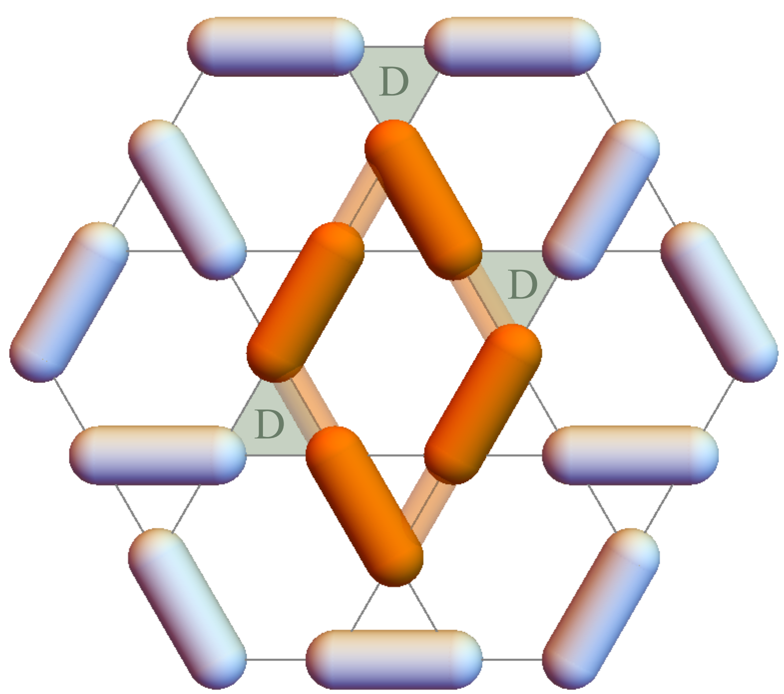
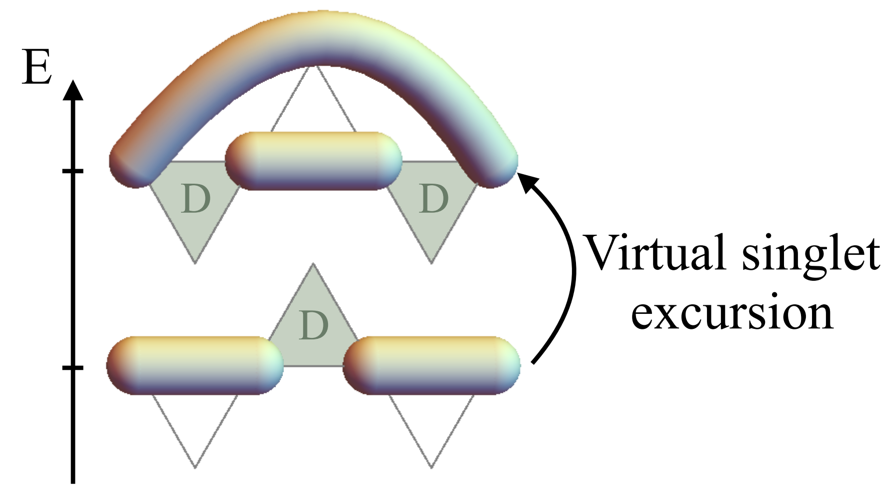
Importance of virtual singlets in RVB theory of Quantum spin Liquids





$$= \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

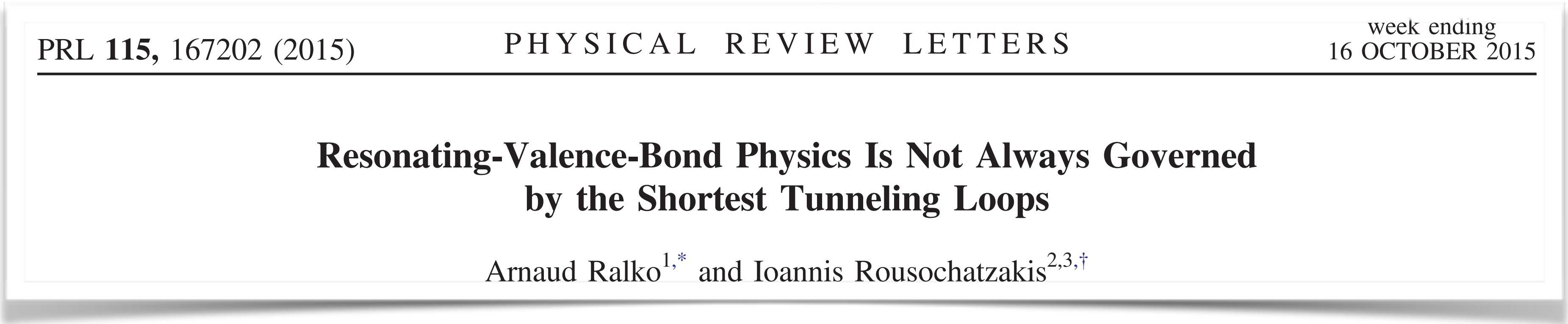
Ioannis Rousochatzakis (Minnesota)

Frédéric Mila (EPFL)

Arnaud **Ralko**, Néel Institute

13 July 2018, UC Davis

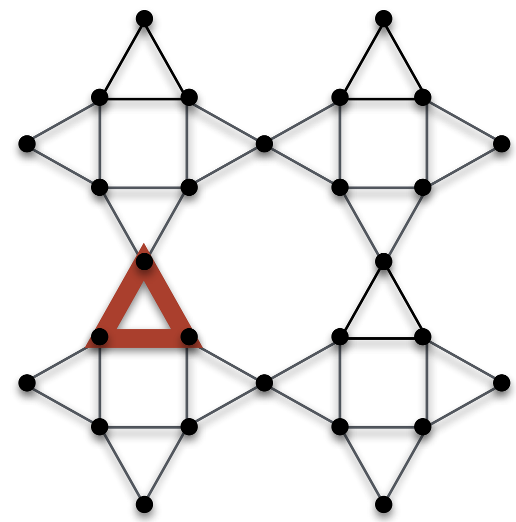
Outline


PRL **115,** 167202 (2015) PHYSICAL REVIEW LETTERS week ending 16 OCTOBER 2015

Resonating-Valence-Bond Physics Is Not Always Governed by the Shortest Tunneling Loops

Arnaud Ralko[1,*] and Ioannis Rousochatzakis[2,3,†]

squa-kagome



unknown singlet phase

Rousochatzakis *et al.* (13)

ED: low-E **singlets**

Richter *et al.* (04, 09)

Siddhartan & Georges (01)

☞ non locality is a key element

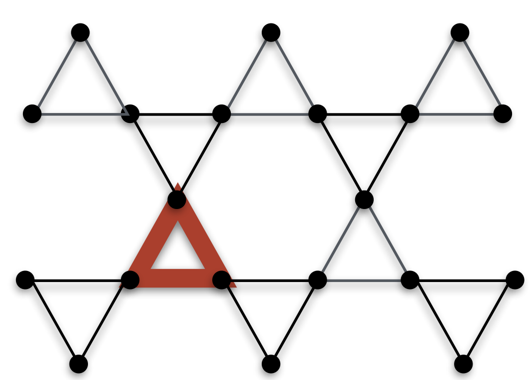
☞ reconcile ED results


PHYSICAL REVIEW B **97**, 104401 (2018)

Microscopic theory of the nearest-neighbor valence bond sector of the spin-$\frac{1}{2}$ kagome antiferromagnet

Arnaud Ralko,[1,*] Frédéric Mila,[2,†] and Ioannis Rousochatzakis[3,‡]

kagome



no magnetic order

Yann *et al.* (11)

ED: low-E **singlets**

Lecheminant *et al.* (94)

☞ microscopic insights

☞ agreement with DMRG

☞ corner-sharing lattices have the **strongest** RVB picture

The Resonating Valence Bond Theory

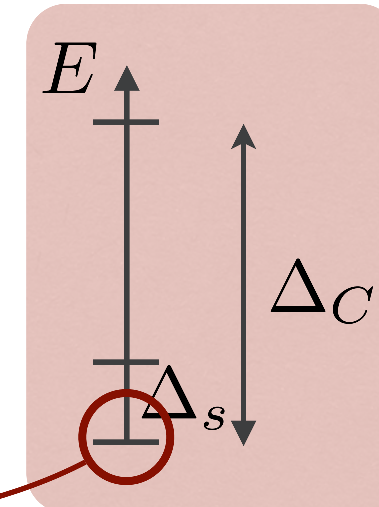
where the disordered magnetic states come from?

