Monte Carlo study of Microscopic Models for Néel-PlaquetteVBS transition in 2D square lattice

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Outline

1. Background: Deconfined Quantum Criticality

2. Construction of our model and DQC

3. Finite temperature “vestigial order”

4. Conclusion and discussions

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Motivation: DQC

Phase transitions:

Classical

Locally defined order parameter
Ginzburg-Landau paradigm

Topological

Topological order defined globally
No locally definable order!

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Phase transitions:

Classical

Locally defined order parameter
Ginzburg-Landau paradigm

Deconfined quantum criticality

Order-to-order transition
= locally defined order parameter
But ***defects*** play dominant role!

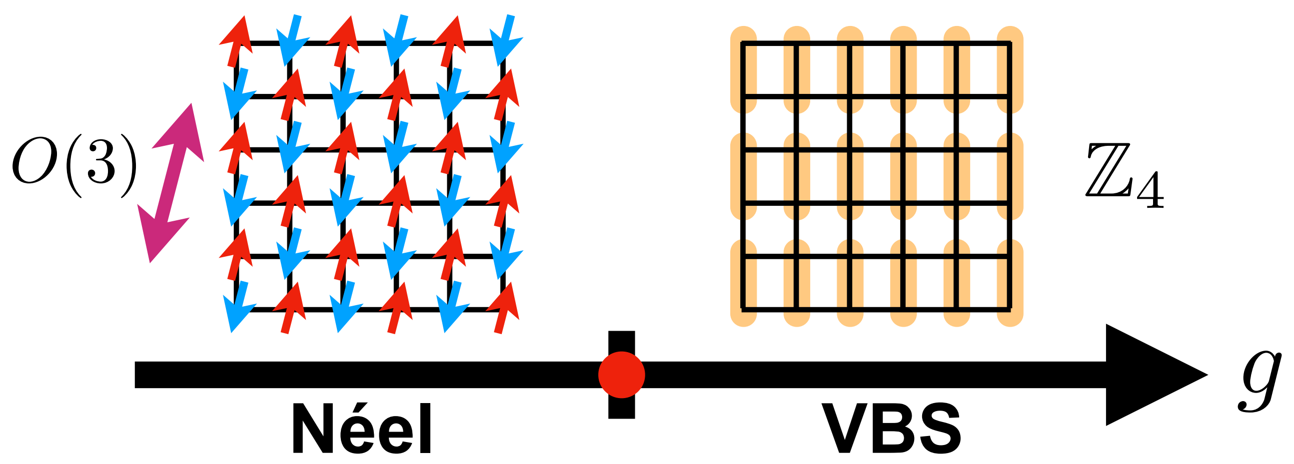
Topological

Topological order defined globally
No locally definable order!

Motivation: DQC

<u>Deconfined quantum criticality (DQC):</u>
<u>Quantum Phase transition beyond Ginzburg-Landau paradigm</u>

[T. Senthil et al., Science (2004)]
[M. Levin & T. Senthil, PRB (2004)]



Deconfined Quantum Criticality

- ✔ **2+1 dimensional**
- ✔ **square lattice**
- ✔ **spin 1/2**

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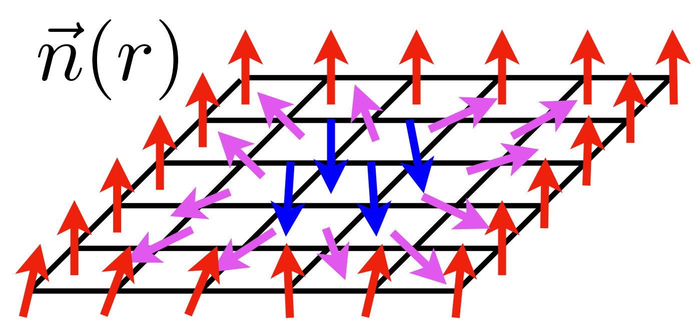
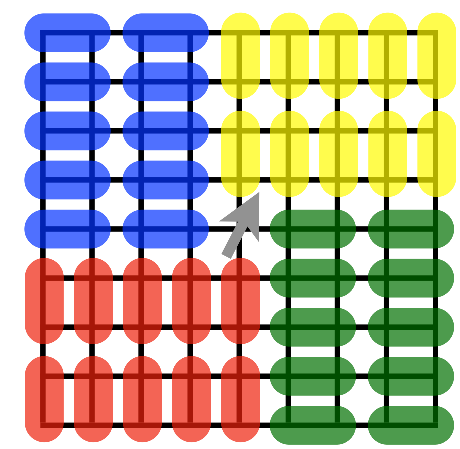
- ✔ spin 1/2

