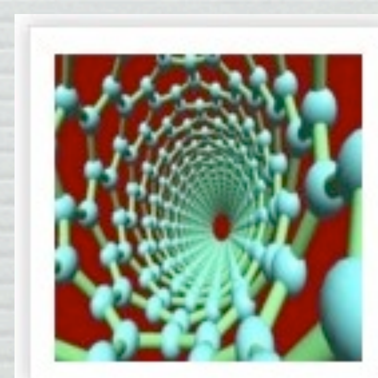
The spin-1 kagome antiferromagnet

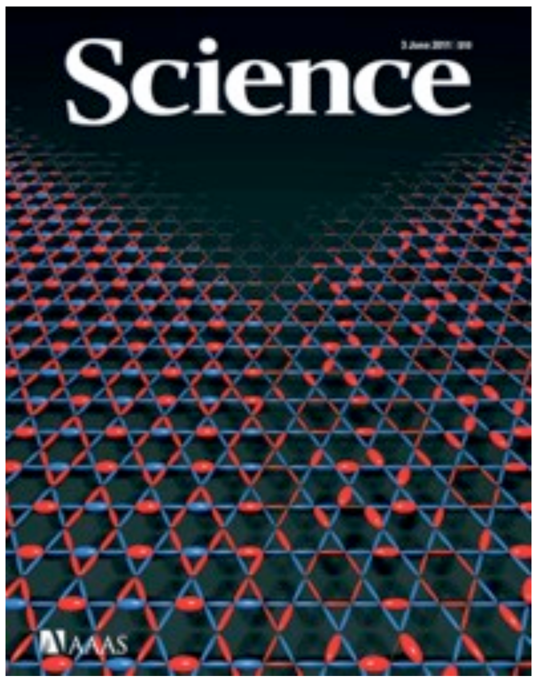
Wei Li
Arnold Sommerfeld Center For Theoretical Physics,
Physics Department, LMU Munich, Germany.

04. 09. 2014
Benasque

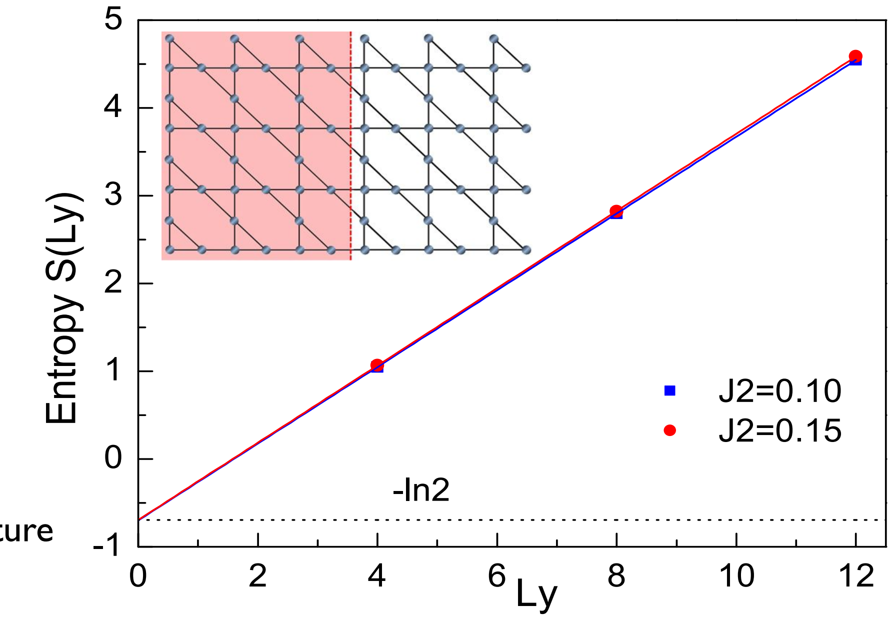


why spin-1 kagome antiferromagnet (KAF)?

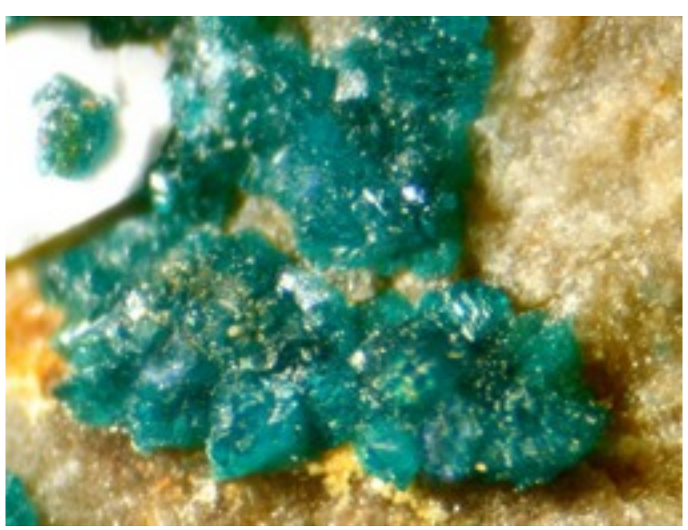
✎ Spin-1/2 kagome antiferromagnets have been intensively studied.



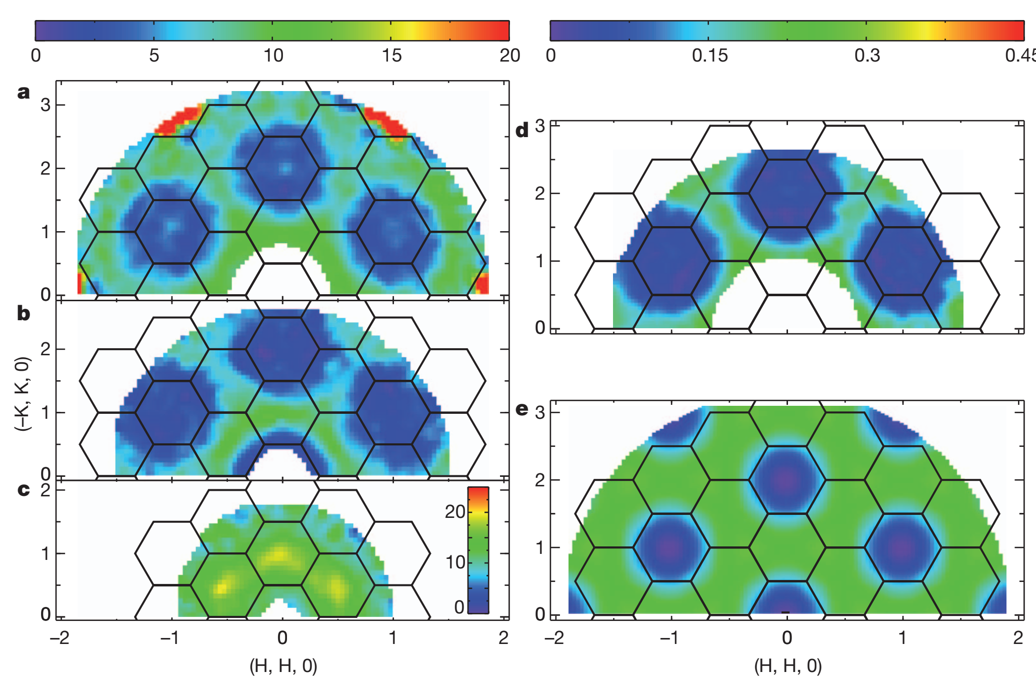
S. Yan, D.A. Huse, & S.R. White, *Spin liquid ground state of the S=1/2 kagome Heisenberg antiferromagnet*. Science **332**, 1173–1176 (2011)



H.-C Jiang, Z.H. Wang & L. Balents, Nature Physics **8**, 902-905 (2012)
S. Depenbrock, et. al, PRL, 2012

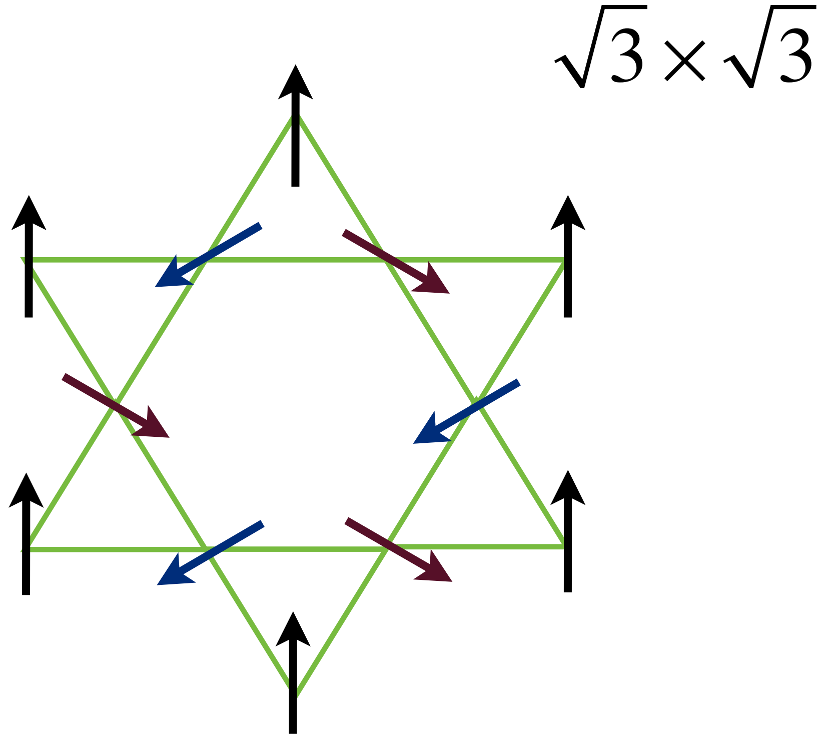


Herbertsmithite



T.-H. Han, et. al, *Fractionalized excitations in the spin-liquid state of a kagome-lattice antiferromagnet*, *Nature* **492**, 406–410 (2012)

✎ Spin-1 KAF are less well studied....

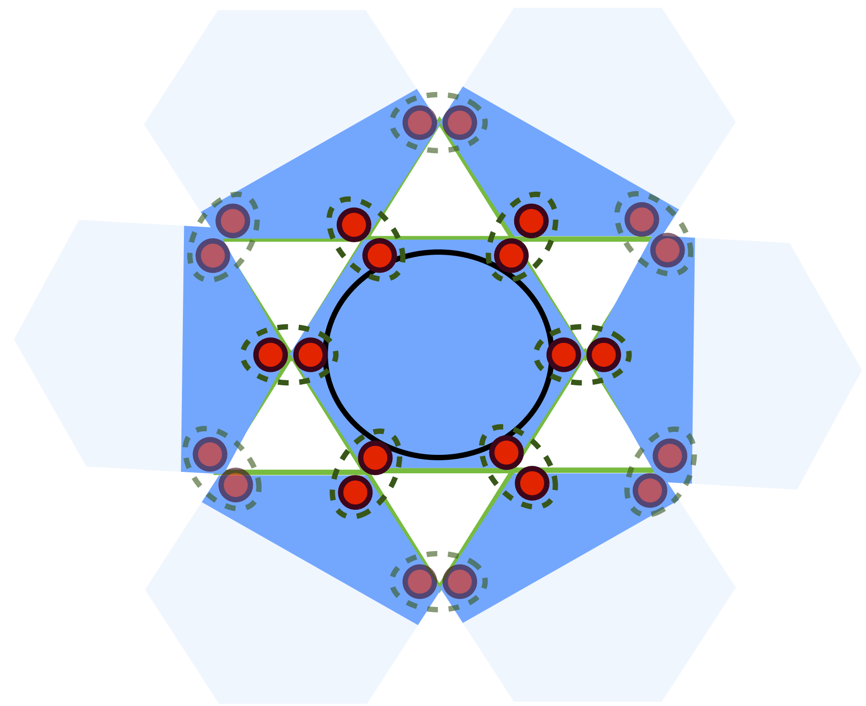


Magnetically ordered?

True for large S limit!
[D.A. Huse et. al, PRB (1992)]
[C.L. Henley et. al, JMMM. (1995)]

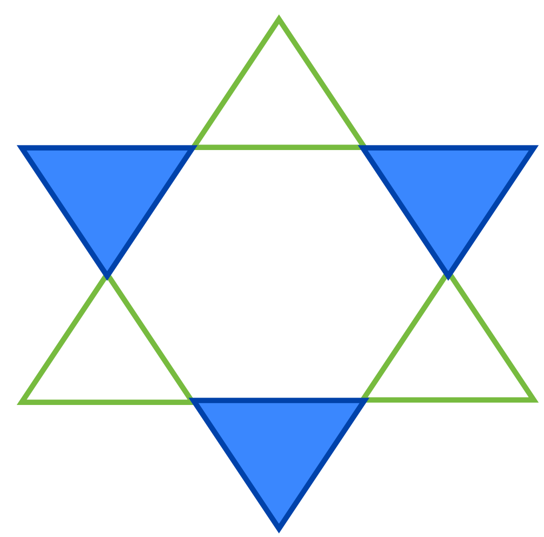
Stable in spin-1 KAF [C. Xu et. al, PRB (2007)]

or



hexagon valence bond solid state?
[K. Hida, 2000]

or



fully trimerized crystal?
[Z. Cai, 2009]

Experimental studies of the spin-1 KAF

	material	reference	comments
I	m-MPYNN $\cdot BF_4$	(a) N. Wada, et. al, JPSJ (1997). (b) T. Matsushita, et. al, JPSJ (2010).	(a) gapped antiferromagnet (b) magnetization curve (0, 1/2 & 3/4 plateaus)
II	$Ni_3V_2O_8$	G. Lawes, et. al, PRL (2004).	kgaome staircase
III	$KV_3Ge_2O_9$	S. Hara, et. al, JPSJ (2012).	
IV	$BaNi_3(OH)_2(VO_4)_2$	D.E. Freedman, et. al, Chem. Commun. (2012).	AF & F couplings

Experiments show:

(a) No magnetic susceptibility peak [I & III] ➙ *no magnetic transition, no SO(3) symmetry breaking*

(b) Low−T susceptibility collapse to zero [I] ➙ *gapped states*

(c) Specific heat has a maximum around J/2 (J the AF coupling) [I] ➙ *phase transition?*

Numerical simulations of the spin-1 KAF was ... *few*

✎ Coupled cluster calculation [Götze et. al., PRB (2012)]

Long-range magnetic order appears only for S>1.

