Title: Resonating valence bond theory of the spin-1/2 kagome Heisenberg antiferromagnet

Date: Apr 18, 2017 03:30 PM

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Abstract: <p>Recent studies of highly frustrated antiferromagnets (AFMs) have demonstrated the qualitative impact of virtual, longer-range singlet excitations on the effective RVB tunneling parameters of the low energy sector of the problem [1,2]. Here, I will discuss the current state of affairs on the RVB description of the spin-1/2 kagome AFM, and present new results that settle a number of issues in this problem [3].</p>

<p> </p>

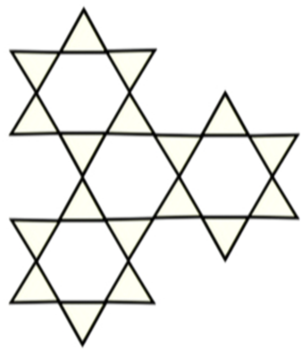
<p>[1] I. Rousochatzakis, Y. Wan, O. Tchernyshyov, and F. Mila, PRB 90,</p>

<p>100406(R) (2014)</p>

<p>[2] A. Ralko and I. Rousochatzakis, PRL 115, 167202 (2015) [3] in preparation.</p>

UNIVERSITY OF MINNESOTA
Driven to Discover

Resonating valence bond theory of the spin-1/2 kagome Heisenberg antifferomagnet



$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Ioannis Rousochatzakis (University of Minnesota)

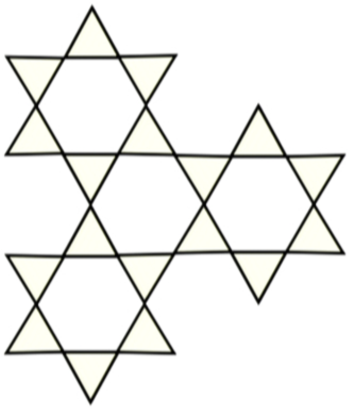
A. Ralko, F. Mila & IR (in preparation)
A. Ralko & IR, PRL **115**, 167202, (2015)
IR, Y. Wan, O. Tchernyshyov, F. Mila, PRB **90**, 100406(R), (2014)

Perimeter Institute,Waterloo, 18 April 2017

Outline of the talk

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

- spin-S kagome AFM: quick review
- spin-1/2 kagome: established results
- microscopic RVB picture: virtual long-range singlets
- comparison to established numerical results
- Outlook



AF Heisenberg model on kagome

Classical limit (S=∞)

1/S

- exponential # of GS's (coplanar + non-coplanar) — Baxter (1970); Chalker *et al* (1991); Ritchey, Chandra, Coleman (1993), ...
- harmonic level: coplanar states selected
- anharmonic level: $\sqrt{3} \times \sqrt{3}$ state selected — Chubukov (1992); Henley & Chan (1995), Sachdev (1992); Götze, Farnell, Bishop, Li & Richter (2011); Chernyshev, Zhitomirsky (2014)
- integer S is qualitative different — van Delft & Henley (1993); Changlani, Läuchli (2015),…

Quantum limit (S=1/2)

AF Heisenberg model on kagome

Classical limit (S=∞)

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Quantum limit (S=1/2)

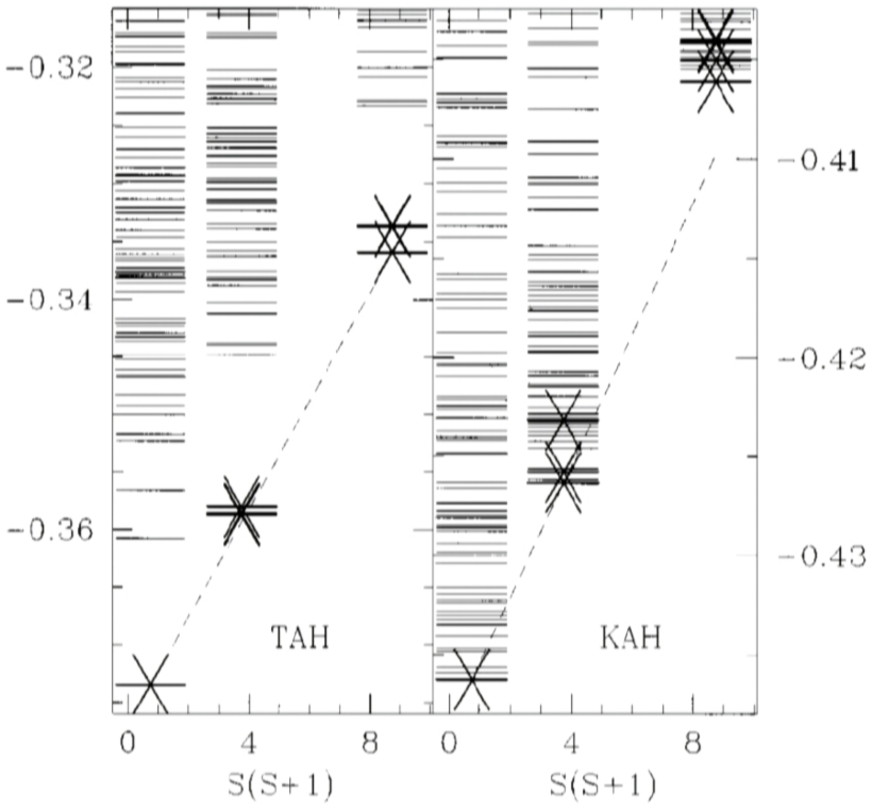
Questions:

1) what are the **established** numerical facts?

2) is there a **simple, microscopic** picture that explains them?

one of the first established facts: low-lying singlets

Lecheminant, Bernu, Lhuillier, Sindzingre, Waldtmann, ... ('97,'98)



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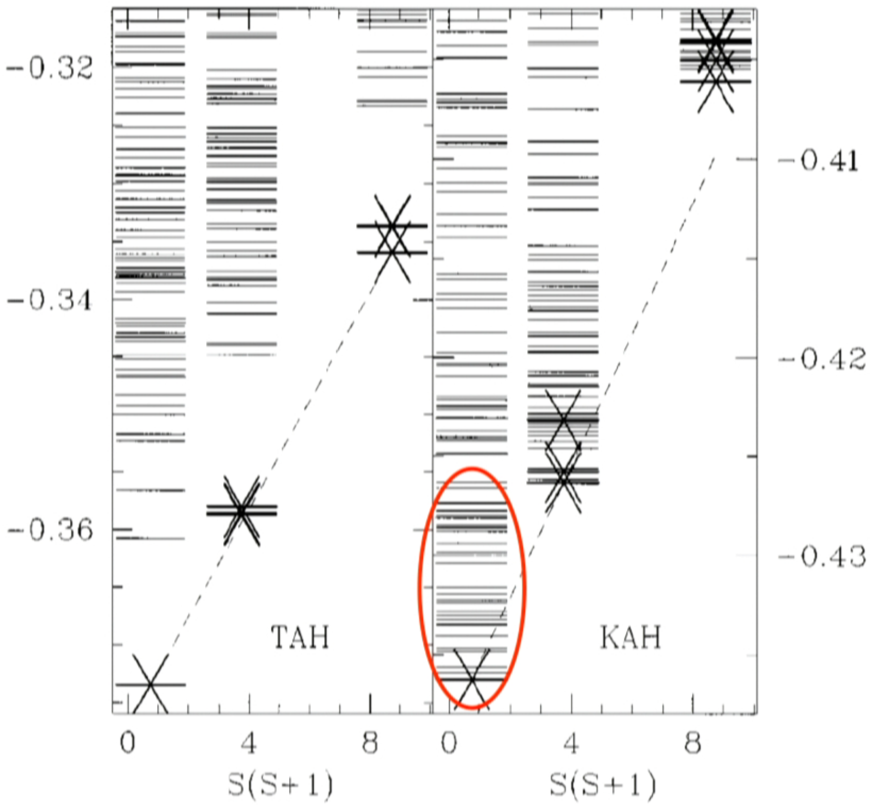

exponential # of low-E singlets

$N_{singlets} \sim 1.15^N$

where do they come from?