✔ **Defects in one phase entails the order of the other phase**



Skyrmions



Spinons

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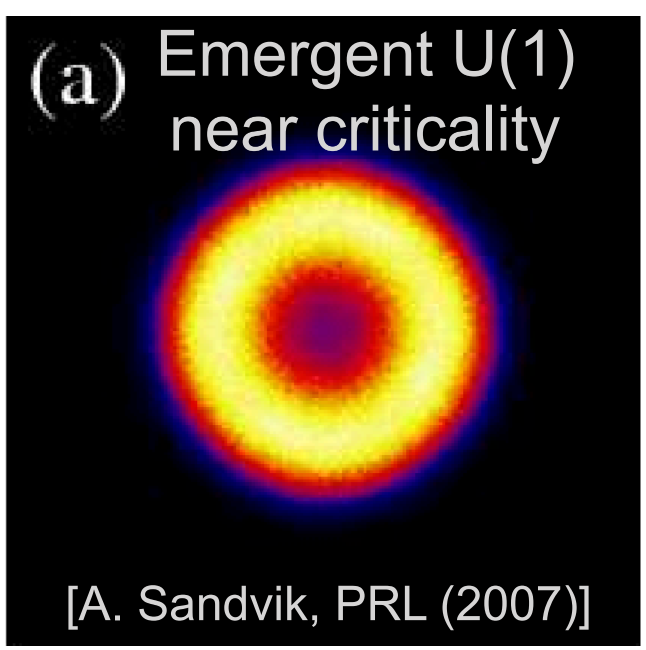
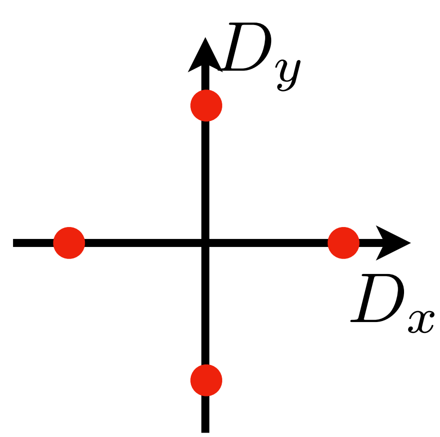


$\mathbb{Z}_4$ order away from criticality

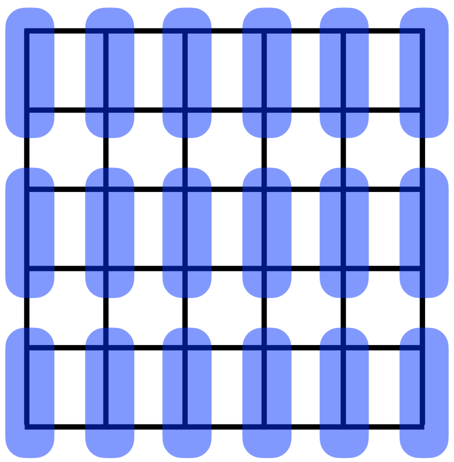


✔ $\mathbb{Z}_4$ **perturbation is (dangerously) irrelevant against U(1) symmetry**

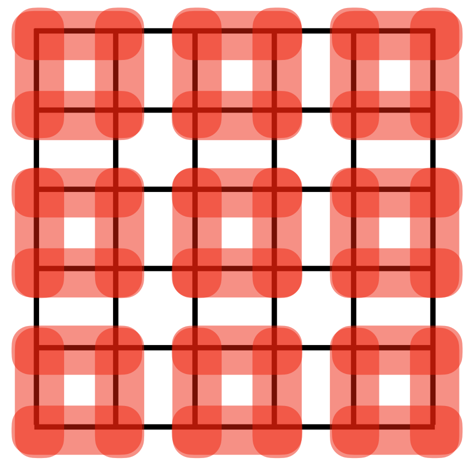
✔ **DQC point is close to U(1) spin-liquid**

Columnar-Plaquette “duality”

