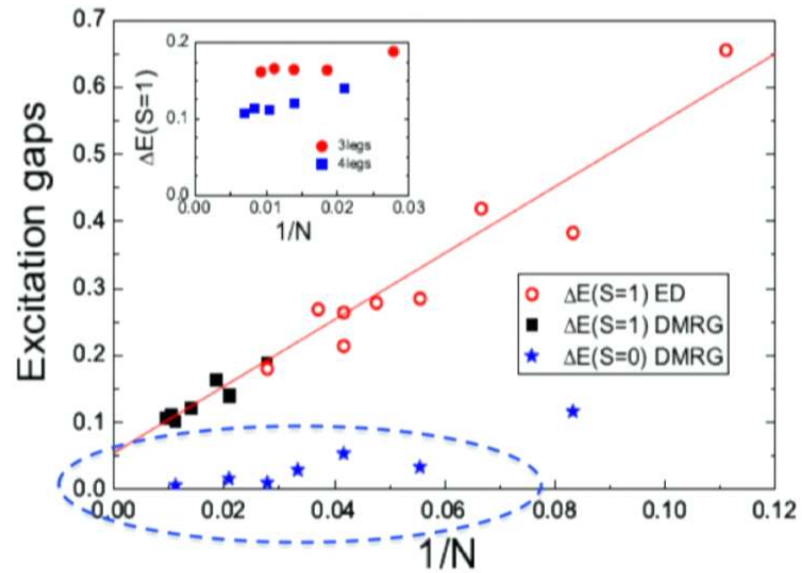


Stefan Depenbrock,<sup>1,\*</sup> Ian P. McCulloch,<sup>2</sup> and Ulrich Schollwöck<sup>1</sup>

# Singlet gap



Yan, Huse, White



Jiang, Weng, Sheng

*Does the singlet gap stay finite in the thermodynamic limit?*

## Contractor Renormalization (CORE)

*Using ED to compute the effective Hamiltonian in the singlets sector for larger lattices*

General Method: C. Morningstar, M. Weinstein, PRD (1996).

Square lattice Hubbard Model: E. Altman and A. A, PRB (2002).

Checkerboard+Pyrochlore: Berg, Altman, AA PRL (2003)

Kagome (first attempt): Budnik, A.A. PRL (2004);

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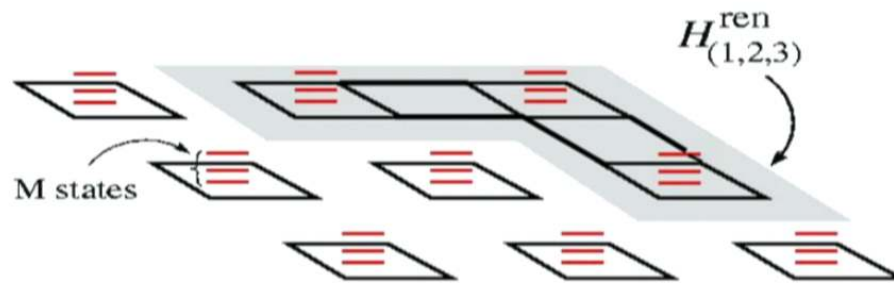
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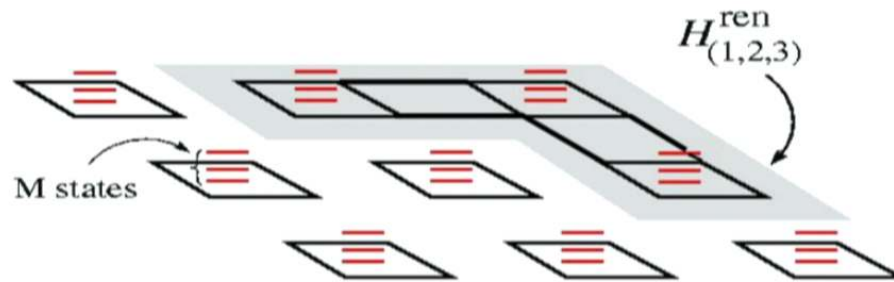
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## Exact Diagonalizations (ED) of connected clusters



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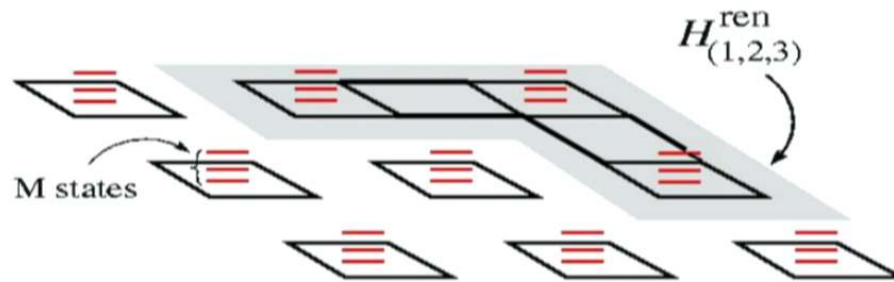


Find low spectrum of  $H$  on the connected cluster.

Project the wavefunctions onto the reduced Hilbert space

$$\varepsilon_n, |\psi_n\rangle \Rightarrow |\tilde{\Psi}_n\rangle \quad |\tilde{\Psi}_n\rangle = \frac{1}{Z_n} \left[ P|\psi_n\rangle - \sum_{n' < n} |\tilde{\Psi}_{n'}\rangle \langle \tilde{\Psi}_{n'} | \psi_n \rangle \right]$$

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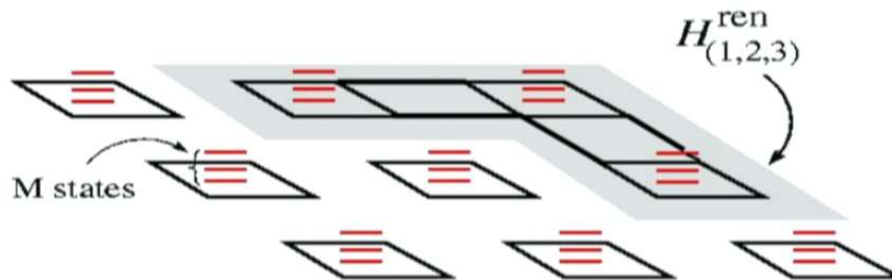
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Construct renormalized cluster hamiltonians:

$$H_{(1,\dots,N)}^{ren} \equiv \sum_{n=1}^{M^N} \varepsilon_n |\tilde{\psi}_n\rangle \langle \tilde{\psi}_n |$$

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$$H_{(1,\dots,N)}^{ren} \equiv \sum_{n=1}^{M^N} \varepsilon_n |\tilde{\psi}_n\rangle \langle \tilde{\psi}_n| \quad \neq \langle \alpha_1, \dots, \alpha_N | H_0 + H' \frac{(1-P_0)}{E-H_0} H' + \dots | \alpha'_1, \dots, \alpha'_N \rangle$$

Old perturbative RG

## CORE effective hamiltonian

1. Effective Interactions  $h_{1,2\dots n}^{(n)} = \mathcal{H}_{1,2\dots n}^{\text{ren}} - \sum_{\text{all sub clusters}} h_{\{1\},\{2\},\dots,\{n-1\}}$

For fast convergence: sum minimally embedding shapes (e.g. rectangles)

E. Altman's thesis.

2. Expansion in interaction **range**

$$H_{\text{eff}} = \sum_i h_i + \sum_{\langle ij \rangle} h_{ij} + \sum_{\langle ijk \rangle} h_{ijk} + \sum_{ijk\dots} h_{ijk\dots} \dots$$

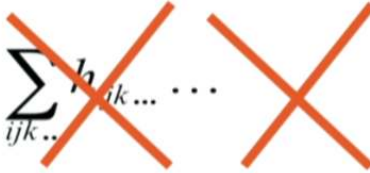
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3. Truncation approximation depends on rapidly decreasing interactions at longer ranges.

