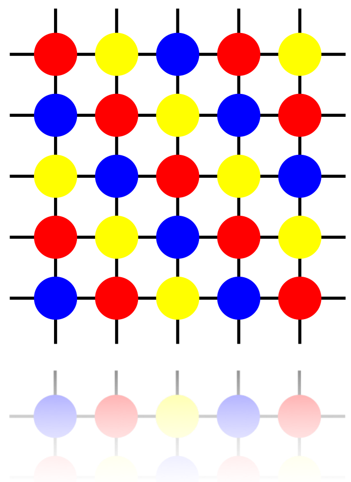

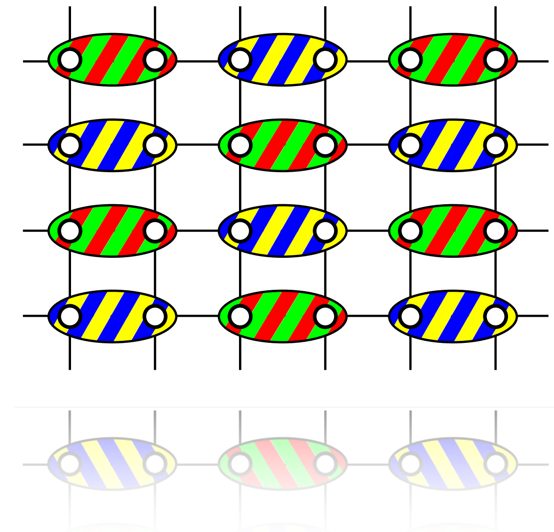

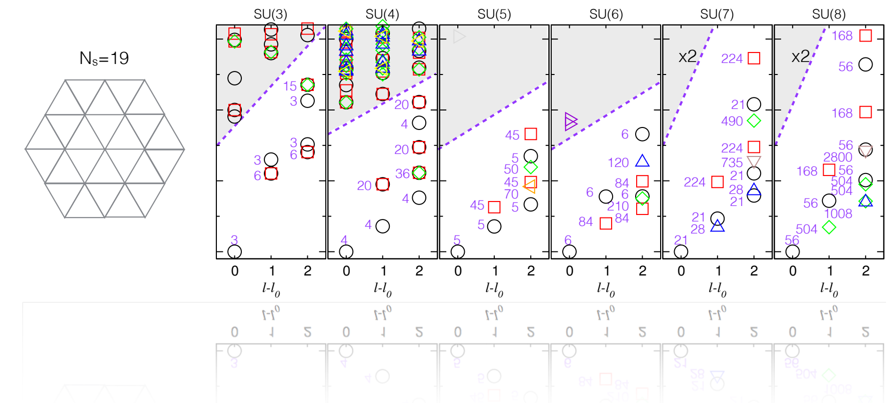

SU(N) Quantum Magnetism: Chiral Spin Liquids / Thermodynamics

Andreas Läuchli
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universität innsbruck
Theoretische Physik

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Quantum Simulations and Numerical Studies in Many-Body Physics
December 9th-11th, 2016, Hsinchu

Outline

- Introduction: Why SU(N) Magnetism ?
- SU(3) Square Lattice
- SU(4) Square Lattice
- SU(N>2) Triangular Lattice with additional TRS breaking term
- Thermodynamics of the SU(N) square lattice Heisenberg model
- Conclusion & Outlook

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SU(N) Magnetism

- Magnetism in Mott insulators in the solid state originates from electron spin
- Interactions (exchange interactions) are typically SU(2) symmetric, for all S
  (disregarding anisotropy effects)
- So far SU(N) models have mostly served as a theoretical playground,
  but no materials were realistically described by SU(N>2) Hamiltonians
  (apart perhaps from idealistic Kugel-Khomskii type spin orbital Hamiltonians)
- Can cold atom systems help us realize SU(N) models and find
  novel quantum phases ?

SU(N) Magnetism with alkaline-earth atoms

- Fermionic alkaline-earth are very promising systems:
  M. Cazallilla et al. NJP 2009, A. Gorshkov et al. Nat. Phys 2010 /
  Experimental work in Kyoto, Florence, at LMU, in Amsterdam, …

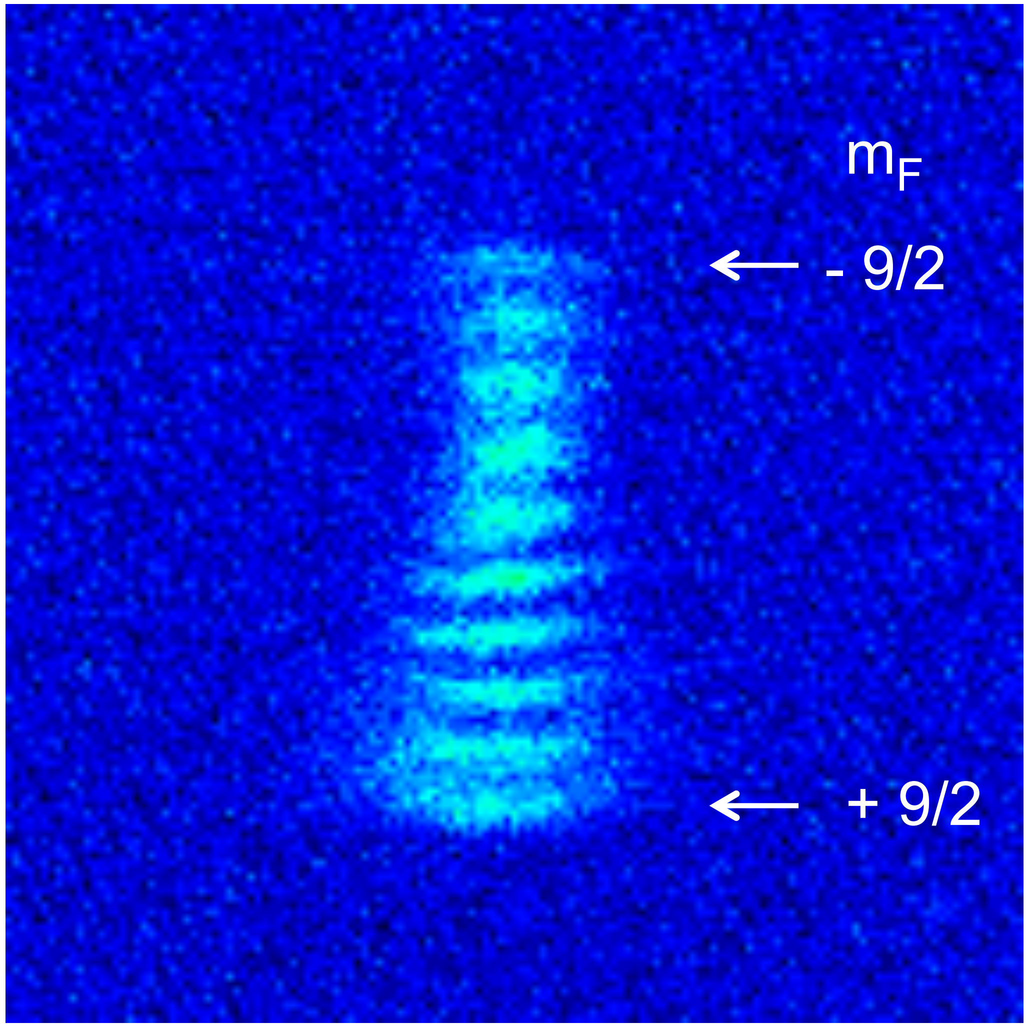
- nuclear spin decoupled from electronic spin

- nuclear spin can be large (up to I=9/2)

- nuclear spin independent scattering length
  ⇛ SU(N) symmetric interactions (N up to 10)!

- What are possible Mott insulating states of SU(N) fermions in an optical lattice ?

- Not so much is known for N>2 !



10 internal states of ^{87}Sr
courtesy of F. Schreck

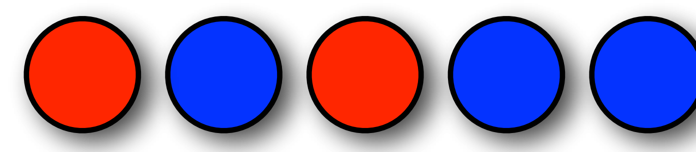
Quantum Magnetism:
Strong coupling limit: Mott Insulator (t<<U)

- Start with N-flavor Hubbard model at filling of **one** particle per site

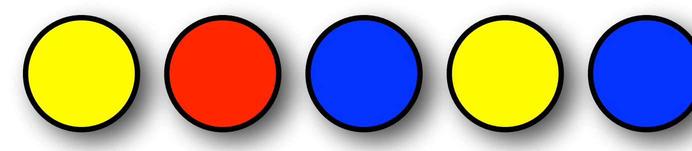
$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \alpha=1}^{N} (c^\dagger_{i,\alpha} c_{j,\alpha} + \mathrm{h.c.}) + U \sum_{i,\alpha=1<\beta}^{N} n_{i,\alpha} n_{i,\beta}$$

- N=2: At second order (t^2/U) : Standard SU(2) Heisenberg model

$$\mathcal{P}^{(2)}_{i,j} = 2\ \mathbf{S}_i \cdot \mathbf{S}_j + 1/2$$



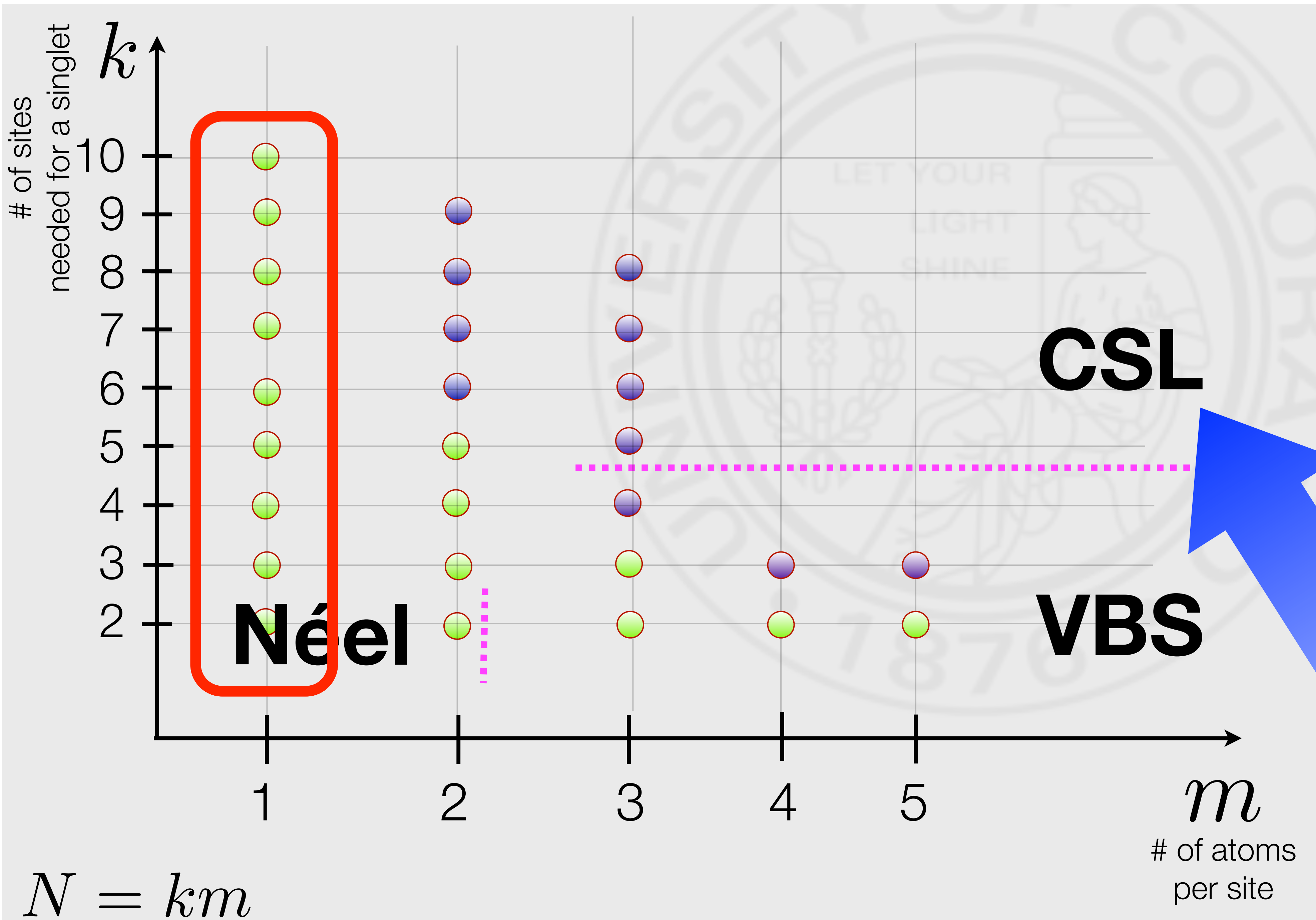
- N=3: At second order (t^2/U) : SU(3) Heisenberg model
(can be cast into a special S=1 bilinear-biquadratic model)



$$\mathcal{P}^{(3)}_{i,j} \sim (\mathbf{S}_i \cdot \mathbf{S}_j) + (\mathbf{S}_i \cdot \mathbf{S}_j)^2 + \mathrm{const}$$

- general N: at second order one obtains a nearest-neighbor *permutation* Hamiltonian with SU(N) symmetry, where the local basis transforms as the fundamental irreducible representation of SU(N).

Theoretical (mean-field) predictions for square lattice with nearest-neighbour permutation



CSL:
Chiral Spin Liquid

VBS:
Valence Bond Crystal

Slide from a talk by V. Gurarie

M. Hermele, V.Gurarie A.M. Rey, PRL 2009

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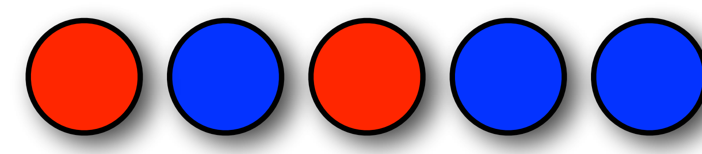

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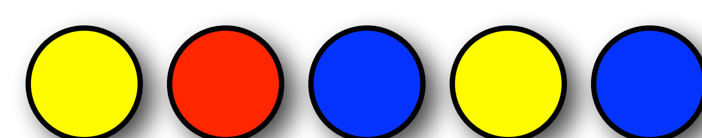
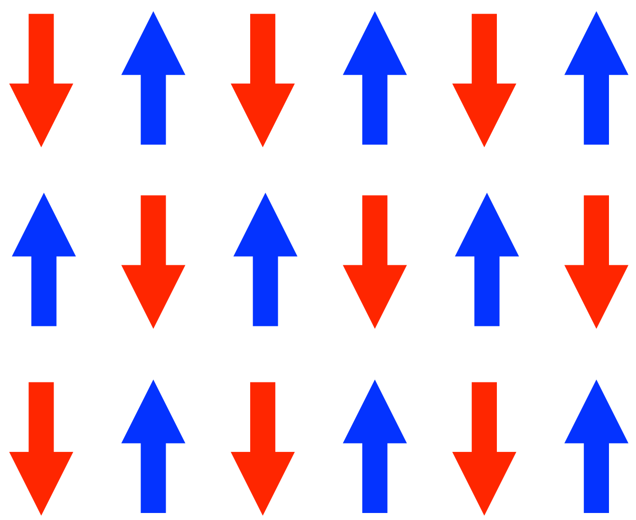
(can be cast as a S=1 Bilinear-Biquadratic model)



$$\mathcal{P}^{(3)}_{i,j} \sim (\mathbf{S}_i \cdot \mathbf{S}_j) + (\mathbf{S}_i \cdot \mathbf{S}_j)^2 + \text{const}$$

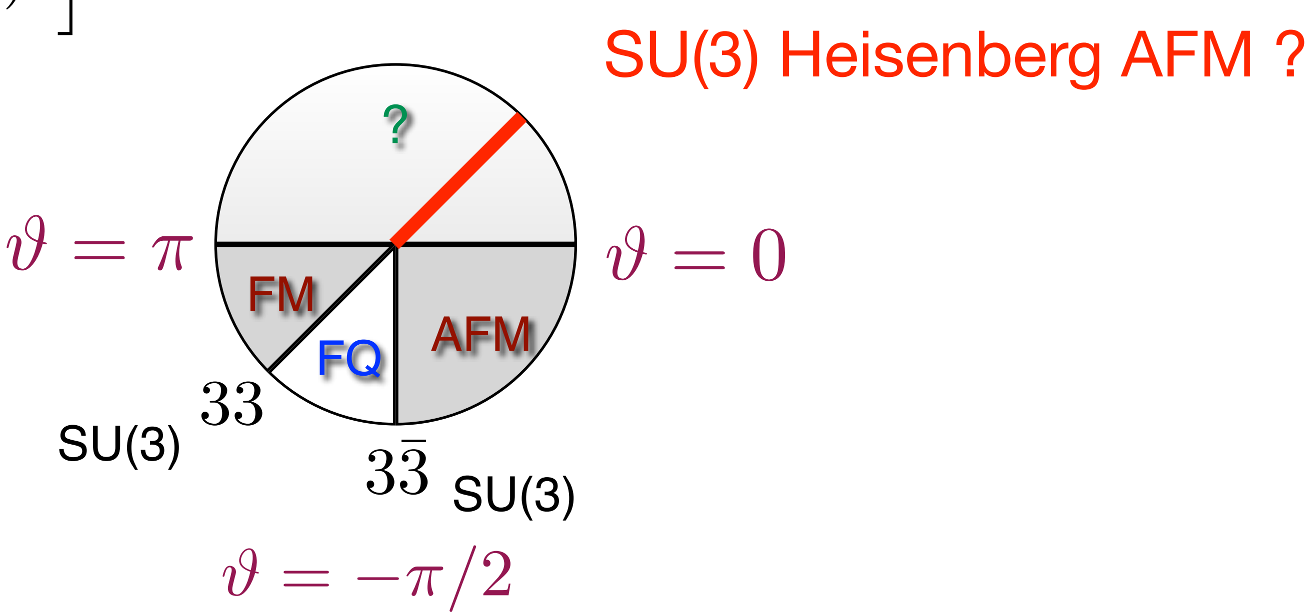
SU(2)/SU(3) Heisenberg models on a square lattice