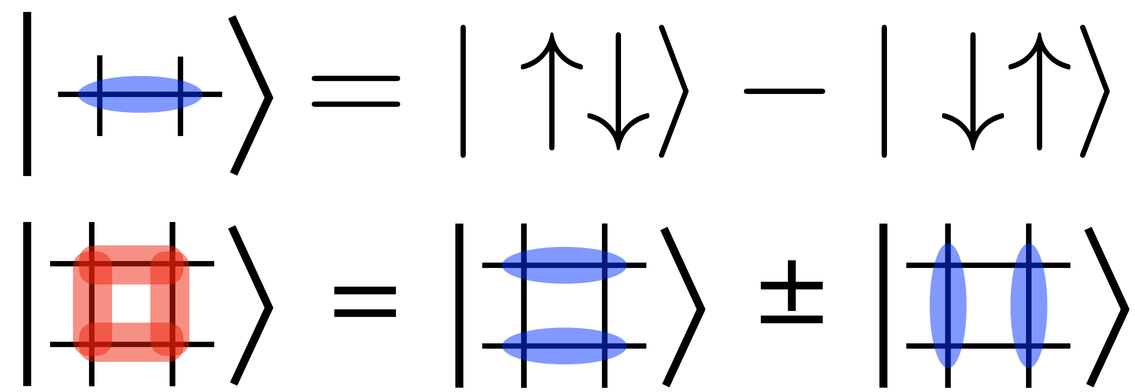
Two types of four-fold degenerate VBS states in square lattice!



Columnar



Plaquette



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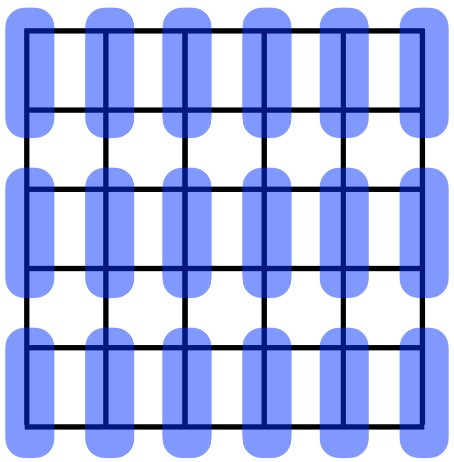
Two types of four-fold degenerate VBS states in square lattice!



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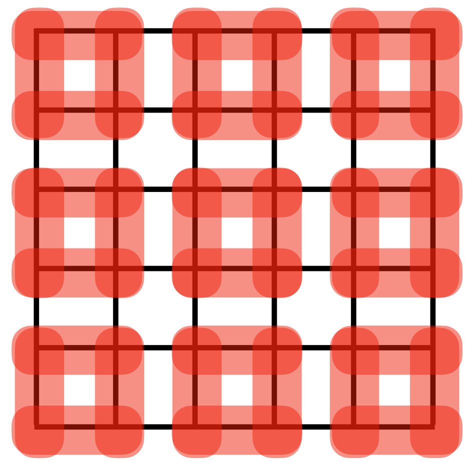

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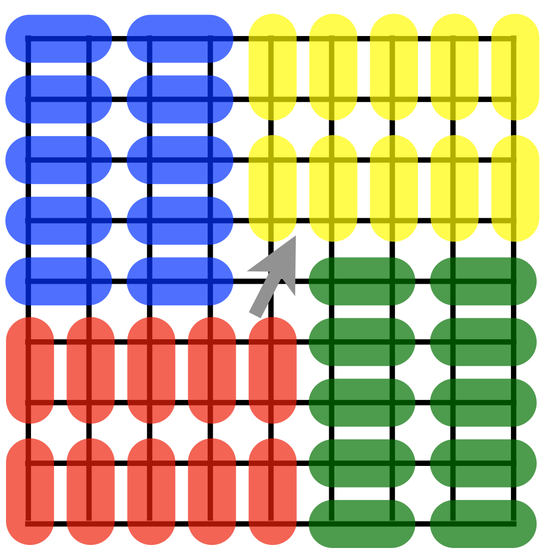