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$\xi_{\text{coherence}}$

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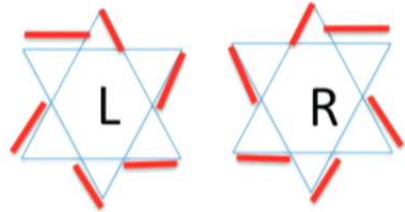
$$H_{\text{eff}} = \sum_i h_i + \sum_{\langle ij \rangle} h_{ij} + \sum_{\langle ijk \rangle} h_{ijk} + \sum_{ijk\dots} h_{ijk\dots} \dots$$

The diagram shows the expansion of the effective Hamiltonian  $H_{\text{eff}}$  in interaction range. The terms are  $\sum_i h_i$ ,  $\sum_{\langle ij \rangle} h_{ij}$ ,  $\sum_{\langle ijk \rangle} h_{ijk}$ , and  $\sum_{ijk\dots} h_{ijk\dots}$ . The last two terms are crossed out with red X's. A green box labeled  $\xi_{\text{coherence}}$  has arrows pointing to the  $h_{ij}$  and  $h_{ijk}$  terms.

3. Truncation approximation depends on rapidly decreasing interactions at longer ranges.

*$H_{\text{eff}}$  may be solved by ED, Variationally, DMRG, or CORE iteration*

# Star of (Magen) David Blocking

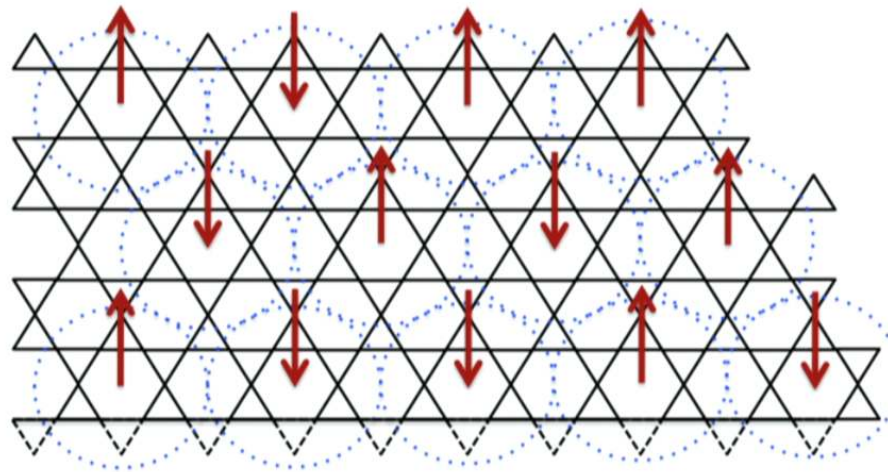


Ground state doublet

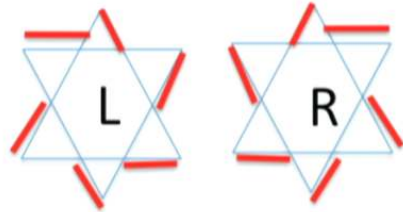
$$|\uparrow\rangle = \frac{1}{\sqrt{2 + 1/16}}(|L\rangle + |R\rangle)$$

$$|\downarrow\rangle = \frac{1}{\sqrt{2 - 1/16}}(|L\rangle - |R\rangle)$$

Pseudospin "Ising" basis



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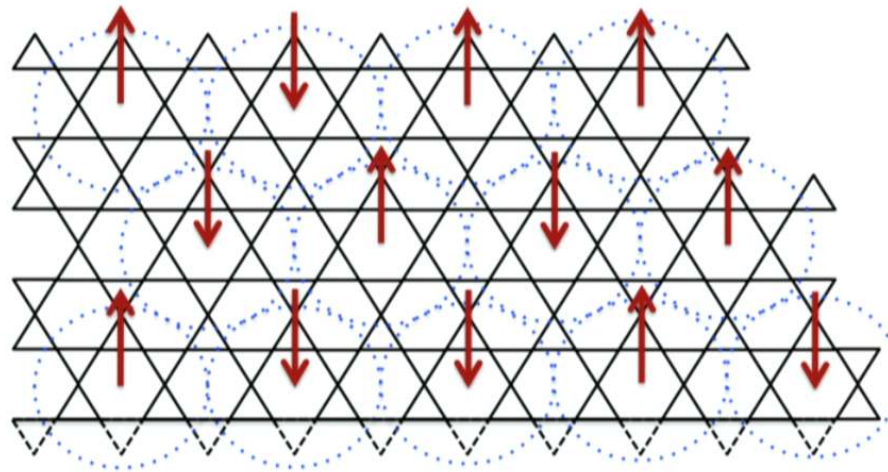


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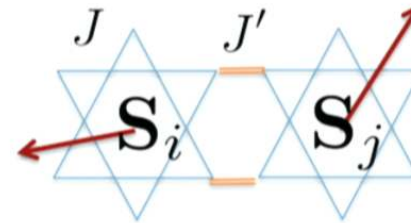


Reduced Hilbert space size:  $2^{N/12} \ll 2^N$

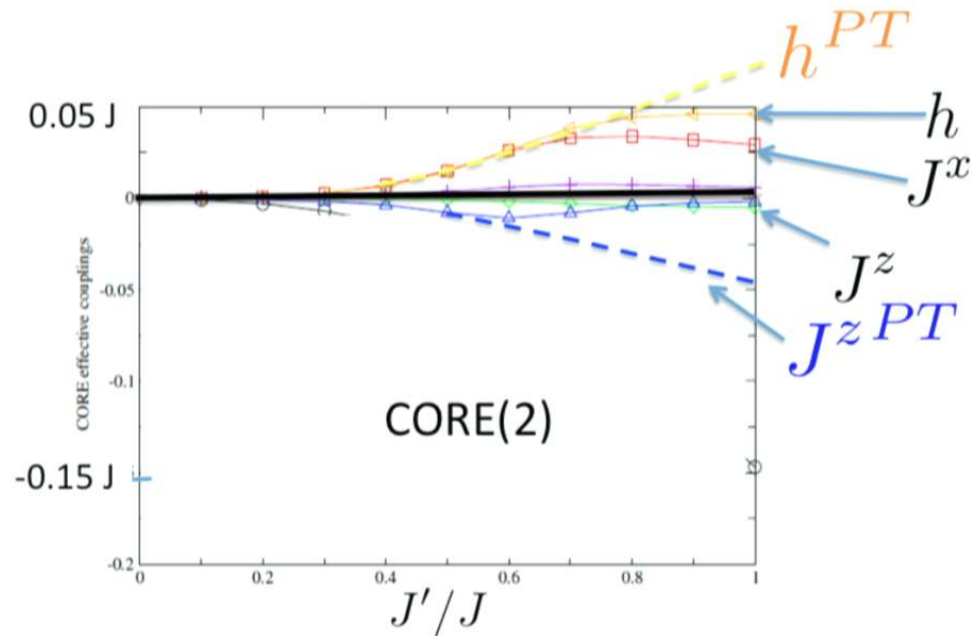
# CORE(2) versus Perturbation Theory

Perturbation Theory (PT)

