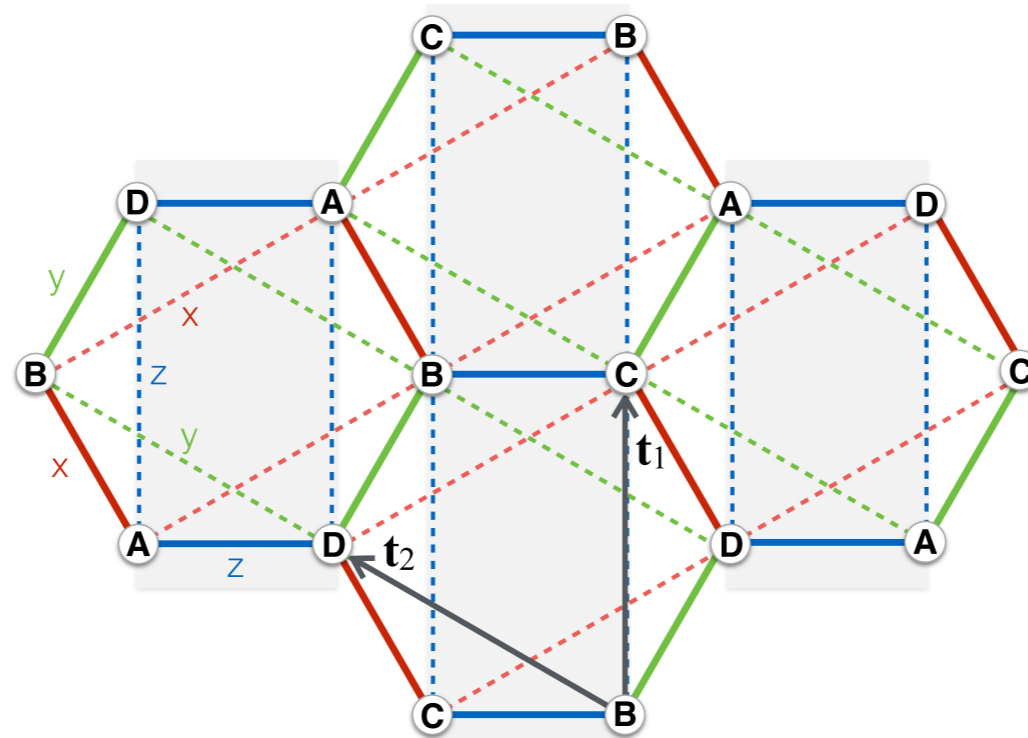




Phase diagram and quantum order-by-disorder in the Kitaev K_1 - K_2 honeycomb magnet



Ioannis Rousochatzakis, University of Minnesota

Spin Orbit Summer School, Quantum Matter Institute, UBC Vancouver, Canada

24 October 2015

Collaborators

- Natalia Perkins (UMN)



- Stephan Rachel (TU Dresden)



- Johannes Reuter (TU Berlin)

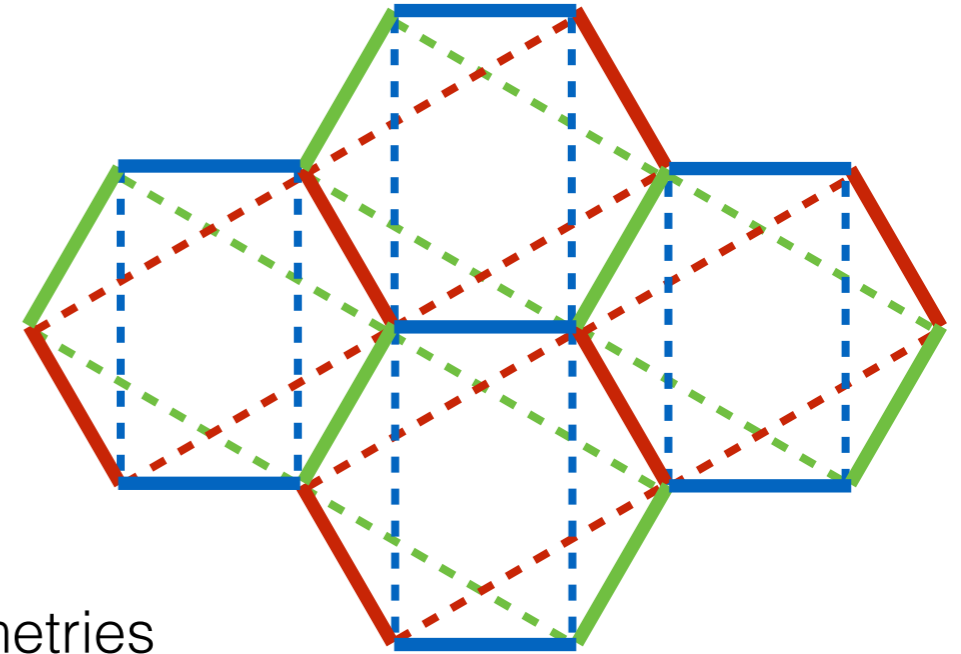


- Ronny Thomale (Wuerzburg University)

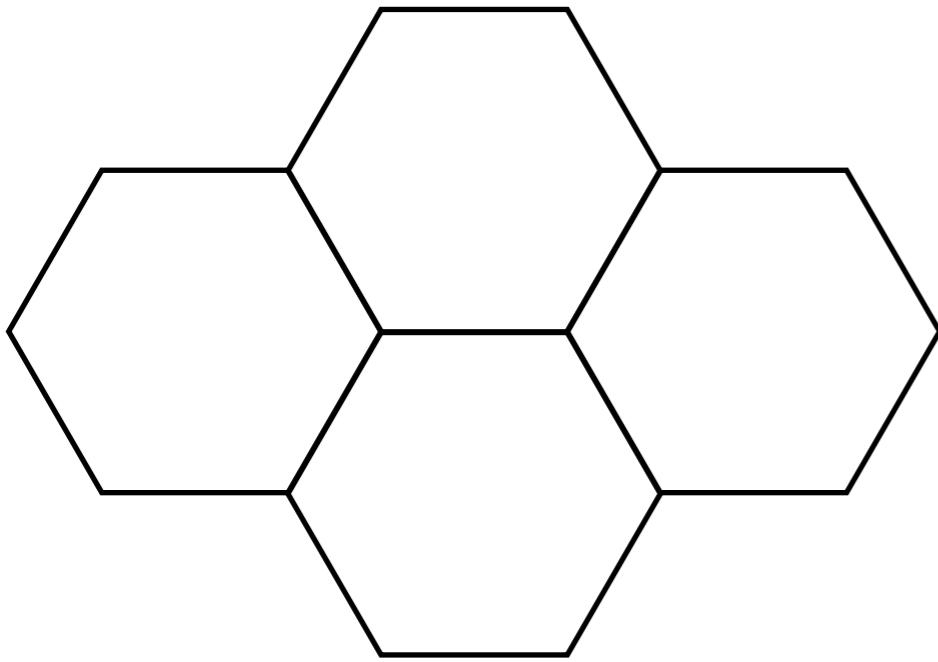


Outline

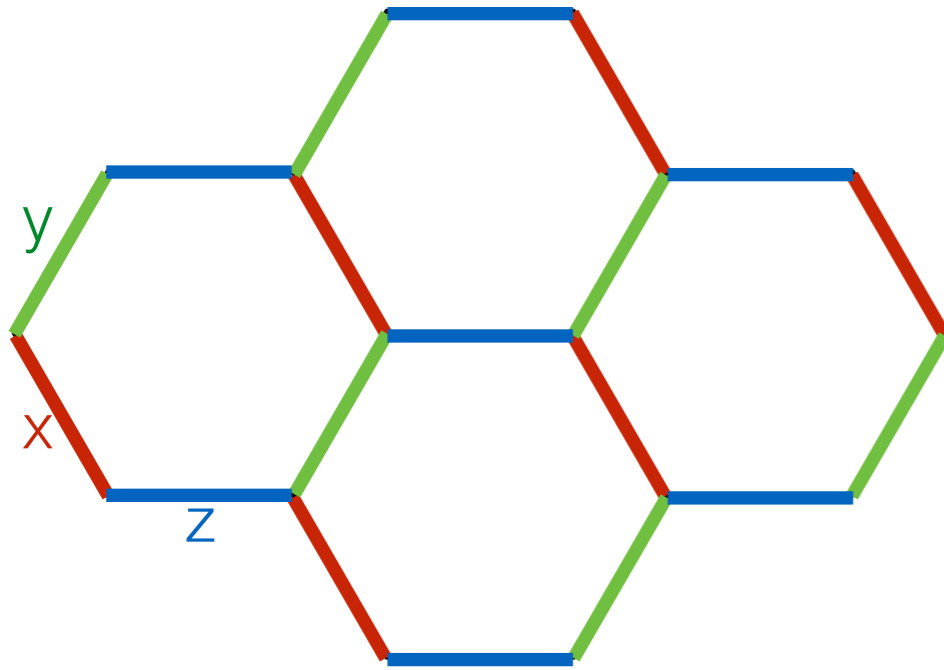
- Motivation: Kitaev spin liquid in real materials
- Na_2IrO_3 : importance of second-neighbor interaction K_2
- Quantum K_1 - K_2 model: *hidden*, gauge-like dualities & symmetries
- Phase diagram from Exact Diagonalizations
- Physical mechanism of instability: Classical vs Quantum spins
- Outlook: back to materials



Kitaev's honeycomb model ($S=1/2$):



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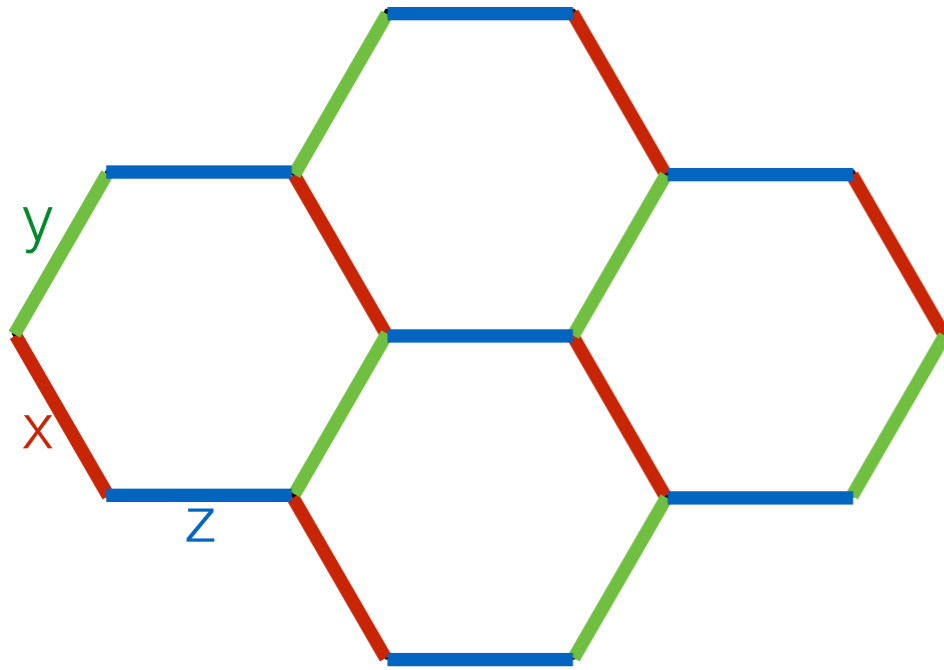


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Main motivation: Kitaev spin liquid

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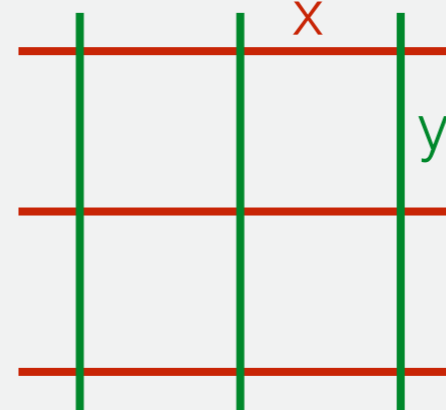
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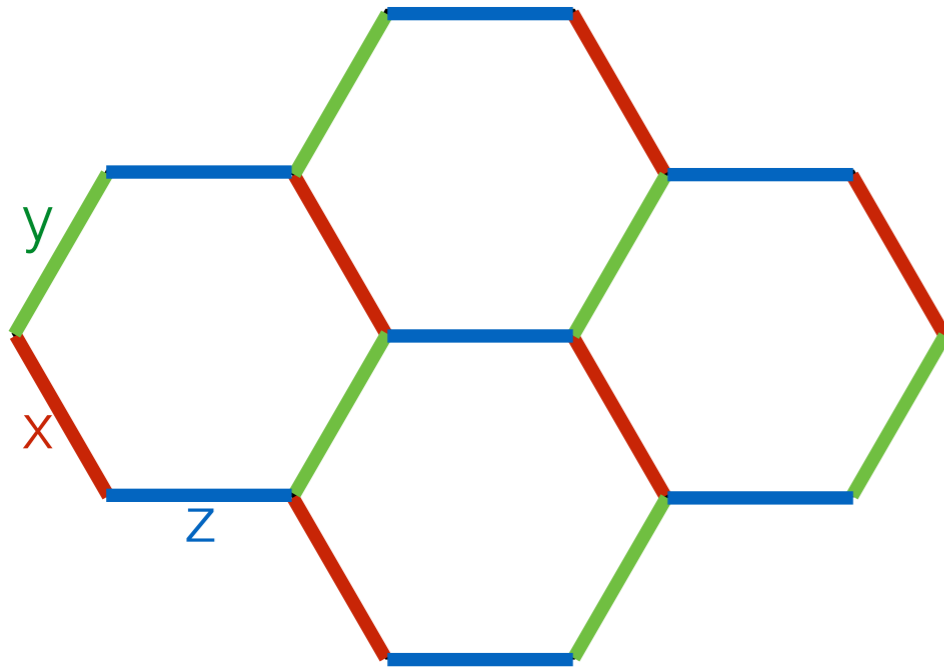
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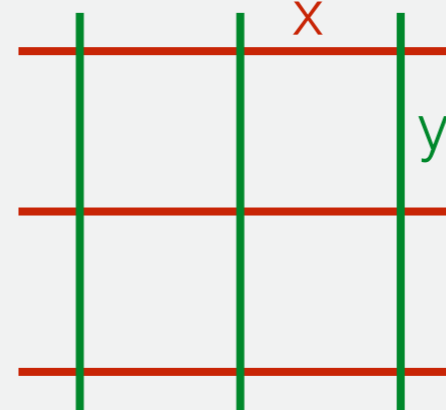
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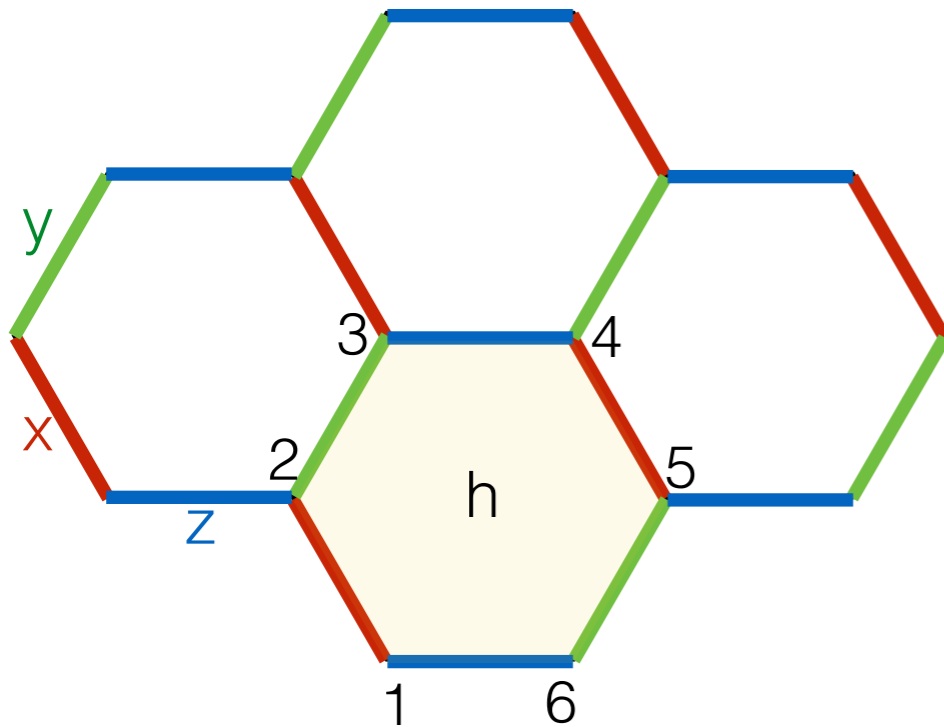


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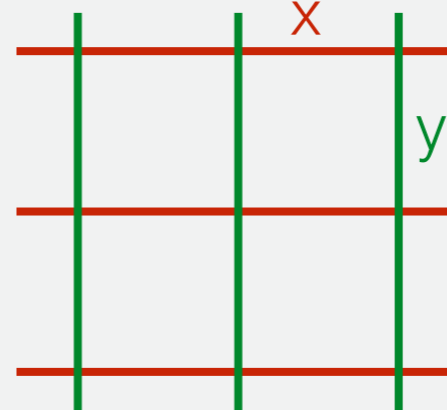
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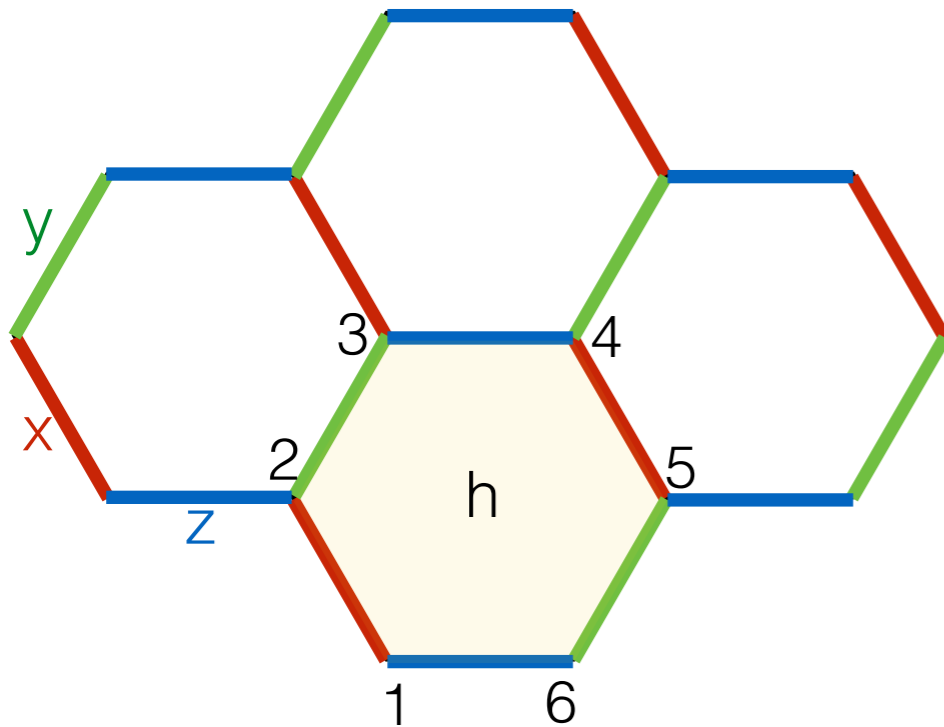
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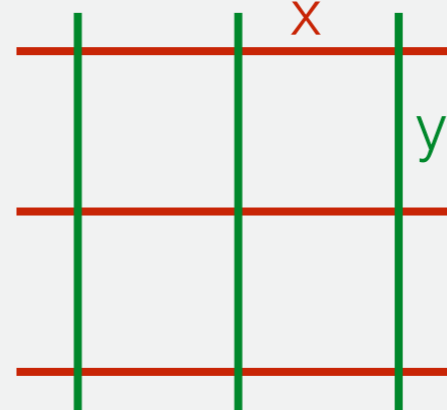
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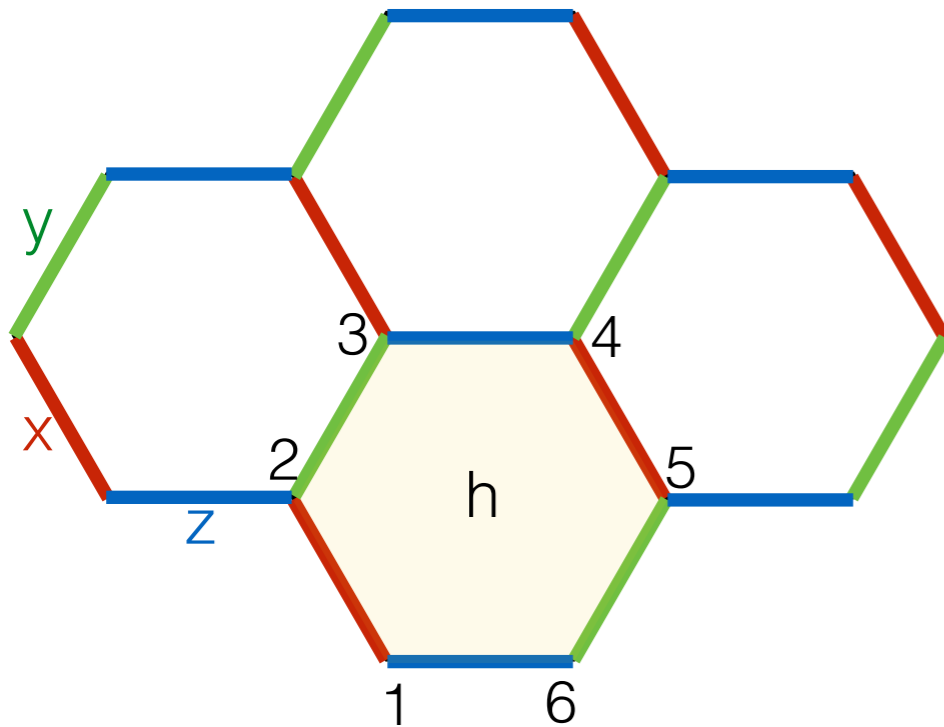
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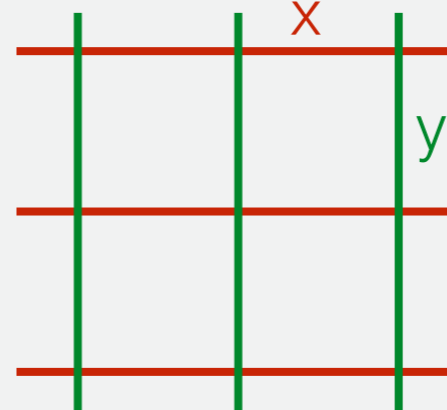
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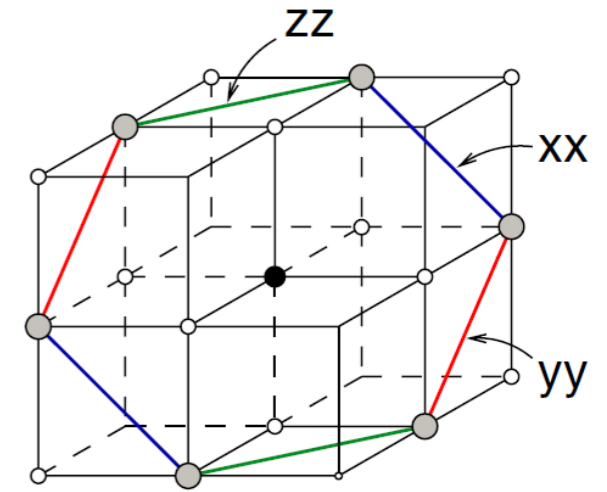
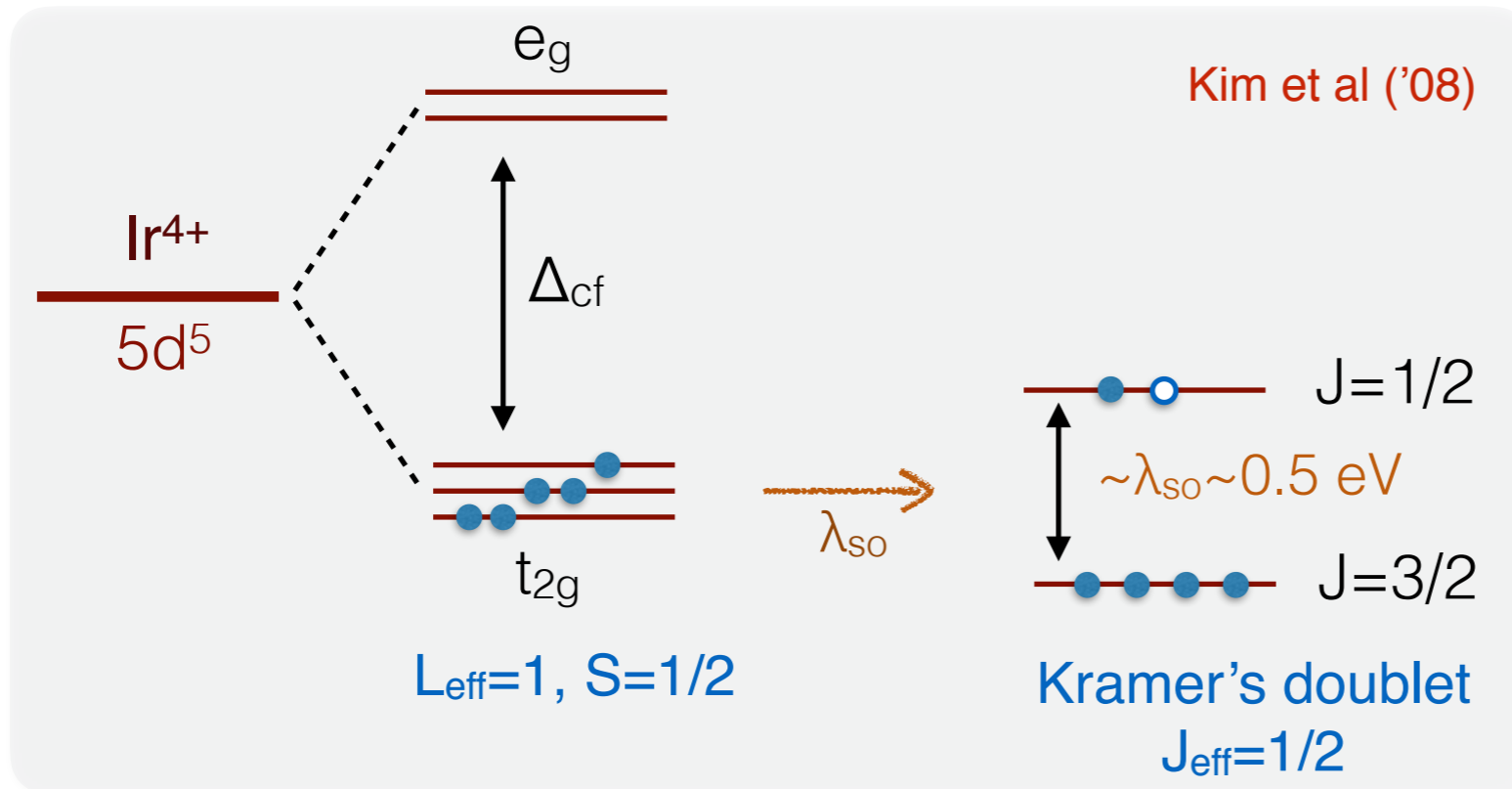
- excitations: gapless Majorana fermions and gapped $W_h = -1$ vortices

Material realizations: strong SOC with 90° oxygen bonding

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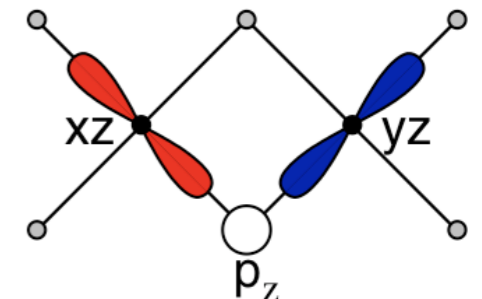
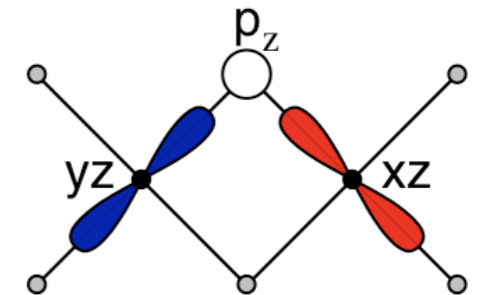
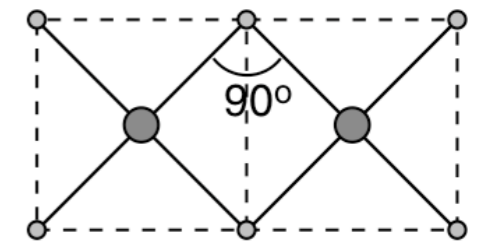
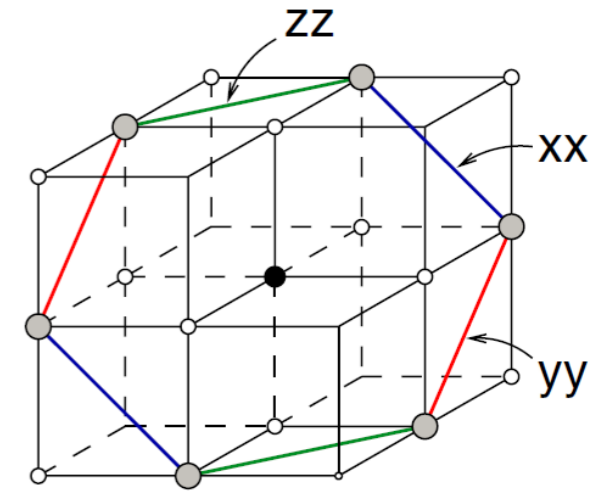
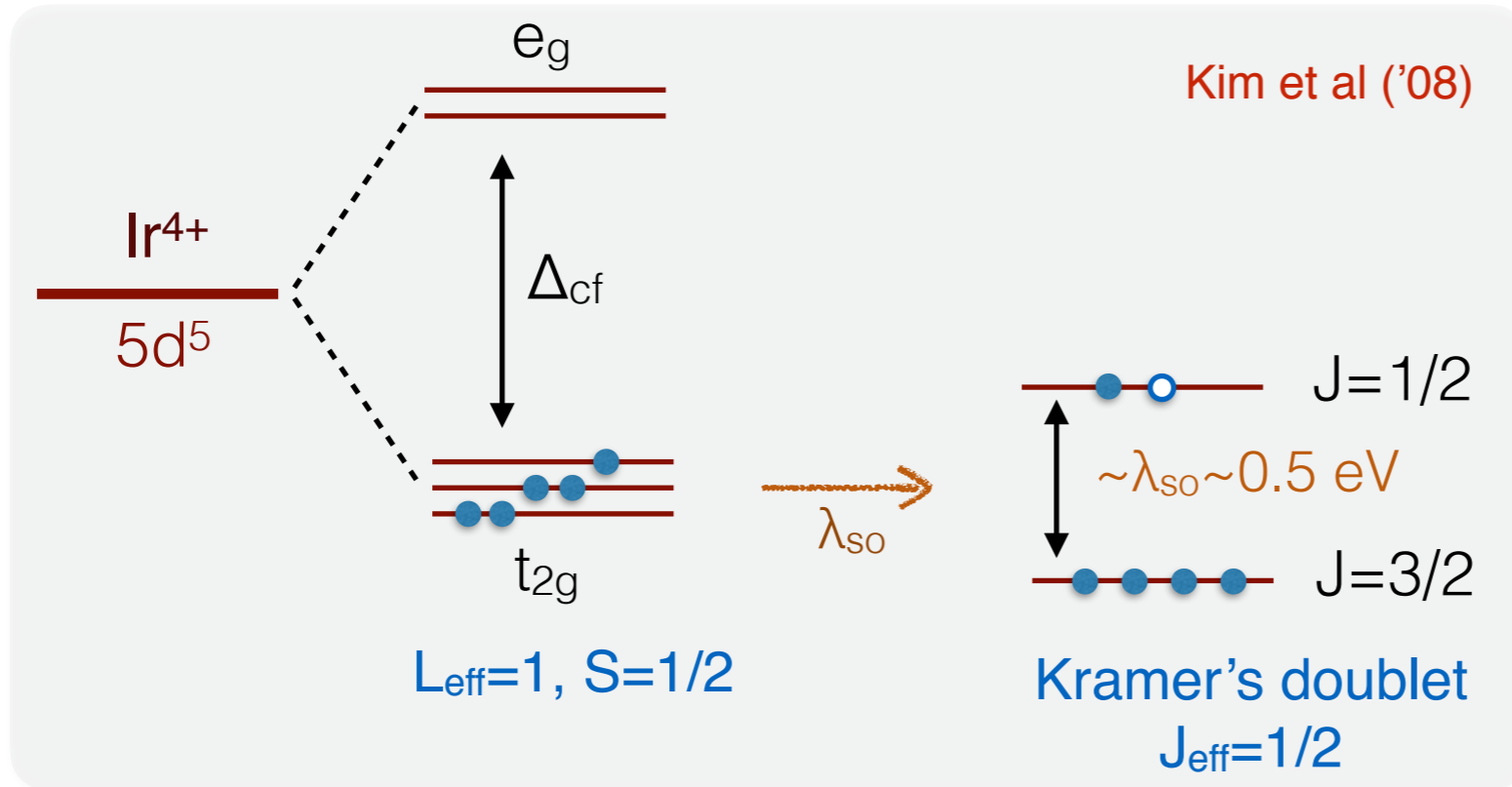
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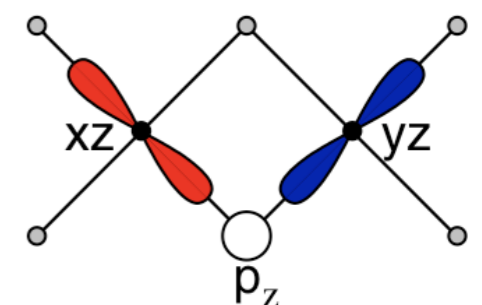
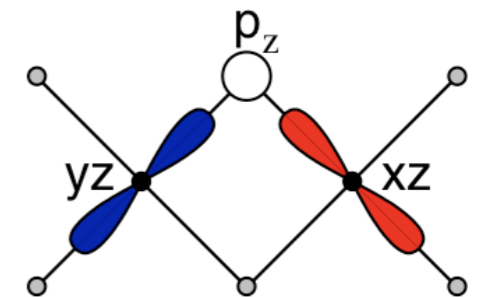
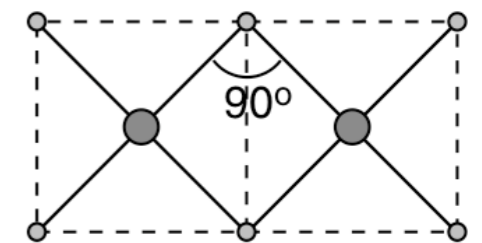
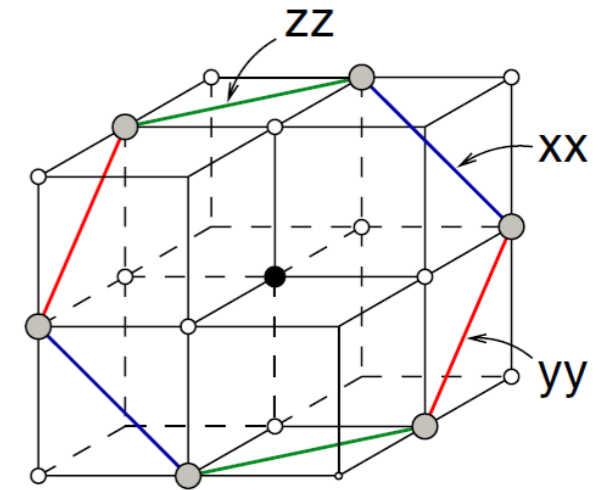
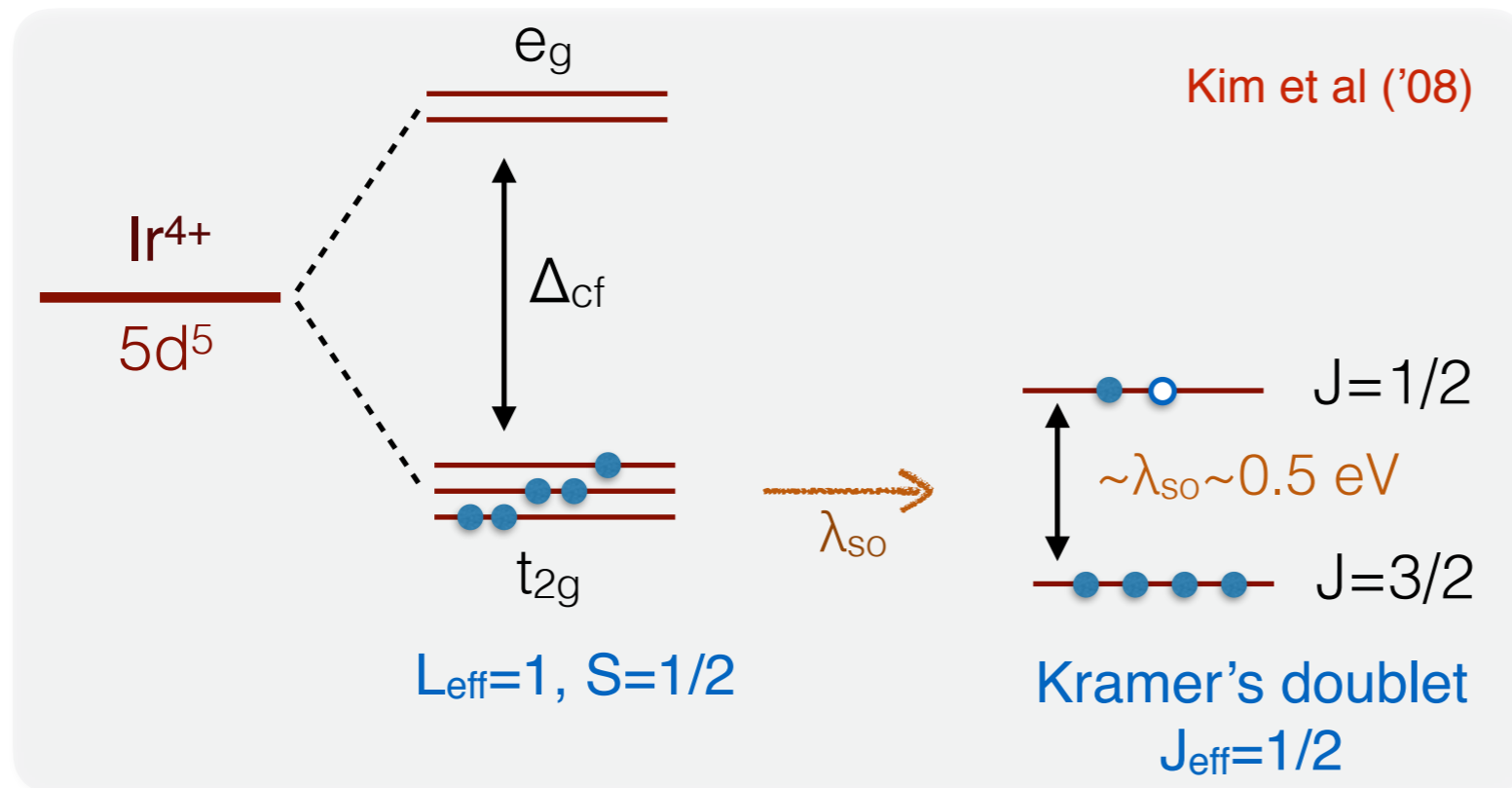