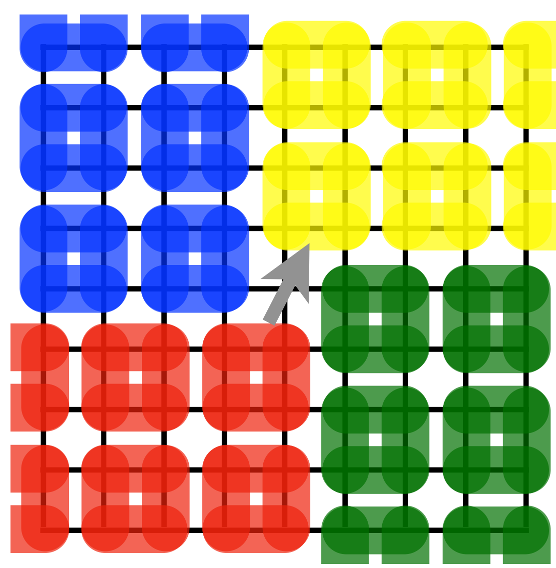

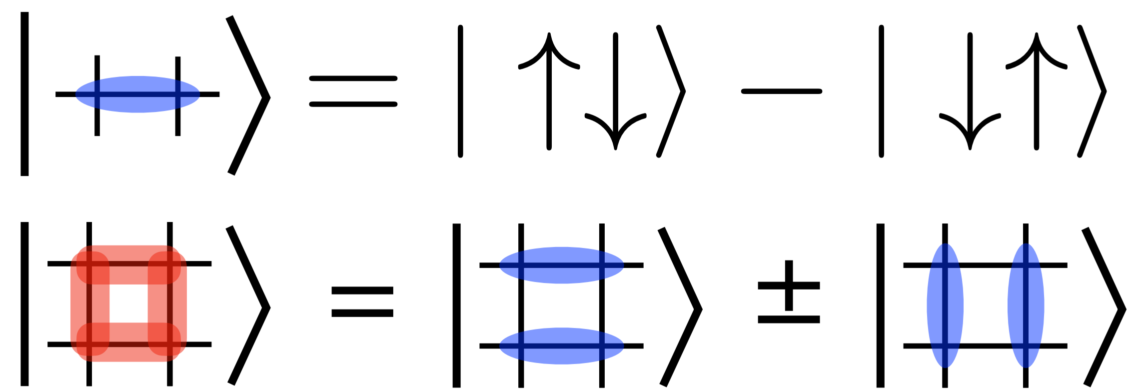

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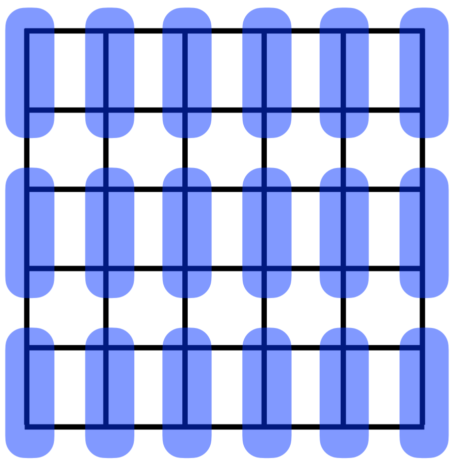

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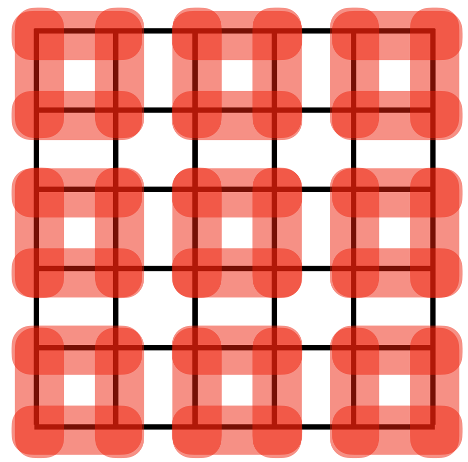

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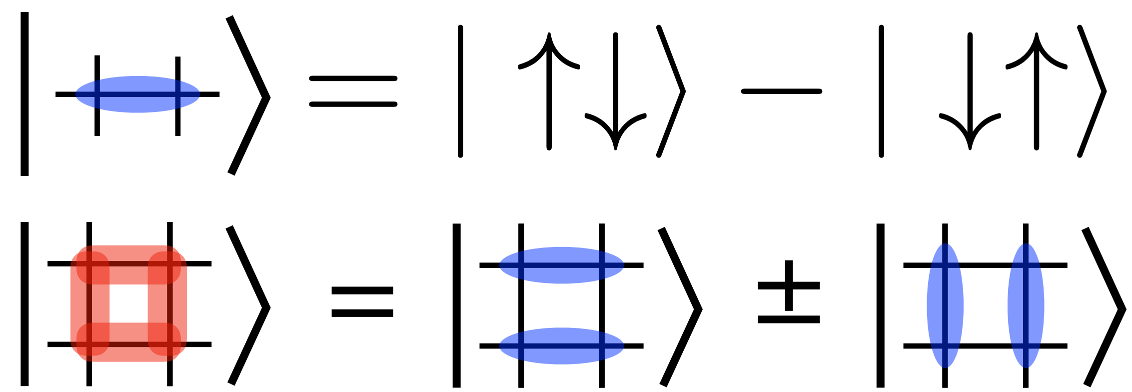