➜ *No* $\sqrt{3}\times\sqrt{3}$ *magnetic order in spin-1 KAF!*

Spin-1 KAF GS energy estimated as $E_0 = -1.4031$

✎ Until this year:

H.J. Changlani and A.M. Läuchli, *Ground state of the spin-1 antiferromagnet on the kagome lattice,* arXiv:1406.4767v1 (2014).

T. Liu, WL, A. Weichselbaum, J. von Delft, and G. Gu, *Simplex valence-bond crystal in the spin-1 kagome Heisenberg antiferromagnet*, arXiv:1406.5905 (2014).

T. Picot, D. Poilblanc, *Nematic and supernematic phases in Kagome quantum antiferromagnets under a magnetic field*, arXiv:1406.7205 (2014).

The Resonating AKLT-loop State

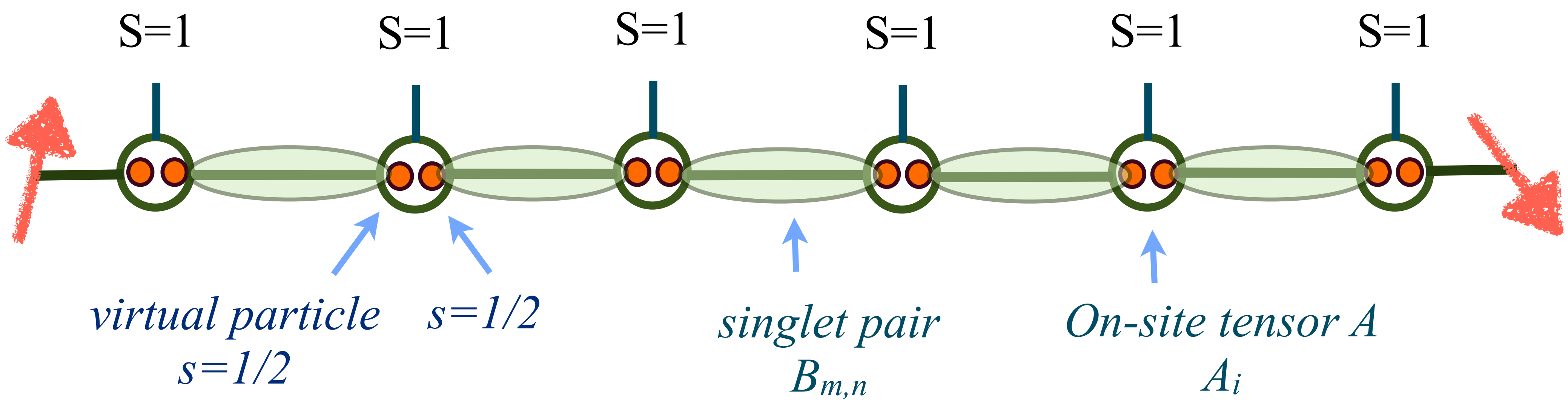
✎ *Topological resonating AKLT-loop states and its PEPS representation*

✎ *The RAL family and its variational energies*

related paper:

WL, S. Yang, M. Cheng, Z.-X. Liu, and H.-H. Tu
Topology and criticality in the resonating Affleck-Kennedy-Lieb-Tasaki loop spin liquid states
Phys. Rev. B 89, 174411 (2014).

Spin-1 system: Affleck-Kennedy-Lieb-Tasaki (AKLT) string state



✎ AKLT-string state has a natural Matrix-Product State representation.

$$|AKLT\rangle = P_{s=1}^{\otimes N} \prod_{i=1} \left|\uparrow_{2i-1}\downarrow_{2i} - \downarrow_{2i-1}\uparrow_{2i}\right\rangle$$

i labels site where physical spin-1 locates

Matrix-Product State, D=2

$$A_i^{m=1} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, A_i^{m=-1} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, A_i^{m=0} = \frac{\sqrt{2}}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

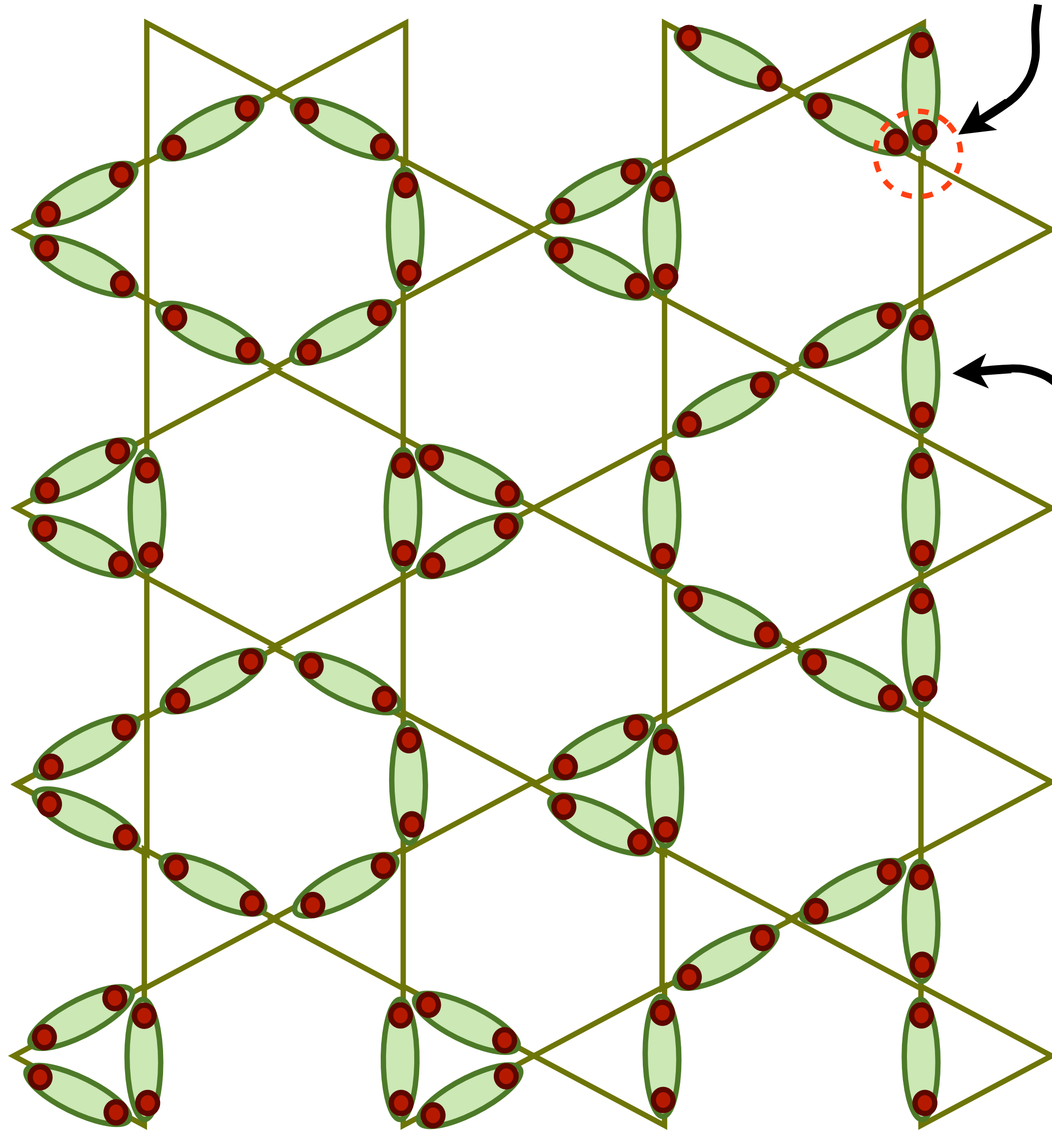
$$B_{2i-1,2i} = \frac{\sqrt{2}}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

✎ *Symmetry-Protected Topological Order:* *spinon carries spin-1/2, symmetry fractionalization*

I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. 59, 799 (1987); Commun. Math. Phys. 115, 477, (1988).

spin-1 systems: *Resonating AKLT-loop (RAL) State*

project $1/2 \otimes 1/2$ => spin-1

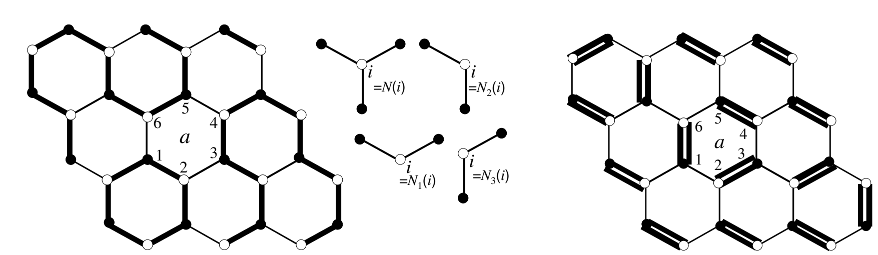


singlet

$$\frac{1}{\sqrt{2}}\left(\left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle\right)$$

$$\left|RAL\right\rangle = \sum_{\text{all loop configs}} \left|L\right\rangle$$

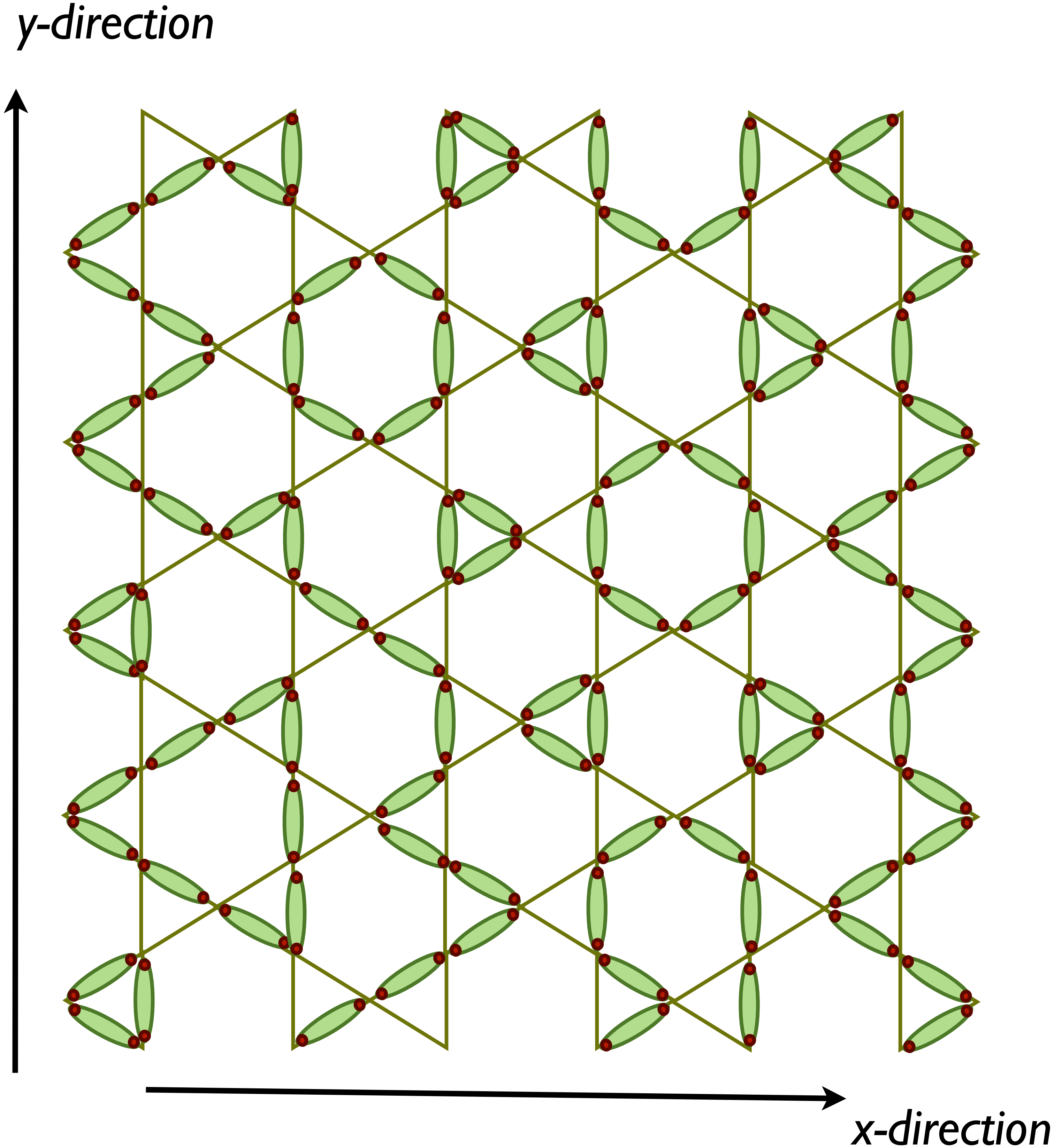
The singlets form a closed loop called <u>AKLT loop</u>.