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- Quantum chemistry data for Na_2OIr_3 : $K_1=-17 \text{ meV}$, $J_1=3 \text{ meV}$,

Katukuri et al (2014)

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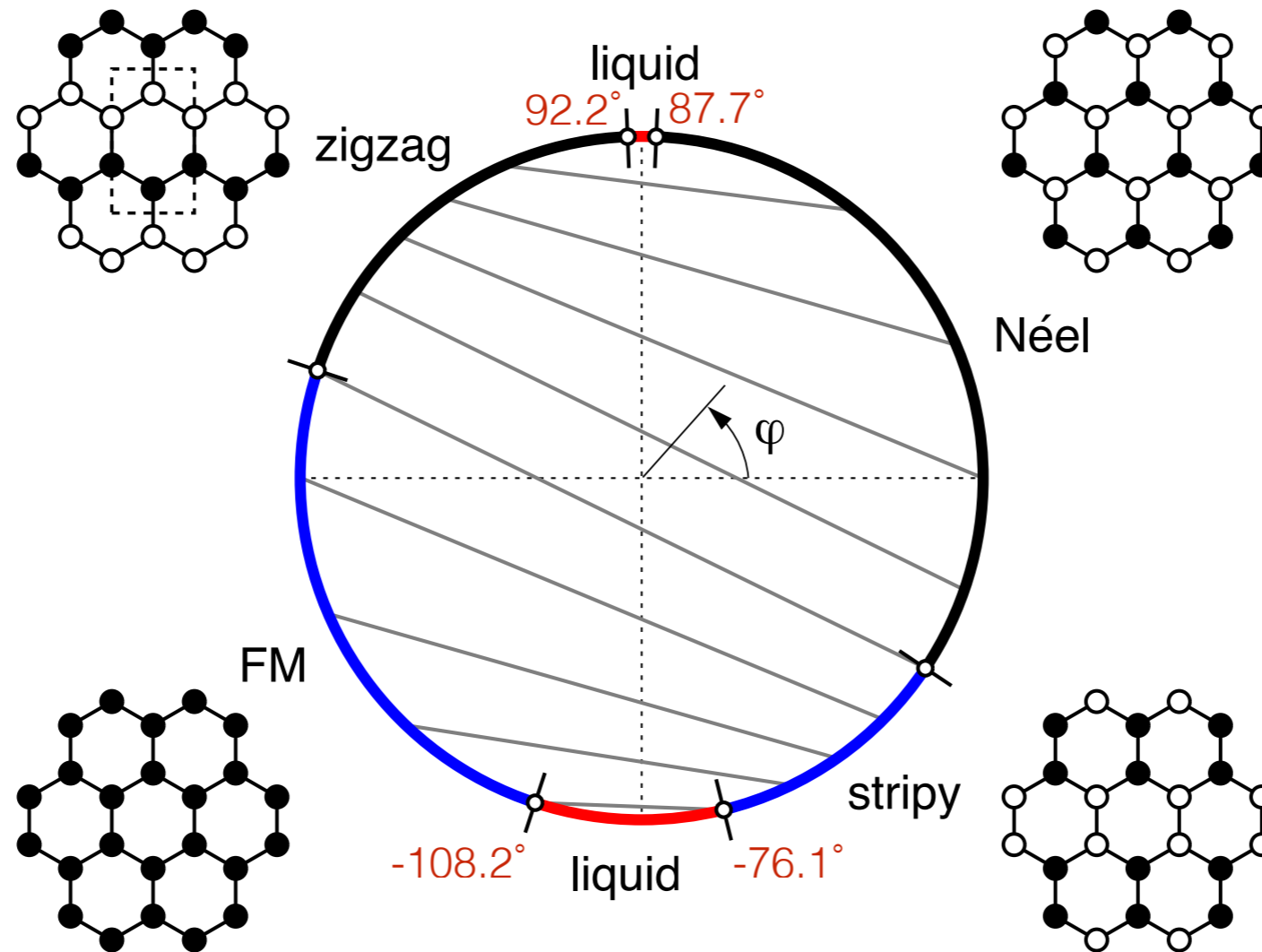
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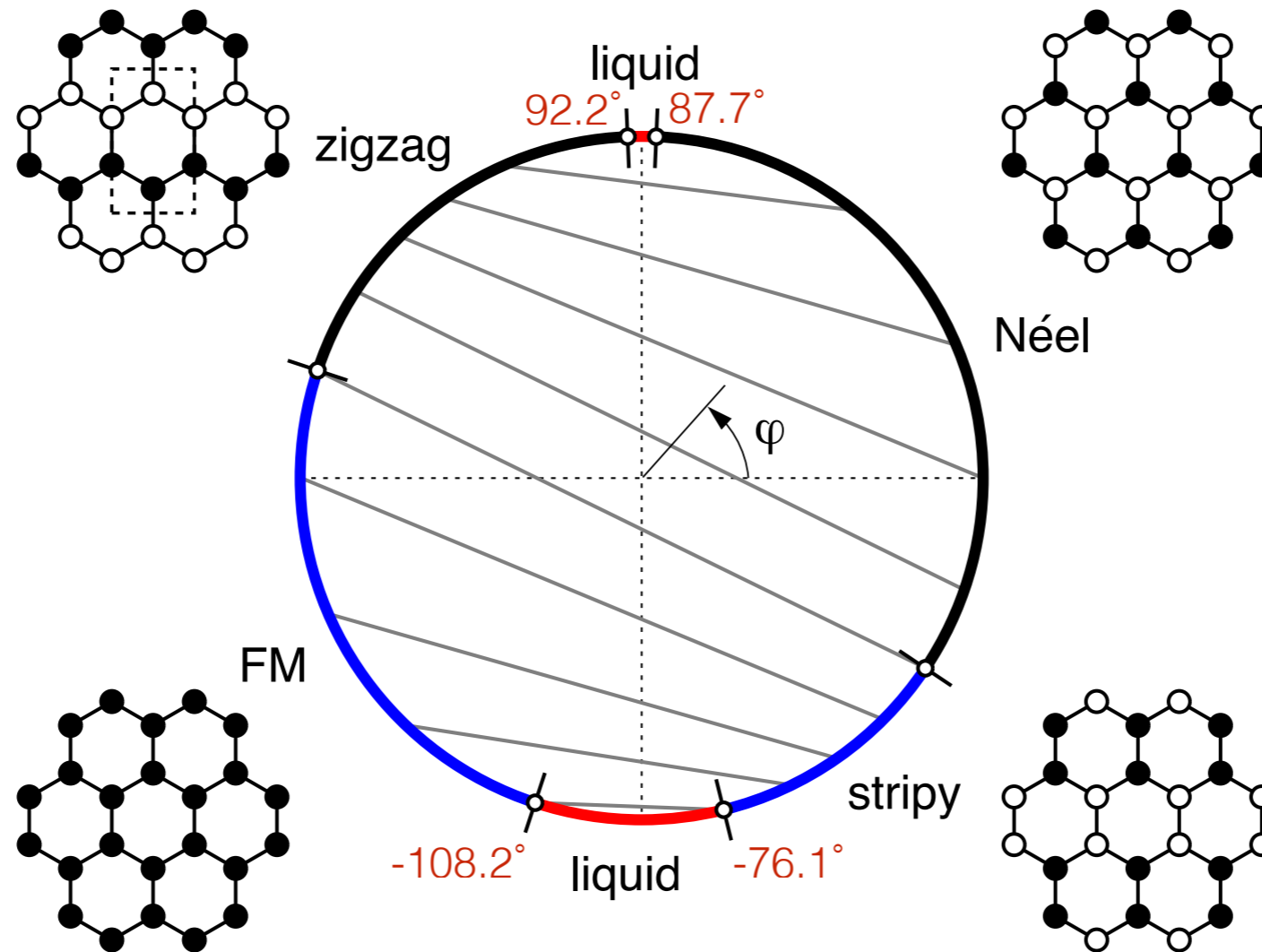


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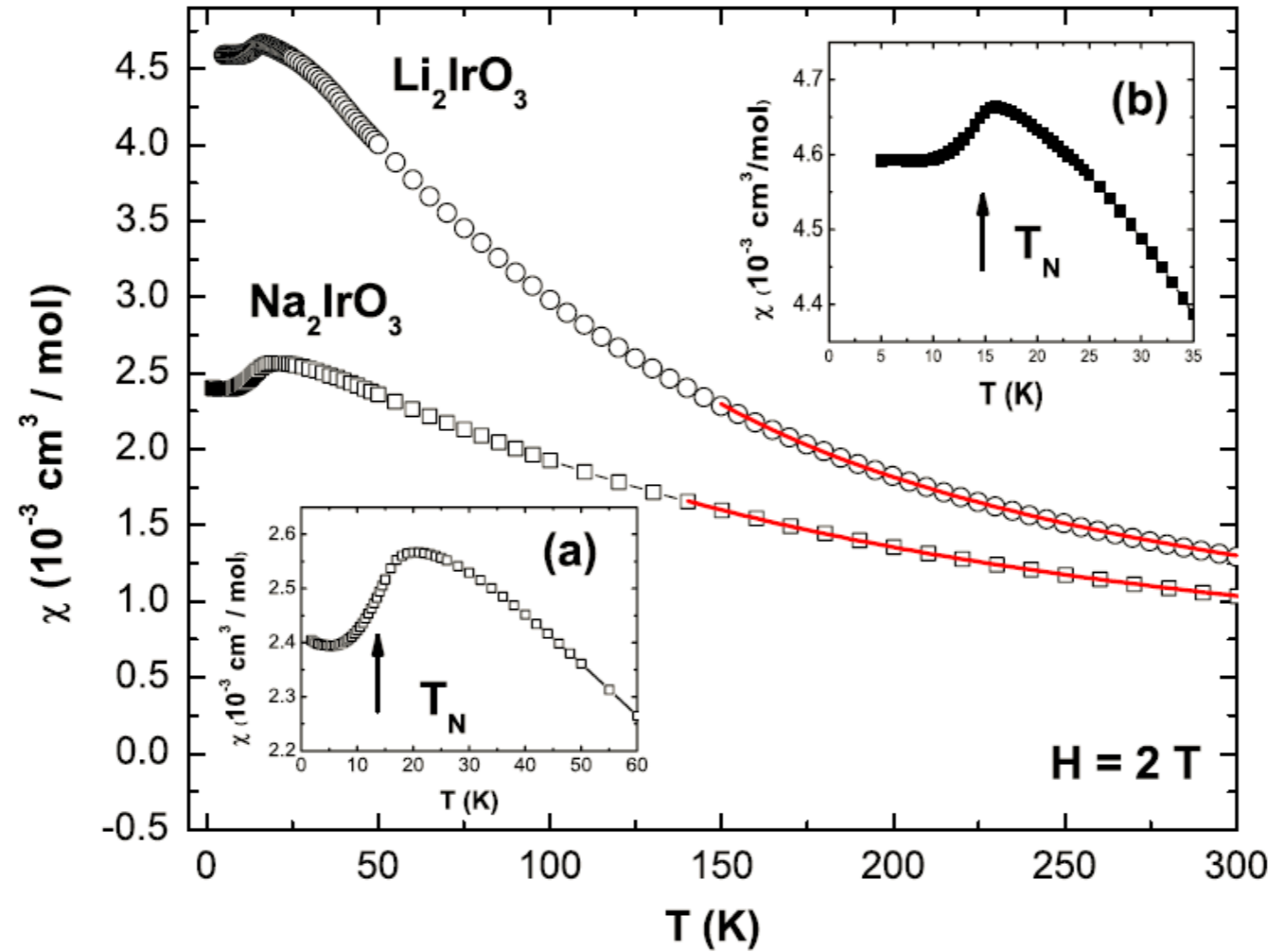


*lines represent a hidden duality

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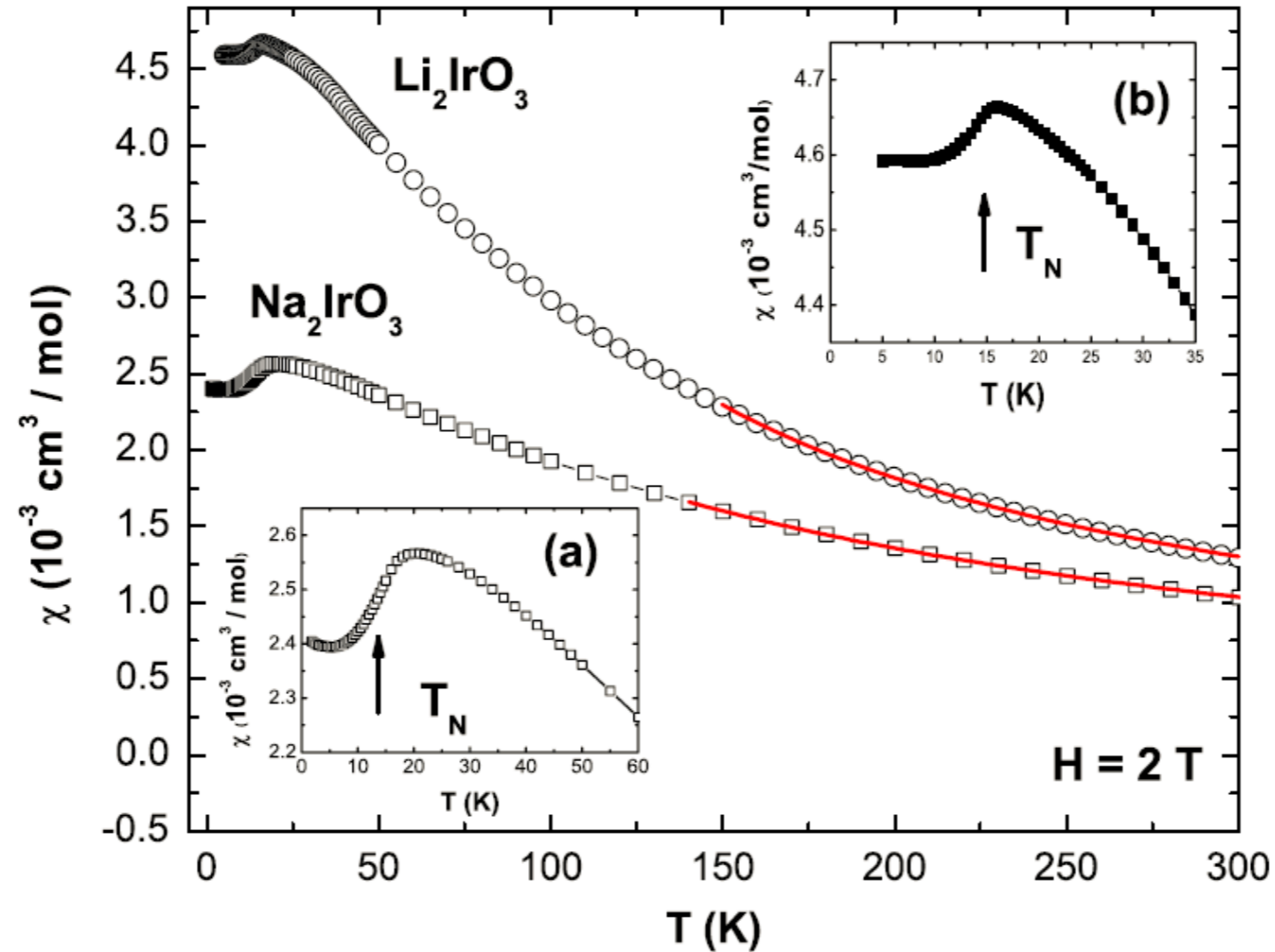
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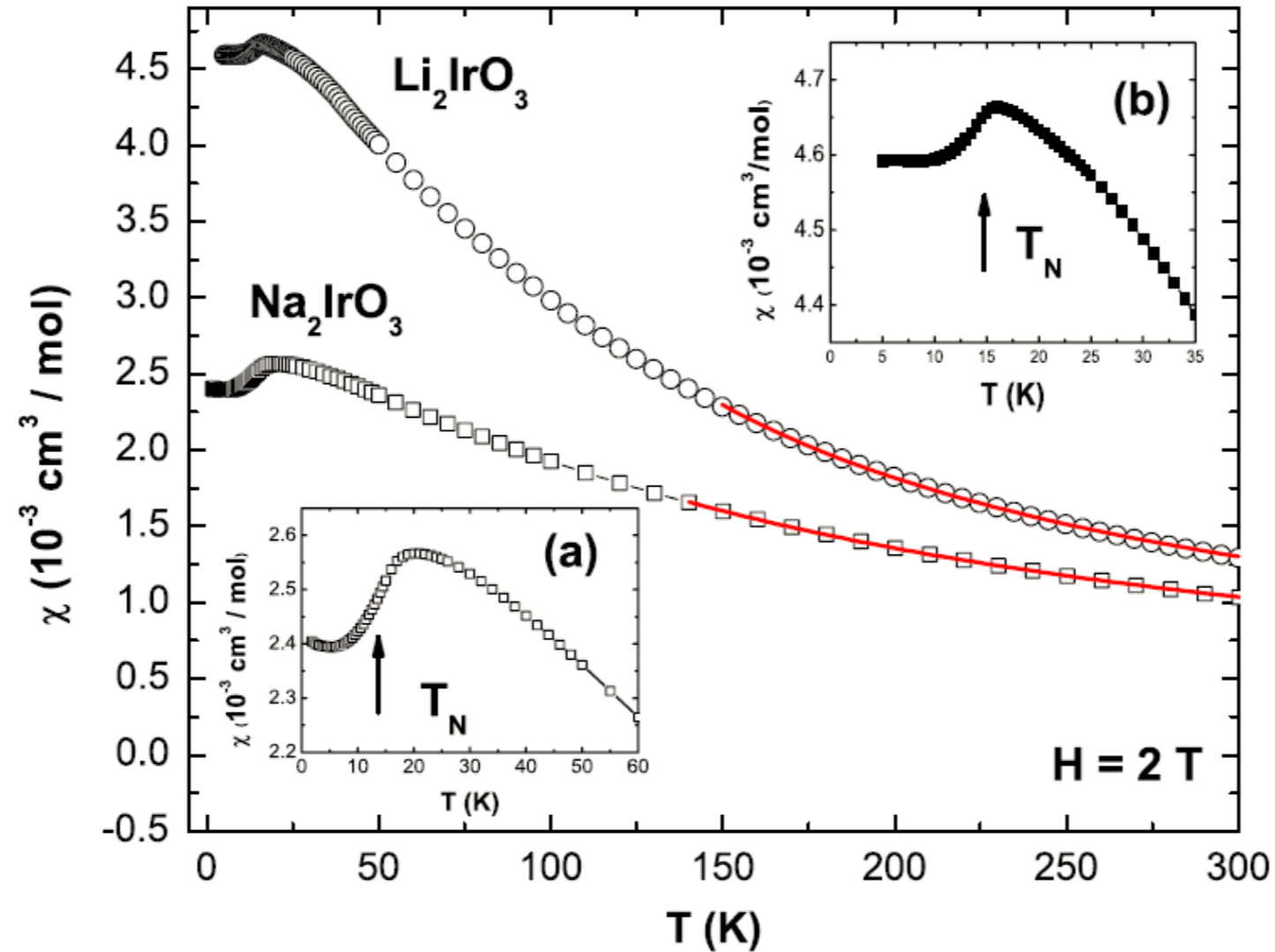


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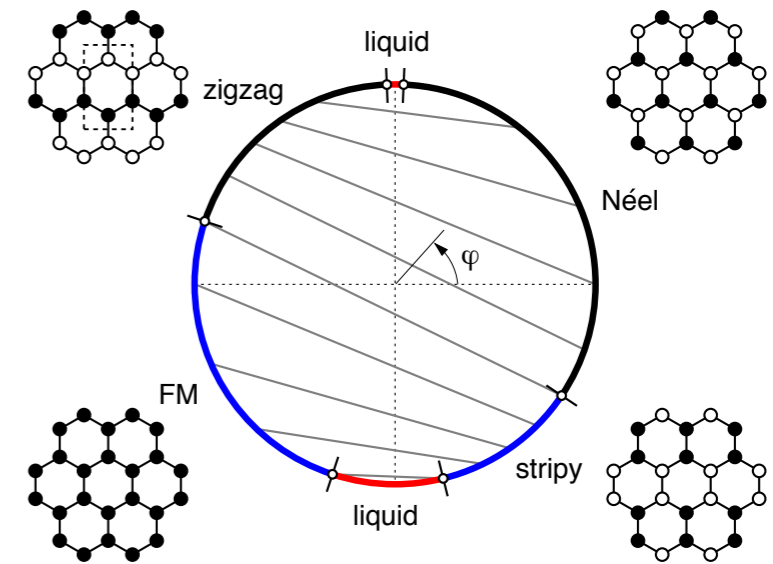
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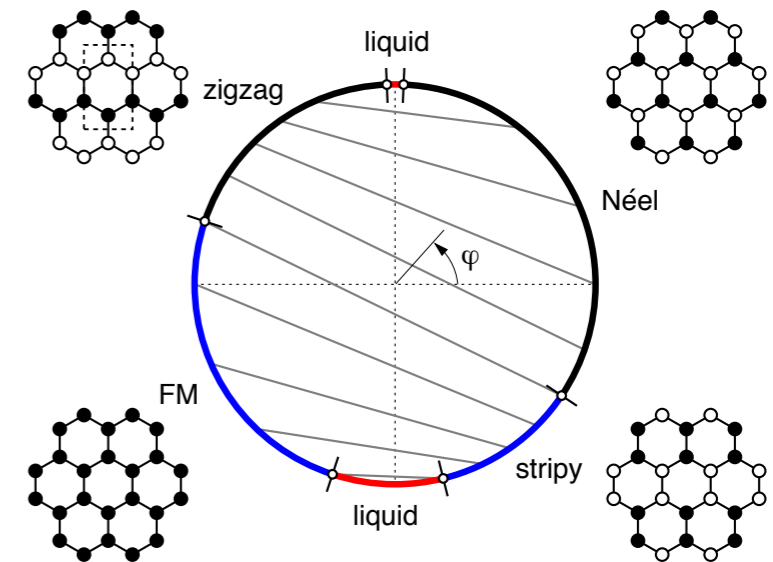
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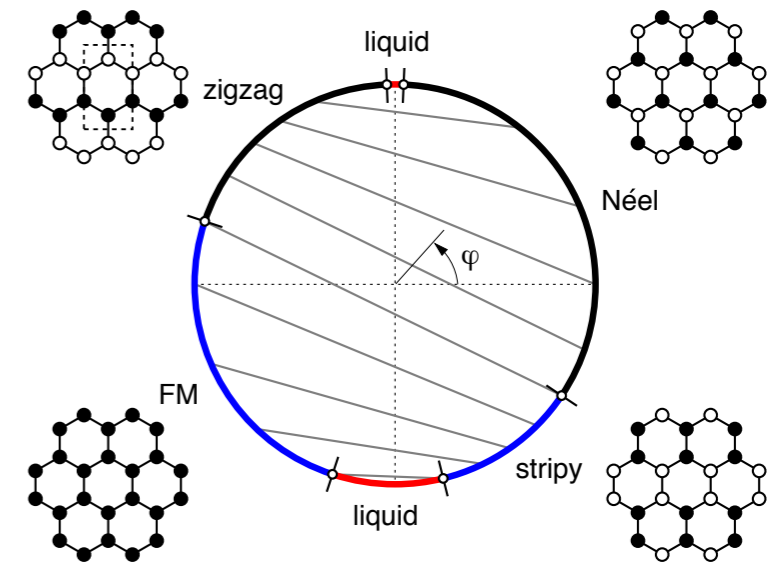
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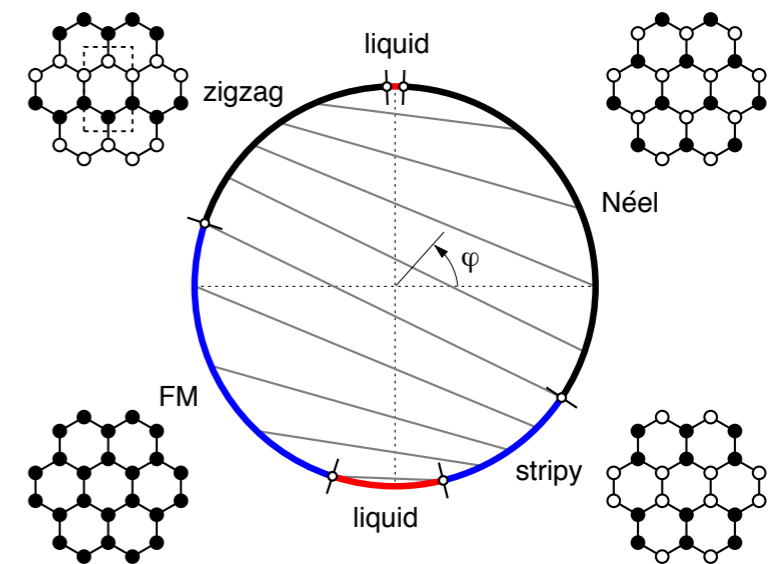
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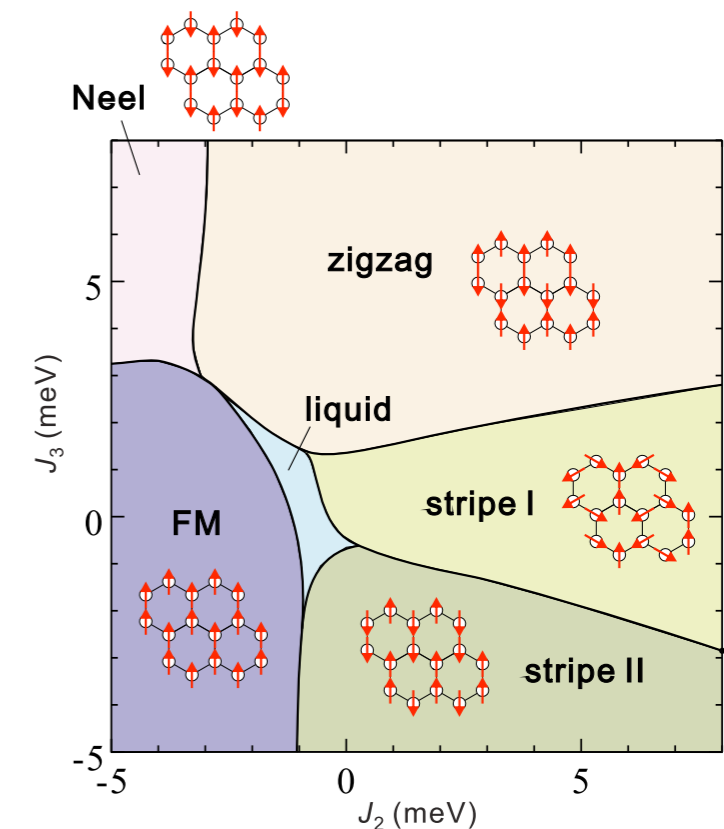
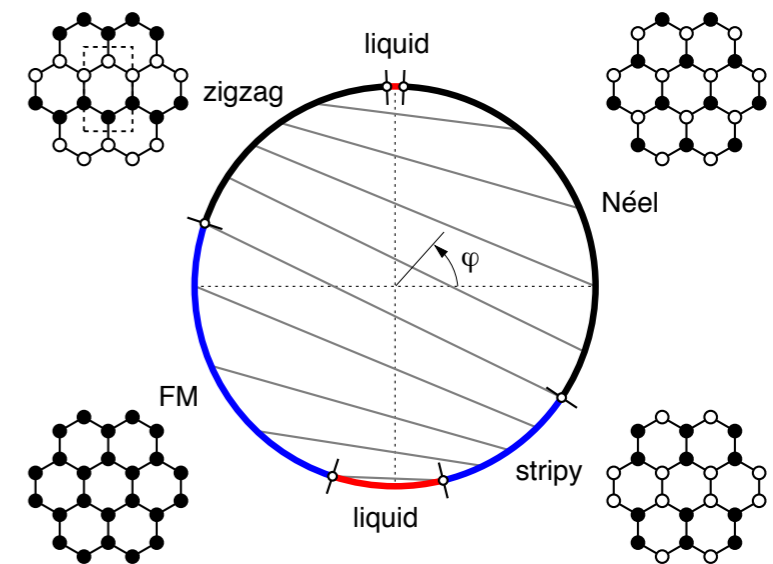
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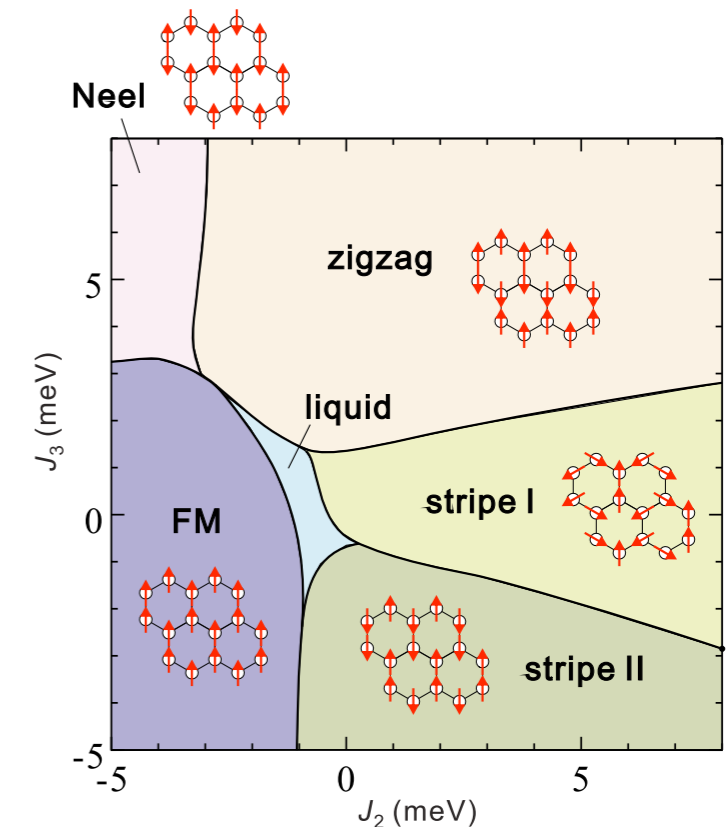
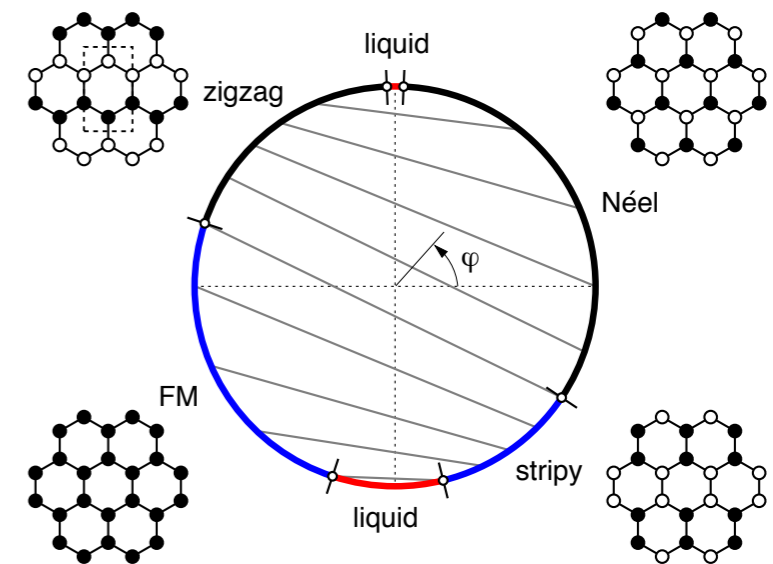
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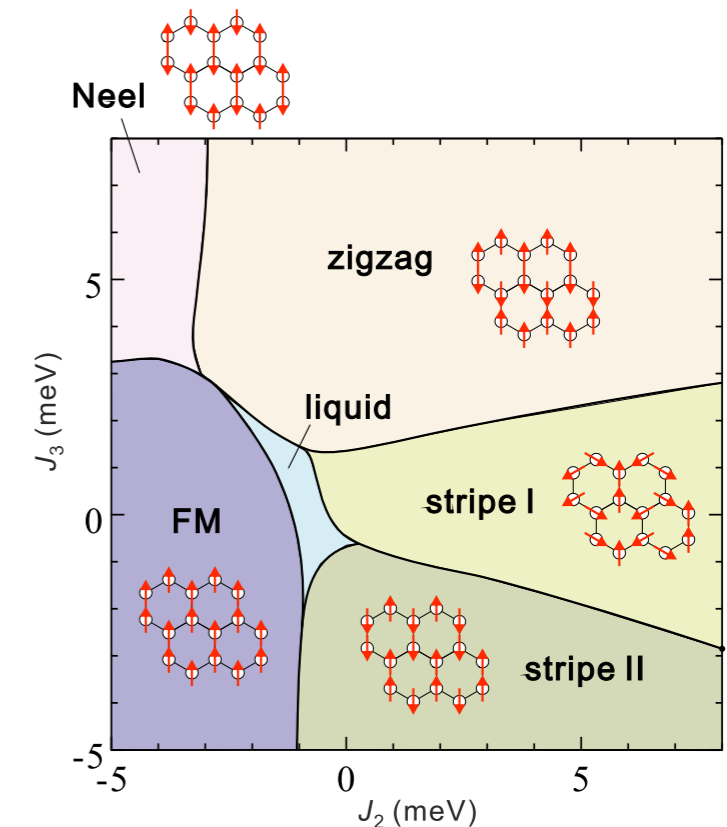
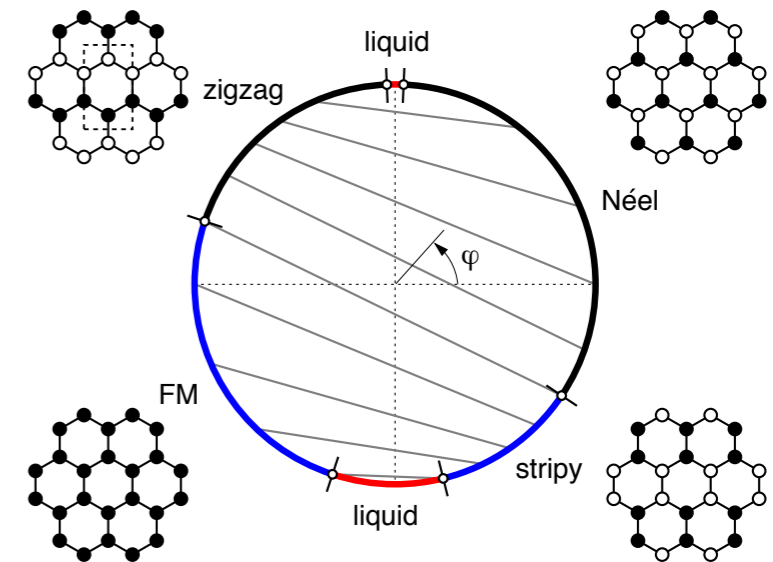
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- superexchange expansion: Sizyuk, Perkins, et al (2014)

- NN Γ is very small in Na_2IrO_3 (consistent with Q. Chem.)