- not related to semiclassics
  I. R., A. Läuchli, F. Mila (2008)
- \`trimerized' limit Mila (1988)
- RVB picture
  Elser (1988)
  Elser & Zeng (1995)
  Mambrini & Mila (2000)
  Misguich et al ('02-'03)
  Poilblanc et al (2010)
  ...

origin of singlets: many competing "towers"? NO

IR, Läuchli, Mila (2008)

symmetry decomposition of all classical coplanar states for 12-site cluster

S	Cuboc. $\mathbf{P}^{\Gamma}_{ABC}(1\times 6)$	N	Cuboc. $\mathbf{P}^{M}_{ABC}(3\times 6)$	N
0	A_{1g}	1	A_{1g},E_g	3
1	A_{2g},E_g	3	$A_{1g},E_g,2T_{2u}$	9
2	$A_{1g},2E_g$	5	$3(A_{1g},E_g),2T_{2u}$	15
3	$A_{1g},2A_{2g},2E_g$	7	$3(A_{1g},E_g),4T_{2u}$	21
4	$2A_{1g},A_{2g},3E_g$	9	$5(A_{1g},E_g),4T_{2u}$	27
5	$A_{1g},2A_{2g},4E_g$	11	$5(A_{1g},E_g),6T_{2u}$	33
6	$3A_{1g},2A_{2g},4E_g$	13	$7(A_{1g},E_g),6T_{2u}$	39

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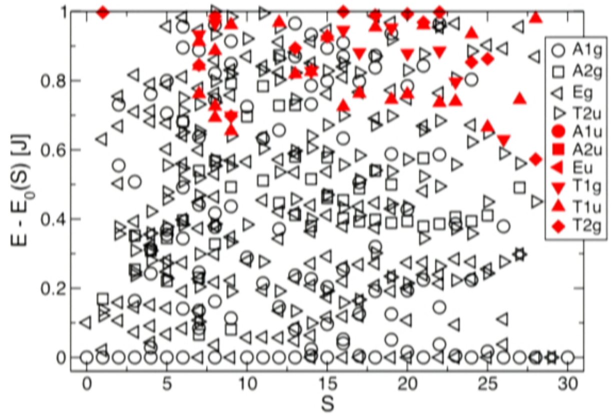
S=5/2



Z_2 spin liquid is one of the competing states

Yan, Huse, White (Science 2011)

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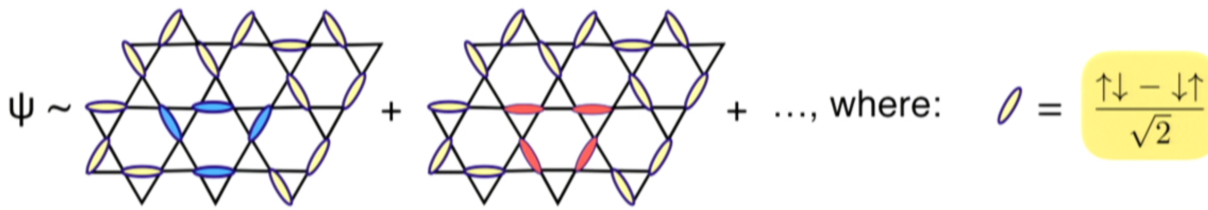
•physical picture: resonating valence bond state Anderson (1973)



•two ingredients for this type of ground state:

1) **infinite** # of **competing** states with very low E (in a variational sense)
2) strong enough quantum-mechanical tunneling

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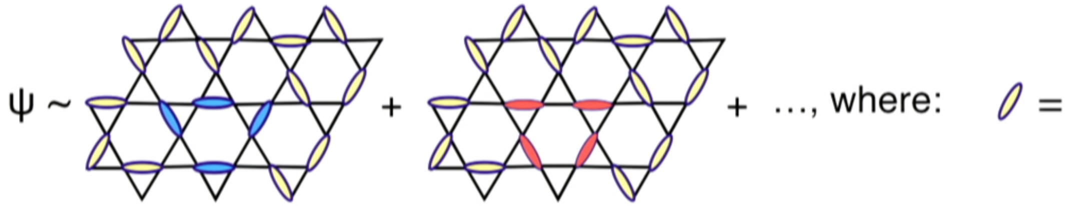

$$\frac{\uparrow\downarrow - \downarrow\uparrow}{\sqrt{2}}$$

•two ingredients for this type of ground state:

1) **infinite** # of **competing** states with very low E (in a variational sense)
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•there are two **integrable** quantum dimer models with this ground state:

Misguich, Serban, Pasquier, PRL **89**, 137202 (2002)

Hao, Inglis, Melko, Nat. Commun. **5**, 5781 (2014)

but both **appear** very far from microscopic models (see below)
→ complexity reduction?

U(1) Dirac spin liquid is another competing state

•physical picture: fermions moving in the background of fluxes

•most recent DMRG study: He, Zaletel, Oshikawa, Pollmann, arXiv:1611.06238v1 (2016)

1) evidence for **gapless** U(1) Dirac spin liquid

- would be consistent with tensor-network methods & VMC

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- first example of a gapless spin liquid in a non-bipartite 2D lattice?
- hard to get in the context of **quantum dimer model**

2) **if not gapless**, then singlet gap is much smaller than anticipated before.

→ very large correlation length (limitation on numerical methods)

→ system is close to a critical point

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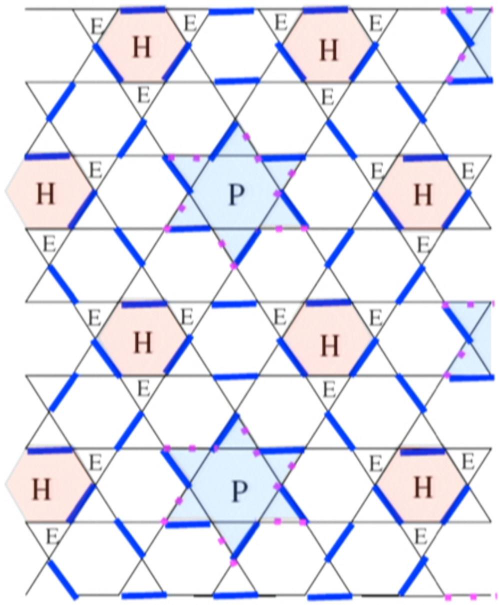
VBC with **shortest** loops (L=6): **not** one of the competing states

Marston & Zeng (1991)
Nikolic & Senthil (2002)
Schwandt, Mambrini & Poilblanc (2010)
Singh & Huse (2007)
Evenbly & Vidal (2010)



next shortest loops (L=8): one of the competing states

- the “diamond VBC” state Yan, Huse, White (Science 2011)