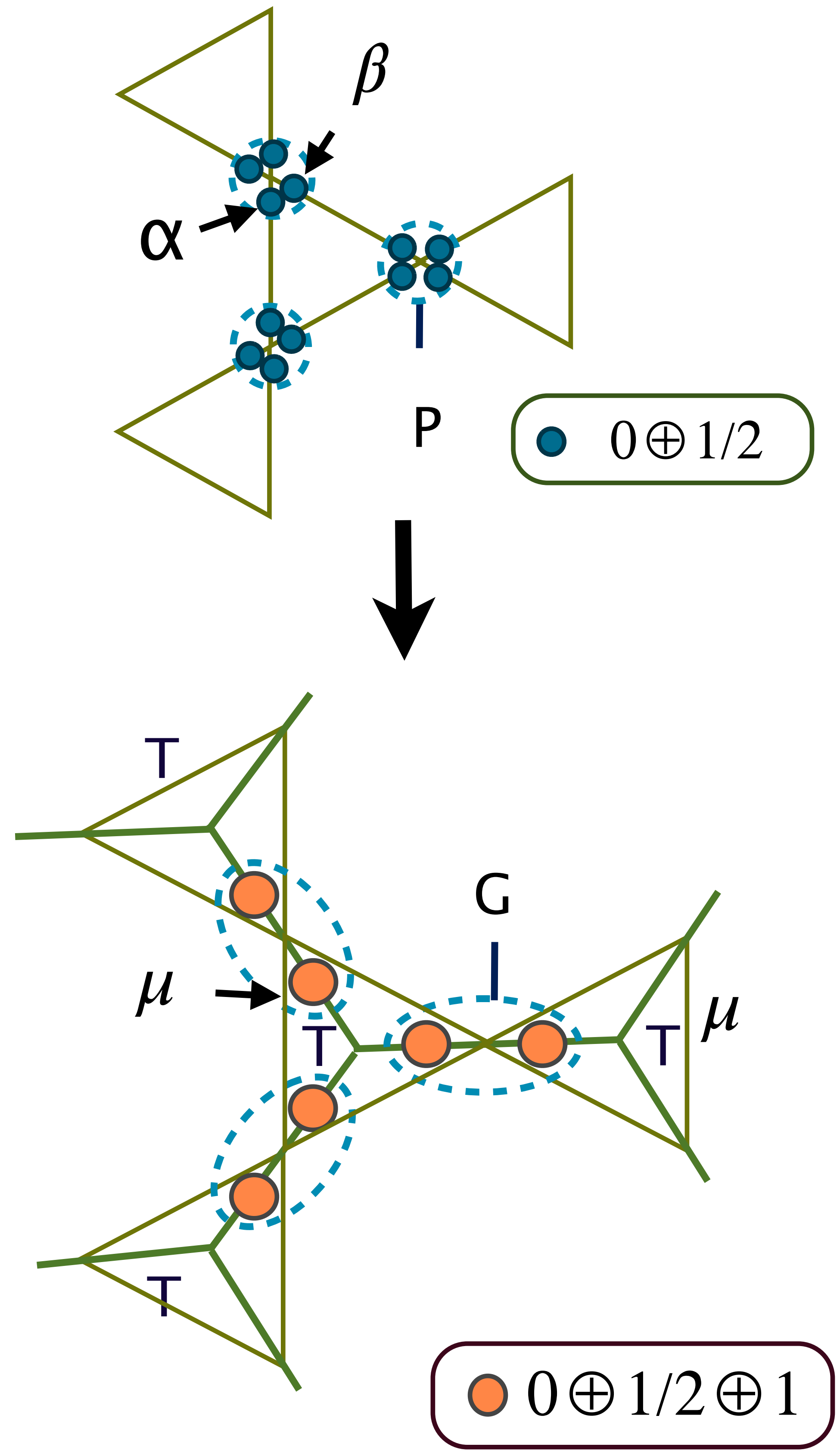
(a) (b)

Hong Yao, Liang Fu, and Xiao-Liang Qi
<u>arXiv:1012.4470</u> (2010).

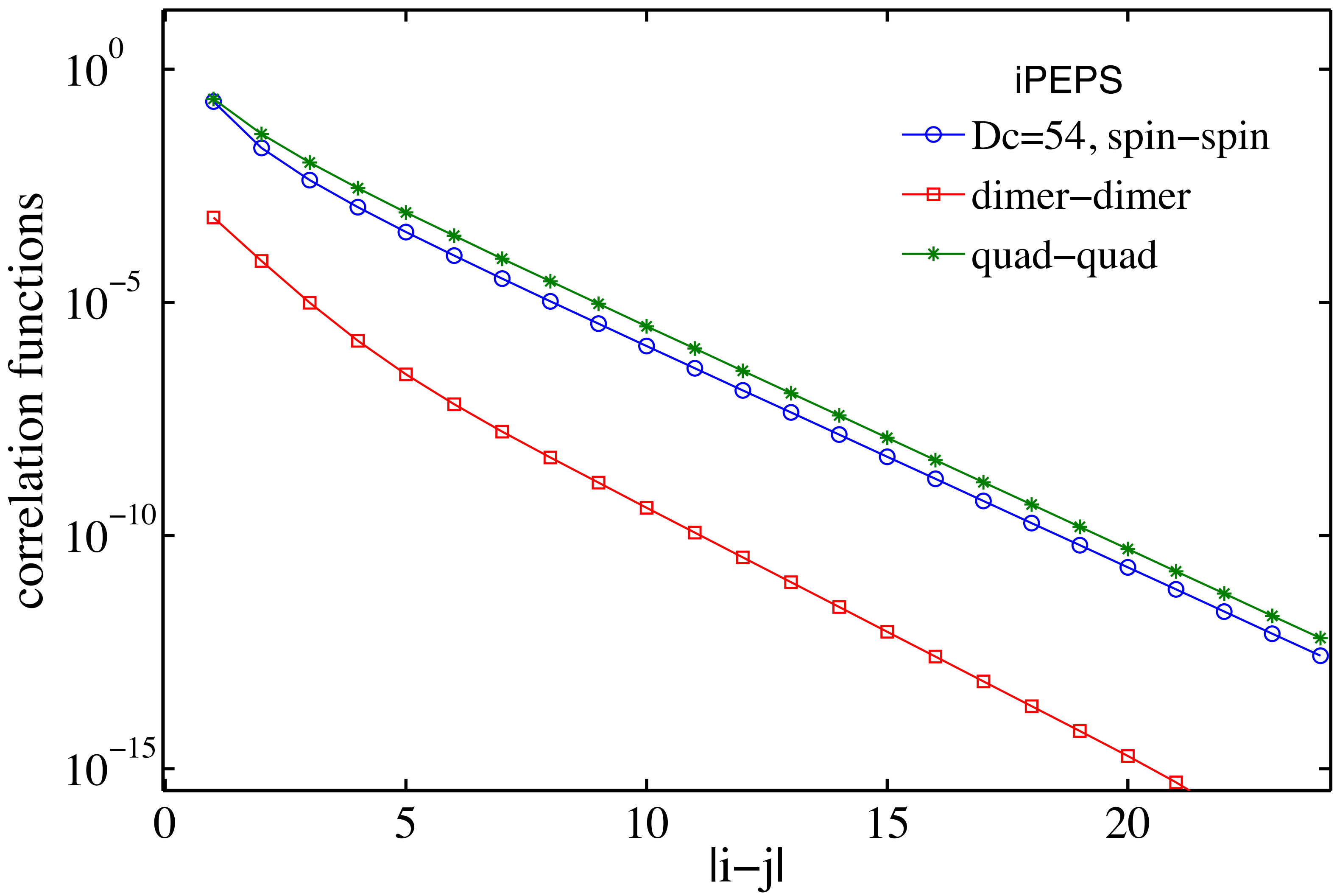
The spin-1 RAL on the kagome lattice



Loop config. on kagome lattice

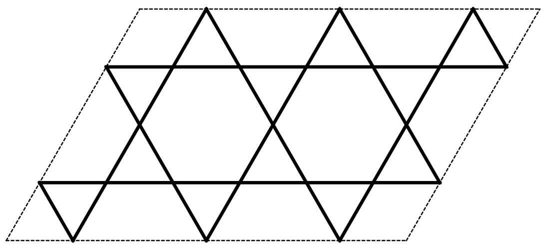


The RAL states on the kagome lattices: gapped spin liquid



Z_2 spin liquid?

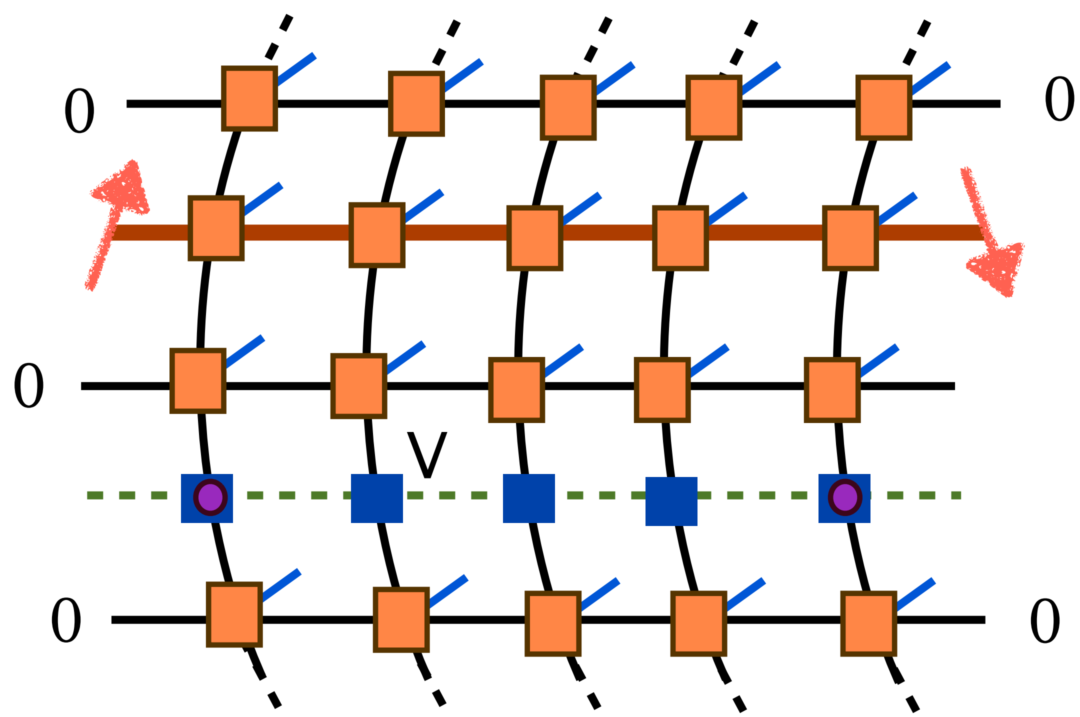
✎ No magnetic, dimer, or quadrupolar order.