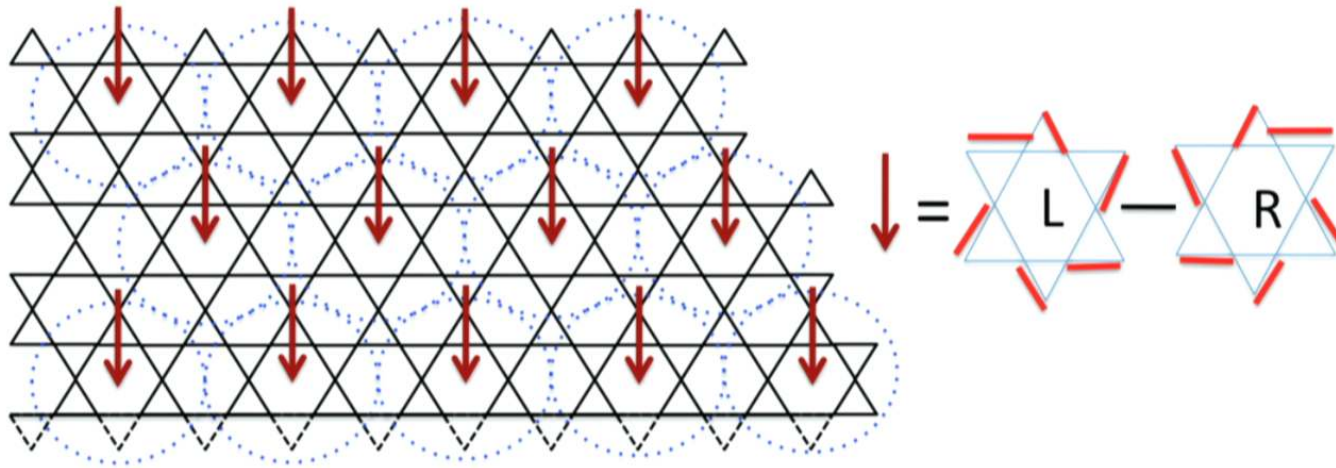
Syromyatnikov, Maleyev, PRB (2002)



$$H^{CORE(2)} = E_0 + h(S_i^z + S_j^z) + J^x S_i^x S_j^x + J^y S_i^y S_j^y + J^z S_i^z S_j^z$$

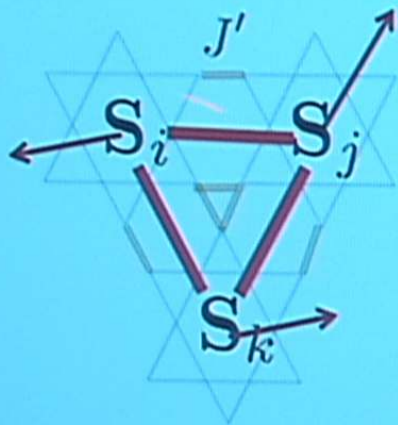


# Groundstate of CORE(2)

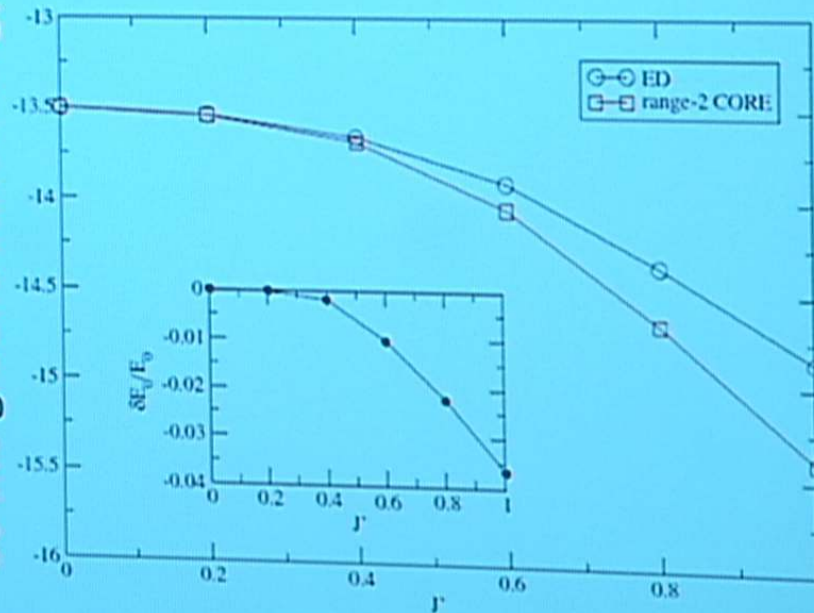


1. Product of *antisymmetric* singlets
2. Broken Lattice translational symmetry (12 site unit cell)
3. Point group symmetry  $p6m$  (triangular lattice)

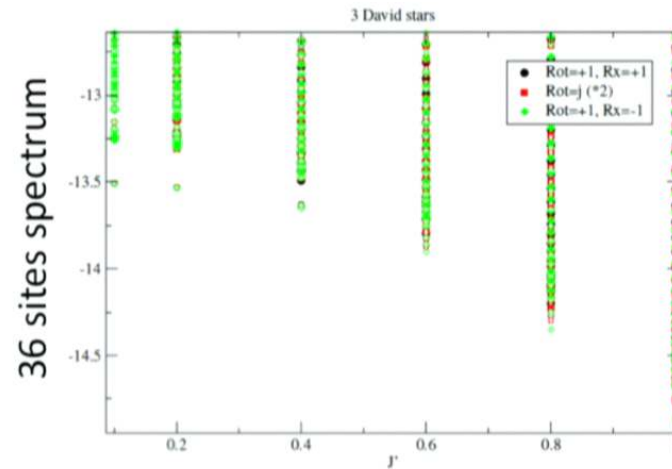
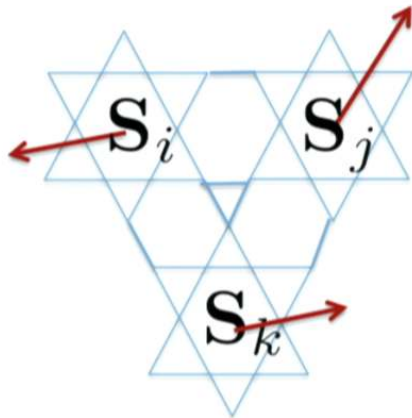
# CORE(2) – not yet converged



36 site ground state energy



# Range 3 computation



Sylvain Capponi:

Lanczos: 36 sites OBC, with point group symmetries  
750\*10<sup>6</sup> configurations. Toulouse CALMIP supercomputer

Ravi Chandra:

Lanczos-SVD algorithm\*: 2 x 18 sites, 200 SVD states  
Desktop PC with 15GB memory; relative precision 10<sup>-4</sup>

\*Weinstein, AA, Ravi Chandra PRE 84 (2011)

# CORE(3) Interaction Parameters

$$H^{CORE(3)} = Nc_0 + \sum_i h\sigma_i^z + \sum_{\langle ij \rangle, \alpha} J_\alpha \sigma_i^\alpha \sigma_j^\alpha + \sum_{\langle ijk \rangle_{\Delta}, \alpha} J_{z\alpha\alpha} \sigma_i^z \sigma_j^\alpha \sigma_k^\alpha$$