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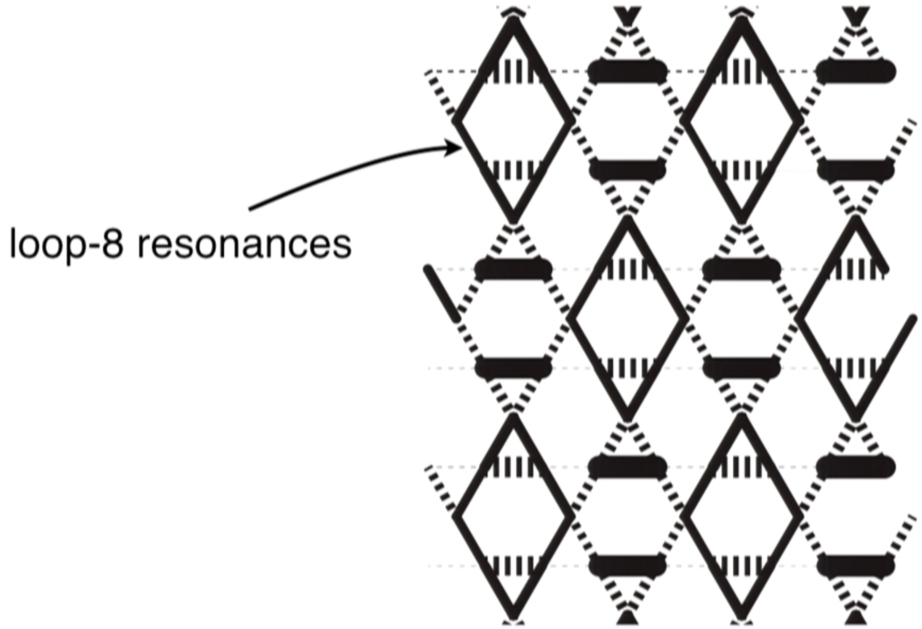
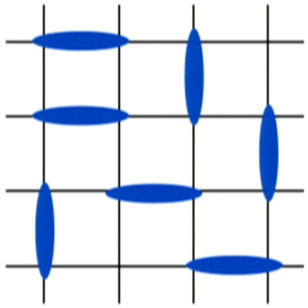


→ L=8 play a much bigger role than L=6

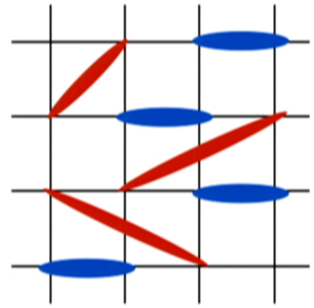
short-range vs. long-range VB states

Liang, Doucot, Anderson (1988); Sandvik (2005)

total singlet manifold is macroscopically large; can be pictured by VB's of arbitrary range



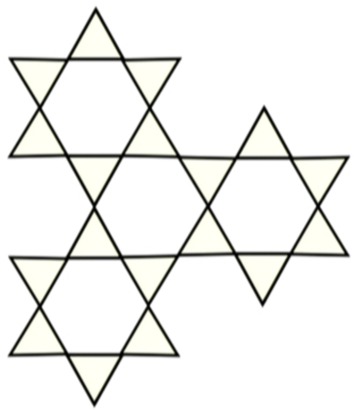
a short-range VB state



a long-range VB state

generic aspect of corner-sharing triangle antiferromagnets

Elser (1988), Elser & Zeng (1995),...



$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2} J \sum_{\Delta} \mathbf{S}_{\Delta}^2 + \text{cst.}$$

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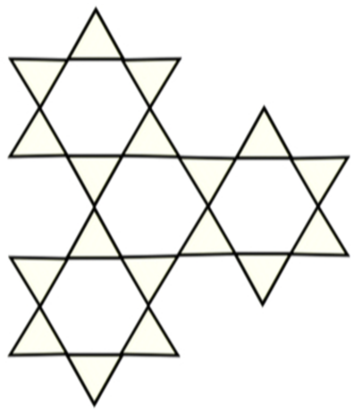

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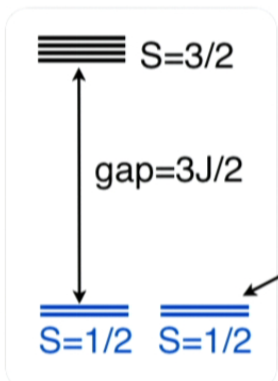
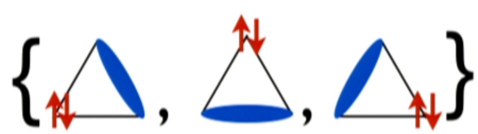
isolated triangle:





only four of them are linearly independent

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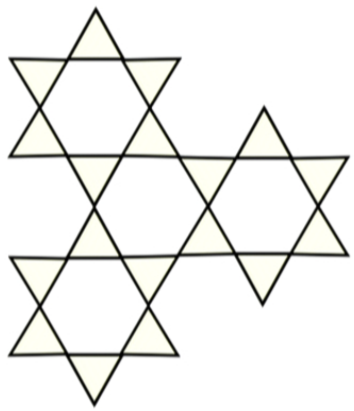

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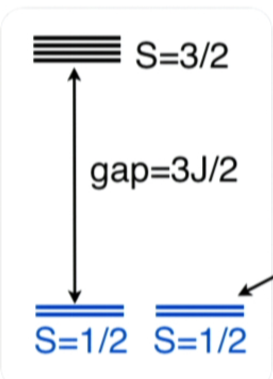
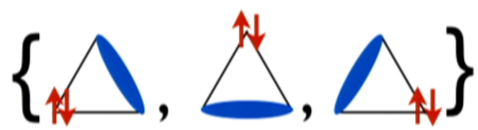
= sum of projectors onto S=1/2 sector

isolated triangle:



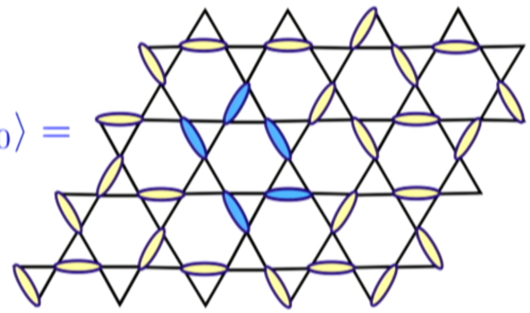


only four of them are linearly independent

Casting RVB idea into a Hamiltonian: the quantum dimer model (QDM)

$$\mathcal{H} \rightarrow \mathcal{H}_{\mathrm{NNVB}} = \left(\mathcal{O}^{-1/2}\mathcal{H}\mathcal{O}^{-1/2}\right)_{\mathrm{NNVB}}$$

$|D_0\rangle =$



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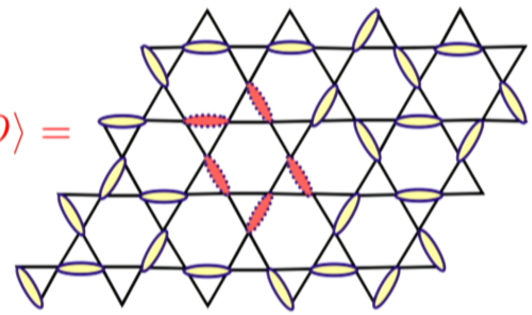

Casting RVB idea into a Hamiltonian: the quantum dimer model (QDM)