- SU(2): Two-sublattice Néel order



- SU(3): special point of bilinear-biquadratic S=1 model

$$\mathcal{H} = J \sum_{i,j} \left[\cos\vartheta \mathbf{S}_i \mathbf{S}_j + \sin\vartheta \left(\mathbf{S}_i \mathbf{S}_j \right)^2 \right]$$



Quantum Monte-Carlo:
K. Harada and N. Kawashima,
Phys. Rev. B 65, 052403 (2002)

First: a variational (semiclassical) approach

- a site-product wave function (similar to Gutzwiller approach for Bosons)

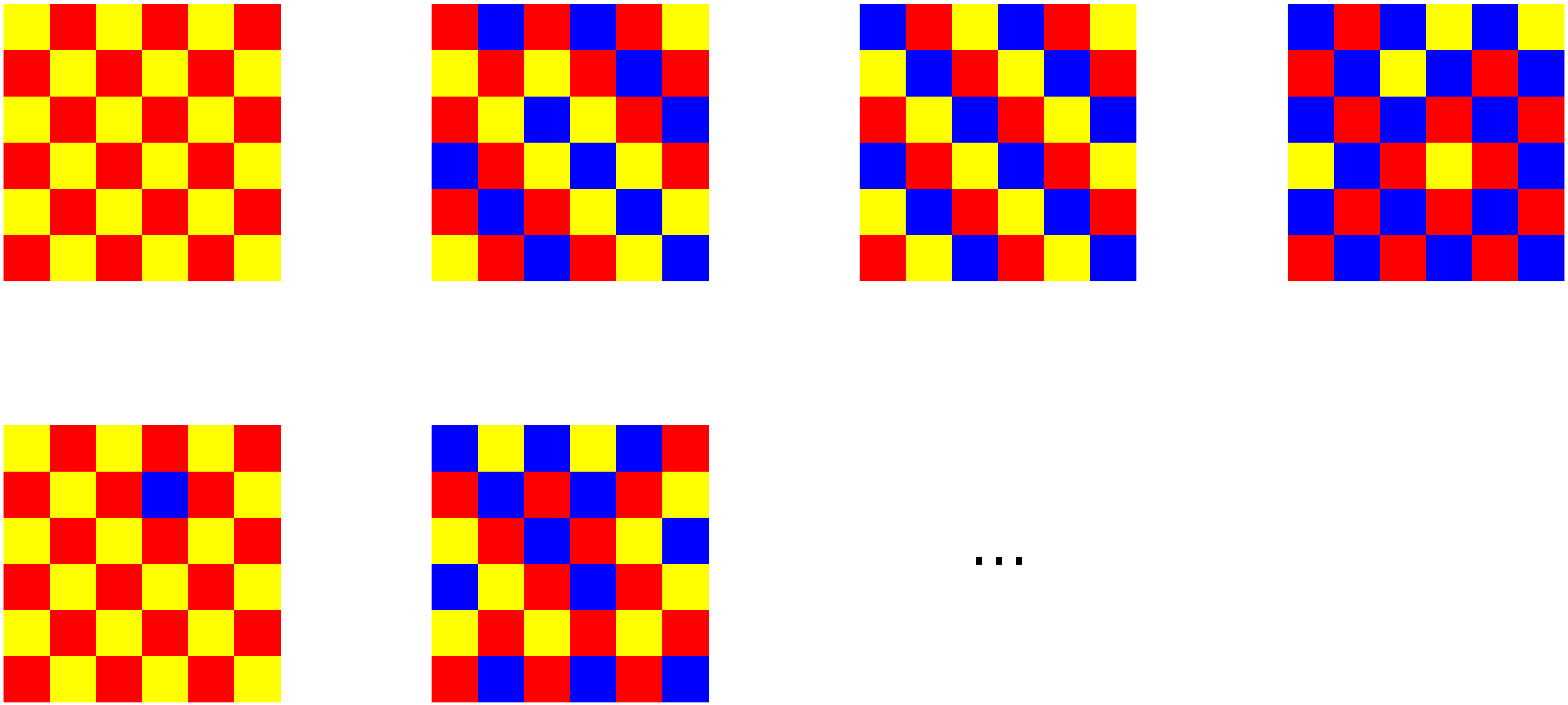
$$|\Psi\rangle = \prod_i |\psi_i\rangle$$

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

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

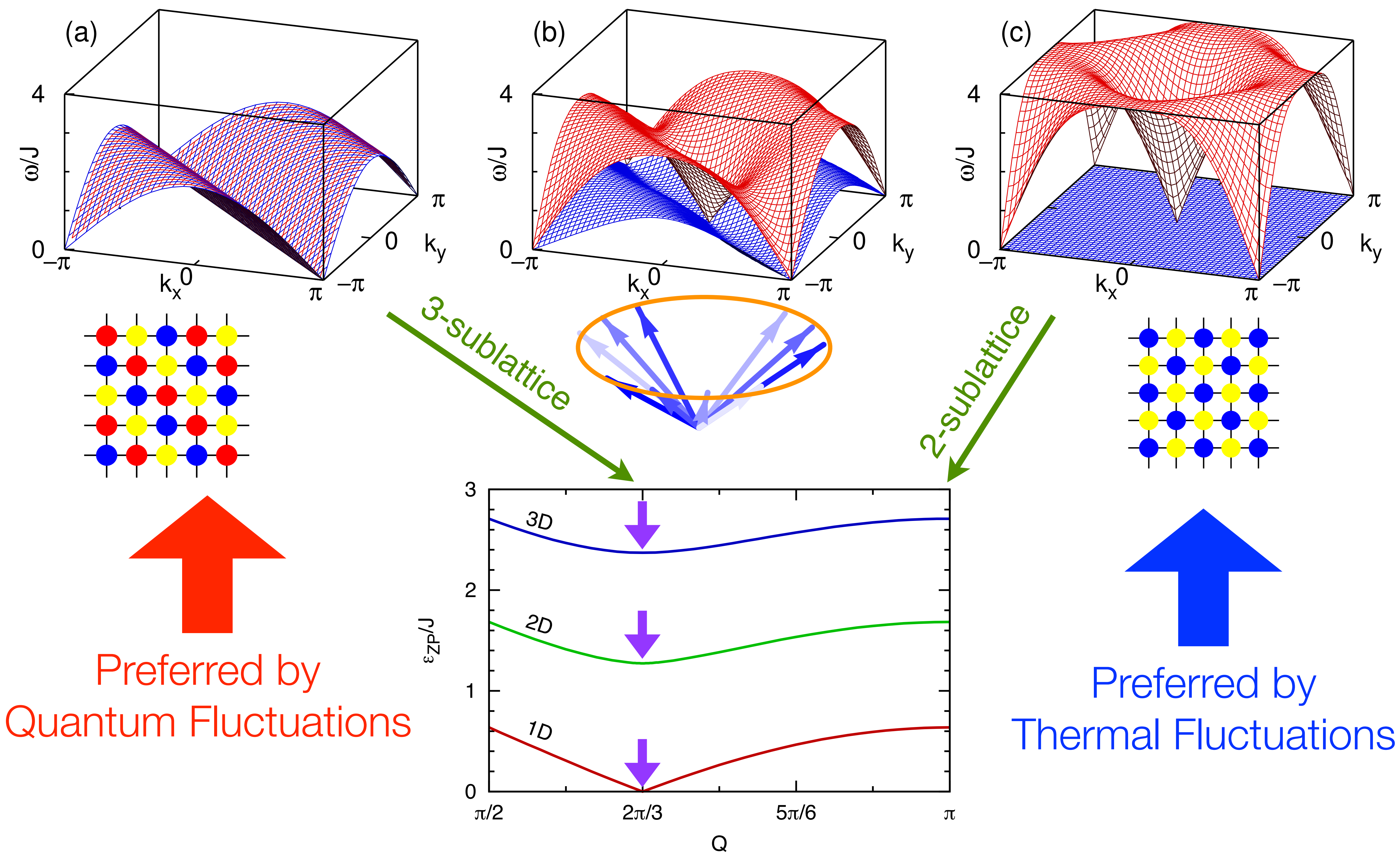
- minimal, when $\mathbf{d}_i$ and $\mathbf{d}_j$ on a bond are orthogonal

SU(3) classical solutions: macroscopic degeneracy



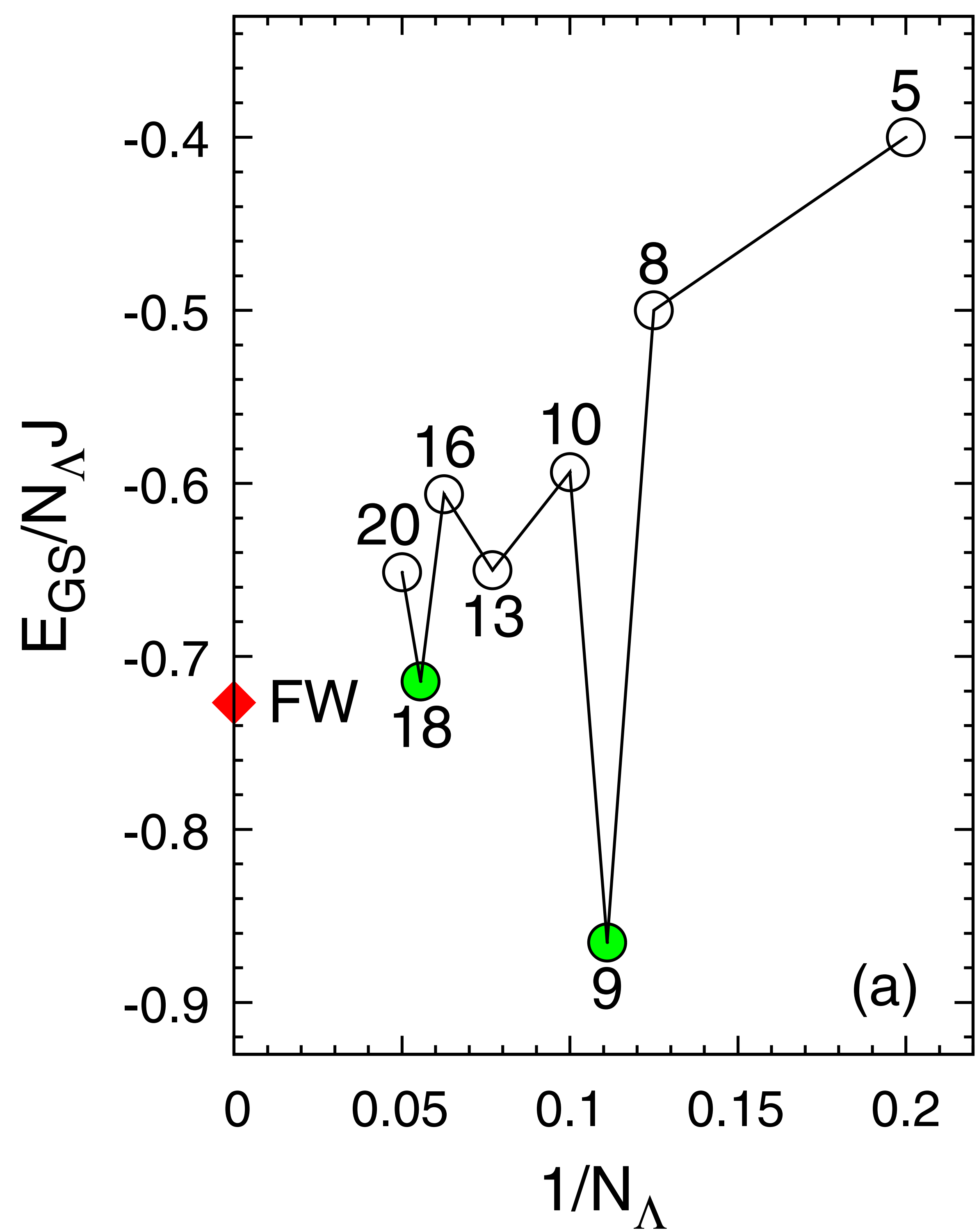
- Degeneracy reminiscent of the 3-state AF Potts model.
- Do quantum fluctuations select a unique state out of the degenerate manifold ?

SU(3) flavor-wave: dispersion and zero-point energy



Unbiased Approach: Exact Diagonalizations

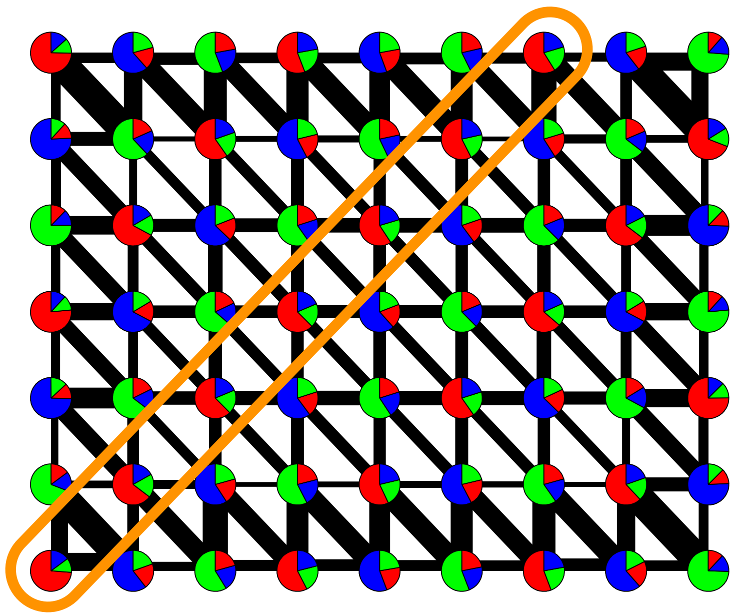
- Square samples up to 20 sites
- Energy per site is lowest for samples with a multiple of 3 sites
- Agreement with energy per site from flavor wave theory



Comparison to large scale DMRG + iPEPS results

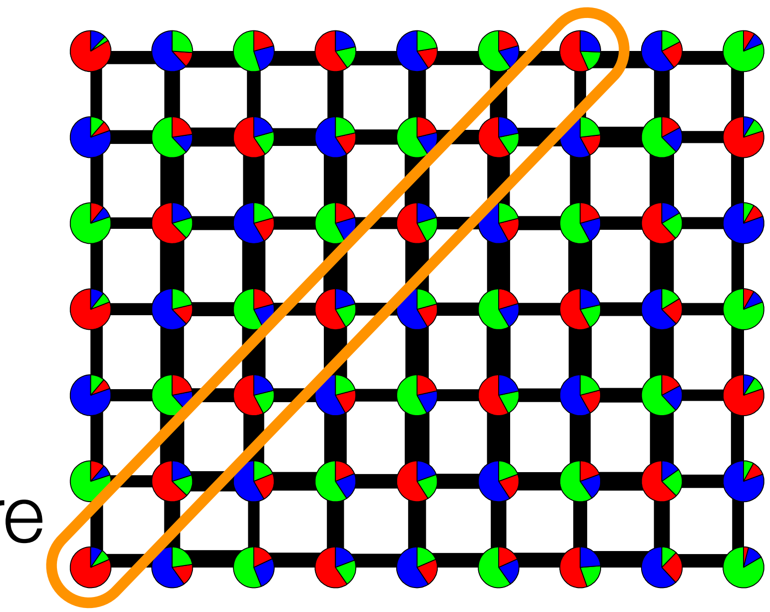
B. Bauer, P. Corboz, AML, L. Messio, K. Penc, M. Troyer, and F Mila,
PRB **85**, 125116 (2012)