Shastry & Sutherland (81)

$$\langle S_i \cdot S_j \rangle \simeq e^{-\frac{|r_i - r_j|}{\xi}}$$

$$\Delta_S = \frac{|r_i - r_j|}{\xi/a}$$

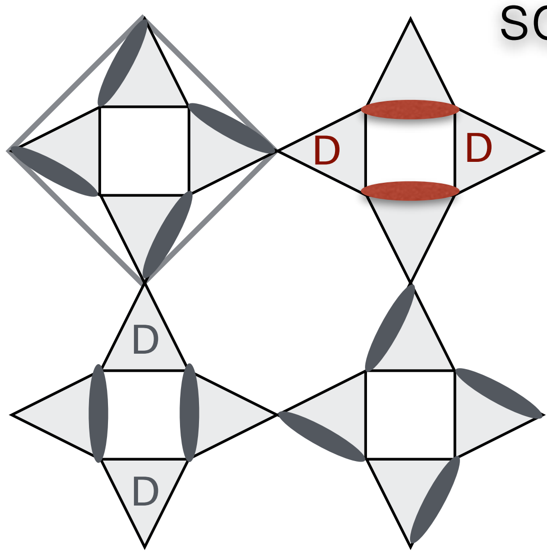
- even at T=0K
- SU(2) is protected
- S=0 singlet coverings!



all spins paired as singlets $= \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$

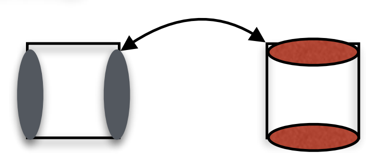
- **N**earest **N**eighbor **V**alence **B**ond coverings

squa-kagome

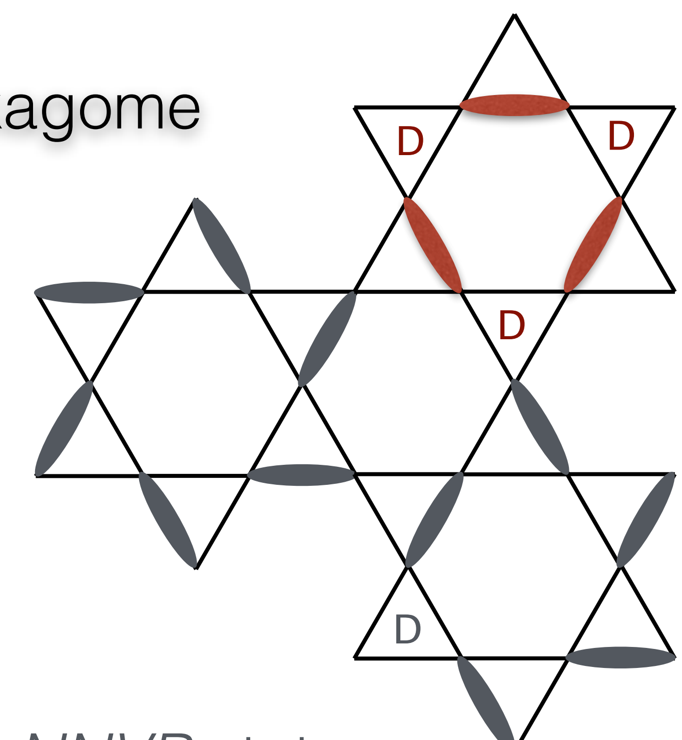


AR & Rousochatzakis (15)

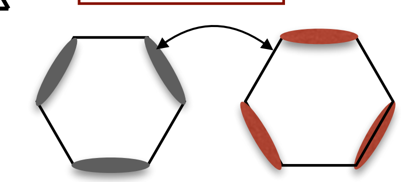
loop 4



kagome



loop 6



# of defect triangles = 1/4 for all *NNVB* states

where the disordered magnetic states come from?

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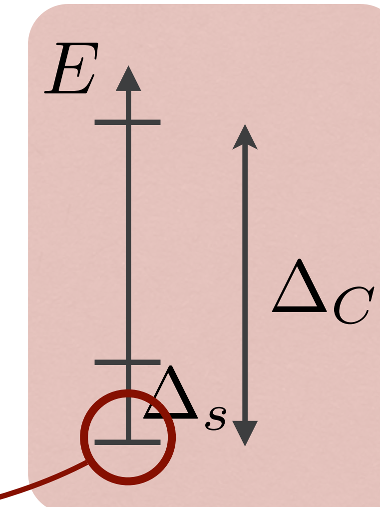
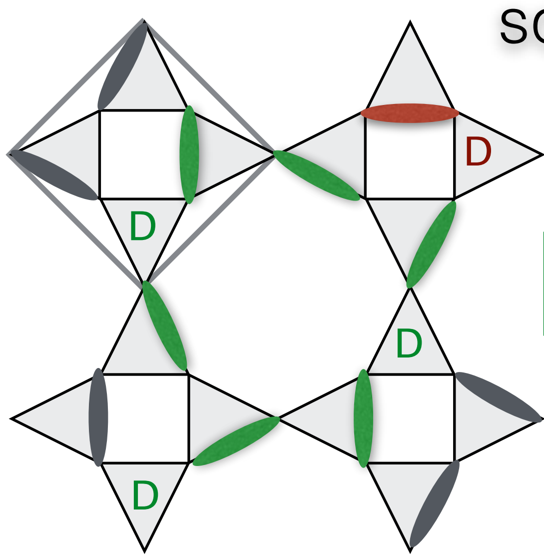


all spins paired as singlets $= \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$

- **N**earest **N**eighbor **V**alence **B**ond coverings

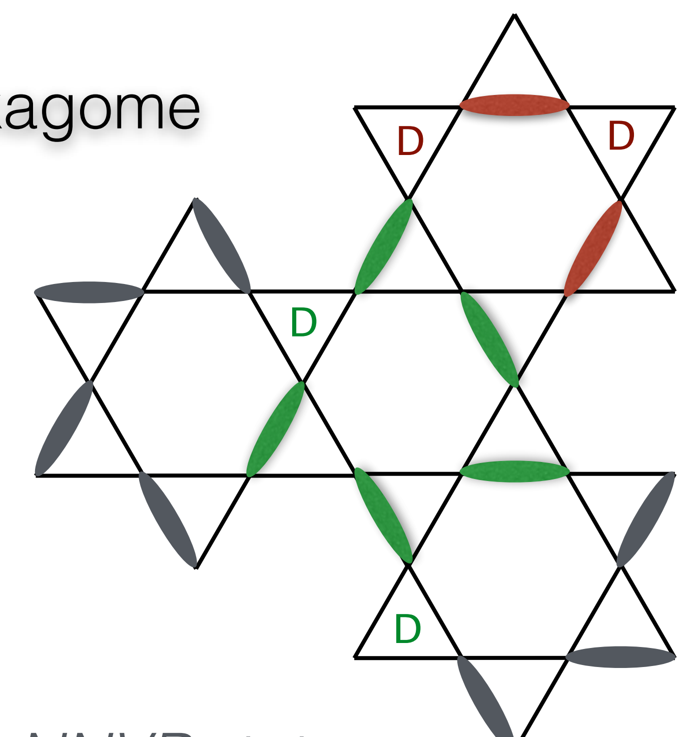
squa-kagome



loop 12

AR & Rousochatzakis (15)

