

Title: Z2 gauge theory for valence bond solids on the kagome lattice

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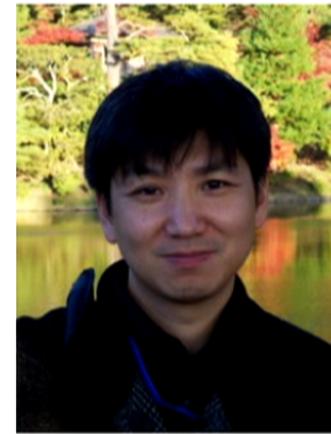
Abstract: <p>We present an effective Z2 gauge theory that captures various competing phases in spin-1/2 kagome lattice antiferromagnets: the topological Z2 spin liquid (SL) phase, and the 12-site and 36- site valence bond solid (VBS) phases. Our effective theory is a generalization of the recent Z2 gauge theory proposed for SL phases by Wan and Tchernyshyov. In particular, we investigate possible VBS phases that arise from vison condensations in the SL. In addition to the 12-site and 36-site VBS phases, there exists 6-site VBS that is closely related to the symmetry-breaking valence bond modulation patterns observed in the recent density matrix renormalization group simulations. We find that our results have remarkable consistency with a previous study using a different Z2 gauge theory. Motivated by the lattice geometry in the recently reported vanadium oxyfluoride kagome antiferromagnet, our gauge theory is extended to incorporate lowered symmetry by inequivalent up- and down-triangles. We investigate effects of this anisotropy on the 12-site, 36-site, and 6-site VBS phases. Particularly, interesting dimer melting effects are found in the 36-site VBS. We discuss the implications of our findings and also compare the results with a different type of Z2 gauge theory used in previous studies.</p>

# Collaborators



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# Kagome lattice antiferromagnet

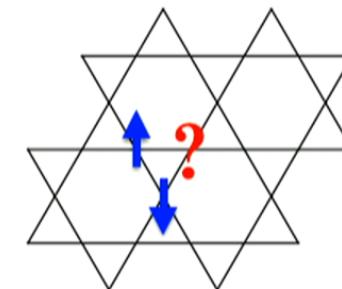
- **Playground of exotic quantum states**

- spin liquid (SL) or valence bond solid (VBS)

- **Spin-1/2 Heisenberg model**

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

*various competing  
low energy states*



<b><math>U(1)</math> SL</b>	VMC
<b><math>Z_2</math> SL</b>	DMRG
<b>12-site VBS</b>	DMRG
<b>36-site VBS</b>	series expansion

# Kagome lattice antiferromagnet

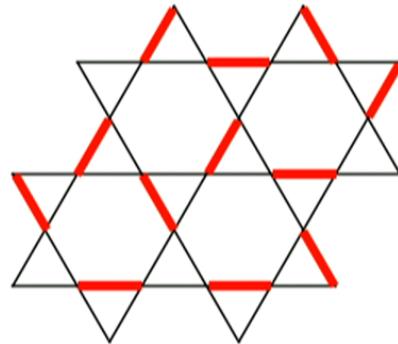
- **Spin liquid**

- resonating valence bonds

*Read & Chakraborty, PRB (1989)*

$$|\Psi\rangle = \left| \begin{array}{c} \text{Kagome lattice} \\ \text{with red bonds} \end{array} \right\rangle + \left| \begin{array}{c} \text{Kagome lattice} \\ \text{with red bonds} \end{array} \right\rangle + \left| \begin{array}{c} \text{Kagome lattice} \\ \text{with red bonds} \end{array} \right\rangle + \dots$$

- spinons ( $s=1/2$ )

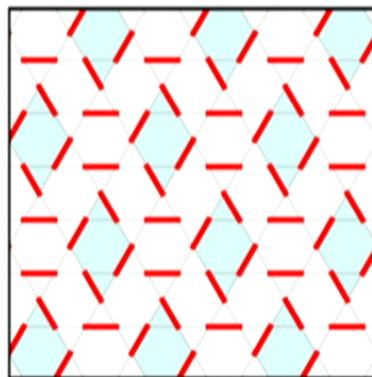


# Kagome lattice antiferromagnet

- **Valence bond solid**

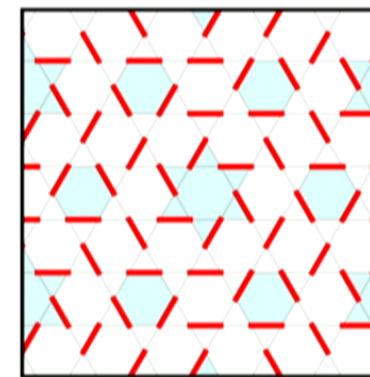
- crystalline order of valence bonds
- spontaneously broken lattice symmetry
- triplons ( $s=1$ )