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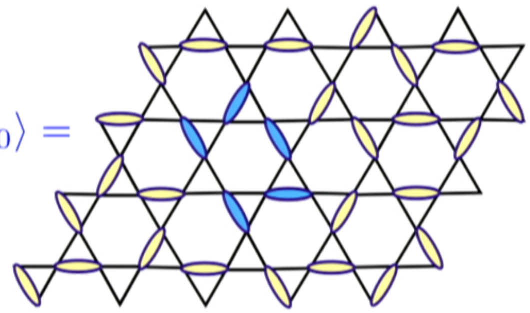

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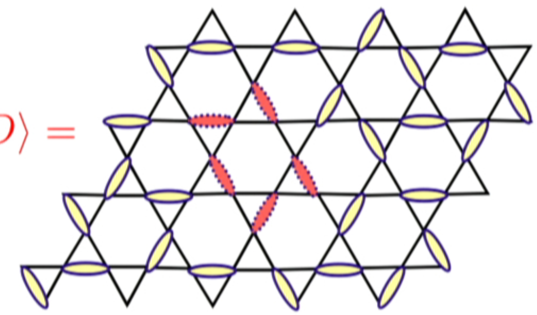
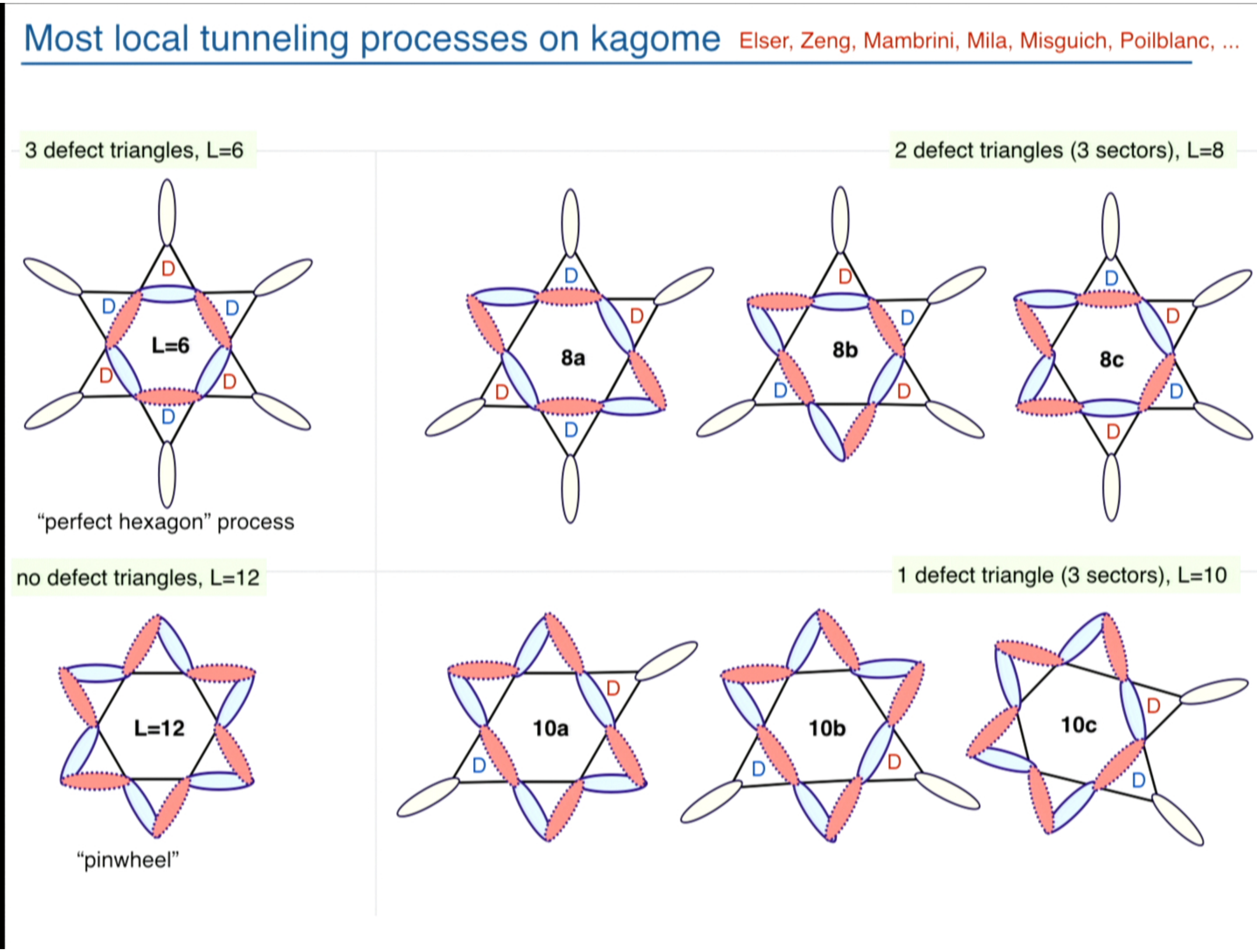
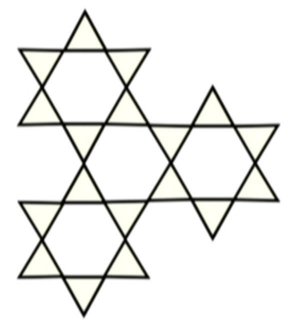



Most local tunneling processes on kagome
Elser, Zeng, Mambrini, Mila, Misguich, Poilblanc, ...
3 defect triangles, L=6
L=6
"perfect hexagon" process
2 defect triangles (3 sectors), L=8
8a
8b
8c
no defect triangles, L=12
L=12
"pinwheel"
1 defect triangle (3 sectors), L=10
10a
10b
10c

How to get the tunneling amplitudes? Traditional approach

Rokhsar & Kivelson (1988)

$$\mathcal{H} \to \mathcal{H}_{\mathrm{NNVB}} = \left(\mathcal{O}^{-1/2}\mathcal{H}\mathcal{O}^{-1/2}\right)_{\mathrm{NNVB}}$$



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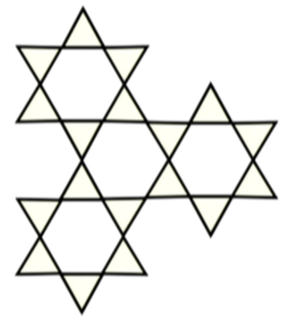
infinite-order, linked-cluster overlap expansion Schwandt, Mambrini & Poilblanc (2010)

→ equivalent with 2x2 NNVB truncation: I.R. *et al*, PRB **90**, 100406(R), (2014)



