



# Order and disorder in SU(3) and SU(4) Heisenberg systems

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## Correlations and coherence in quantum systems

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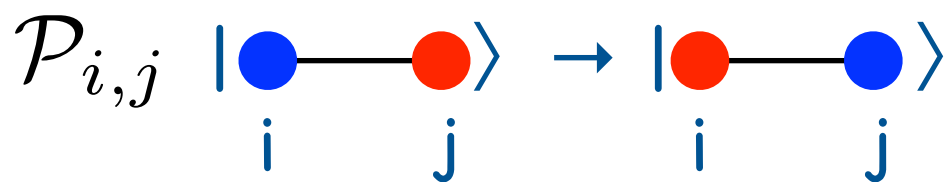
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Tamás A. Tóth, Laura Messio Frédéric Mila	EPF Lausanne
Bela Bauer, Philippe Corboz, Matthias Troyer	ETH Zürich
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Supported by: Hungarian OTKA and Swiss National Foundation

# What are the $SU(N)$ symmetric Heisenberg models that we are interested in?

$$\mathcal{H} = \sum_{i,j} \mathcal{P}_{i,j} \quad \mathcal{P}_{i,j} \text{ is the transposition operator}$$



$N$  species on each site  
that are treated equally.

$$\mathcal{P}_{ij} |\beta_i \alpha_j\rangle = |\alpha_i \beta_j\rangle$$

simplest example:

$SU(2)$   $S=1/2$  (fundamental representation)

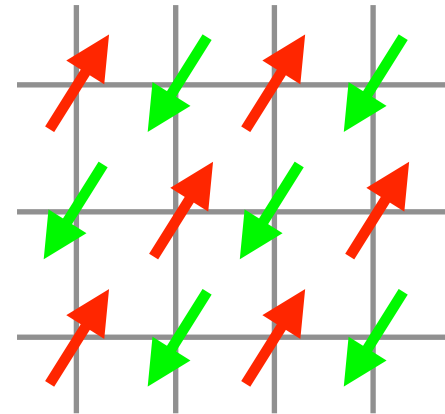
[but not the  $S=1$  !]

# Why do we care about $SU(3)$ or $SU(4)$ Heisenberg models?

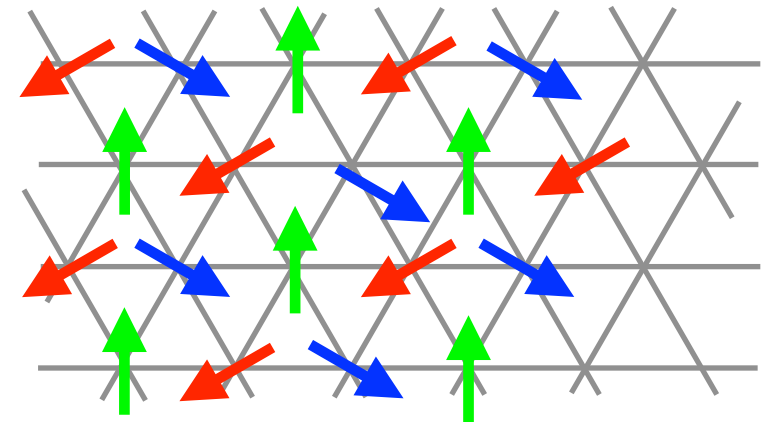
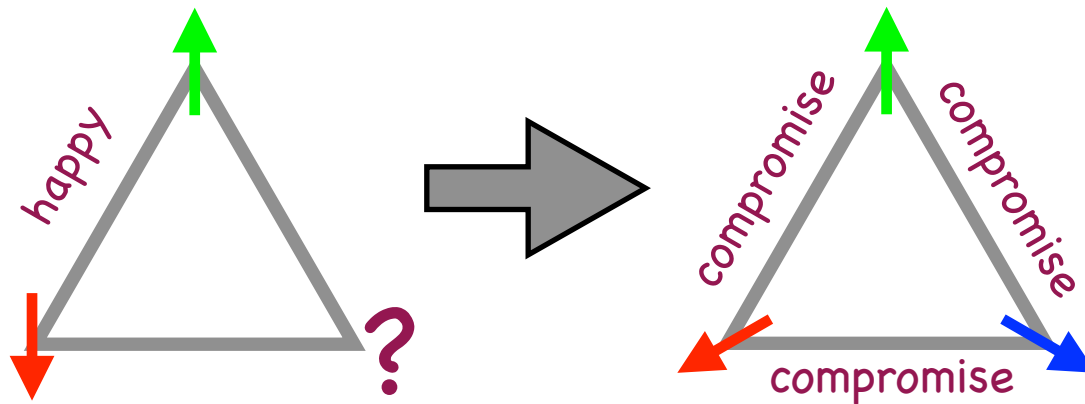
- (i) They are interesting and intellectually challenging  
( funding agencies ?)
- (ii) Nostalgia from our youthhood, when we all wanted  
to become particle physicist ( $SU(3)$  and quarks)
- (iii) Cold atomic gases
- (iv) Spin models
- (v) Spin-orbital models ( $SU(4)$ )

# SU(2) quantum Heisenberg models

square and honeycomb  
(bipartite) lattices:  
happy (mean field)  
antiferromagnets



triangular lattice:  
frustrated antiferromagnet

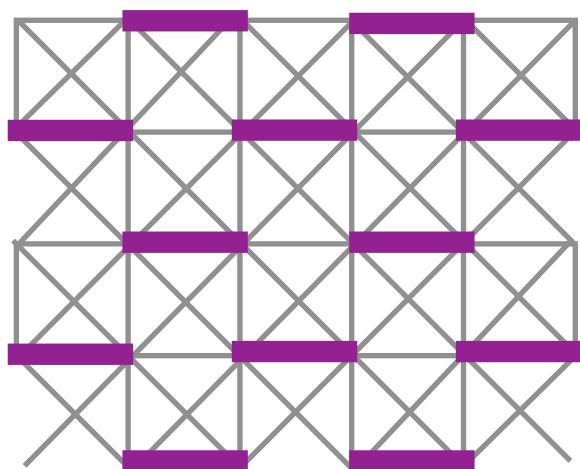
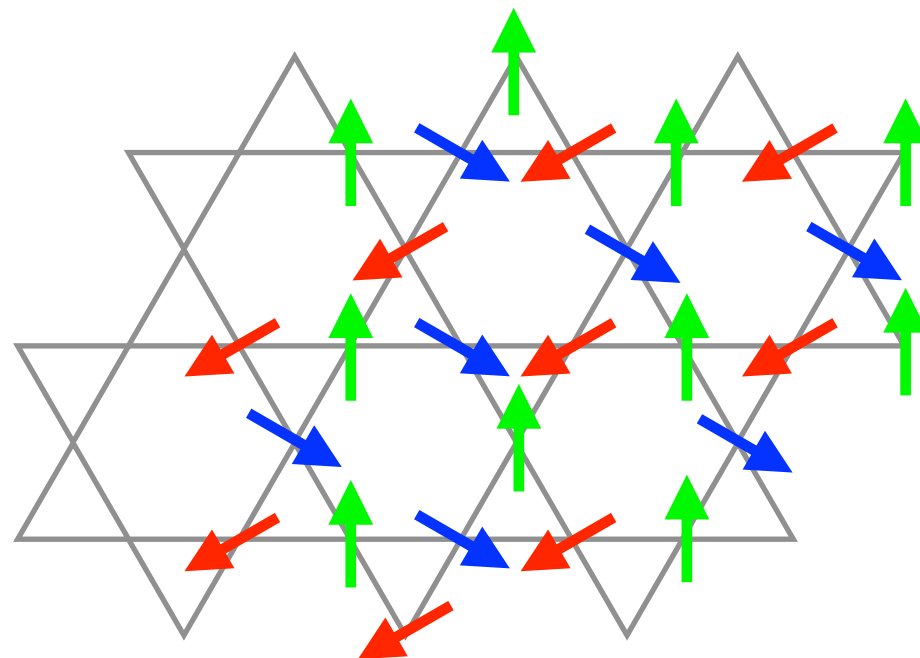


3-sublattice 120 degree state

# SU(2) quantum Heisenberg models

kagome lattice: highly frustrated antiferromagnet, mean field ground state macroscopically degenerate.

Ground state debated, likely a  $Z_2$  spin liquid



frustrated square lattice: dimerized state

# SU(2) vs. SU(3) - two sites



$$\mathcal{P}_{12}(|\alpha\beta\rangle - |\beta\alpha\rangle) = -(|\alpha\beta\rangle - |\beta\alpha\rangle) \quad E = -1, \text{ odd wave function}$$

$$\mathcal{H} = \mathcal{P}_{12} \quad \mathcal{P}_{12}(|\alpha\beta\rangle + |\beta\alpha\rangle) = +(|\alpha\beta\rangle + |\beta\alpha\rangle) \quad E = +1, \text{ even wave function}$$

## Addition of two $S=1/2$ SU(2) spins:

$$1/2 \otimes 1/2 = 0 \oplus 1$$

using Young diagrams:

$$2 \times 2 = 1 + 3$$

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

$\square$   $\uparrow$  or  $\downarrow$  spin

$\begin{array}{|c|} \hline \square \\ \hline \end{array}$   $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$  singlet, odd  
(anti-symmetrical)

$\begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}$   $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$  triplet  
even (symmetrical)

## Addition of two SU(3) spins:

$$3 \times 3 = 3 + 6$$

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

$\square$   $|a\rangle, |b\rangle, \text{ and } |c\rangle$ .

$\begin{array}{|c|} \hline \square \\ \hline \end{array}$   $|\ab\rangle - |\ba\rangle, |\ac\rangle - |\ca\rangle,$   
 $|\bc\rangle - |\cb\rangle$ : odd (anti-  
symmetrical).

$\begin{array}{|c|c|} \hline \square & \square \\ \hline \end{array}$   $|\aa\rangle, |\bb\rangle, |\cc\rangle, |\ab\rangle + |\ba\rangle,$   
 $|\ac\rangle + |\ca\rangle, \text{ and } |\bc\rangle + |\cb\rangle.$   
even (symmetrical)

# SU(3) irreps on 3 sites

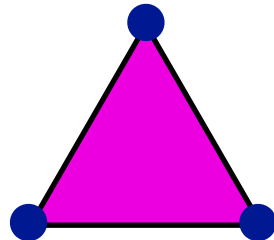
Addition of three SU(3) spins (27 states):

$$\begin{aligned}
 3 \times 3 \times 3 &= 1 + 2 \times 8 + 10 \\
 \square \otimes \square \otimes \square &= \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} \oplus 2 \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} \oplus \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \square \\ \hline \end{array}
 \end{aligned}$$

SU(3) singlet

$$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} = |ABC\rangle + |CAB\rangle + |BCA\rangle - |BAC\rangle - |ACB\rangle - |BCA\rangle$$

spins fully antisymmetrized



in the SU(3) singlet the spins are fully entangled:  
we cannot write it in a product form



# What methods do we use?

- (i) Variational - site factorized wave function
- (ii) Flavor wave calculations
- (iii) Exact diagonalization of small clusters
- (iv) iPEPS: infinite project entangled pair states (variational approach based on tensor ansatz)
- (v) Variational: Gutzwiller projected fermionic wave functions

# Variational (classical) approach

a site-product wave function for SU(3):

$$|\Psi\rangle = \prod_i |\psi_i\rangle$$

$$|\psi_i\rangle = d_{A,i}|A\rangle_i + d_{B,i}|B\rangle_i + d_{C,i}|C\rangle_i$$

$$E_{\text{var}} = \frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = J \sum_{\langle i,j\rangle} |\mathbf{d}_i \cdot \bar{\mathbf{d}}_j|^2$$

minimal, when the  $\mathbf{d}_i$  and  $\mathbf{d}_j$  on the bond are orthogonal

**two different colors on a bond**

# SU(3) flavour-wave theory

N. Papanicolaou, Nucl. Phys. B **305**, 367 (1988)

A. Joshi *et al.* PRB **60**, 6584 (1999)



We enlarge the fundamental to the fully symmetric representation of  $M$  boxes.

States in the fully symmetric multiplet can be represented by 3 Schwinger bosons  $a_A, a_B$  and  $a_C$

$$a_{A,i}^\dagger a_{A,i} + a_{B,i}^\dagger a_{B,i} + a_{C,i}^\dagger a_{C,i} = M$$

$$\mathcal{P}_{ij} = \sum_{\mu, \nu \in \{A, B, C\}} a_{\mu,i}^\dagger a_{\nu,j}^\dagger a_{\nu,i} a_{\mu,j}$$

The site product wave function is the “classical” solution (no quantum entanglement between sites)

$$|\Psi\rangle = \prod_i |\psi_i\rangle$$

$$|\psi_i\rangle = d_{A,i} |A\rangle_i + d_{B,i} |B\rangle_i + d_{C,i} |C\rangle_i$$

cf. SU(2) spin coherent state for SU(2)

$$|\vartheta, \varphi\rangle = \cos \frac{\vartheta}{2} |\uparrow\rangle + \sin \frac{\vartheta}{2} e^{i\varphi} |\downarrow\rangle$$

# SU(3) flavour-wave theory

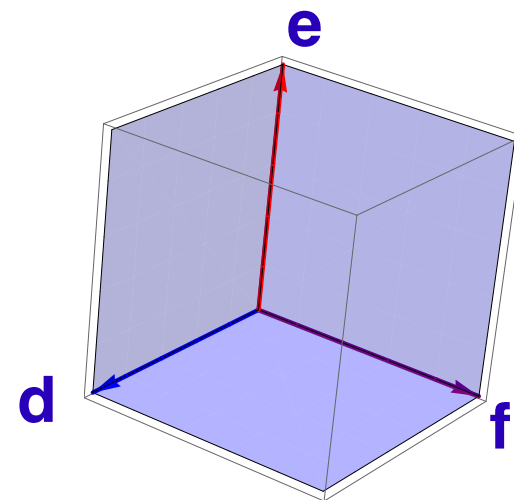
Local coordinate system

$$|\Psi\rangle = \prod_i \left( \tilde{a}_i^\dagger \right)^M |\tilde{0}\rangle$$

$$\tilde{a}_{A,j}^\dagger = \sum_\mu d_{\mu,j} a_{\mu,j}^\dagger$$

$$\tilde{a}_{B,j}^\dagger = \sum_\mu e_{\mu,j} a_{\mu,j}^\dagger$$

$$\tilde{a}_{C,j}^\dagger = \sum_\mu f_{\mu,j} a_{\mu,j}^\dagger$$



1/M expansion:

$$\begin{aligned} \tilde{a}_{A,i}^\dagger, \tilde{a}_{A,i} &\rightarrow \sqrt{M - \tilde{a}_{B,i}^\dagger \tilde{a}_{B,i} - \tilde{a}_{C,i}^\dagger \tilde{a}_{C,i}} \\ &\rightarrow \sqrt{M} - \frac{1}{2\sqrt{M}} \left( \tilde{a}_{B,i}^\dagger \tilde{a}_{B,i} + \tilde{a}_{C,i}^\dagger \tilde{a}_{C,i} \right) + \dots \end{aligned}$$