- wide cylinders with DMRG, pinned boundary sites on the left/right ends

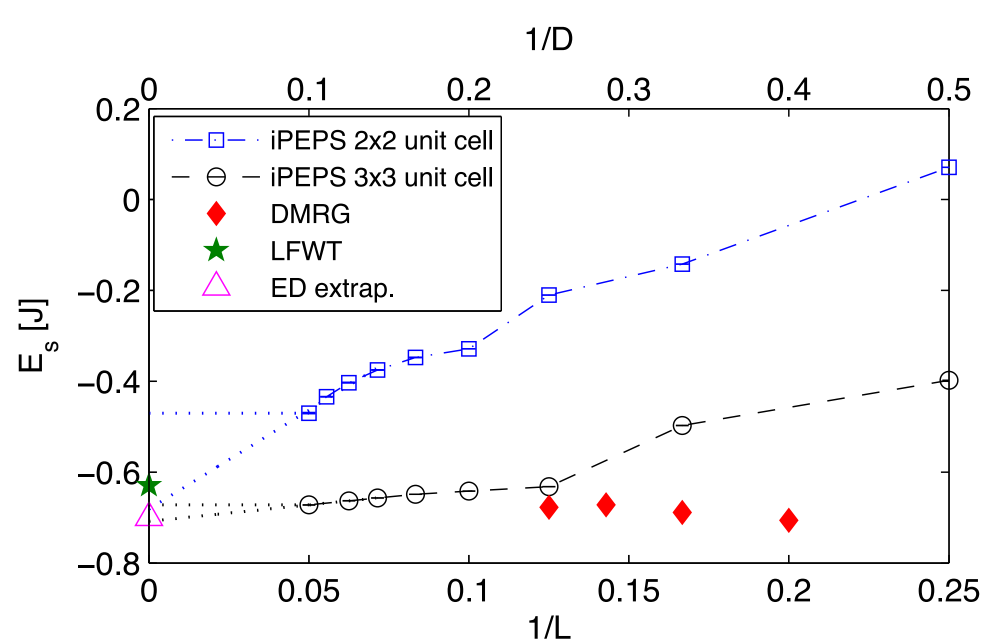


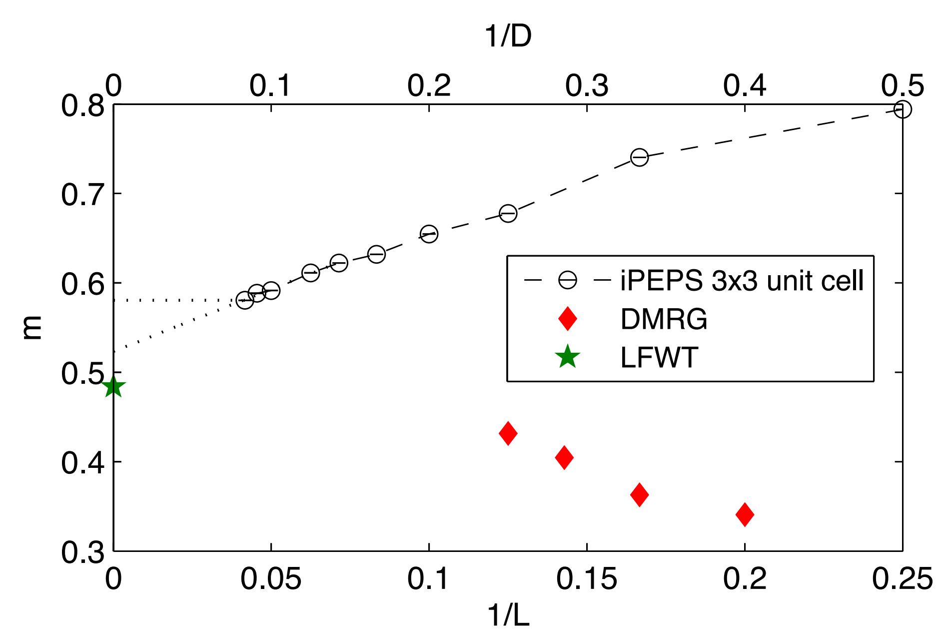
triangular

square



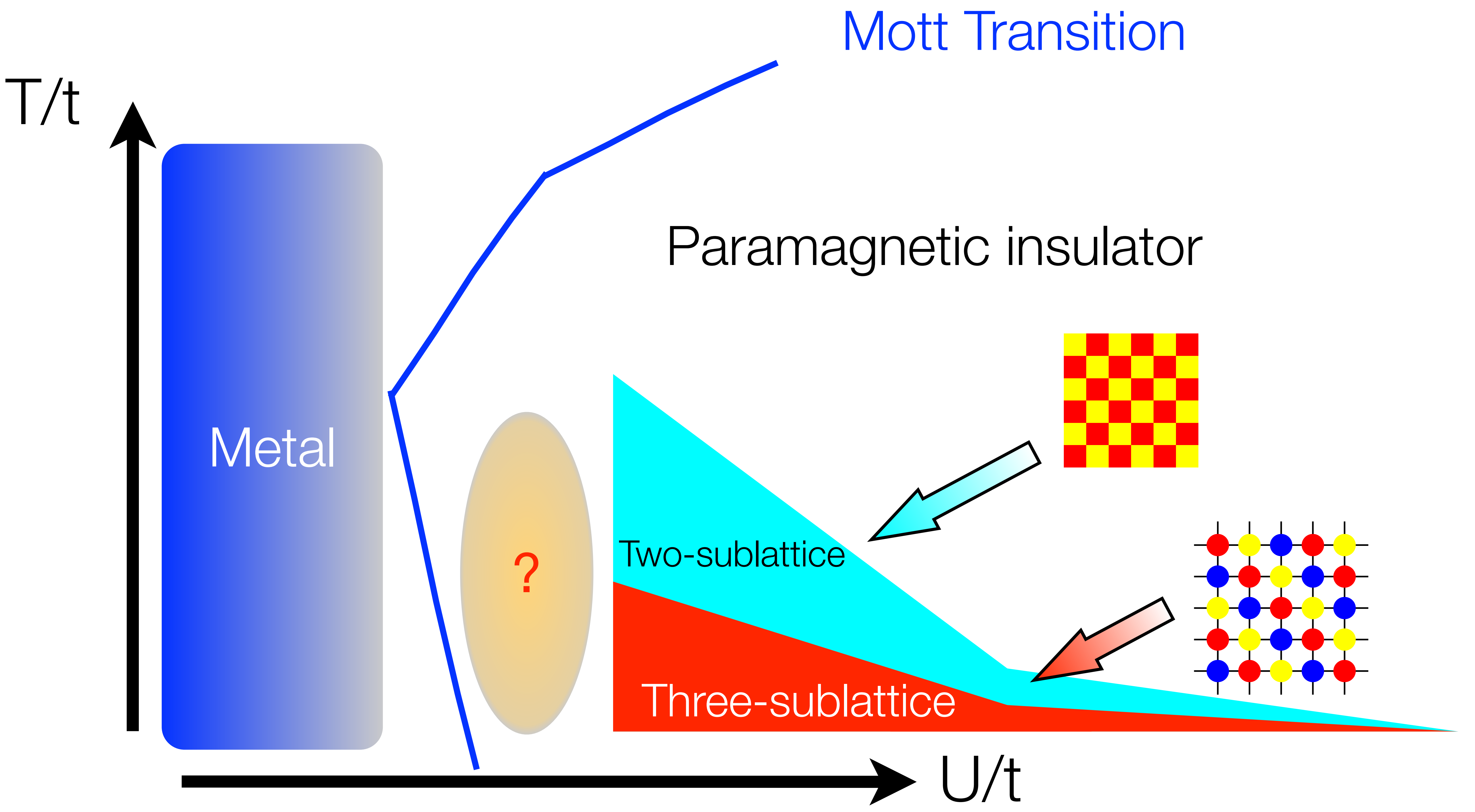
- iPEPS



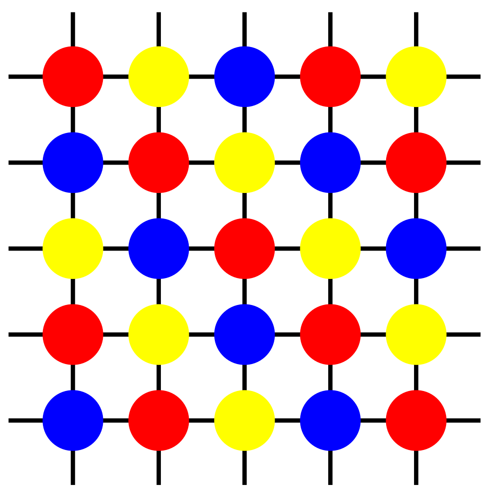


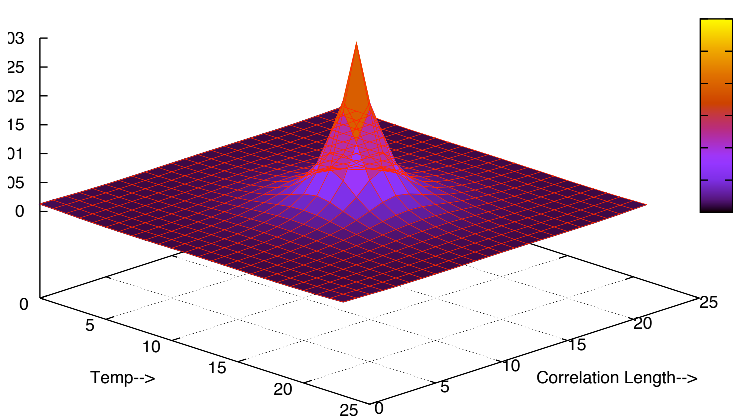
(Speculative) phase diagram of N=3, ρ=1/3 Hubbard model

Square/Cubic lattice



Intermediate Conclusions





- Quantum fluctuations select a three-sublattice flavor ordered state as the ground state of the ρ=1/3 Mott insulator on square and cubic lattices
- Thermal fluctuations select a two-sublattice Néel configuration. Finite temperature transition in three dimensions before entering the three sublattice state ?
- What happens for N>3 ? Is flavor ordering still possible or are spin liquids taking over ?
- If order by disorder is too demanding for current experiments, then resort to SU(3) triangular lattice !

T. Tóth, AML, F. Mila, K. Penc, PRL 2010

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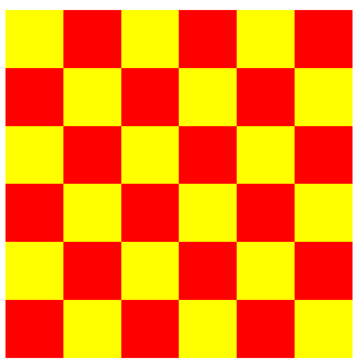
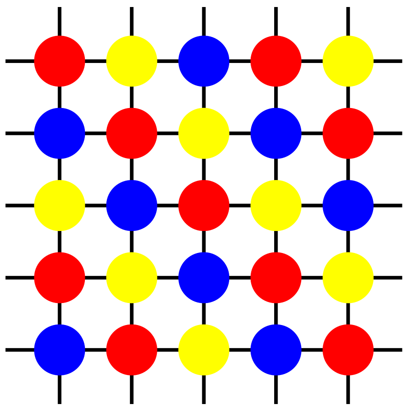
Ground state of the SU(4) Square lattice model ?

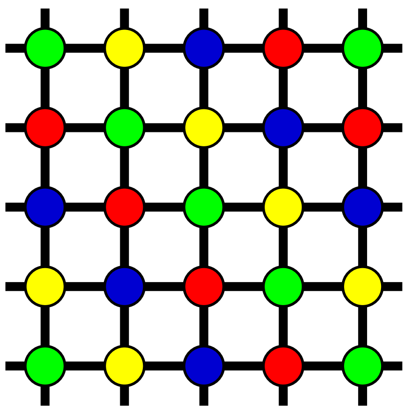
- Simple (2π/N,2π/N) magnetic ordering ?



SU(2)

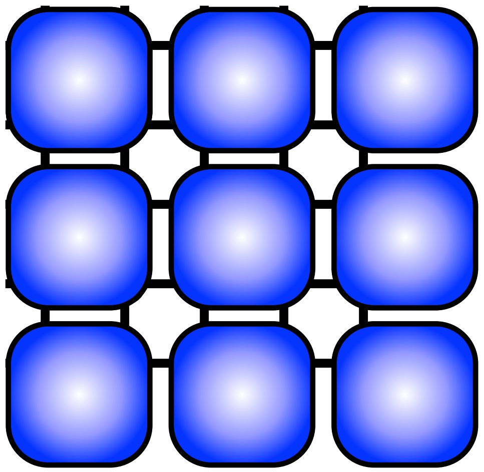


SU(3)



SU(4) ??

- Singlet ground state ?

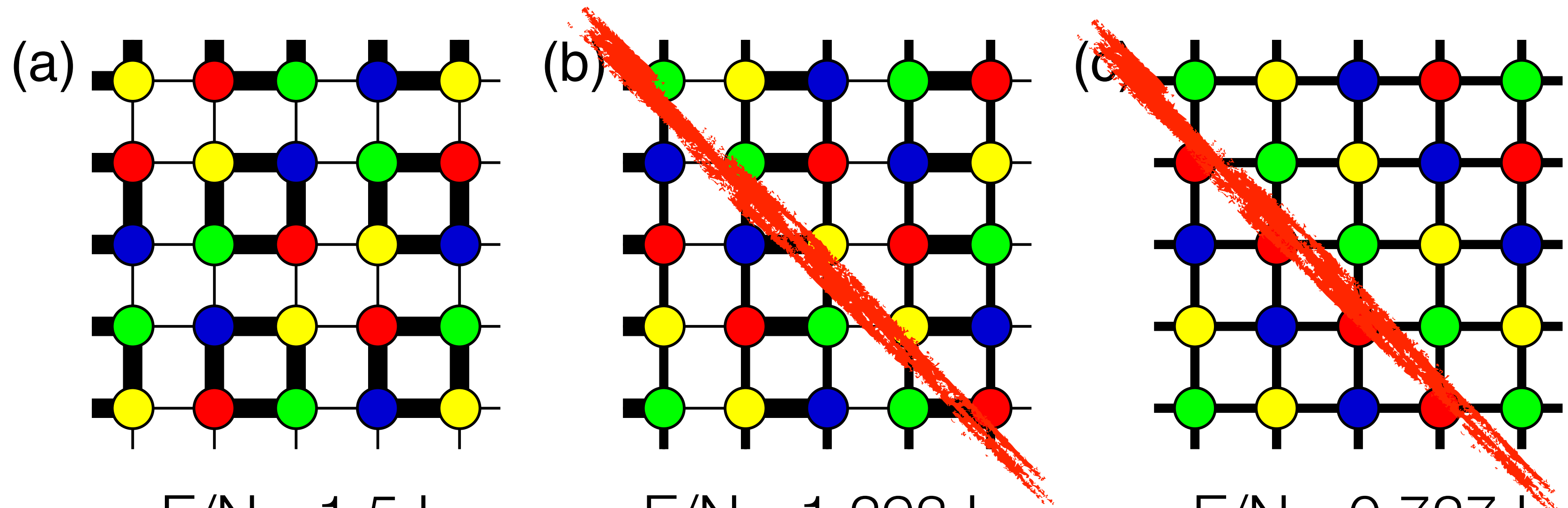


Plaquette ground state
van den Bossche EPJB 2000

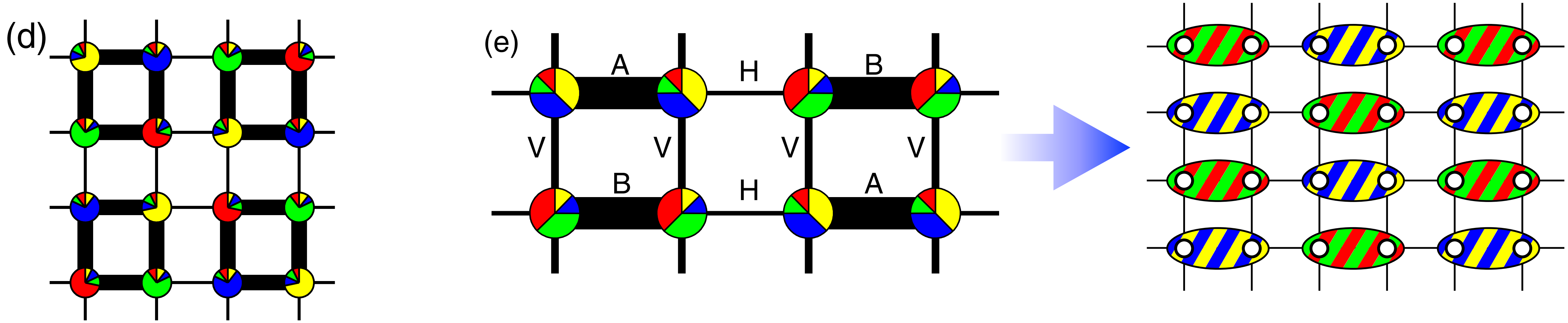
- or something else ?

Ground state of the SU(4) Square lattice model ?

- large semiclassical degeneracy: what does LFWT tell us ?