$|\phi_b\rangle =$  , $|\phi_r\rangle =$ 

$$\mathcal{O} = \begin{pmatrix} 1 & -1/4 \\ -1/4 & 1 \end{pmatrix}, \quad \mathcal{H} = \begin{pmatrix} -9/4 & +9/8 \\ +9/8 & -9/4 \end{pmatrix}$$

tunneling t_{NNVB}

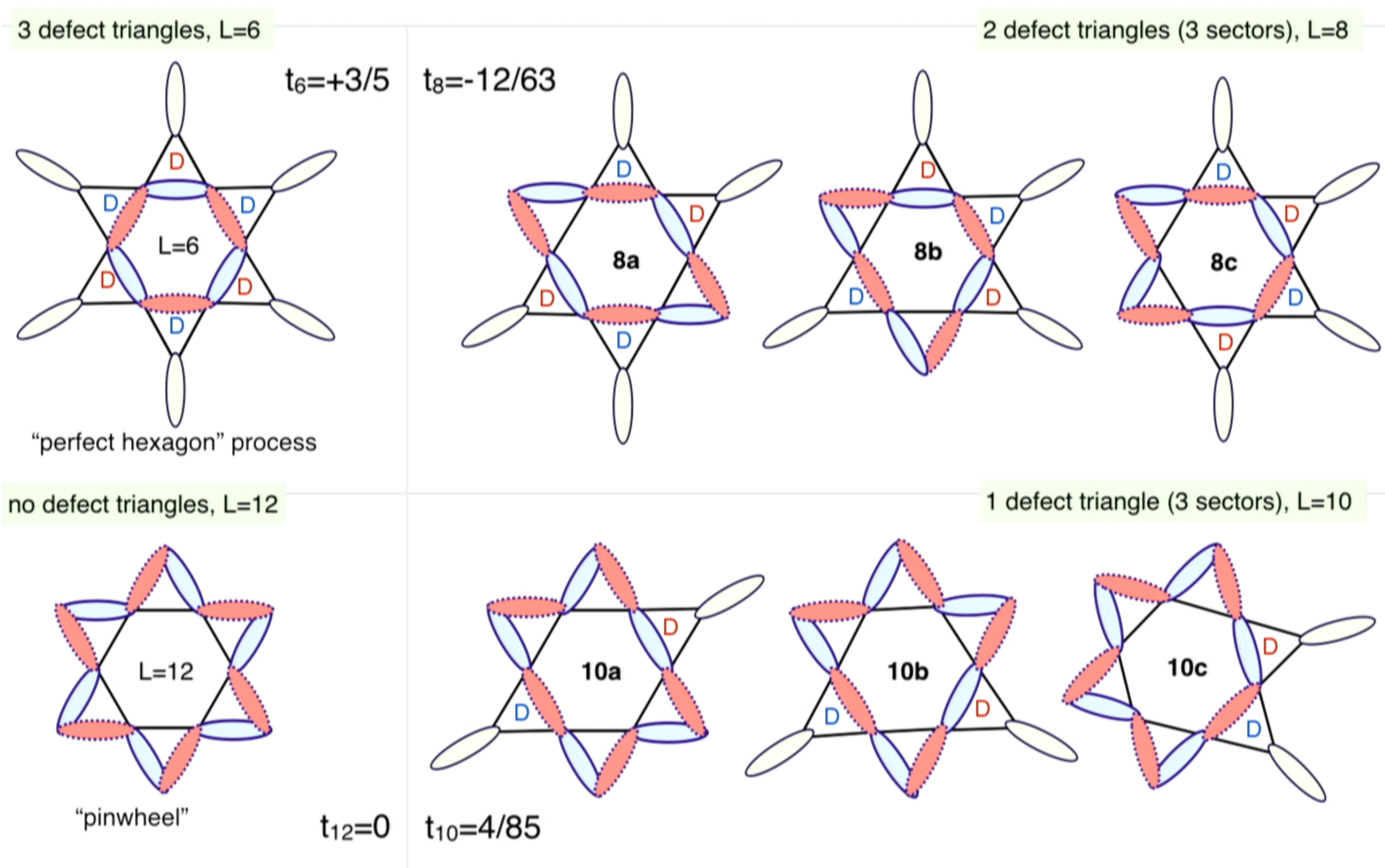
$$\mathcal{H}_{\mathrm{NNVB}} = \left(\mathcal{O}^{-1/2}\mathcal{H}\mathcal{O}^{-1/2}\right)_{\mathrm{NNVB}} = \begin{pmatrix} -21/10 & +3/5 \\ +3/5 & -21/10 \end{pmatrix}$$

general formula: $t_{\mathrm{NNVB}} = \dfrac{v - E_0\omega}{1-\omega^2}$

- drops exponentially with loop length
- contains no info about lattice embedding

2x2 NNVB tunneling amplitudes

Schwandt, Mambrini & Poilblanc (2010)



another problem: Z_2 spin liquid appears very far in parameter space

comparison with the two integrable models:

	t_6	V_6	t_8	V_8	t_{10}	V_{10}	t_{12}	V_{12}
minimal QDM:	**3/5**	**3/20**	**-4/21**	**1/42**	**4/85**	**1/340**	0	0
integrable model #1 Misguich, Serban, Pasquier, PRL **89**, 137202 (2002)	**-1**	0	**-1**	0	**-1**	0	**-1**	0
integrable model #2 Hao, Inglis, Melko, Nat. Commun. **5**, 5781 (2014)	0	0	**-1**	**1**	0	0	0	0

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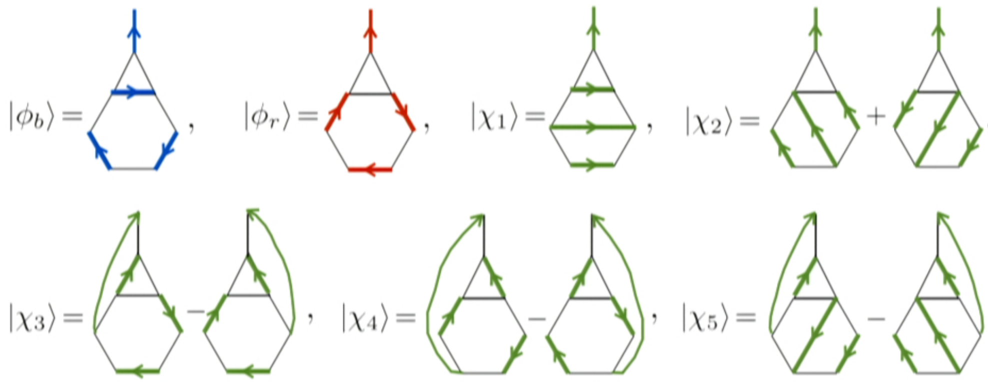
what is missing from the traditional approach?



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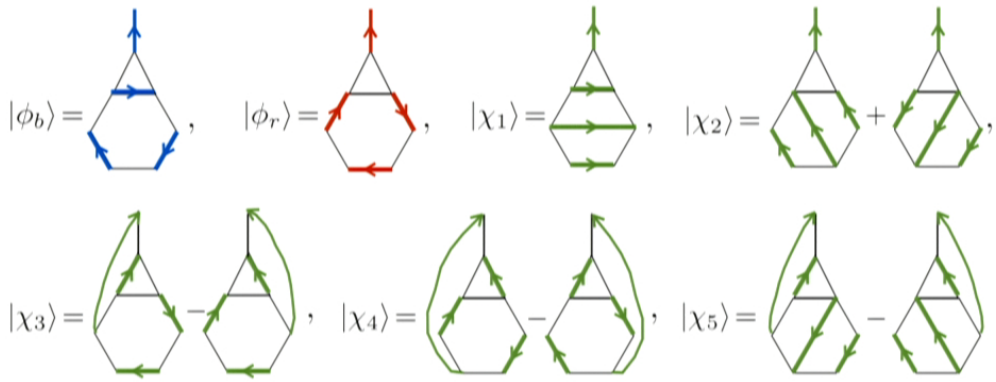