The kagome RAL states: the topological sectors

spinon line
"electric" Wilson loop

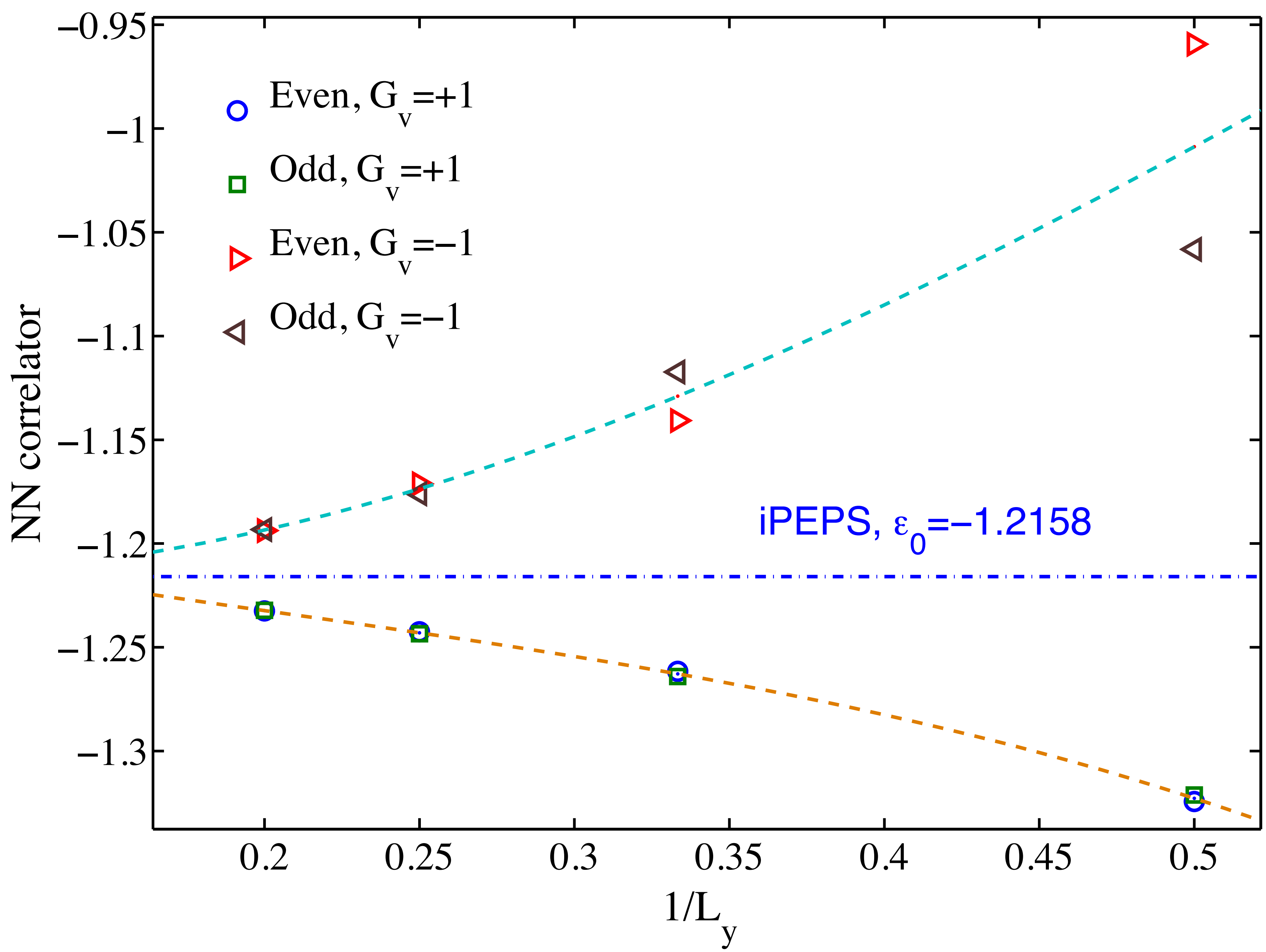
flux (vison) line
"magnetic" Wilson loop



V=diag(1,−1,−1,1,1,1)

One can constructed 4 topological sectors on infinite cylinder, they are labeled by $\{P_V = \text{even/odd}, G_V = \pm 1\}$.

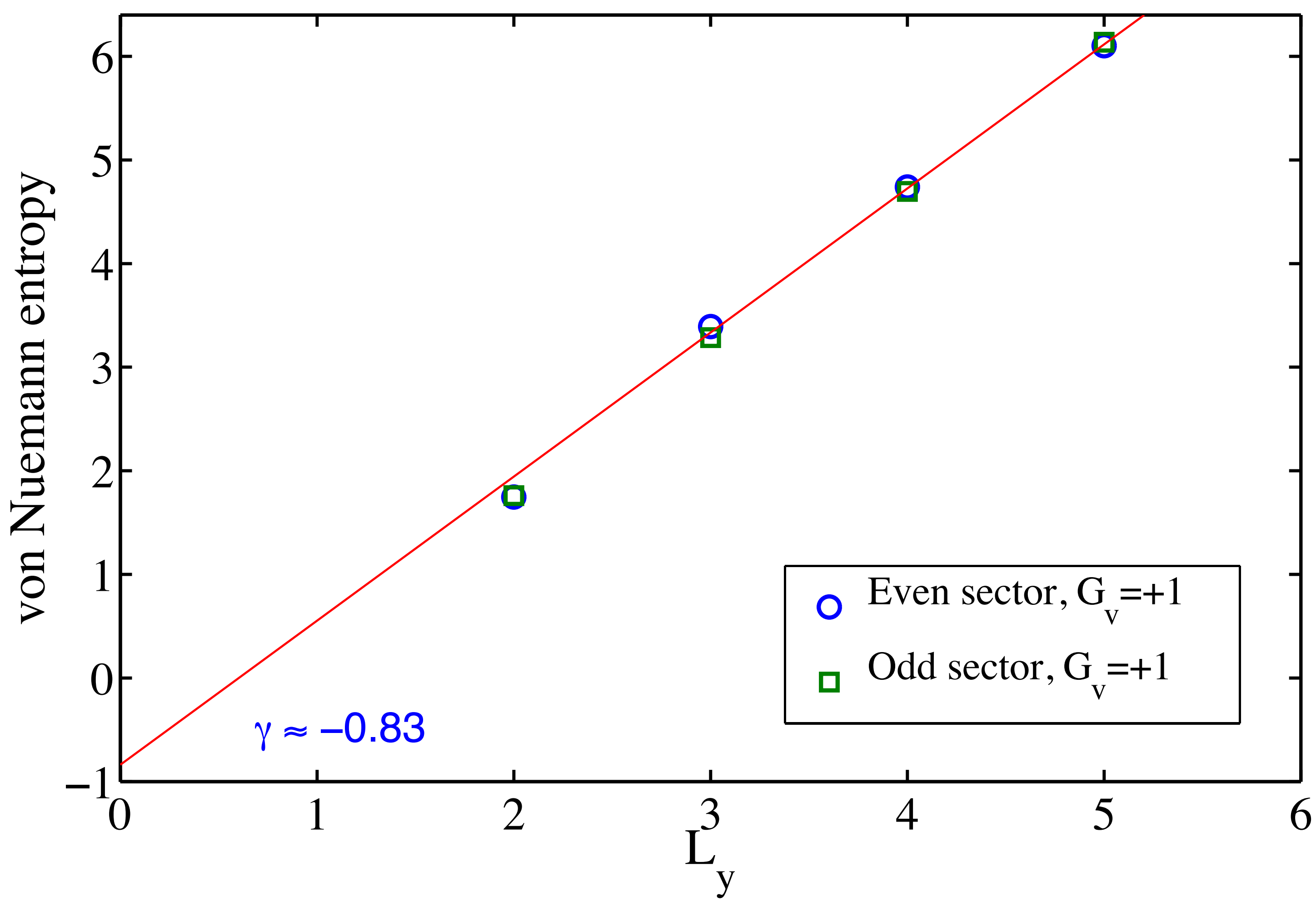
Variational energies of four topological sectors



✎ Four constructed states are degenerate in the thermodynamic limit.

D. Poilblanc, et al, PRB **86**, 014404 (2012)
D. Poilblanc, et al, PRB **87**, 140407 (2013)

Topological Entanglement Entropy



$$S_E = \alpha L - \gamma + \ldots$$

Leading term, proportional to entanglement surface.

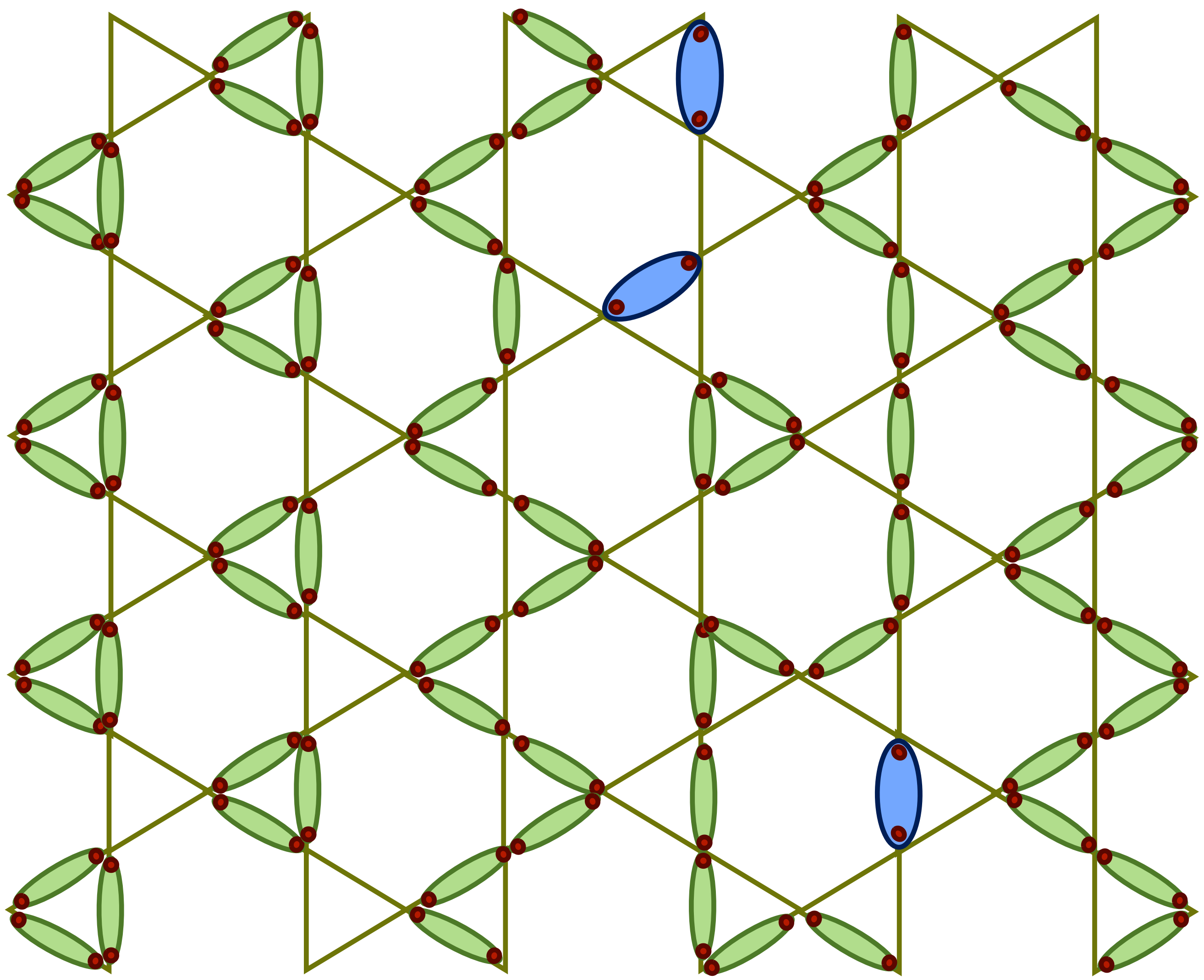
sub-leading term, owing to long range entanglement.

✎ $\gamma \approx \ln(2)$ verifies the existence of $\mathbb{Z}_2$ *topological order.*

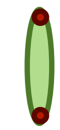
Alexei Kitaev and John Preskill, Phys. Rev. Lett. 96, 11404 (2006).
Michael Levin and Xiao-Gang Wen, Phys. Rev. Lett. 96, 110405 (2006).
Hong-Chen Jiang, ZhenghanWang and Leon Balents, Nat. Phys. **8**, 902 (2012).

The mixed RAL states:

allow spin-1 dimer (L=2 loop) to appear

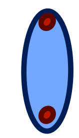


mixed RAL configuration



spin-1/2 dimer

$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$



spin-1 dimer

$|+1,-1\rangle - |0,0\rangle + |-1,+1\rangle$

The mixed RAL state as a PEPS:

bond state for mix RAL

$$|\varepsilon_{mix}\rangle = |0,0\rangle + |1,2\rangle - |2,1\rangle + |4,6\rangle - |5,5\rangle + |6,4\rangle$$