Holstein-Primakoff bosons

$$\begin{aligned} \mathcal{P}_{ij} &\rightarrow M \left[ (\bar{\mathbf{e}}_i \cdot \mathbf{d}_j) \tilde{a}_{B,i}^\dagger + (\bar{\mathbf{f}}_i \cdot \mathbf{d}_j) \tilde{a}_{C,i}^\dagger + (\bar{\mathbf{d}}_i \cdot \mathbf{e}_j) \tilde{a}_{B,j} + (\bar{\mathbf{d}}_i \cdot \mathbf{f}_j) \tilde{a}_{C,j} \right] \\ &\times \left[ (\mathbf{e}_i \cdot \bar{\mathbf{d}}_j) \tilde{a}_{B,i} + (\mathbf{f}_i \cdot \bar{\mathbf{d}}_j) \tilde{a}_{C,i} + (\mathbf{d}_i \cdot \bar{\mathbf{e}}_j) \tilde{a}_{B,j}^\dagger + (\mathbf{d}_i \cdot \bar{\mathbf{f}}_j) \tilde{a}_{C,j}^\dagger \right] - M \end{aligned}$$

quadratic in operators: we know how to diagonalize it (spin wave)

$$\mathcal{H} = -MJL + M \sum_\nu \sum_{\mathbf{k}} \omega_\nu(\mathbf{k}) \left( \alpha_\nu^\dagger(\mathbf{k}) \alpha_\nu(\mathbf{k}) + \frac{1}{2} \right)$$

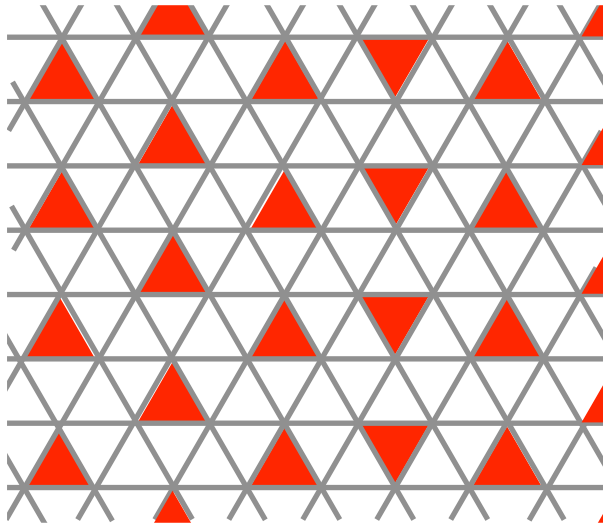
# The models

- (i)  $SU(3)$  model on the triangular lattice
- (ii)  $SU(3)$  model on the square lattice
- (iii)  $SU(4)$  model on the square and cubic lattice
- (iv)  $SU(4)$  model on the honeycomb lattice

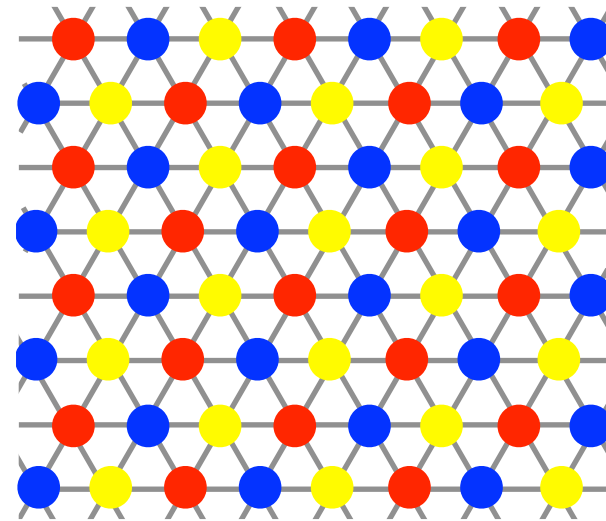
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# The fate of SU(3) on triangular lattice



crystal of singlets?

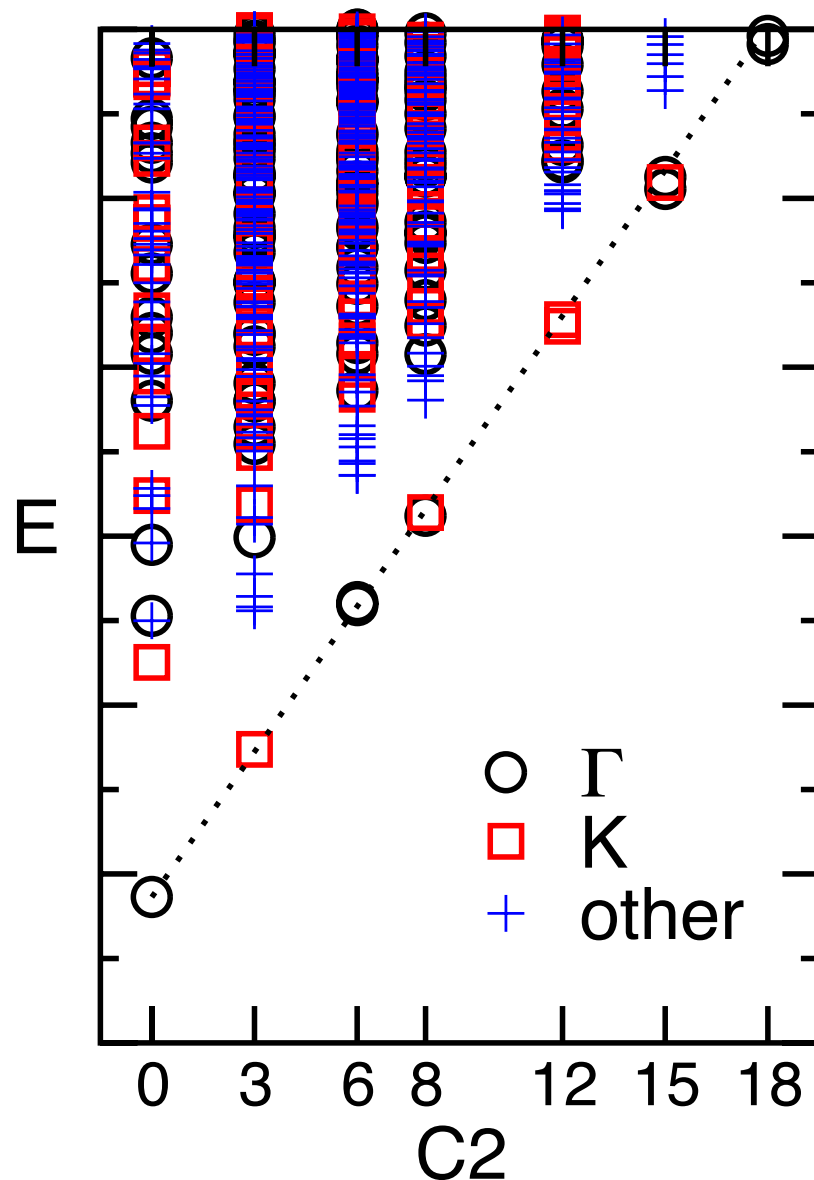


“classical” solution?

SU(3) classical state is perfectly happy on the triangular lattice - the 3 mutually perpendicular  $\mathbf{d}$ 's form a 3 sublattice structure.

SU(2) frustrated!

# SU(3) on triangular lattice - exact diagonalization

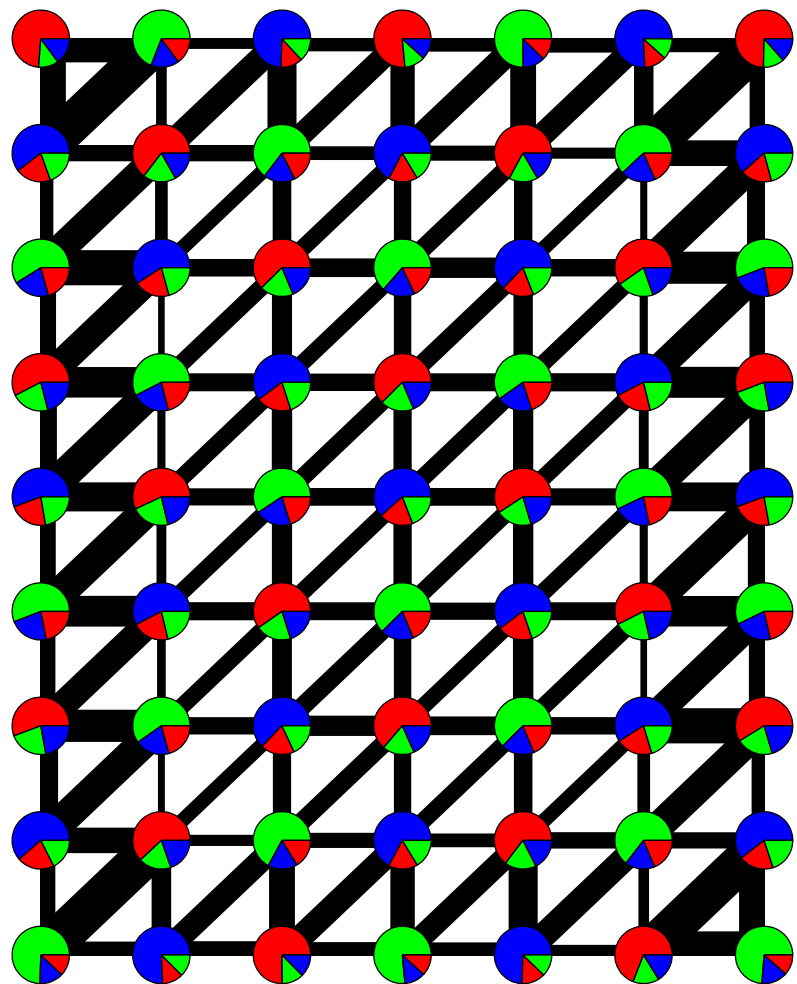


Signature of SU(3) breaking  
in the excitation spectrum:  
Anderson towers compatible  
with 3 sublattice order

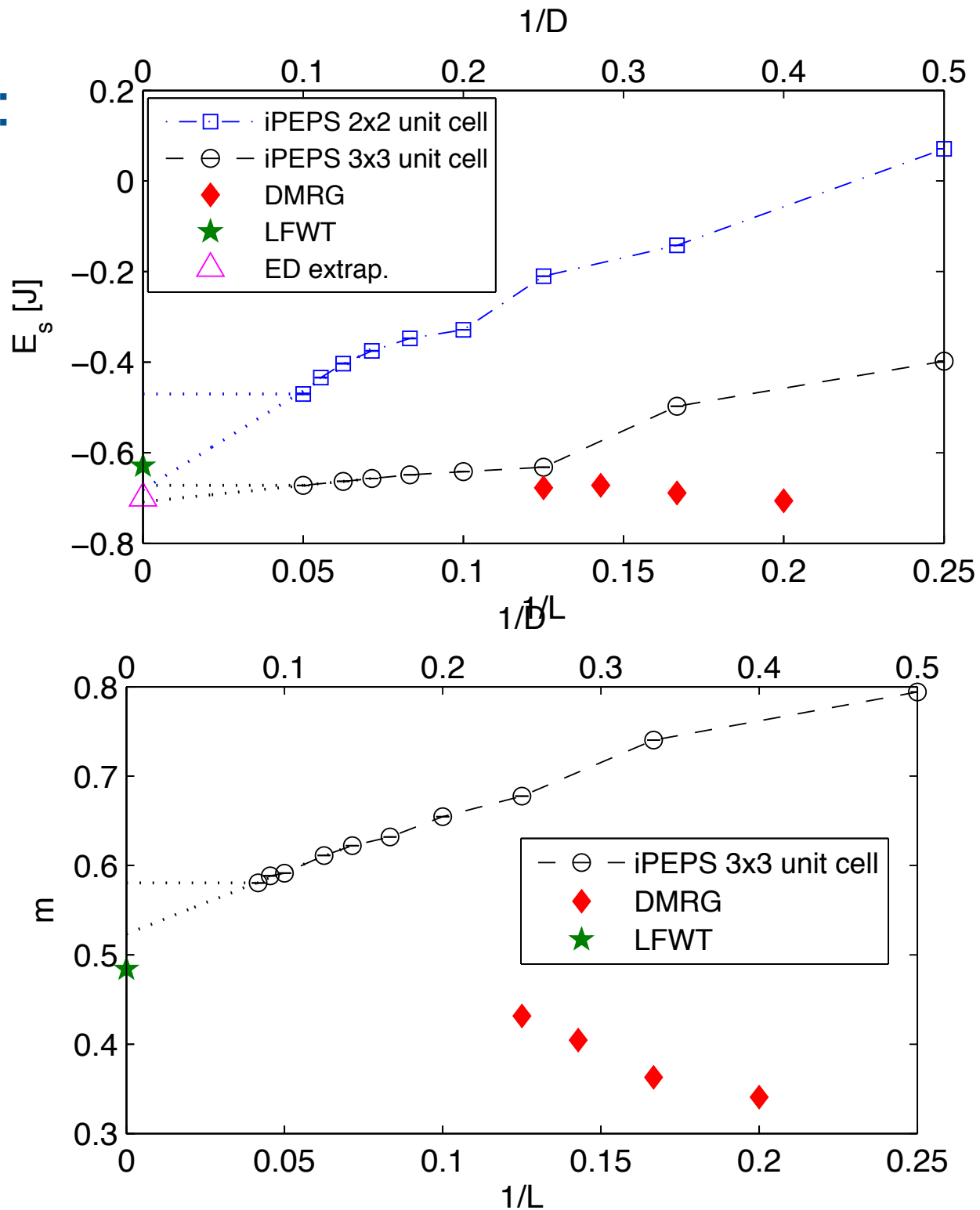
C2 - Casimir operator, analog  
of the total spin  $S^2$



# Unbiased calculation: iPEPS, DMRG



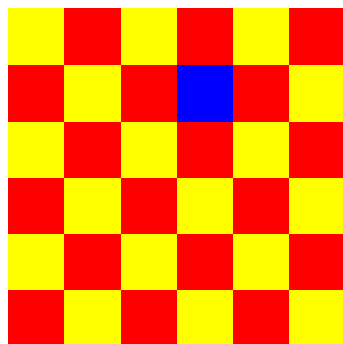
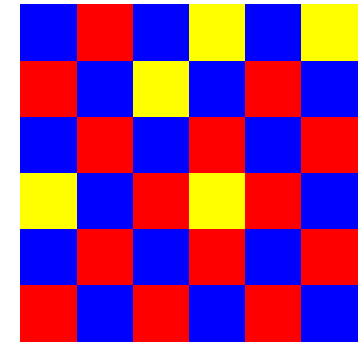
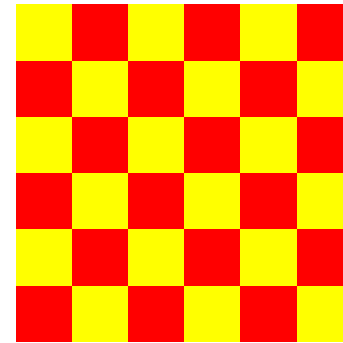
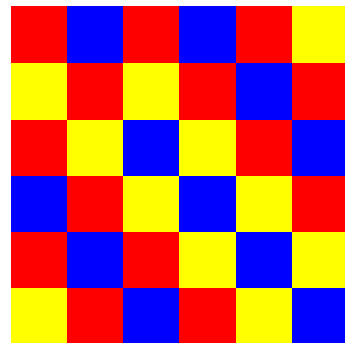
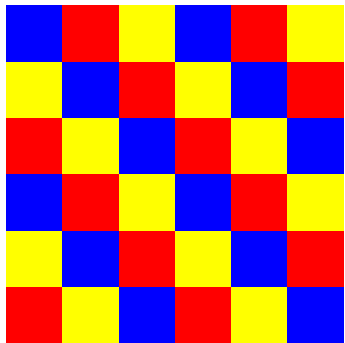
B. Bauer, P. Corboz, A. M. Läuchli, L. Messio,  
K. Penc, M. Troyer, F. Mila:  
Phys. Rev. B **85**, 125116/1-11 (2012)