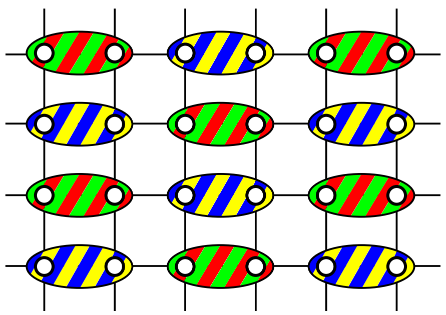
E/N=-1.5J E/N=-1.293J E/N=-0.727J

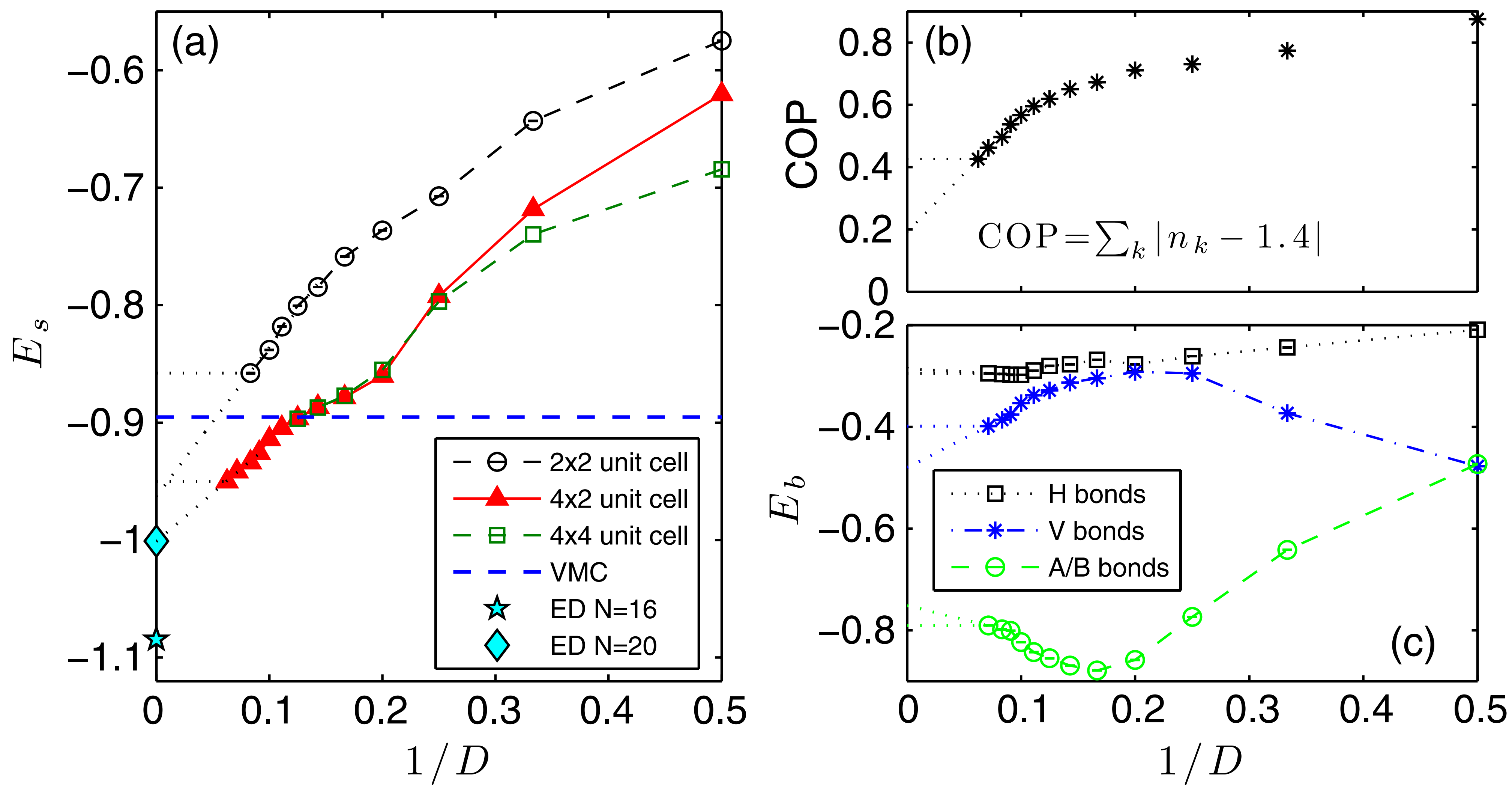


iPEPS D=2 iPEPS D=12 !

P. Corboz, AML, K. Penc, M.Troyer, F. Mila, PRL 2011

iPEPS Ground state



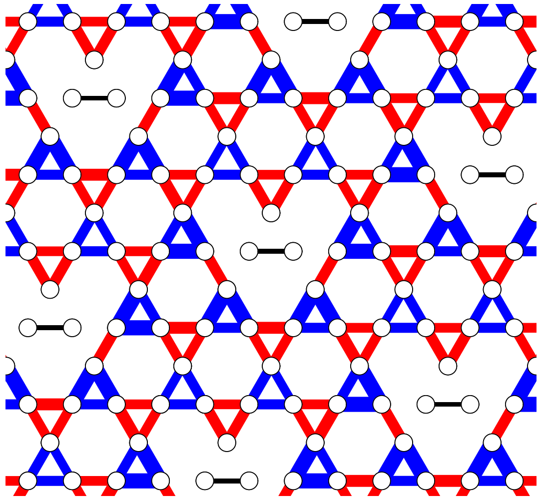


- iPEPS energy substantially lower than best variational energy
- stable “dimerization” in the thermodynamic limit
- finite color order parameter: “Néel” order of $SU(4)_6$ on top of the dimer background.

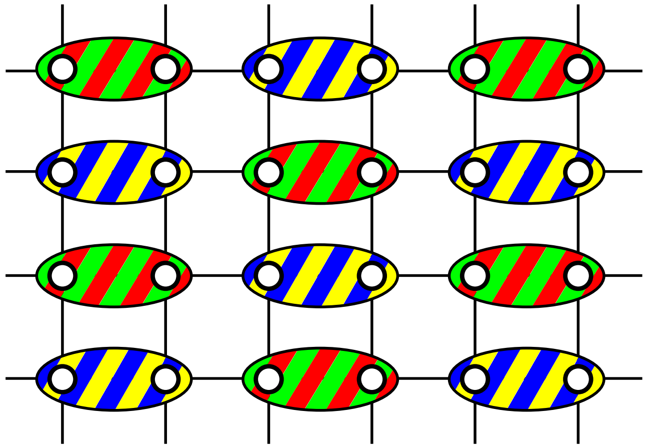
P. Corboz, AML, K. Penc, M.Troyer, F. Mila, PRL 2011

P. Corboz, K. Penc, F. Mila, AML, PRB 2012
B. Bauer, P. Corboz, AML, L. Messio, K. Penc, M.Troyer, F. Mila, PRB 2012
P. Corboz, AML, K. Penc, M.Troyer, F. Mila, PRL 2011
T. Tóth, AML, F. Mila, K. Penc, PRL 2010
AML, F. Mila, K. Penc, PRL 2006

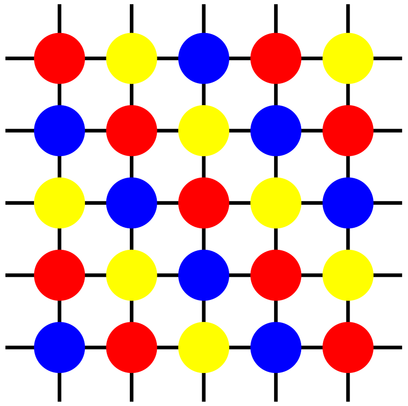
Intermediate conclusion (2)



VBS analogues
SU(3) kagome &
SU(4) checkerboard



peculiar magnetic order
SU(4) on square lattice



Order by disorder,
competition between
quantum fluctuations and
thermal fluctuations
SU(3) on square lattice

SU(N) spin liquids ?

at larger N ?

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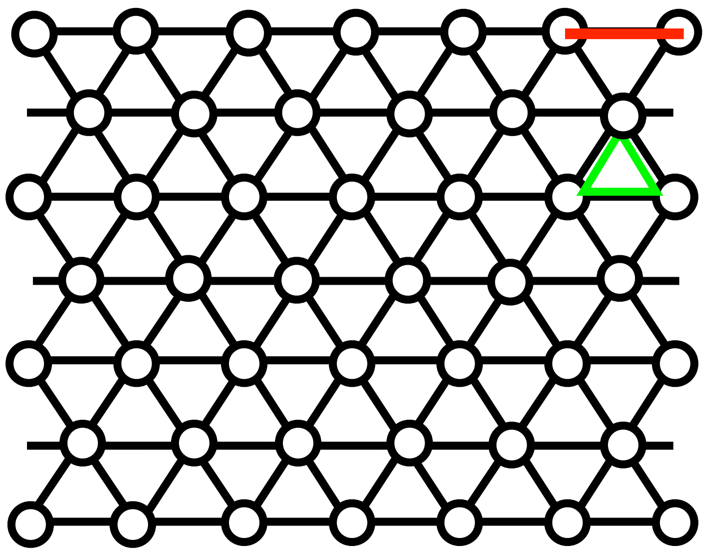
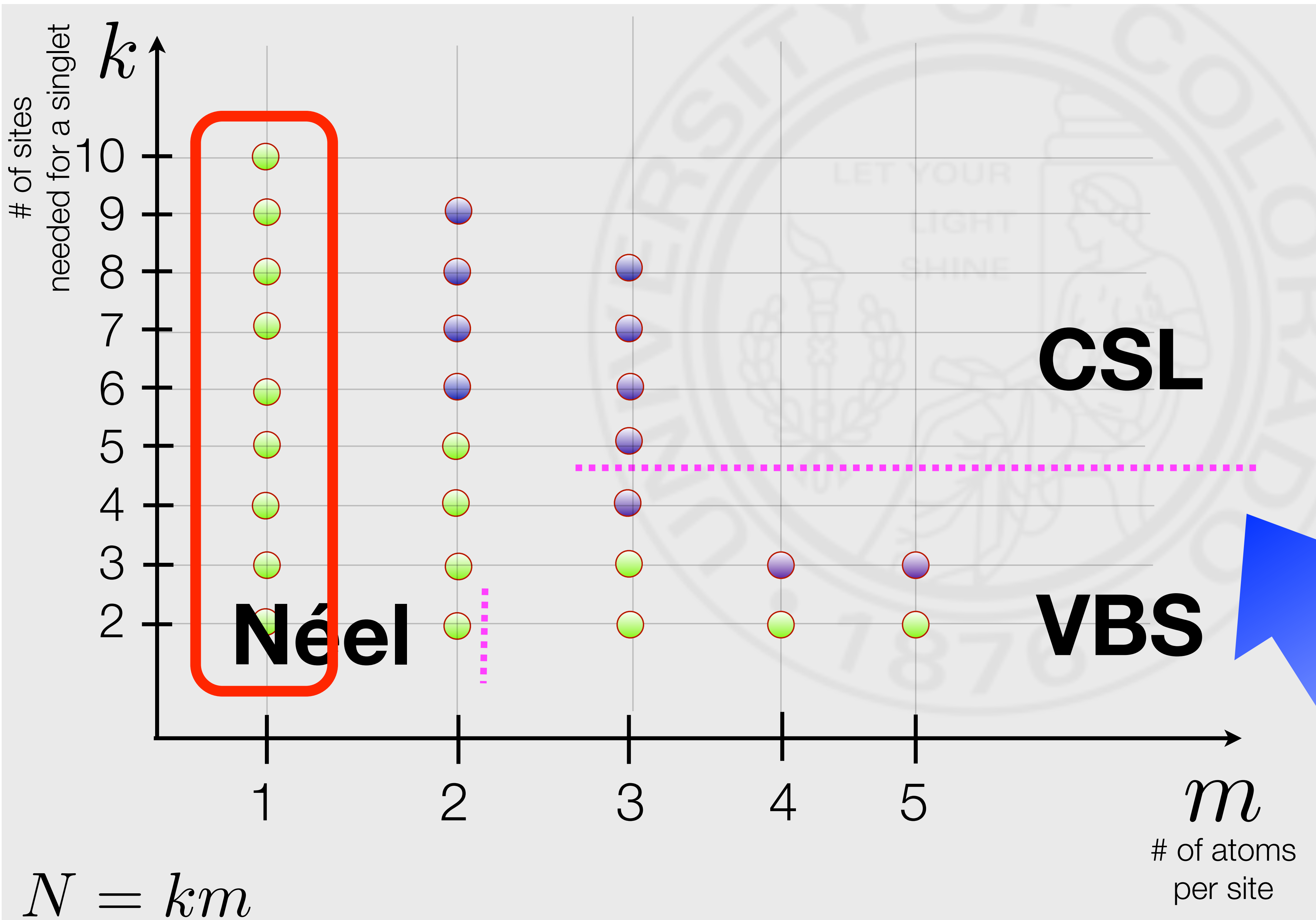
SU(N) Chiral Spin Liquids on the Triangular Lattice

$$\mathcal{H} = \cos(\theta) \sum_{\langle i,j \rangle} P_2(i,j) + \sin(\theta) \sum_{i,j,k \in \triangle} \Im P_3(i,j,k)$$



P. Nataf, M. Lajko, A. Wietek, K. Penc, F. Mila, and AML, PRL (2016)

Theoretical predictions for Square Lattice



CSL:
Chiral Spin Liquid
(spontaneous TRS breaking)

VBS:
Valence Bond Crystal

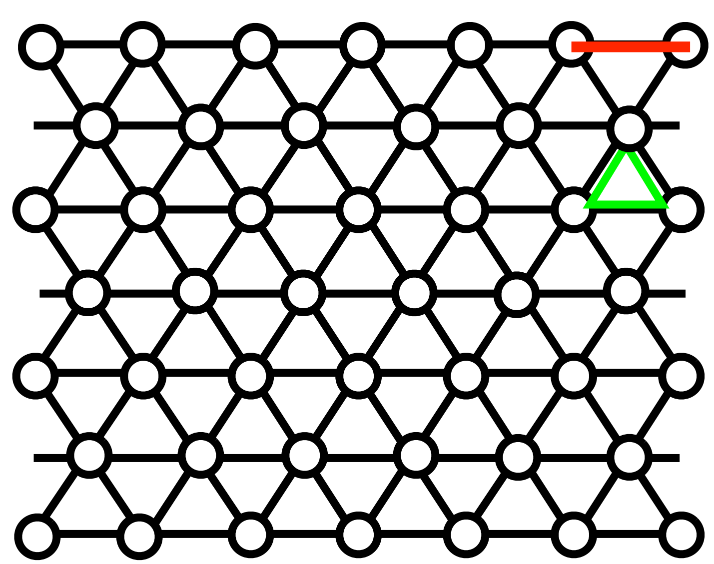
Slide from a talk by V. Gurarie

M. Hermele, V.Gurarie A.M. Rey, PRL 2009

Can we stabilise a CSL by a chiral term ?

- We focus on the triangular lattice for now:

$$\mathcal{H} = \cos(\theta) \sum_{\langle i,j \rangle} P_2(i,j) + \sin(\theta) \sum_{i,j,k \in \triangle} \Im P_3(i,j,k)$$



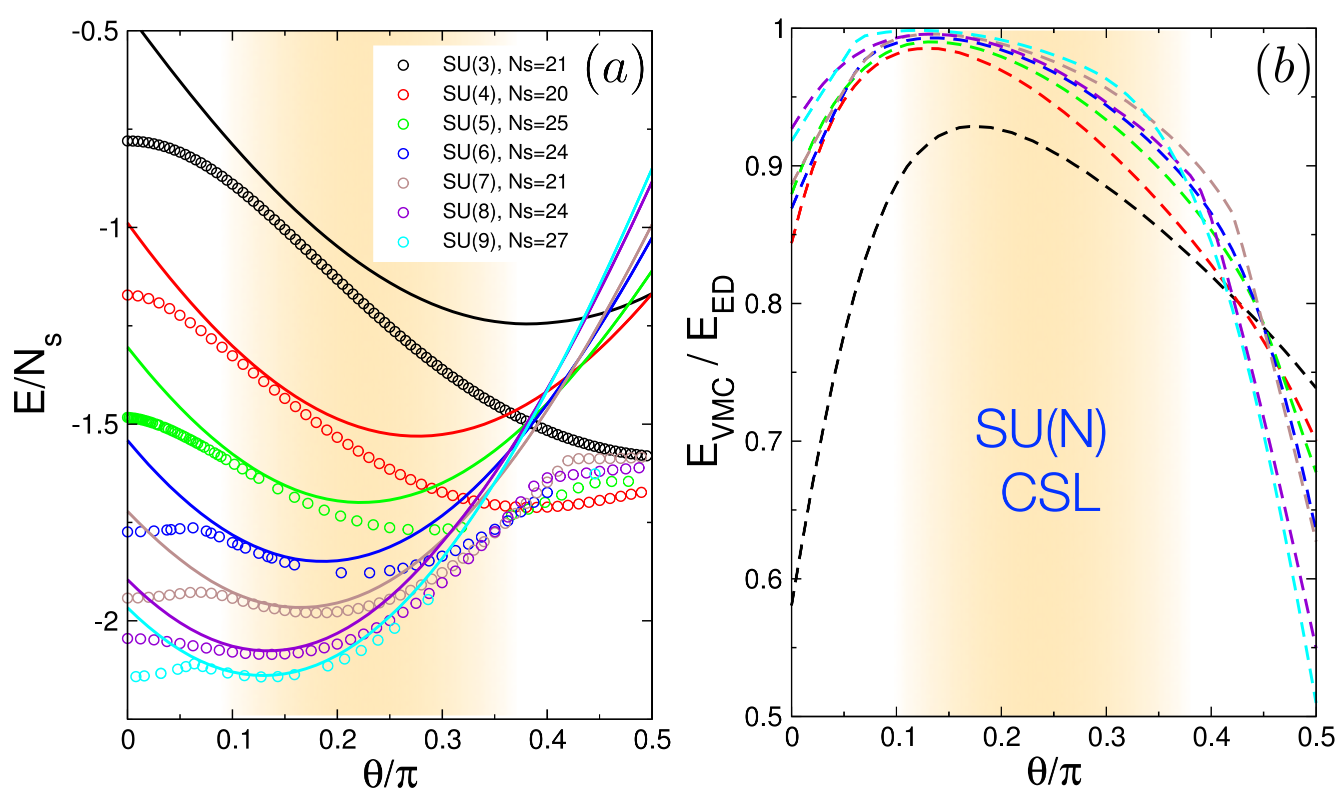
- ImP3 can be generated by 3rd order perturbation theory for Pi/2 Flux per plaquette.