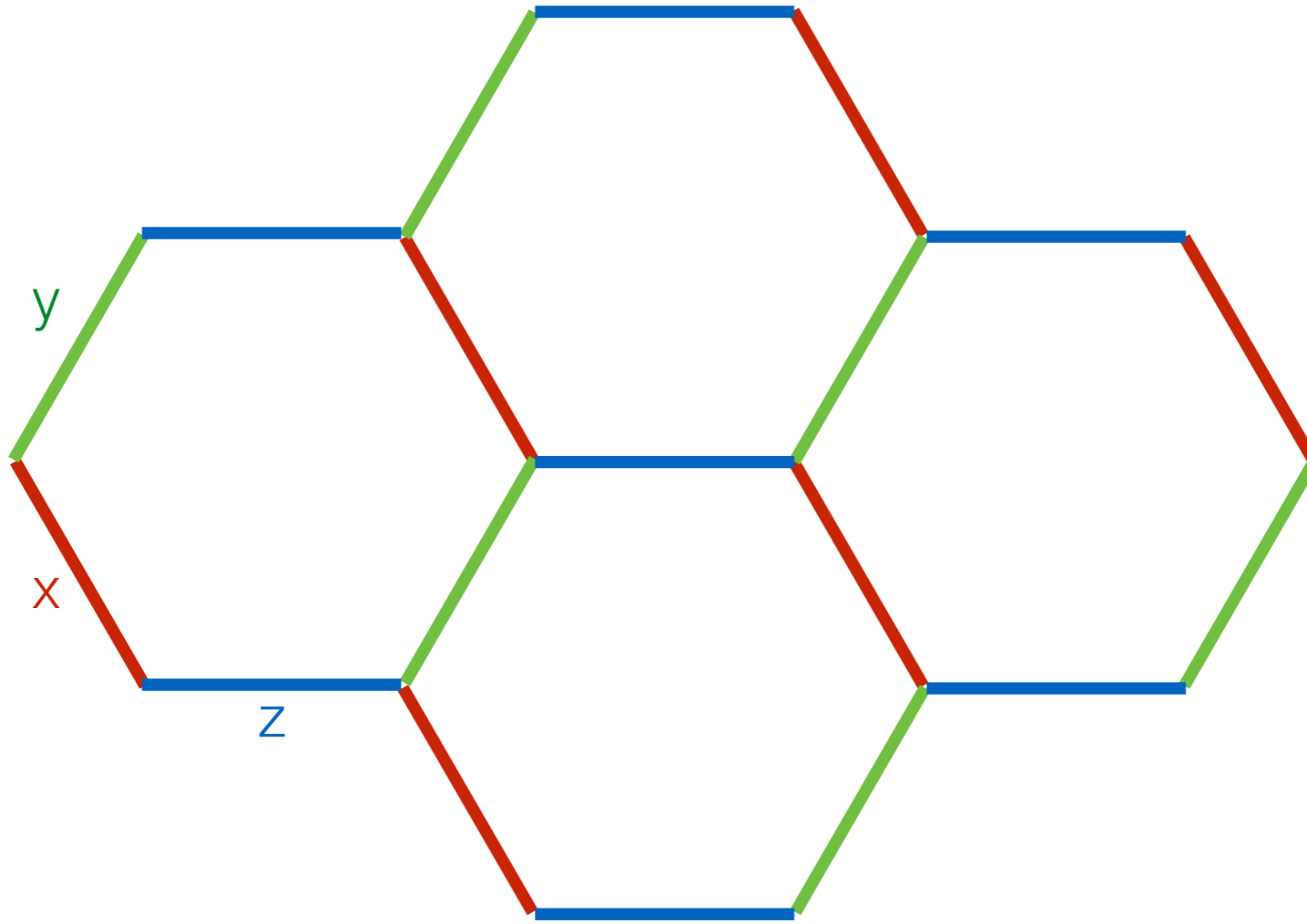
- K_2 is the largest coupling after K_1

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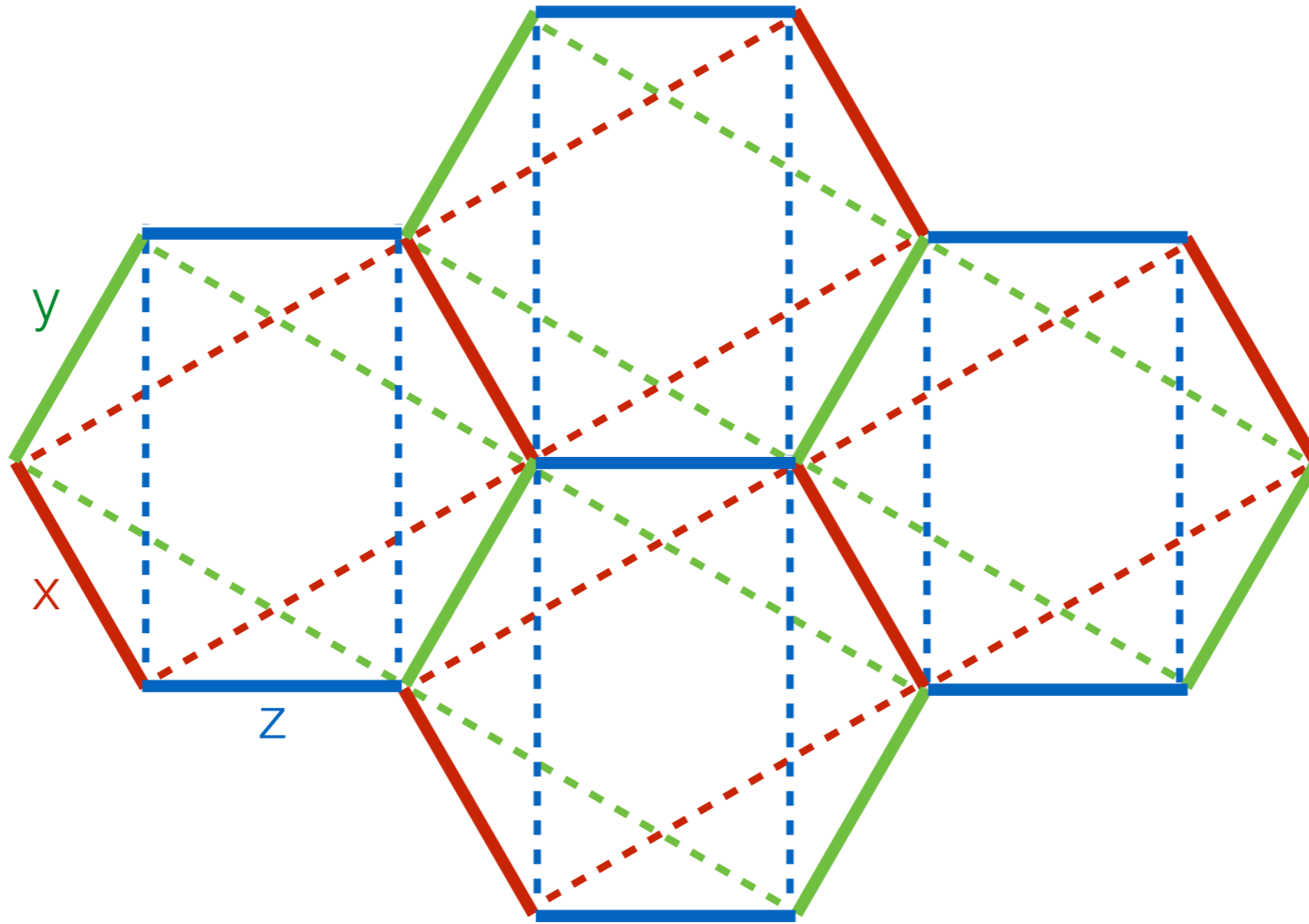


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The quantum K_1 - K_2 model: general

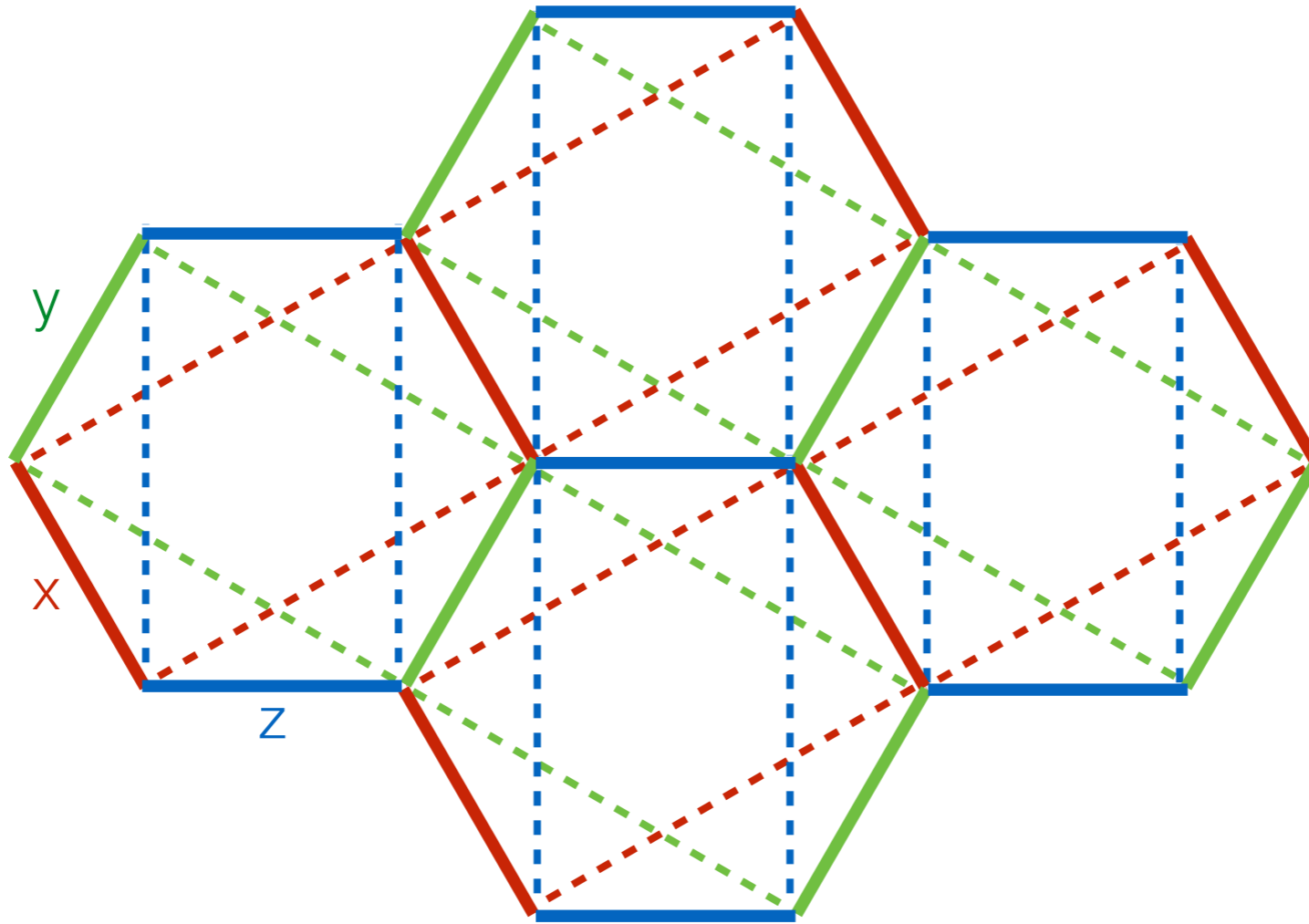


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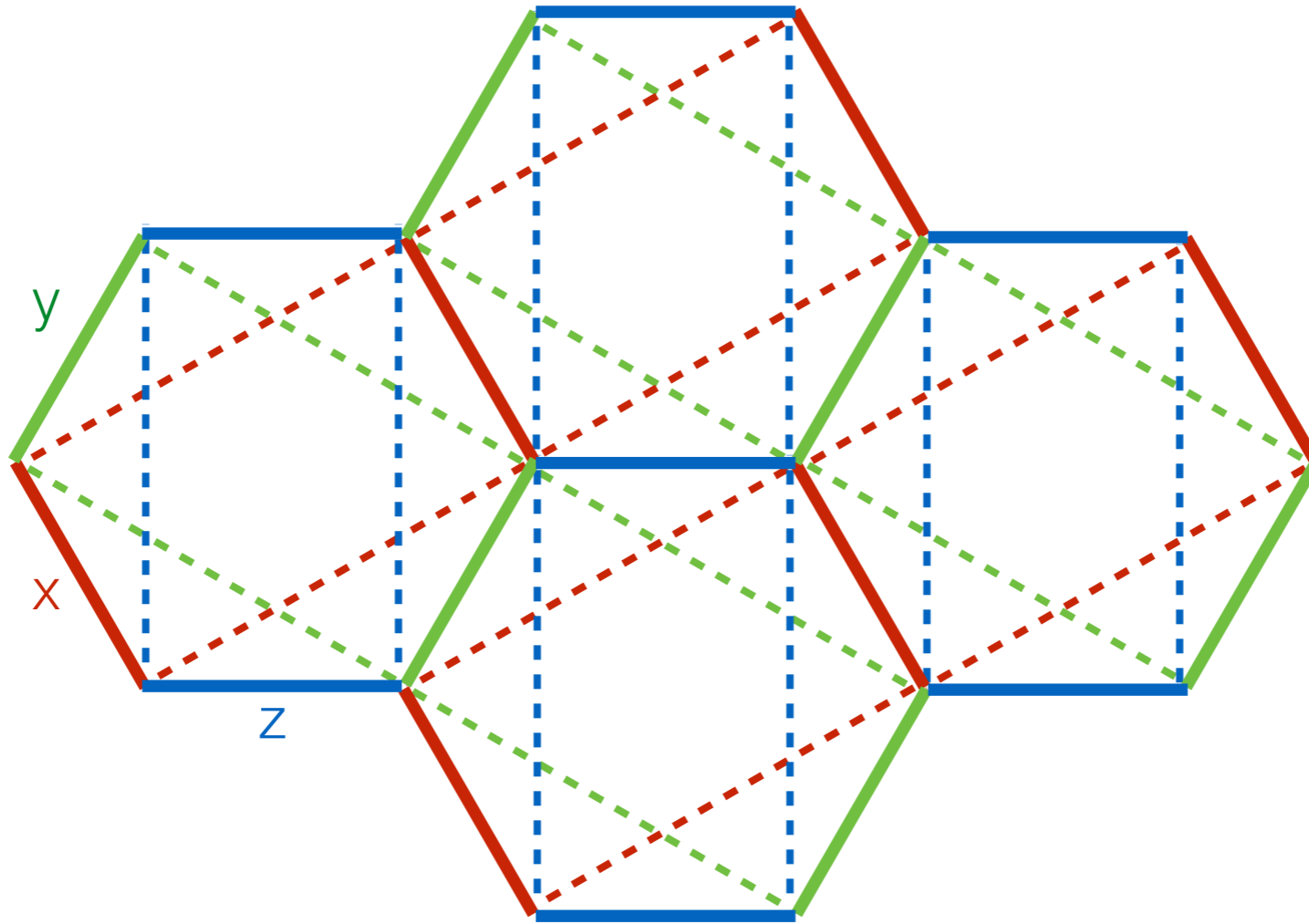


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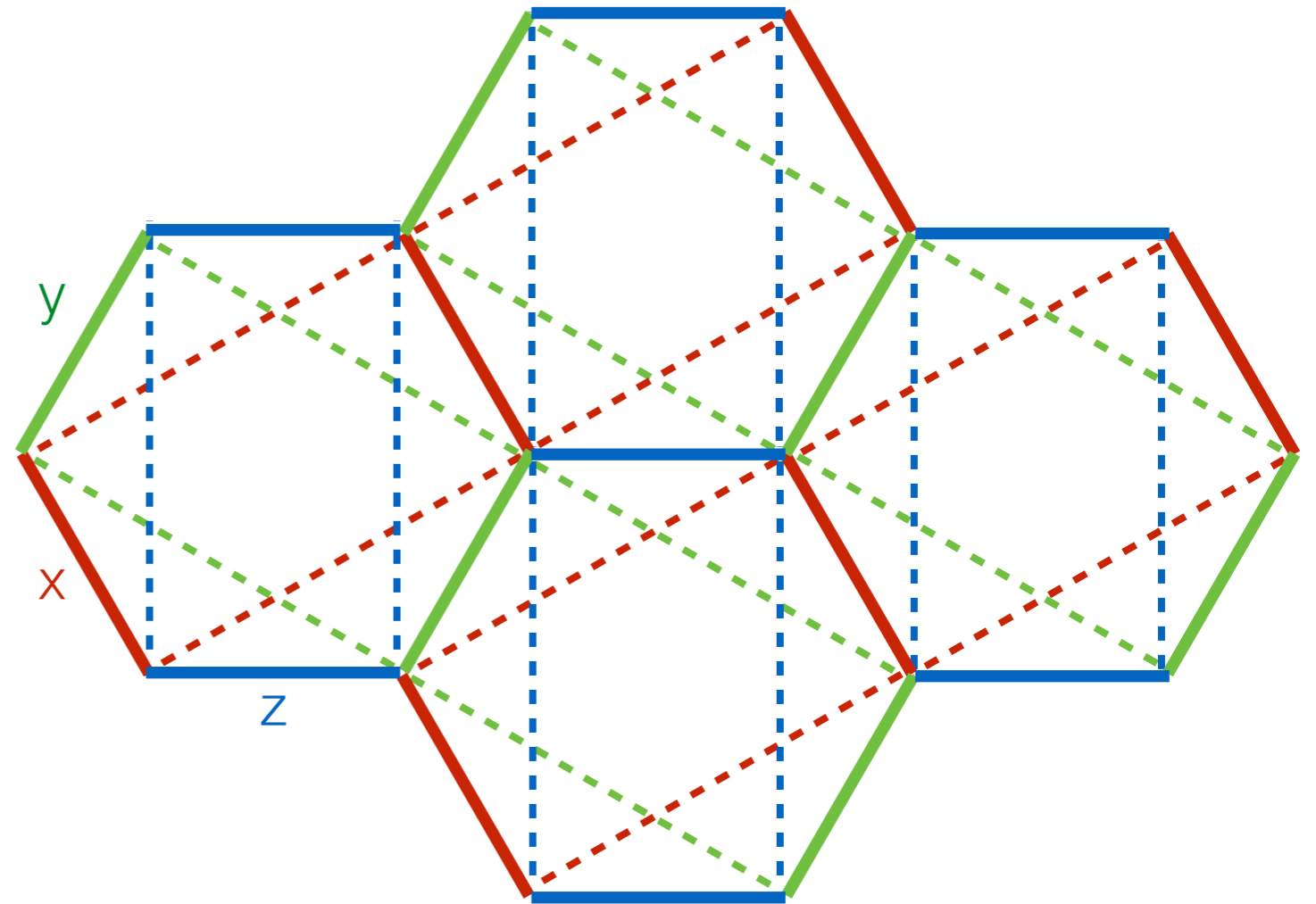
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- K_2 kills the exact solvability: W_h are no longer conserved

The quantum K_1 - K_2 model: hidden duality & symmetries

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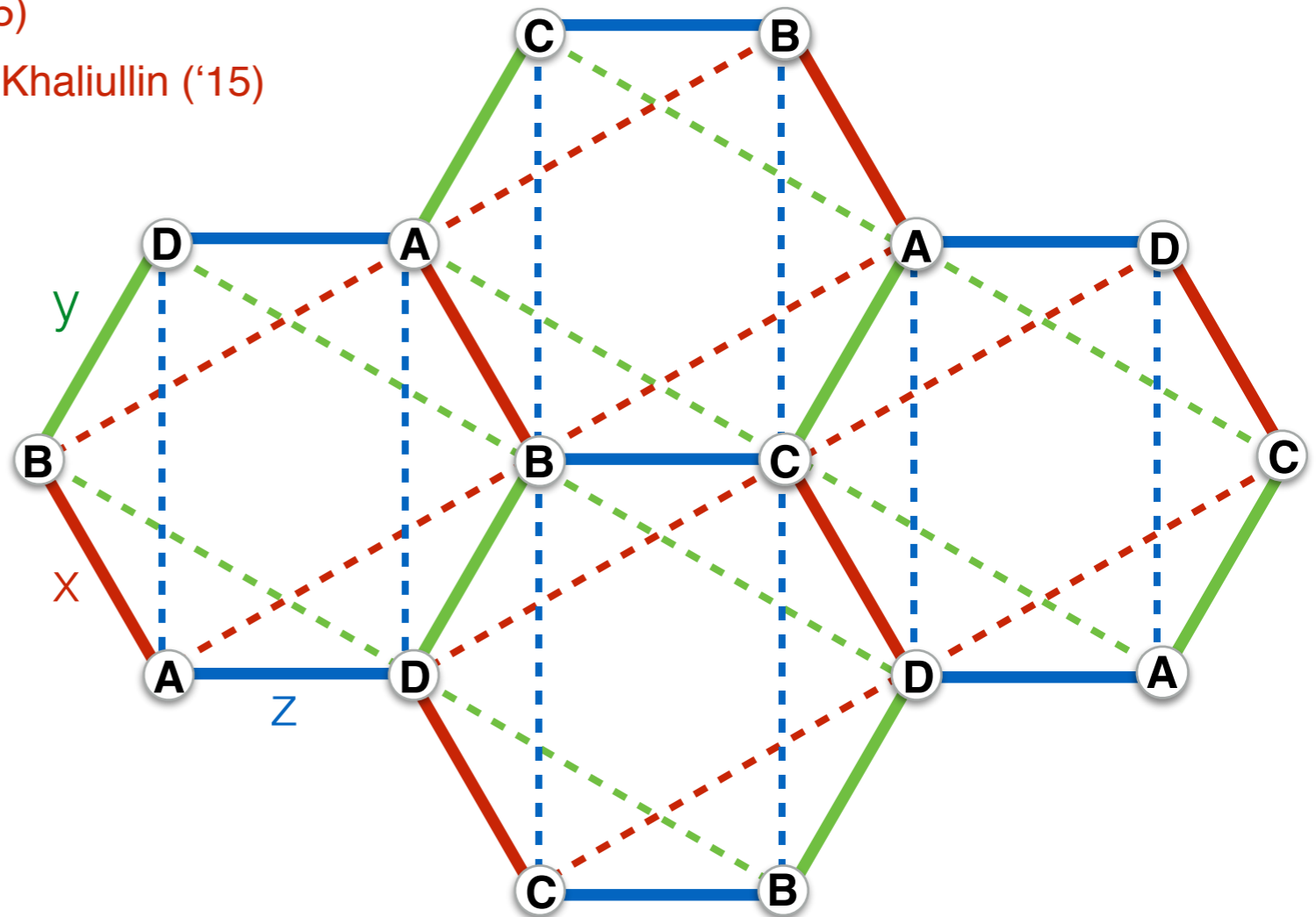
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Khaliullin ('05)

Chaloupka & Khaliullin ('15)



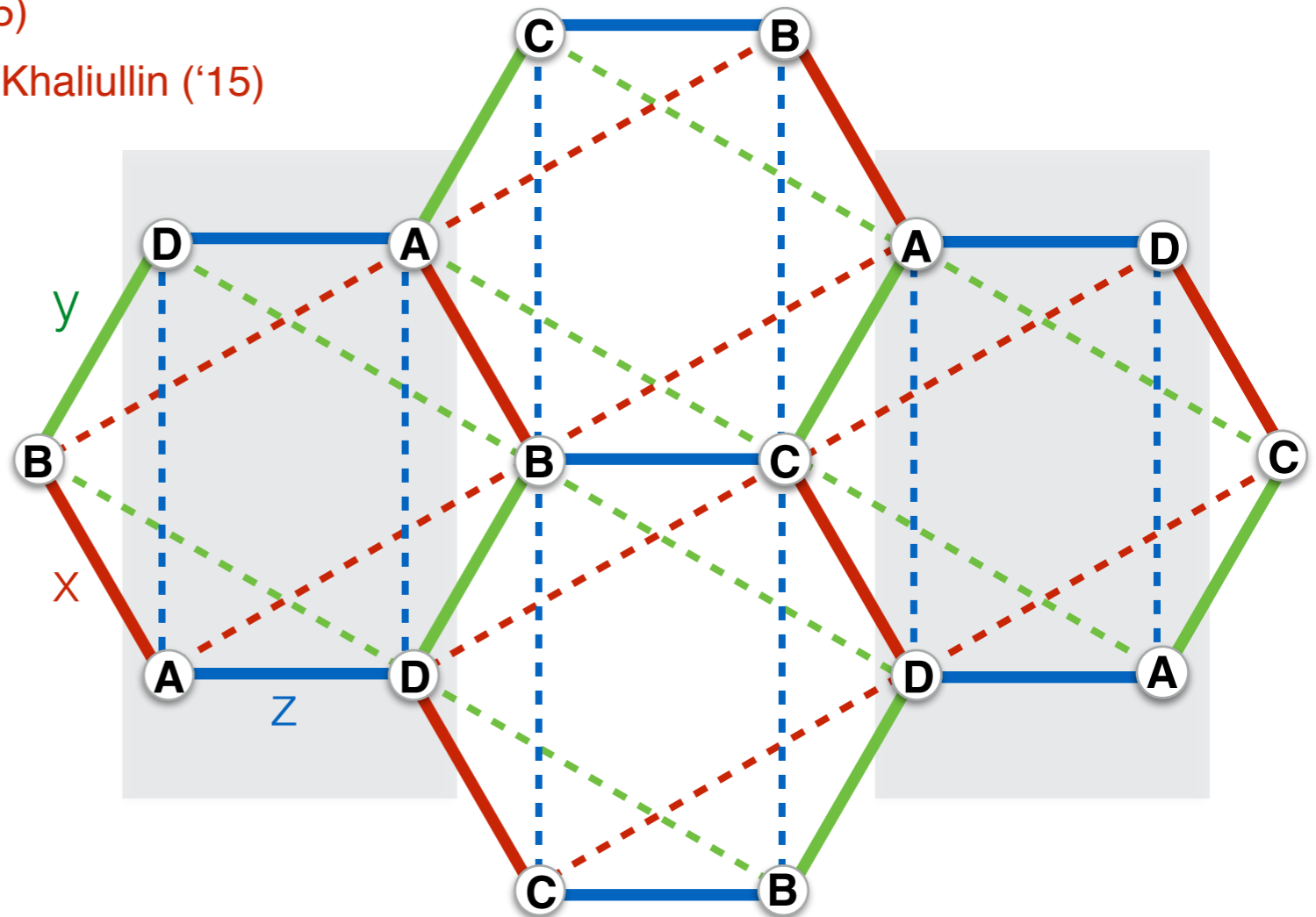
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The quantum K_1 - K_2 model: hidden duality & symmetries

- global symmetry in real+spin space: double cover of C_{3v}

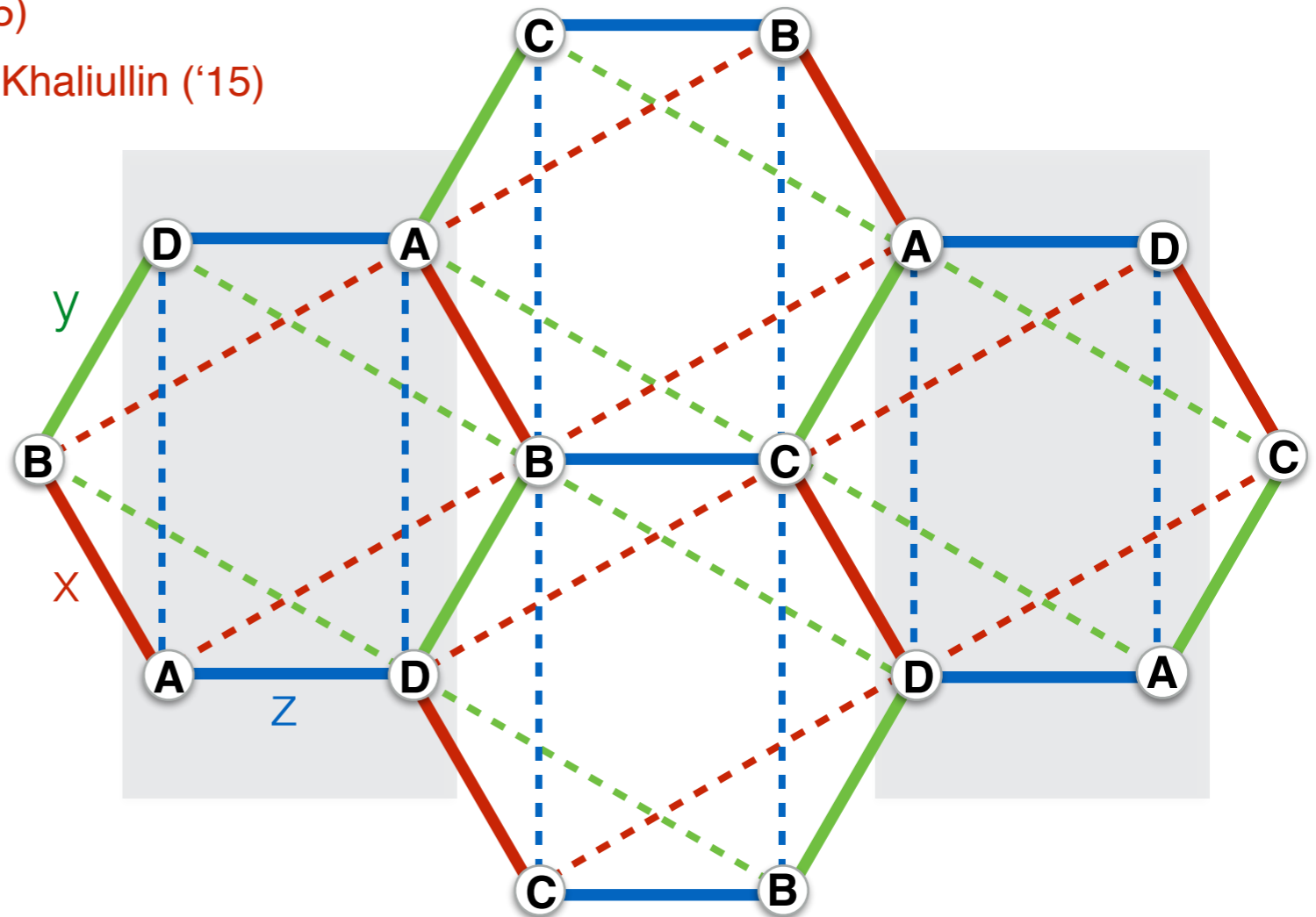
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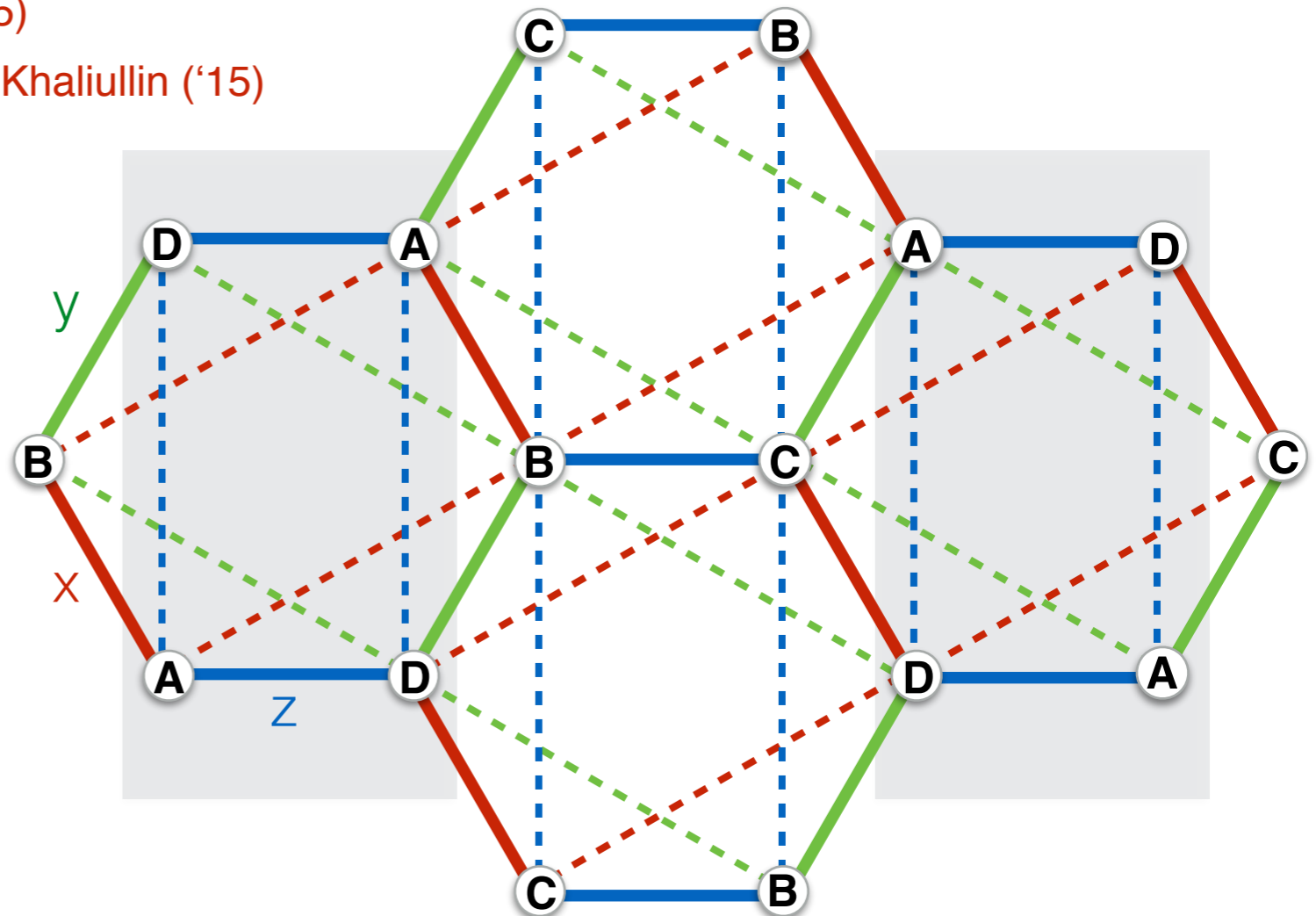
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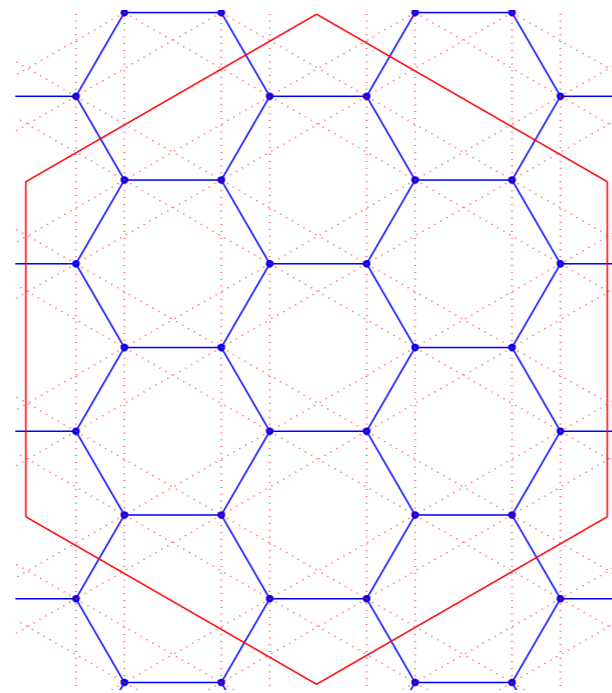
- gauge-like symmetry

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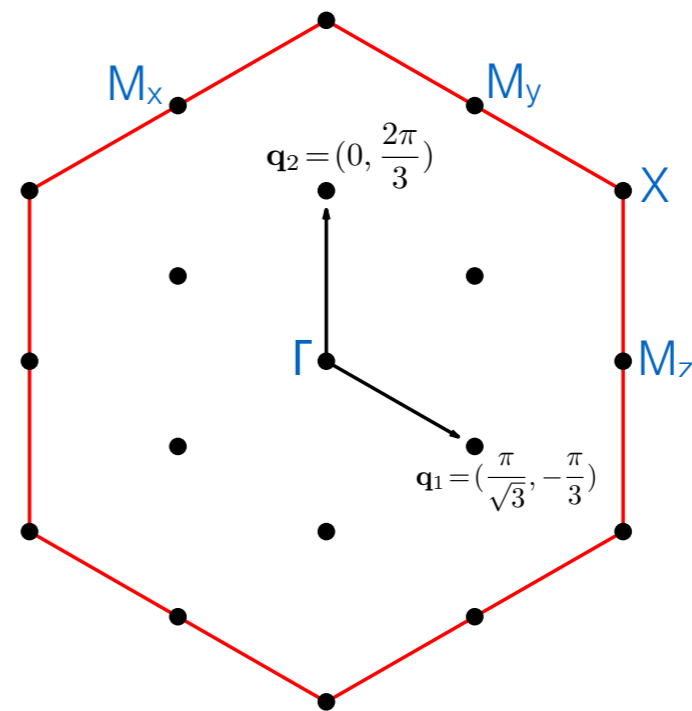


Exact diagonalizations: finite-size clusters

24-sites

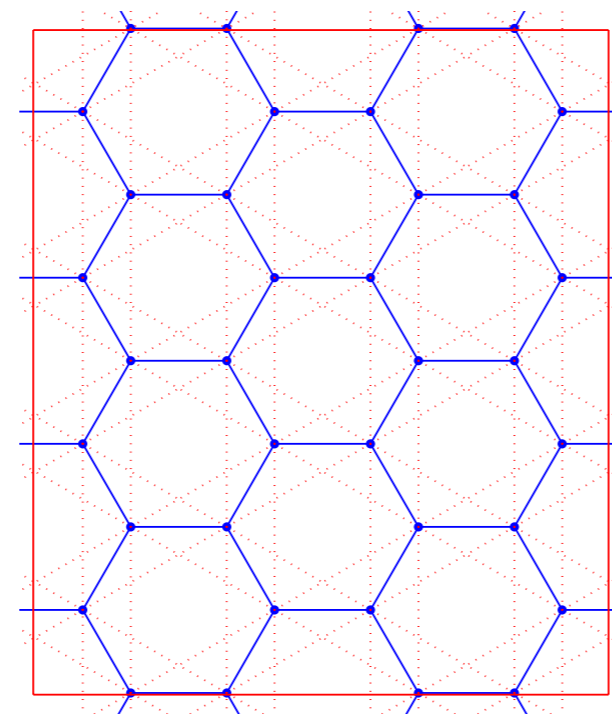


(a)