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- (iv)  $SU(4)$  model on the honeycomb lattice

# SU(3) classical solutions: macroscopically degenerate

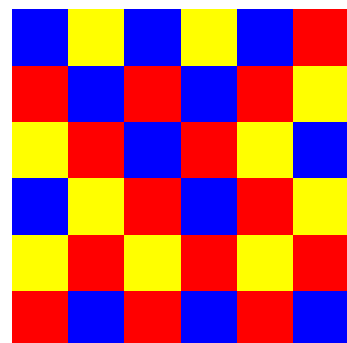


All bonds happy at the mean field level,  
frustration due to abundance of choices

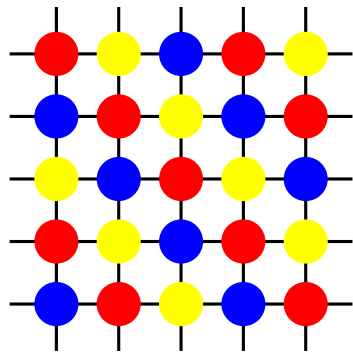
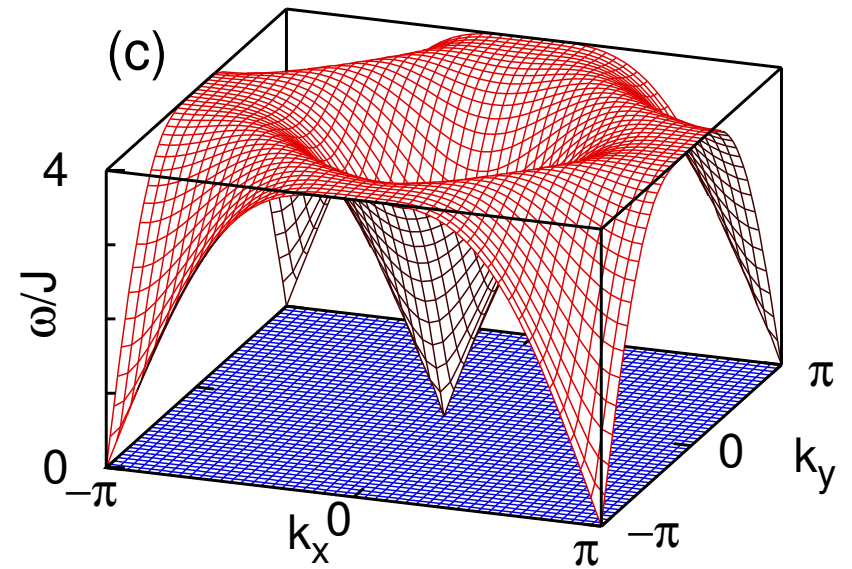
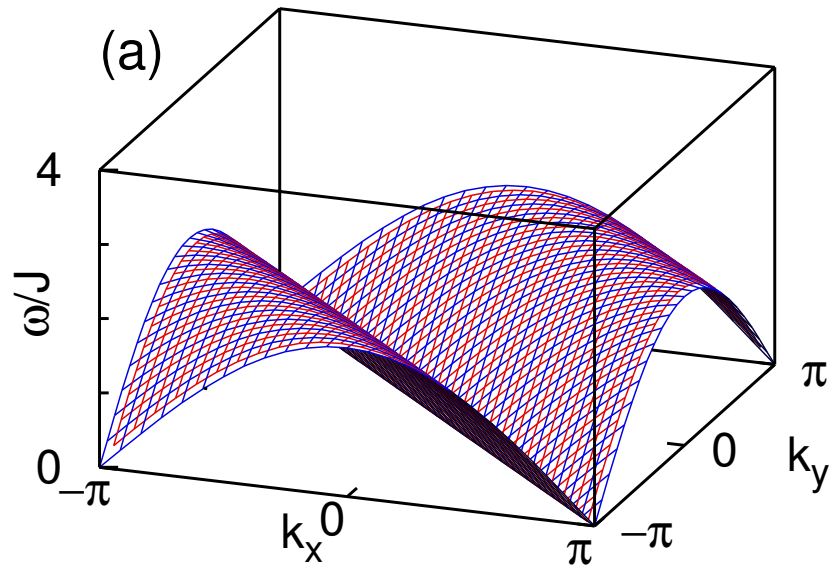
Order by disorder:

quantum fluctuations select the  
ground state

$$E_{ZP} = \frac{M}{2} \sum_{\nu} \sum_{\mathbf{k}} \omega_{\nu}(\mathbf{k})$$

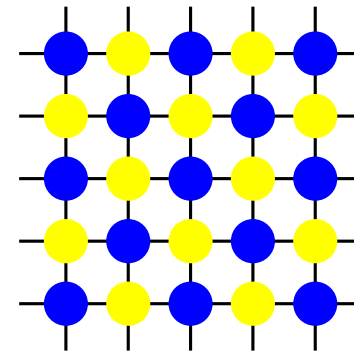


# SU(3) flavour-wave: dispersions, zero point energy



$$E_{ZP} = 1.27$$

The winner !

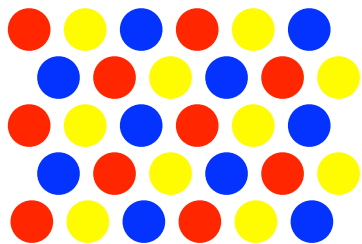
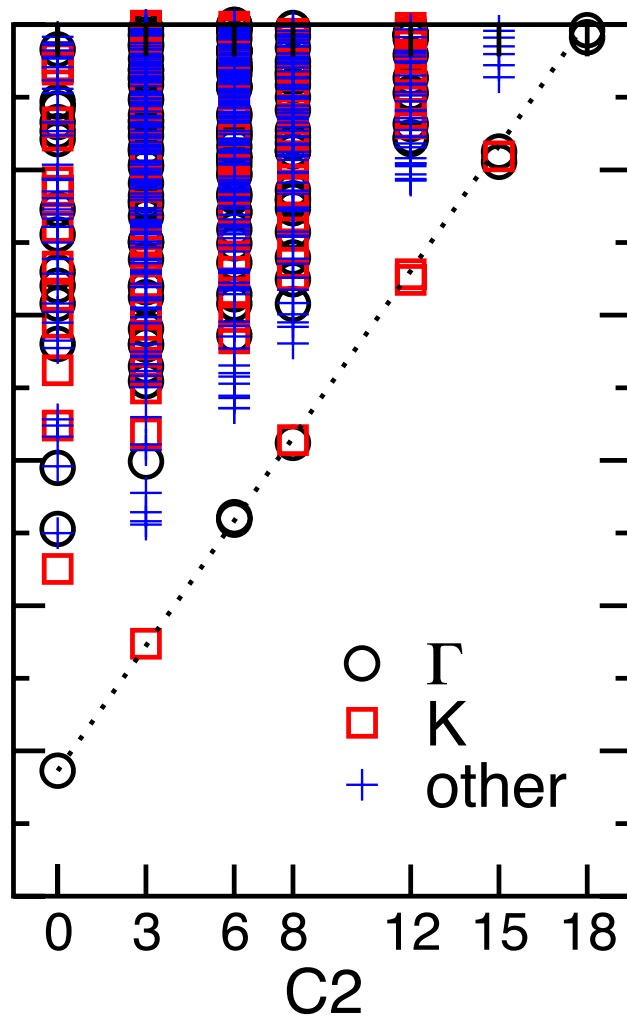


$$E_{ZP} = 1.68$$

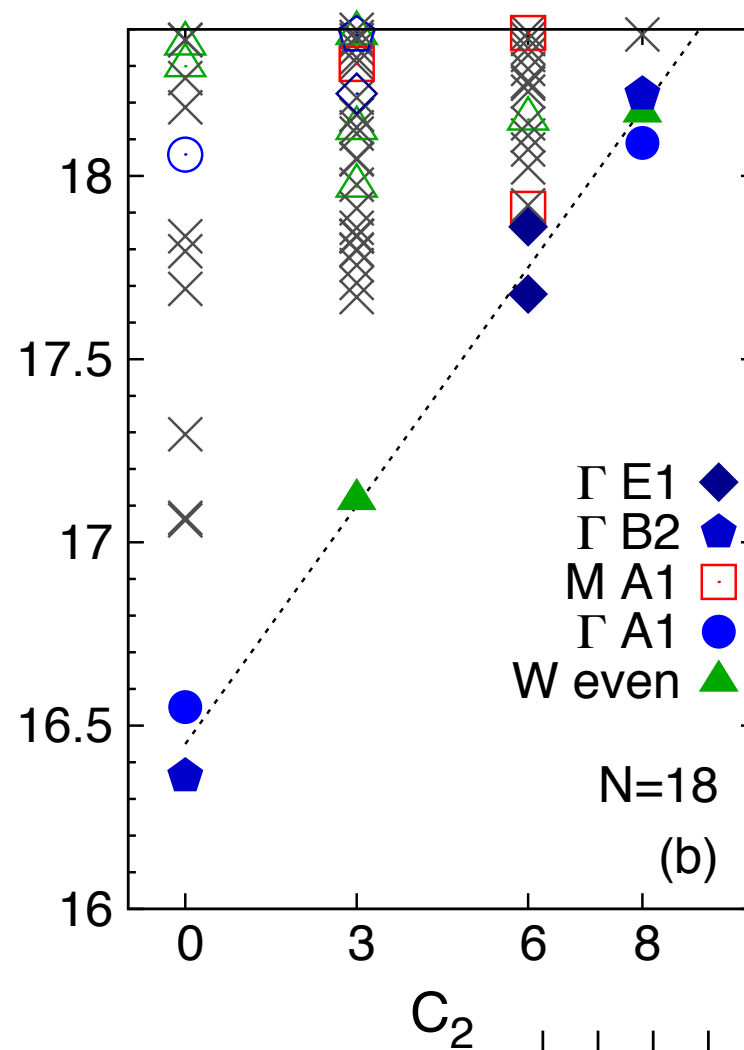
T. A. Tóth, A. M. Läuchli, F. Mila, and K. Penc:  
PRL 105, 265301 (2010).