kagome



loop 10

\# of defect triangles = 1/4 for all *NNVB* states

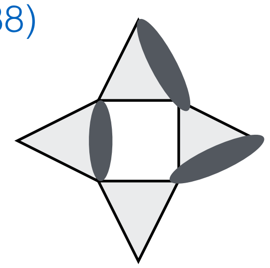
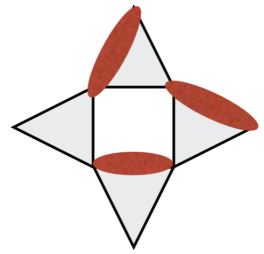
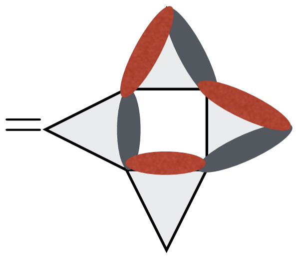
- non-trivial dynamics comes from the defect triangles
- need of a systematic procedure to extract effective model

casting the RVB idea into hamiltonian

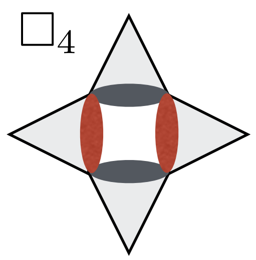
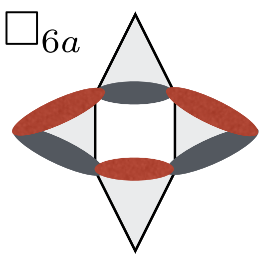
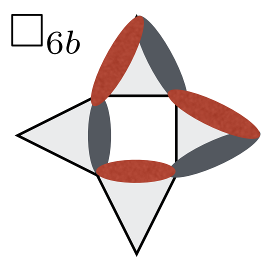
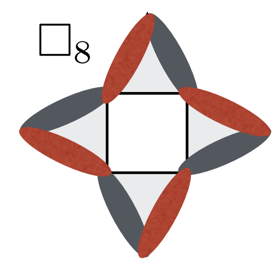
the NNVB description

- analytical expression of the transition graph made of loops

Sutherland (88)

$|1_p\rangle =$  $|2_p\rangle =$  $\omega_p = \langle 1_p | 2_p \rangle =$  $= (-1)^{\frac{L_p}{2}} 2^{1-\frac{L_p}{2}}$

non-orthogonality ⇒ **exponential decaying**

$\square_4$  $\square_{6a}$  $\square_{6b}$  $\square_8$  + 18 **octagon** processes

- explicit calculation of the hamiltonian for each NNVB process p **AR** & Rousochatzakis (15)

$$\mathcal{H}_{\mathrm{eff}} = \mathcal{O}^{-\frac{1}{2}} \mathcal{H}_{\mathrm{Heis}} \mathcal{O}^{+\frac{1}{2}}$$

$$\begin{aligned} \omega_p &= \langle 1_p | 2_p \rangle \\ o_p &= \langle 1_p | \mathcal{H}_{\mathrm{Heis}} | 2_p \rangle \\ d_p &= \langle 1_p | \mathcal{H}_{\mathrm{Heis}} | 1_p \rangle = \langle 2_p | \mathcal{H}_{\mathrm{Heis}} | 2_p \rangle \end{aligned}$$

$$\mathcal{H}^p_{\mathrm{NNVB}} = \begin{pmatrix} 1 & \omega_p \\ \omega_p & 1 \end{pmatrix}^{-\frac{1}{2}} \begin{pmatrix} d_p & o_p \\ o_p & d_p \end{pmatrix} \begin{pmatrix} 1 & \omega_p \\ \omega_p & 1 \end{pmatrix}^{\frac{1}{2}} = \begin{pmatrix} V_p & t_p \\ t_p & V_p \end{pmatrix}$$

⇒ identical to infinite-order diagram expansion **AR** *et al.* (09), Schwandt *et al.* (10)

the NNVB description

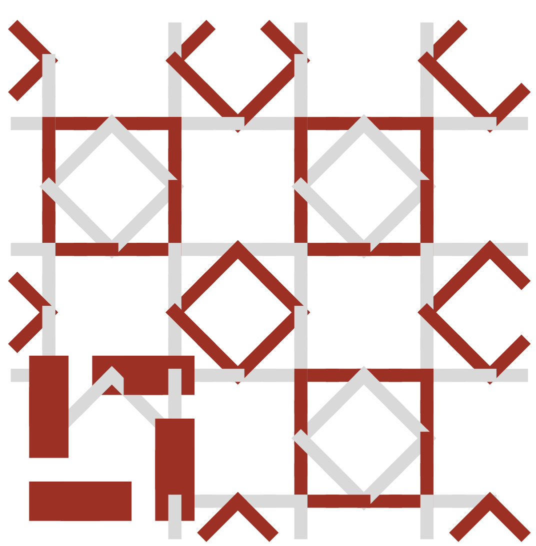
$$\mathcal{H}_{\mathrm{NNVB}} = \sum_p t_p \left(|1_p\rangle\langle 2_p| + h.c. \right) + V_p \left(|1_p\rangle\langle 1_p| + |2_p\rangle\langle 2_p| \right)$$

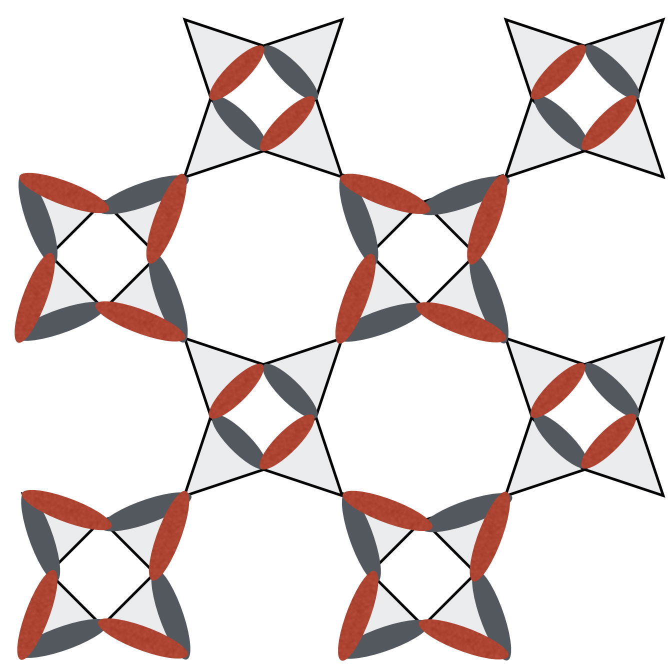
void plaquette	process	t_p	V_p
AA-square	$\square_4$	-1	$+\frac{1}{2}$
	$\square_{6a,b}$	$+\frac{1}{5}$	$+\frac{1}{20}$
	$\square_8$	0	0

$|t_4| = 1 \gg |t_6| = 0.2$ x5 larger !

$\Rightarrow$ physics dominated by the shortest loop

- connected dimer-dimer correlations by ED up to 48 sites





pinwheel state

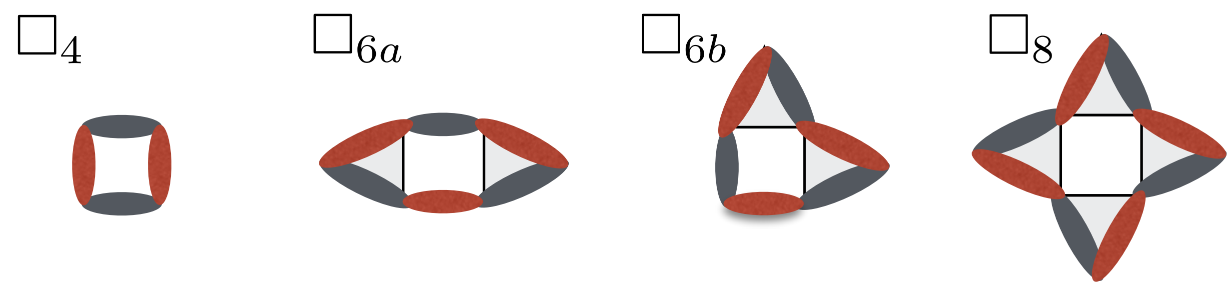
$\Rightarrow$ not compatible with SU(2) model