What is a Chiral Spin Liquid ?

- Topological State of Matter with *intrinsic* topological order (not just a SPT phase):
- Topological ground state degeneracy on the torus (N fold), but not on the disk.
- Gap to bulk excitations.
- Chirality either through spontaneous TRS & parity breaking, or externally imposed.
- Gapless chiral edge states with open boundaries.
  Structure of energy spectrum characteristic for the type of topological order (anyons)
- Let us check these requirements in our numerical simulations.

Systematic study in N from 3 to 9 !

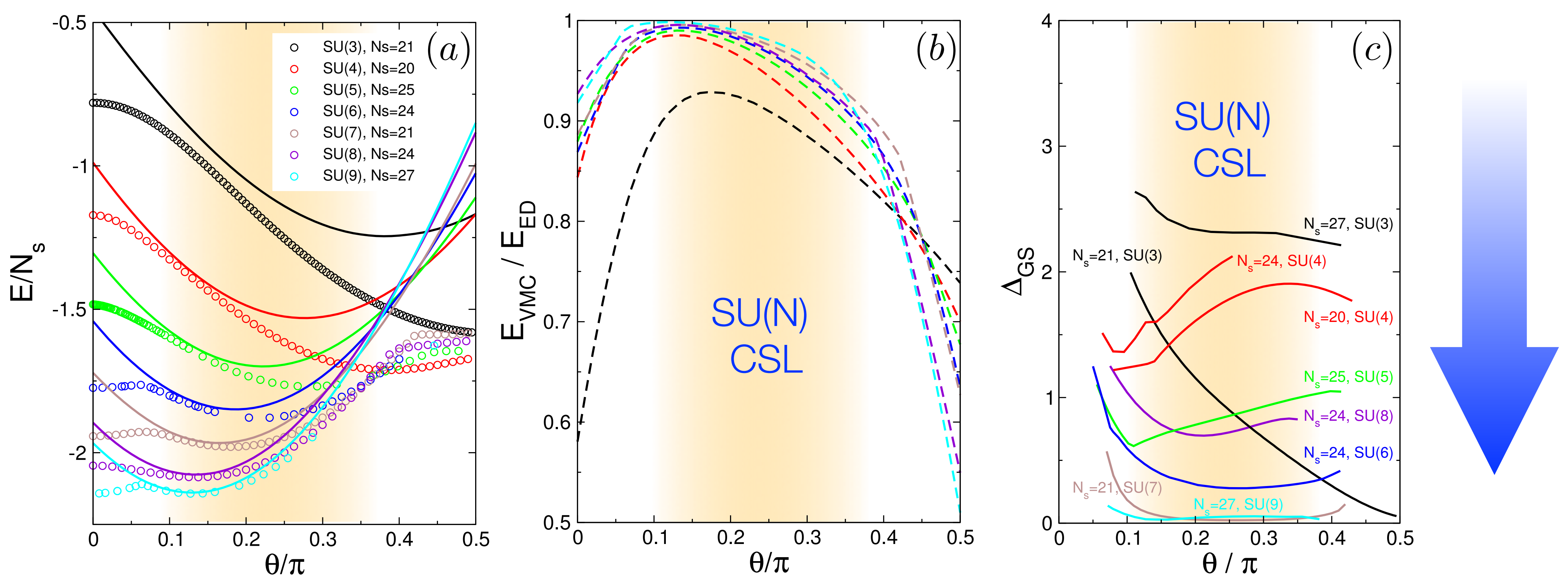
- Using standard ED + SU(N) multiplet ED (P. Nataf & F. Mila, PRL 2014)



- Energy per site / Comparison to model wave function “à la Laughlin state”

Systematic study in N from 3 to 9 !

- Using standard ED + SU(N) multiplet ED (P. Nataf & F. Mila, PRL 2014)



- Energy per site / Comparison to VMC
- GS Manifold ?

Systematic study in N from 3 to 9 !

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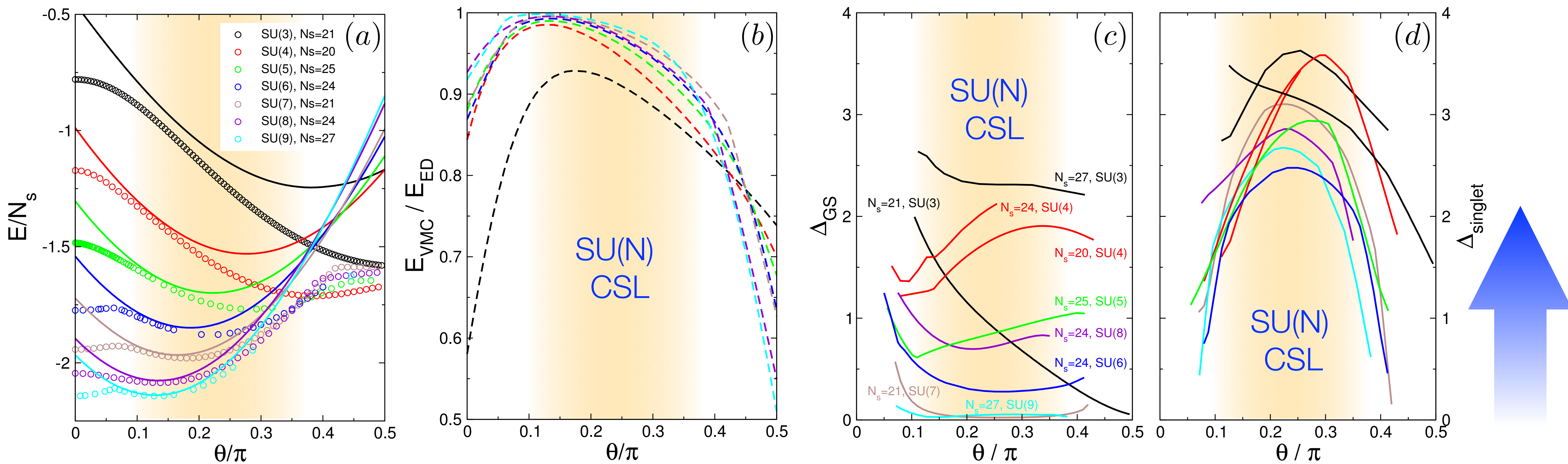
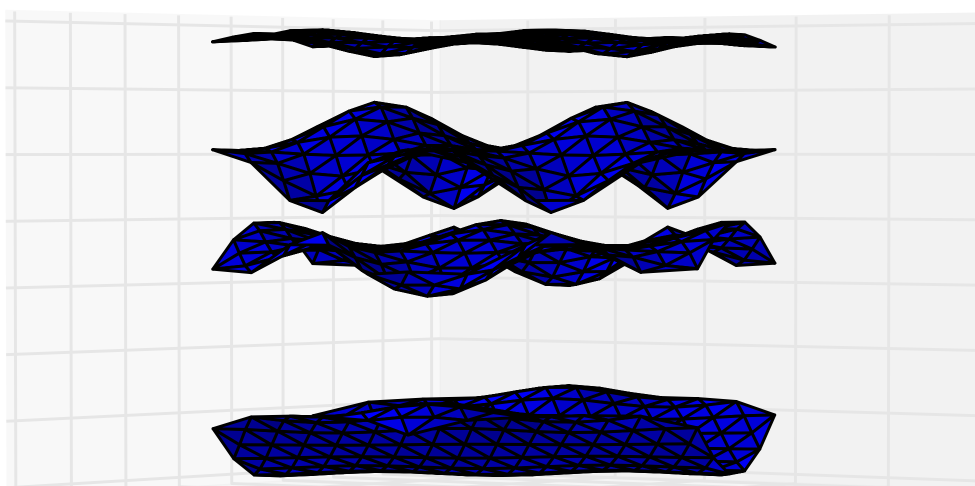


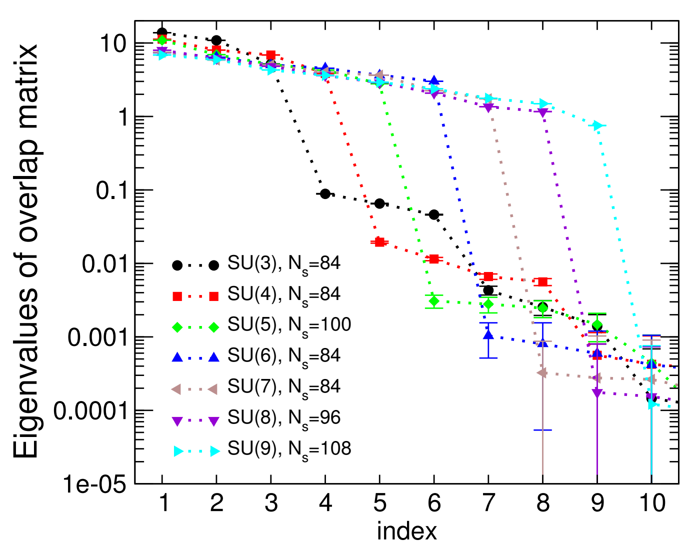
- Energy per site / Comparison to VMC
- GS Manifold ?
- Gap above GS ?

Nature of model wave function:

- Abelian SU(N) Chiral spin liquid wave function:

Band structure $\pi/4$ model





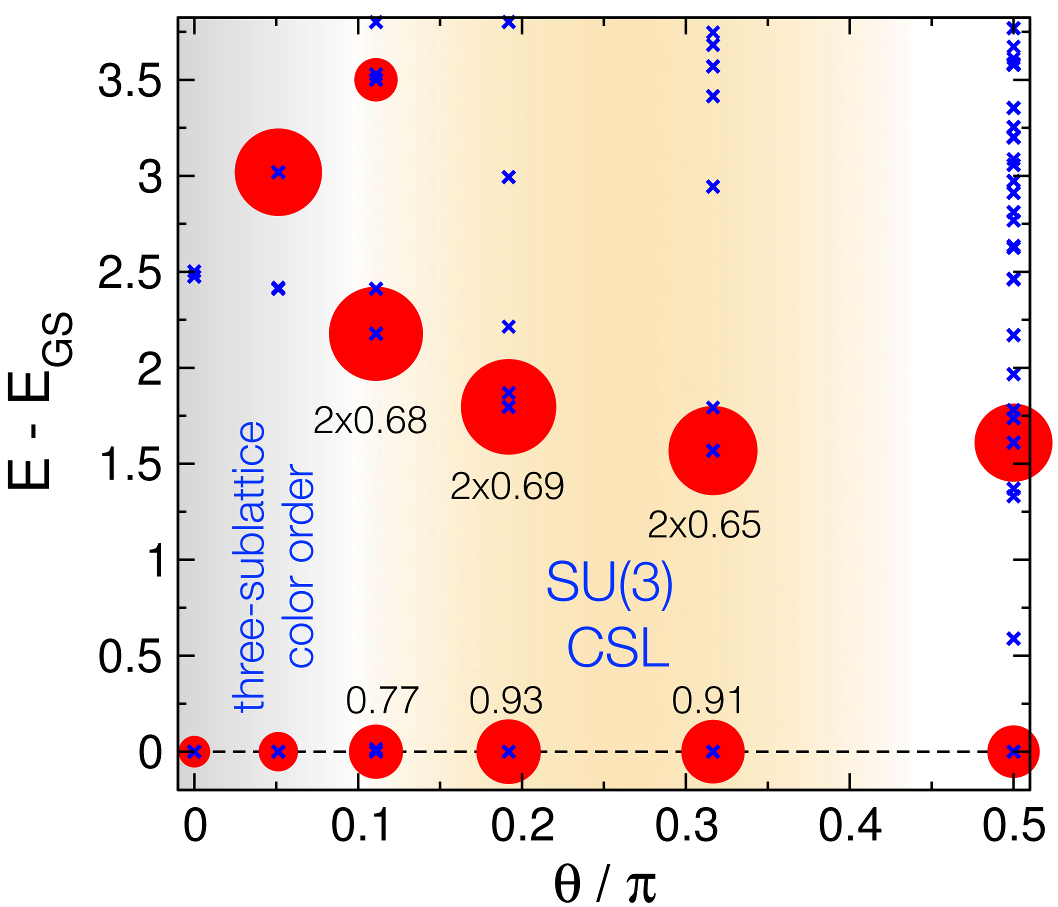
- Gutzwiller projection of one filled band with N fermions per orbital. (parton construction / X.G. Wen)

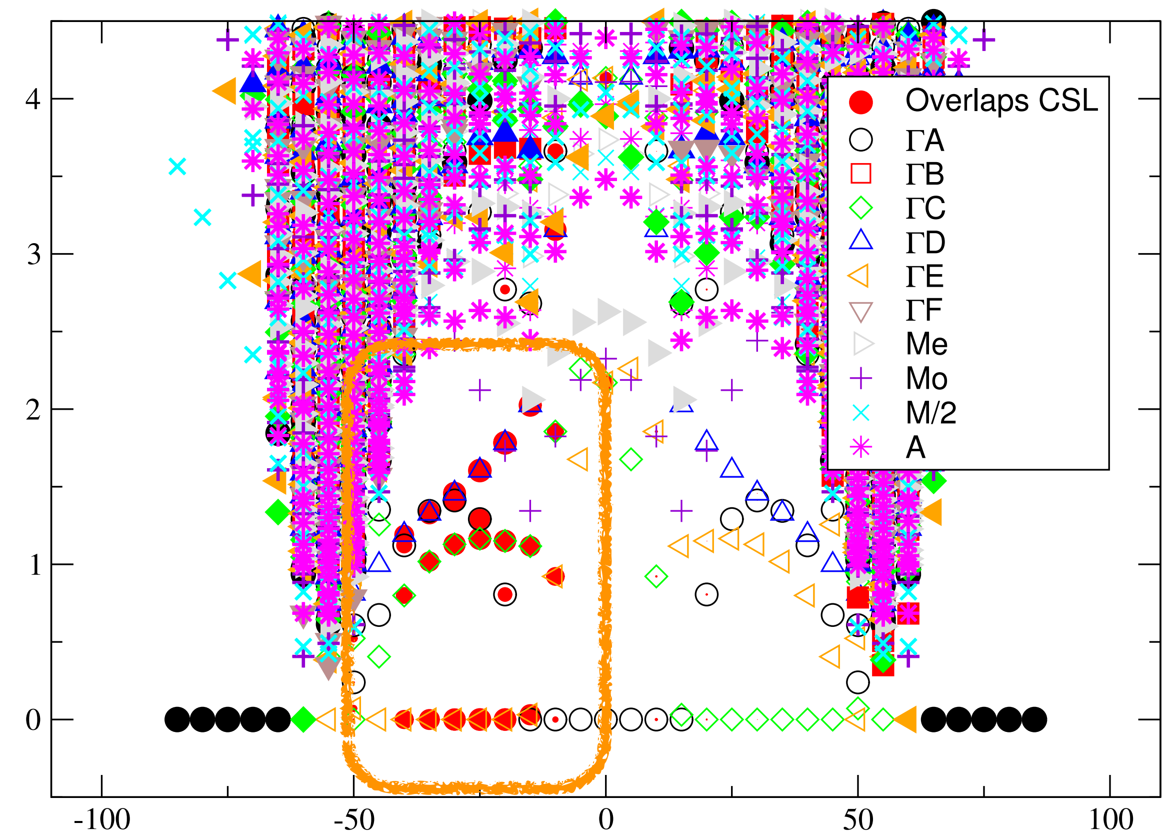
- lowest band has Chern number 1 (Hofstadter Hamiltonian with uniform flux of Pi/N per triangular plaquette)

- Despite unique non-projected Band-Insulator, one obtains N distinct spin states after projection when changing boundary conditions ➡ topological degeneracy

Overlaps with VMC model states

- ED overlaps for SU(3)/12 sites and SU(4) 16 sites:
- Overlaps up to 90% in total !



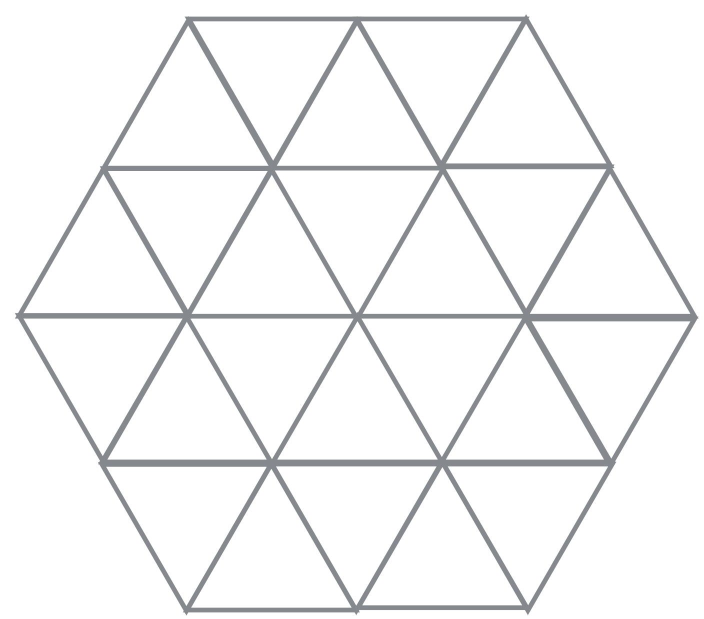


Chiral Edge States

- Nature of the edge states ? Edge states can diagnose bulk topological order !