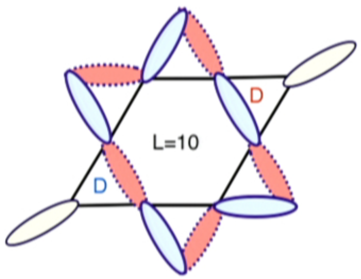
$$\mathcal{O} = \begin{pmatrix} 1 & -1/4 & -1/2 & -1 & 1/4 & 1/2 & -1/2 \\ -1/4 & 1 & 1/2 & 1 & -1 & -1/2 & 1/2 \\ -1/2 & 1/2 & 1 & 1/2 & -1/2 & -1/4 & 1/4 \\ -1 & 1 & 1/2 & 5/2 & -1 & -5/4 & 5/4 \\ 1/4 & -1 & -1/2 & -1 & 5/2 & 5/4 & -5/4 \\ 1/2 & -1/2 & -1/4 & -5/4 & 5/4 & 7/4 & -1 \\ -1/2 & 1/2 & 1/4 & 5/4 & -5/4 & -1 & 7/4 \end{pmatrix} \qquad \mathcal{H} = \begin{pmatrix} -3 & 21/16 & 15/8 & 15/4 & -21/16 & -15/8 & 15/8 \\ 21/16 & -3 & -15/8 & -15/4 & 15/4 & 9/4 & -9/4 \\ 15/8 & -15/8 & -9/4 & -21/8 & 15/8 & 21/16 & -21/16 \\ 15/4 & -15/4 & -21/8 & -57/8 & 9/2 & 69/16 & -69/16 \\ -21/16 & 15/4 & 15/8 & 9/2 & -51/8 & -63/16 & 63/16 \\ -15/8 & 9/4 & 21/16 & 69/16 & -63/16 & -63/16 & 3 \\ 15/8 & -9/4 & -21/16 & -69/16 & 63/16 & 3 & -51/16 \end{pmatrix}$$

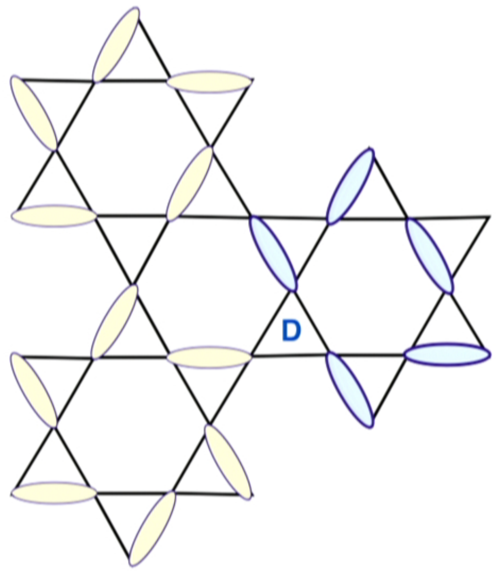
$$\mathcal{H}_{\mathrm{NNVB+}} = \left(\mathcal{O}^{-1/2}\mathcal{H}\mathcal{O}^{-1/2}\right)_{\mathrm{NNVB+}} \to t = 0.578$$

compare to: t=0.6513

Systematically enlarge the `NNVB+' basis: Numerical cluster approach

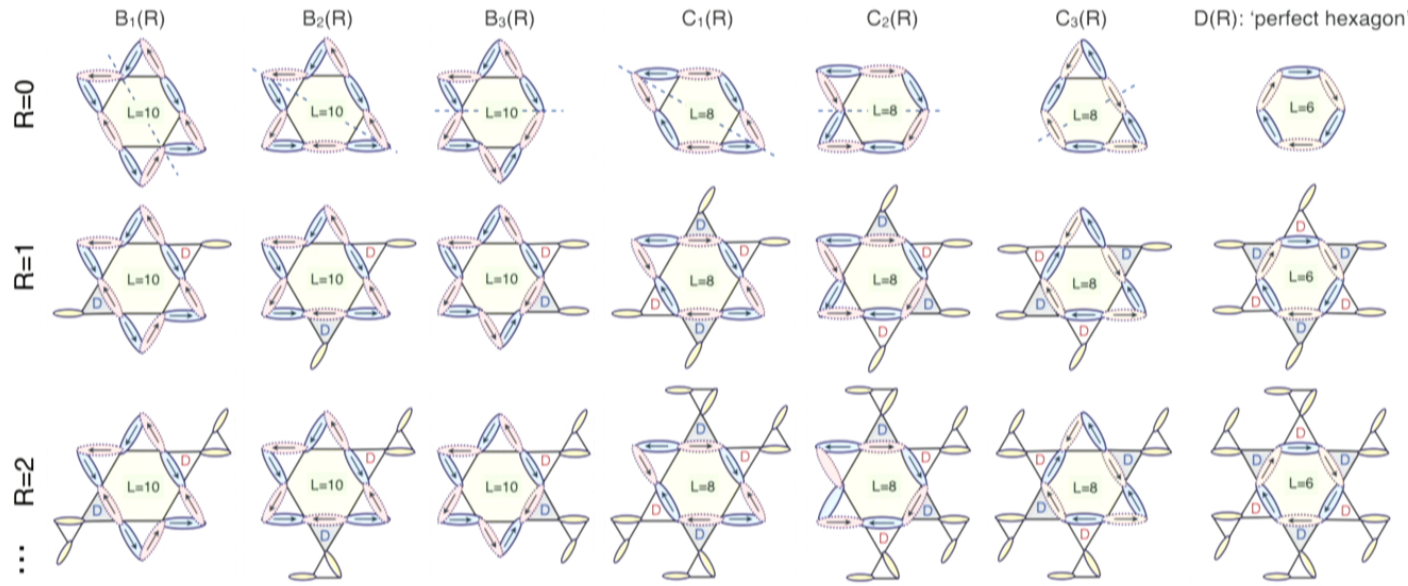
How to capture the dominant virtual corrections in a systematic way?