$J_2$	$J_2 = 0$ (Kagomé)	$J_2 = +0.1$	$J_2 = -0.1$
$c_0$	-5.24629	-5.17068	-5.48631
$h$	-0.0692243	0.0593234	-0.362797
$J_x$	-0.00909679	-0.0154208	0.00112276
$J_y$	-0.0118789	0.00183224	-0.0176992
$J_z$	0.0210562	0.00368622	0.0201406
$J_{zxx}$	-0.02792	-0.0196486	-0.0282832
$J_{zyy}$	0.00455018	-0.00474948	0.00452468
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# Truncation Error CORE(3)

Comparing ground state energy of CORE(3) to DMRG on large lattices



number of stars	$E_0^{CORE_3}$	$E_0^{DMRG}$	Error
$2 \times 2$	-0.418452	-0.417213	-0.001239
$2 \times 3$	-0.423953	-0.422336	-0.001617
$3 \times 4$	-0.431150	-0.428046	-0.003104
$3 \times 5$	-0.432688	-0.429191	-0.003497

Ranges  $> 3$  effective interactions are very small!  
 $\rightarrow$  CORE(3) converges well.

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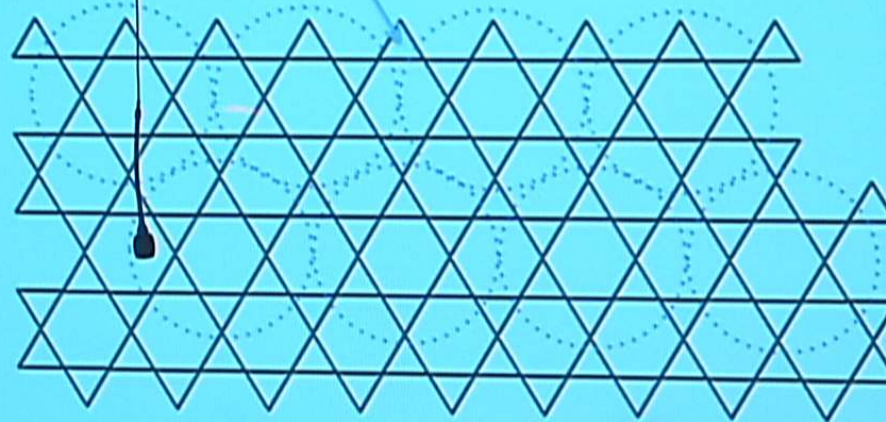


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# Is the GS a Spin Liquid?

$$H^\delta = \frac{1}{2} \sum_{\Delta} (S_{\Delta}^2 - 9/4) + \delta \frac{1}{2} \sum_{\Delta_{inter}} (S_{\Delta}^2 - 9/4)$$



$$E_{\Delta_{inter}} = \frac{dE_0}{d\delta}$$

$$E_{\Delta} = -0.687J$$

$$E_{\Delta_{inter}} = -0.665J$$

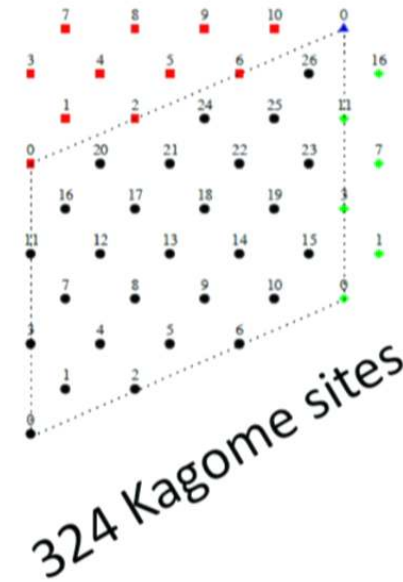
< 3% modulation  
consistent with truncation error

# Singlets spectra of large lattices

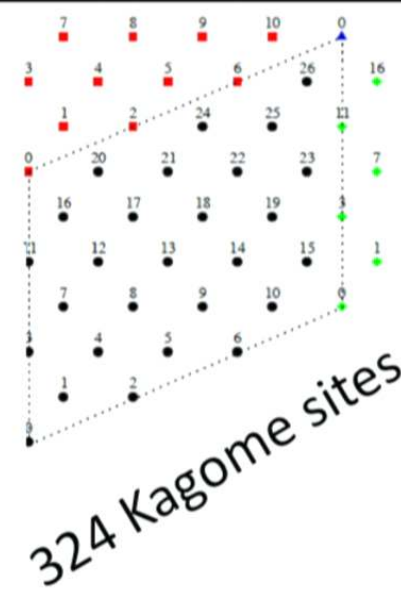
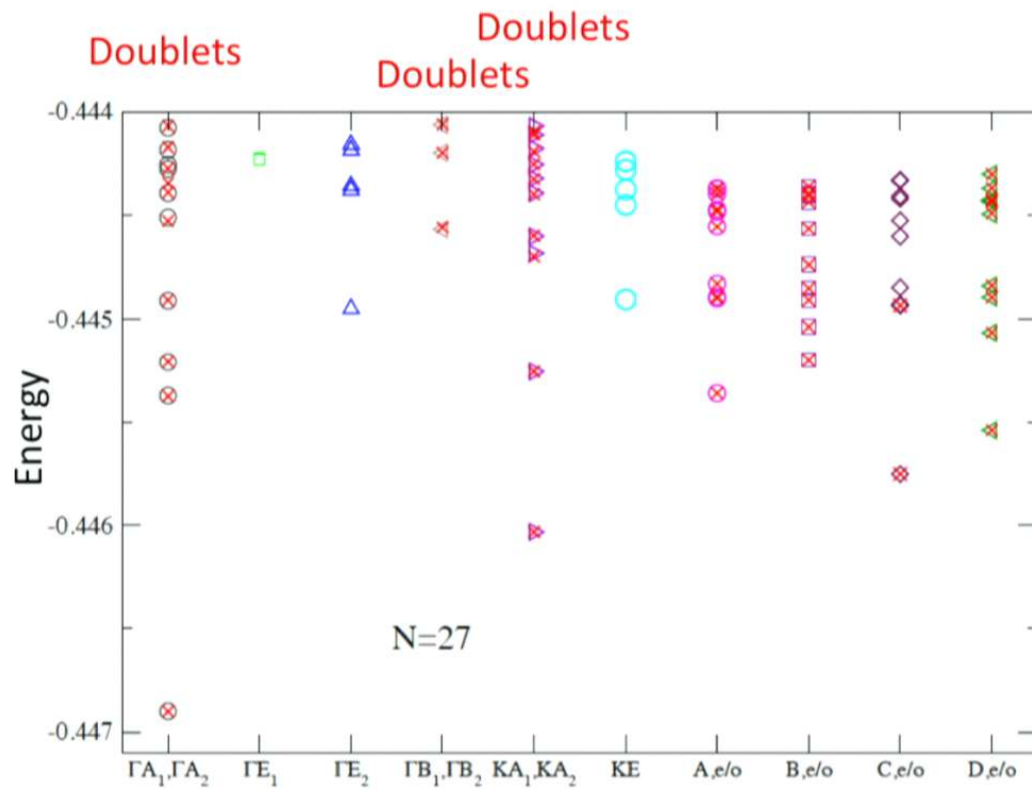
3x4 MD's