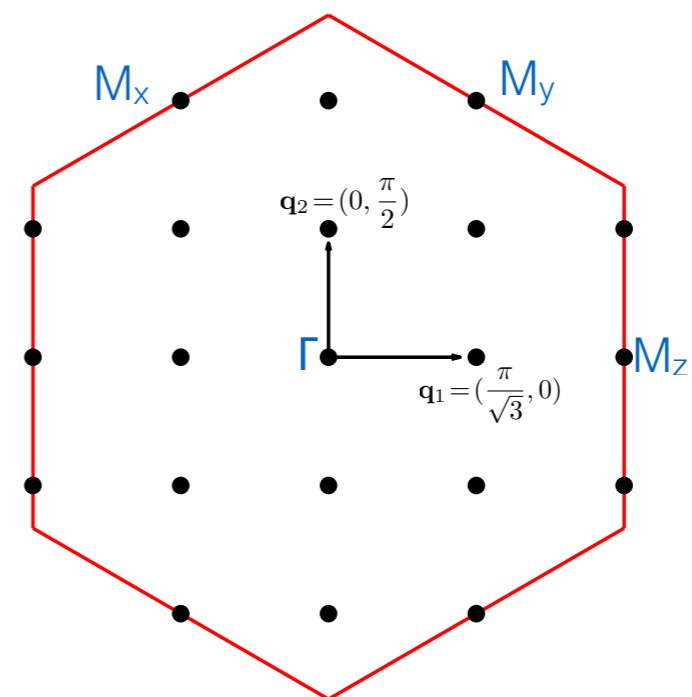


(b)

32-sites

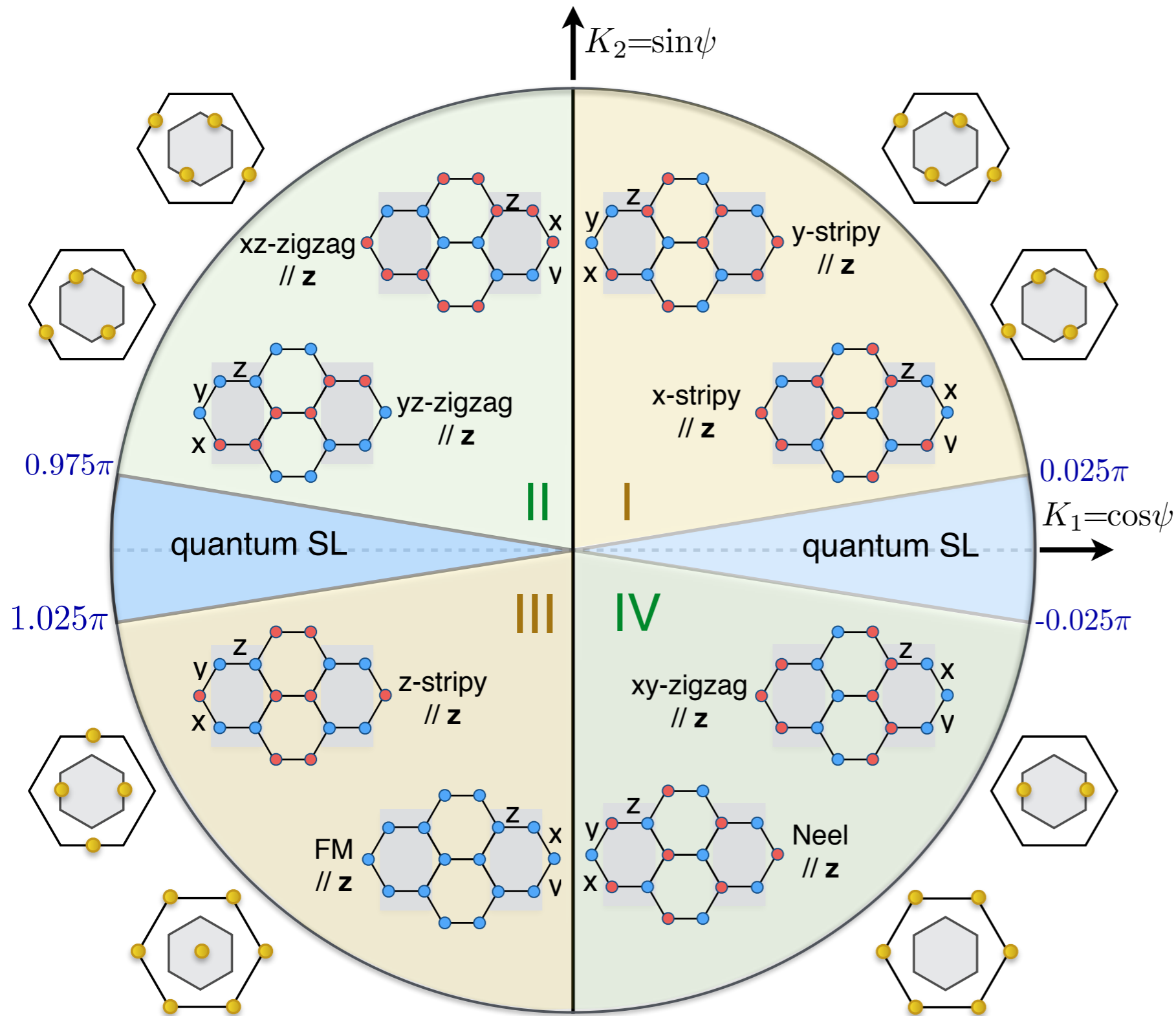


(c)



(d)

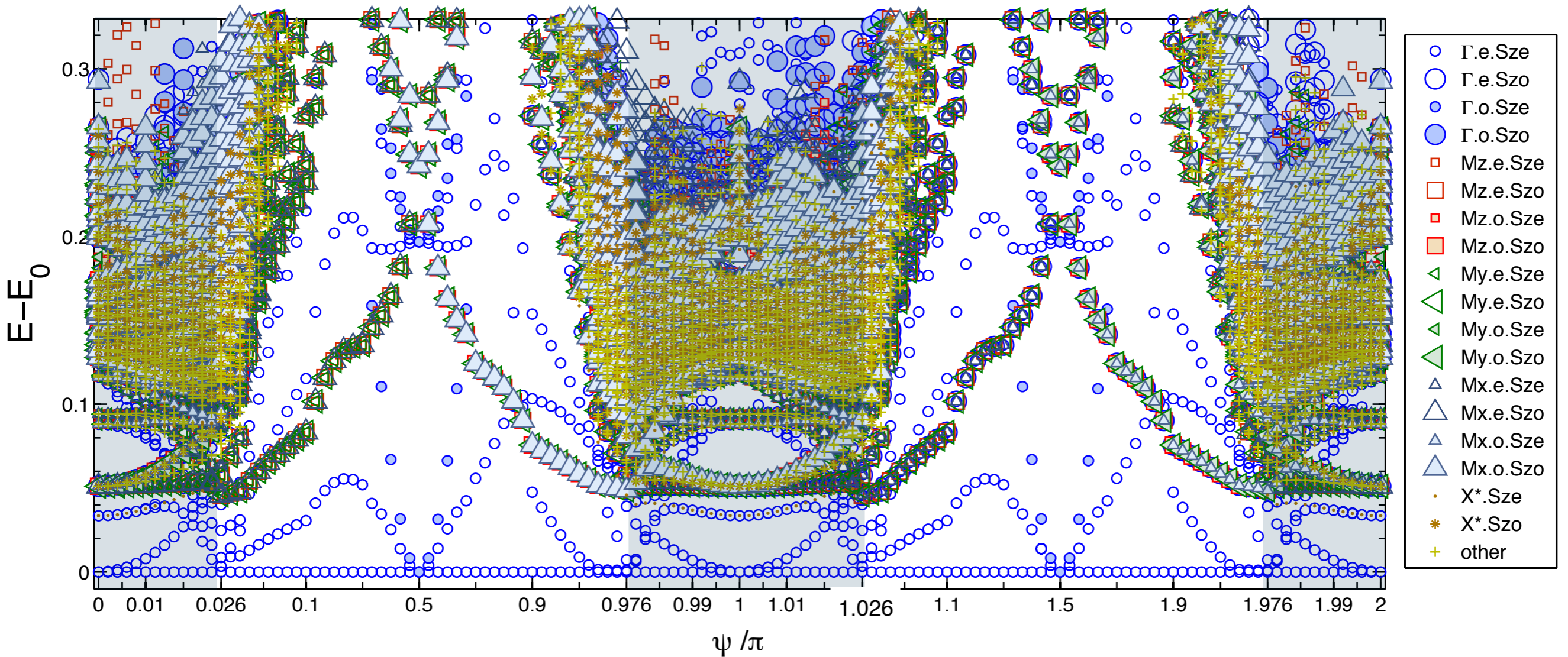
The quantum K_1 - K_2 model: phase diagram obtained from ED



- QSL is very fragile !
- 4 magnetic LRO regions; related by duality
- zigzag in Na213
- 12 GS's in each region; some are very different !

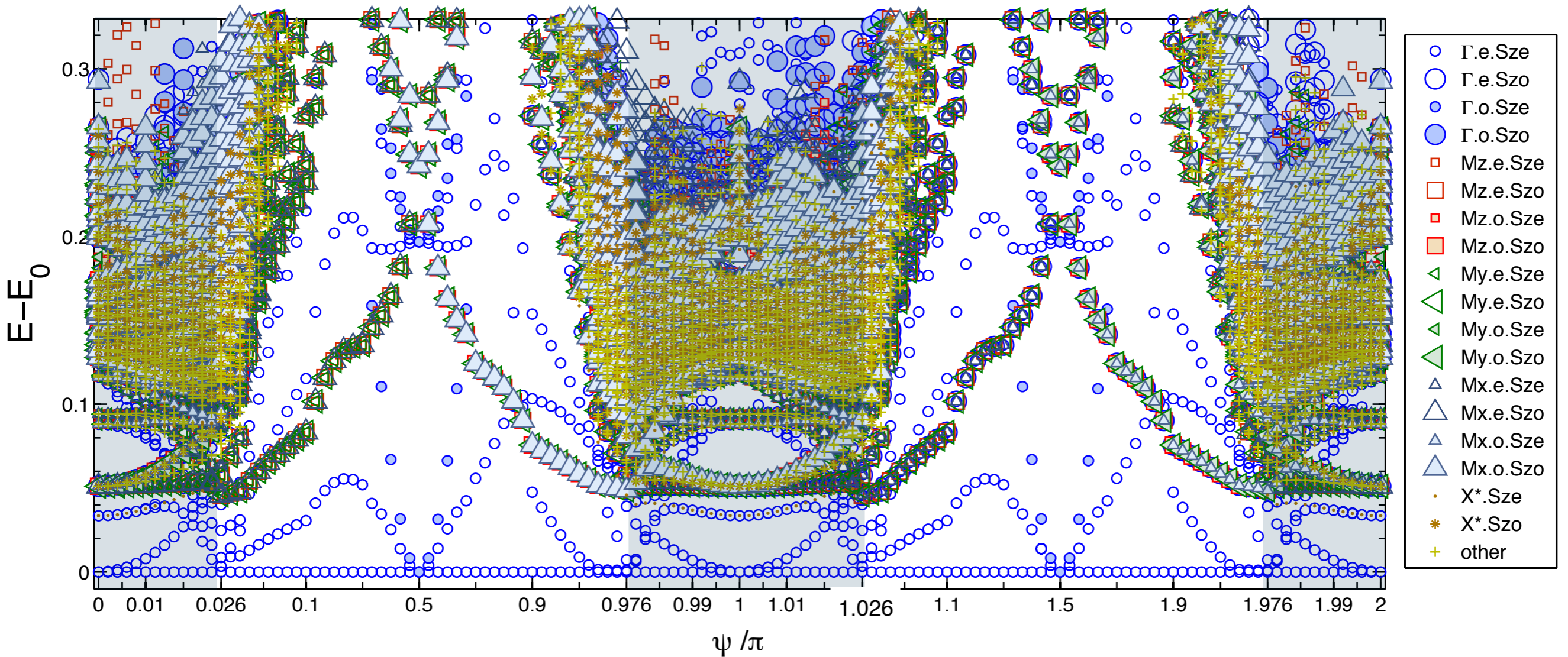
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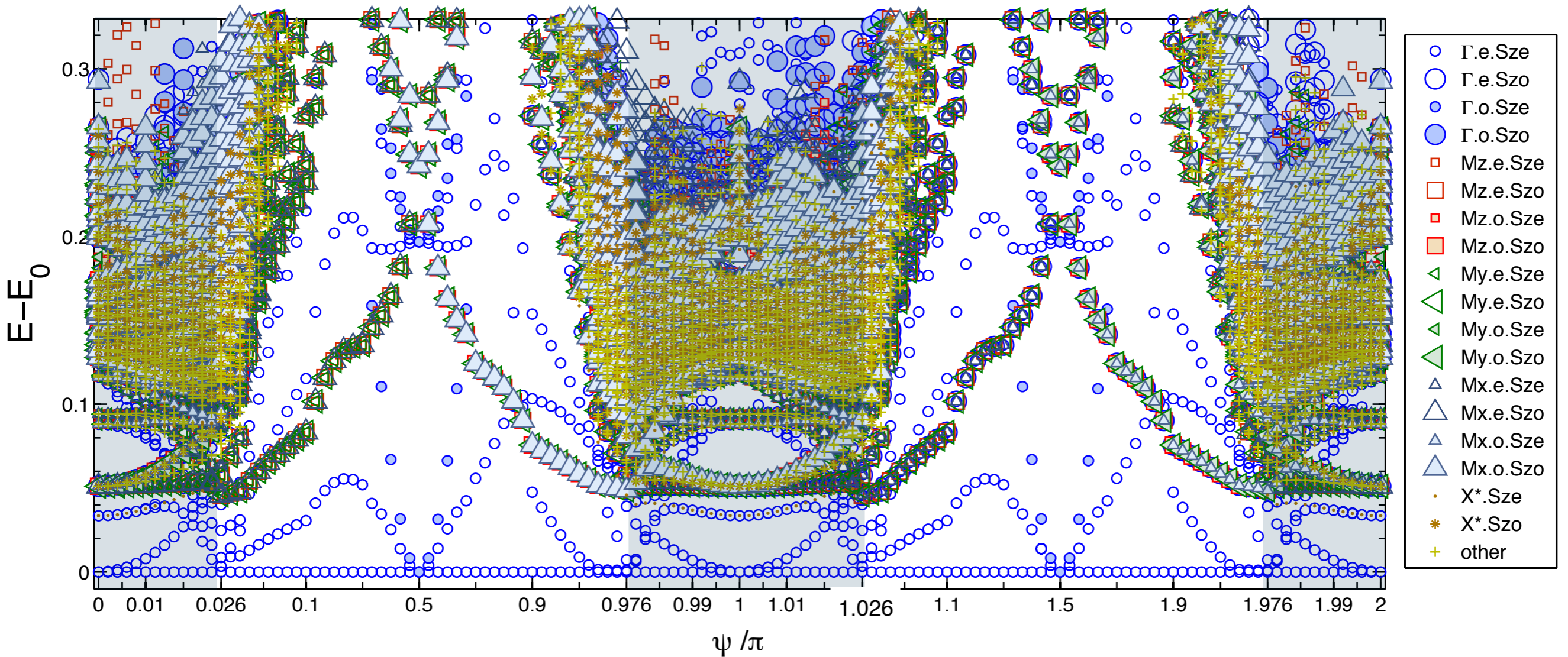
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- Kitaev spin liquid regions: very dense spectra !

The quantum K_1 - K_2 model: “low-energy spectroscopy”

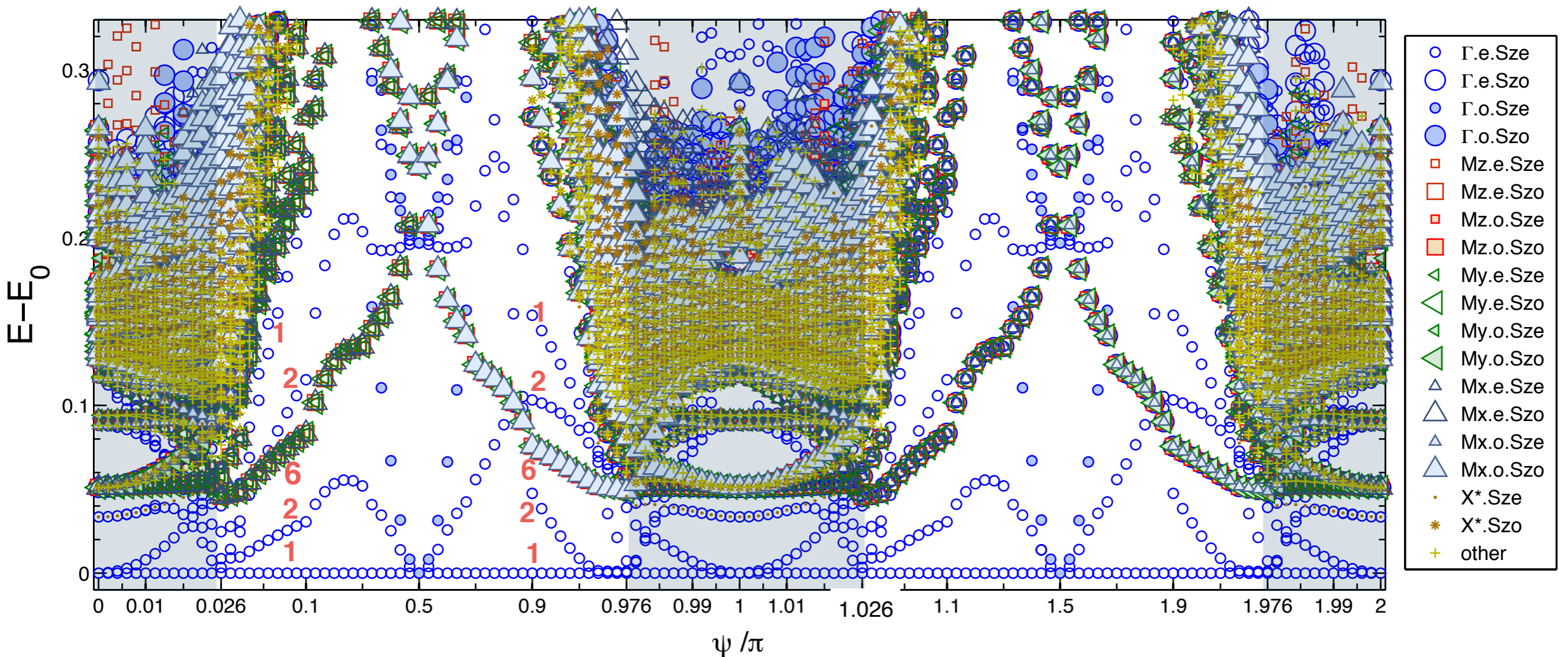
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- Kitaev spin liquid regions: very dense spectra !
- Magnetic LRO regions: small number of low-lying states
- low-energy spectroscopy: multiplicity & symmetry quantum numbers; large spin gap

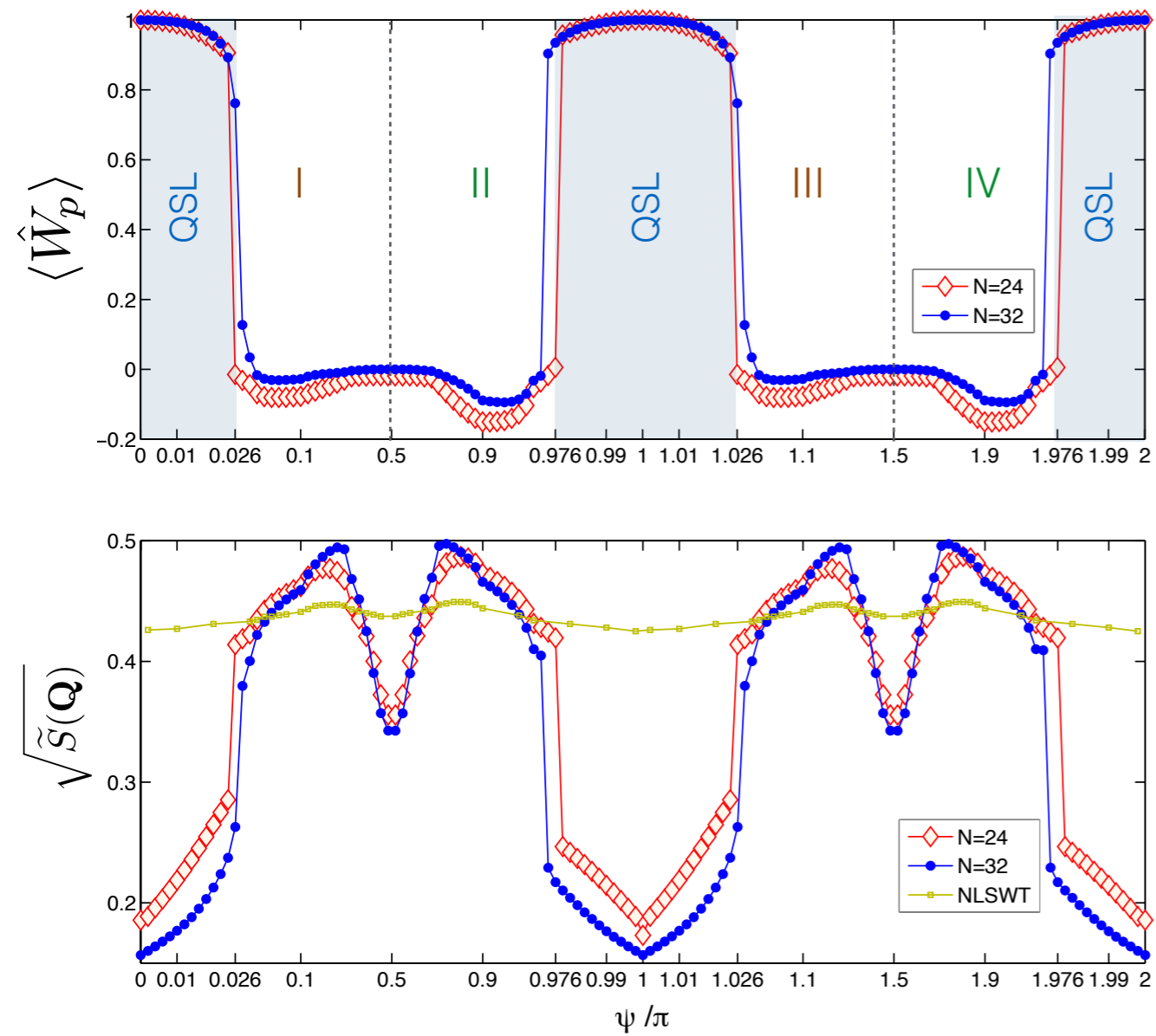
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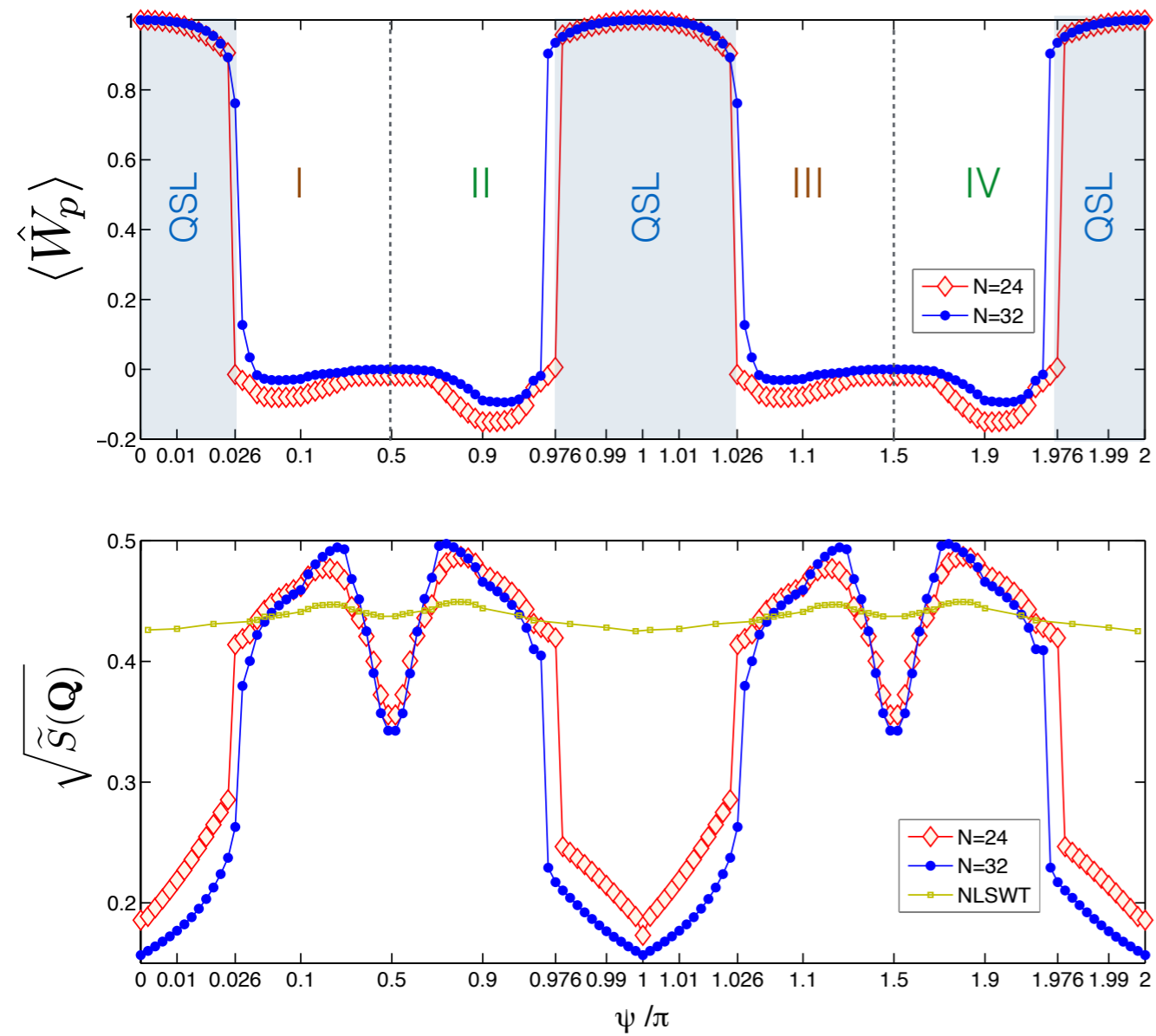
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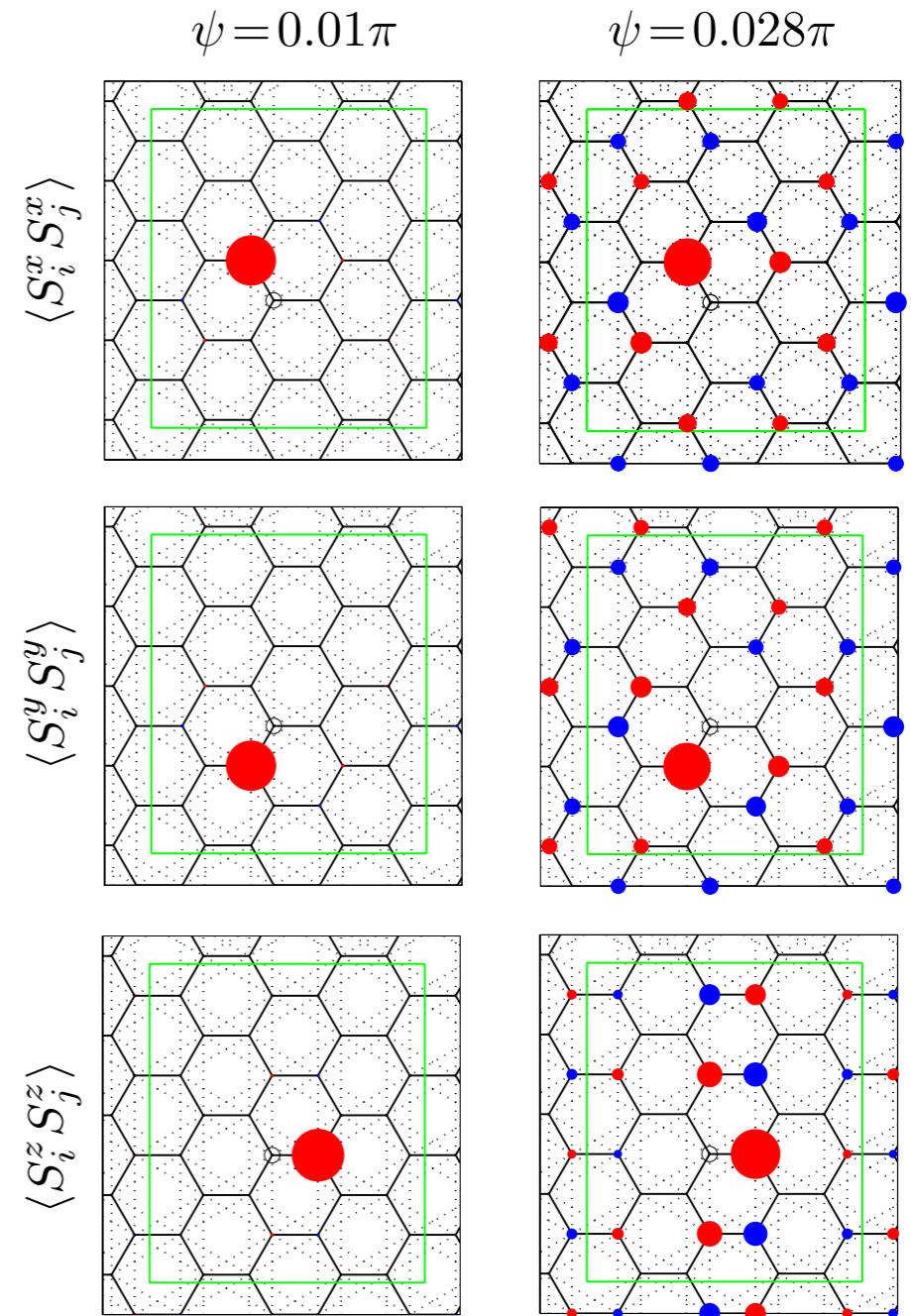
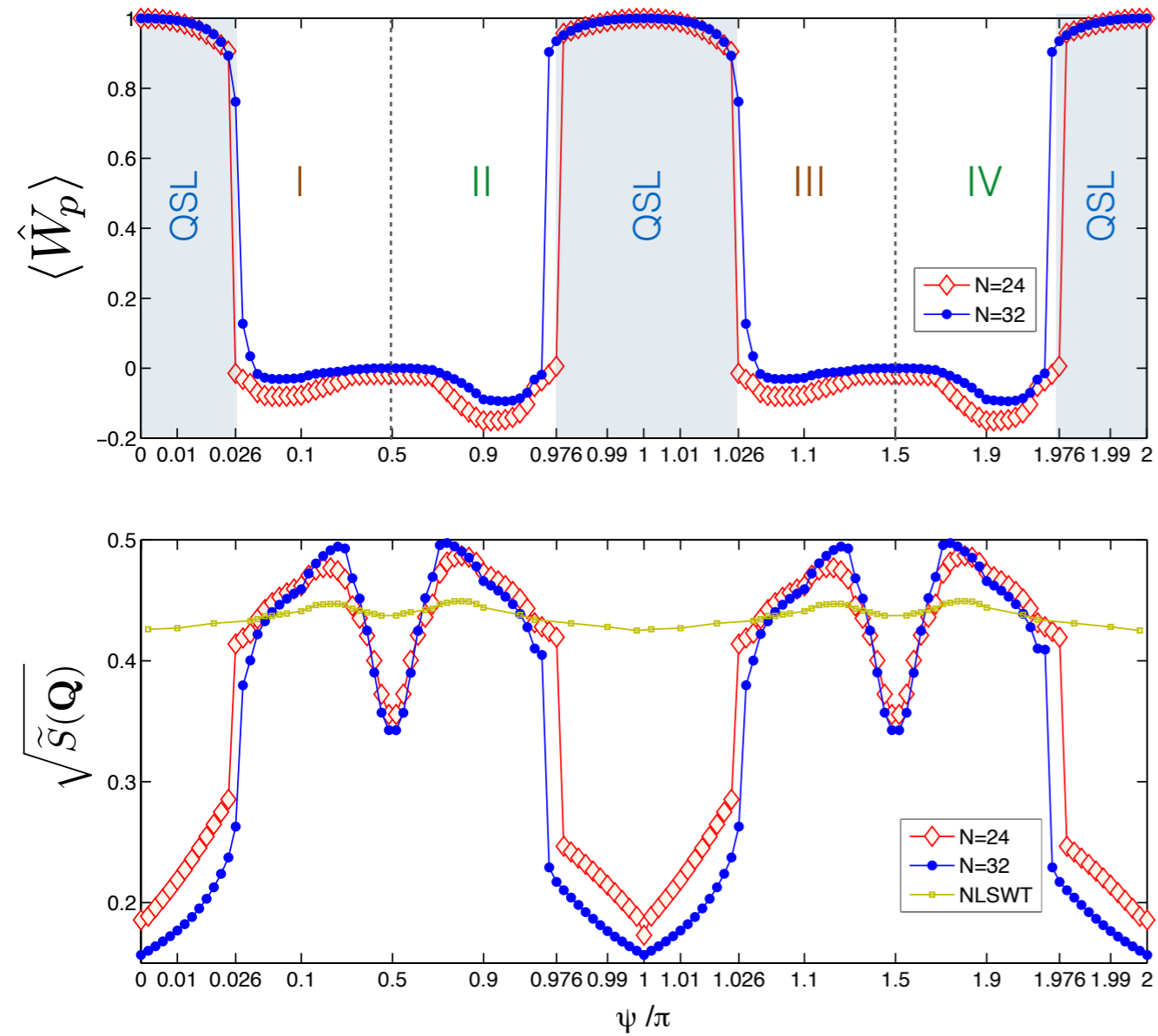
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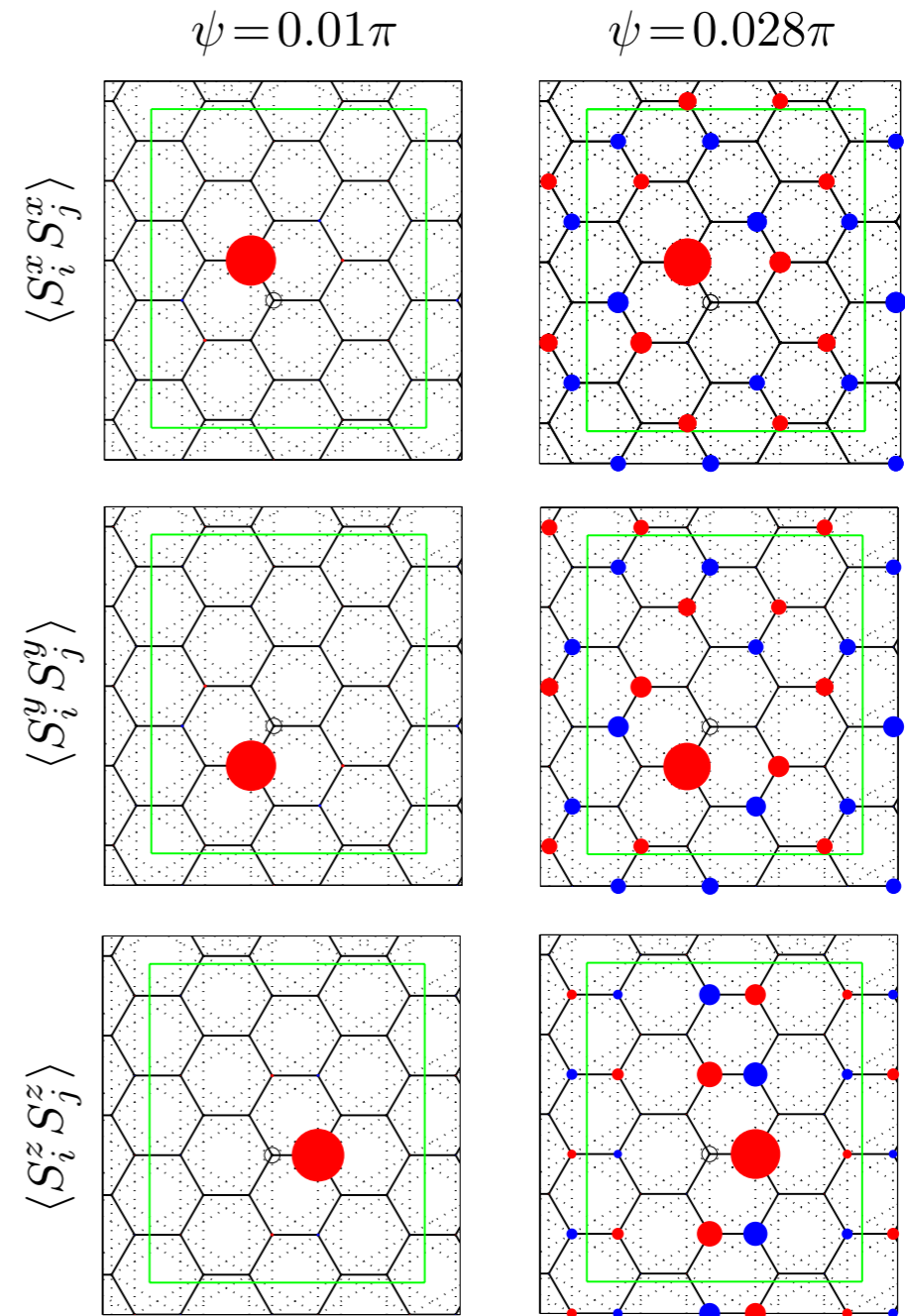
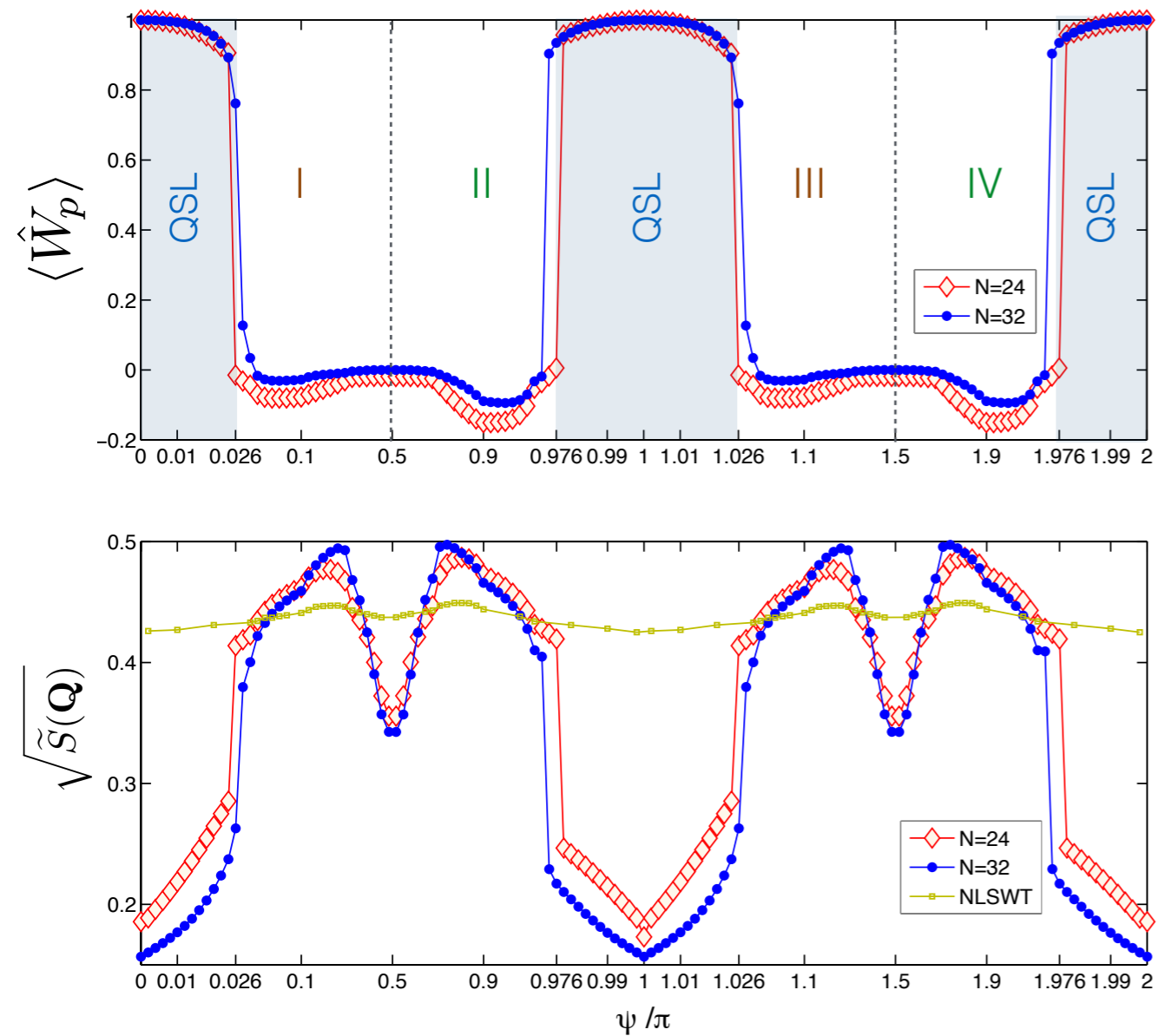
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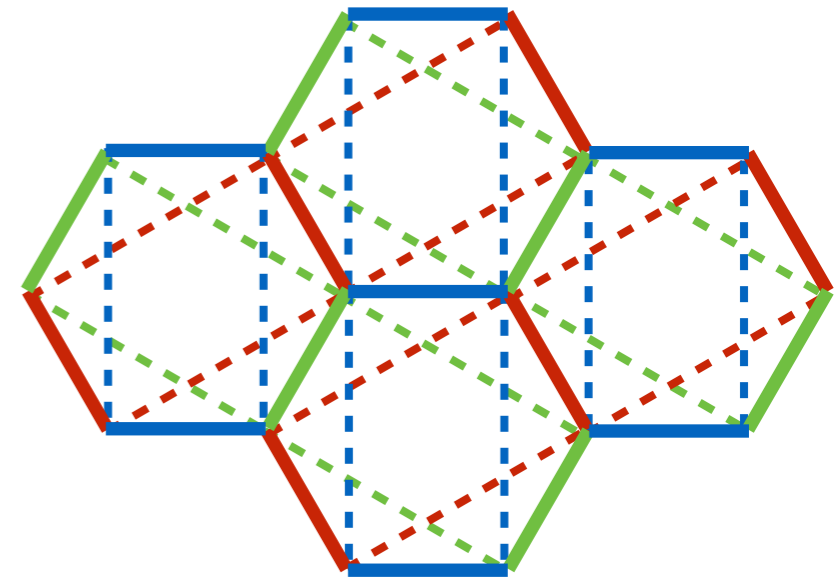
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- short vs. long-range ordering
- local spin length is very close to $1/2$; states seem very classical !