Numerical cluster approach

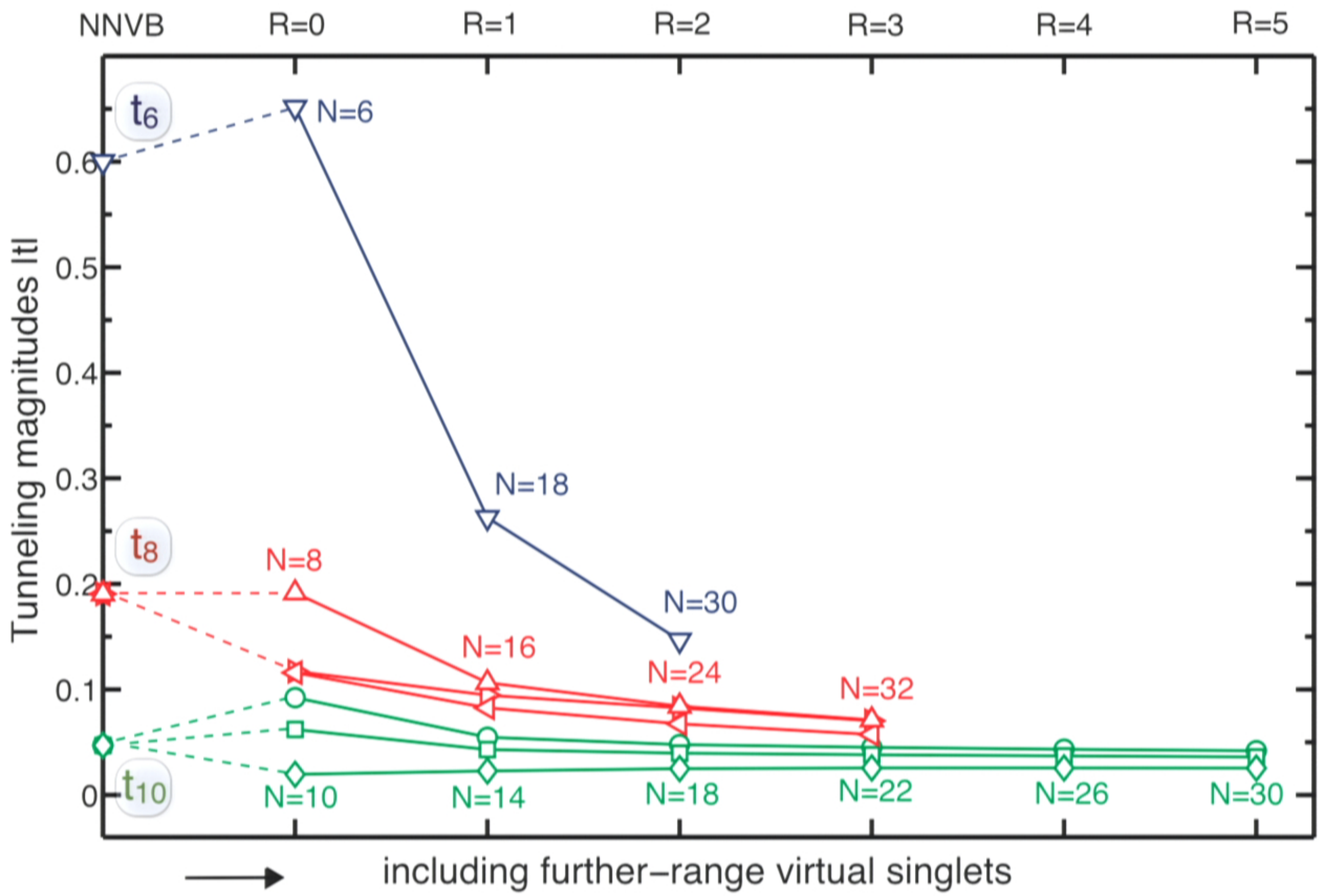
IR, Wan, Tchernyshyov, Mila, PRB **90**, 100406(R), (2014)



- start from minimal clusters that accommodate only the two relevant NNVB states
- systematically enlarge clusters to accommodate longer and longer range singlets
- extract tunneling amplitudes from the exact Heisenberg spectra
- check convergence with R
- analogy: compare with method of extracting J from 2-site Hubbard model

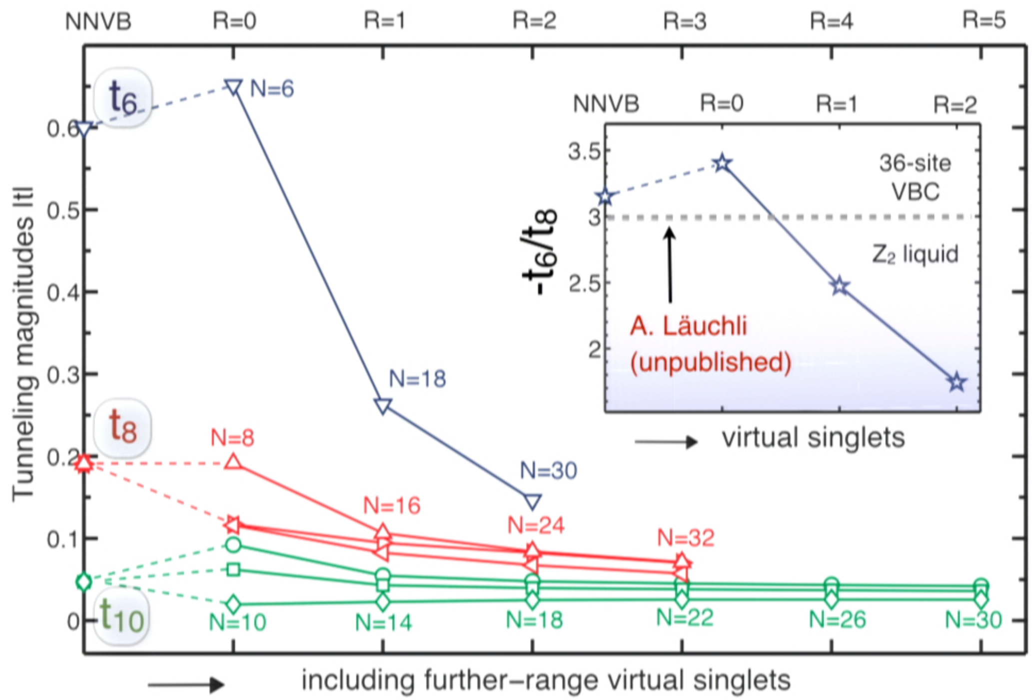
Renormalized tunneling amplitudes

IR, Wan, Tchernyshyov, Mila, PRB **90**, 100406(R), (2014)



Sensitivity to t_6 and nearby Z_2 spin liquid

IR, Wan, Tchernyshyov, Mila (2014)



tunneling depends not only on type of loop, but also on **environment** of the loop

IR, Wan, Tchernyshyov, Mila (PRB, 2014)

A. Ralko & IR (PRL, 2015)

A. Ralko, F. Mila & IR (in preparation)

- consider the VB environment closest to L=8 loops:

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- consider the VB environment closest to L=8 loops:

→ **9** parameters for L=8

- similarly, we get **29** parameters for L=10.
- including L=6, we get a model with **40** parameters! all implemented in numerics

→**result:** diamond VBC state, but close to Z_2 spin liquid

Simplified loop-8 model with a single parameter x

A. Ralko, F. Mila & IR, in preparation

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

(t8=v8)=(-1,0) point of model by Hao *et al* (2014) ↑ $\mathcal{H}_{\rm T8}$

full model without loop-6 and 10 ↑ $\mathcal{H}'_{\rm T8}$

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

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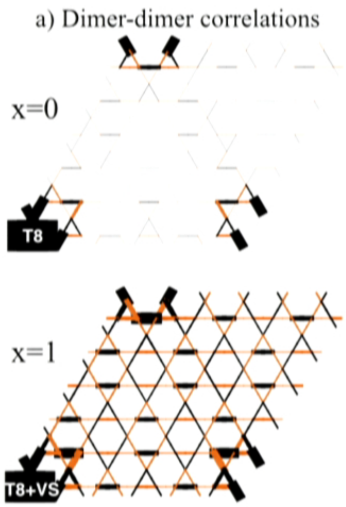

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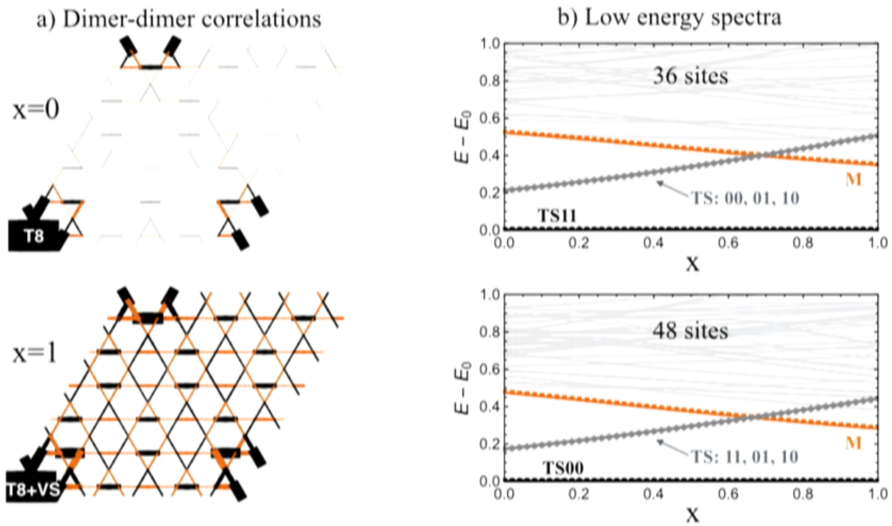
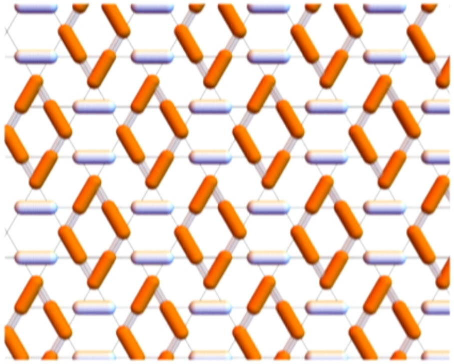