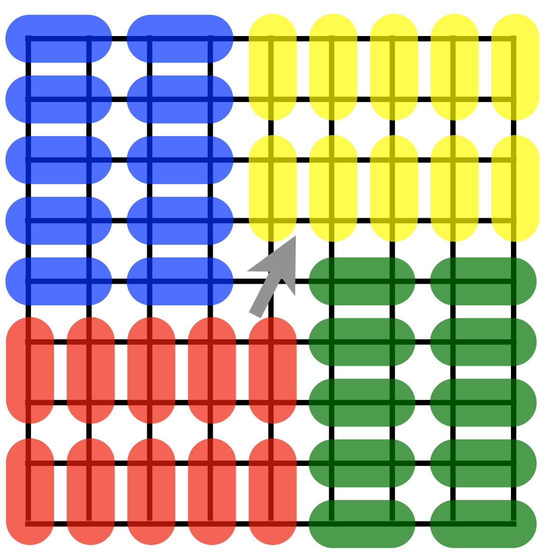

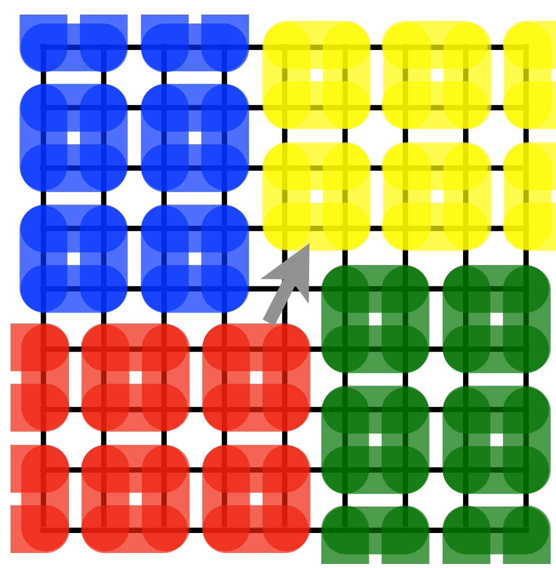

$$D_x := \frac{1}{N} \sum_{r=(x,y)} (-1)^x \hat{S}_{x,y} \hat{S}_{x+1,y}$$

$$\Pi_A = \frac{2}{N} \sum_{\substack{(i,j,k,l)\in p \\ p\in A}} (-1)^{i_x} \hat{P}_{[\hat{S}_i+\hat{S}_j+\hat{S}_k+\hat{S}_l=0]}$$

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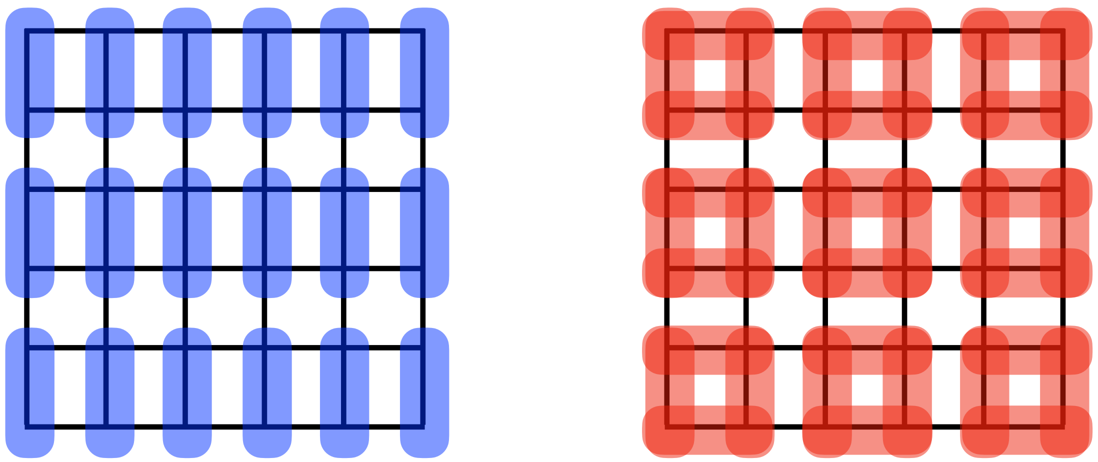