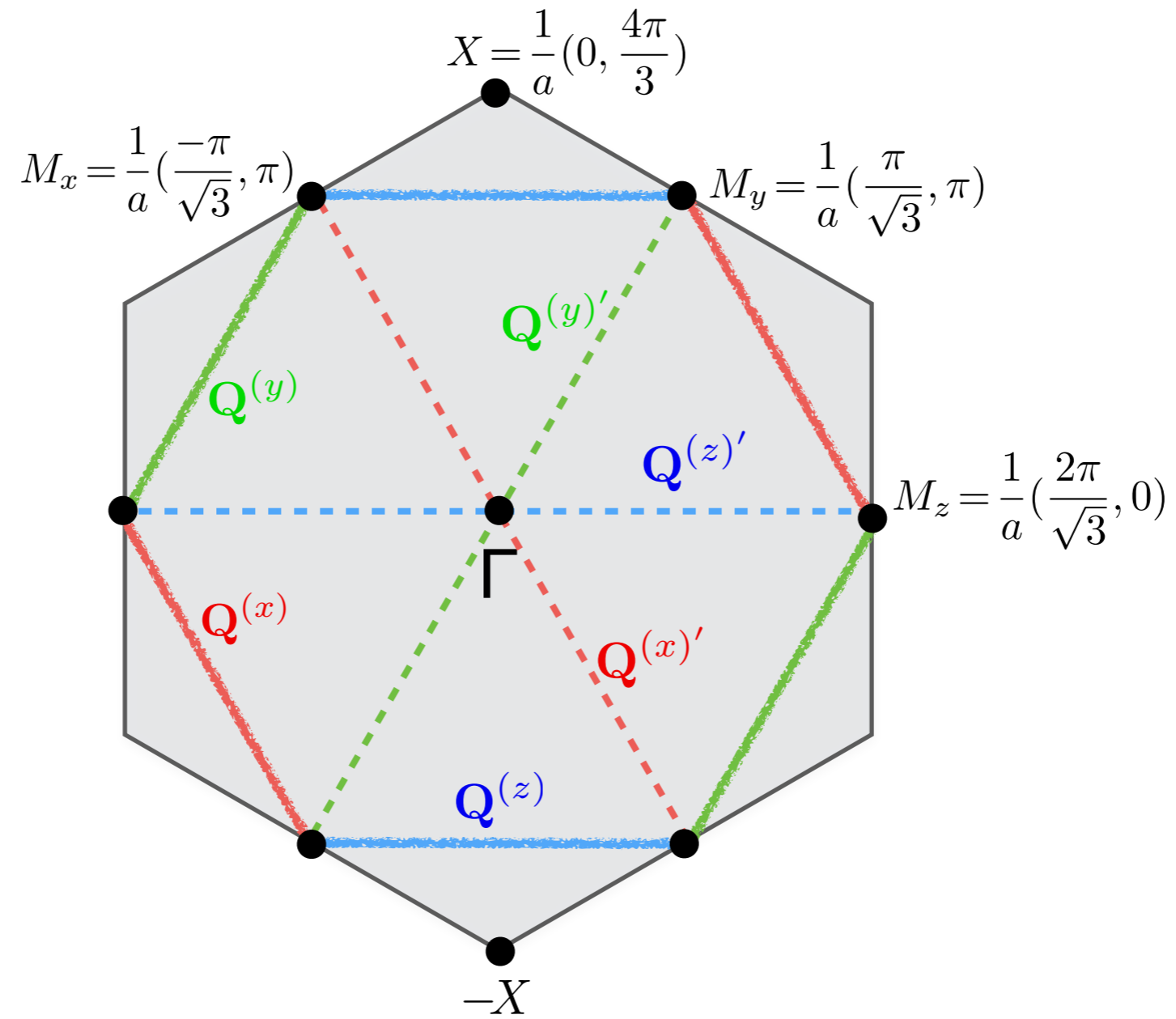
What is the physical mechanism of instability?

Striking aspect:

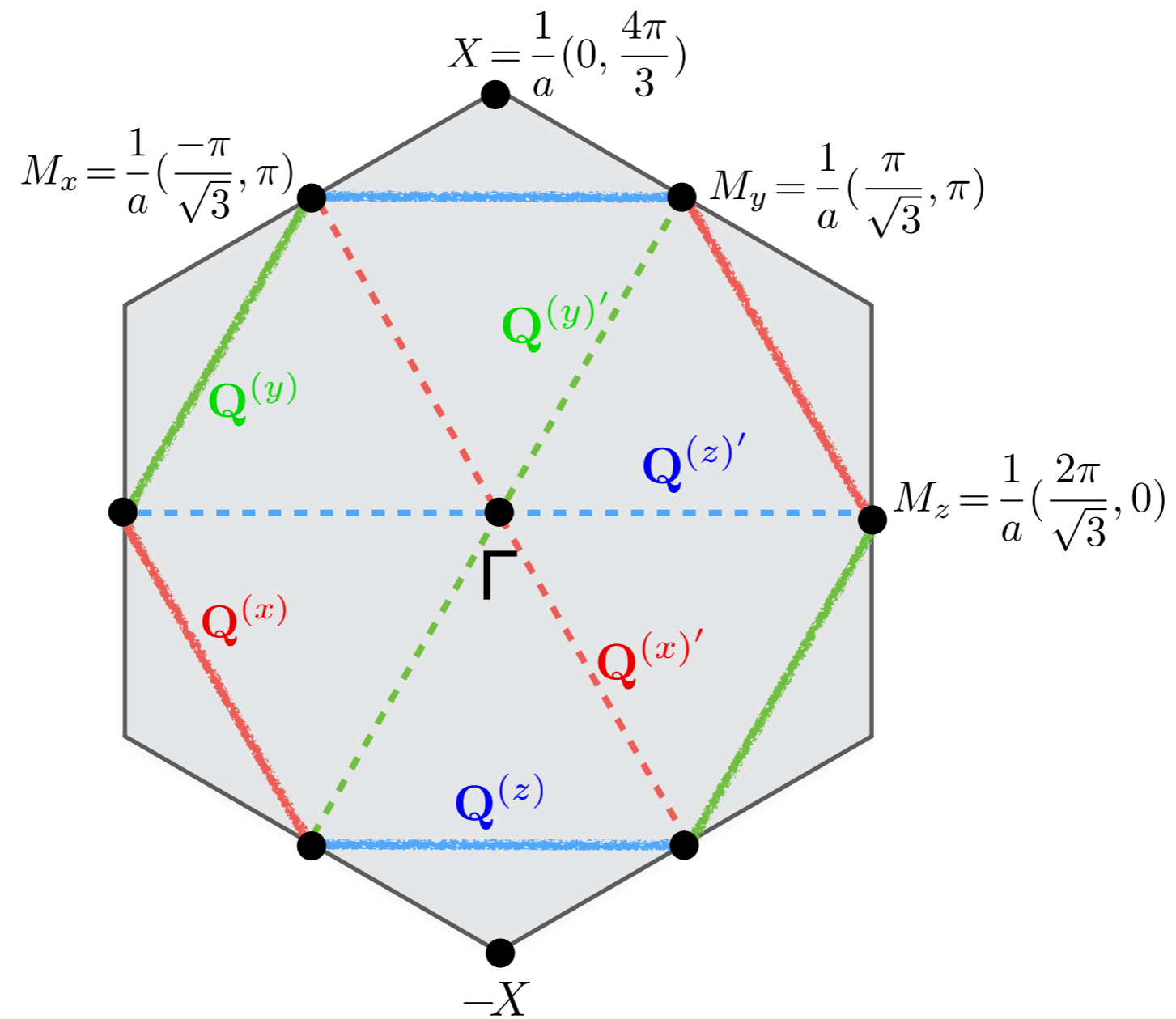
States **seem** very classical (local spin length almost $1/2$, large spin gap, etc).

Yet, classical limit hosts **qualitatively** different physics !

Classical minima form lines in momentum space



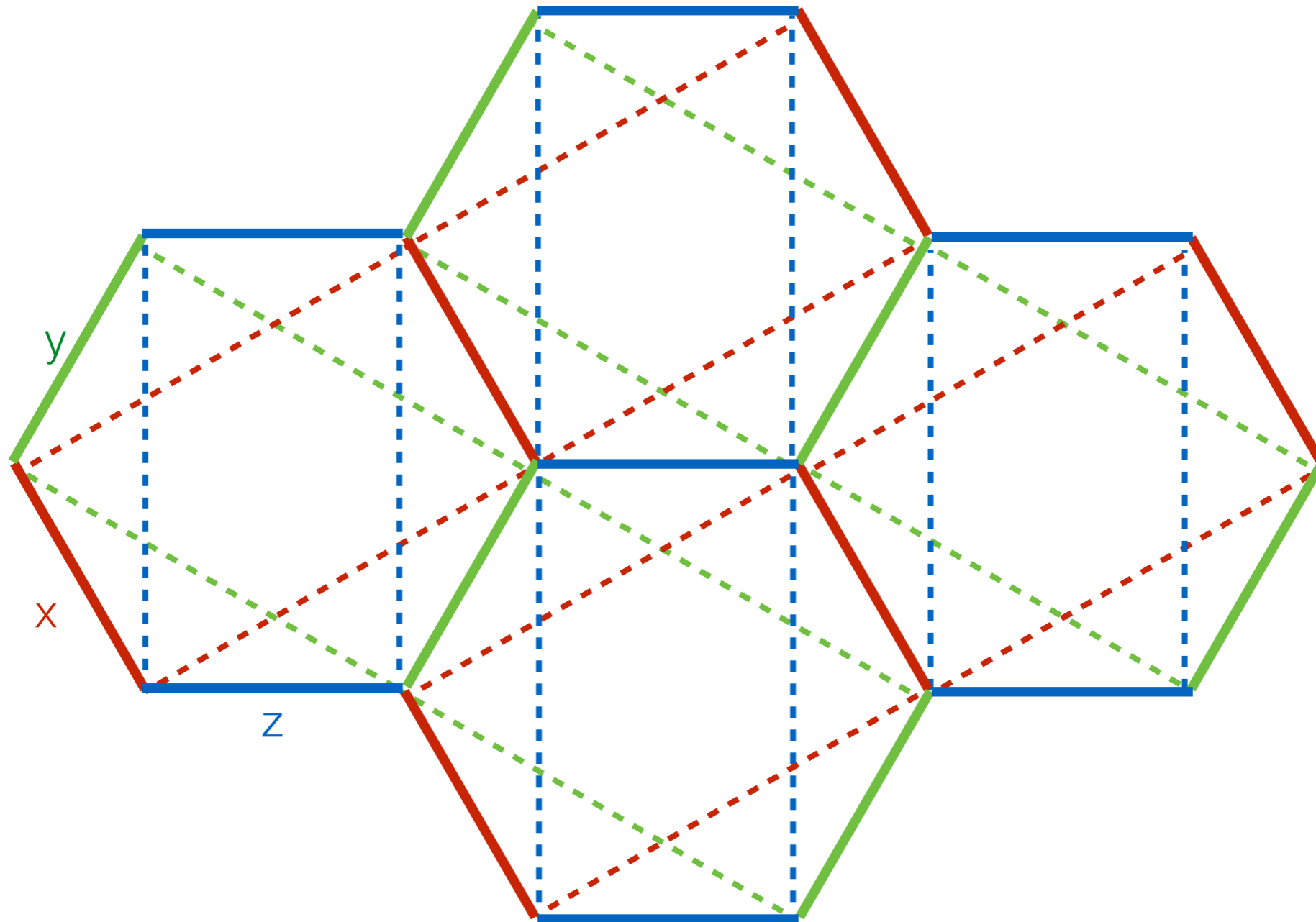
Classical minima form lines in momentum space



→ sub-extensive number of classical GS's

Origin of sub-extensive degeneracy: *sliding* symmetries

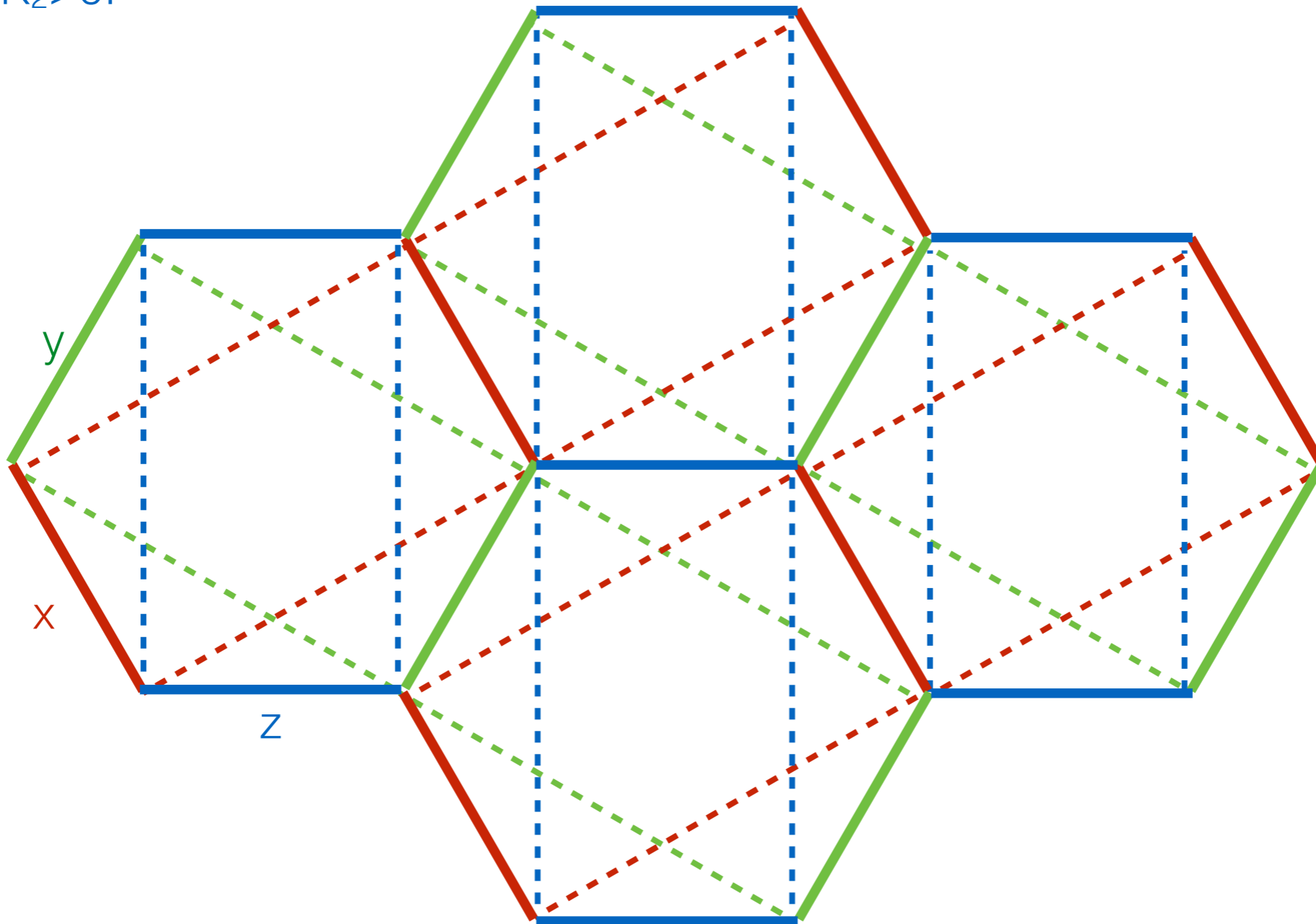
Batista & Nussinov (2005)