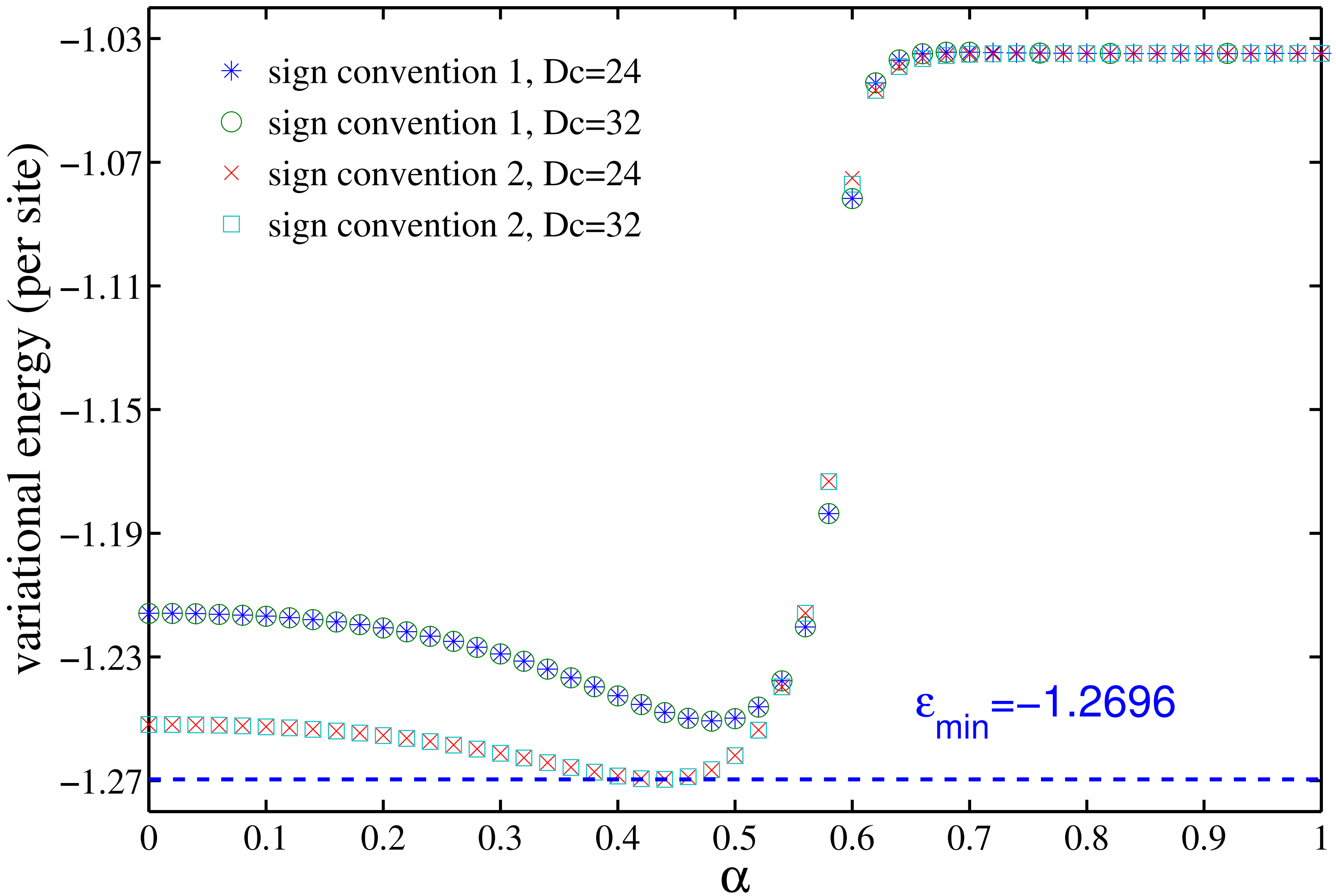
$$P' = (1-\alpha)P + \alpha W, \qquad W = \sum_{l=1}^{4} W_l,$$

$$W_1 = \sum_{m} \sum_{\mu_1\mu_2\mu_3\mu_4} C^m_{\mu_1,0}\delta_{\mu_2,0}\delta_{\mu_3,0}\delta_{\mu_4,0}|m\rangle\langle\mu_1,\mu_2,\mu_3,\mu_4|.$$

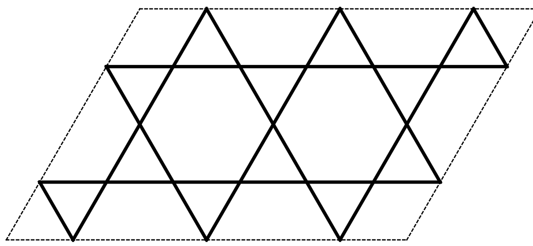
✎ *mRAL state interpolate the RAL and spin-1 RVB states (controlled by parameter α).*

Variational Energies of the RAL states

$$\boxed{H = \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j}$$



✎ By exploring $\boldsymbol{\alpha}$ in the family of RAL states, we provide an upper bound for spin-1 kagome HAF model.



The RAL states: conclusions

✎ Resonating AKLT-loop state: a family of states with natural PEPS representation.

✎ The kagome RAL states have *no magnetic order, no dimer crystal order*, or any other symmetry breaking orders, but they are *topologically ordered*.

✎ The RAL states serve as variational wavefunctions of the spin-1 KAF.

✎ However, the variational energy is still high, Eg = -1.2696.

✎ Tune more parameters in the RAL family ➜ lowest Eg ~-1.38

PEPS simulations of the spin-1 KAF

✎ *Simple update & (double-triangle) cluster update*

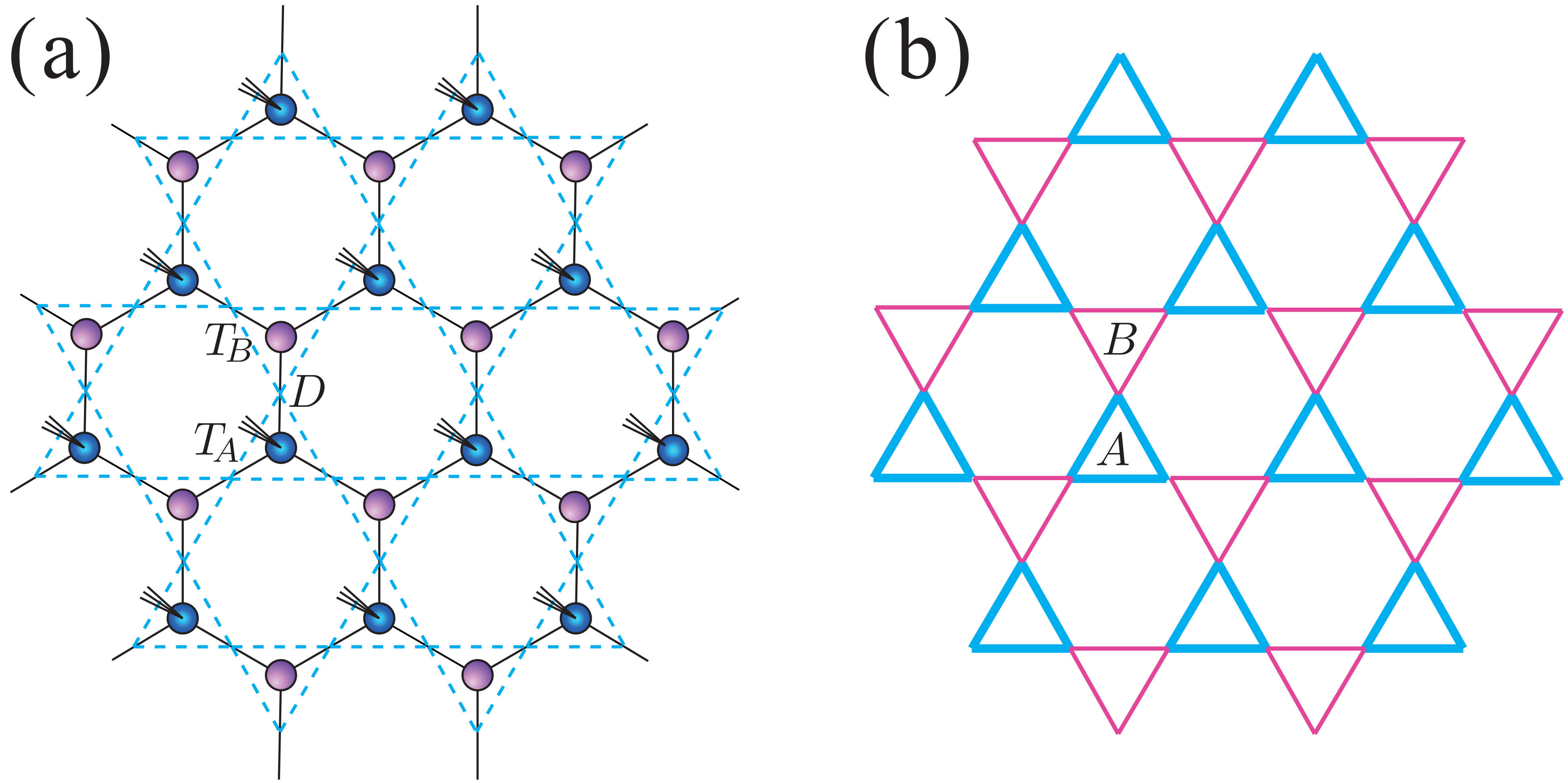
✎ *Non-abelian symmetry in PEPS*

✎ *Ground state properties*

Related paper:

T. Liu, WL, A. Weichselbaum, J. von Delft, and G. Su
Simplex valence-bond crystal in the spin-1 kagome Heisenberg antiferromagnet
arXiv:1406.5905 (2014).

Tensor network states

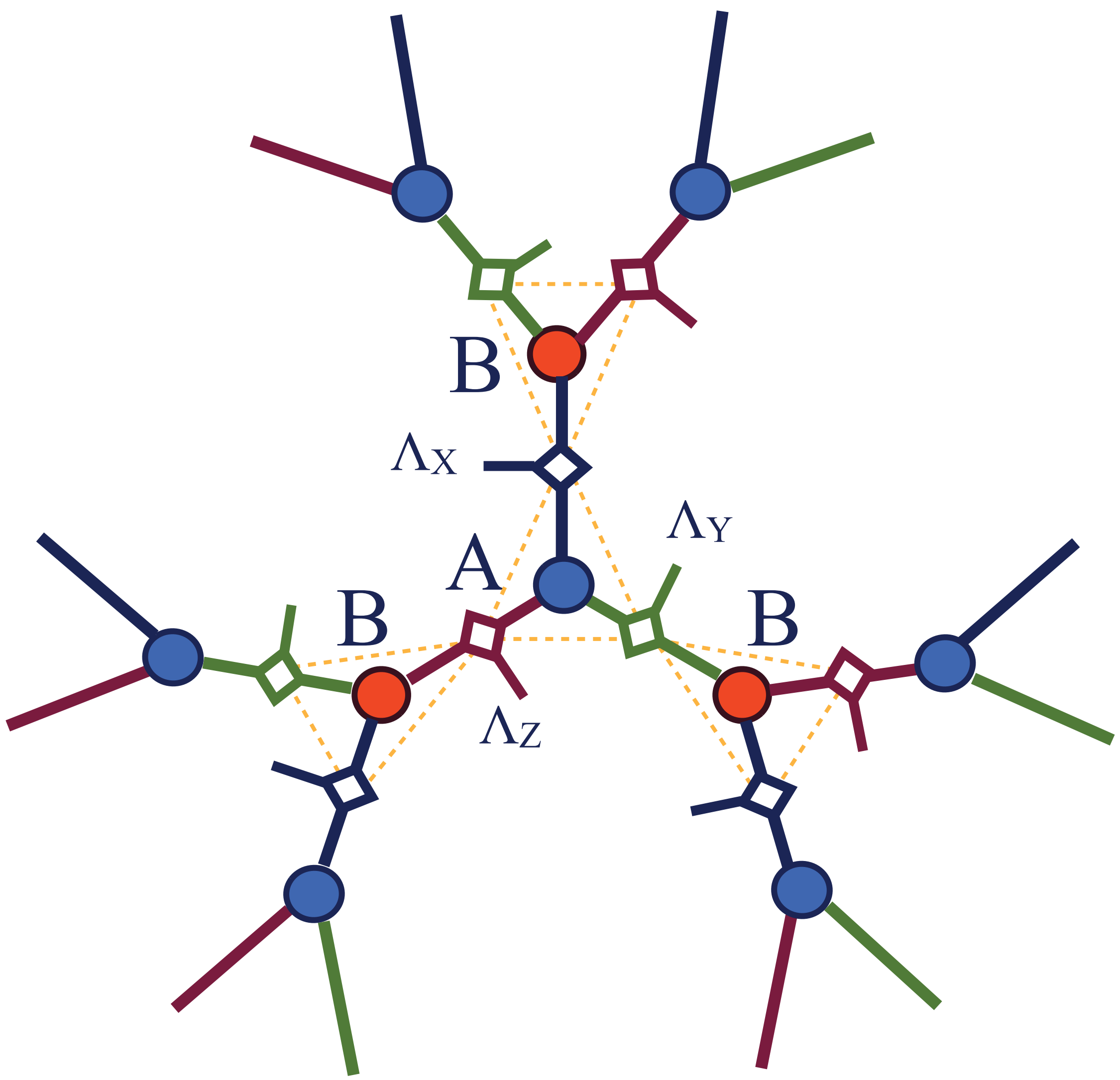


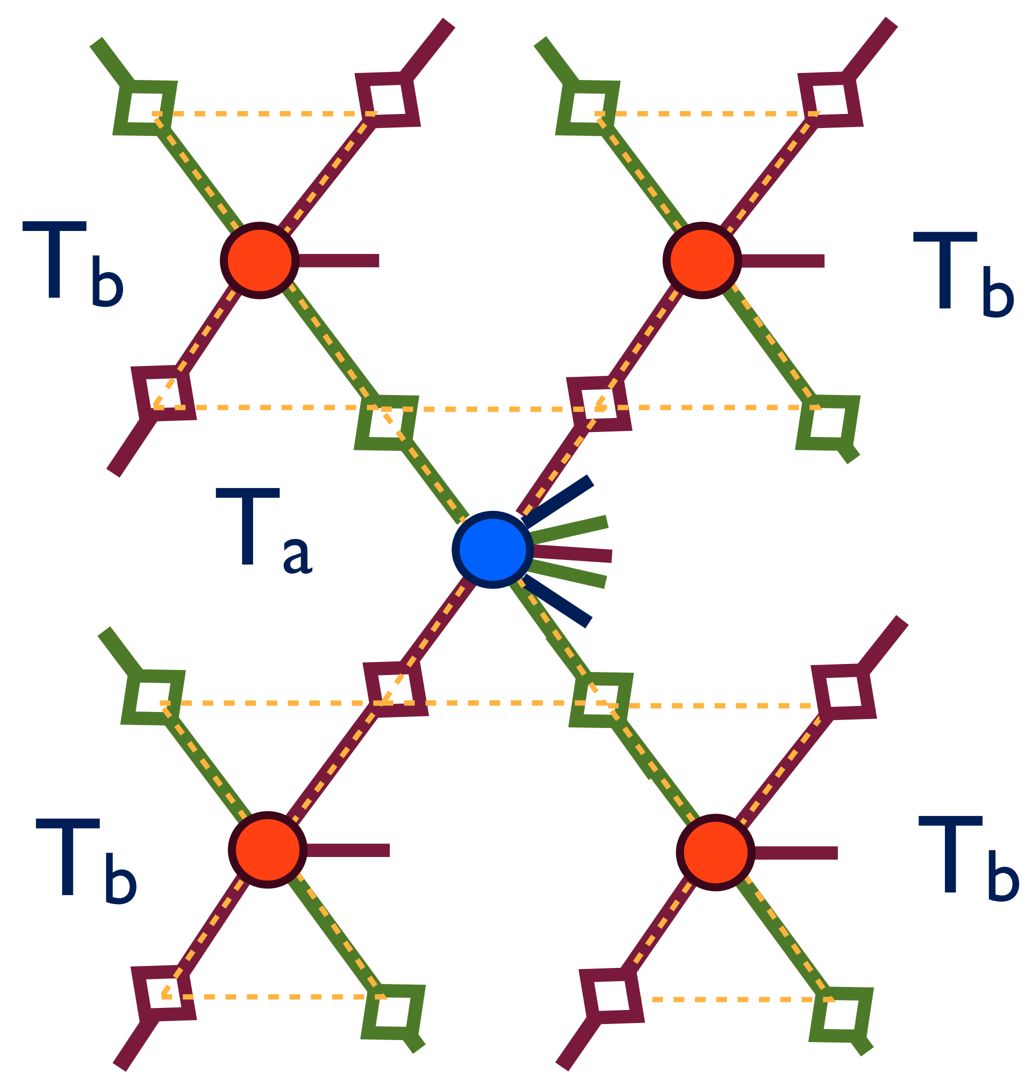
✎ Take the RAL state as a *starting point* of further optimizations.