RVB description cannot be local

from NNVB to cluster approach

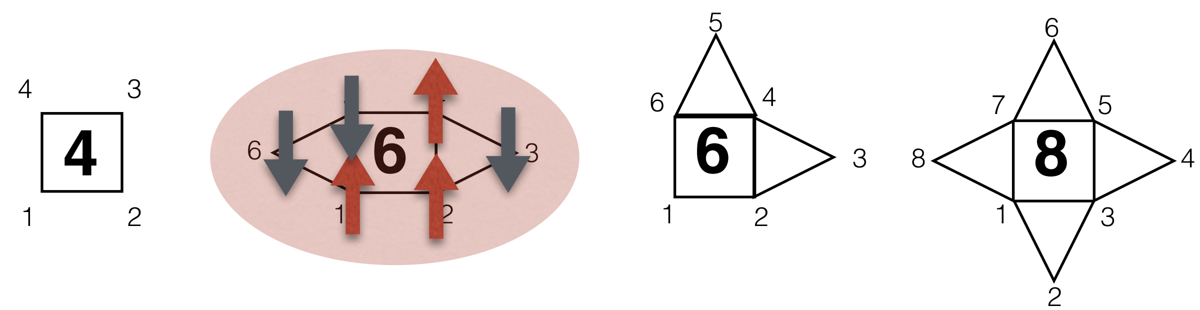
AR & Rousochatzakis (15)

- take small clusters compatible with each process

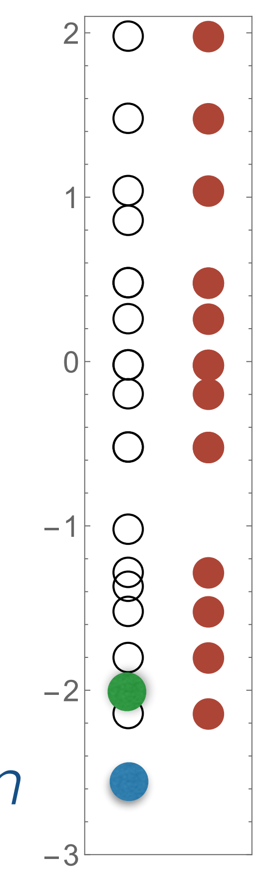


+ octagons

- clusters:

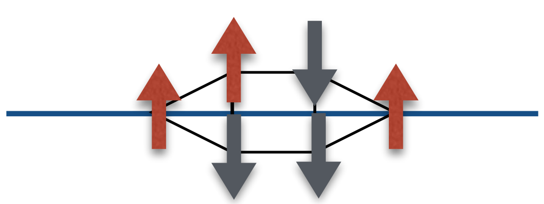


spectrum

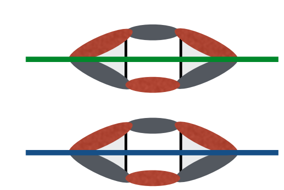


Sz=0 1

- diagonalize the **spin 1/2 Heisenberg** model

x=1  GS in the S = 0 sector

- reflection symmetry ⇒ splitting ***even*** / ***odd*** of the loop



odd

even

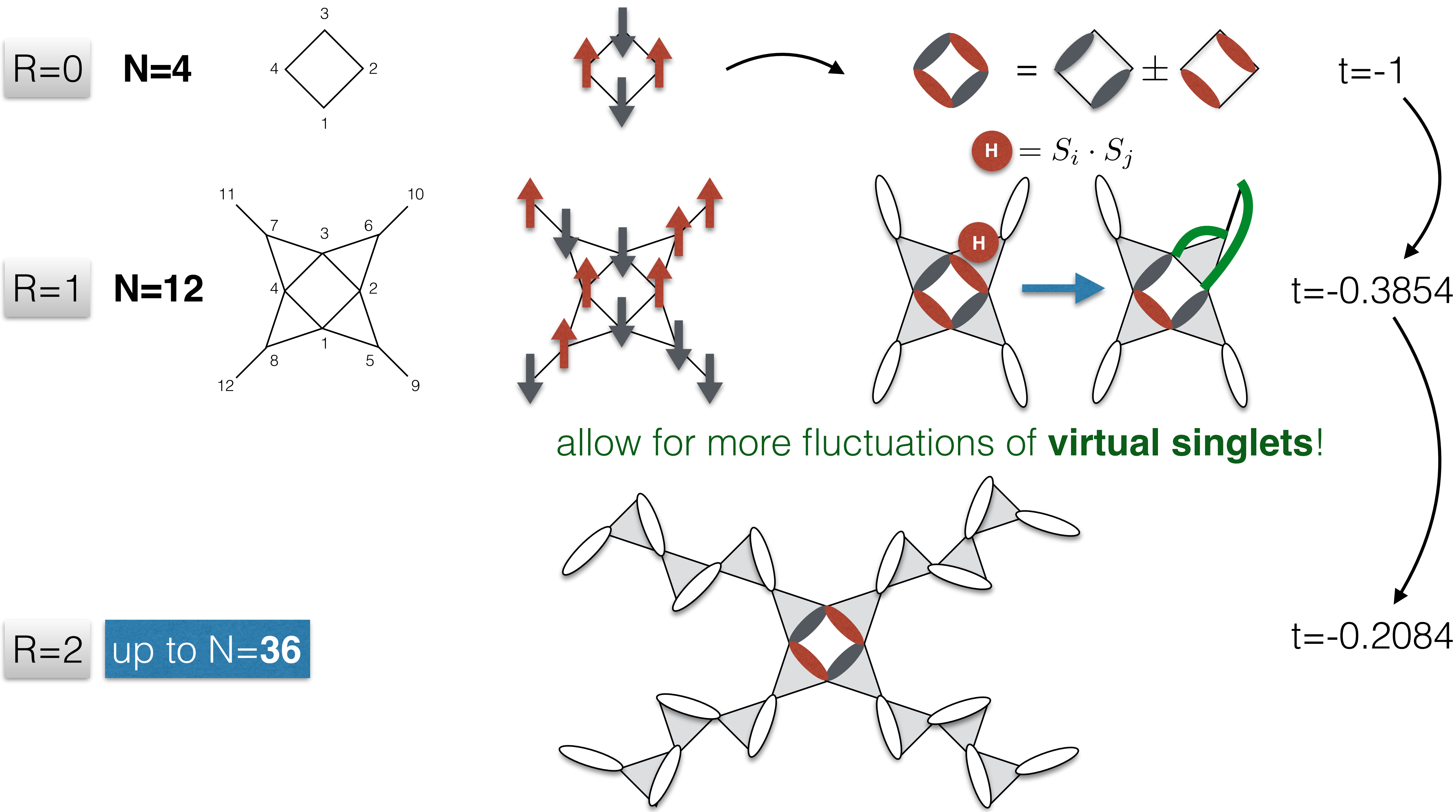
- extract the tunnelling amplitude

$$t_p = \frac{E_{\text{odd}} - E_{\text{even}}}{2}$$

role of virtual singlets

AR & Rousochatzakis (15)

- enlarging the cluster size (R) allows for virtual long-range singlet fluctuations