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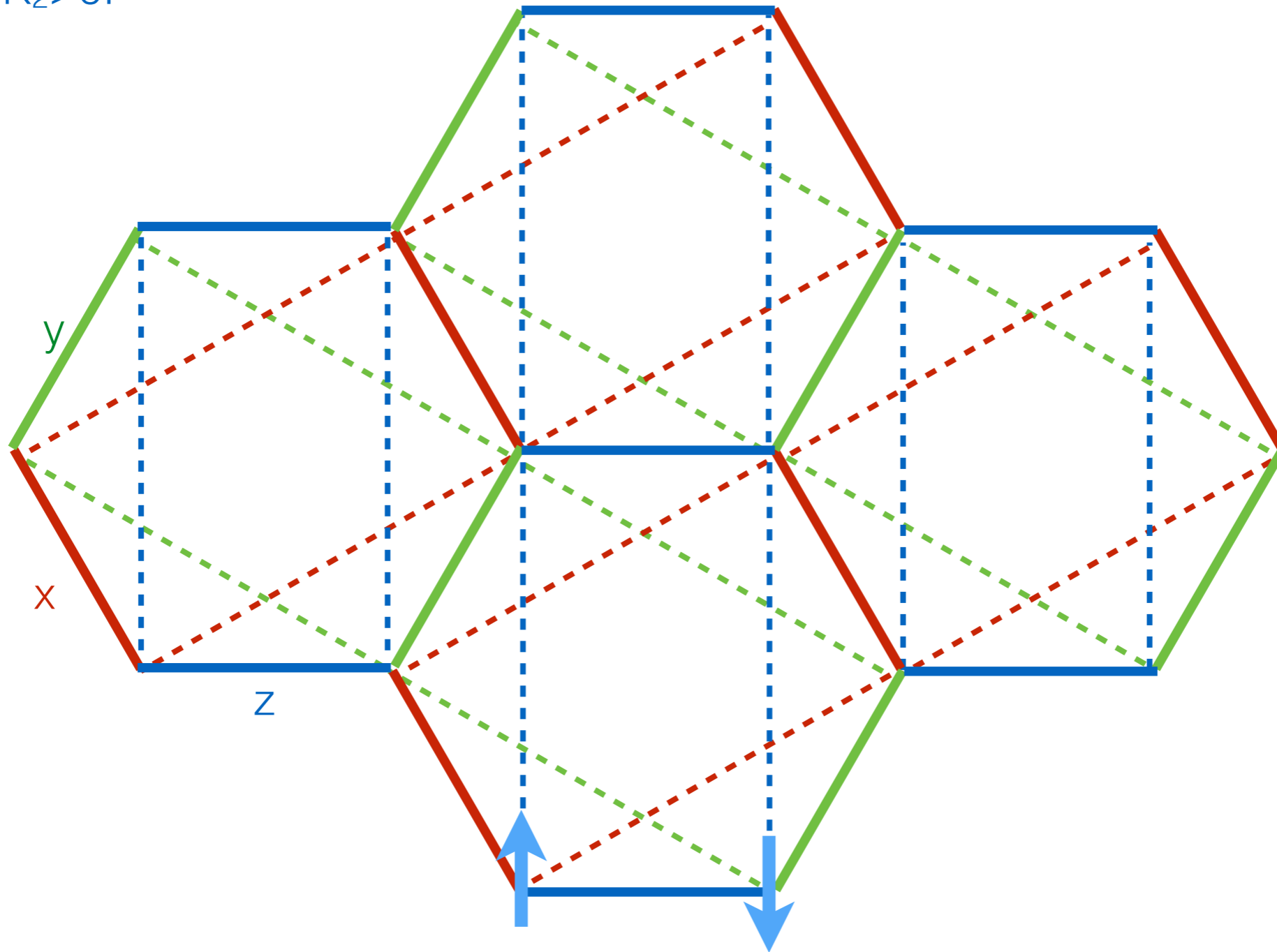
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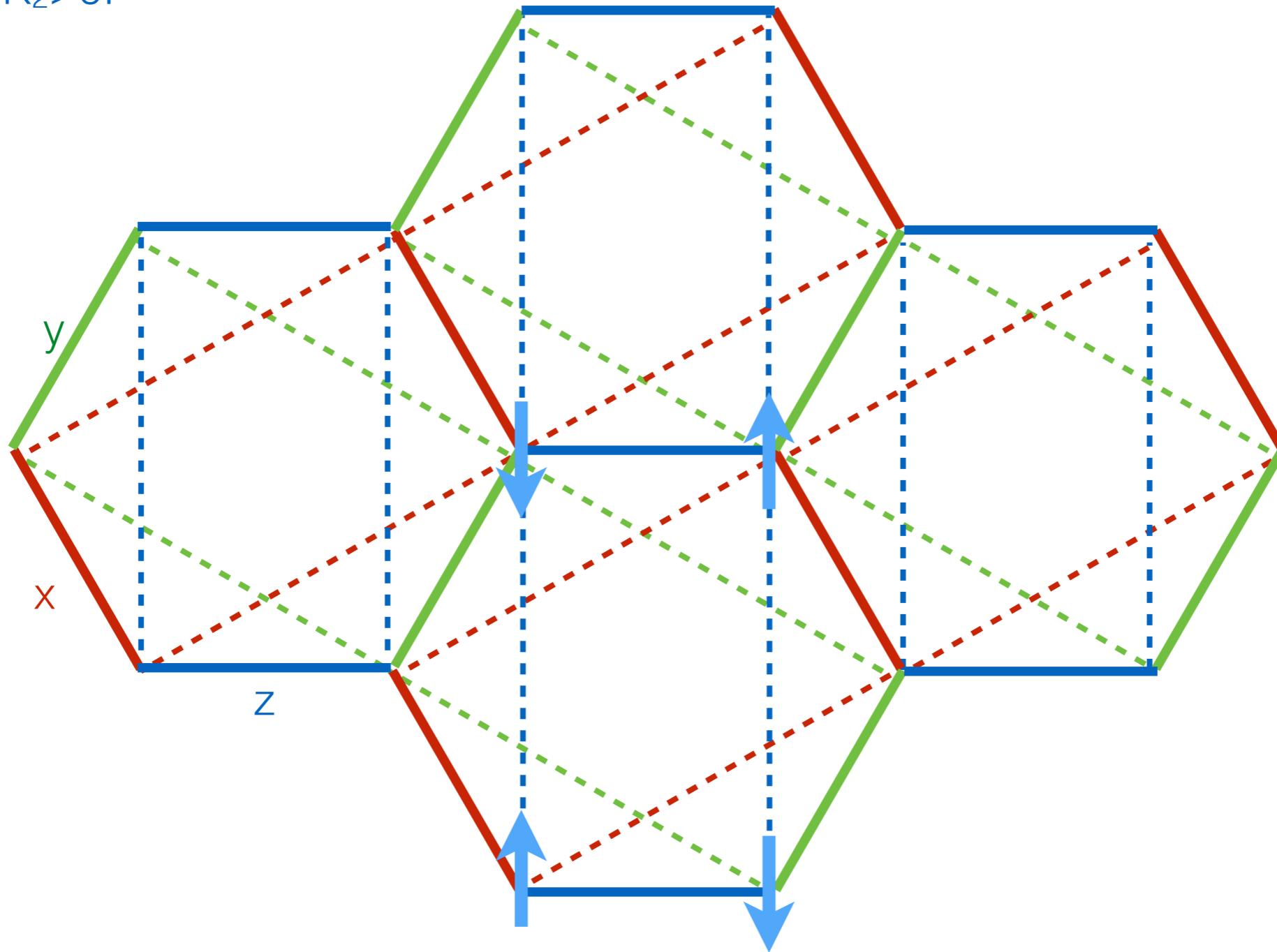
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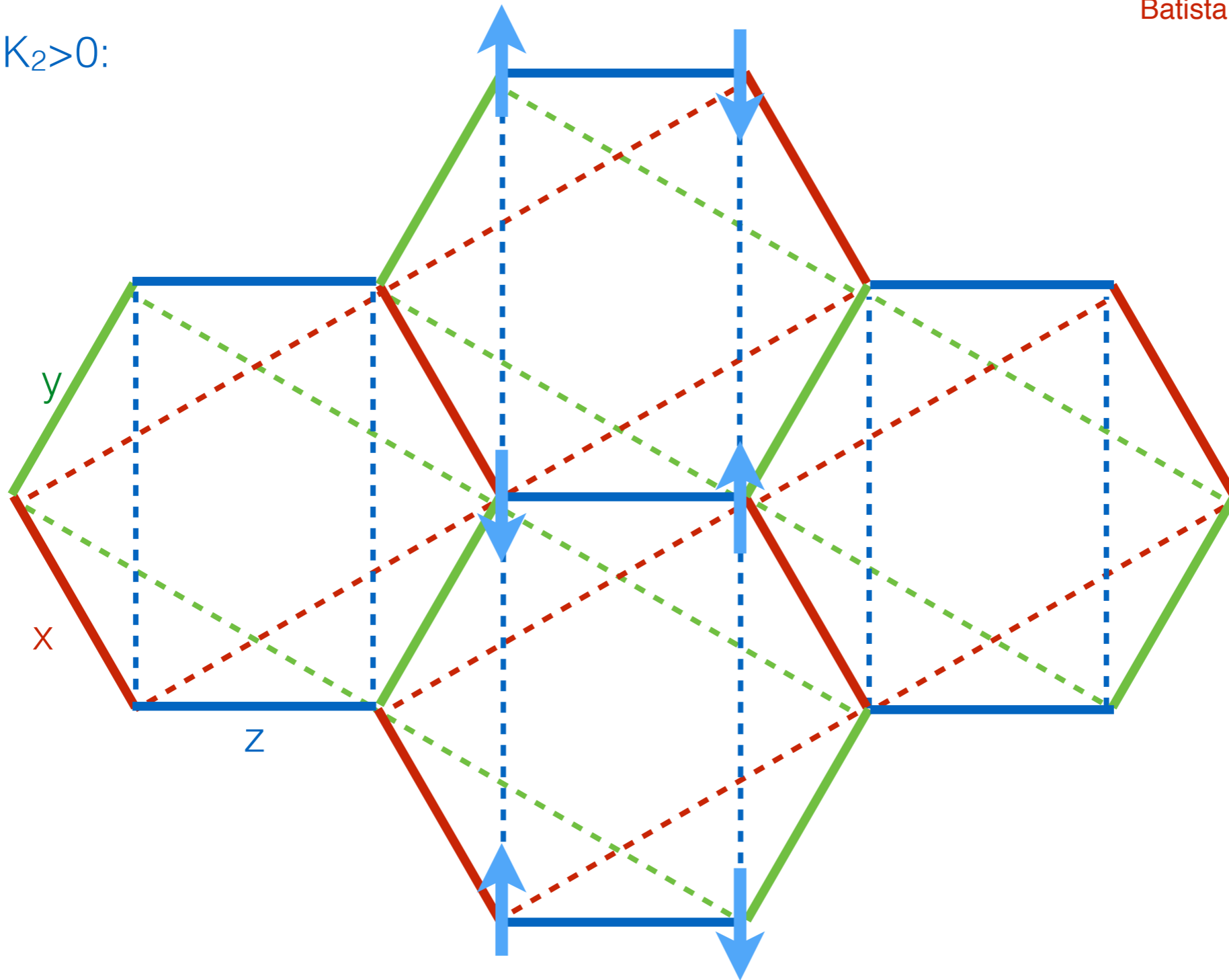
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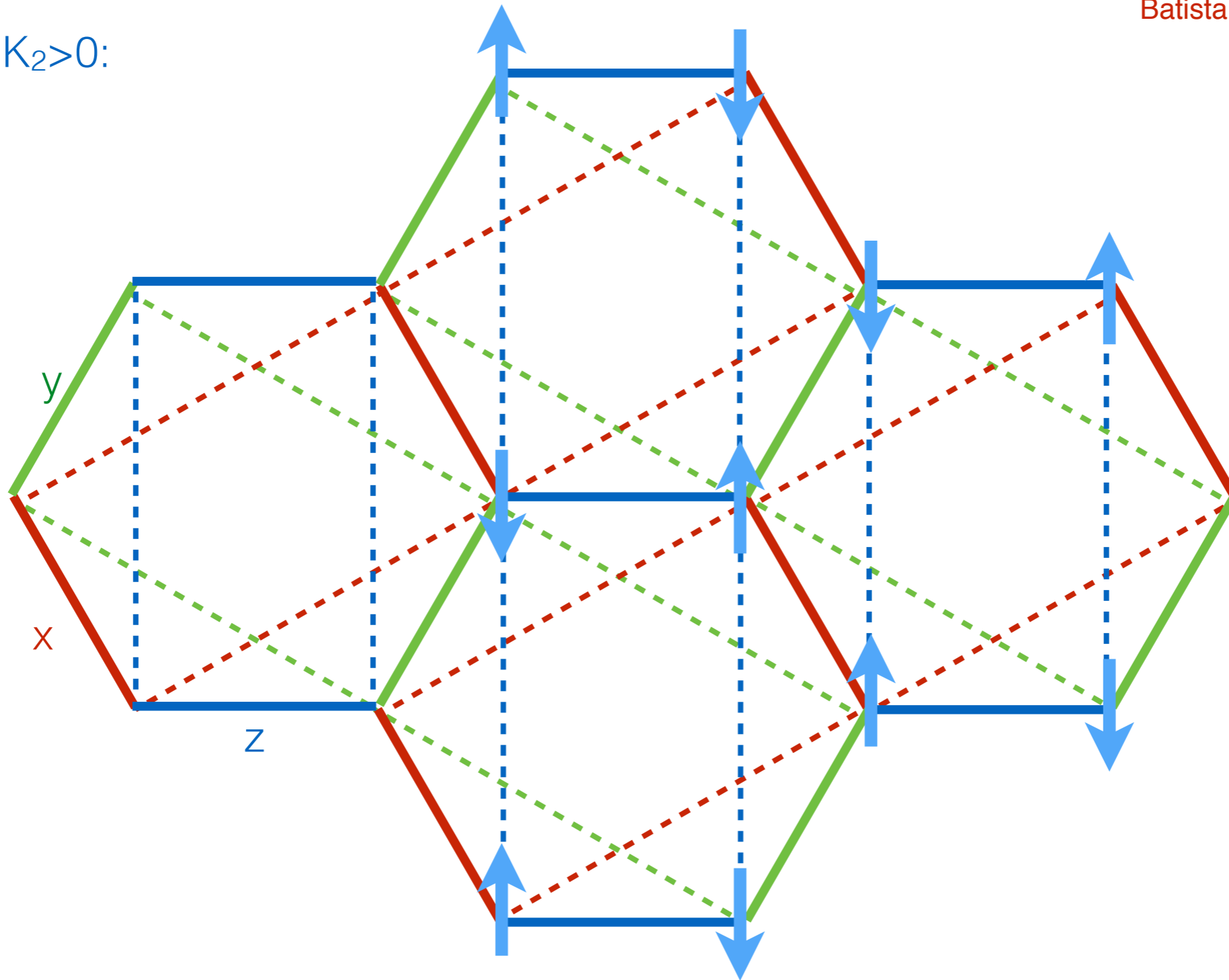
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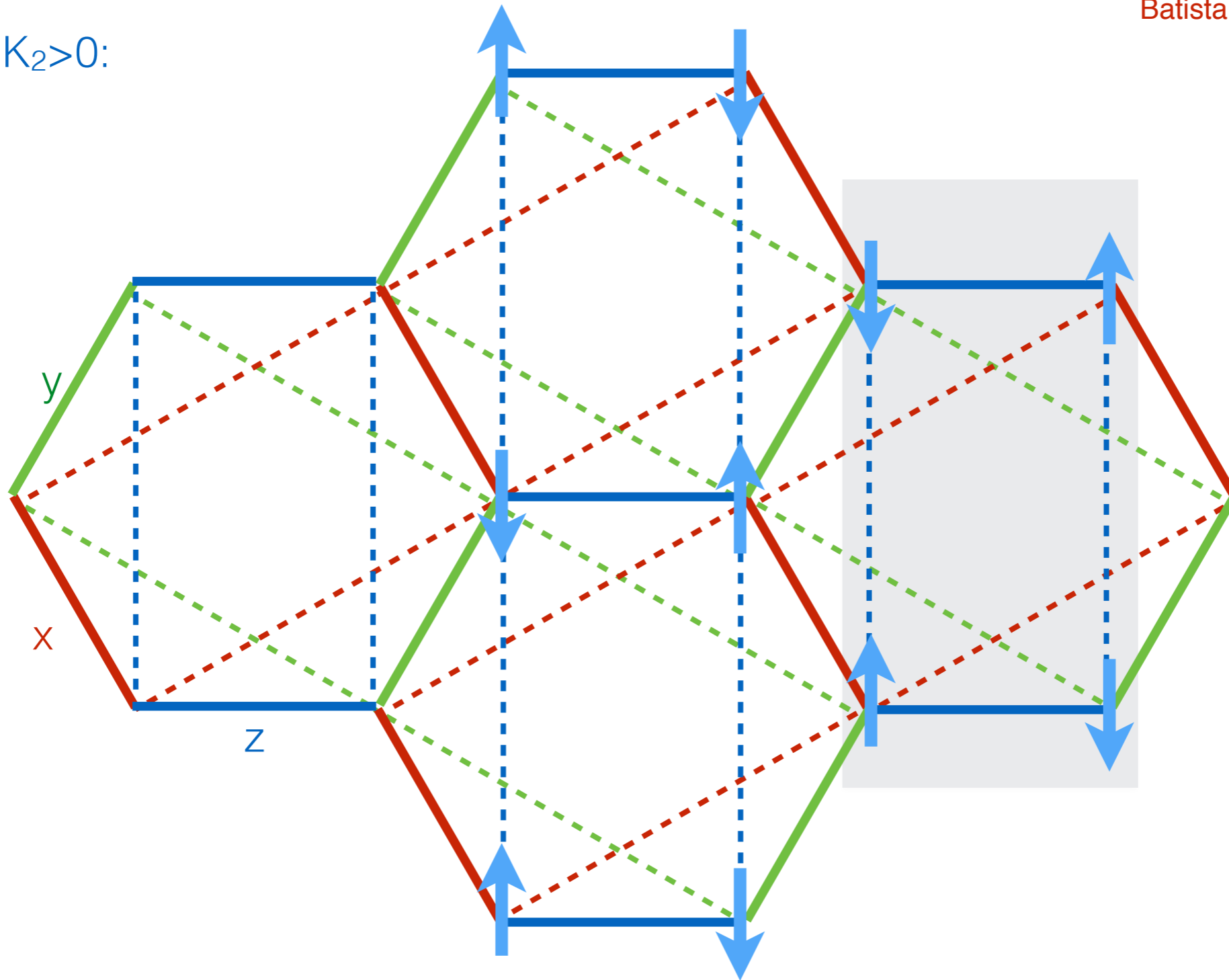
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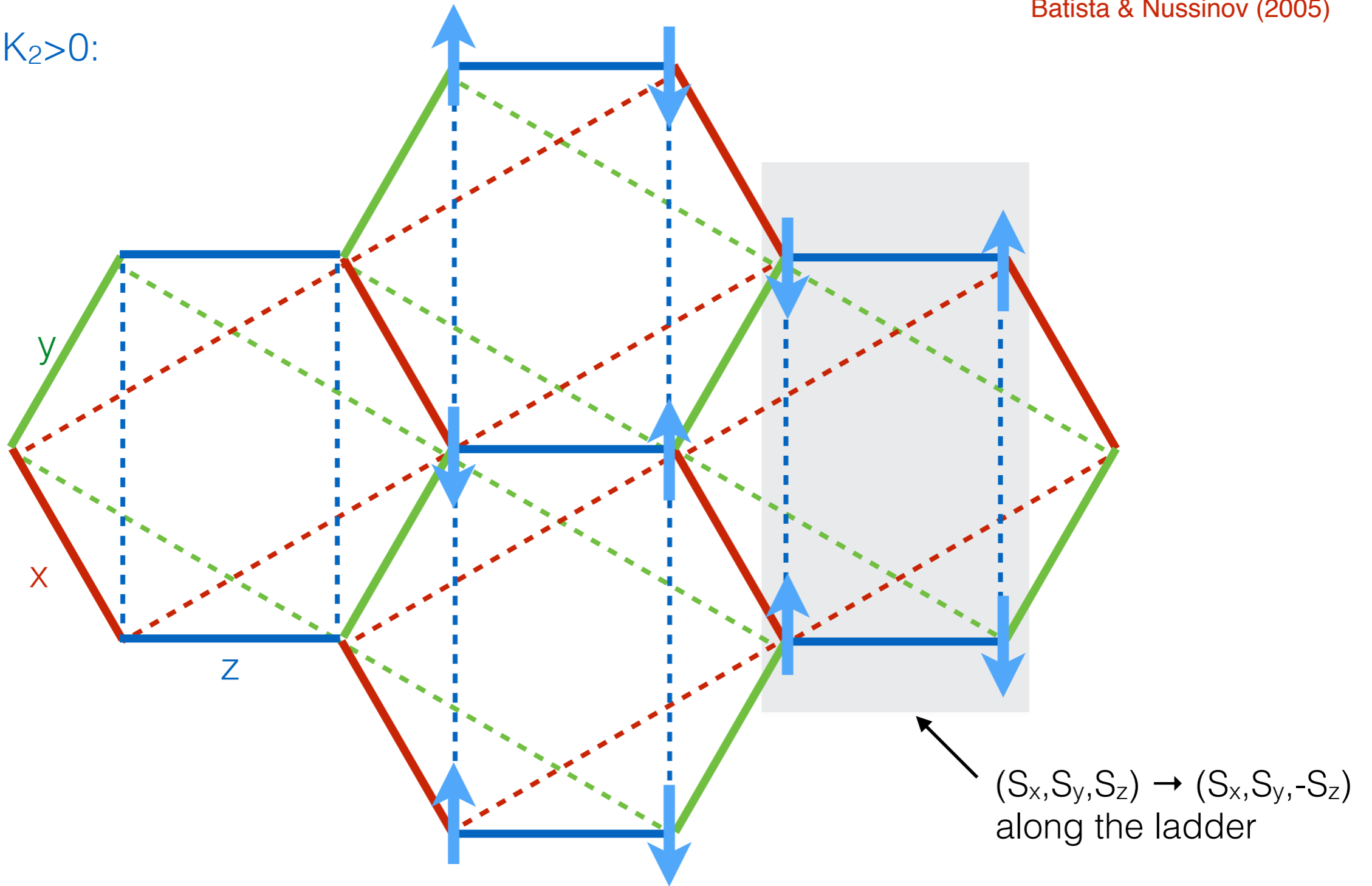
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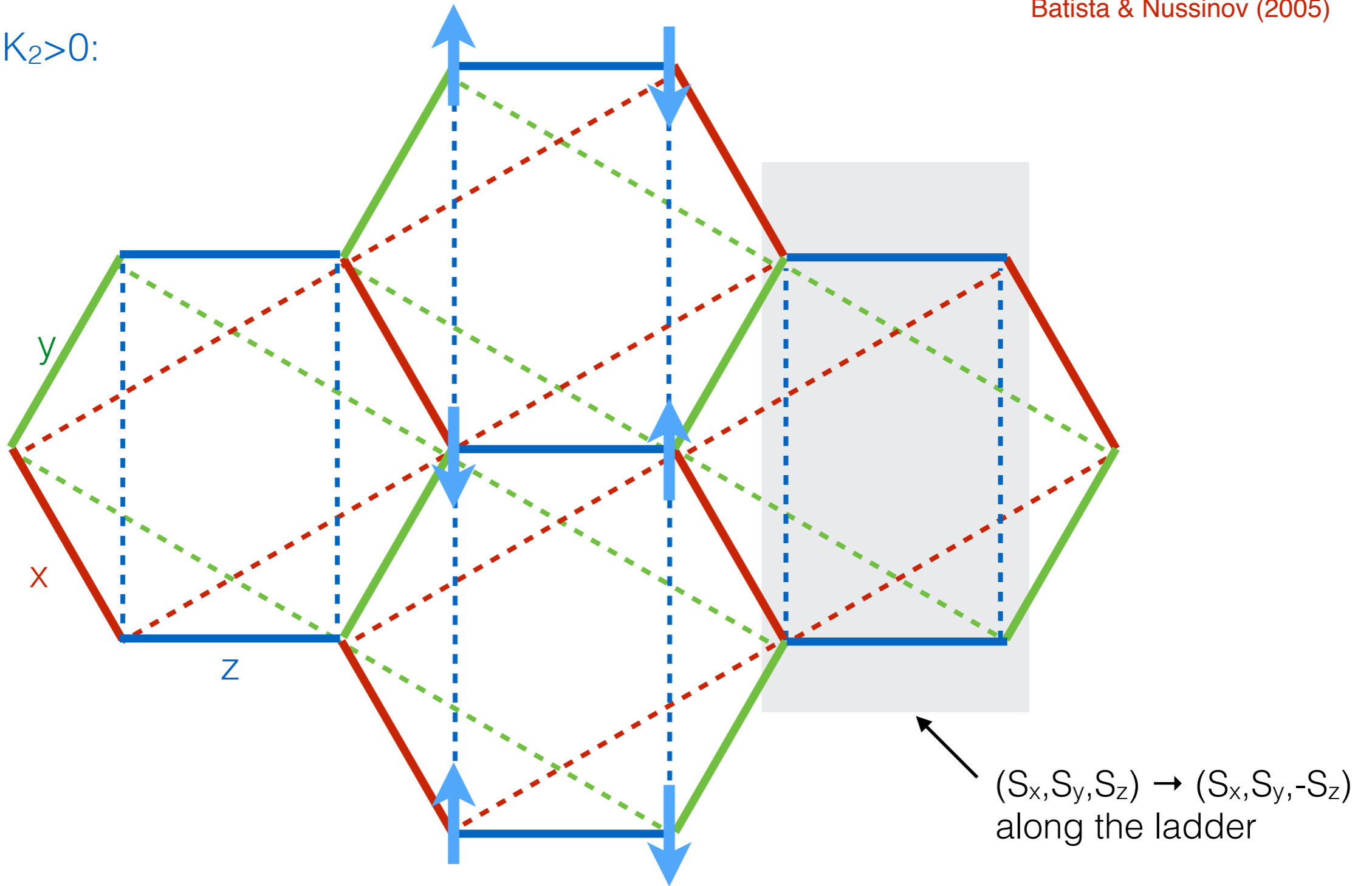
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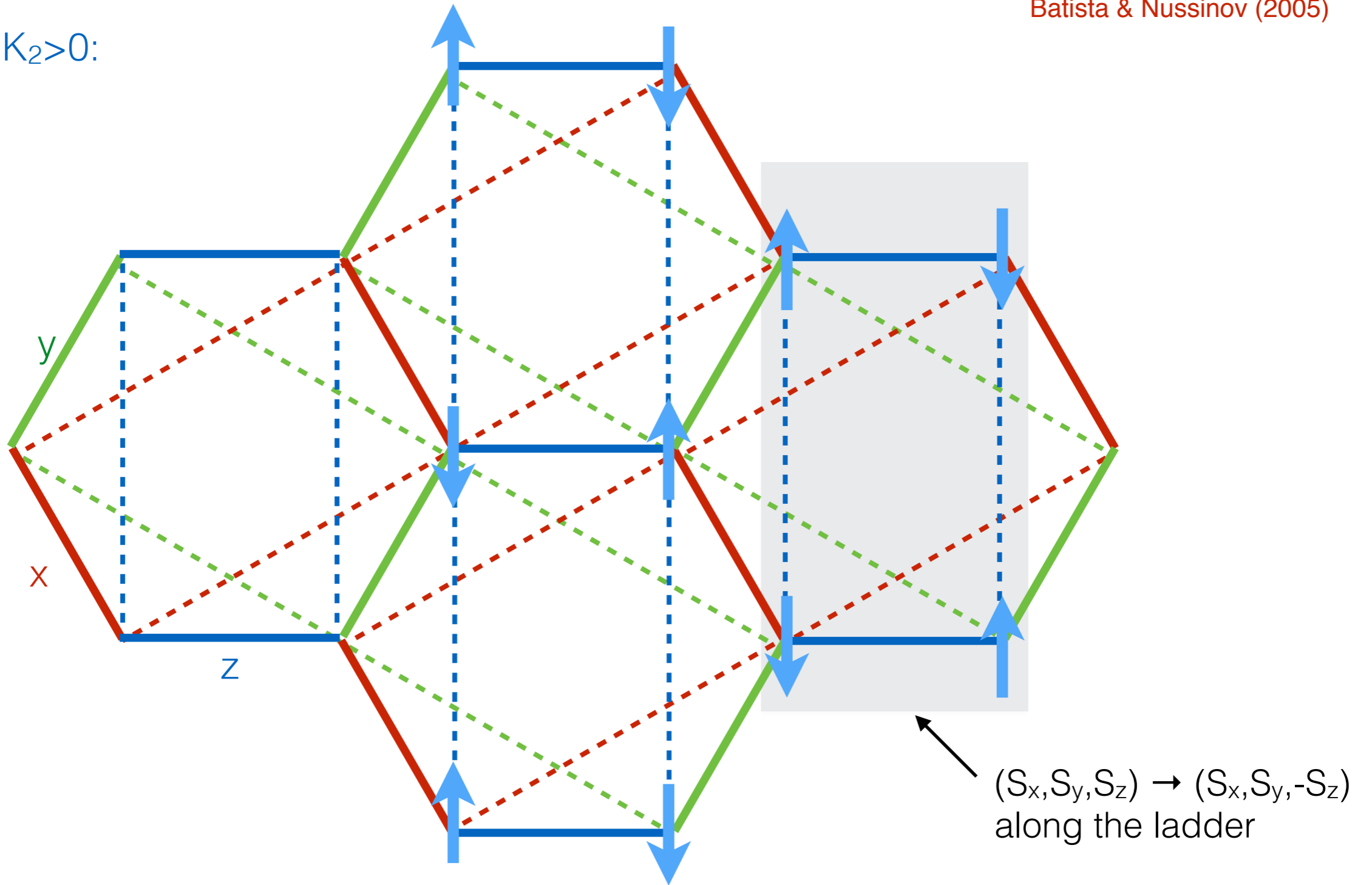
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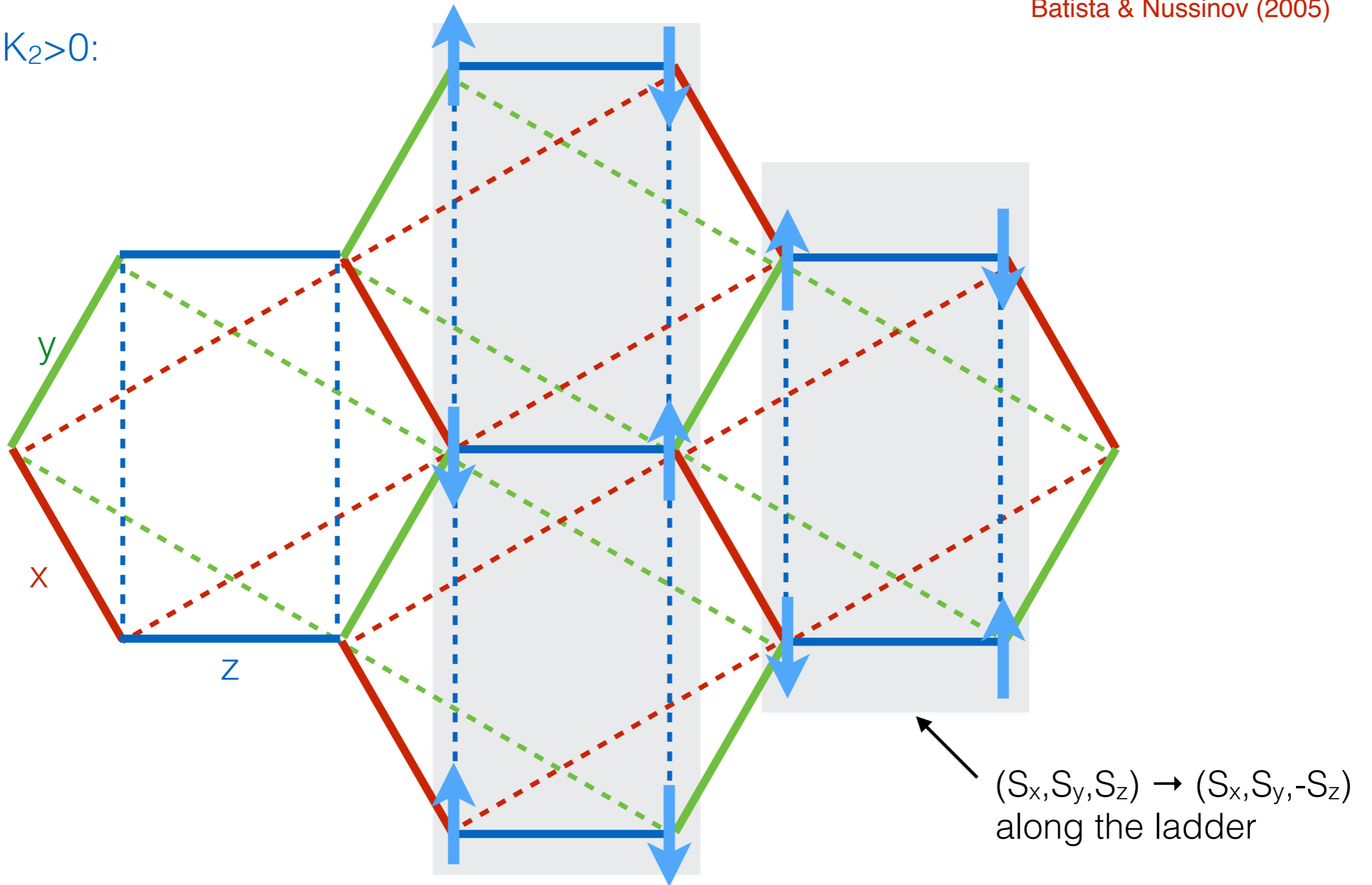
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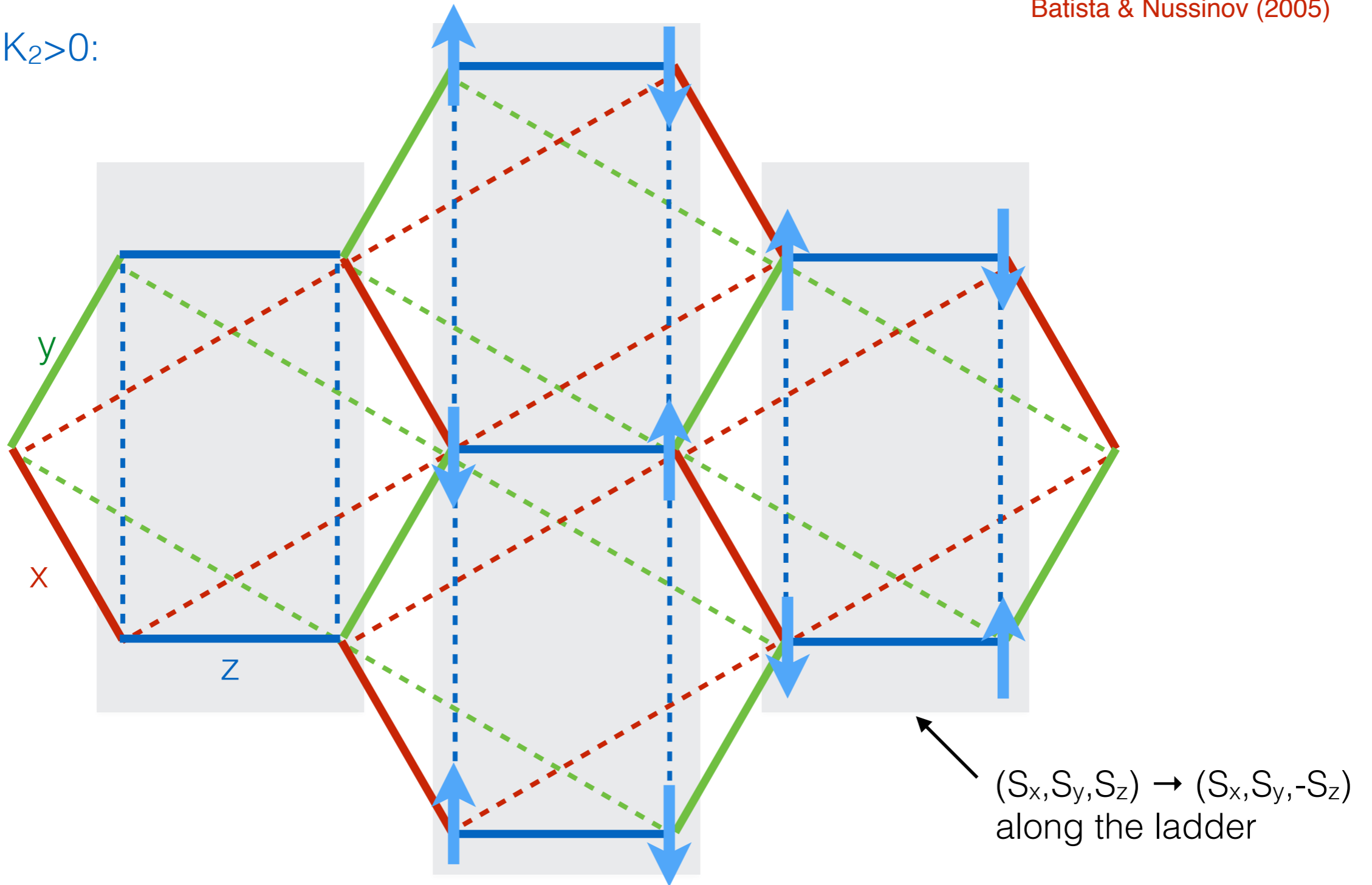
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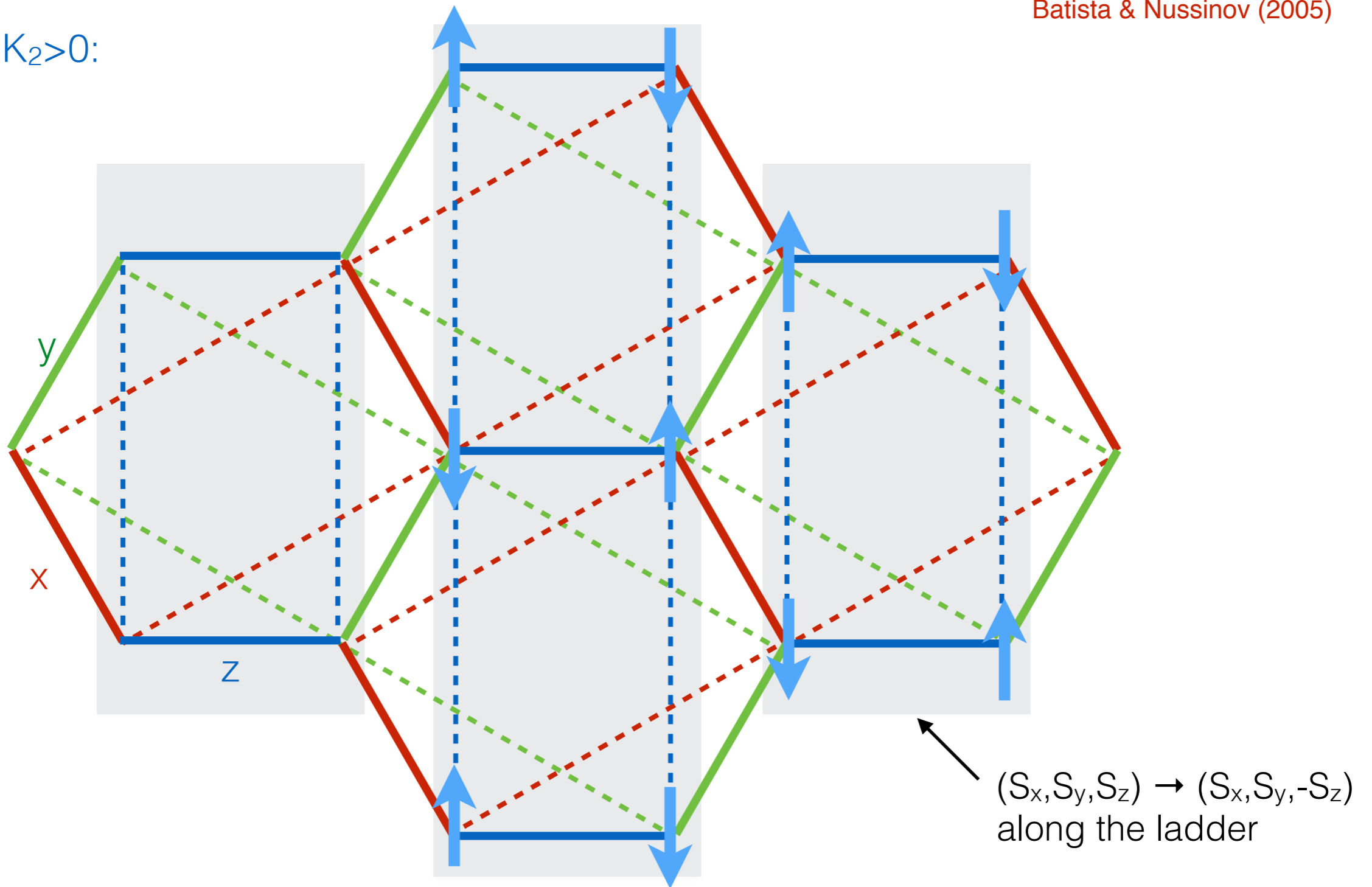
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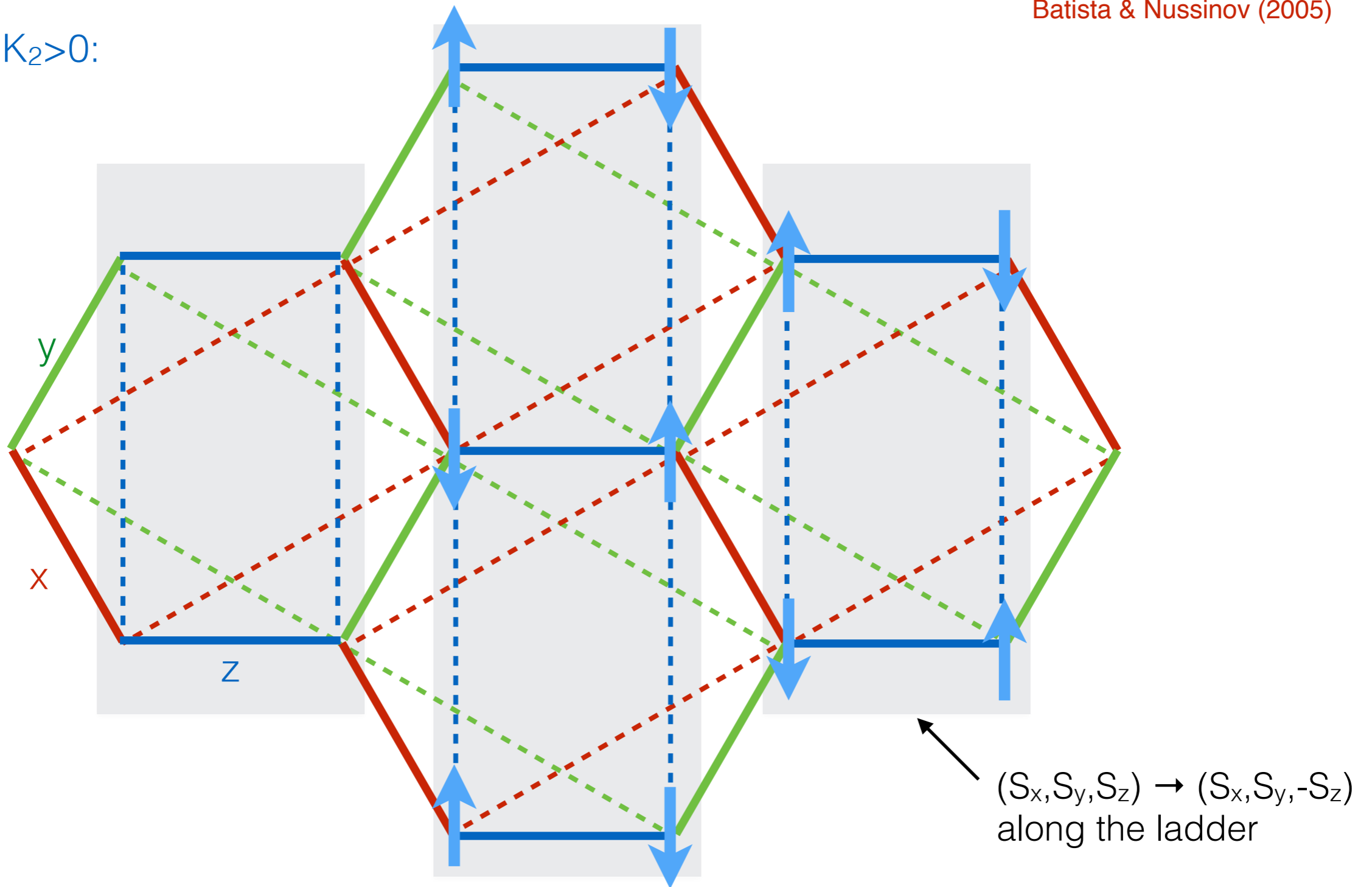


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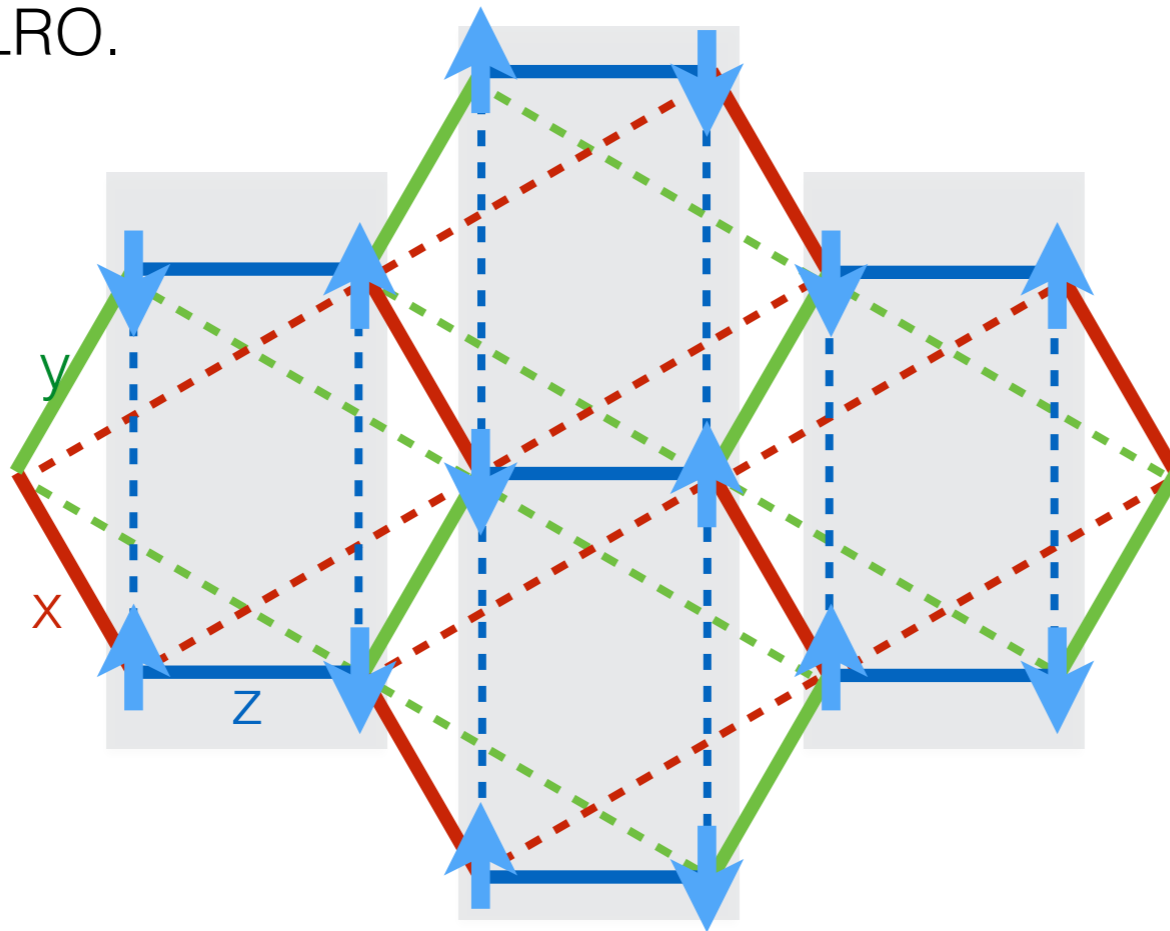
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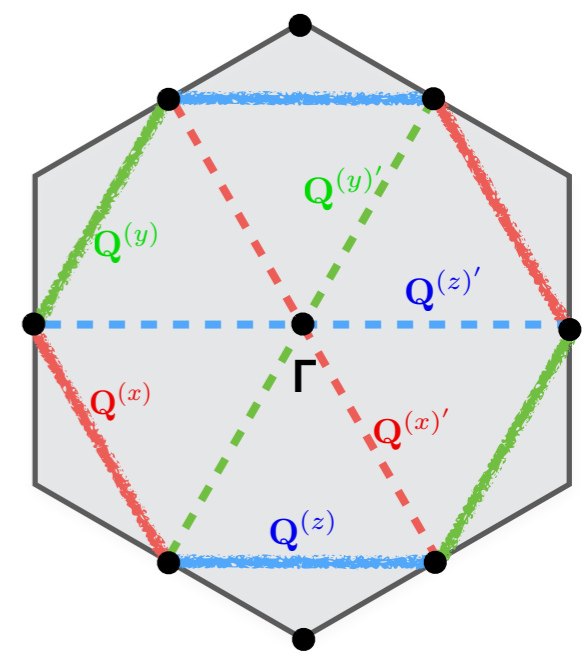
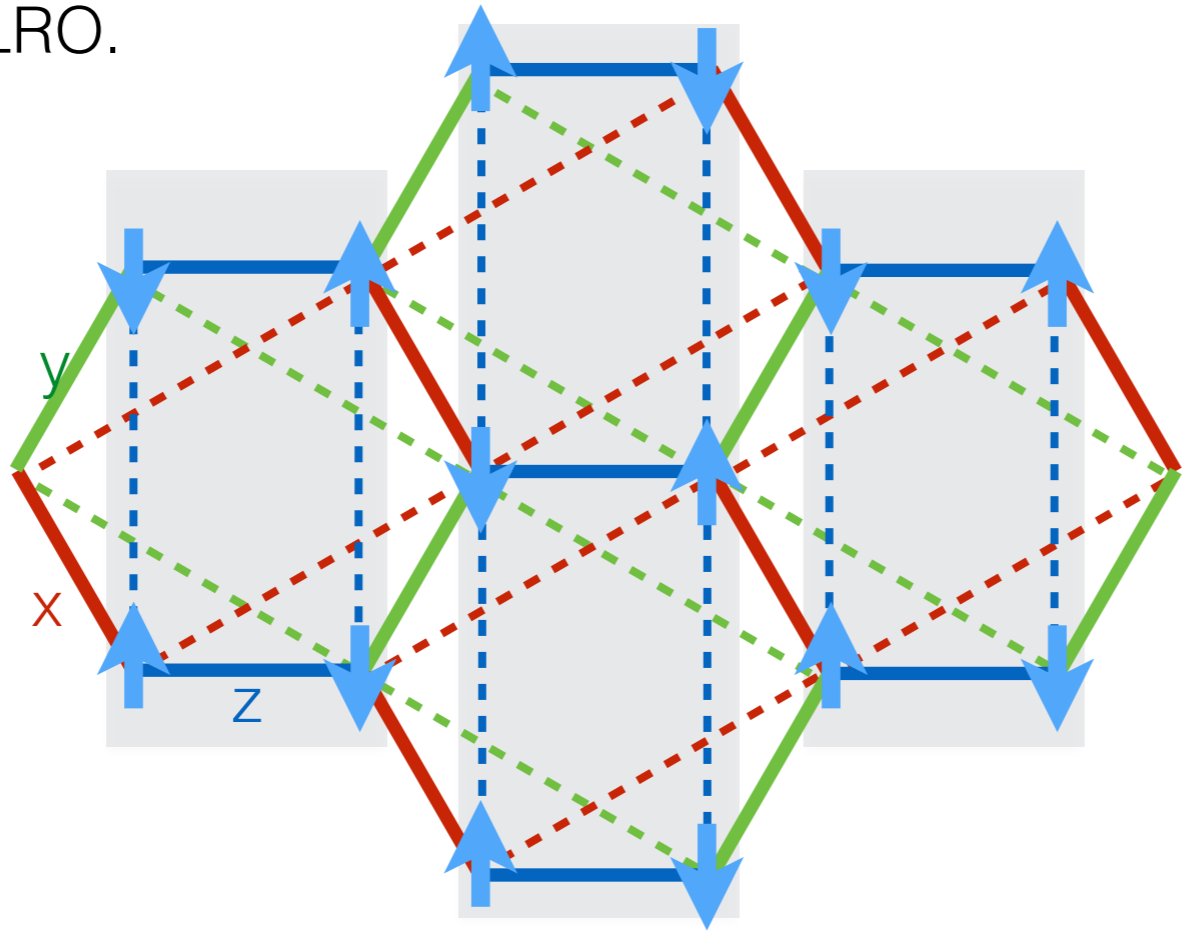
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- $T=0$: sliding symmetries can break, but in all possible ways!
→ no isolated Bragg peaks as we found with ED