**(a) 12-VBS**



*Yan, Huse, White, Science (2011)  
Huh, Punk, Sachdev, PRB (2013)*

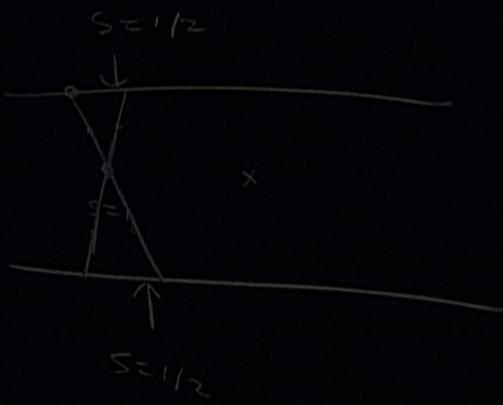
**(b) 36-VBS**



*Nikolic & Senthil, PRB (2003)  
Singh & Huse, PRB (2007,2008)*

$\sqrt{4^+}$  ( $s = 1/2$ )

$\downarrow$  ( $s = 1$ )



# Kagome lattice antiferromagnet

- **Material systems**

Herbertsmithites $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$	U(1) SL or $Z_2$ SL?
Deformed kagome antiferromagnet $\text{Rb}_2\text{Cu}_3\text{SnF}_{12}$	12-site VBS
Vanadium oxyfluoride $(\text{NH}_4)_2(\text{C}_7\text{H}_{14}\text{N})(\text{V}_7\text{O}_6\text{F}_{18})$	?

Han et al., Nature (2012)

Pilon et al., PRL (2013)

Martan et al., Nat. Phys. (2010)

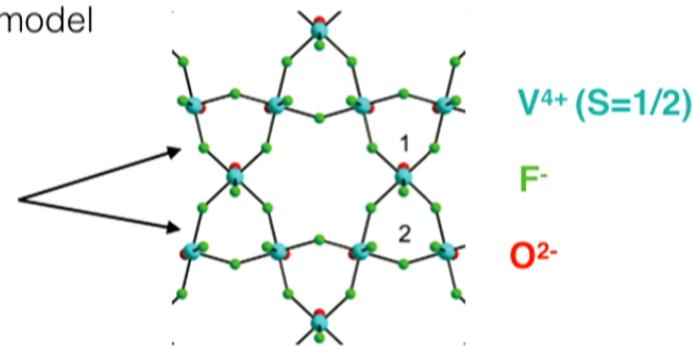
Aidoudi et al., Nat. Chem. (2011)

Clark et al., PRL (2013)

- perturbations to the ideal Heisenberg model

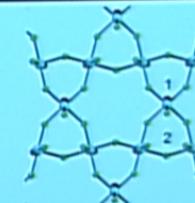
Vanadium oxyfluoride

Up- and down-triangles are  
**not equivalent.**



## Motivation for effective theory

Q2: Effects of the lower symmetry ( $\triangle \neq \nabla$ )  
on spin liquids and valence bond solids?



Vanadium oxyfluoride

Previous studies focus on the further neighbor Heisenberg interactions  
and Dzyaloshinskii-Moriya interactions.

## Motivation for effective theory

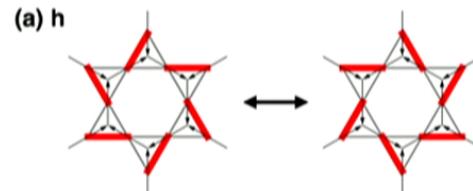
- Focusing on the VBS phases found in our effective theory, we investigate the lower symmetry effects on the phases.
- We find interesting dimer melting effects in the 36-site VBS phase.