# A1	# A2
1 -64.37144334047481208927	1 -64.36732936063638987889
2 -63.96754639332078085090	2 -63.86789783887156346509
3 -63.79832541628604047901	3 -63.84784614830449811507
4 -63.75933331555023642068	4 -63.70772139593811544955
5 -63.62067587174262683902	5 -63.57801300230658370083
6 -63.51830836371206601143	6 -63.51410861653796757764

# CORE(3) on 27 MD's



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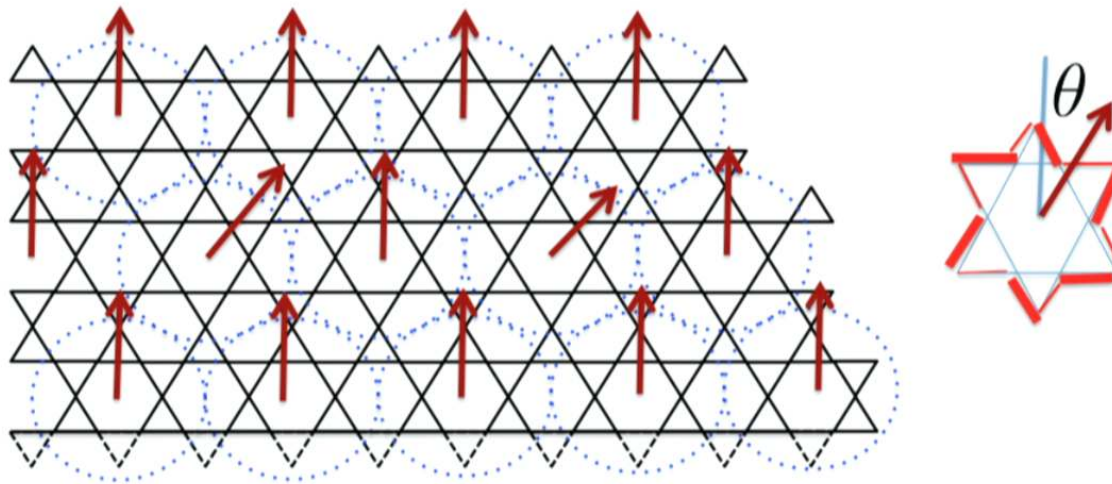
# Mean field theory-HVBC

$$E^{FM} = Nc_0h \sum_i \cos \theta + \sum_{\langle ij \rangle} J_x \sin \theta_i \sin \theta_j + J_z \cos \theta_i \cos \theta_j \\ + \sum_{\langle ijk \rangle} J_{zxx} \cos \theta_i \sin \theta_j \sin \theta_k + 2J_{zzz} \cos \theta_i \cos \theta_j \cos \theta_k$$

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$$+ \sum_{\langle ijk \rangle} J_{zxx} \cos \theta_i \sin \theta_j \sin \theta_k + 2J_{zzz} \cos \theta_i \cos \theta_j \cos \theta_k$$



# Uniform Chiral State

$$E^{FM}(\theta)/N - c_0 = h \cos \theta + 3J_x \sin^2 \theta + 3J_z \cos^2 \theta \\ + 6J_{xx} \cos \theta \sin^2 \theta + 2J_{zz} \cos^3 \theta$$

# Uniform Chiral State

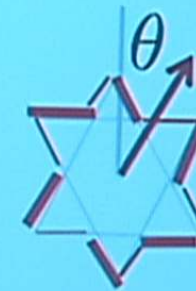
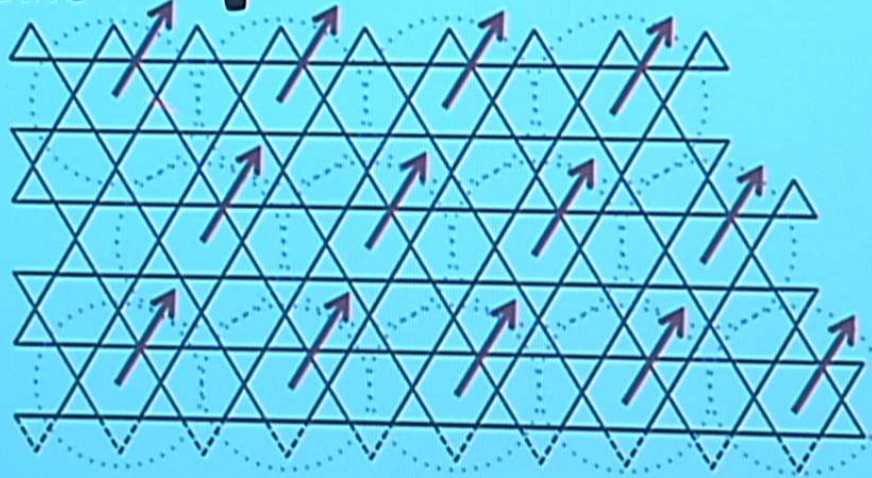
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Dominant, negative  
terms

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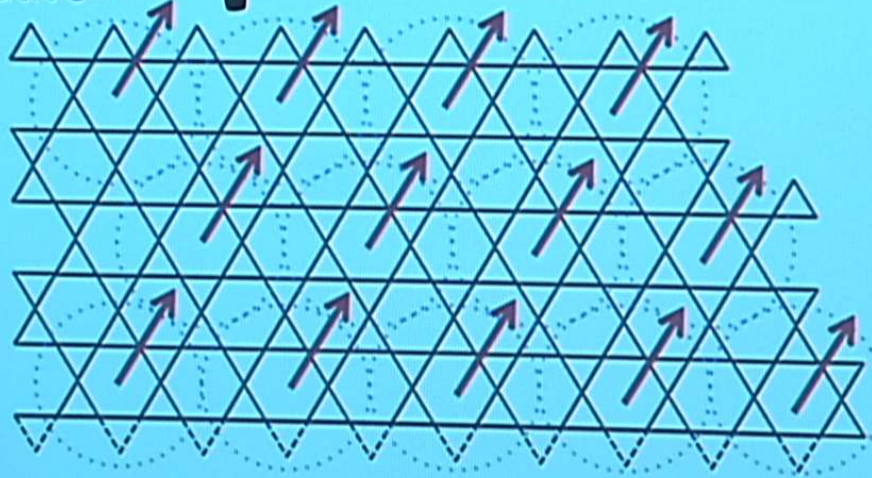
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Dominant, negative terms