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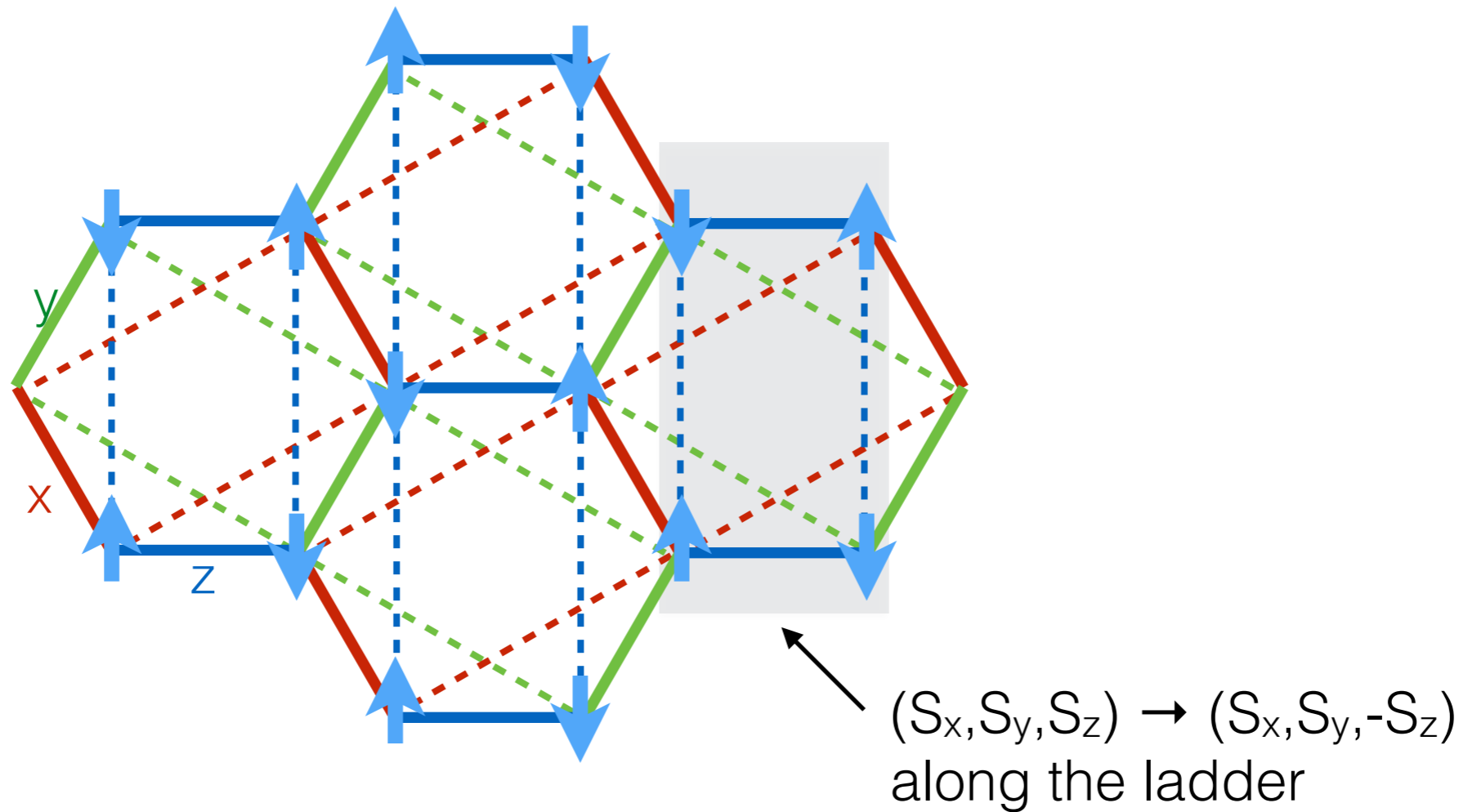
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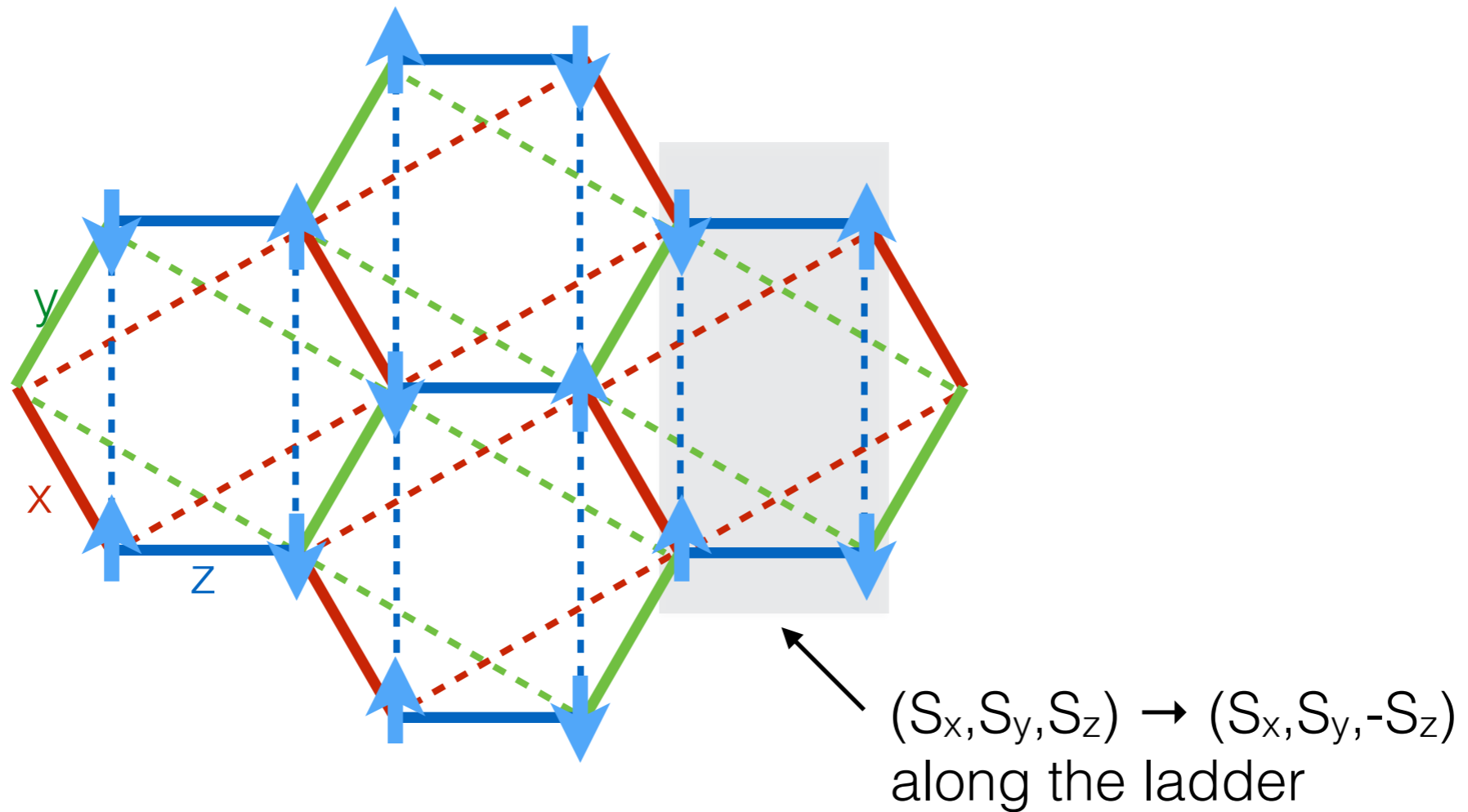
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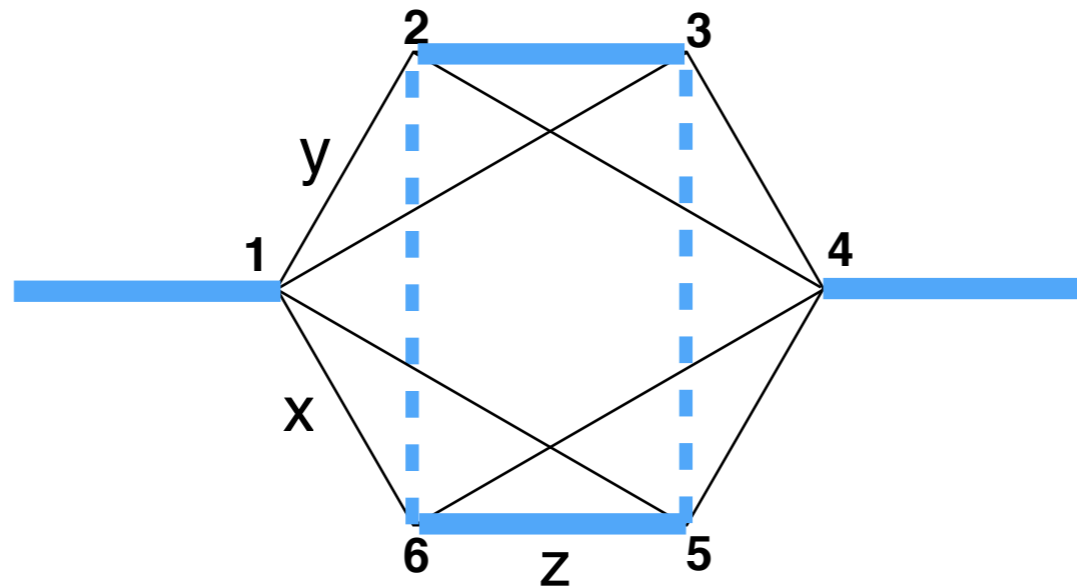


→ different ladders must talk to each other via quantum fluctuations !

Quantum order-by-disorder: strong coupling expansion

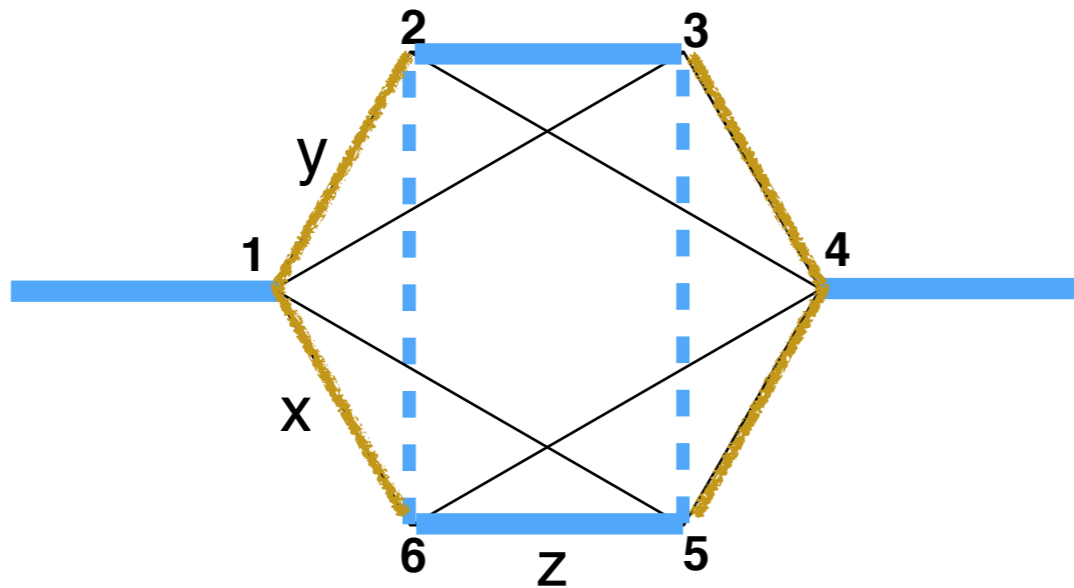
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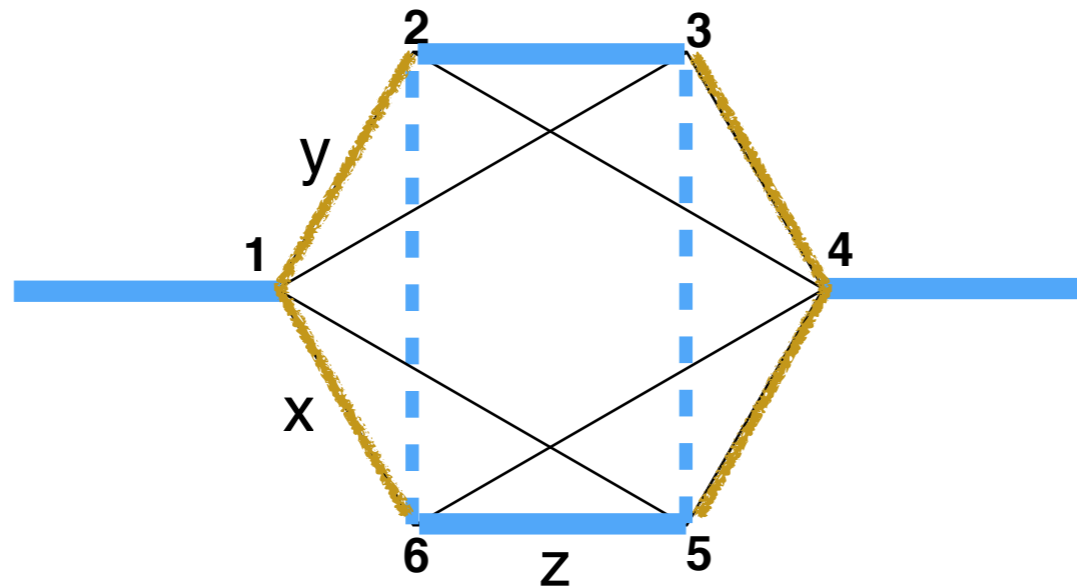
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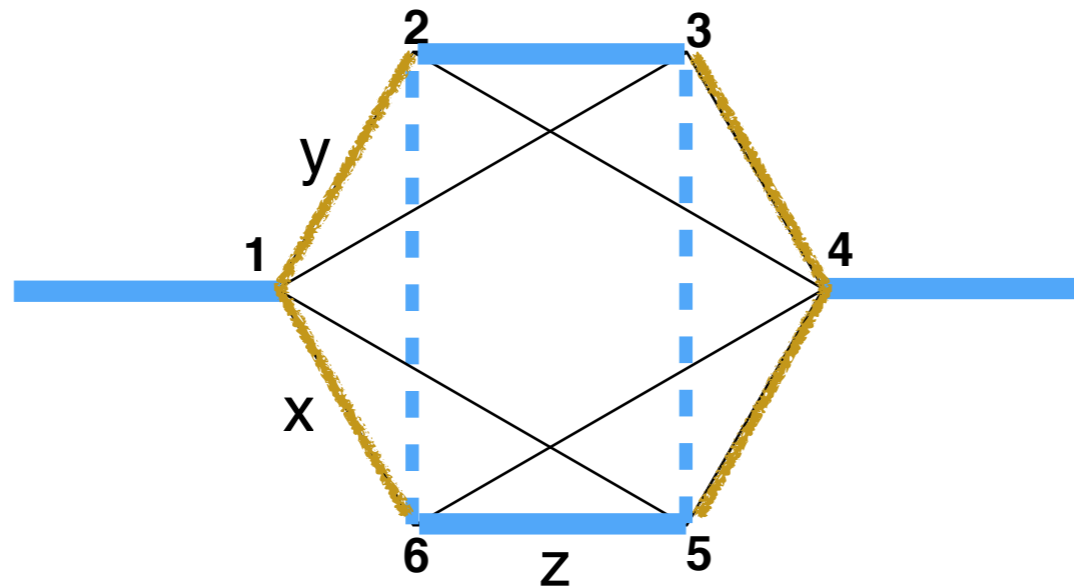


- *effective* term is a flux operator: $J_W \hat{W}_h = 2^6 J_W S_1^z S_2^x S_3^y S_4^z S_5^x S_6^y$

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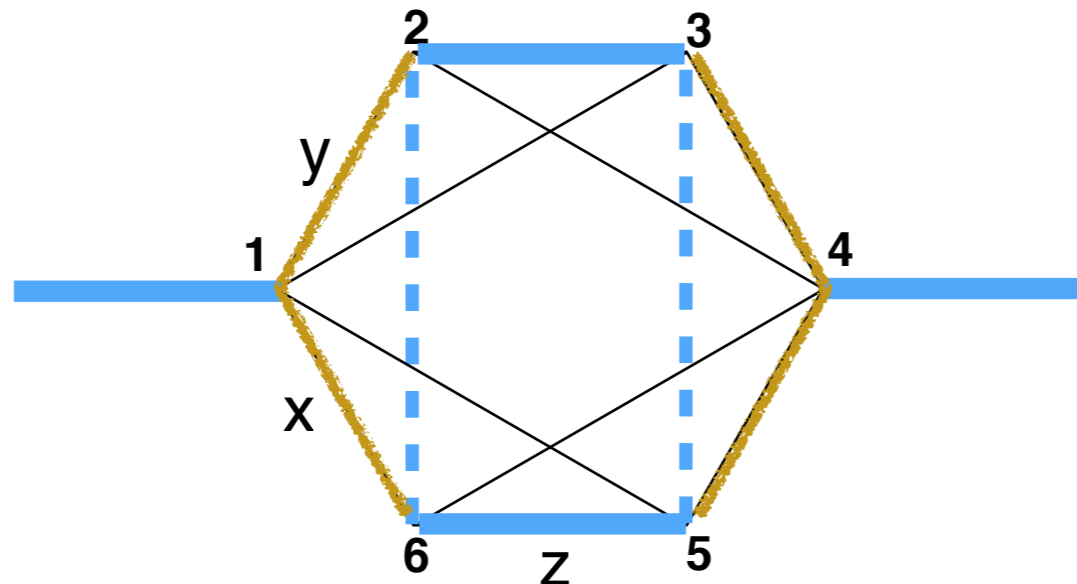


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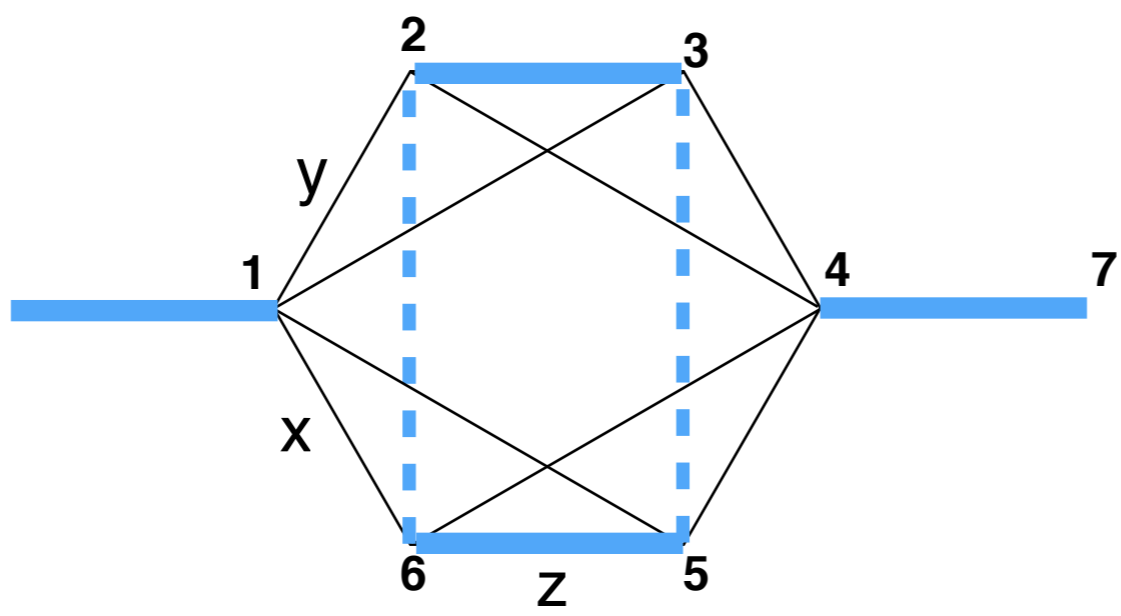
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- this term maps to the so-called **Toric code model** in the square lattice

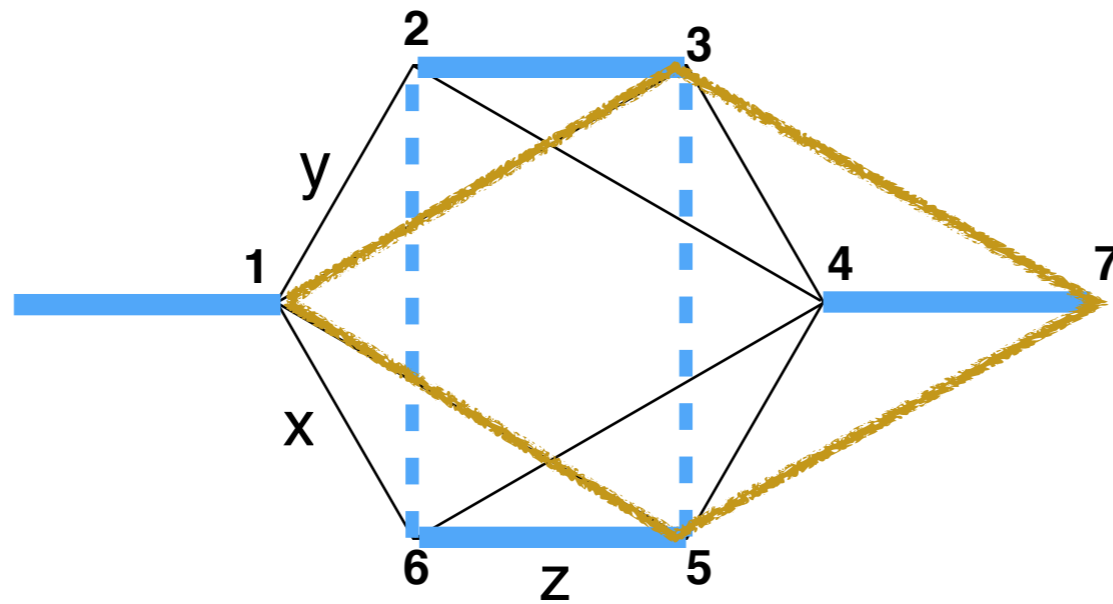
A. Kitaev ('03, '06)

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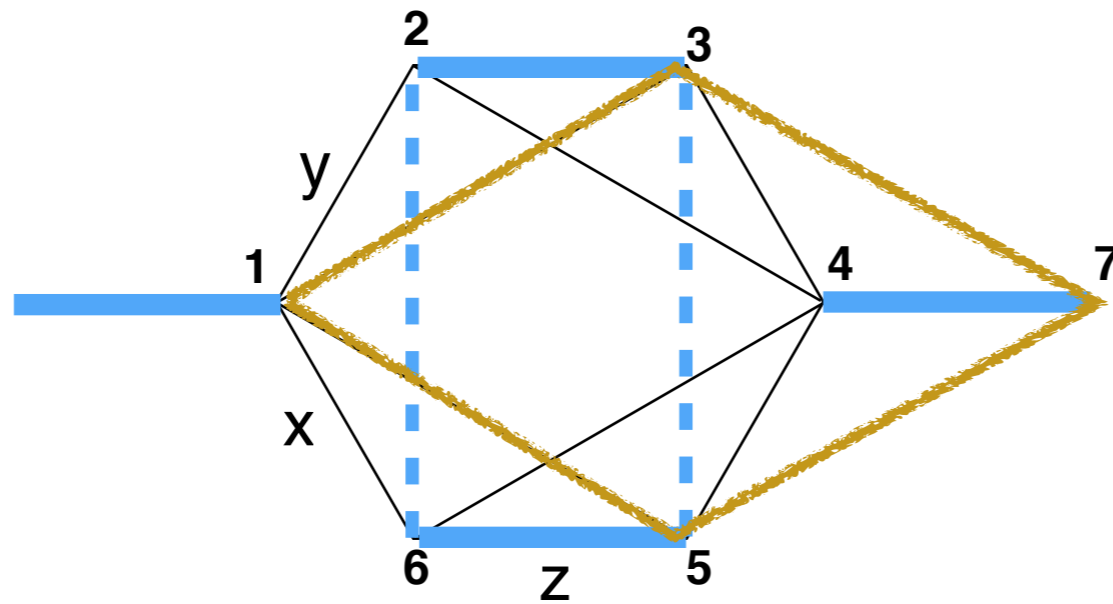
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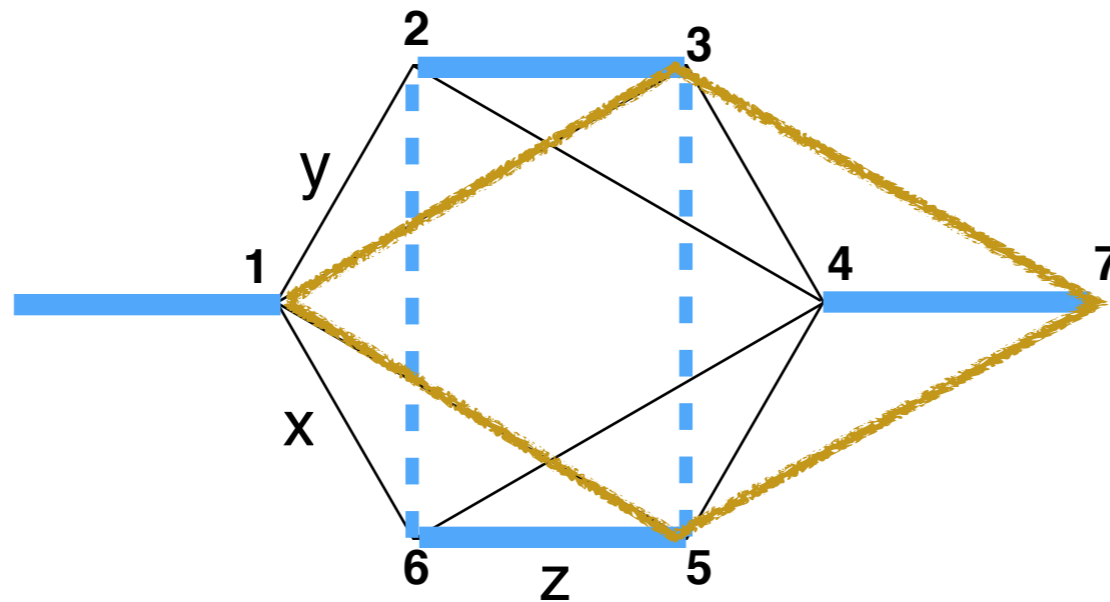


- *effective* Ising coupling J_1 between NNN ladders:

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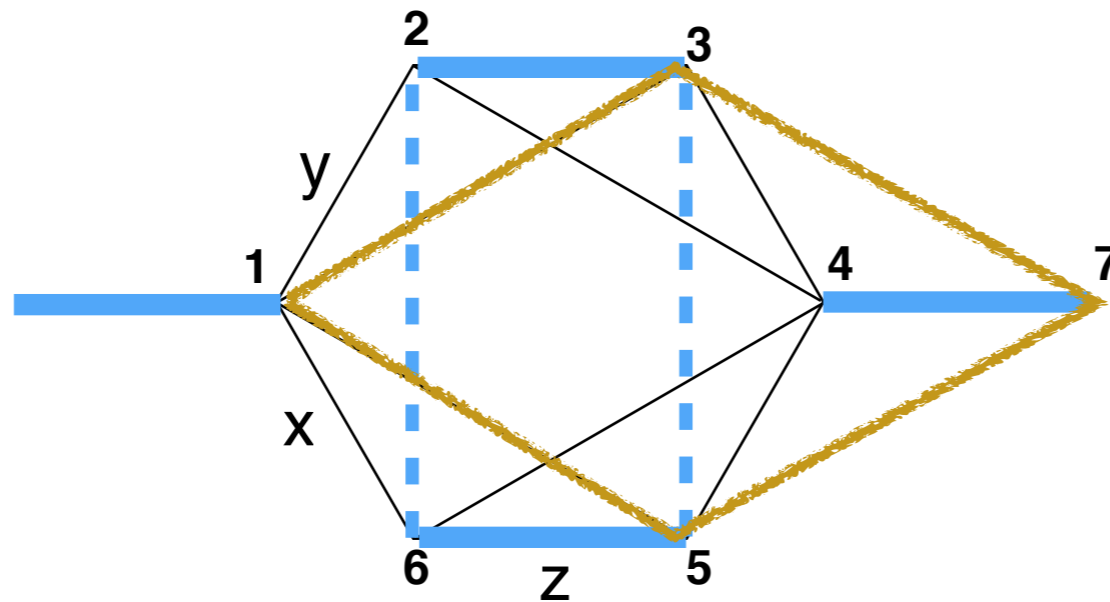


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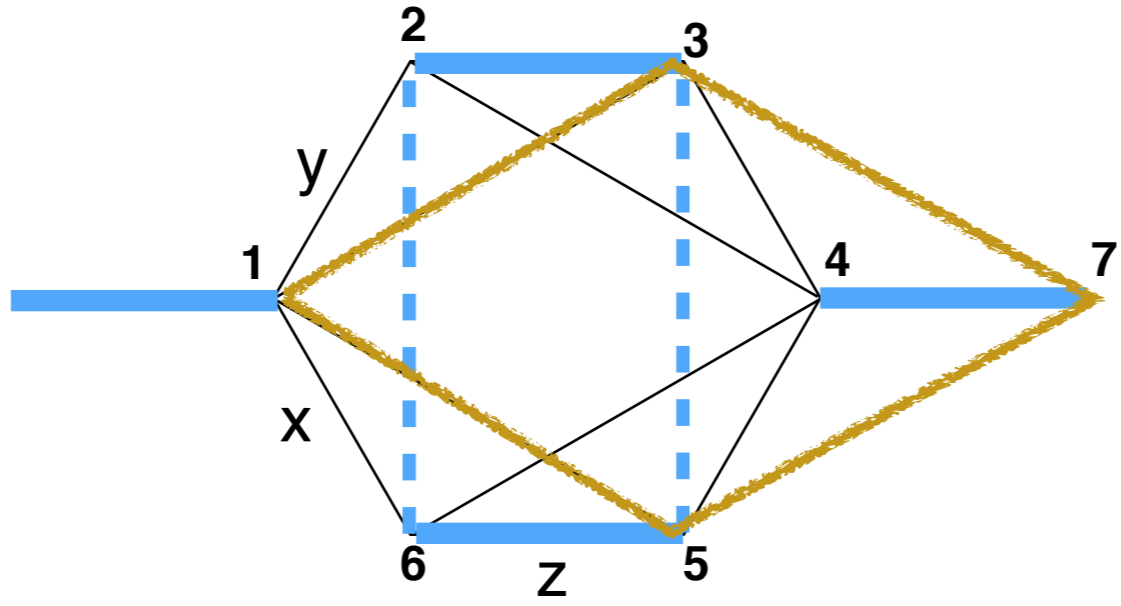


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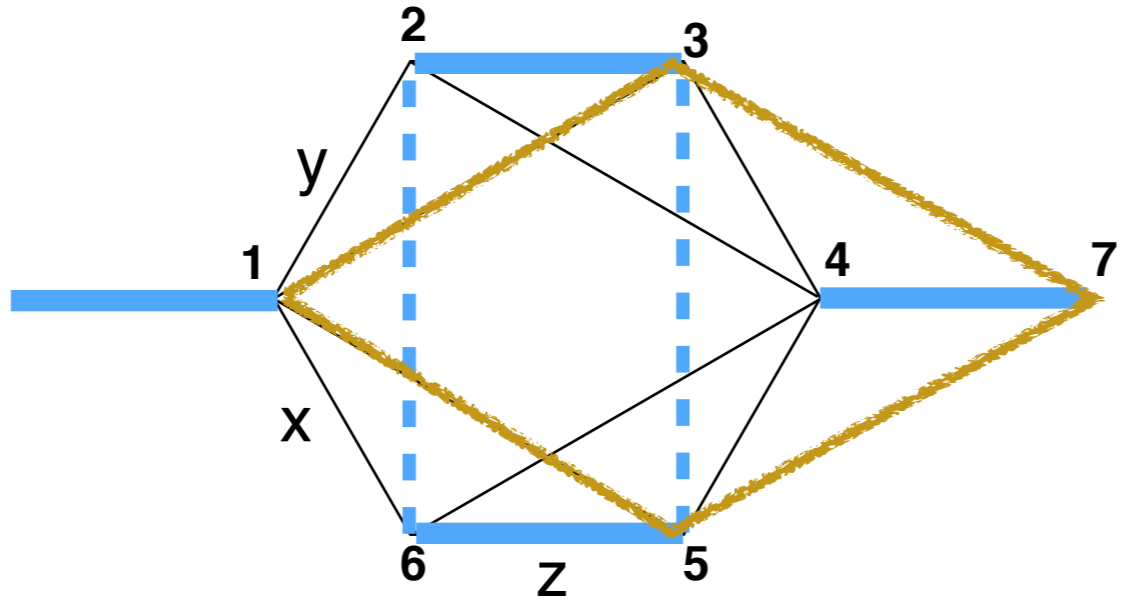
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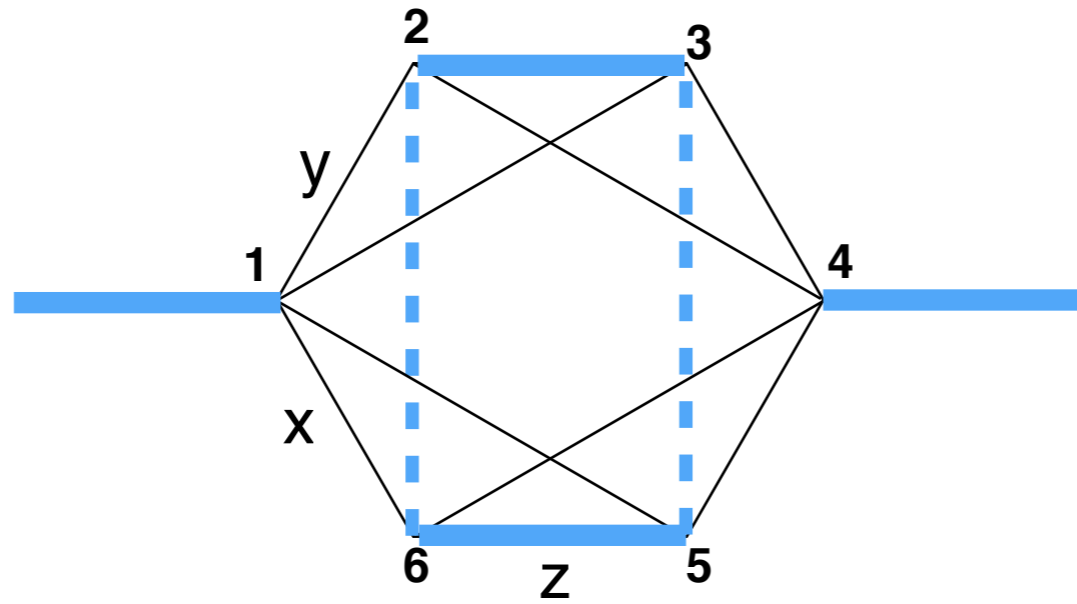
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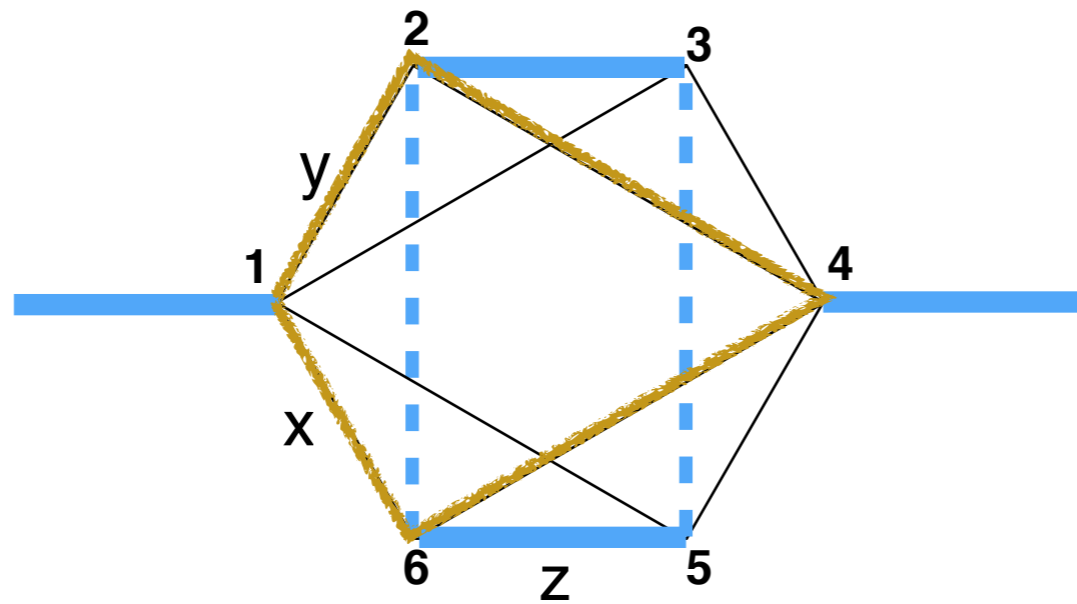
- same process in the triangular Kitaev model Jackeli & Avella(2015)