# Quantum dimer model

- Our  $\mathbb{Z}_2$  gauge theory is exactly equivalent to a quantum dimer model.

$$H_{\text{QDM}} = -h \sum_{D \in \mathcal{D}} |\bar{D}\rangle\langle D| + K \sum_{D \in \mathcal{D}} \epsilon_D |D\rangle\langle D|$$

$h$ : dimer motion



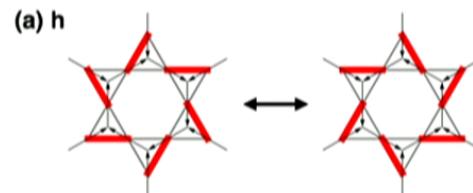
Length	Transition graph and $ D\rangle$	Multiplicity	$\epsilon_D$
6		1	3
8		3	-3
8		6	-1
8		6	1
10		6	-1
10		6	1
10		3	3
12		1	-3

# Quantum dimer model

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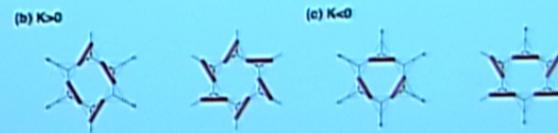
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## Quantum dimer model

- Our  $Z_2$  gauge theory is exactly equivalent to a quantum dimer model.

$$H_{QDM} = -h \sum_{D \in \mathcal{D}} |\tilde{D}\rangle\langle D| + K \sum_{D \in \mathcal{D}} \epsilon_D |D\rangle\langle D|$$

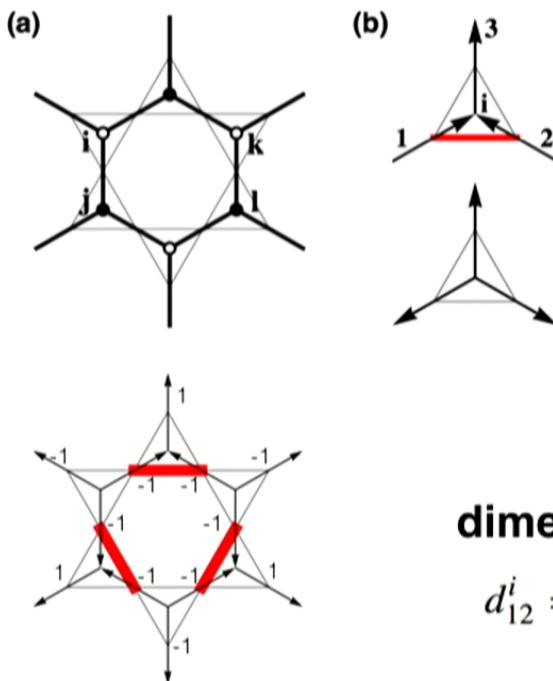
$K$ : dimer interaction



Length	Transition graph and $\langle D \rangle$	Multiplicity	$\epsilon_D$
6		1	+
8		1	-8
9		1	-9
10		1	+
11		1	-4
12		1	+
13		1	-8

# $Z_2$ Gauge theory

- Dimer-arrow mapping



dimer: 2-in-1-out

arrow:  $\sigma^x (= \pm 1)$

**hardcore dimer constraint**

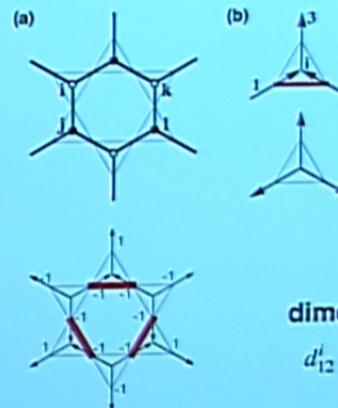
$$Q_i = \sigma_{i1}^x \sigma_{i2}^x \sigma_{i3}^x = \begin{cases} +1 & (i \in A) \\ -1 & (i \in B) \end{cases}$$

**dimer occupation**

$$d_{12}^i = \frac{1}{4} (\sigma_{i3}^x - \sigma_{i1}^x - \sigma_{i2}^x) Q_i + \frac{1}{4} = \begin{cases} 1 & (\text{occupied}), \\ 0 & (\text{empty}). \end{cases}$$