- sawtooth construction until convergence

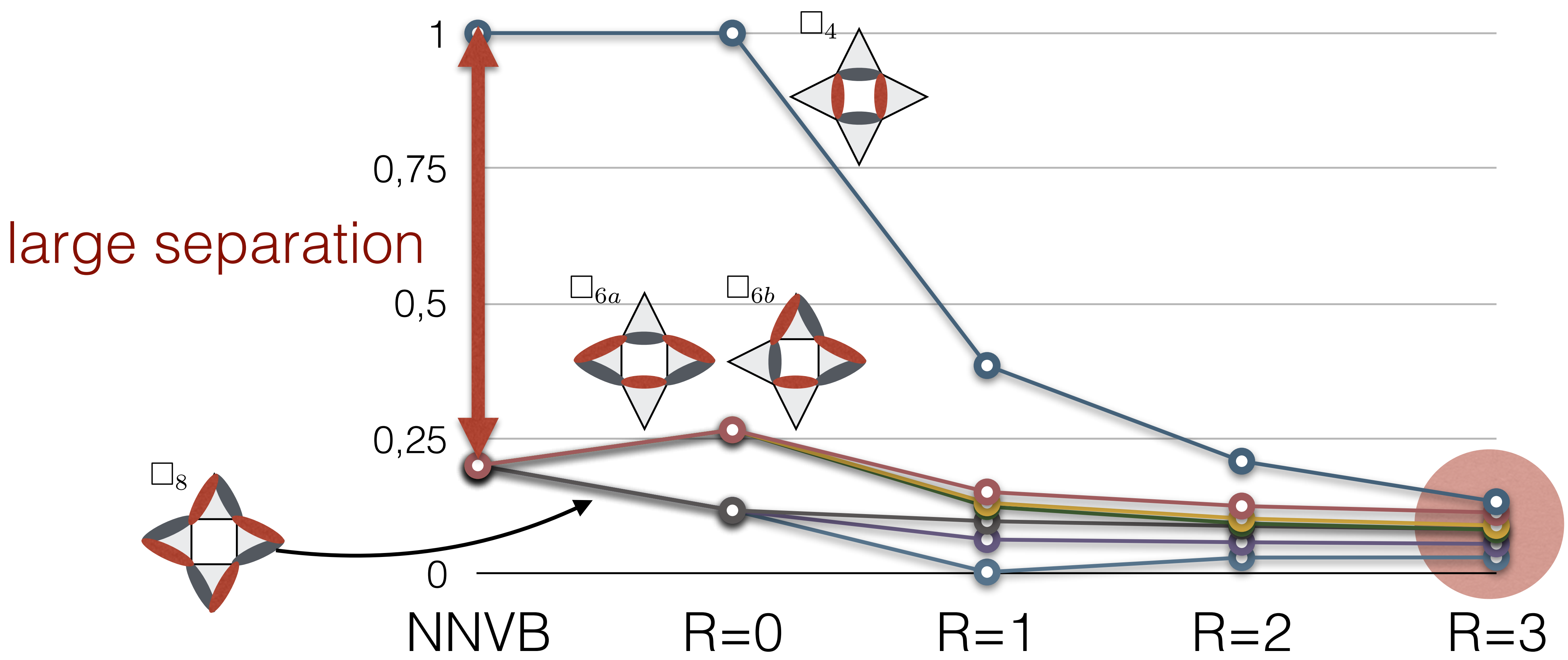
Hao & Tchernyshyov (09), Rousochatzakis *et al.* (14)

huge reduction of ~80%!!!

virtual singlet description

AR & Rousochatzakis (15)

- evolution of the extracted parameters by increasing the minimal cluster sizes
- allow for excursion of excitations out of the target space
- quick convergence, huge effect on smallest loops



RVB physics **not** always controlled by the shortest loops

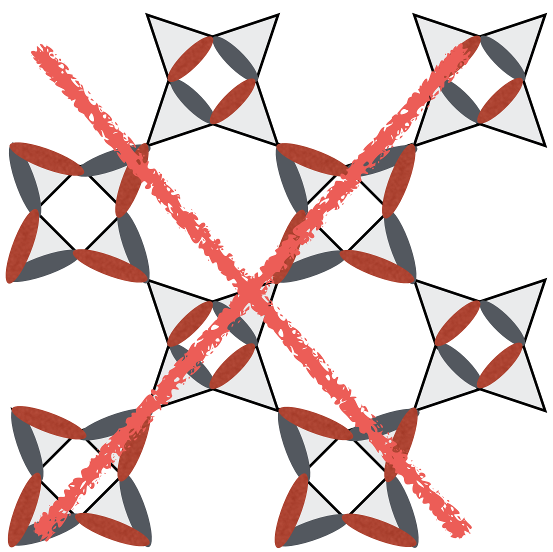
virtual singlet description

AR & Rousochatzakis (15)

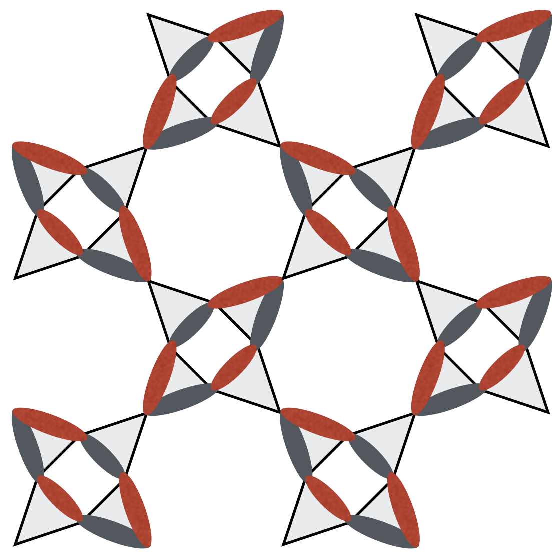
$$\mathcal{H}_{\mathrm{QDM}} = \sum_{\ell,e} t_\ell^e (|1_\ell^e\rangle\langle 2_\ell^e| + \mathrm{h.c.}) + V_\ell^e (|1_\ell^e\rangle\langle 1_\ell^e| + |2_\ell^e\rangle\langle 2_\ell^e|)$$

each process now depends on the environment

- real-space dimer-dimer correlations



NNVB



virtual singlets

- complete change of the properties!
- unexpected resonating loop-6 VBC
- compatible with the SU(2) results!

Rousochatzakis *et al.* (13)