# Unbiased calculation: ED, Anderson towers

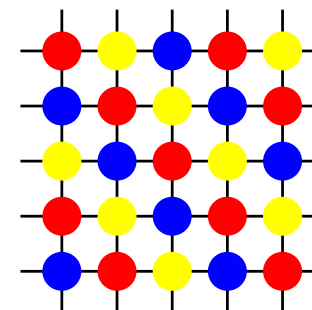
triangular lattice



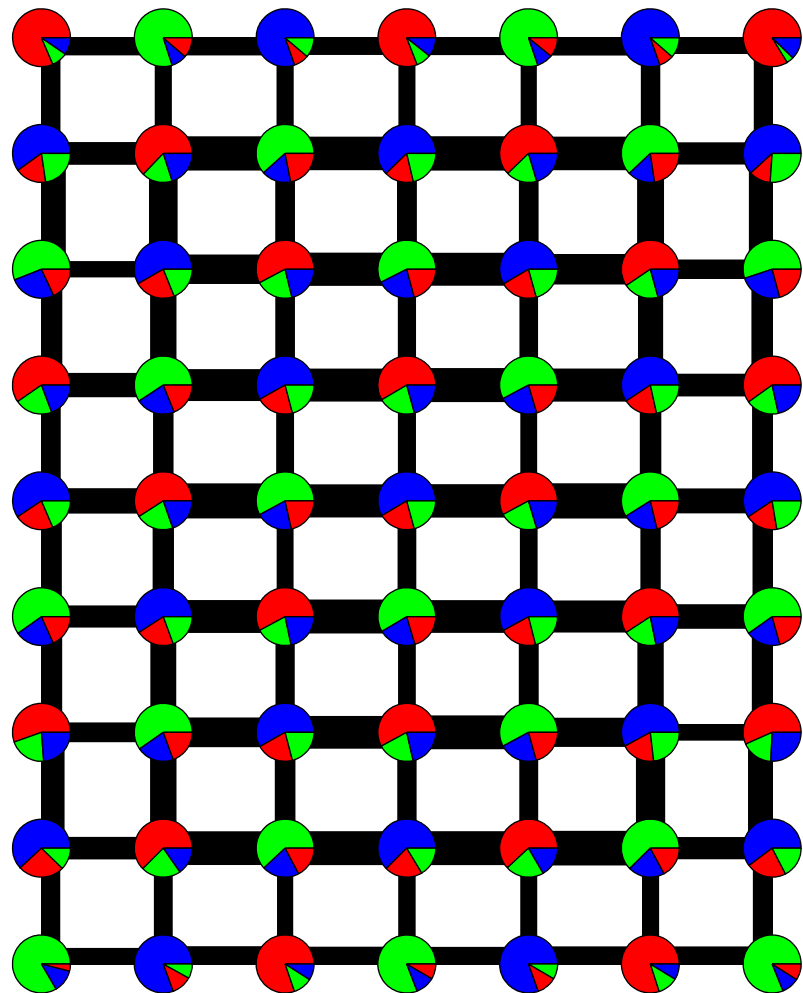
square lattice



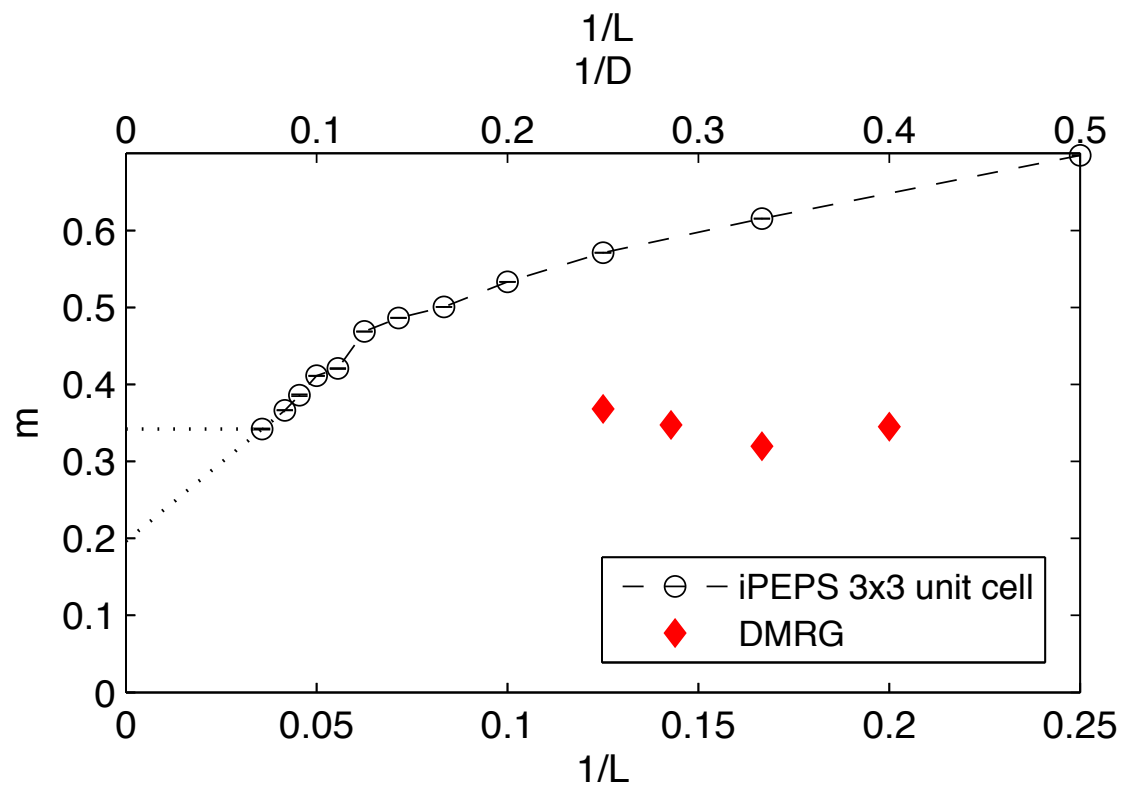
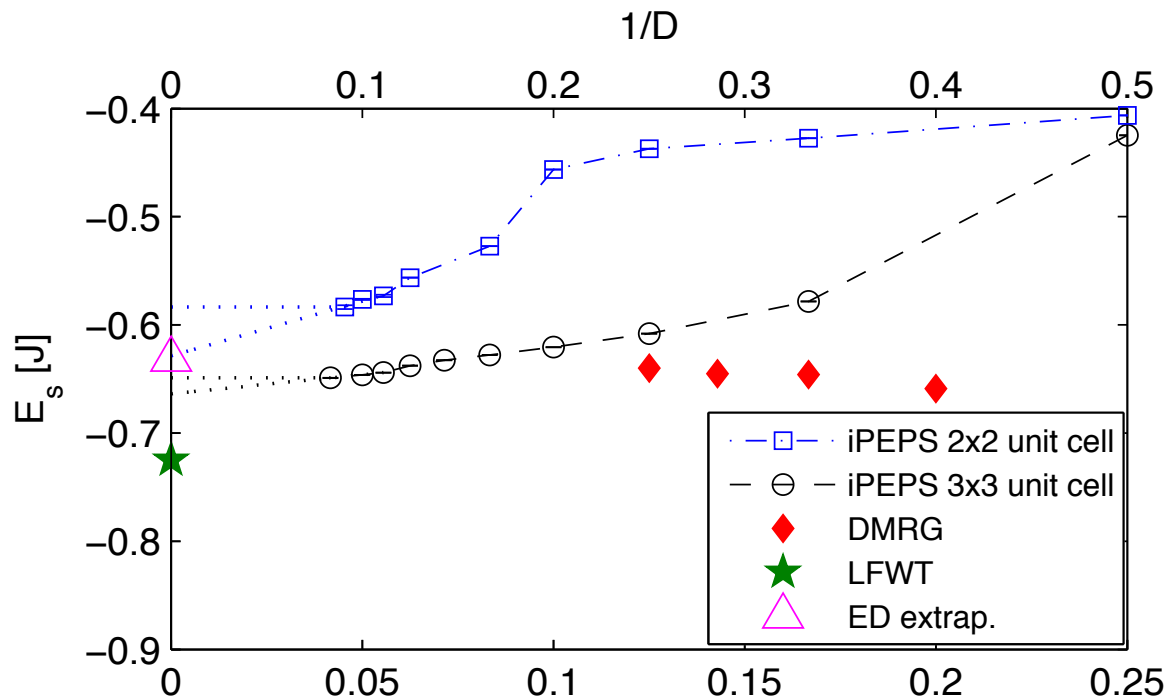
additional Z<sub>2</sub>  
 symmetry



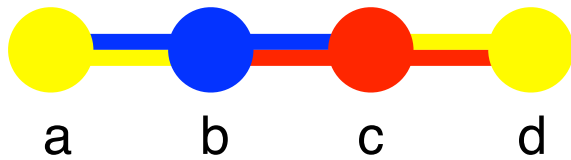
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B. Bauer, P. Corboz, A. M. Läuchli, L. Messio,  
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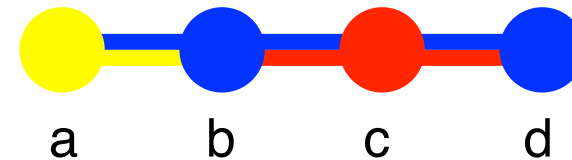
# structure of the flavor wave Hamiltonian



$$\mathcal{H} = (a^\dagger + b)(b^\dagger + a) + (b^\dagger + c)(c^\dagger + b) + (c^\dagger + d)(d^\dagger + c)$$

each term separately  $E_{ZP} = 0$

nearest neighbor also of different color



$$\mathcal{H} = (a^\dagger + b)(b^\dagger + a) + (b^\dagger + c)(c^\dagger + b) + (c^\dagger + d)(d^\dagger + c)$$

the 3-site term gives  $E_{ZP} > 0$

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# SU(4) irreps on 4 sites

Addition of four SU(4) spins (256 states):

$$4 \times 4 \times 4 \times 4 = 1 + 3 \times 15 + 2 \times 20 + 3 \times 45 + 35$$

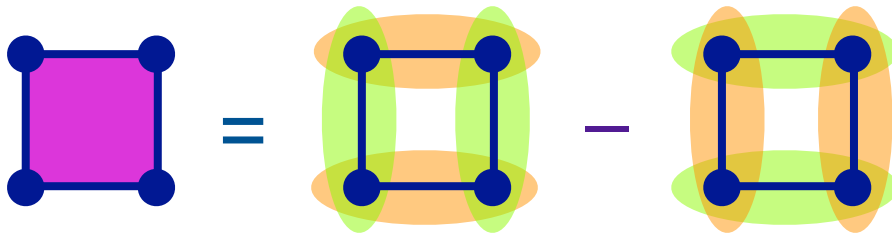
$$\square \otimes \square \otimes \square \otimes \square = \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} \oplus 3 \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \oplus 2 \times \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \square \\ \hline \end{array} \oplus 3 \times \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & & \\ \hline \end{array} \oplus \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \end{array}$$

multiplets

SU(4) singlet

$$\begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} = |\text{abcd}\rangle - |\text{bacd}\rangle + |\text{badc}\rangle - |\text{bdac}\rangle - \dots$$

spins fully antisymmetrized



spin singlet bond:

$$\begin{array}{|c|} \hline \bullet \text{---} \bullet \\ \hline \end{array} = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

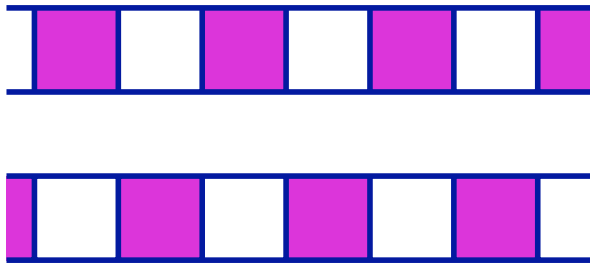
orbital singlet bond:

$$\begin{array}{|c|} \hline \bullet \text{---} \bullet \\ \hline \end{array} = \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right\rangle - \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right\rangle$$

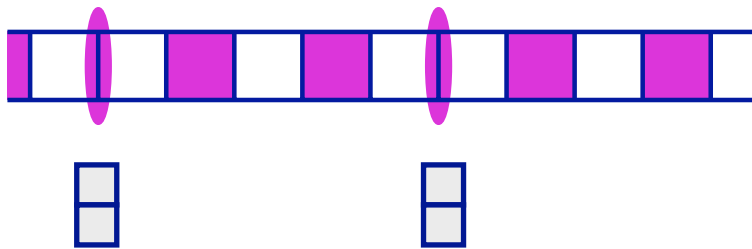
SU(4) singlet plaquette  
entangled spins and orbitals

# SU(4) ladder

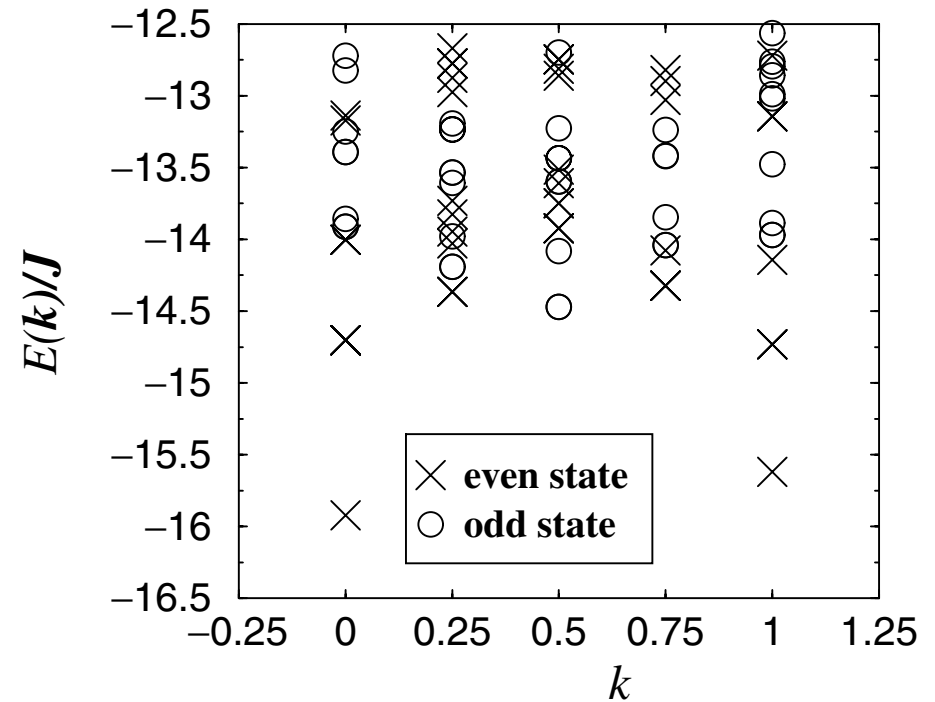
GS twofold degenerate  
(translational invariance broken):



gapped excitation spectrum,  
situation similar to  
 $J_1$ - $J_2$  SU(2) Heisenberg chain:

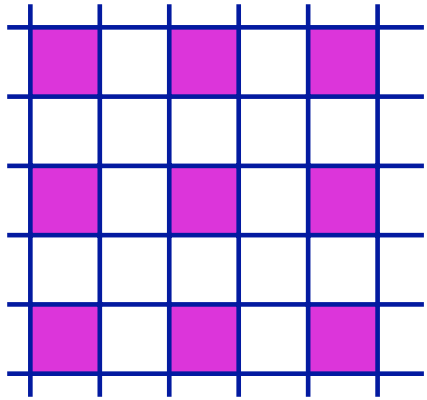


M. van den Bossche et al.,  
Phys. Rev. Lett. **86**, 4124 (2001).



# SU(4) on 2D-square lattice

Ground state 4-fold degenerate?



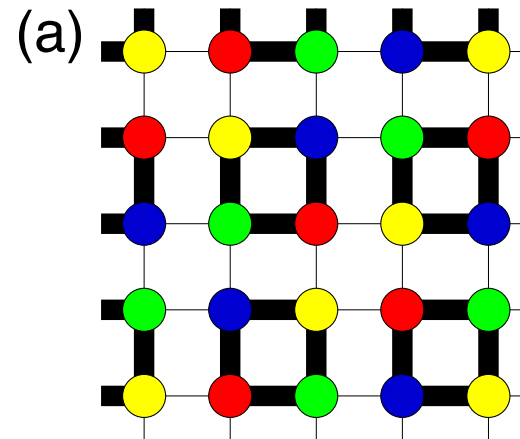
Z<sub>2</sub> liquid ?  
Wang & Viswanath (PRB 2009)

# SU(4) on 2D-square lattice: breaking SU(4)?

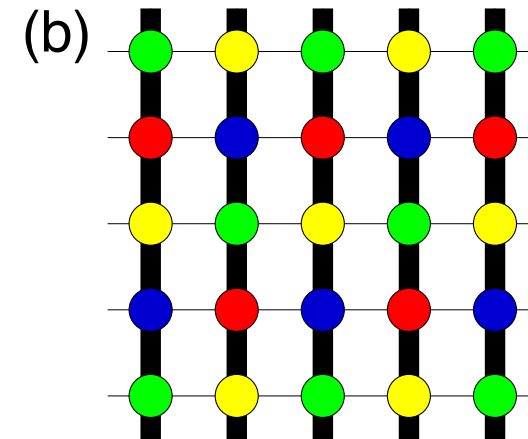
The number of good mean field solution is highly degenerate.

## Order by disorder:

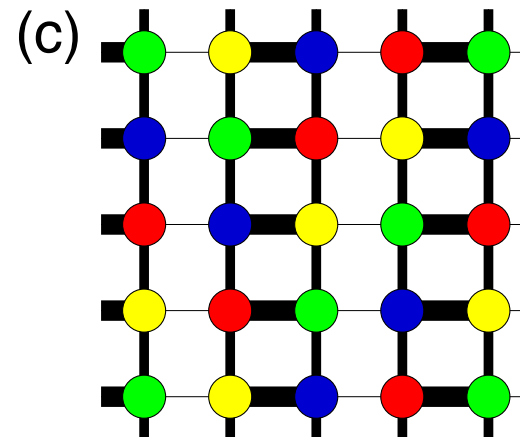
Assuming on-site long range order, which configuration has the lowest zero-point energy?