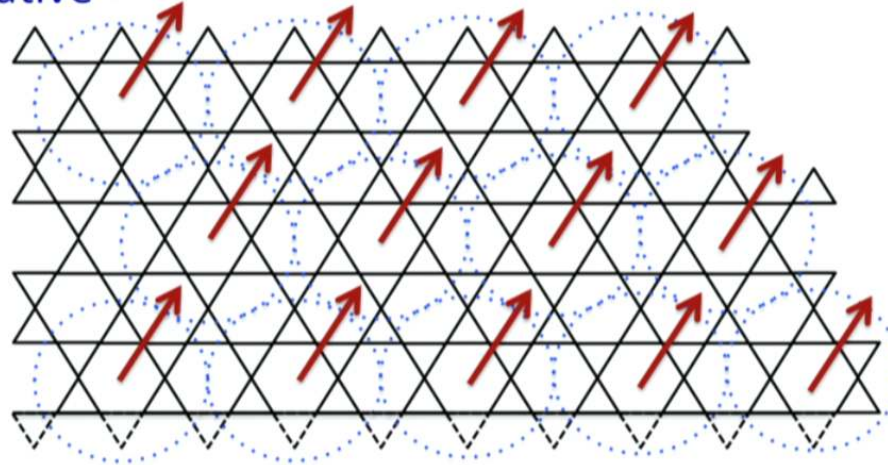


consistent with p6 (2D chiral) Spin Liquid

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Dominant, negative terms

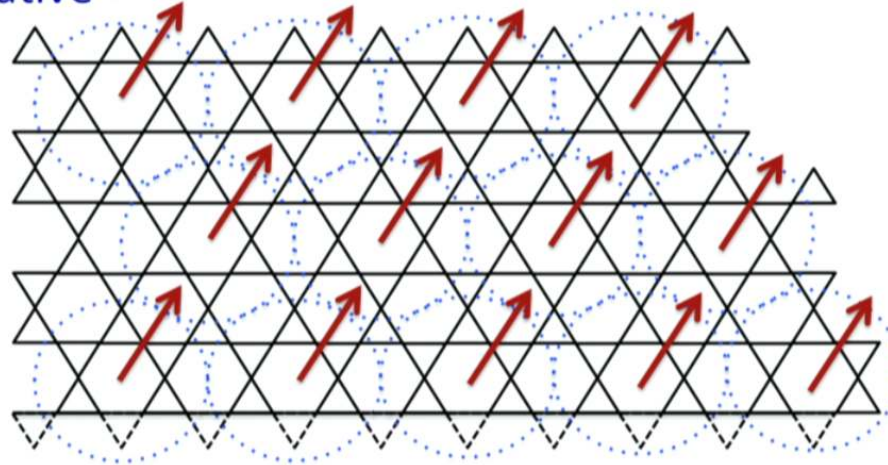


consistent with p6 (2D chiral) Spin Liquid

# Uniform Chiral State

$$E^{FM}(\theta)/N - c_0 = h \cos \theta + 3J_x \sin^2 \theta + 3J_z \cos^2 \theta + 6J_{zxx} \cos \theta \sin^2 \theta + 2J_{zzz} \cos^3 \theta$$

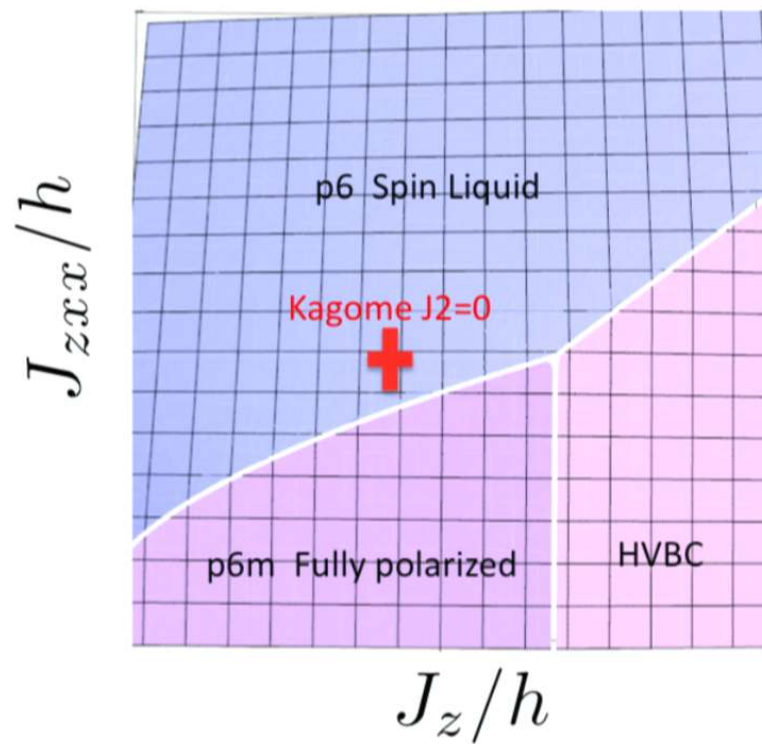
Dominant, negative terms



consistent with p6 (2D chiral) Spin Liquid

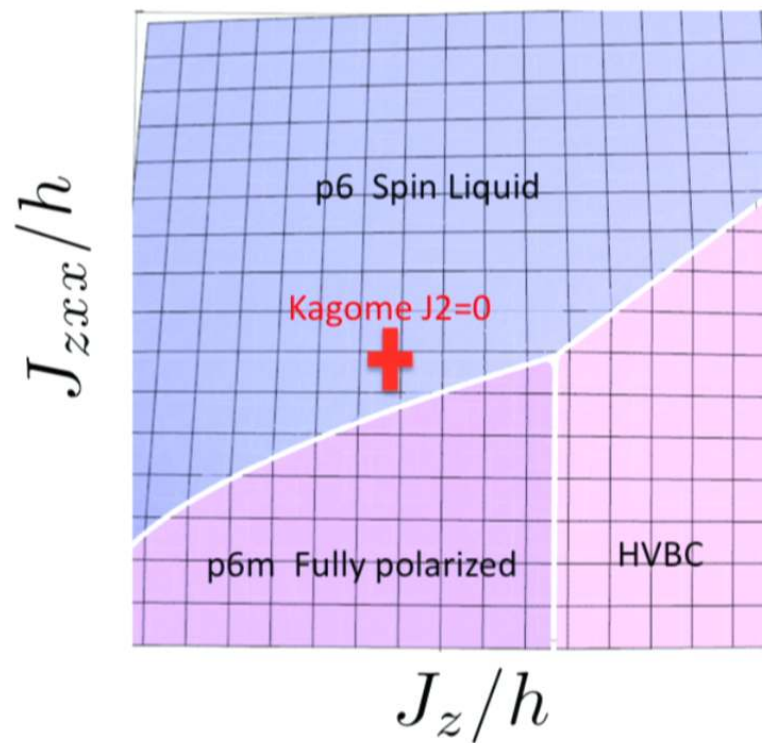
# Projected Phase diagram

$$H = h \sum_i S_i^z + J^z \sum_{\langle ij \rangle} S_i^z S_j^z + J^{zxx} \sum_{ijk} S_i^z S_j^x S_k^x$$