Update the tensors

✎ Adopt the same tensor-network structure as the RAL state.

✎ Take imaginary time evolution for updating the tensors.

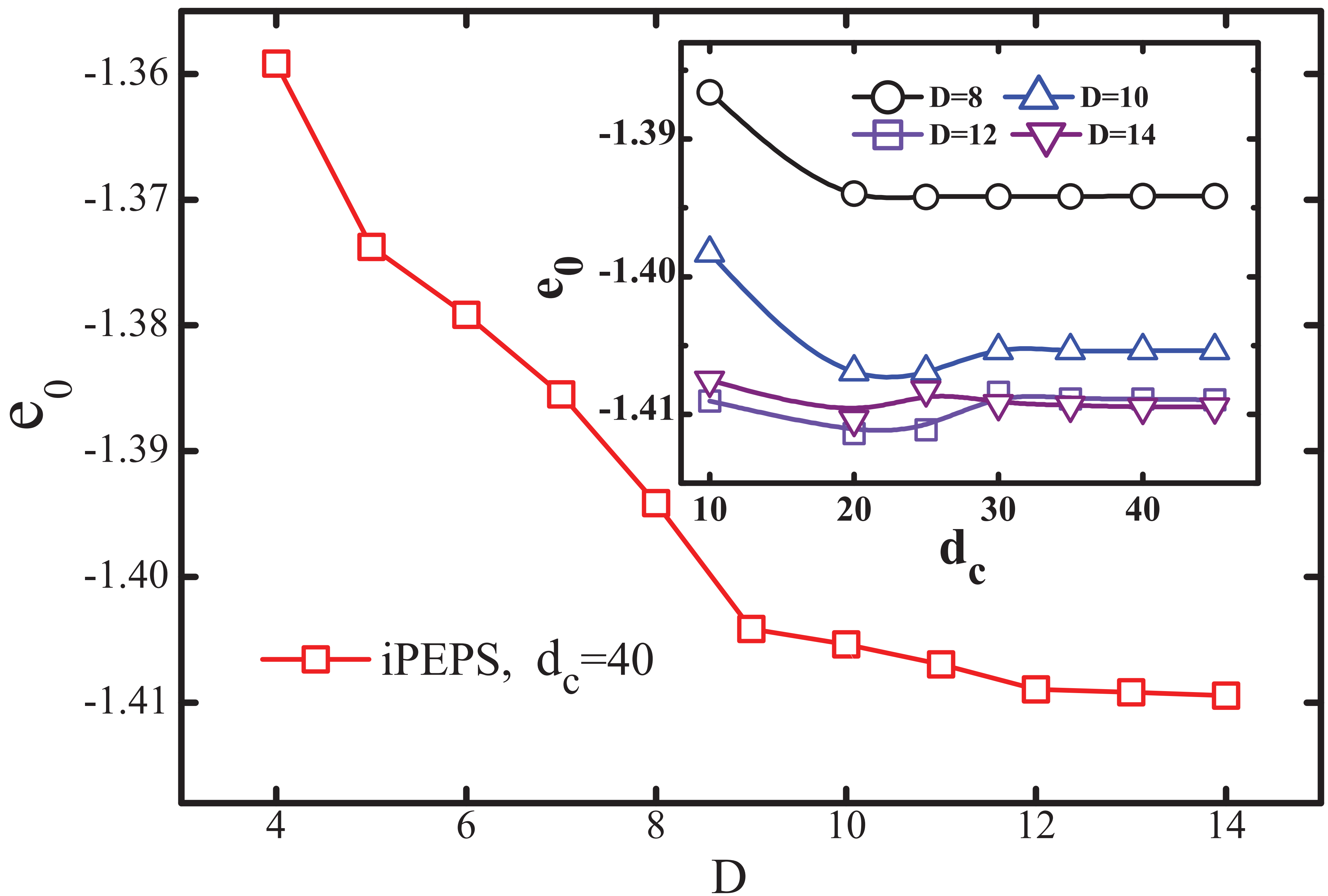




H.-C. Jiang, Z.-Y. Weng, and T. Xiang, PRL, 2008.
WL, J. von Delft, and T. Xiang, PRB, 2012.

Z.-Y. Xie, J. Chen, J.-F. Yu, X. Kong, B. Normand, T. Xiang, PRX, 2014.
T. Liu, S.-J. Ran, WL, X. Yan, Y. Zhao and G. Su, PRB, 2014.

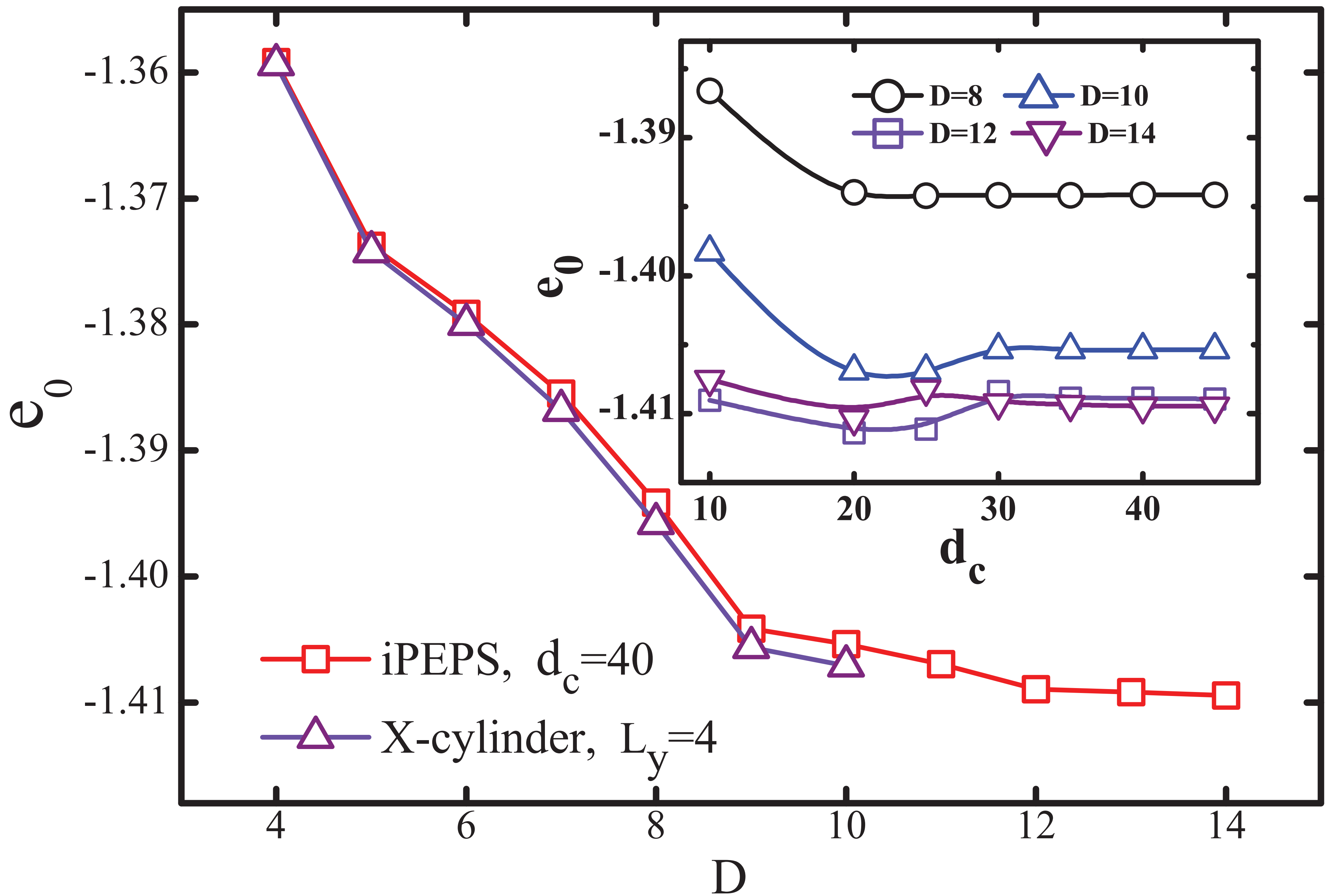
Variational energy (per site)



✎ eg ≃ -1.409 [with D=14, dc=40]

✻ Lower than the CC result [-1.4031, Götze et al. PRB (2012)]

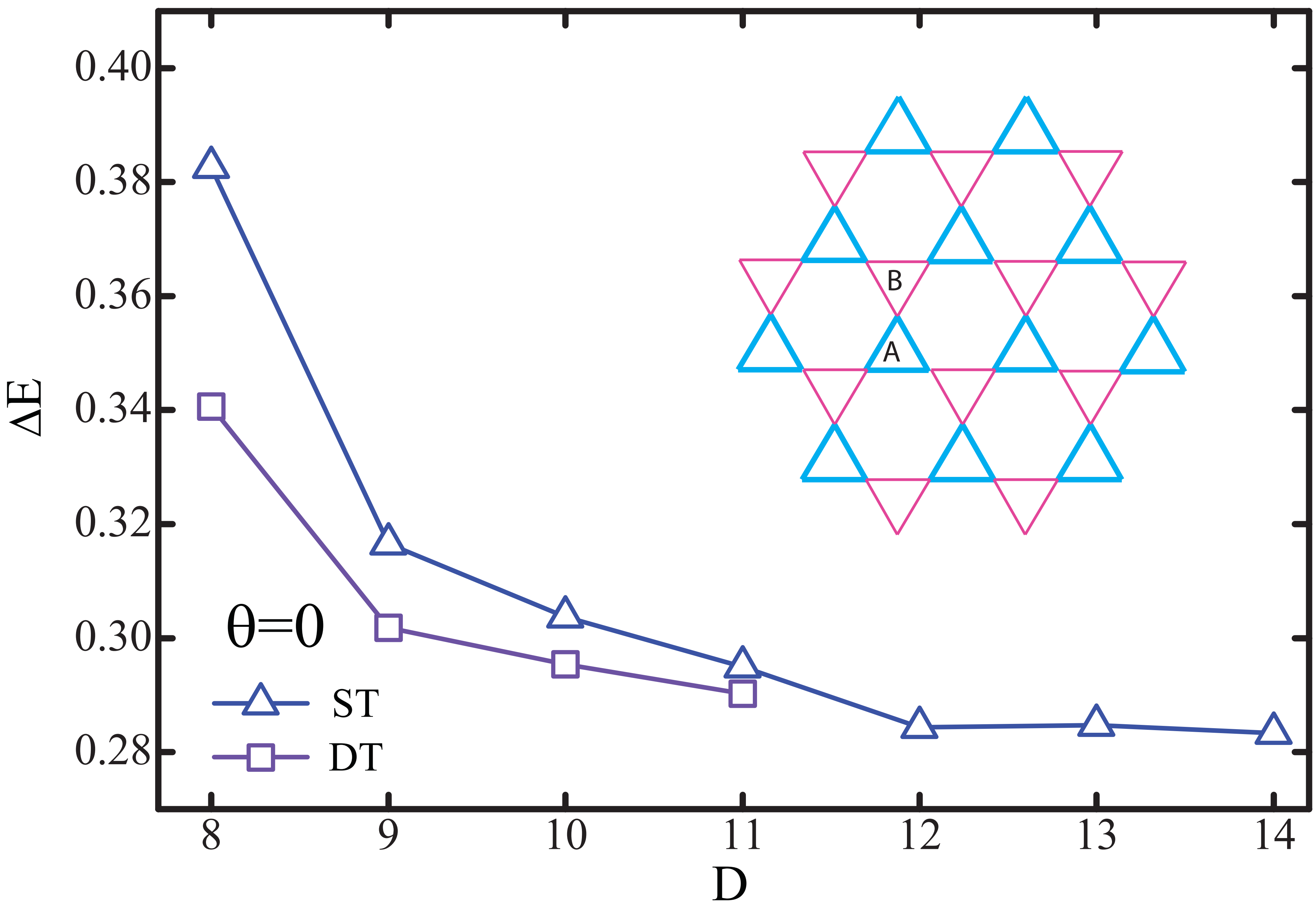
Variational energy (per site)



✎ Roll the wavefunction on a cylinder and perform exact contractions.