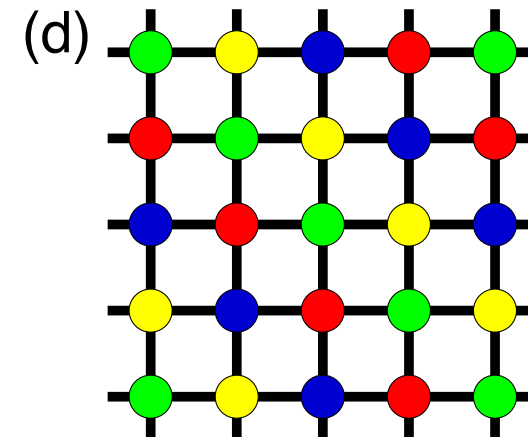
$$E/N = -3/2 J$$



$$E/N = -1.363 J$$

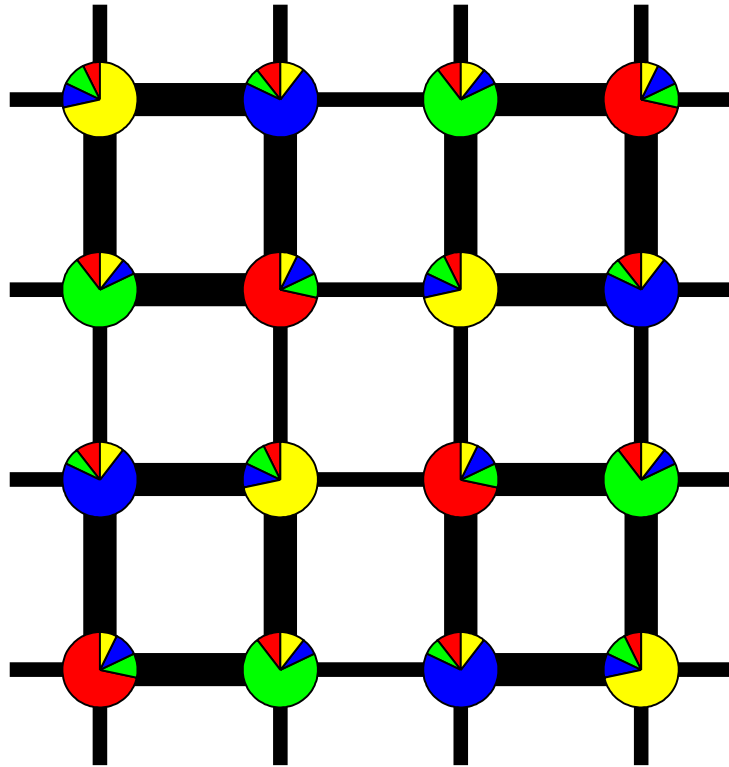


$$E/N = -1.293 J$$



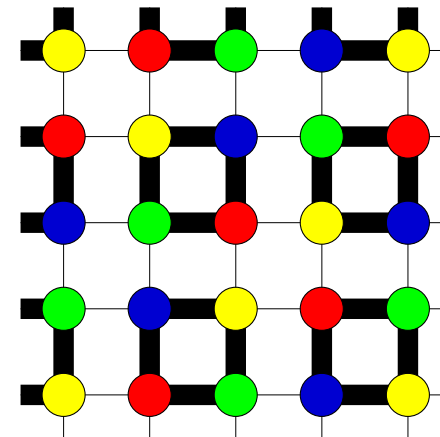
$$E/N = -0.727 J$$

# SU(4) on 2D-square lattice: iPEPS

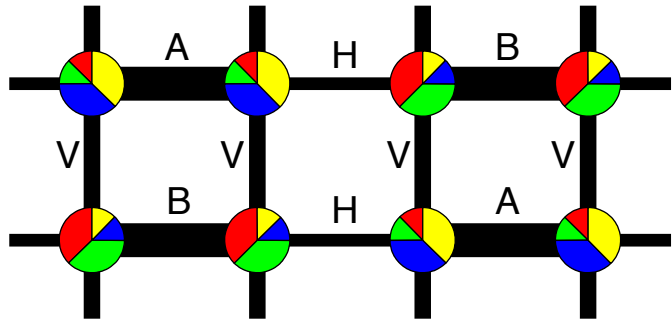


Tensor network method, with  $D$ -dimensional links between sites.

$D = 2$  and a unit cell  $4 \times 4$ . The bond-energy pattern of the ground state is similar to that of the plaquette state selected by LFWT.



# SU(4) on 2D-square lattice: iPEPS



$D = 12$  and a unit cell  $4 \times 2$

dimerization and Neel-like state:  
both spatial and the SU(4)  
symmetry is broken

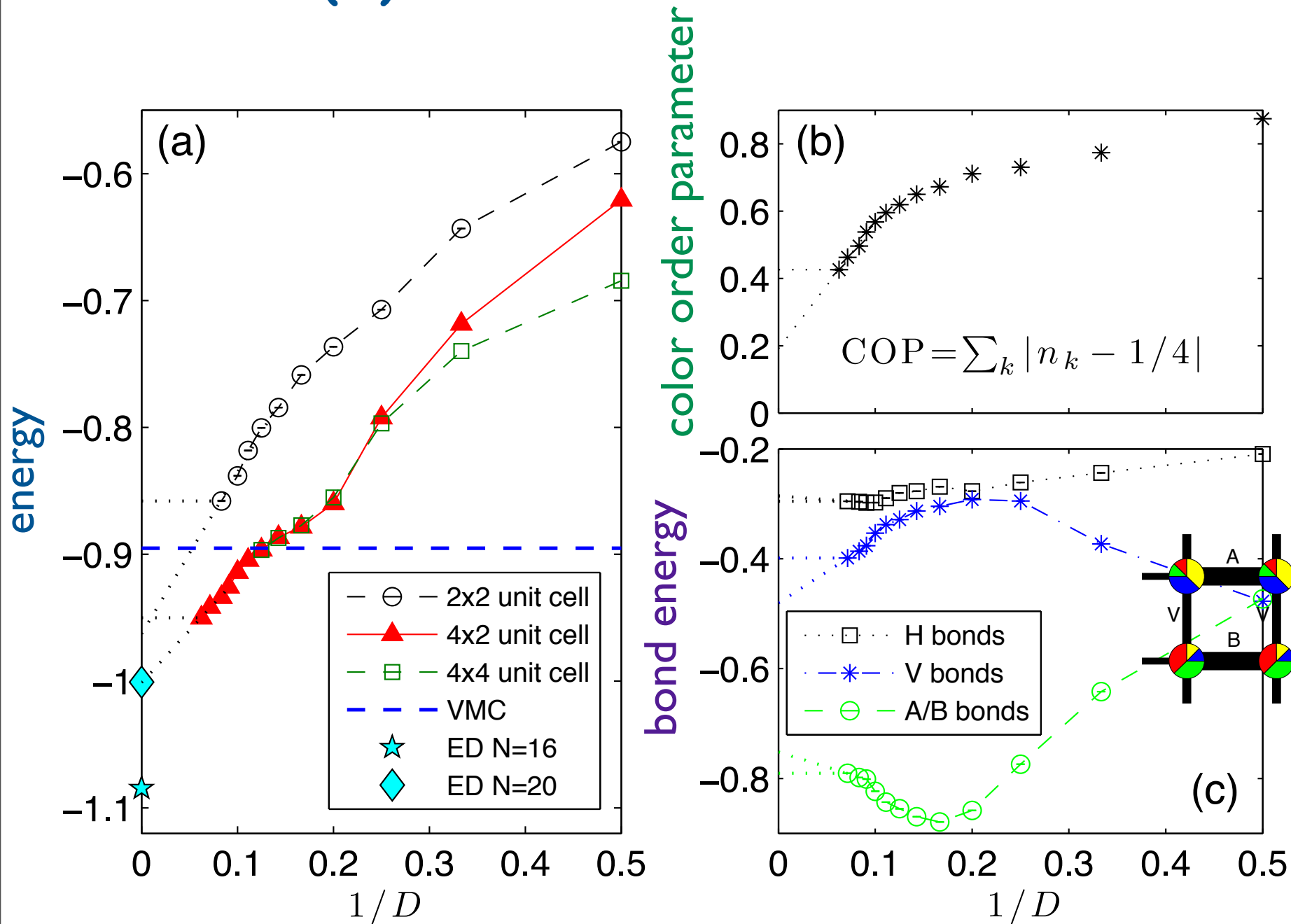
$$4 \times 4 = 6 + 10$$

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

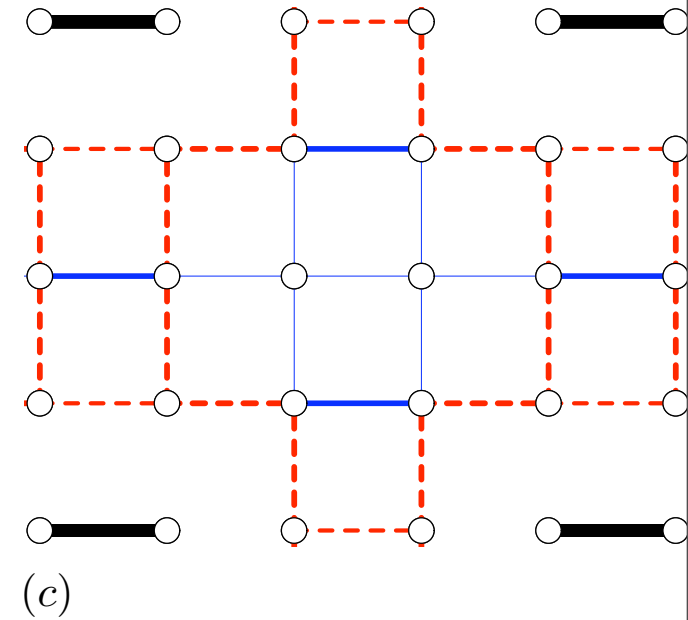
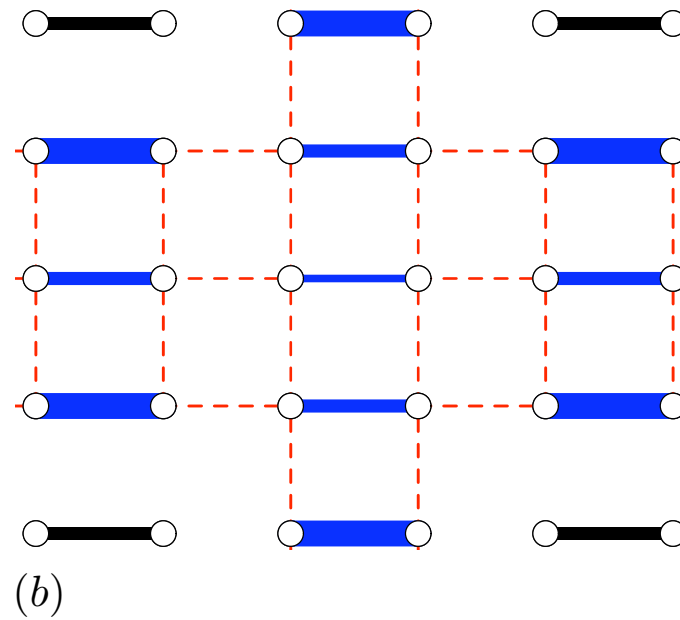
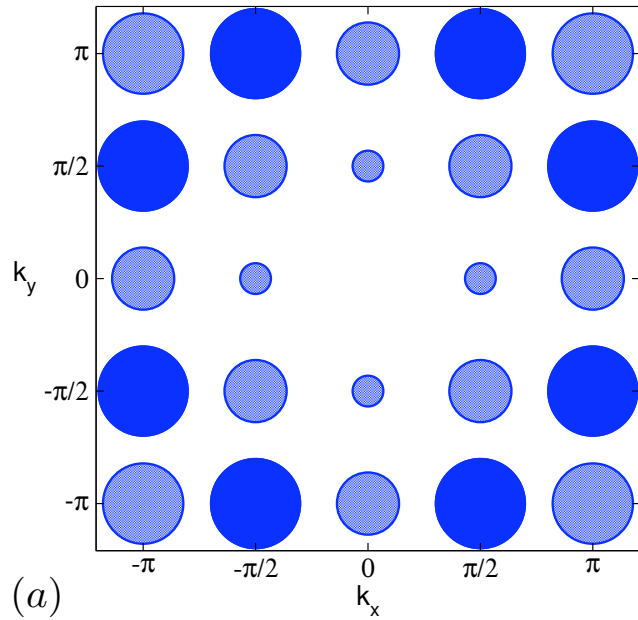


the 6 dimensional irreducible  
representation is realized on the  
dimers, can Neel order

# SU(4) on 2D-square lattice: iPEPS



# SU(4) on 2D-square lattice: ED



Color structure factor

bond energy correlations

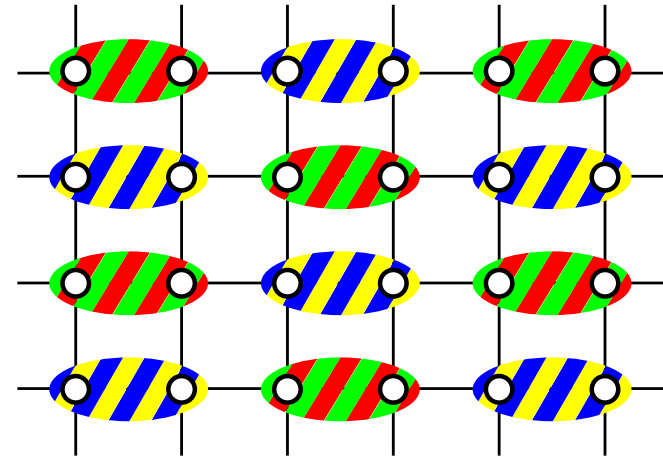
$$\langle P_{ij}P_{kl} \rangle - \langle P_{ij} \rangle^2$$

$$\langle P_{(i,j)}(a,b)P_{(k,l)}(a,b) \rangle$$



# SU(4) on 2D-square lattice: our scenario

Dimerization: 6-dimensional irreps are formed, they can Néel order



P. Corboz, A. M. Läuchli, K. Penc, M. Troyer, F. Mila, PRL **107**, 215301 (2011).

**SU(4) can be lowered to Sp(4) in cold atoms:**

H. Hung, Y. Wang, and C. Wu, Phys. Rev. B **84**, 054406 (2011).

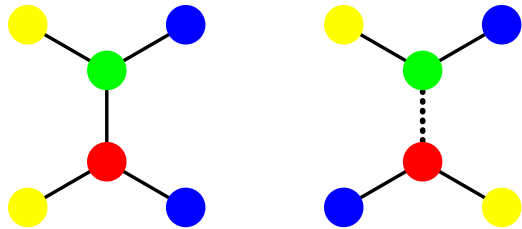
E. Szirmai and M. Lewenstein, EPL **93**, 66005 (2011).