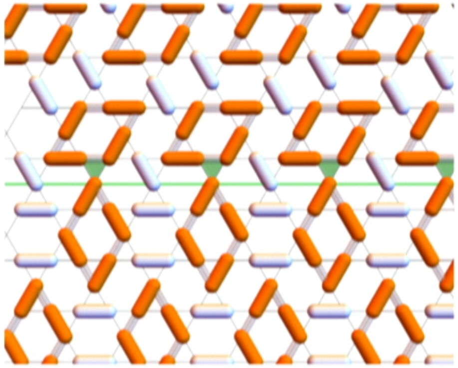
excitations in terms of domain walls & vortices

A. Ralko, F. Mila & IR, in preparation

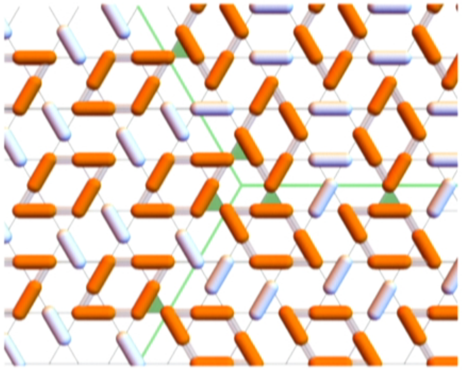
uniform diamond VBC



domain wall excitation



“vortex” excitation



- energy cost of domain wall & vortex states: proportional to x !

→transition to Z_2 spin liquid: melting of VBC via condensation of domain walls & vortices

- actual system is close to transition (on the VBC side):

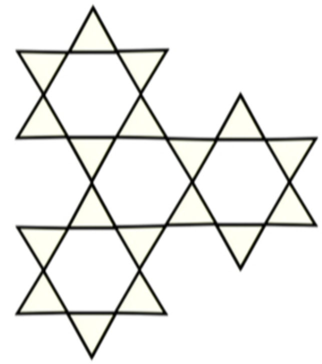
subextensive # of domain walls + extensive # of vortices are present at low energies

Outlook

•RVB theory: offers a simple **microscopic** picture that accounts for established numerical results + **new insights** to the problem

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

- low-lying singlets → proximity to critical point, vortices + domain walls
- irrelevance of shortest resonance loops
- proximity to diamond VBC
- proximity to Z_2 spin liquid



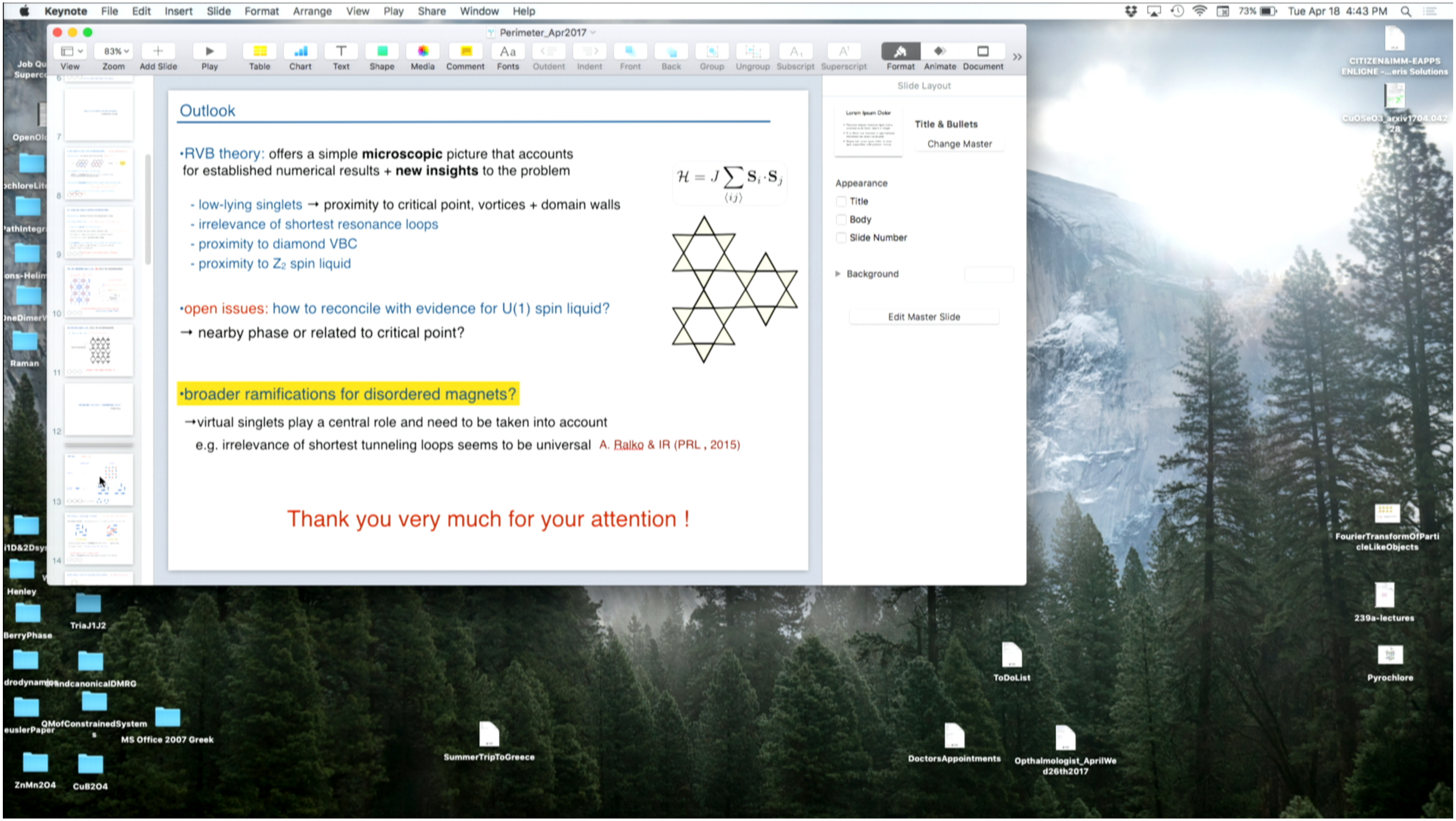
•open issues: how to reconcile with evidence for U(1) spin liquid?

→ nearby phase or related to critical point?

•broader ramifications for disordered magnets?

→virtual singlets play a central role and need to be taken into account

e.g. irrelevance of shortest tunneling loops seems to be universal A. Ralko & IR (PRL , 2015)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Thank you very much for your attention !