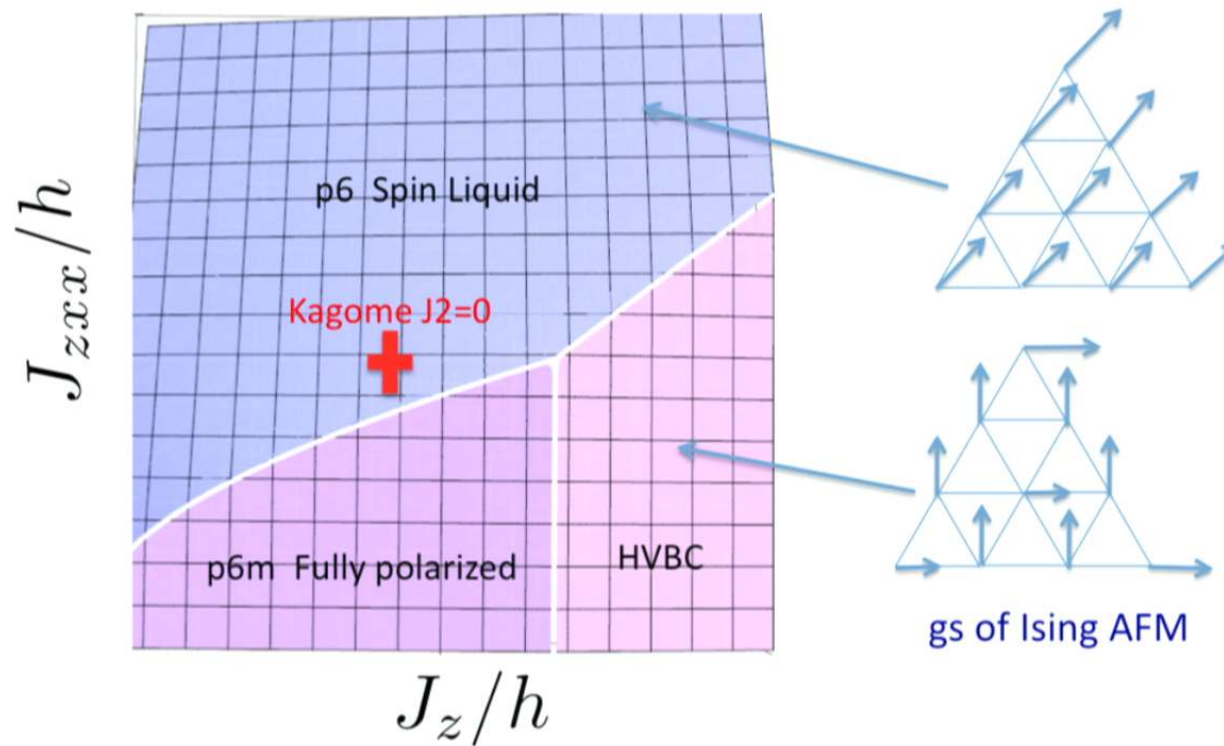
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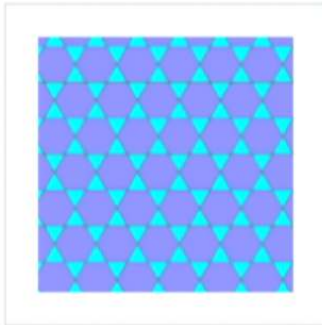
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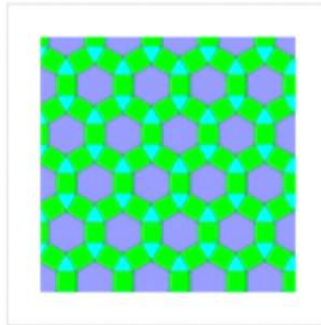


# Wall paper groups (6-fold rotations)

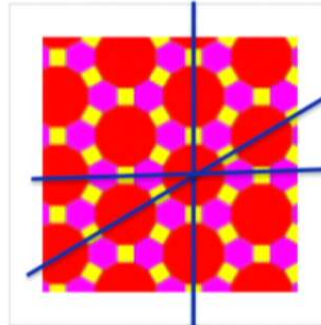
$p6m$  has reflections in three distinct directions.



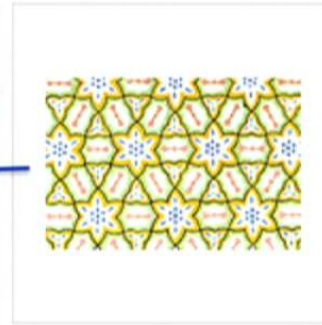
one of the 8 semi-regular tessellations



another semi-regular tessellation



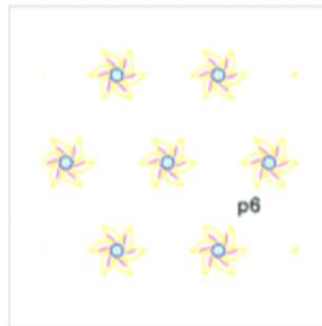
another semi-regular tessellation



Persian glazed tile

Examples of group  $p6$  has **no** reflections or glide reflections.

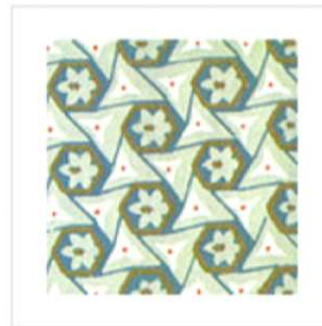
$p6$



Computer generated

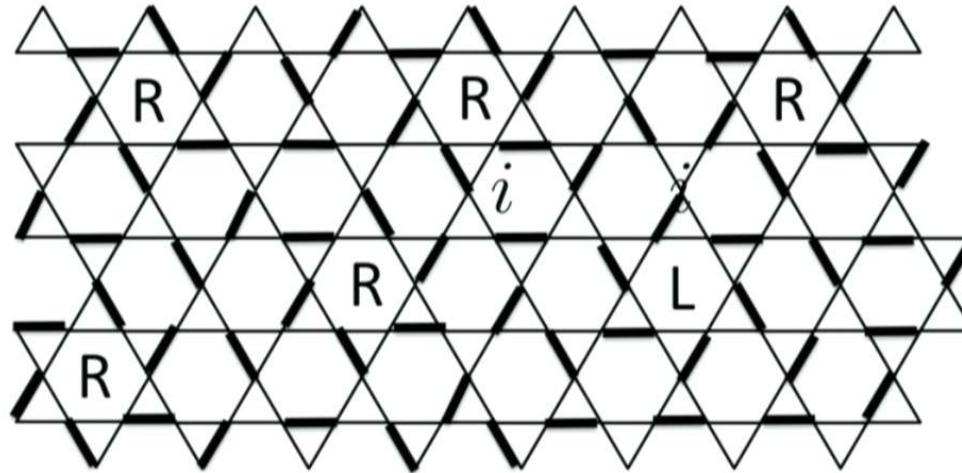


Wall panelling, the Alhambra, Spain



Persian ornament

# Chiral Order Parameter



Chiral Dimer Configuration

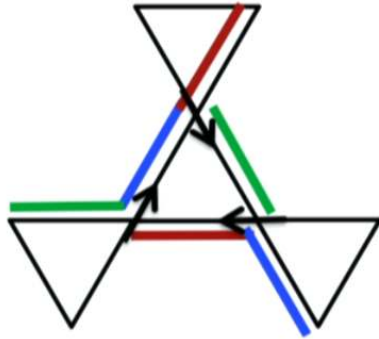
$$C_i = \text{[Diagram of right-handed dimer]} - \text{[Diagram of left-handed dimer]}$$

The diagram shows two dimer configurations. The first is a right-handed dimer (R) and the second is a left-handed dimer (L). The right-handed dimer is defined as the difference between the right-handed and left-handed configurations.

$$C_i = \sum_{\mathbf{d}} (\mathcal{S}_{\mathbf{d}} \mathcal{S}_{\eta^r(\mathbf{d})} - \mathcal{S}_{\mathbf{d}} \mathcal{S}_{\eta^l(\mathbf{d})})$$

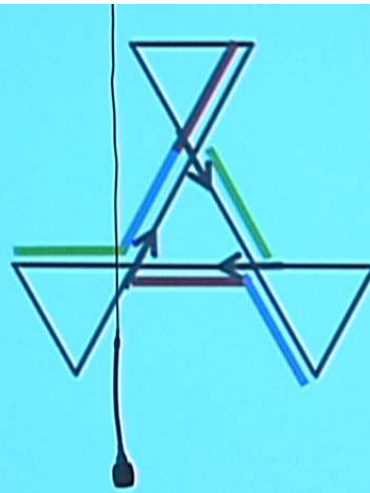
$$m_c = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \langle C_i \rangle$$