## $Z_2$ Gauge theory

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arrow:  $\sigma^x (= \pm 1)$

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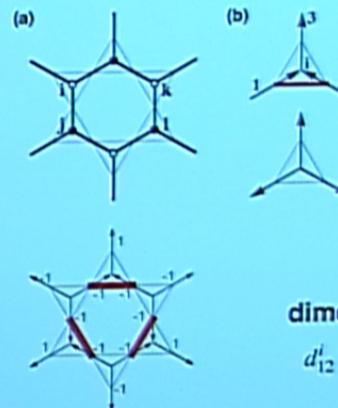
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dimer occupation

$$d_{i2}^i = \frac{1}{4} (\sigma_{i3}^x - \sigma_{i1}^x - \sigma_{i2}^x) Q_i + \frac{1}{4} = \begin{cases} 1 & (\text{occupied}), \\ 0 & (\text{empty}). \end{cases}$$

## $Z_2$ Gauge theory

- Dimer-arrow mapping



dimer: 2-in-1-out  
arrow:  $\sigma^x (= \pm 1)$

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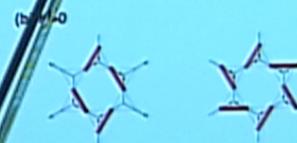
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## $Z_2$ Gauge theory

- Hamiltonian

$$H_{ZGT} = -h \sum_{\alpha} F_{\alpha}^z + K \sum_{\langle ij \rangle // \langle kl \rangle} \sigma_{ij}^x \sigma_{kl}^x + A \sum_{\langle ij \rangle} \sigma_{ij}^x$$



## $Z_2$ Gauge theory

- Hamiltonian

$$H_{\text{ZGT}} = -h \sum_{\alpha} F_{\alpha}^z + K \sum_{\langle ij \rangle // \langle kl \rangle} \sigma_{ij}^x \sigma_{kl}^x + A \sum_{\langle ij \rangle} \sigma_{ij}^x$$

(b)  $K>0$



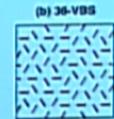
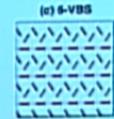
(c)  $K<0$



## Quantum dimer model

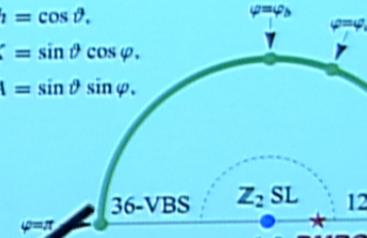
- Phase diagram

$$H_{QDM} = -h \sum_{D \in \mathcal{D}} |\tilde{D}\rangle\langle D| + K \sum_{D \in \mathcal{D}} \epsilon_D |D\rangle\langle D| + A \sum_{T \in \mathcal{T}} \eta_T |T\rangle\langle T|$$

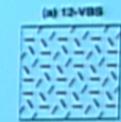


Misguich, Evenbly, Pasquier, PRL (2002)

$$h = \cos \vartheta, \\ K = \sin \vartheta \cos \varphi, \\ A = \sin \vartheta \sin \varphi.$$



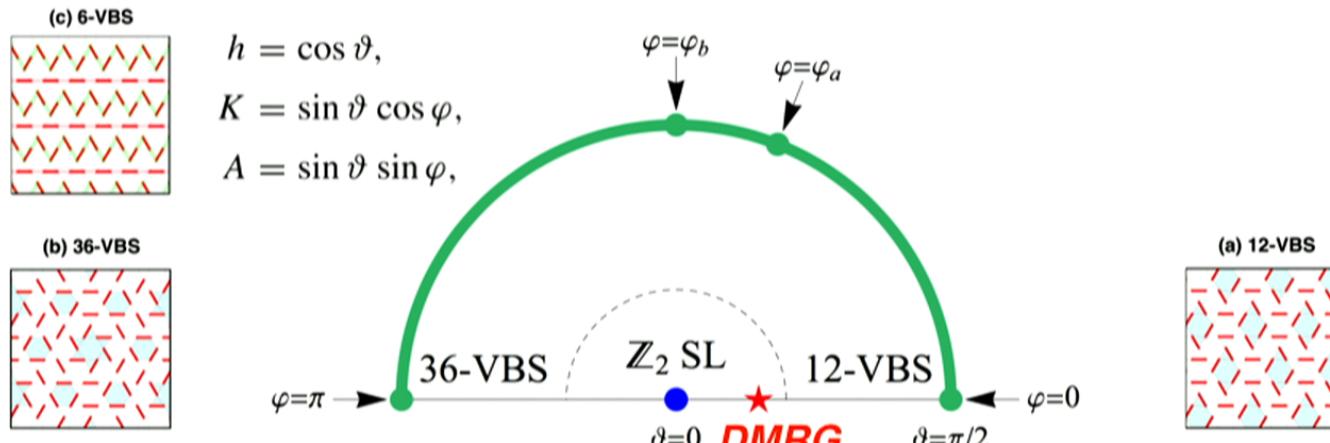
Yan, Huse, White, Science (2011)  
Wan & Tchernyshyov, PRB (2013)