# The models

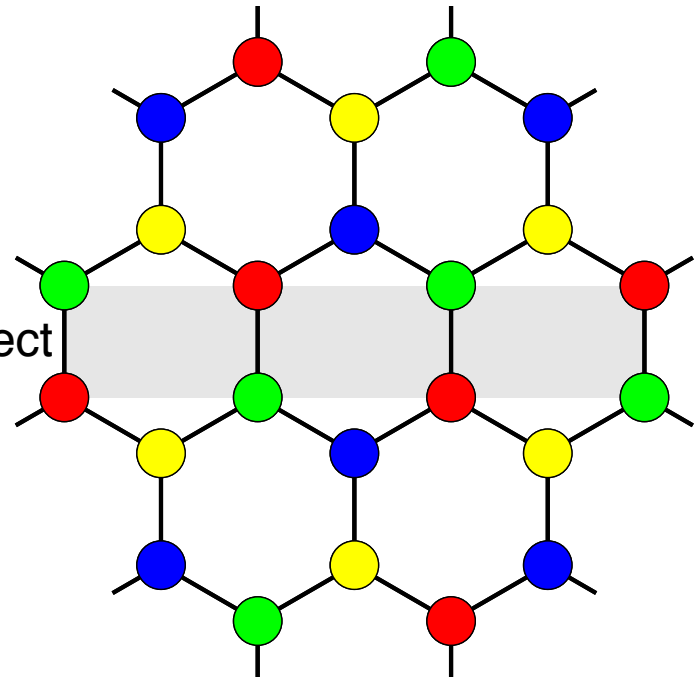
- (i)  $SU(3)$  model on the triangular lattice
- (ii)  $SU(3)$  model on the square lattice
- (iii)  $SU(4)$  model on the square and cubic lattice
- (iv)  $SU(4)$  model on the honeycomb lattice

# Lifting of the degeneracy in flavor wave theory

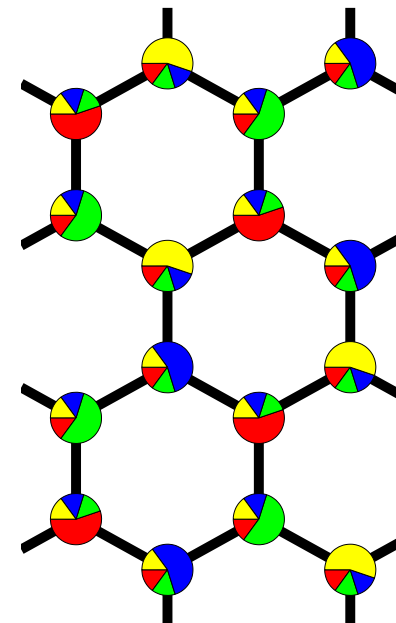
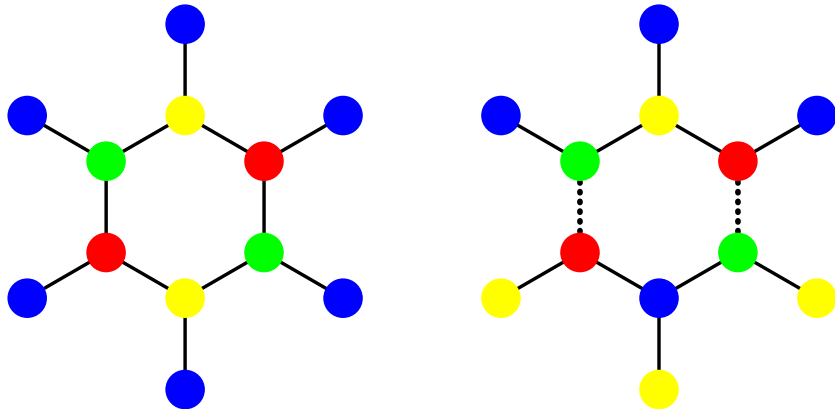
Basic building blocks:  
nearest (mean field) and next nearest  
(fluctuations) neighbor colors different.



A linear defect

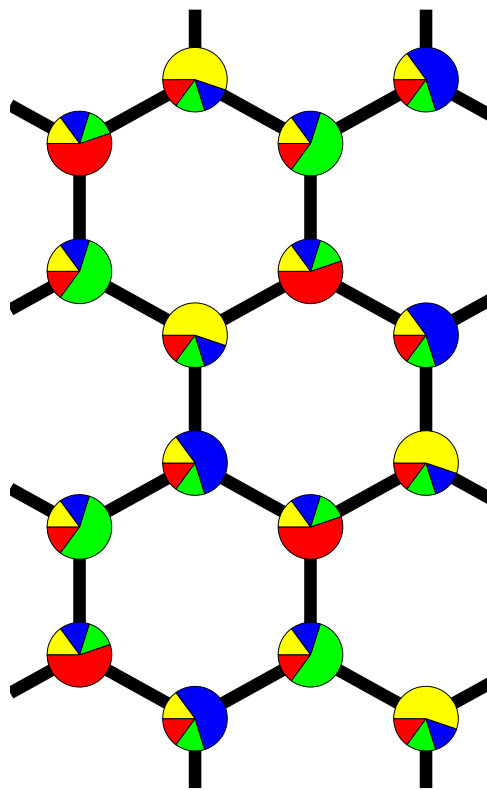
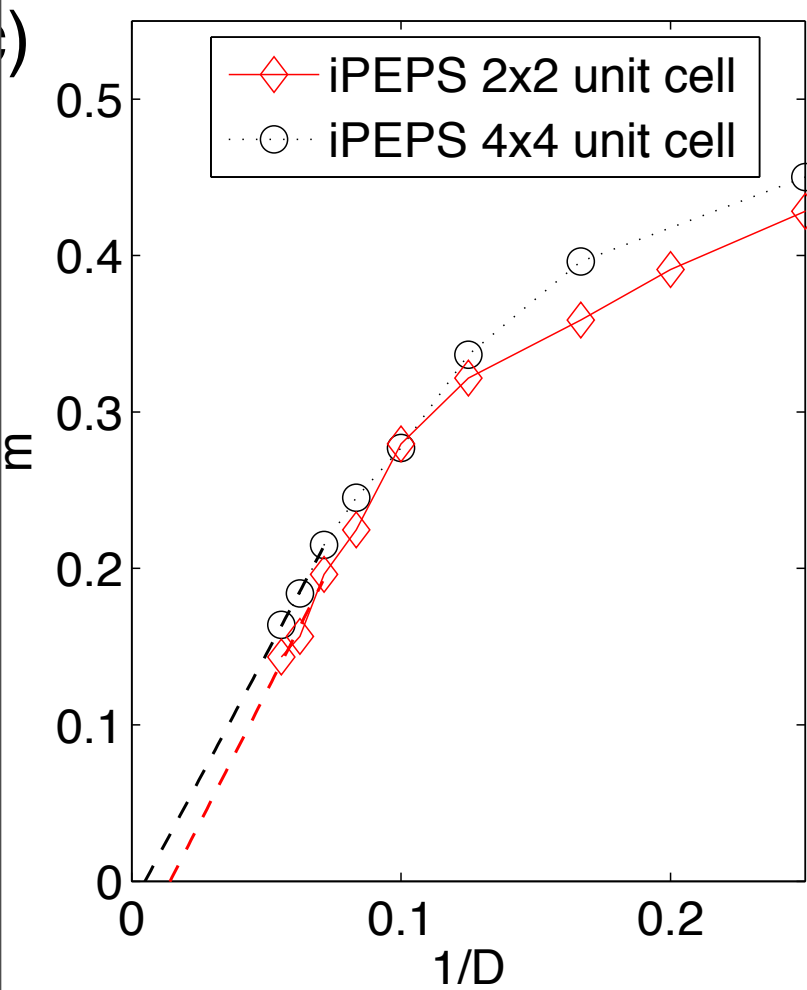


The allowed 9-spin configurations,  
not lifted in harmonic approximation:

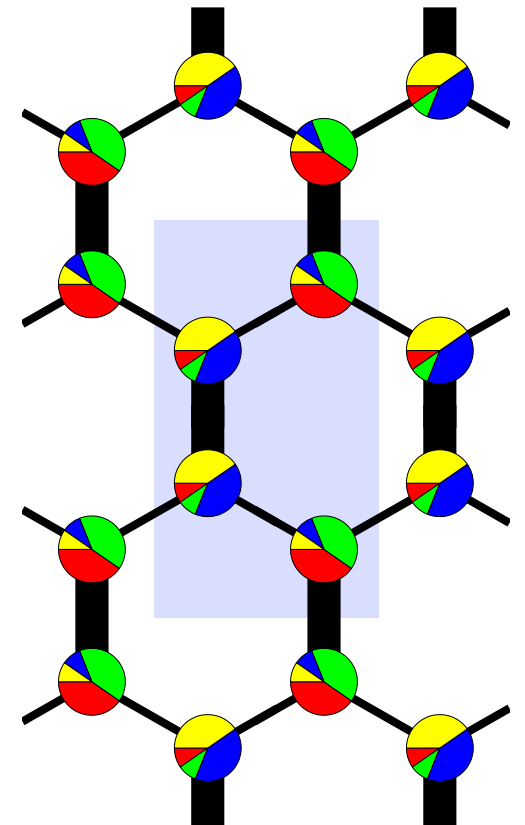


iPEPS,  
D=6

# iPEPS - local magnetization vanishes

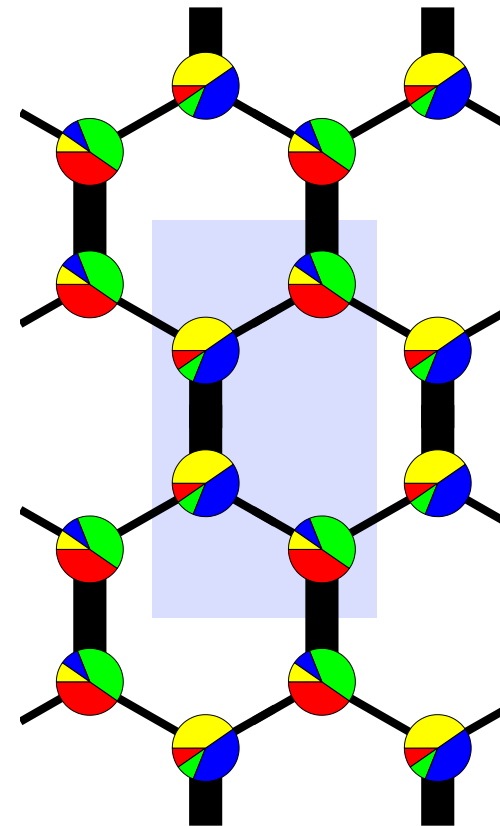
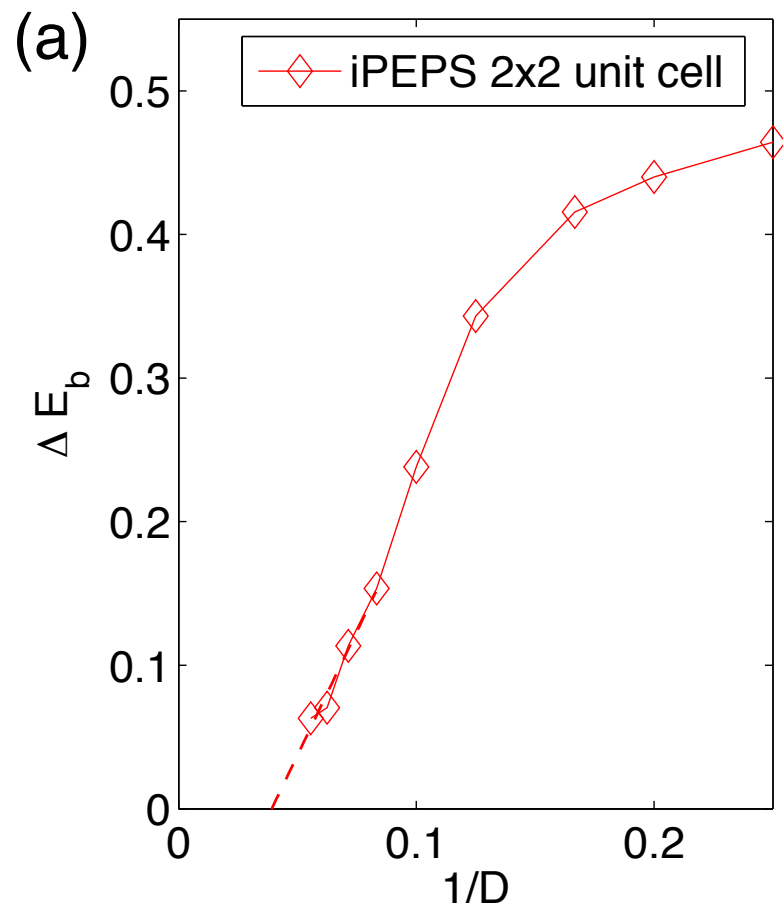


4x4 unit cell,  
D=6



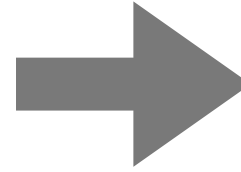
2x2 unit cell,  
D=6

# iPEPS - dimerization vanishes



2x2 unit cell,  
 $D=6$

local magnetization vanishes,  
no translational symmetry breaking



flavor liquid?

we use the fermionic  
representation:

$$\mathcal{P}_{ij} = \sum_{\mu, \nu \in \text{colors}} f_{\alpha, i}^{\dagger} f_{\beta, i} f_{\beta, j}^{\dagger} f_{\alpha, j}$$

$$\begin{aligned} \mathcal{P}_{ij}^{\text{MF}} &= \sum_{\alpha, \beta \in \text{colors}} \langle f_{\beta, i} f_{\beta, j}^{\dagger} \rangle f_{\alpha, i}^{\dagger} f_{\alpha, j} \\ &= - \sum_{\alpha \in \text{colors}} t_{ij}^{\alpha} f_{\alpha, i}^{\dagger} f_{\alpha, j} \end{aligned}$$