❋ Variational energy on cylinder.

Trimerization Order



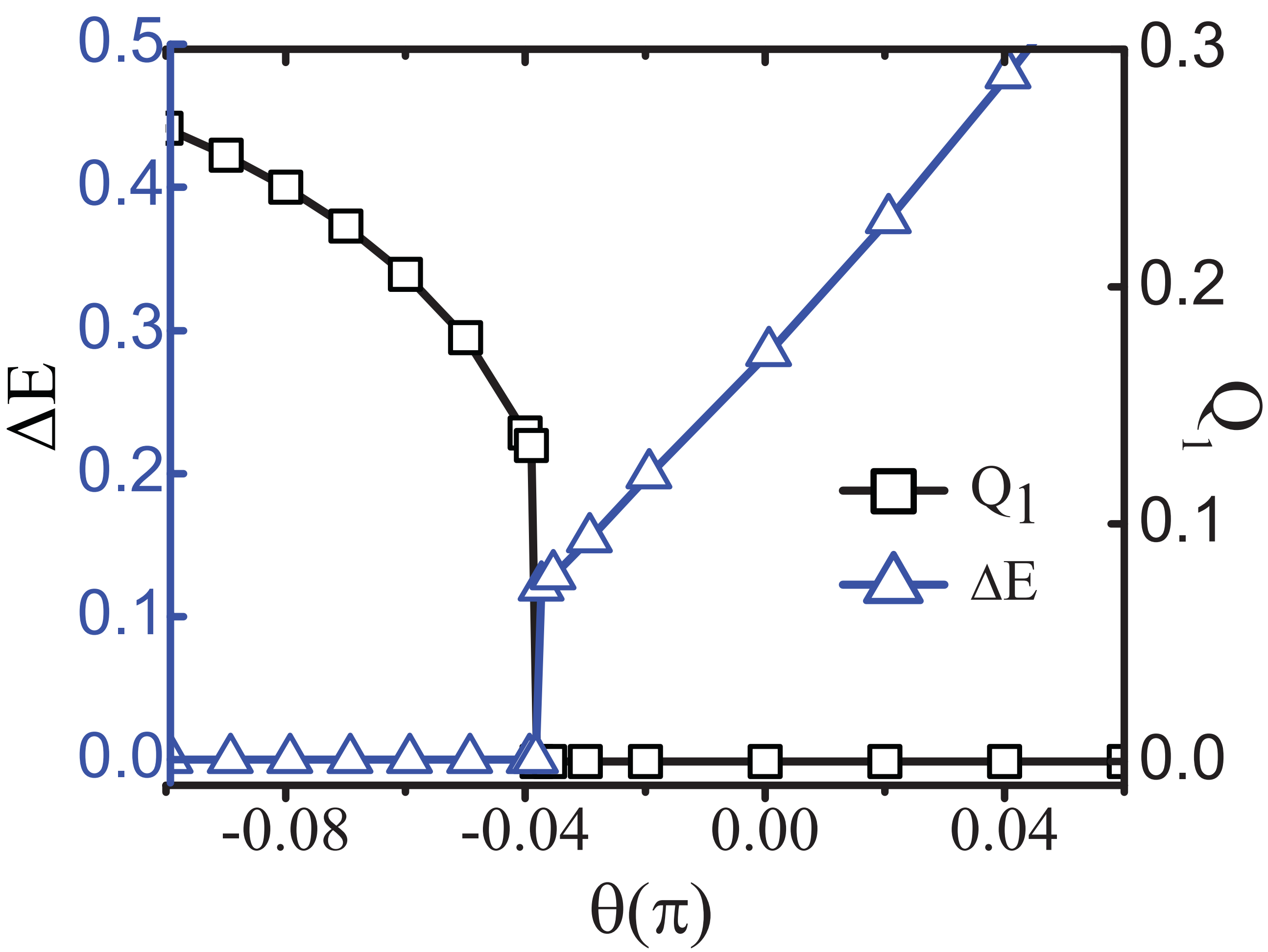
✎ The ground state breaks the lattice symmetry.

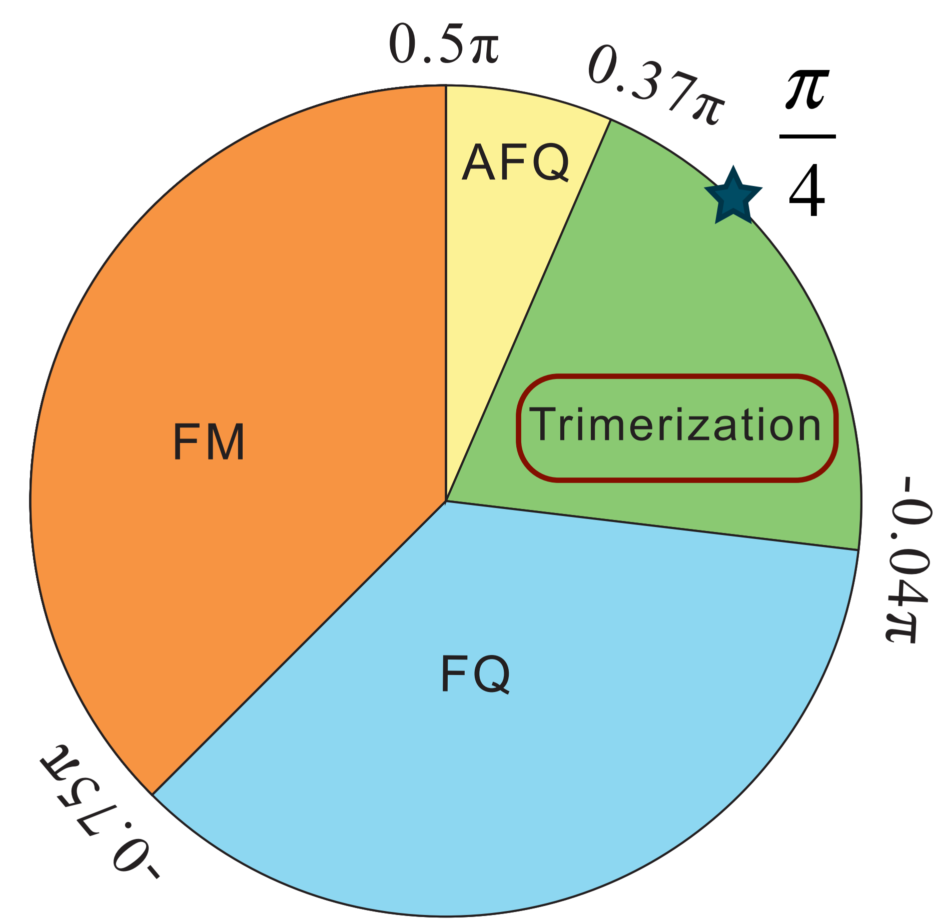
❋ A simplex (triangle) valence bond crystal (SVBC).

The SVBC phase

The bilinear biquadratic model:

$$H = \sum_{<ij>} [\cos\theta\,(\mathbf{S}_i \cdot \mathbf{S}_j) + \sin\theta\,(\mathbf{S}_i \cdot \mathbf{S}_j)^2]$$





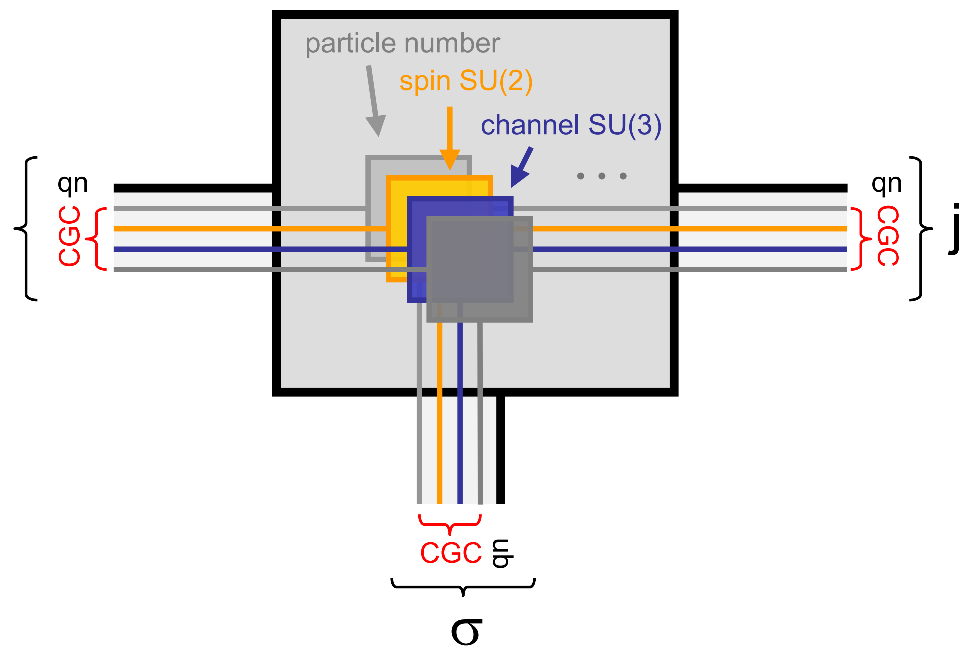
✎ The SVBC order is rather robust, and extends to a phase.

SU(3) point with trimerization order
[P. Corboz, et al, PRB 2012]

QSpace tensor library
& the SU(2) PEPS algorithm

A. Weichselbaum, Annals of Physics 327, 2972 –3047 (2012).

$$A_\nu \otimes \{\mathrm{C}\}_\nu \equiv A_\nu \otimes \Big(\bigotimes_{s=1}^{m} \mathrm{C}_{s;\nu}\Big)$$



Elementary ingredients: (i) state space decomposition:

$$|Q'n';Q'_z\rangle = \sum_{Qn;Q_z} \sum_{\tilde{Q}\tilde{n};\tilde{Q}_z} (A^{[\tilde{Q}]}_{QQ'})^{[\tilde{n}]}_{nn'} \cdot C^{[\tilde{Q}_z]}_{Q_zQ'_z} \, |Qn;Q_z\rangle|\tilde{Q}\tilde{n};\tilde{Q}_z\rangle$$

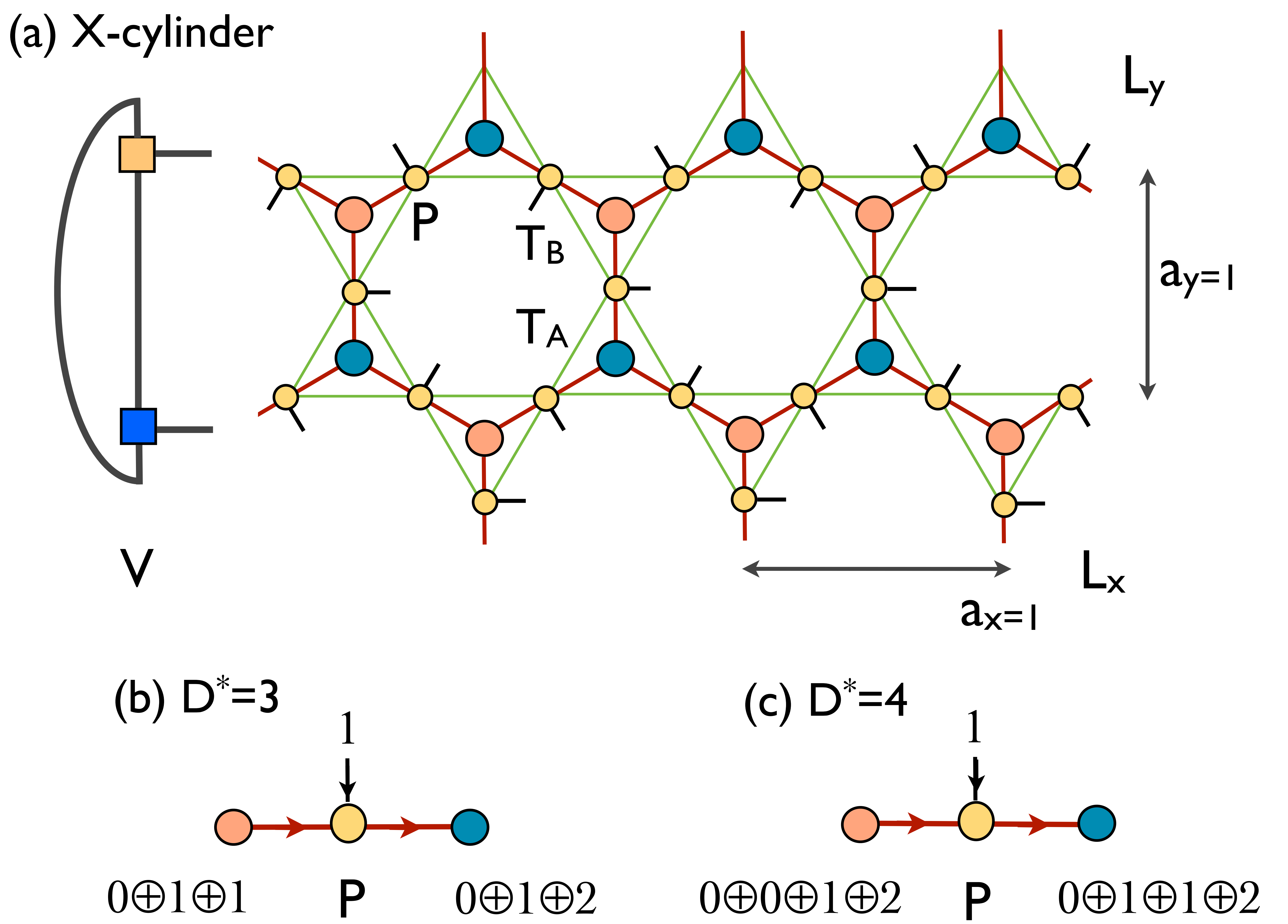
(ii) operator representation (cf. Wigner-Eckart theorem):

$$\langle Q'n';Q'_z|\hat{F}^{\tilde{Q}}_{\tilde{Q}_z}|Qn;Q_z\rangle = (F^{[\tilde{Q}]}_{QQ'})^{[1]}_{nn'} \cdot C^{[\tilde{Q}_z]}_{Q_zQ'_z},$$