⇒ the virtual singlets drastically change the physical picture

☞ non-locality is a key element

☞ controlled procedure

☞ applicable to a large class of systems

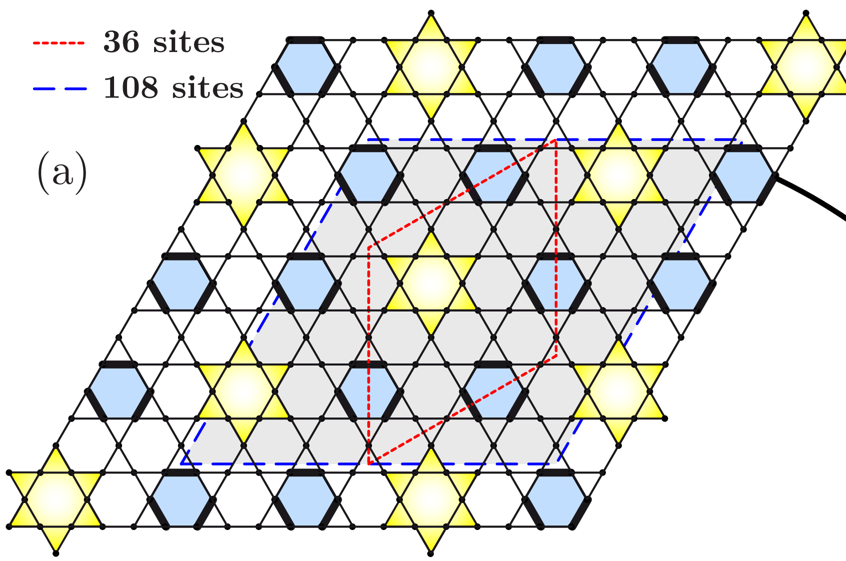
Virtual singlets on the Kagome

back to the kagome lattice

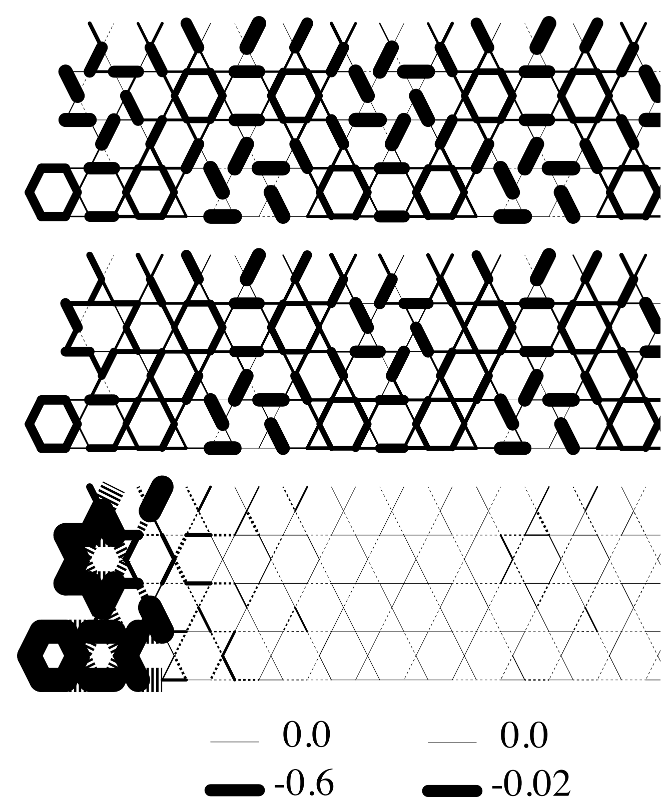
- the question of the RVB description of KAFM runs for more than 20 years

NNVB

Schwandt *et al.* (10)
Poilblanc *et al.* (10)



no spin liquid ⇒ 36-site VBC



Z2 spin liquid

but…

SU(2)

Yan, Huse & White (11)

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i \cdot S_j$$

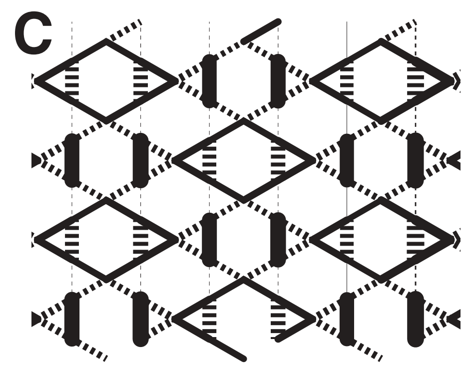
Spin-Liquid Ground State of the $S = 1/2$ Kagome Heisenberg Antiferromagnet

Simeng Yan,[1] David A. Huse,[2,3] Steven R. White[1]*

We use the density matrix renormalization group to perform accurate calculations of the ground state of the nearest-neighbor quantum spin $S = 1/2$ Heisenberg antiferromagnet on the kagome lattice. We study this model on numerous long cylinders with circumferences up to 12 lattice spacings. Through a combination of very-low-energy and small finite-size effects, our results provide strong evidence that, for the infinite two-dimensional system, the ground state of this model is a fully gapped spin liquid.

back to the kagome lattice

- response of the SL to small perturbations
  Yan, Huse & White (11)



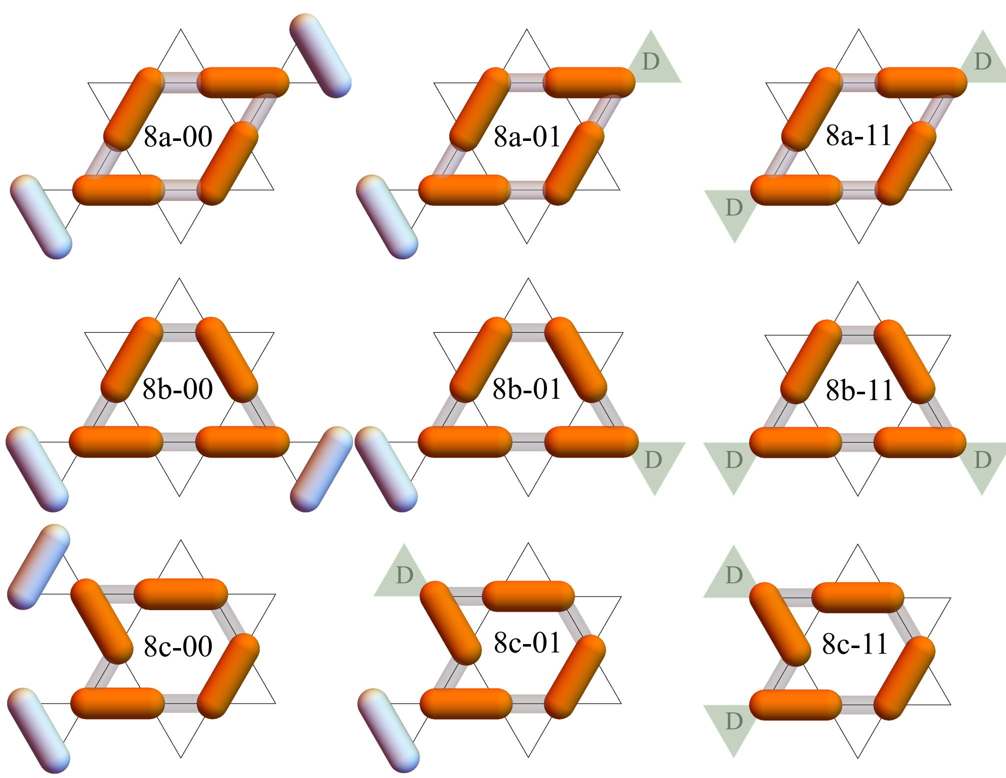
NOT the 12-site VBC of Hao (14)

* same translations
* different PGS

⇒ diamond pattern very close

* not reachable with NNVB

- consider the VB environment close to Loop 8 **AR**, Mila & Rousochatzakis (18)



⇒ **9** parameters

* **29** for L=10

* Including L=6, **40** parameters!

⇒ all implemented in numerics

☞ result: Diamond VBC state very close to Z2 liquid

simplified loop-8 model with single parameter

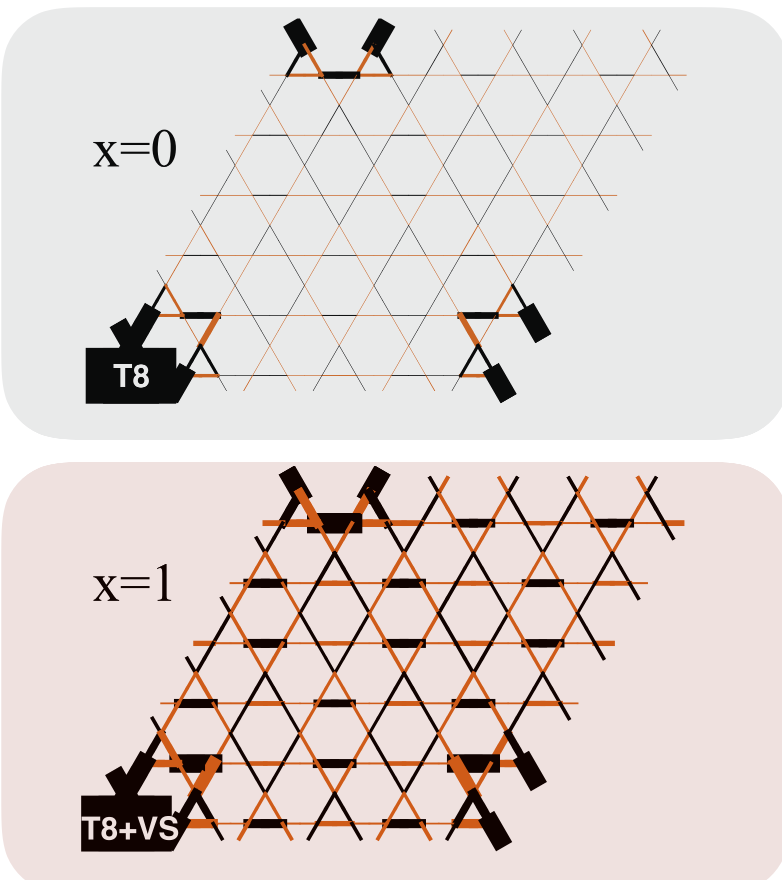
AR, Mila & Rousochatzakis (18)

$$\mathcal{H}_{\mathrm{s}}(x) = (1\text{-}x)\underbrace{\mathcal{H}_{\mathrm{T8}}}_{\uparrow} + x\underbrace{\mathcal{H}'_{\mathrm{T8}}}_{\uparrow}$$