# Quantum dimer model

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Misguich, Serban, Pasquier, PRL (2002)

Yan, Huse, White, Science (2011)

Wan & Tchernyshyov, PRB (2013)

## Ginzburg-Landau theory for VBS phases

- Order parameter: vison condensation

*vison condensation*

$Z_2$  SL      VBS

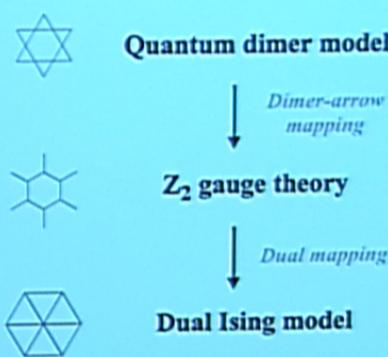
Senthil & Fisher, PRB (2000)

Nikolic & Senthil, PRB (2003)

Xu & Balents, PRB (2011)

Huh, Punk, Sachdev, PRB (2013)

## Mappings in the effective theory



vison

topological vortex

flux excitation  
in the gauge field

local Ising spin  
on the dual lattice

Read & Chakraborty, PRB (1989)

Senthil & Fisher, PRB (2000)

Nikolic & Senthil, PRB (2003)



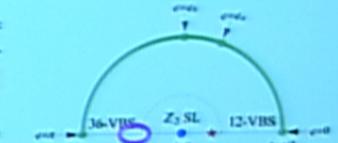
## Landau theories for VBS orders

- **Soft spin model**

- hopping Hamiltonian for the visons in the  $Z_2$  SL
- soft vison modes + PSG analysis

Wen, PRB (2002)

case	range	position	degeneracy	N
1	$\varphi = 0$	$\pm Q$	2	4
2	$\varphi = \pi$	$Q_{1,2}$	2	8
3	$0 <  \varphi  \leq \frac{\pi}{2}$	$\pm Q$	2	4
4	$\frac{\pi}{2} \leq  \varphi  < \pi$	$\pm Q_{1,2}$	1	4



- **Ginzburg-Landau theories**

- Ginzburg-Landau functional using the soft modes and vison PSG

Huh, Punk, Sachdev, PRB (2013)



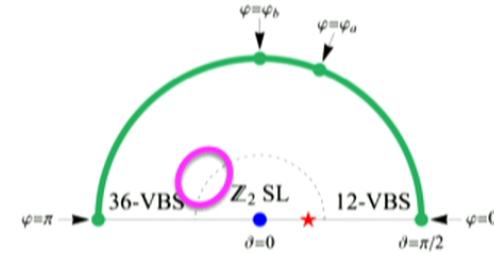
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4	$\frac{\pi}{2} \lesssim  \varphi  < \pi$	$\pm \mathbf{Q}_{1,2}$	1	4

Wen, PRB (2002)



- **Ginzburg-Landau theories**

- Ginzburg-Landau functional using the soft modes and vison PSG

Huh, Punk, Sachdev, PRB (2013)