Quantum order-by-disorder: strong coupling expansion



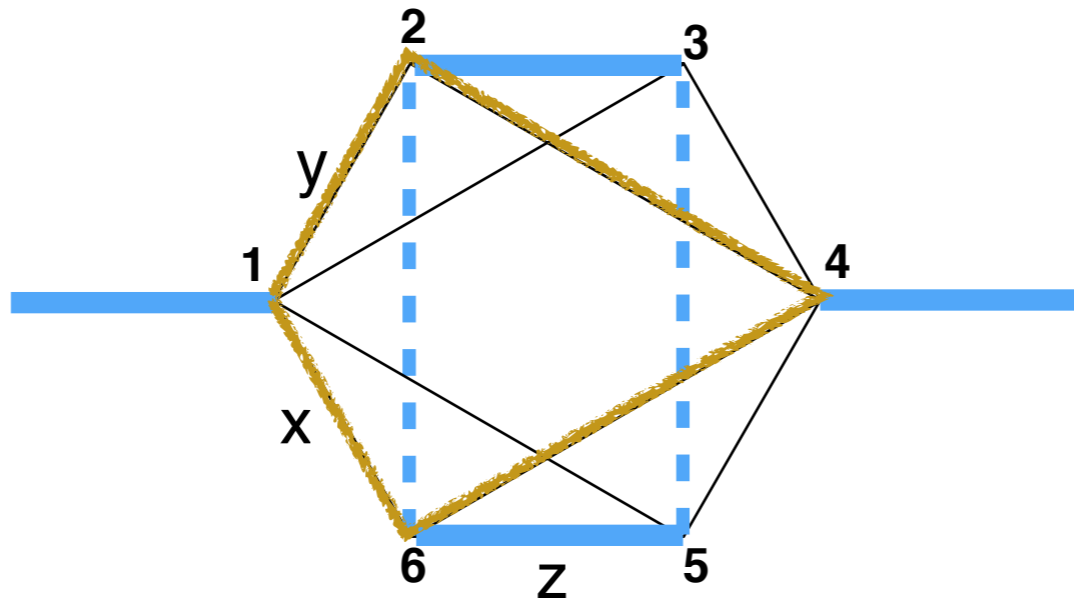
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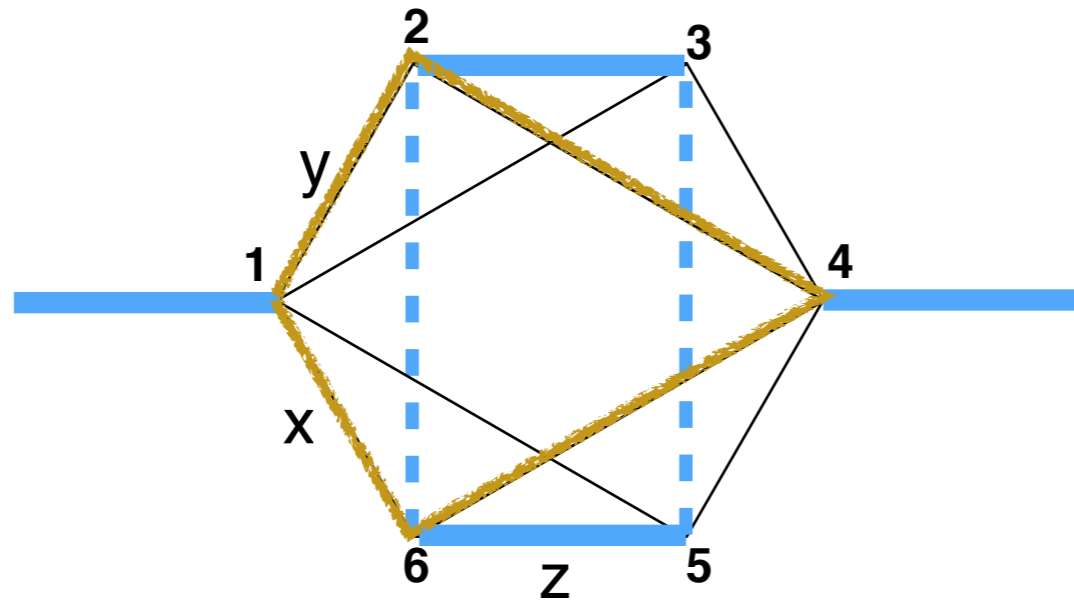


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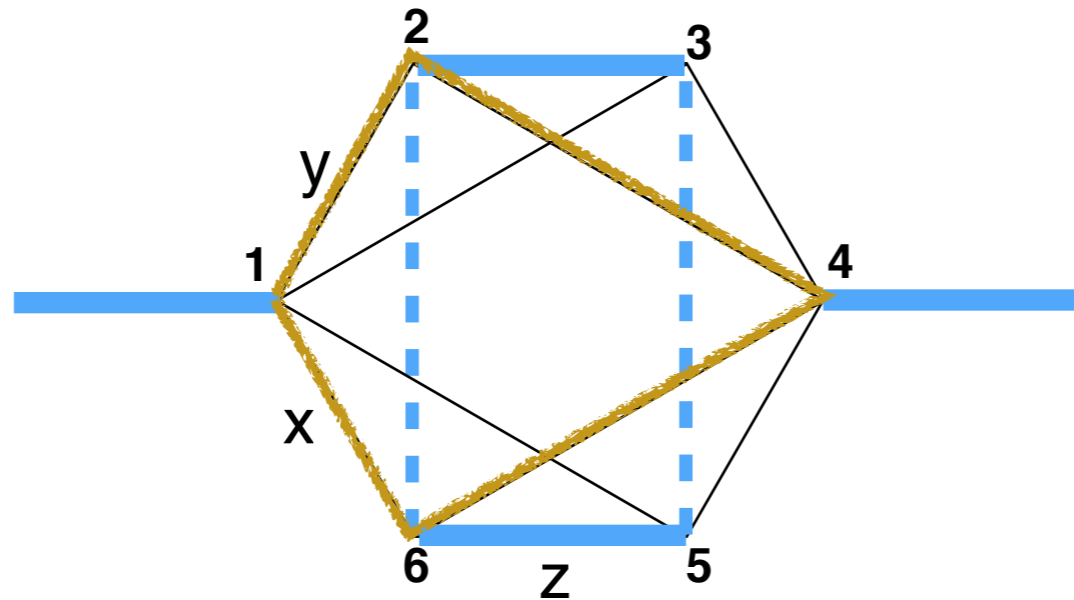
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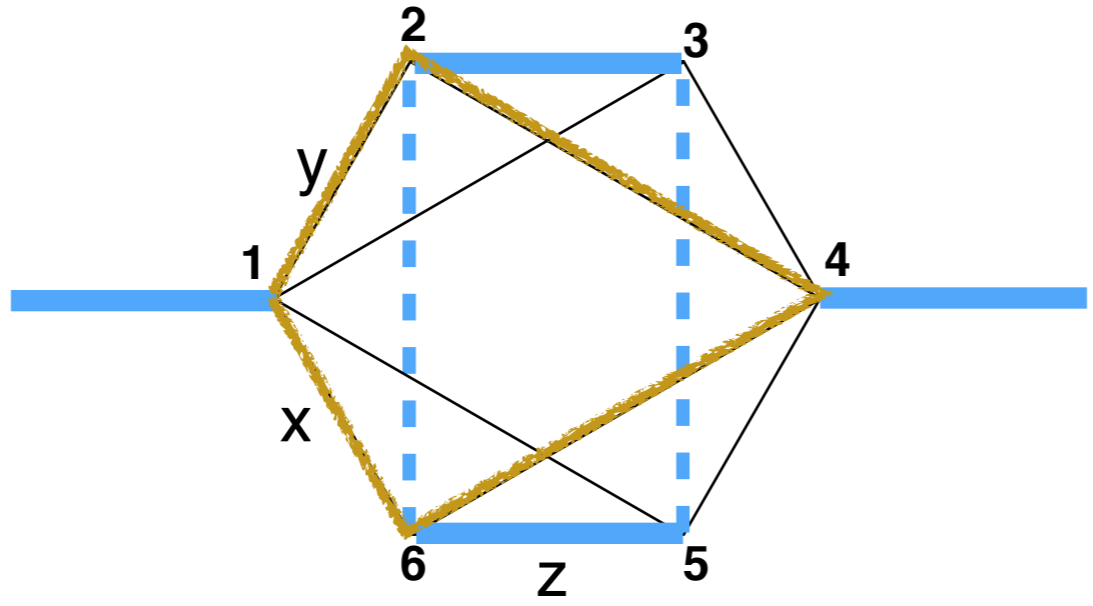


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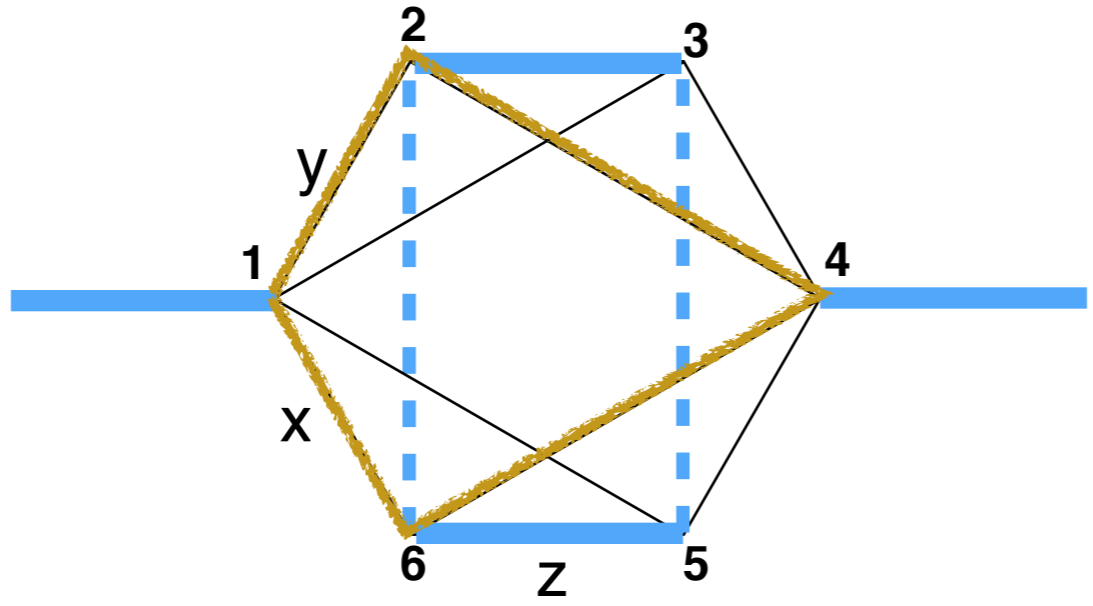
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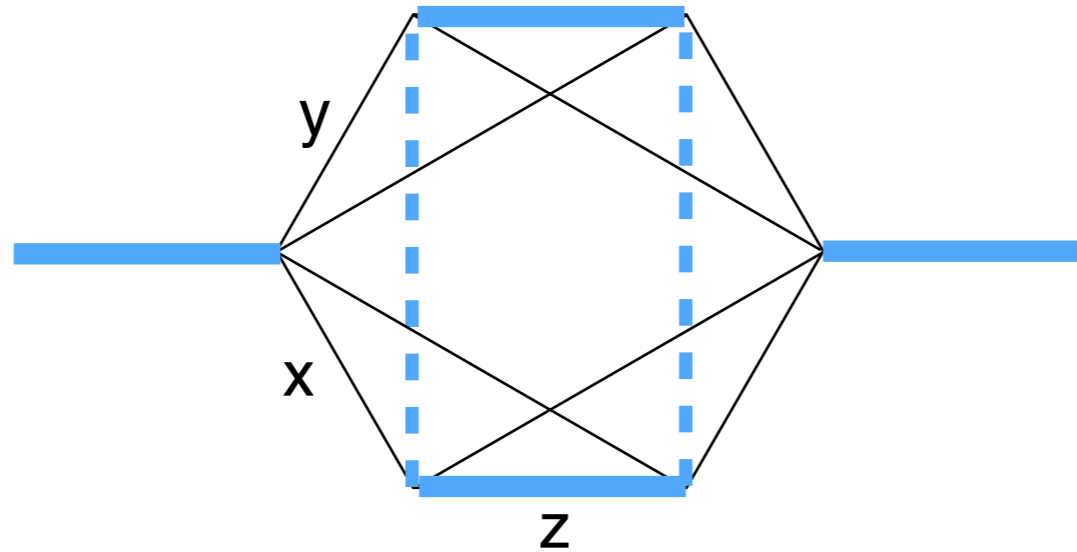
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large for $\psi = \pi/4, 3\pi/4, 5\pi/4, 7\pi/4$

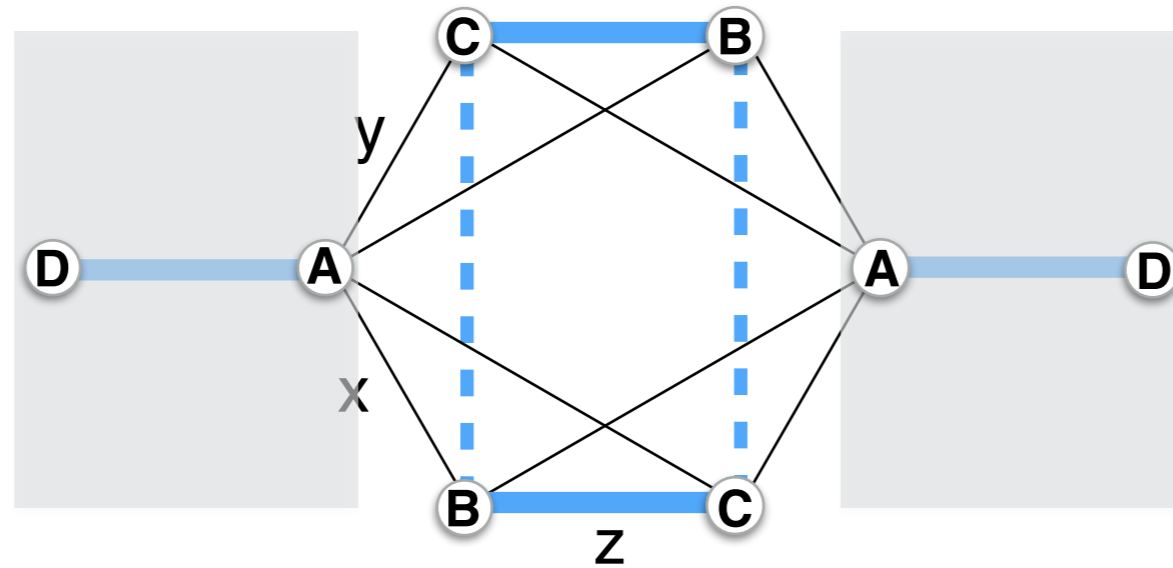
Quantum order-by-disorder: no coupling between NN ladders

- NN ladders do not talk to each other: true to all orders in pert. theory



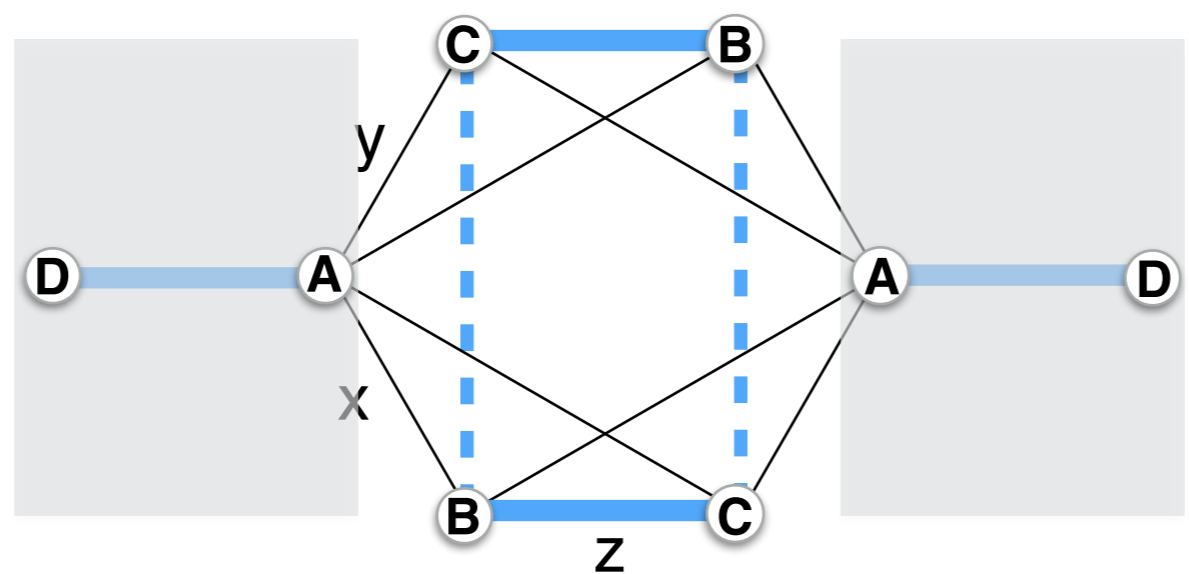
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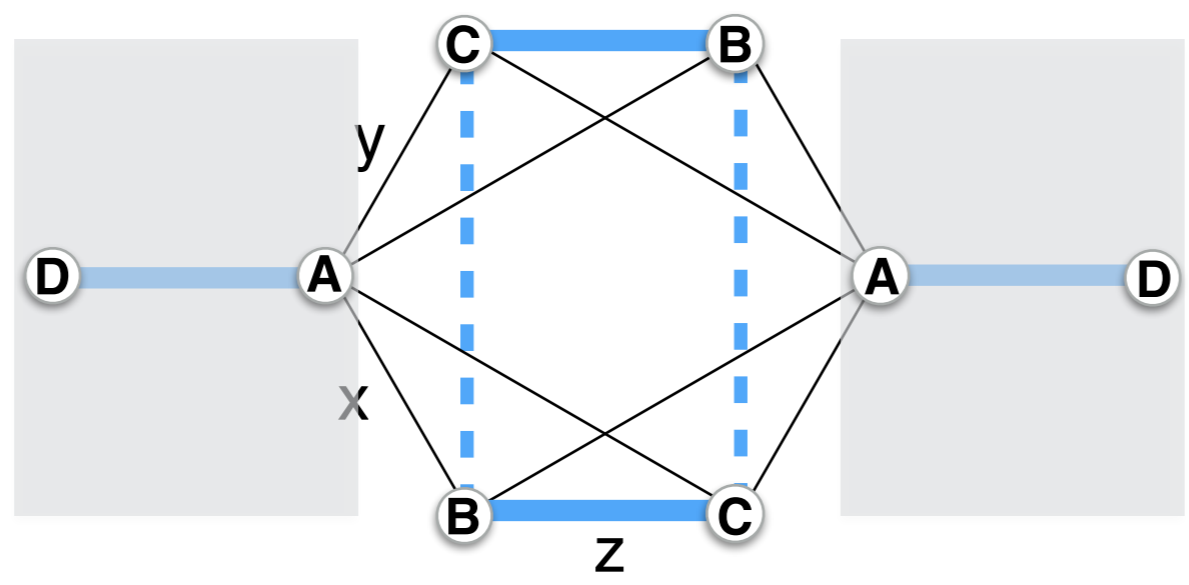
- gauge-like symmetry: $S_{xyz} = \begin{pmatrix} A & B & C & D \\ \mathbf{1} & C_{2x} & C_{2y} & C_{2z} \end{pmatrix}$

$(A_x, A_y, A_z) \rightarrow (A_x, A_y, A_z)$
 $(D_x, D_y, D_z) \rightarrow (-D_x, -D_y, D_z)$

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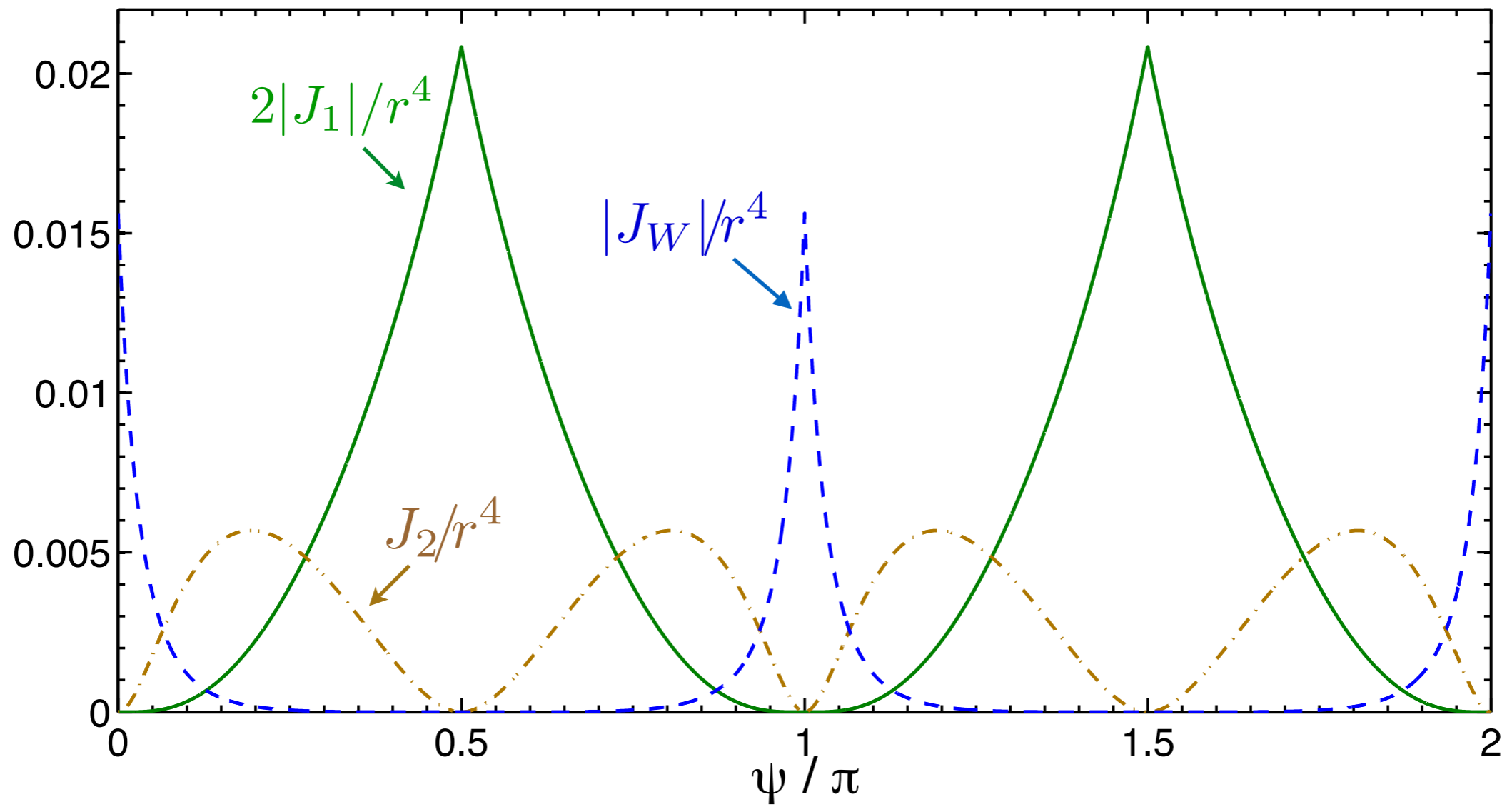
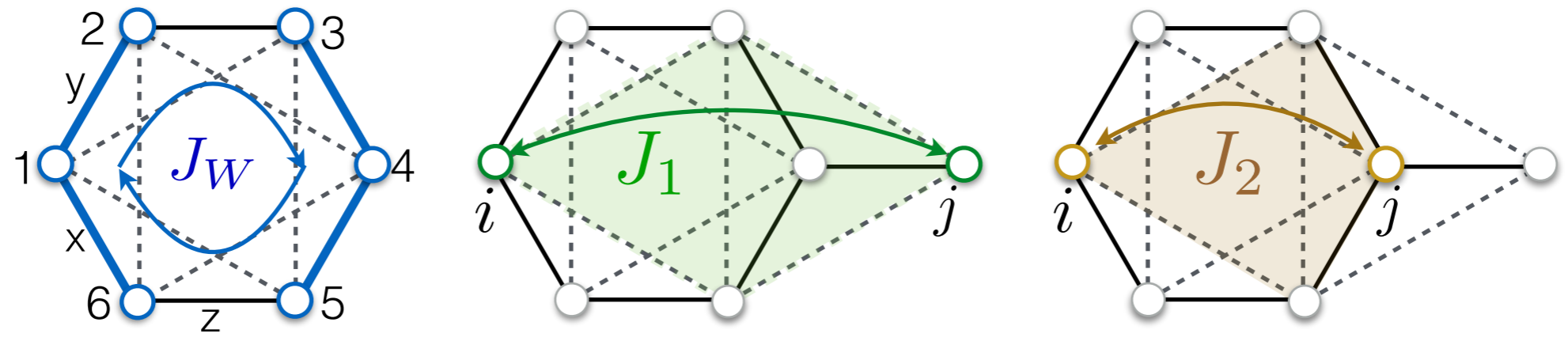
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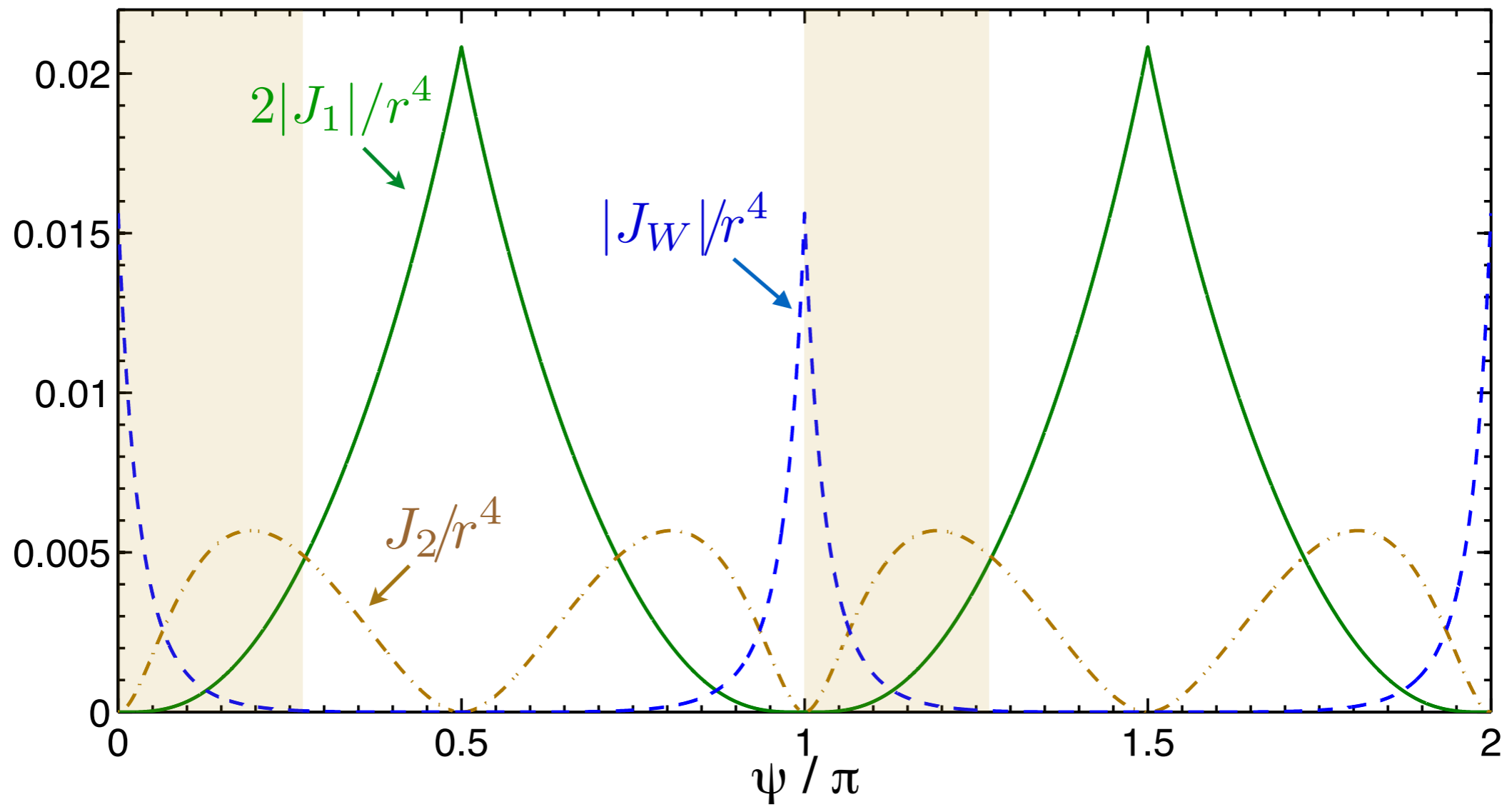
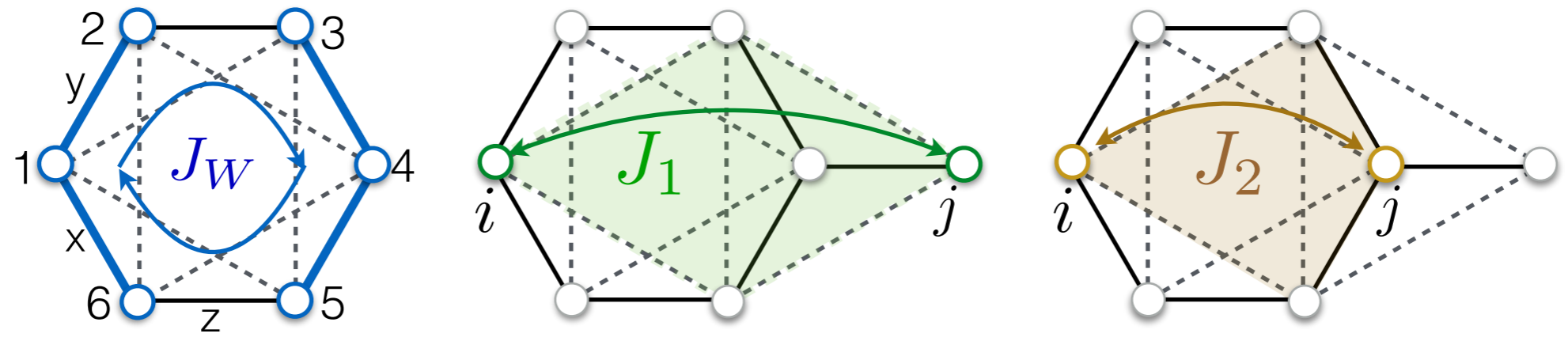
$$J_{nn} A_z B_z \rightarrow -J_{nn} A_z B_z, \text{ so } J_{nn} \text{ must vanish identically !}$$

Quantum order-by-disorder: strong coupling expansion



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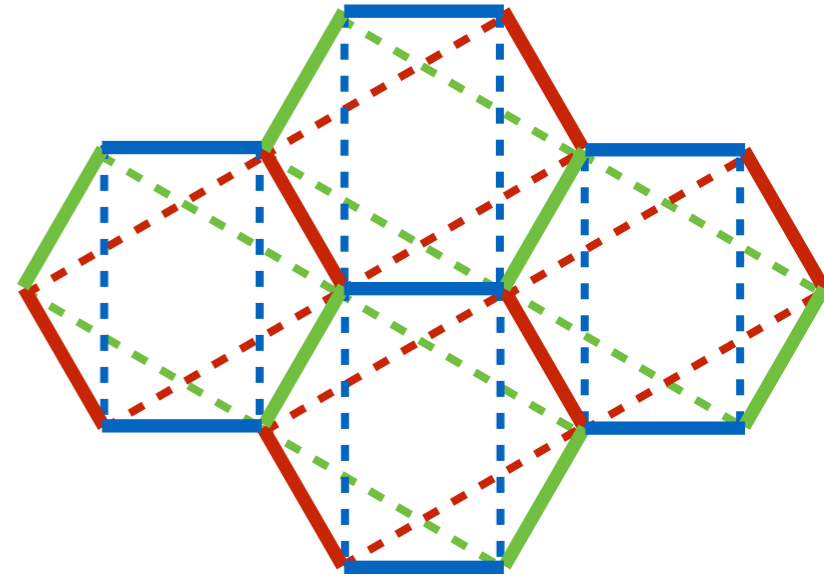


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Take home messages

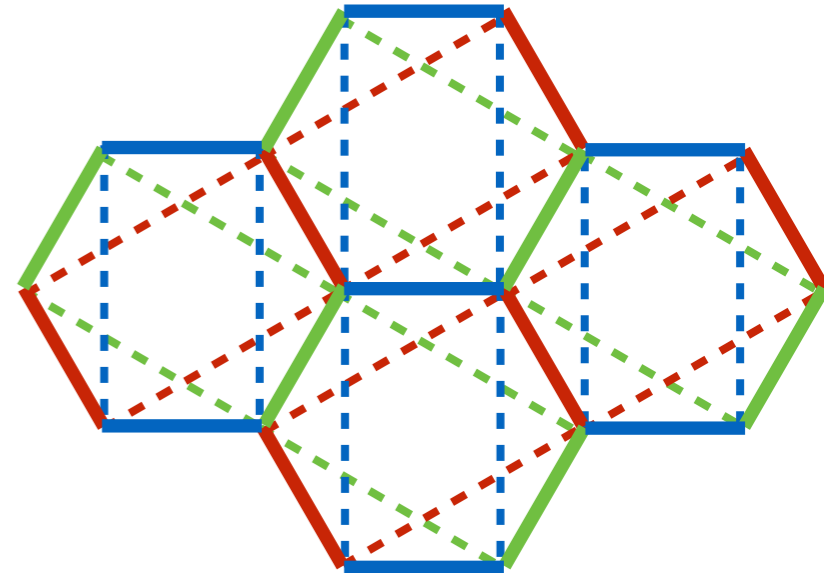
Take home messages

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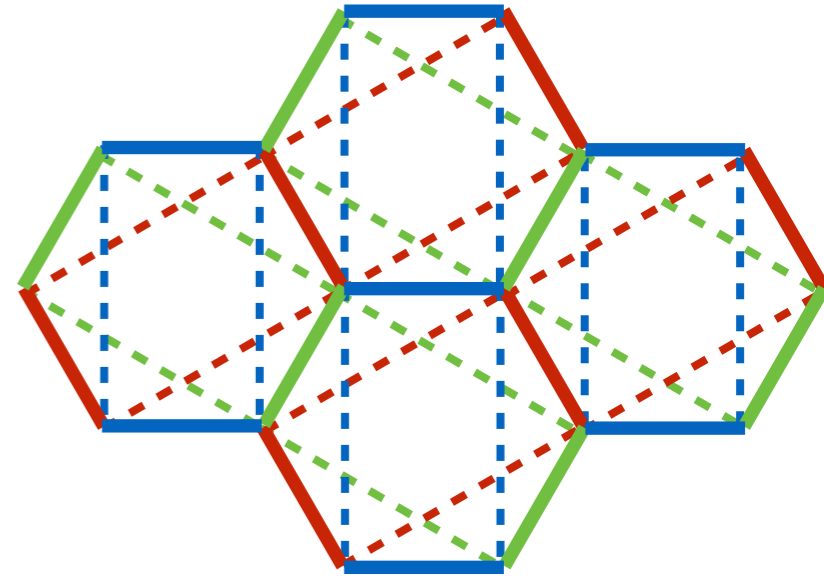
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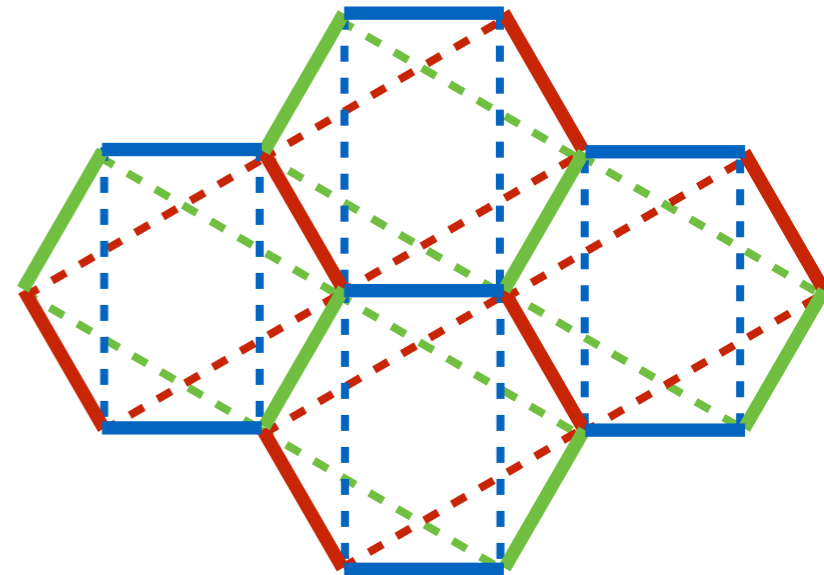
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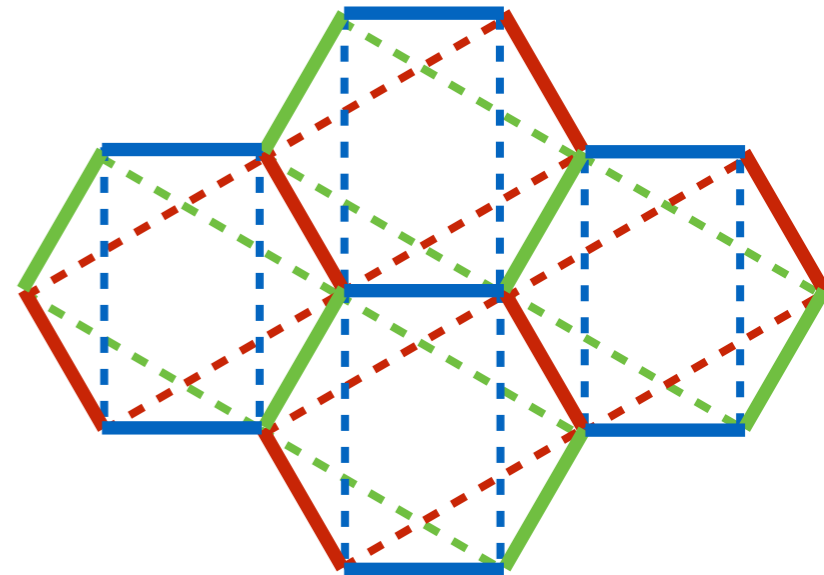
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Thank you very much for your attention !