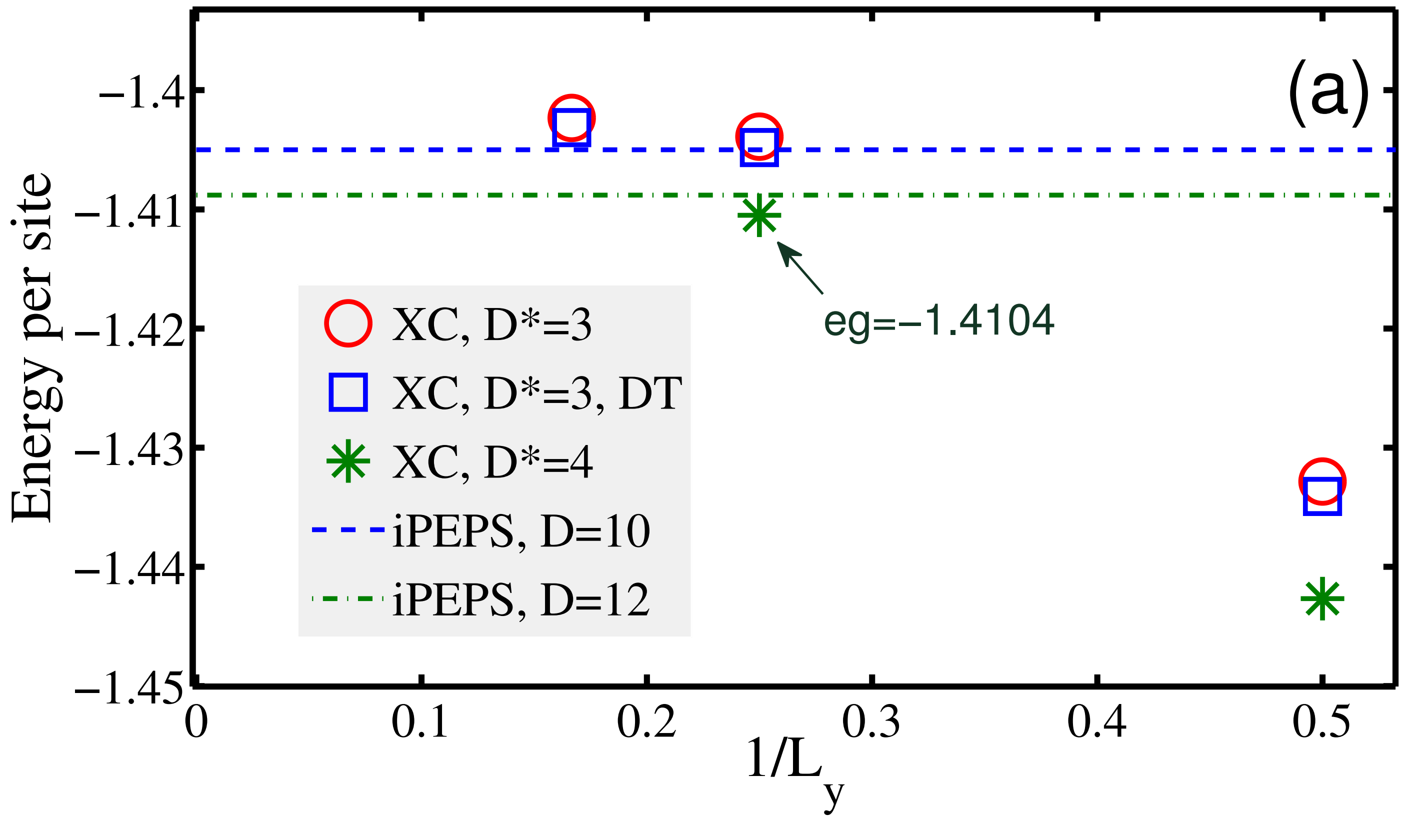
The *benefits* of using SU(2)$_{\text{spin}}$ symmetric tensors:

✎ A clearly *more efficient* numerical simulation [the numerical cost of PEPS on a 2D lattice scales like O(D$^{10\sim12}$)!]

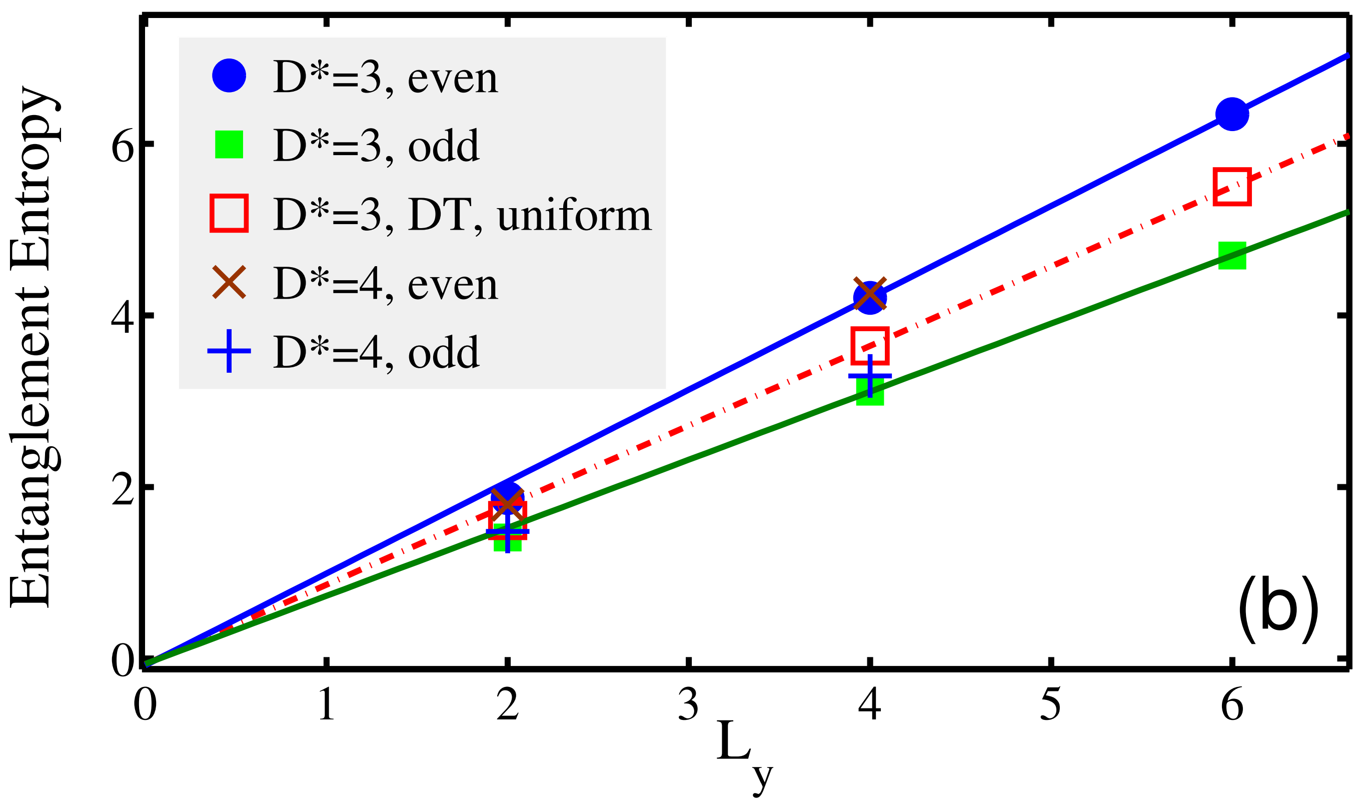
✎ Detailed information also about the *multiplet structure* along the bonds, obtained variationally through update methods.


(a) X-cylinder
V
P
T_B
T_A
L_y
$a_{y=1}$
L_x
$a_{x=1}$
(b) $D^*=3$
1
$0\oplus1\oplus1$
P
$0\oplus1\oplus2$
(c) $D^*=4$
1
$0\oplus0\oplus1\oplus2$
P
$0\oplus1\oplus1\oplus2$

Energy & Entanglement on cylinders



In agreement with previous PEPS calculation without symmetry implementation.



$\gamma \approx 0$ suggests a topologically trivial state.

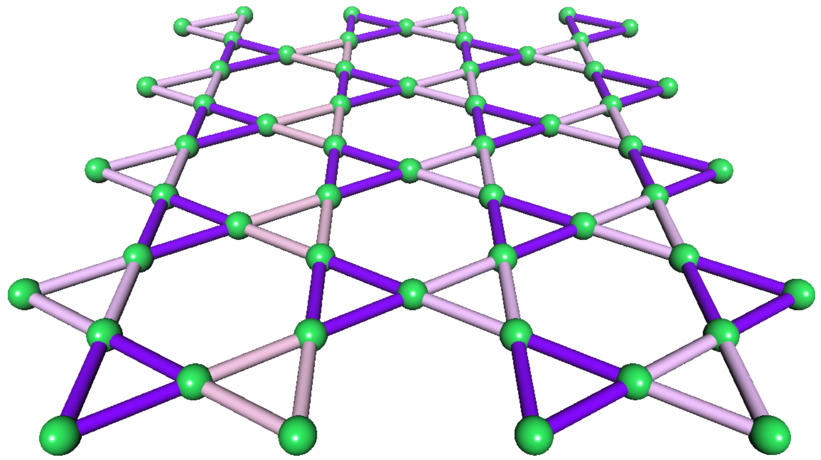
Conclusions

- We employ the tensor network algorithm (with/without SU2 symmetry) to perform a variational study of the spin-1 KAF model.

  ☀ 1st (?) example that SU2 symmetry pays off in PEPS calculations.

  Just in its beginning!

- The ground state has a simplex valence-bond crystal order, with GS energy determined as Eg ≃ -1.409.



☀ SVBC picture is consistent with experimental observations: ***gapped***, ***non-magnetic***, & ***symmetry breaking*** *low-T phase*

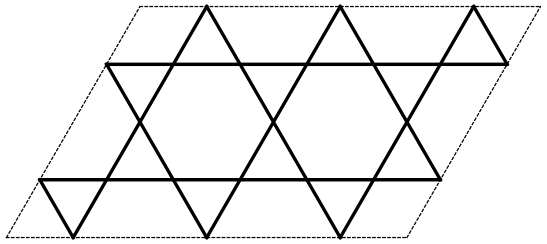
Collaborators of the RAL project

Shuo Yang
MPQ, Germany
moving to PI, Canada

Hong-Hao Tu
MPQ, Germany

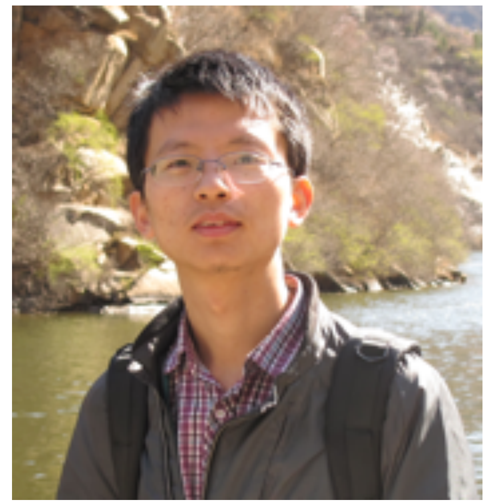
Zheng-Xin Liu
Tsinghua

Meng Cheng
Station-Q, US



spin-1 kagome numerical project

University of Chinese Academy of Sciences, Beijing, China



Tao Liu

Gang Su

LMU Munich, Germany

Andreas Weichselbaum

Jan von Delft

Thanks for your attention!