- Compute Hamiltonian Edge Spectrum of “disc” type cluster with discrete rotation symmetry:

N_S=19
C_6



Chiral Edge States

- Theoretical prediction: chiral SU(N)$_1$ WZNW CFT:

$SU(2)_1$ sector	N_s mod 2	$l=0$	$l=1$	$l=2$	$l=3$
$\bullet$ (1)	0	$\bullet$	$\yng(2)$	$\bullet \oplus \yng(2)$	$2\times\bullet \oplus \yng(2)$
$\square$ (2)	1	$\square$	$\square$	$\square \oplus \yng(3)$	$2\times\square \oplus \yng(3)$

$SU(3)_1$ sector	N_s mod 3	$l=0$	$l=1$	$l=2$	$l=3$
$\bullet$ (1)	0	$\bullet$	$\yng(2,1)$ (8)	$\bullet \oplus 2\times \yng(2,1)$	$2\times\bullet \oplus 3\times\yng(2,1) \oplus \yng(3)(10) \oplus \yng(3,3)(\bar{10})$
$\square$ (3)	1	$\square$	$\square \oplus \yng(2,2)$ $(\bar{6})$	$2\times\square \oplus \yng(2,2) \oplus \yng(3,1)$ (15)	$3\times\square \oplus 3\times\yng(2,2) \oplus 2\times\yng(3,1)$
$\yng(1,1)$ $(\bar{3})$	2	$\yng(1,1)$	$\yng(1,1) \oplus \yng(2)$ (6)	$2\times\yng(1,1) \oplus \yng(2) \oplus \yng(3,2)$ $(\bar{15})$	$3\times\yng(1,1) \oplus 3\times\yng(2) \oplus 2\times\yng(3,2)$

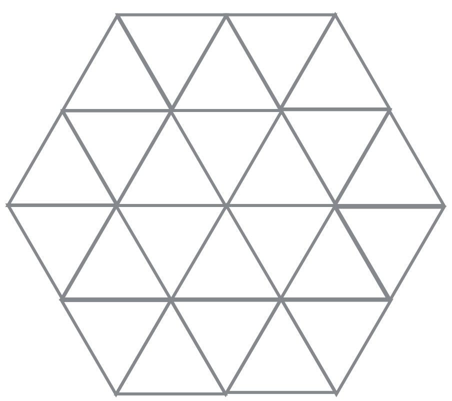
$SU(4)_1$ sector	N_s mod 4	$l=0$	$l=1$	$l=2$
$\bullet$ (1)	0	$\bullet$	$\yng(2,1,1)$ (15)	$3\times\yng(2,1,1)$
$\square$ (4)	1	$\square$	$\square \oplus \yng(2,2,1)$ $(\bar{20})$	$2\times\square \oplus 2\times\yng(2,2,1) \oplus \yng(3,1,1)$ (36)
$\yng(1,1)$ (6)	2	$\yng(1,1)$	$\yng(1,1) \oplus \yng(2)(10) \oplus \yng(2,2,2)(\bar{10})$	N/A
$\yng(1,1,1)$ $(\bar{4})$	3	$\yng(1,1,1)$	$\yng(1,1,1) \oplus \yng(2,1)$ (20)	$2\times\yng(1,1,1) \oplus 2\times\yng(2,1) \oplus \yng(3,2,2)$ $(\bar{36})$

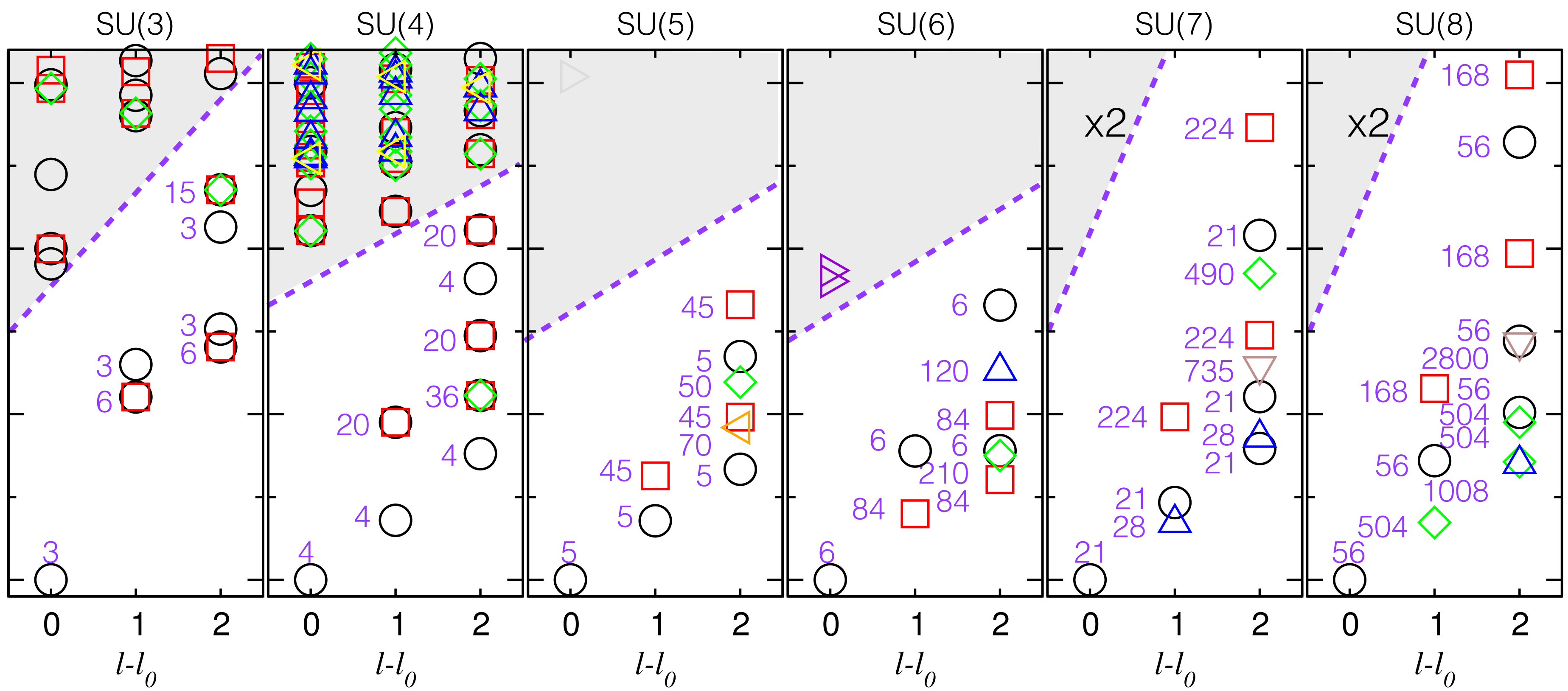
P. Nataf, M. Lajko, A. Wietek, K. Penc, F. Mila, and AML, PRL 2016

From SU(3) to SU(8):

- Numerics:

N_s=19





- SU(N)$_1$ WZNW predictions:

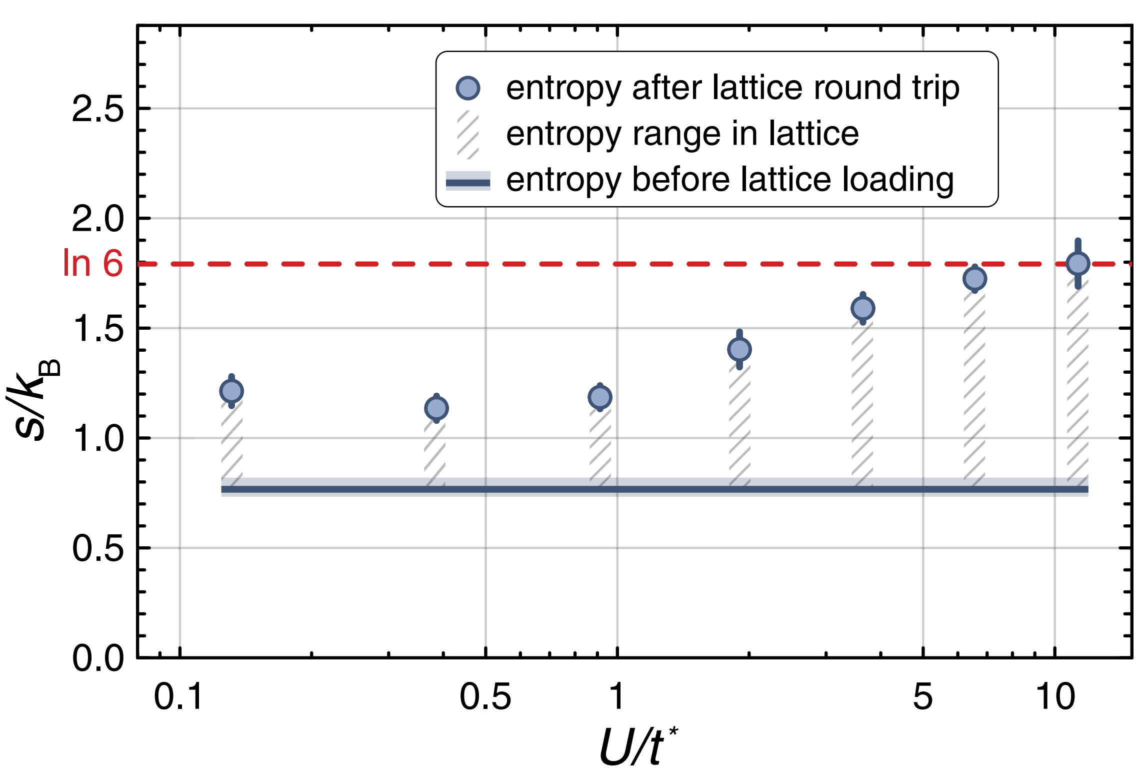
N in SU(N)	N_s mod N	$l=0$	$l=1$	$l=2$
2	1	□ (2)	□	□ ⊕ (4)
3	1	□ (3)	□ ⊕ ($\bar{6}$)	2 × □ ⊕ ⊕ (15)
4	3	($\bar{4}$)	⊕ (20)	2 × ⊕ 2 × ⊕ ($\bar{36}$)
5	4	($\bar{5}$)	⊕ (45)	2 × ⊕ 2 × ⊕ (50) ⊕ ($\bar{70}$)
6	1	□ (6)	□ ⊕ ($\bar{84}$)	2 × □ ⊕ 2 × ⊕ (120) ⊕ ($\bar{210}$)
7	5	($\bar{21}$)	⊕ ($\bar{28}$) ⊕ (224)	3 × ⊕ ⊕ 2 × ⊕ (490) ⊕ ($\bar{735}$)
8	3	(56)	⊕ (168) ⊕ ($\bar{504}$)	3 × ⊕ 2 × ⊕ 2 × ⊕ ($\bar{1008}$) ⊕ (2800)
9	1	□ (9)	□ ⊕ ($\bar{315}$)	2 × □ ⊕ 2 × ⊕ (396) ⊕ ($\bar{2700}$)

Outline

- Introduction: Why SU(N) Magnetism ?
- SU(3) Square Lattice
- SU(4) Square Lattice
- SU(N>2) Triangular Lattice with additional TRS breaking term
- Thermodynamics of the SU(N) square lattice Heisenberg model
- Conclusion & Outlook

Thermodynamics of the SU(N) Heisenberg model

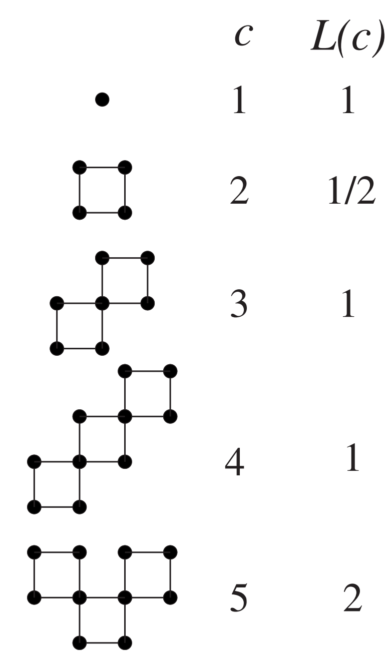
- A number of interesting ground states in SU(N) Heisenberg models revealed
- However experiments are at finite entropy / temperature
- What will be visible in experiments ?



C. Hofrichter et al., PRX 2016

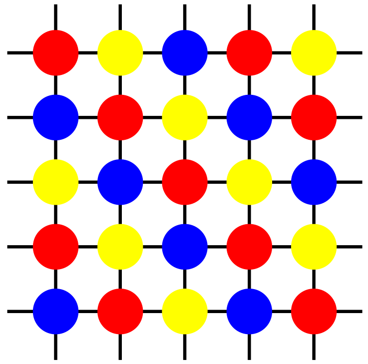
How to obtain finite-T results ?

- Exact diagonalizations exploiting SU(N) symmetry P. Nataf & F. Mila, PRL 2014
  - Complete diagonalization of PBC clusters: SU(3) 18 sites, SU(4) 16 sites
  - NLCE (Numerical linked cluster expansion) 4-5 squares
    M. Rigol et al, PRL 2006, PRE 2007

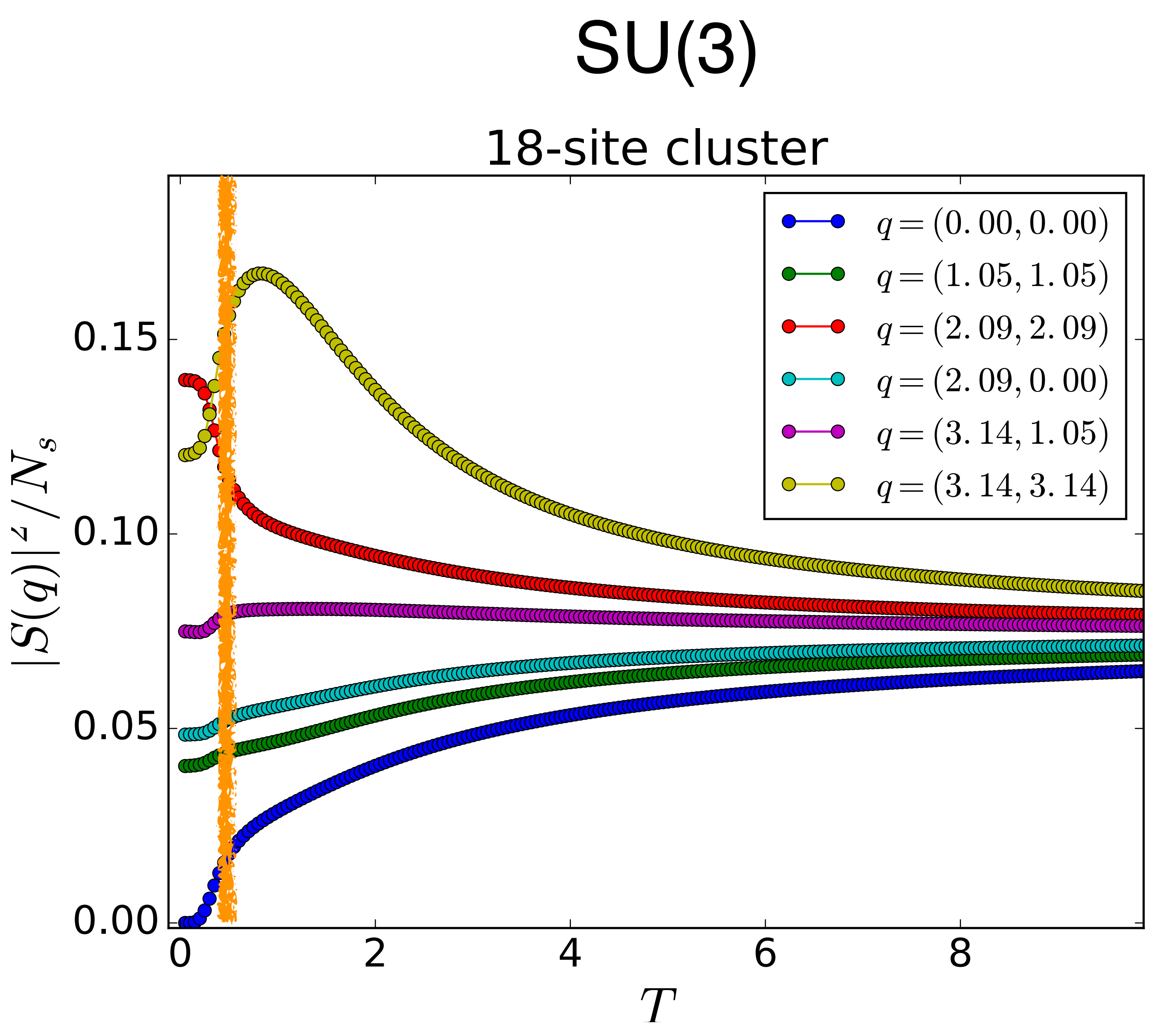


- Analytical high-temperature expansions (analytical N dependence)

Complete diagonalization SU(3)

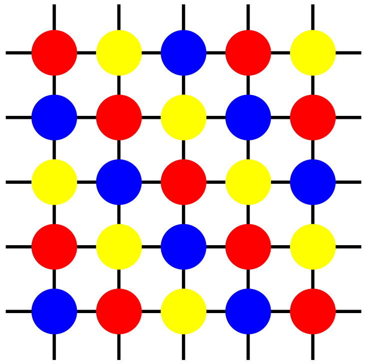


- SU(3) Square lattice: distinct high-T and low-T regime in spin structure factor !