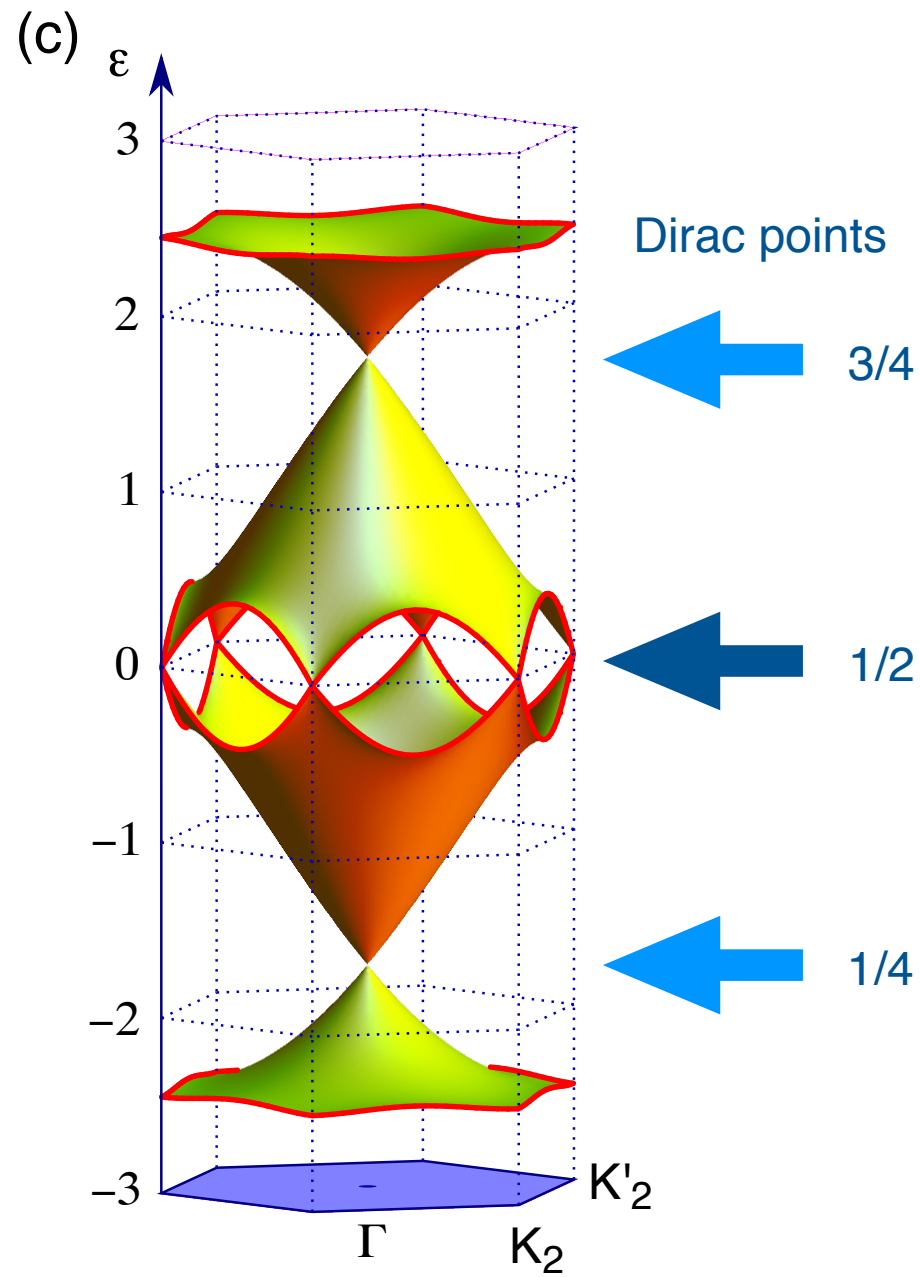
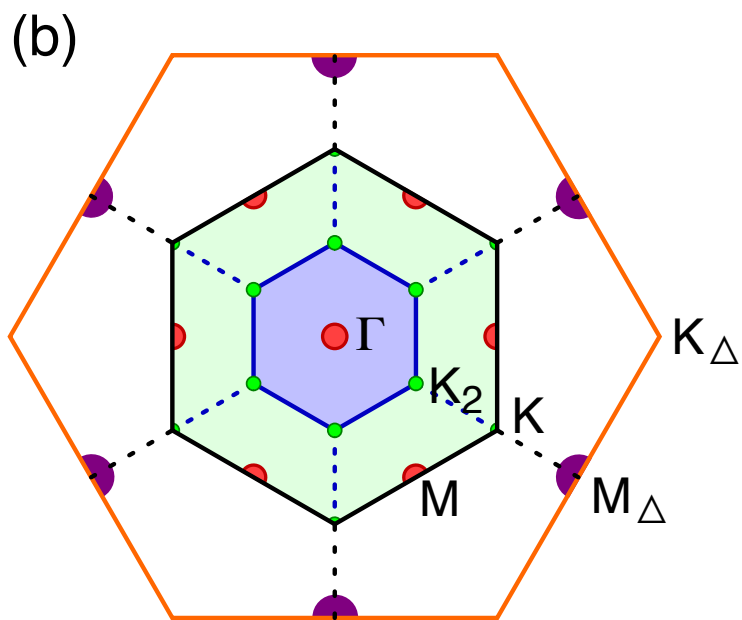
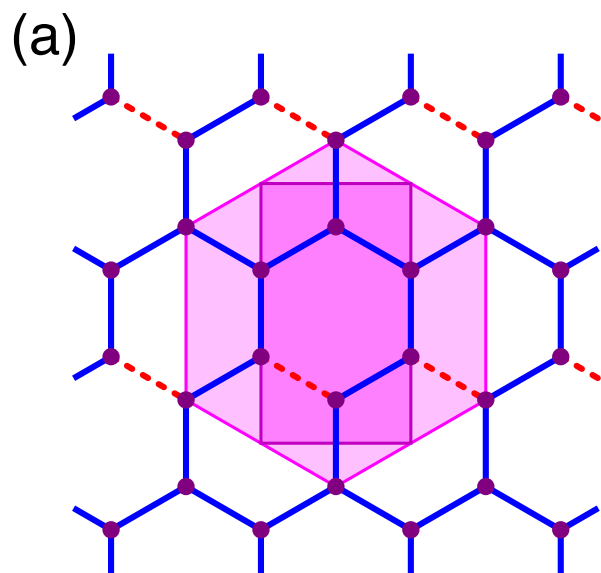
Mean-field decoupling of the  
fermionic Hamiltonian gives a  
hopping Hamiltonian and a  
variational wave function

$$|\Psi_{\text{vari}}\rangle = P_{\text{Gutzwiller}} |\Psi_{\text{FS}}\rangle$$

Using different Ansätze for the  
hoppings, we evaluate the  
expectation value of the  
Hamiltonian

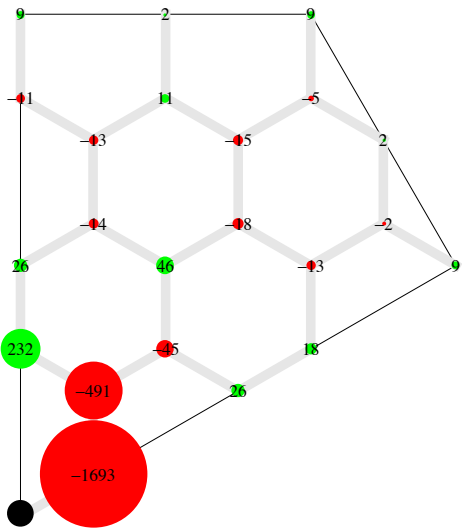
$$E_{\text{vari}} = \frac{\langle \Psi_{\text{vari}} | \mathcal{H} | \Psi_{\text{vari}} \rangle}{\langle \Psi_{\text{vari}} | \Psi_{\text{vari}} \rangle}$$