## Landau theories for VBS orders

- Case2: K<0 and A=0

$$\Psi = (\psi_1, \psi_2, \psi_3, \psi_4, \psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*)$$

$$\mathcal{L} = |\partial \Psi|^2 + r|\Psi|^2 + u|\Psi|^4 + \sum_{m=1}^4 a_m \mathcal{I}_m$$

$$\begin{aligned}\mathcal{I}_1 &= \rho_1^2 \rho_2^2 + \rho_1^2 \rho_3^2 + \rho_2^2 \rho_4^2 + \rho_3^2 \rho_1^2 \\&\quad - \rho_1^2 \rho_2^2 [1 + \cos(2\theta_1 + \theta_3)] \\&\quad - \rho_2^2 \rho_3^2 [1 + \cos(2\theta_2 + \theta_4)],\end{aligned}$$

$$\begin{aligned}\mathcal{I}_2 &= \rho_1^2 \rho_2^2 + \rho_1^2 \rho_3^2 \\&\quad - \rho_1 \rho_2 \rho_3 \rho_4 (\sin(\theta_1 - \theta_2 - \theta_3 + \theta_4) \\&\quad - \rho_1 \rho_2 \rho_3 \rho_4 \sqrt{3} \sin(\theta_1 - \theta_2 - \theta_3 + \theta_4)),\end{aligned}$$

$$\begin{aligned}\mathcal{I}_3 &= \rho_1^2 \rho_2^2 \cos(2\theta_1 + \theta_3 + \theta_4) \\&\quad + (-2 + \sqrt{3}) \sin(2\theta_1 + \theta_3 + \theta_4) \\&\quad + \rho_1^2 \rho_2^2 \cos(2\theta_2 + \theta_4 + \theta_3),\end{aligned}$$

$$\begin{aligned}\mathcal{I}_4 &= \rho_1^2 \rho_2^2 \cos(2\theta_1 + \theta_3 + \theta_4) \\&\quad + \rho_1^2 \rho_2^2 \cos(2\theta_2 + \theta_4 + \theta_3) \\&\quad + \cos(\theta_1 - \theta_2 + 2\theta_3) \\&\quad + \cos(2\theta_1 - \theta_3 + \theta_4 + 2\theta_2) \\&\quad + \cos(2\theta_2 - \theta_4 + \theta_3 + 2\theta_1) \\&\quad + \cos(2\theta_3 - \theta_1 + \theta_2 + 2\theta_4).\end{aligned}$$

$$\begin{aligned}\mathcal{I}_1 &= \sqrt{3} \rho_1 + \sqrt{3} \rho_2 + 13 \sqrt{3} \rho_3 \\&\quad - 4 \sqrt{3} \rho_4,\end{aligned}$$

$$\begin{aligned}\mathcal{I}_2 &= -\sqrt{3} + 13 \rho_1 + \sqrt{3} \rho_2 + 4 \sqrt{3} \rho_4,\end{aligned}$$

$$\begin{aligned}\mathcal{I}_3 &= \sqrt{3} \cos(2\theta_1 + \theta_3 + \theta_4) \\&\quad + (-2 + \sqrt{3}) \sin(2\theta_1 + \theta_3 + \theta_4) \\&\quad + \sqrt{3} \cos(2\theta_2 + \theta_4 + \theta_3),\end{aligned}$$

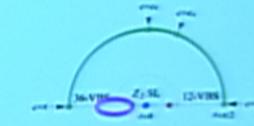
$$\begin{aligned}\mathcal{I}_4 &= \sqrt{3} \cos(2\theta_1 + \theta_3 + \theta_4) \\&\quad + \sqrt{3} \cos(2\theta_2 + \theta_4 + \theta_3) \\&\quad + \cos(\theta_1 - \theta_2 + 2\theta_3) \\&\quad + \cos(2\theta_1 - \theta_3 + \theta_4 + 2\theta_2) \\&\quad + \cos(2\theta_2 - \theta_4 + \theta_3 + 2\theta_1) \\&\quad + \cos(2\theta_3 - \theta_1 + \theta_2 + 2\theta_4).\end{aligned}$$

$$\begin{aligned}\mathcal{J}_1 &= \{ \rho_1^2 \rho_2^2 + \rho_1^2 \rho_3^2 + \rho_2^2 \rho_4^2 + \rho_3^2 \rho_1^2 \\&\quad - \rho_1^2 \rho_2^2 [1 + \cos(2\theta_1 + \theta_3)] \},\end{aligned}$$

$$\begin{aligned}\mathcal{J}_2 &= \{ \rho_1^2 \rho_2^2 + \rho_1^2 \rho_3^2 \\&\quad - \rho_1 \rho_2 \rho_3 \rho_4 (\sin(\theta_1 - \theta_2 - \theta_3 + \theta_4) \\&\quad - \rho_1 \rho_2 \rho_3 \rho_4 \sqrt{3} \sin(\theta_1 - \theta_2 - \theta_3 + \theta_4)),\end{aligned}$$