2-Dimer Chiral Order Parameter



$$\delta\rho_d > 0$$

$$\langle C \rangle > 0$$



$$\delta\rho_d > 0$$

$$\langle C \rangle > 0$$

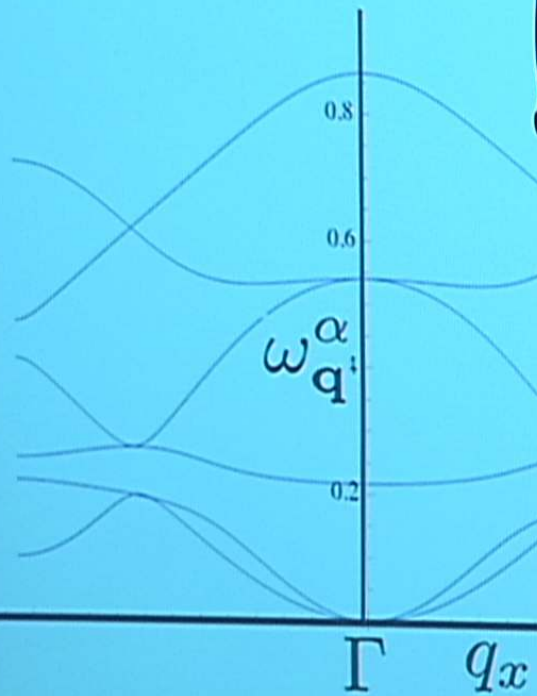
$$\mathcal{L}_d = \frac{1}{2} \int d^2x \frac{1}{2} (\partial_t^2 - \omega_d^2) \delta\rho_d^2(\mathbf{x})$$

$$\mathcal{L}_{d-ion} = -\gamma |\langle C \rangle| \int d^2x \delta\rho_d^2(\mathbf{x}) \mathbf{v}^r \cdot \mathbf{u}(\mathbf{x})$$

$$\mathbf{v}^r = \frac{1}{\sqrt{3}} \left( \cos\left(\frac{\pi}{3}\right), \sin\left(\frac{\pi}{3}\right), -1, 0, \cos\left(\frac{\pi}{3}\right), -\sin\left(\frac{\pi}{3}\right) \right)$$

p6m

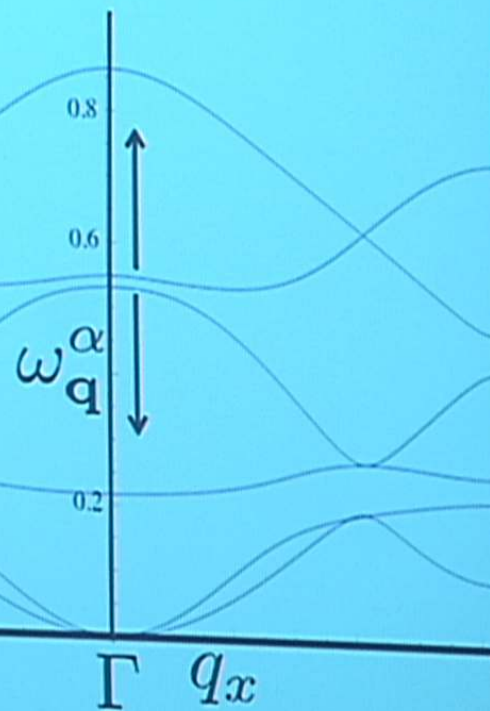
$$m_c = 0$$



$$D^{chiral}(\mathbf{q}) = D(\mathbf{q}) - \frac{\gamma^2 |\langle \mathcal{C} \rangle|^2}{\omega_d} \mathbf{v}^r \mathbf{v}^r$$

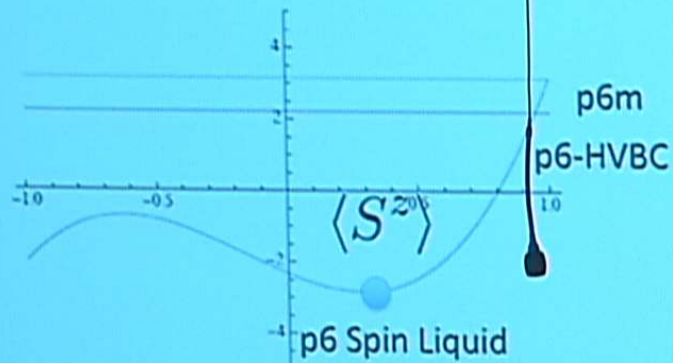
p6

$$m_c > 0$$

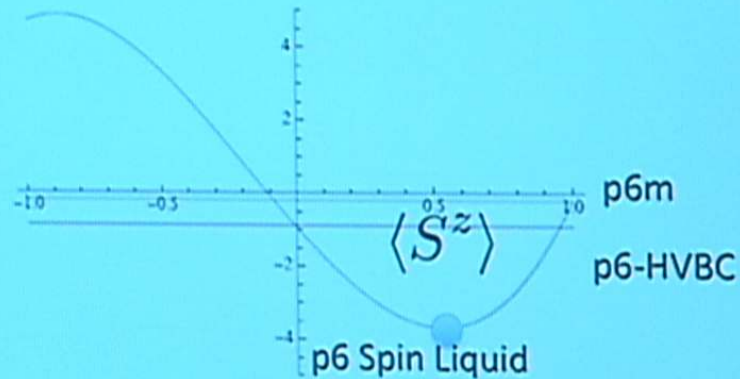


# Varying $J_2$ – work in progress

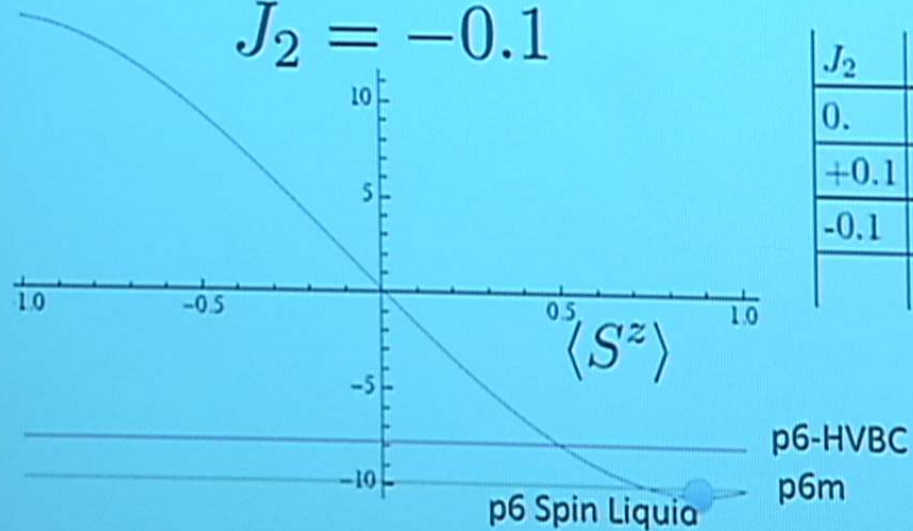
$J_2 = 0.1$



$J_2 = 0.$



$J_2 = -0.1$



$J_2$	$M_z^{MF}$	$M_z^{ED}$	$M_x^{MF}$
0.	0.26473		0.42417
+0.1	0.13904	+0.14756	0.48028
-0.1	0.43511	0.4999	0.246325

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- *CORE is proving useful...*