# The fermionic wave function of the pi-flux state



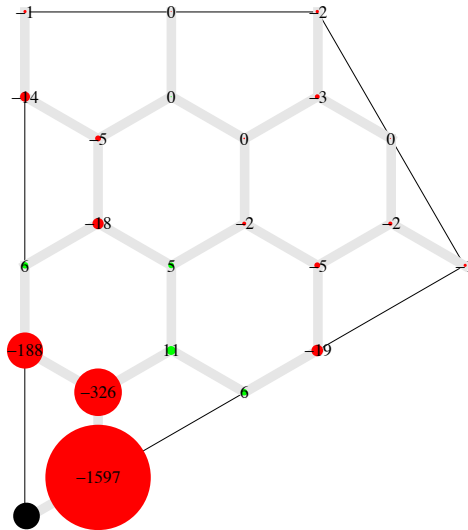
two-fold degenerate bands

# 96-site cluster - real space correlations from Gutzwiller projected wavefunction



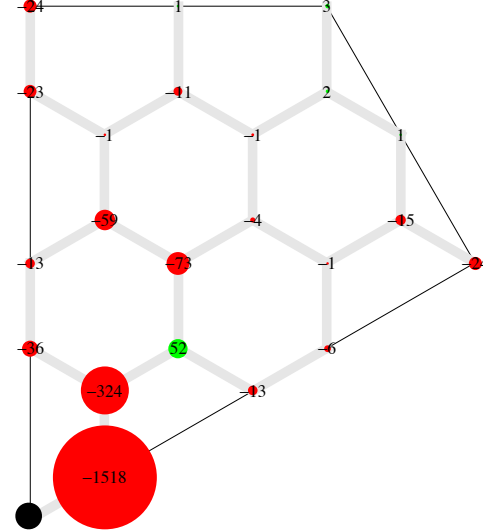
Pi-flux

$$E/N = -0.89466$$



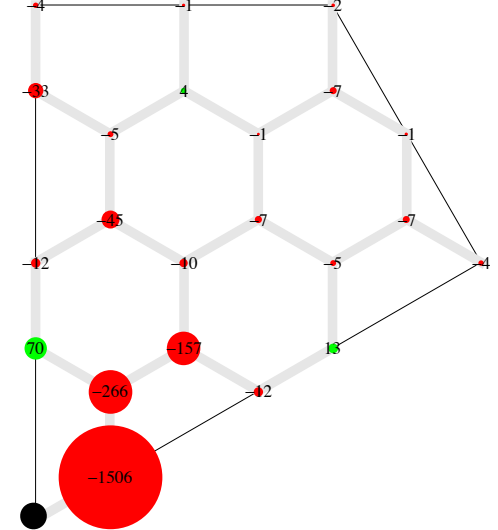
Majorana 0-flux

$$E/N = -0.822479$$



0-flux

$$E/N = -0.763304$$



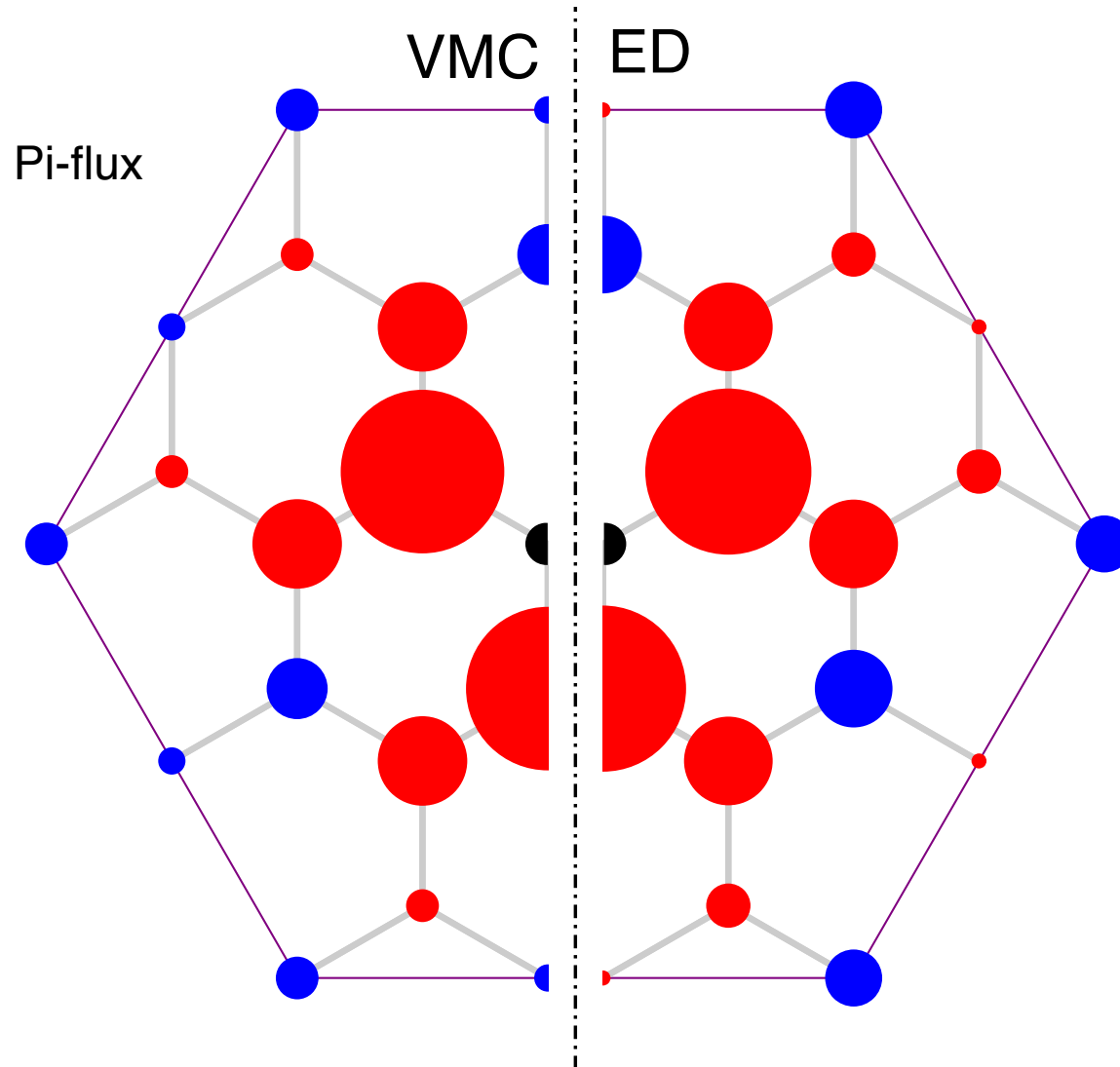
Majorana Pi-flux

$$E/N = -0.754662$$

marked differences in  
3rd neighbor correlations

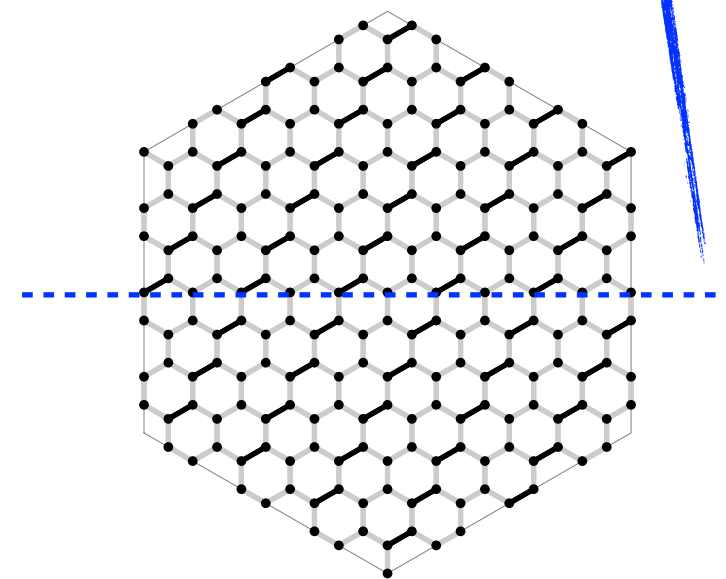
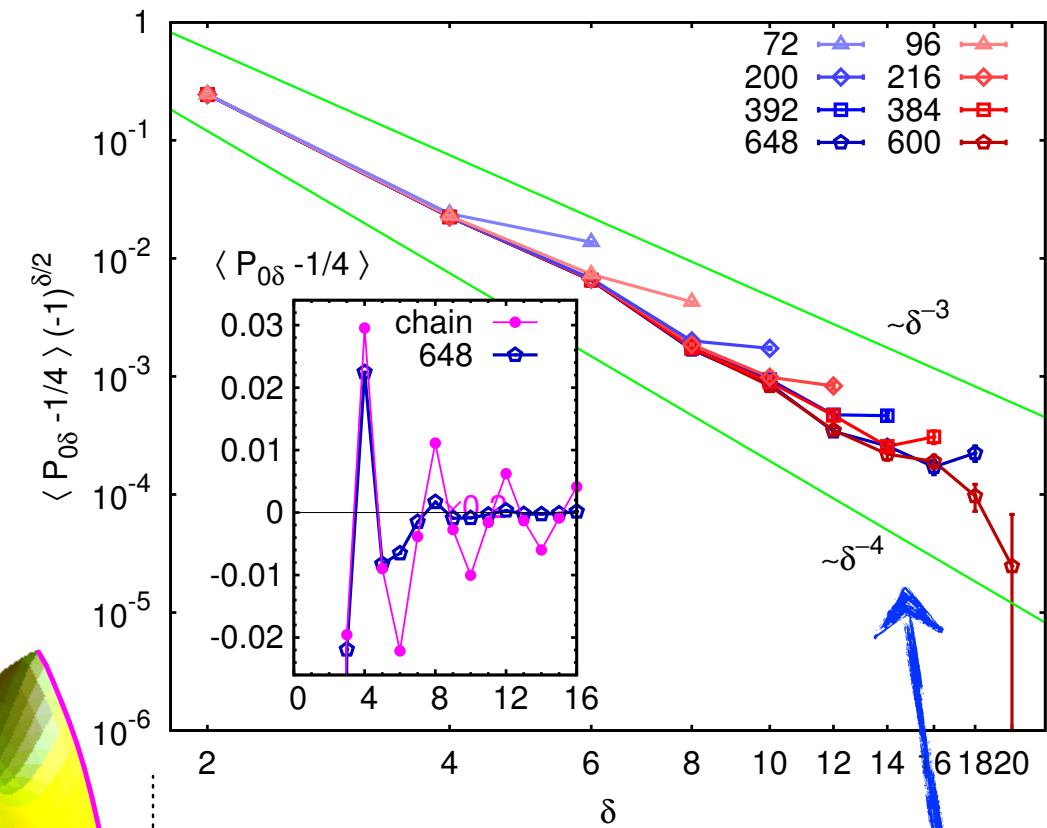
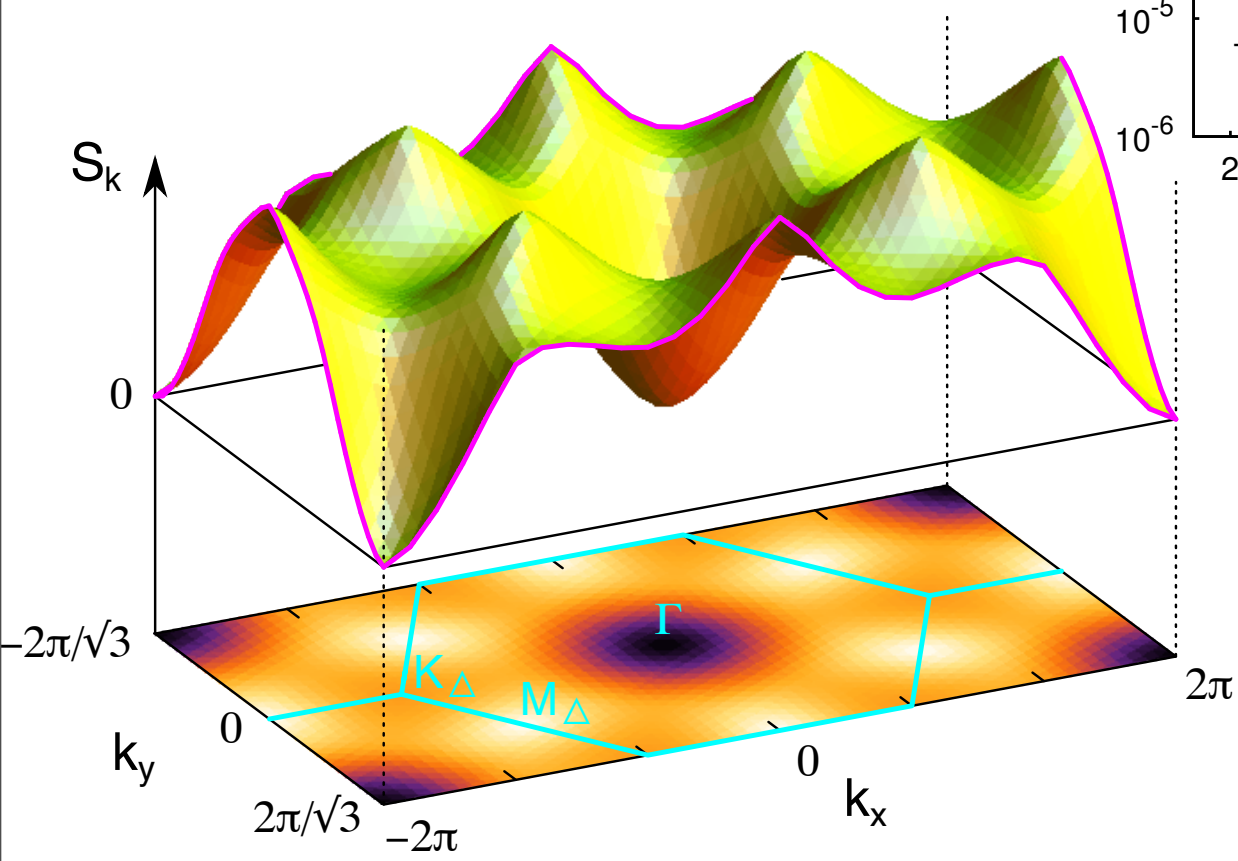


# 24-site cluster - real space correlations

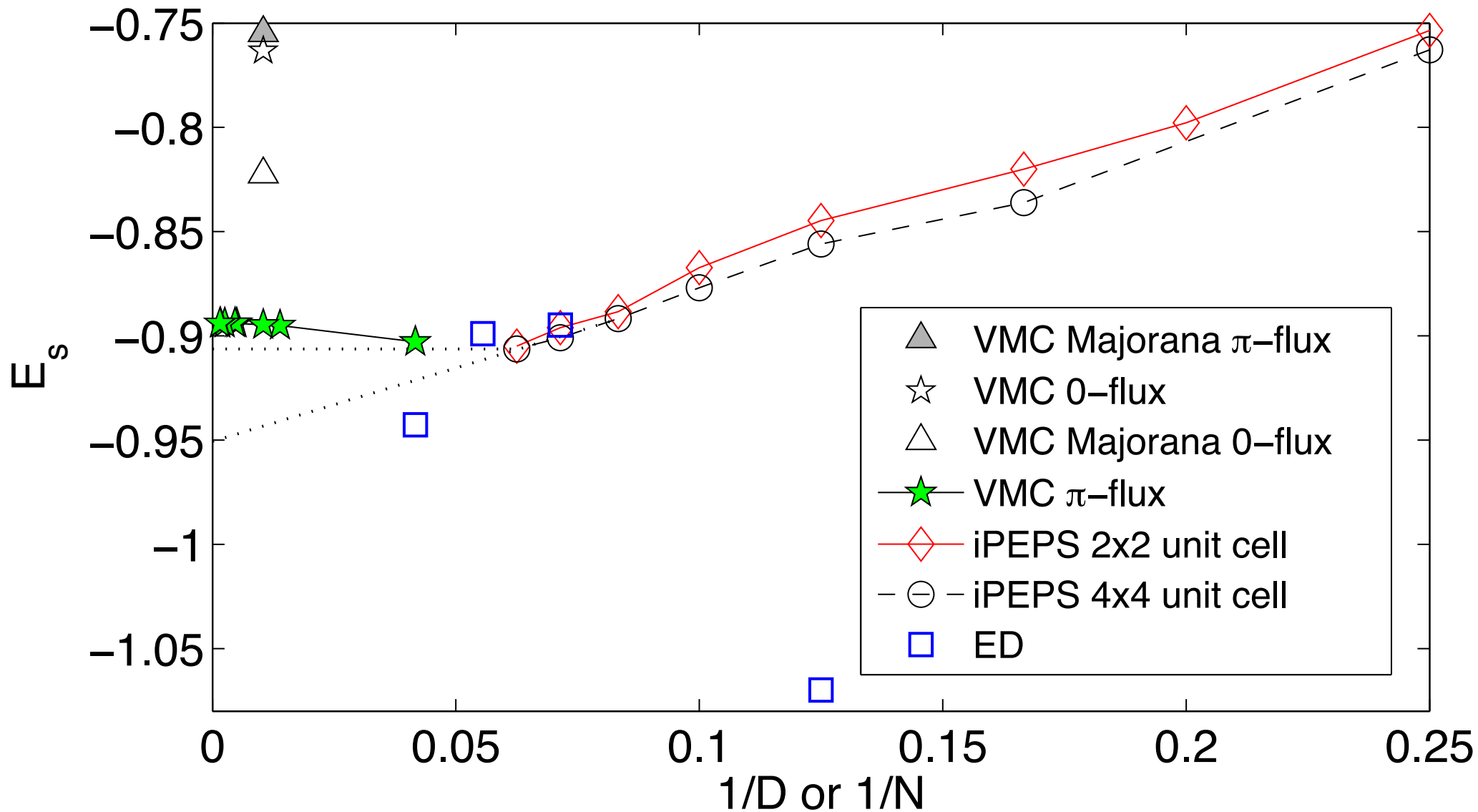


Dimension of the Hilbert space is  $24!/(6!)^4 = 2\,308\,743\,493\,056$   
using symmetries makes it tractable

# algebraic correlations and structure factor

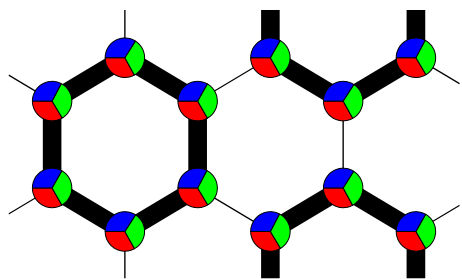


# Ground state energy from different methods



# SU(N) on honeycomb

SU(2) is a Néel state



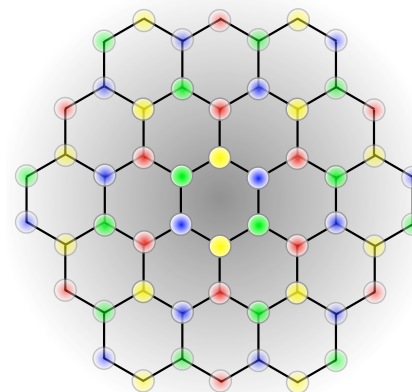
P. Corboz, unpublished

SU(3) is a plaquette state

[Y.-W. Lee and M.-F. Yang, Phys. Rev. B **85**, 100402 (2012).  
H.H.Zhao,C.Xu,Q.N.Chen,Z.C.Wei,M.P.Qin,G.M. Zhang, and T. Xiang,  
Phys. Rev. B **85**, 134416 (2012).]

SU(4) is most probably an  
algebraic flavor liquid

[P. Corboz, M. Lajkó, A. M. Läuchli, K.  
Penc, F. Mila, [arXiv:1207.6029](https://arxiv.org/abs/1207.6029)]



SU(6) is likely a chiral flavor liquid

[G. Szirmai E. Szirmai, A. Zamora, and M.  
Lewenstein, Phys. Rev. A **84**, 011611 (2011)],

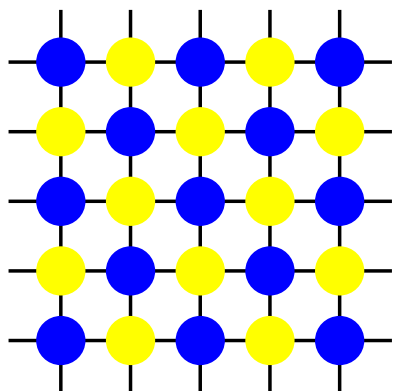
similarly, SU(N) is also a chiral liquid

[extending the results of M. Hermele, V. Gurarie, & A.  
M. Rey, Phys. Rev. Lett. **103**, 135301 (2009)]

honeycomb optical lattices can be realized, see  
poster of Johannes Hecker-Denschlag

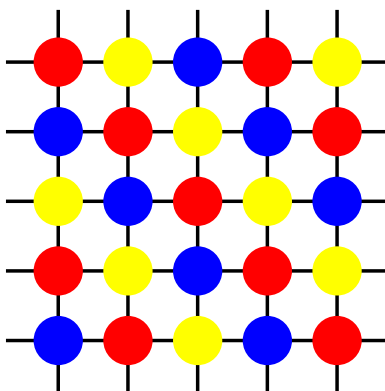
# Conclusions

SU(2)



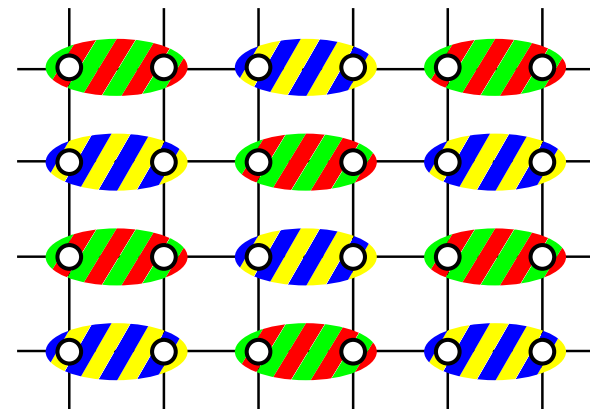
happy

SU(3)



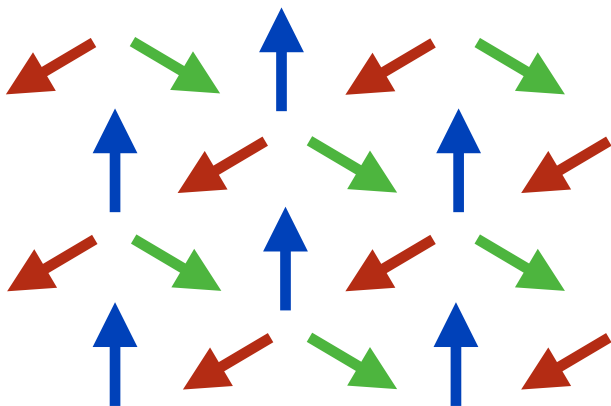
fluctuation stabilized

SU(4)

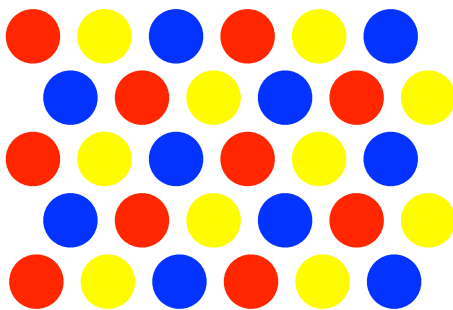


dimerization+Neel

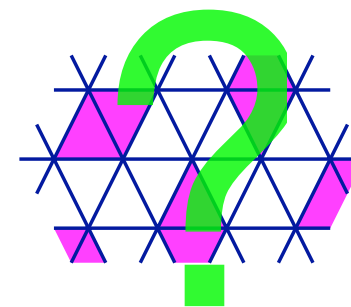
triangular



frustrated



happy



resonating  
liquid



Many happy returns of  
the day to you, Jose!

Many happy workshops in Evora!

the end