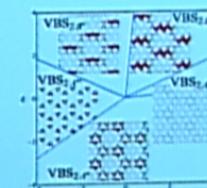
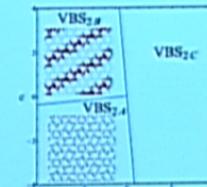
$$\begin{aligned}\mathcal{J}_3 &= \{ \rho_1^2 \rho_2^2 \cos(2\theta_1 + \theta_3 + \theta_4) \\&\quad + (-2 + \sqrt{3}) \sin(2\theta_1 + \theta_3 + \theta_4) \\&\quad + \rho_1^2 \rho_2^2 \cos(2\theta_2 + \theta_4 + \theta_3),\end{aligned}$$

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## Landau theories for VBS orders

- Case2:  $K<0$  and  $A=0$



### VBS 2B, 2B', 2B''

different kind of  
36-site VBS

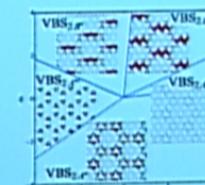
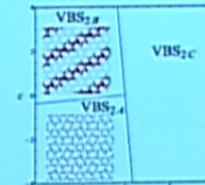
zigzag and parallel  
dimer structures

dimer modulations  
on top of the 6-site VBS



## Landau theories for VBS orders

- Case2:  $K < 0$  and  $A = 0$



### VBS 2B, 2B', 2B''

*different kind of  
36-site VBS*

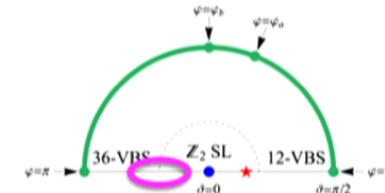
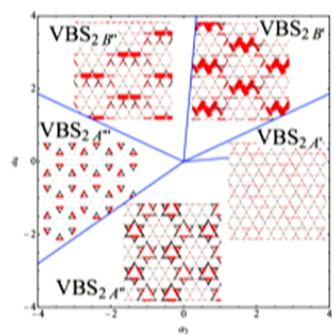
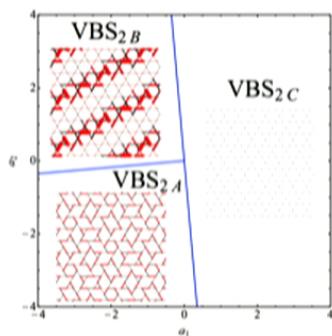
*zigzag and parallel  
dimer structures*

*dimer modulations  
on top of the 6-site VBS*



# Landau theories for VBS orders

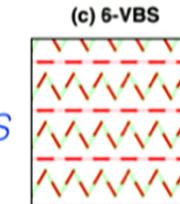
- Case2:  $K<0$  and  $A=0$



**VBS 2B, 2B', 2B''**

*different kind of  
36-site VBS  
zigzag and parallel  
dimer structures*

*dimer modulations  
on top of the 6-site VBS*



## Summary and future work

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- We presented a simple but generic  $Z_2$  gauge theory exactly equivalent to a quantum dimer model.
- The effective theory captures previously proposed various phases:  $Z_2$  SL, 12-site VBS, 36-site VBS. Wan & Tchernyshyov, PRB (2013)
- Our results are remarkably consistent with the results of a previous (conventional)  $Z_2$  gauge theory approach. Huh et al. PRB 87, 235108 (2013)
- We found interesting dimer melting effects on the 36-site VBS under the anisotropic triangular geometry.
- It would be interesting to investigate which microscopic spin Hamiltonian is mapped into our effective theory with the triangular anisotropy. The simplest one will be  $J_1-J_2$  Heisenberg model.