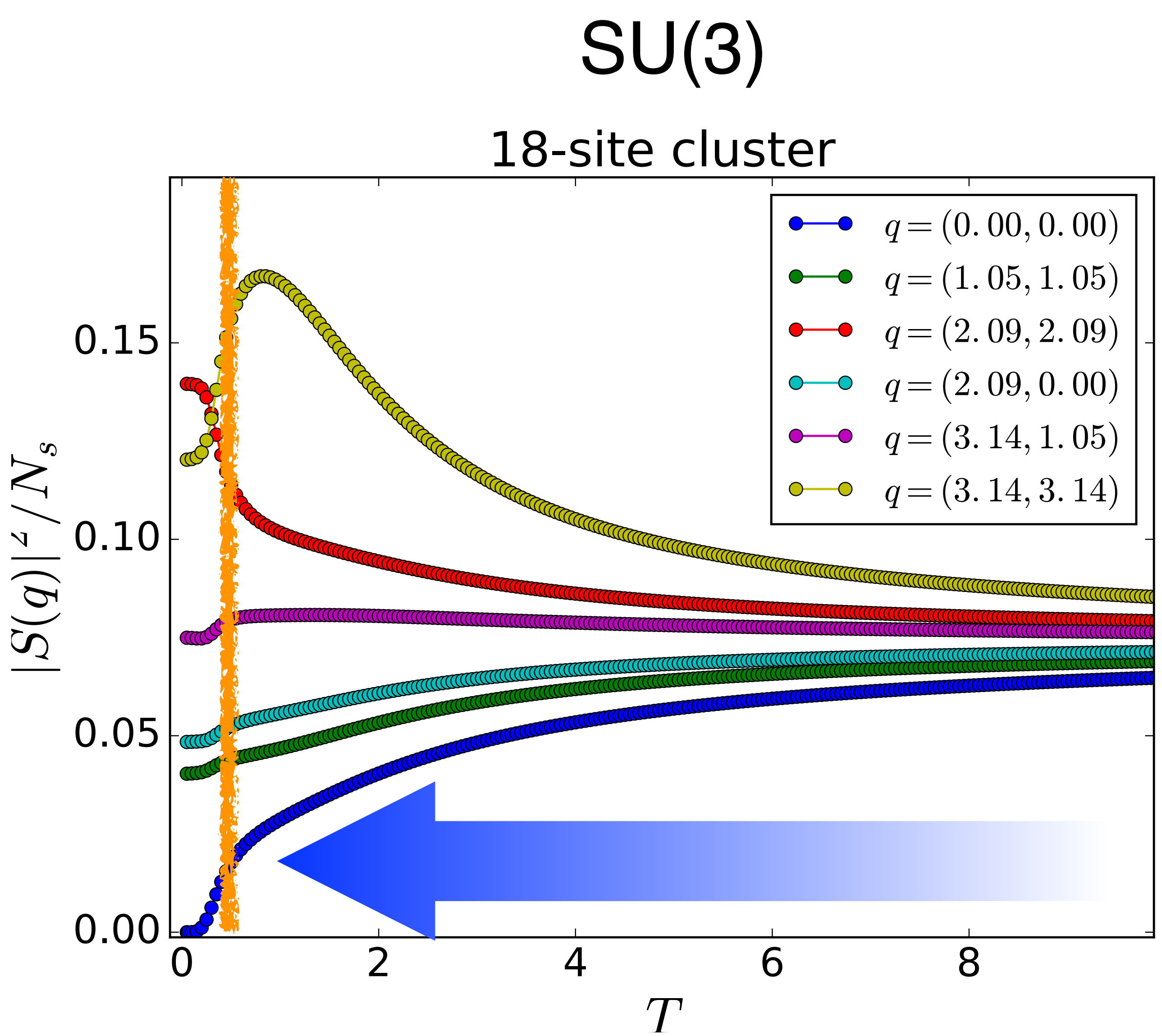


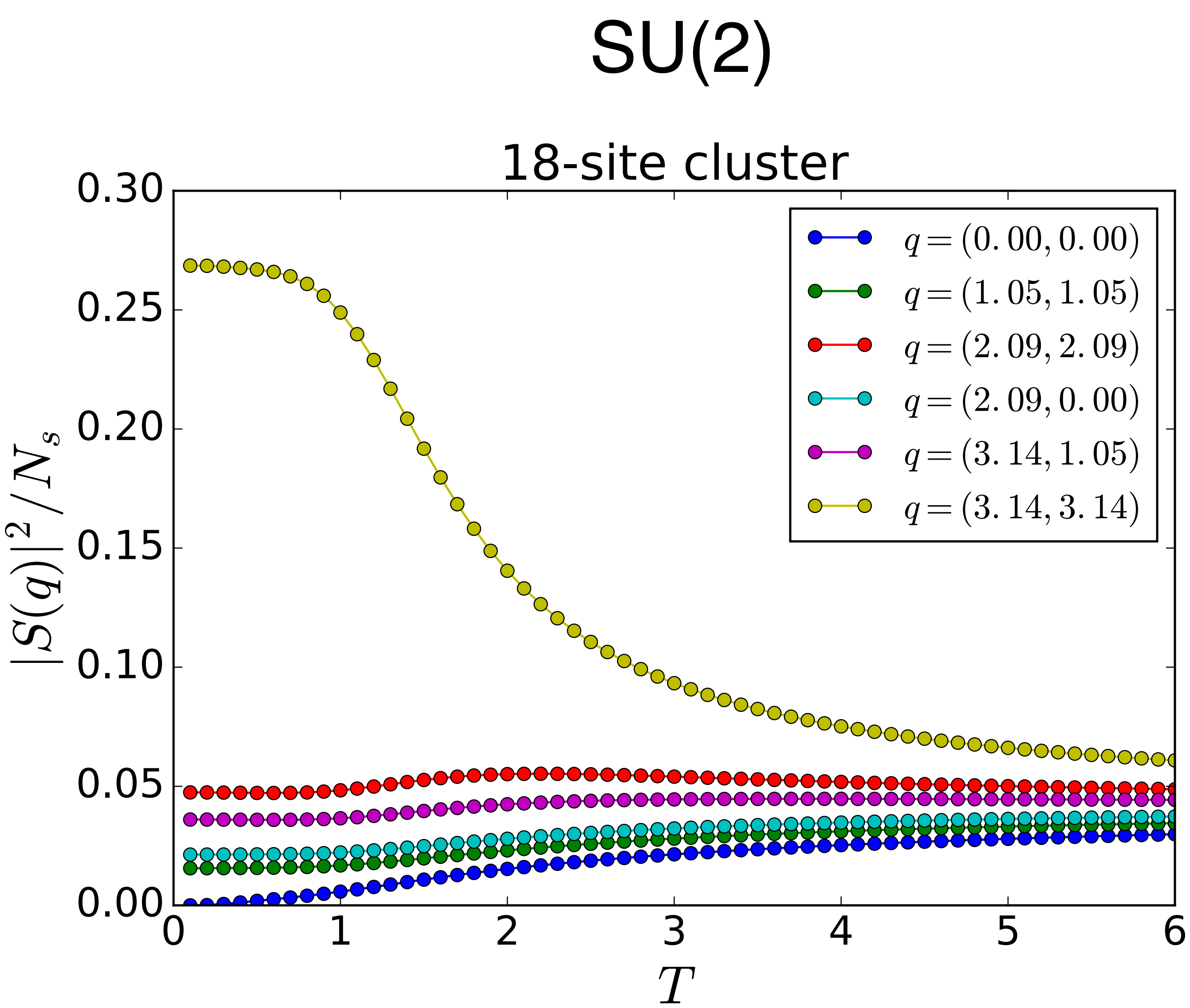
Complete ED, 387’420’489 states, largest matrix dim ~787’000

Complete diagonalization SU(3)



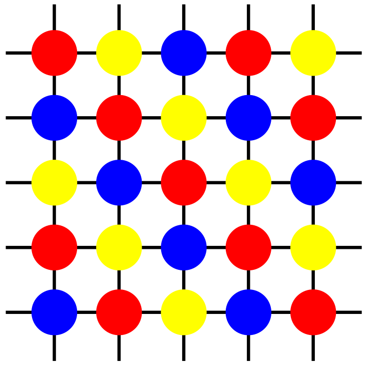
- SU(3) Square lattice: distinct high-T and low-T regime !



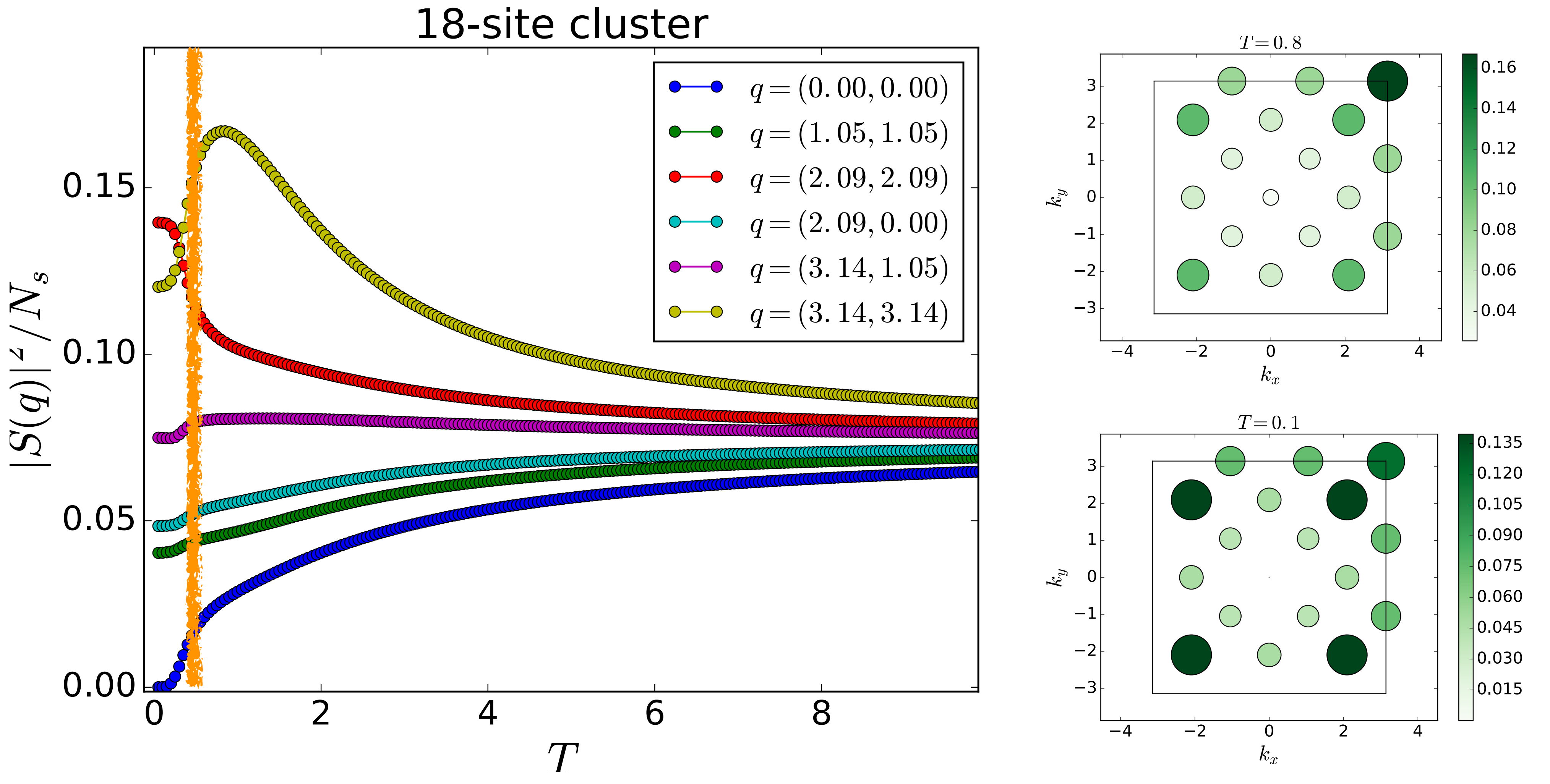


- High-T regime exhibits 2 sublattice fluctuations as SU(2), but short-ranged

Complete diagonalization SU(3)

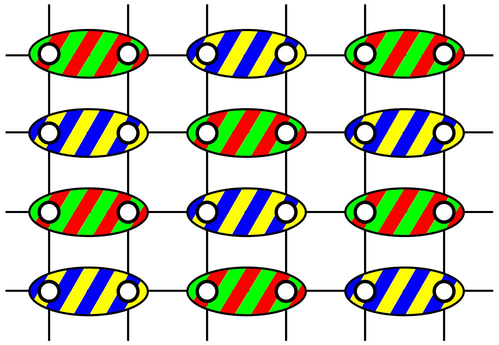


- SU(3) Square lattice: distinct high-T and low-T regime !



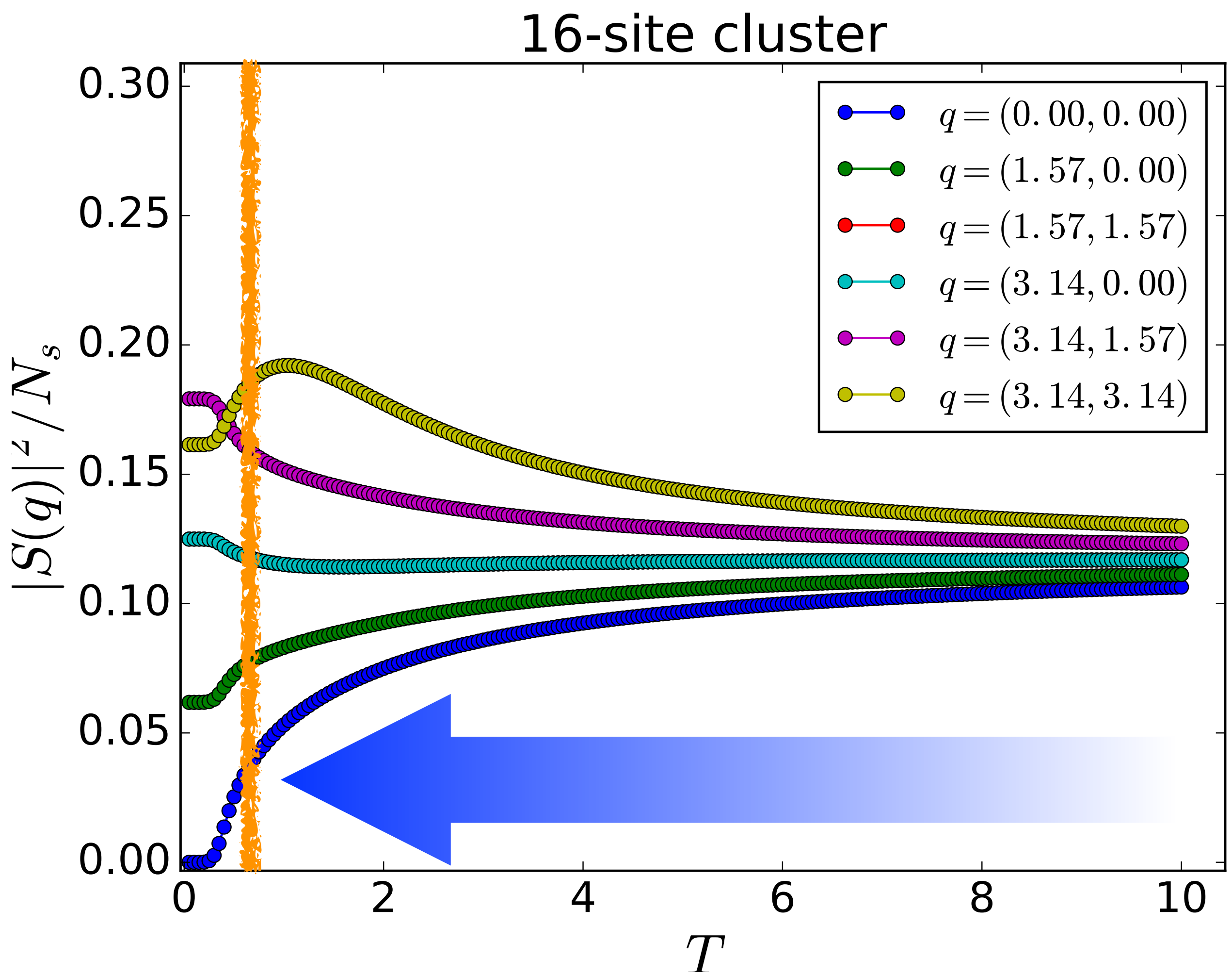
- Low-T regime exhibits 3 sublattice structure