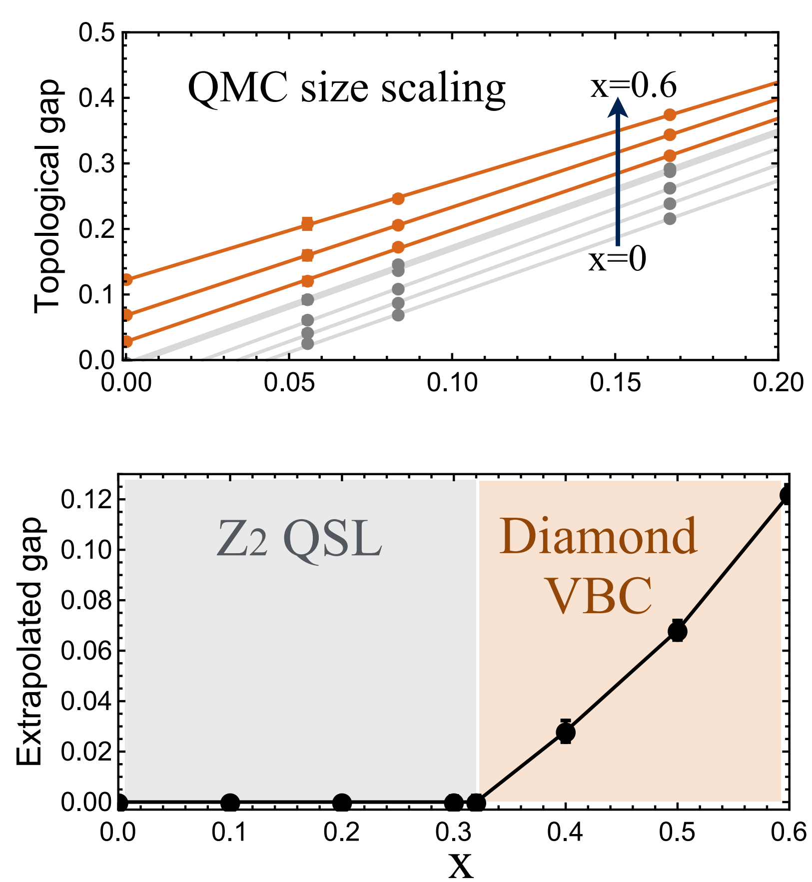
QSL connected to Hao *et al* (2014) full model without loop-6 and 10

- parameter x : encapsulates the total effect of **virtual singlets** on loop-8

dimer-dimer correlations



topological gap

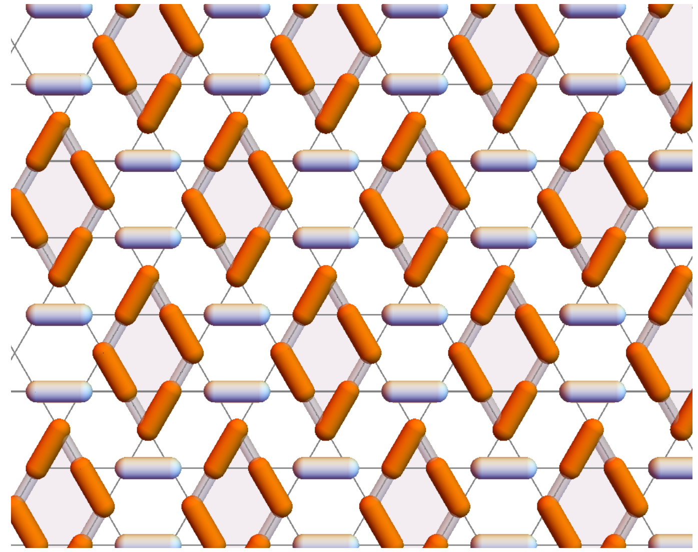


- remaining 31 terms (loop-6 & 10): do not change this picture qualitatively

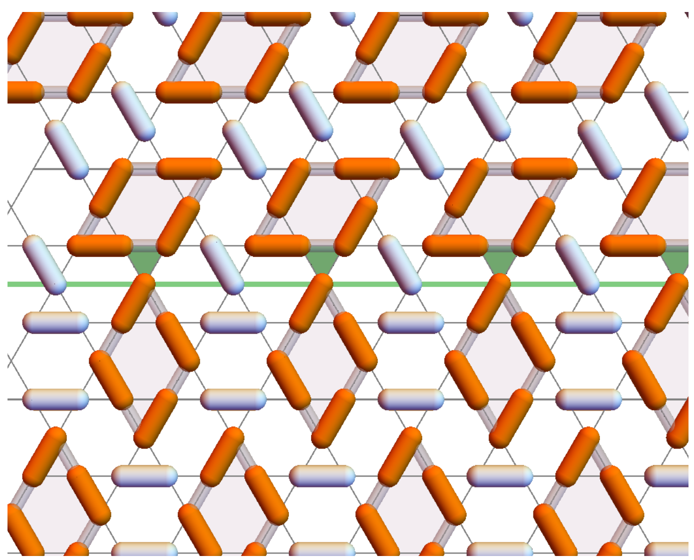
excitations in terms of domain walls and vortices

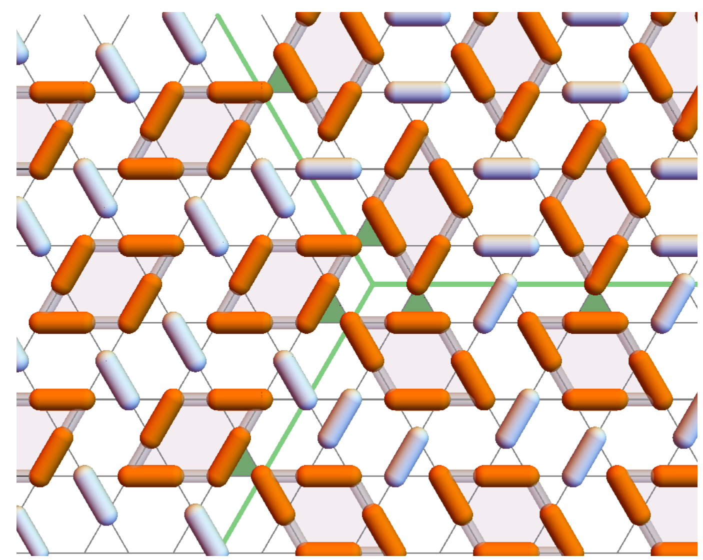
AR, Mila & Rousochatzakis (18)

Uniform Diamond



Single domain wall



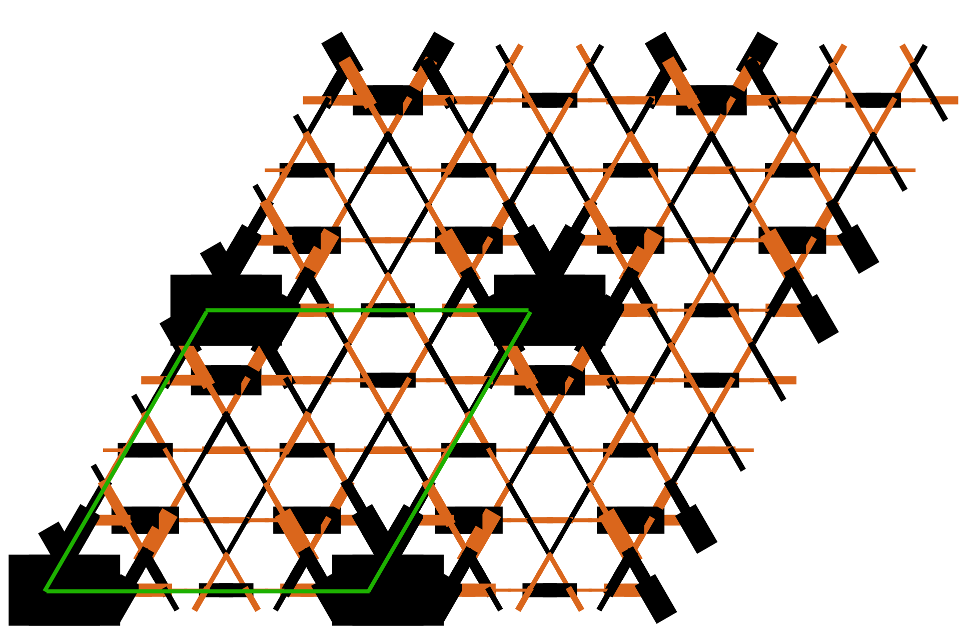


Vortex excitation

- energy cost of domain wall & vortex states: proportional to x !!!
- transition to Z2 liquid by melting of VBC via condensation of domains
- checked numerically: diamond patterns visible in dimer correlations of low-E excitations