Complete diagonalization SU(4)



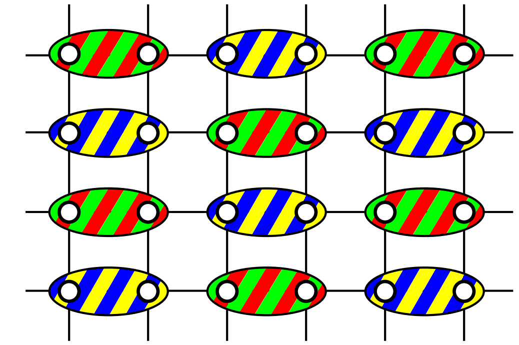
- SU(4) Square lattice

Complete ED, 4’294’967’296 states, largest matrix dim ~512’000

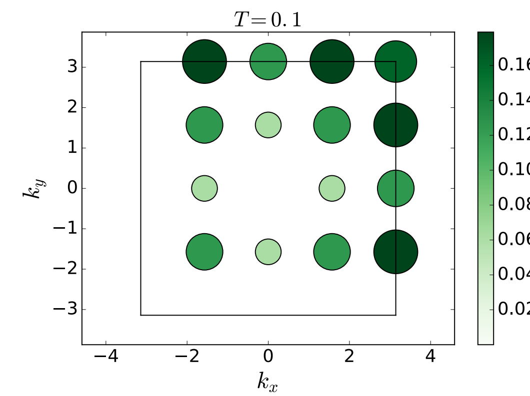


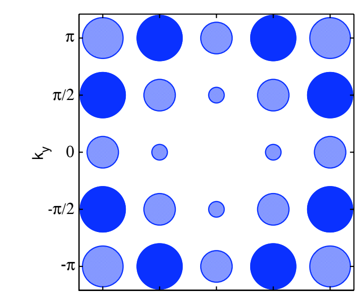
- High-T regime exhibits 2 sublattice fluctuations as SU(2), but short-ranged

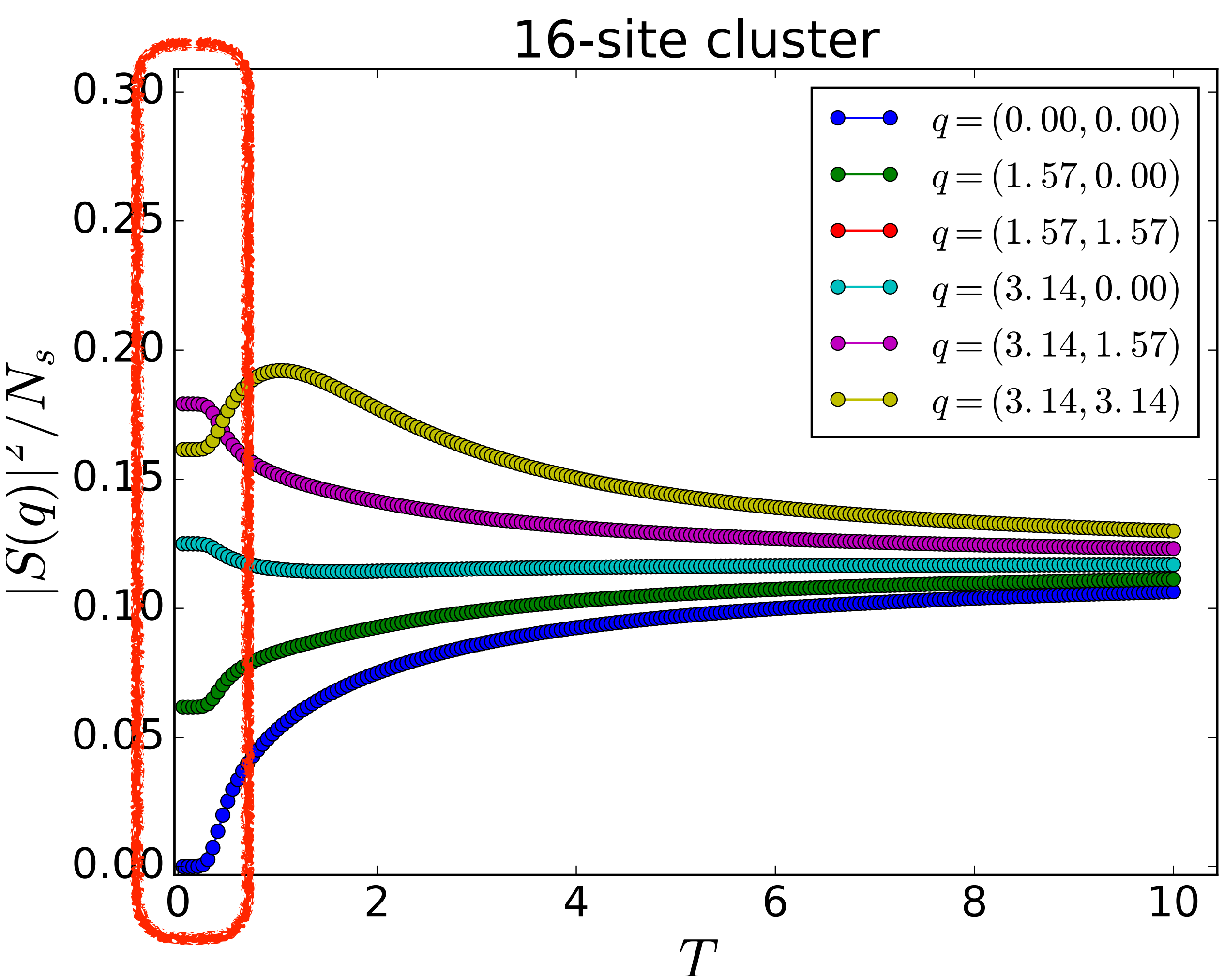
Complete diagonalization SU(4)

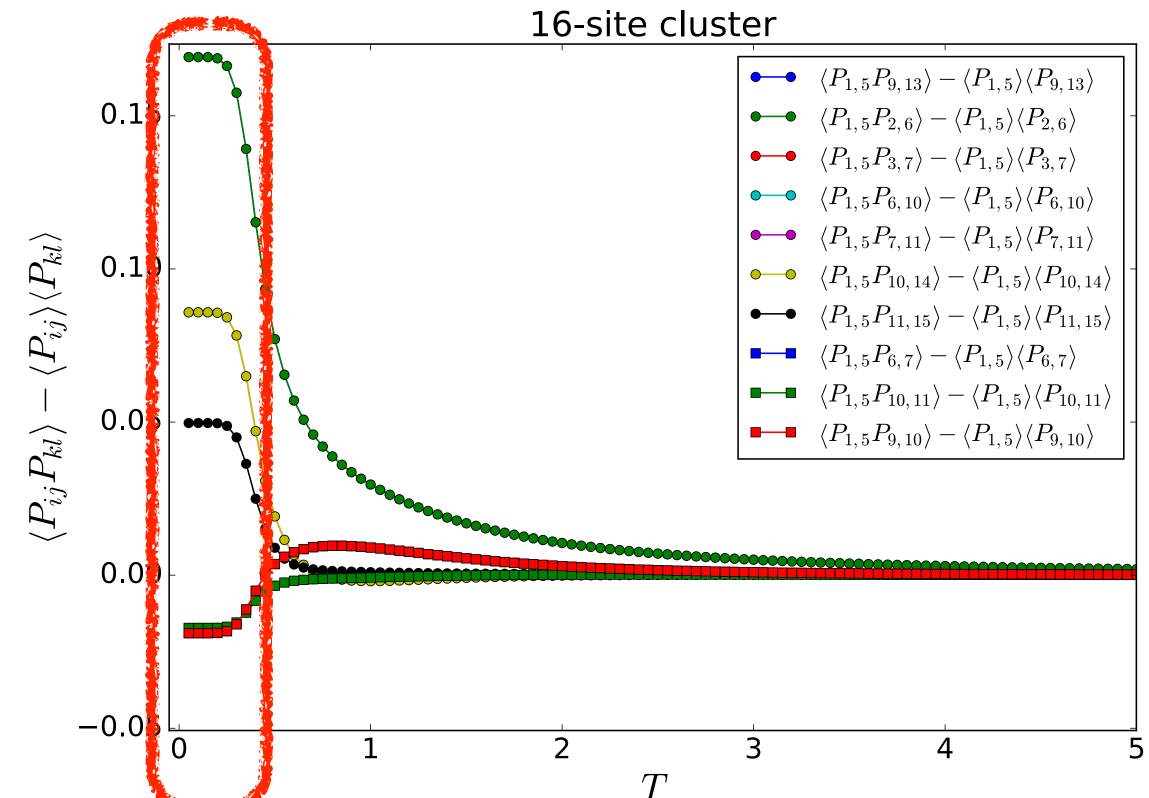


- SU(4) Square lattice





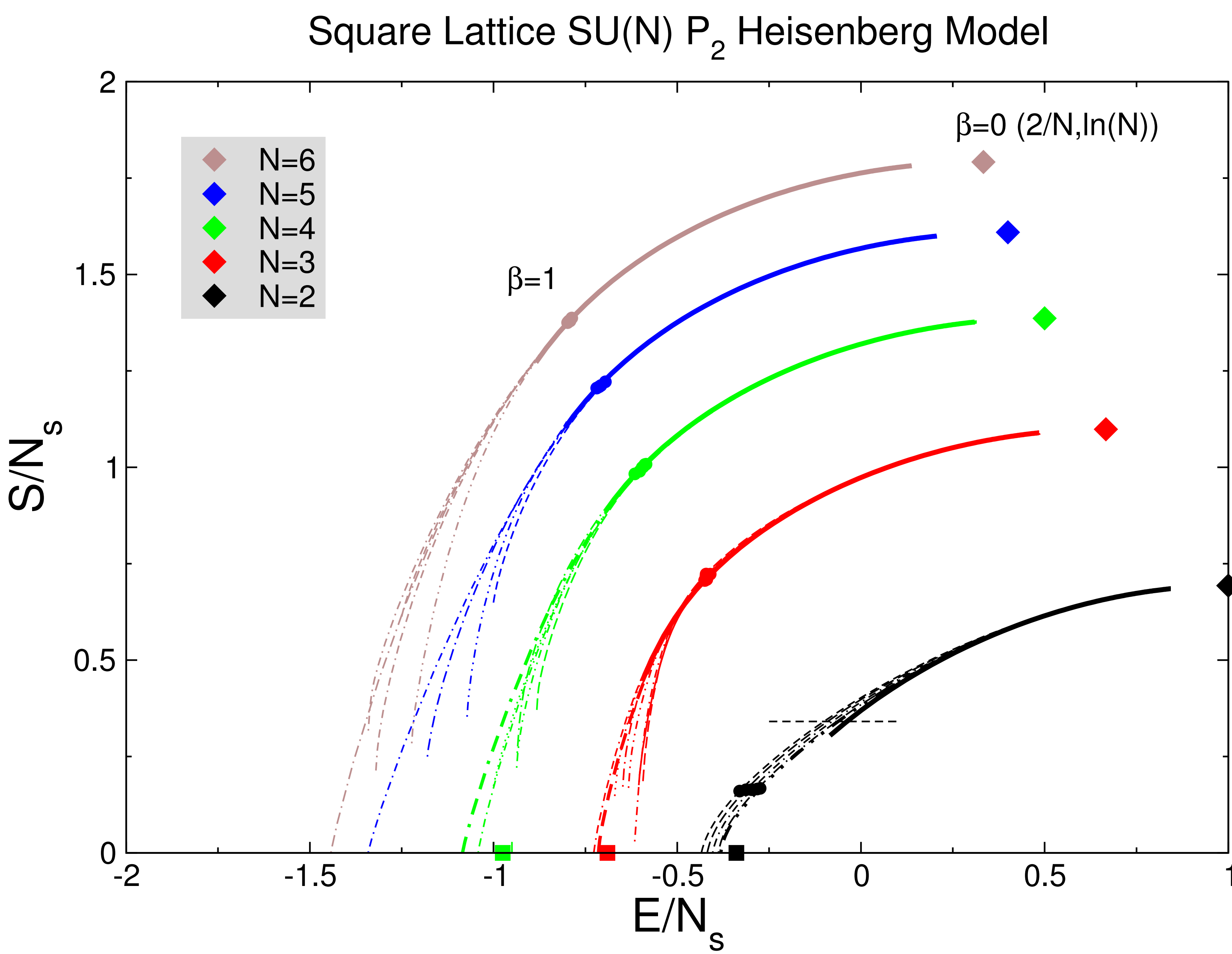




- Low-T regime exhibits dimerised state, with particular Neel order of bond variables.

Microcanonical Thermodynamics: S(E)

- S as a function of energy from finite size ED and NLCE and HTSE (low order)

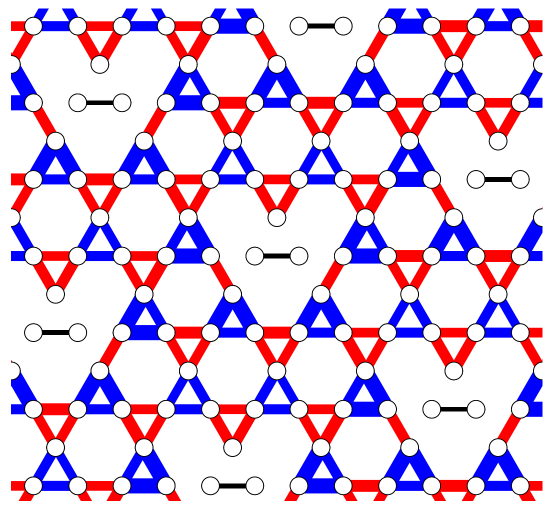


- (Almost) common thermodynamics for N>2 and high temperature !
- same absolute entropy reduction leads to same T in high T regime
- Typically rather distinct low-T regime (unlike the SU(2) case) with substantially lower entropy.

C. Romen and AML, work in progress

Conclusions

P. Corboz, K. Penc, F. Mila, AML, PRB 2012

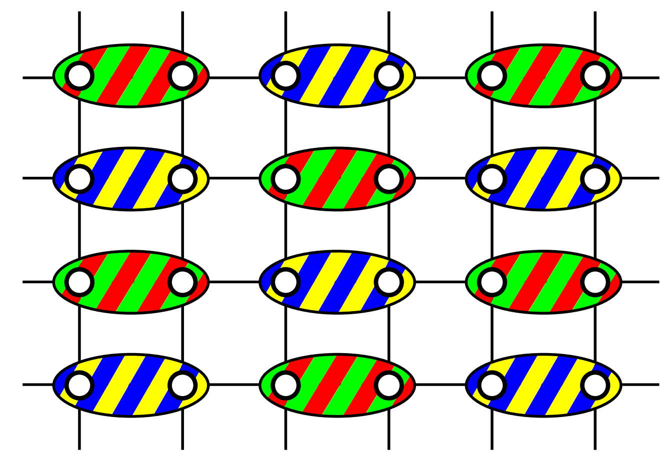


VBS analogues

SU(3) kagome &

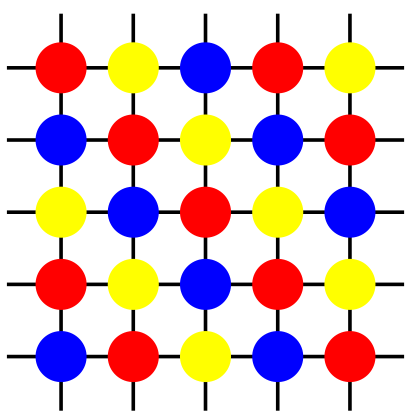
SU(4) checkerboard

P. Corboz, AML, K. Penc, M.Troyer, F. Mila, PRL 2011



peculiar magnetic order

SU(4) on square lattice



Order by disorder,

competition between

quantum fluctuations and

thermal fluctuations

SU(3) on square lattice

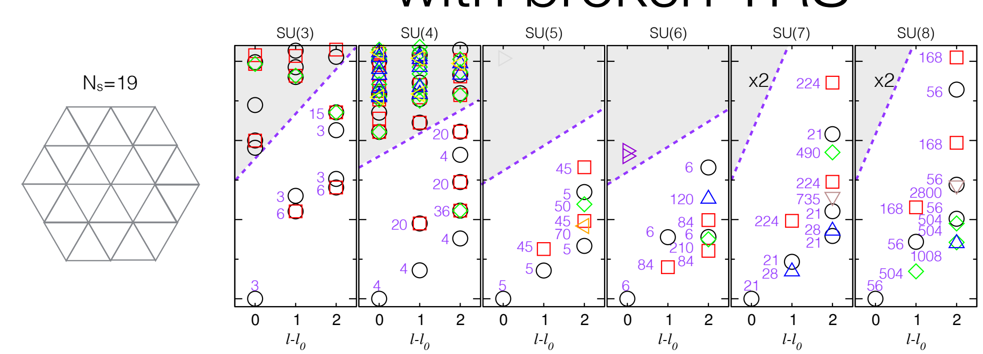
T. Tóth, AML, F. Mila, K. Penc, PRL 2010

B. Bauer, et al., PRB 2012

chiral spin liquids

SU(N>2) on triangular lattice

with broken TRS



P. Nataf, M. Lajko, A. Wietek, K. Penc, F. Mila, and AML, PRL 2016

Thank you for your attention !