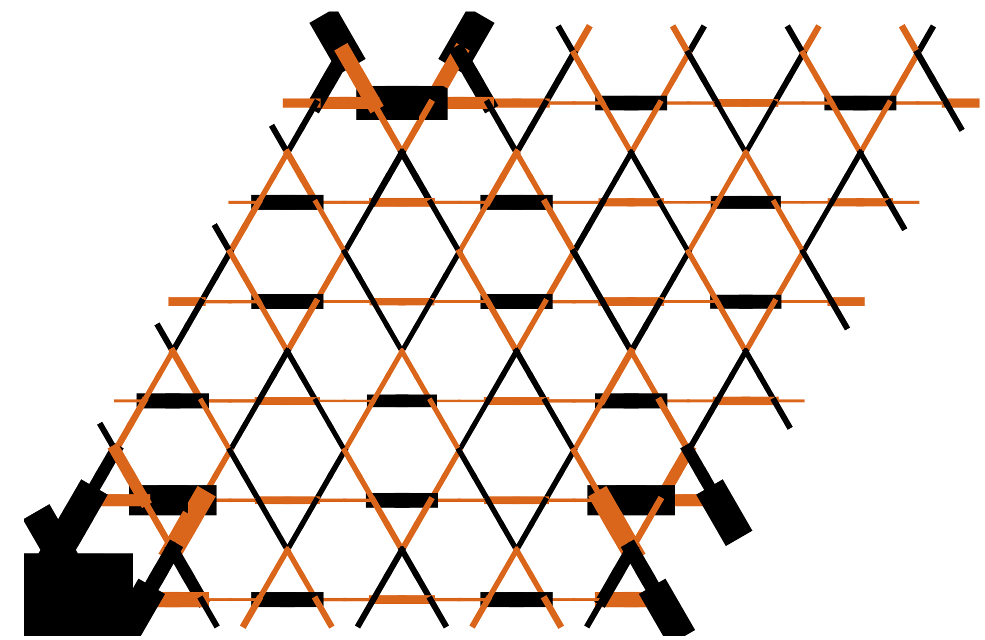
Virtual singlet description

- Dimer-Dimer correlations of the virtual singlet



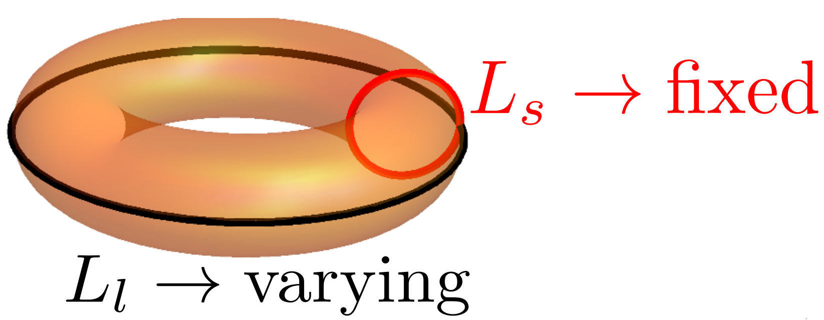
Without loop-10

⇒ Diamond VBC state



Full virtual singlet QDM

- Comparison with DMRG: Importance of cylinder geometry

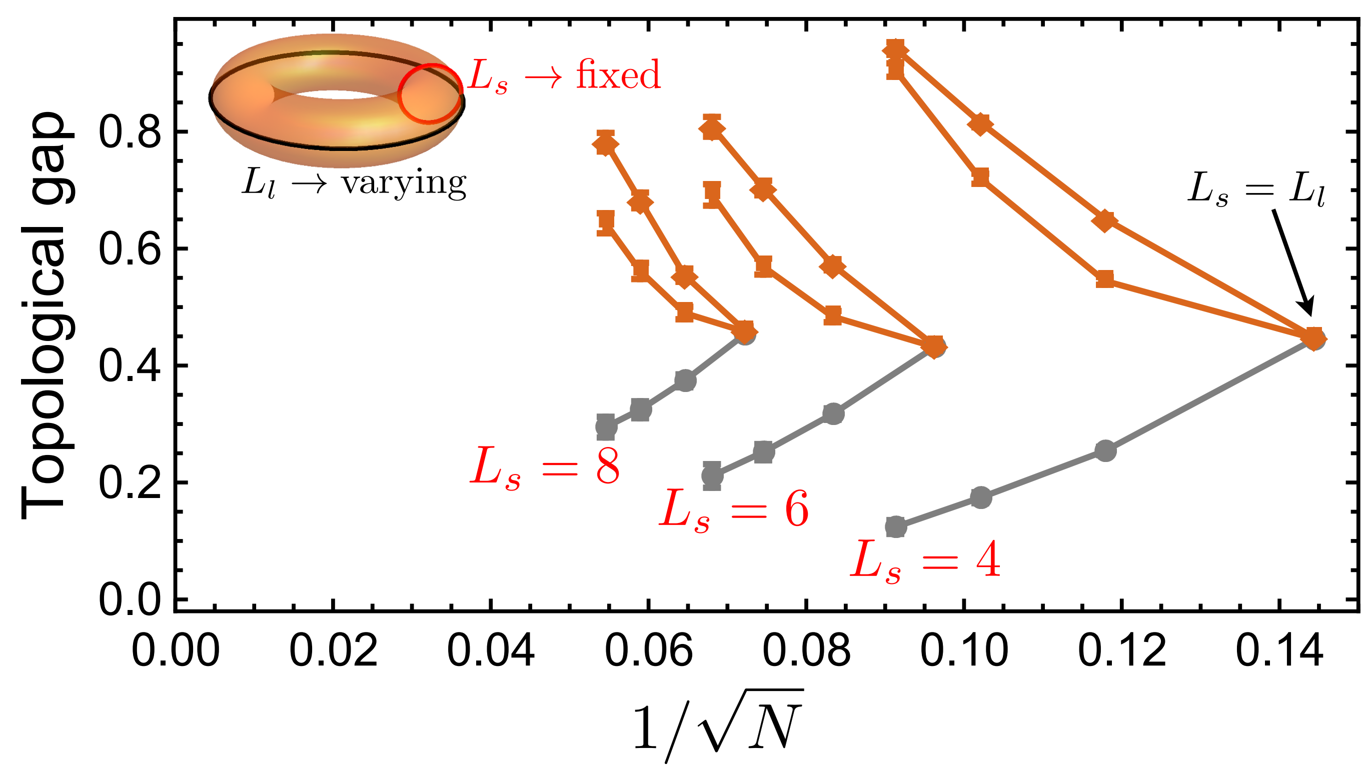


4 topological sectors

Green's function QMC simulations

Z2-QSL at the thermodynamic limit !

For a small enough perimeter



conclusion

- virtual singlets very promising for the description of SU(2) models
- integrate non-local processes at the origin of strong renormalisation

  ⇒ shortest loops are not always governing the physics

- squa-kagome worst case scenario, reconciles with SU(2)
- kagome provides microscopic insights about the SU(2) physics