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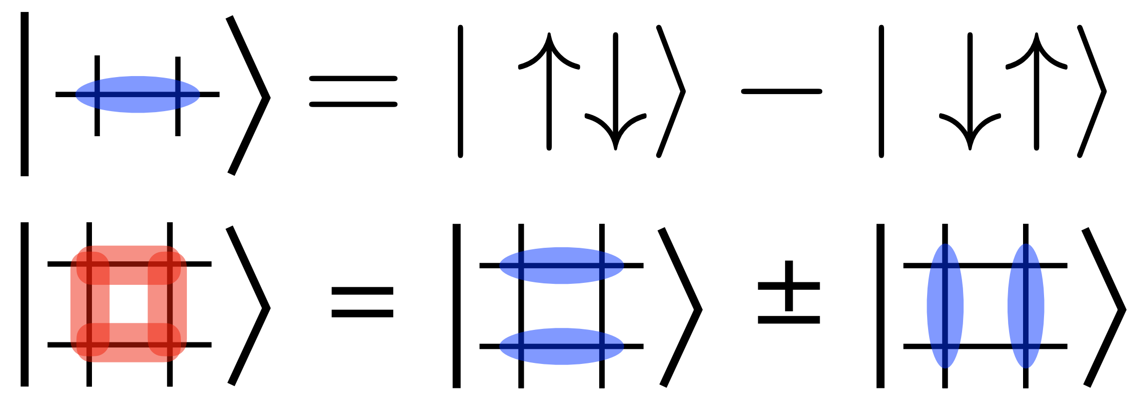

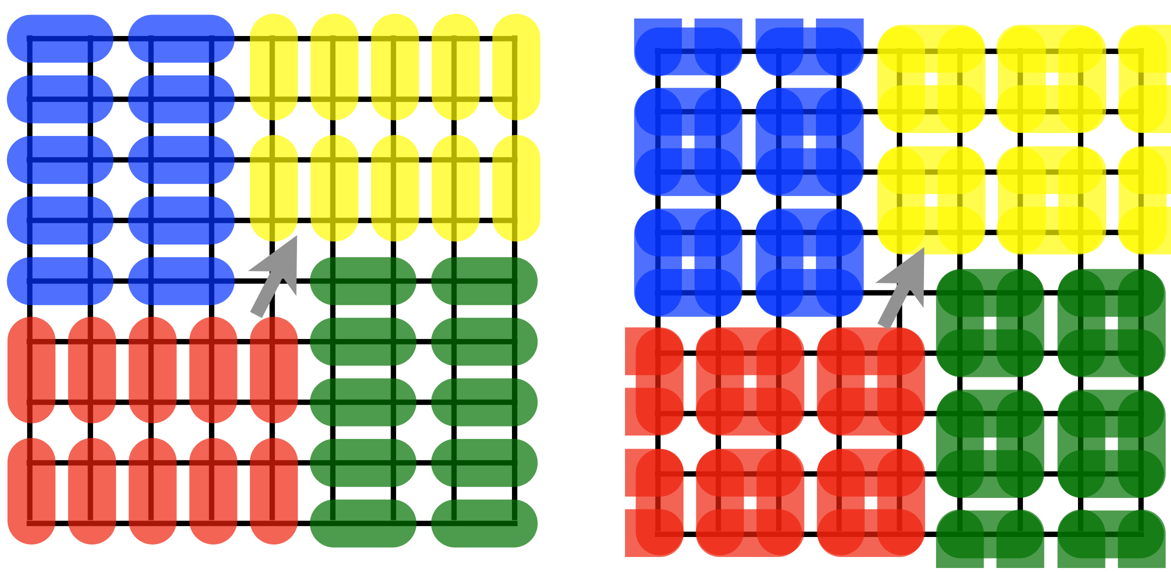

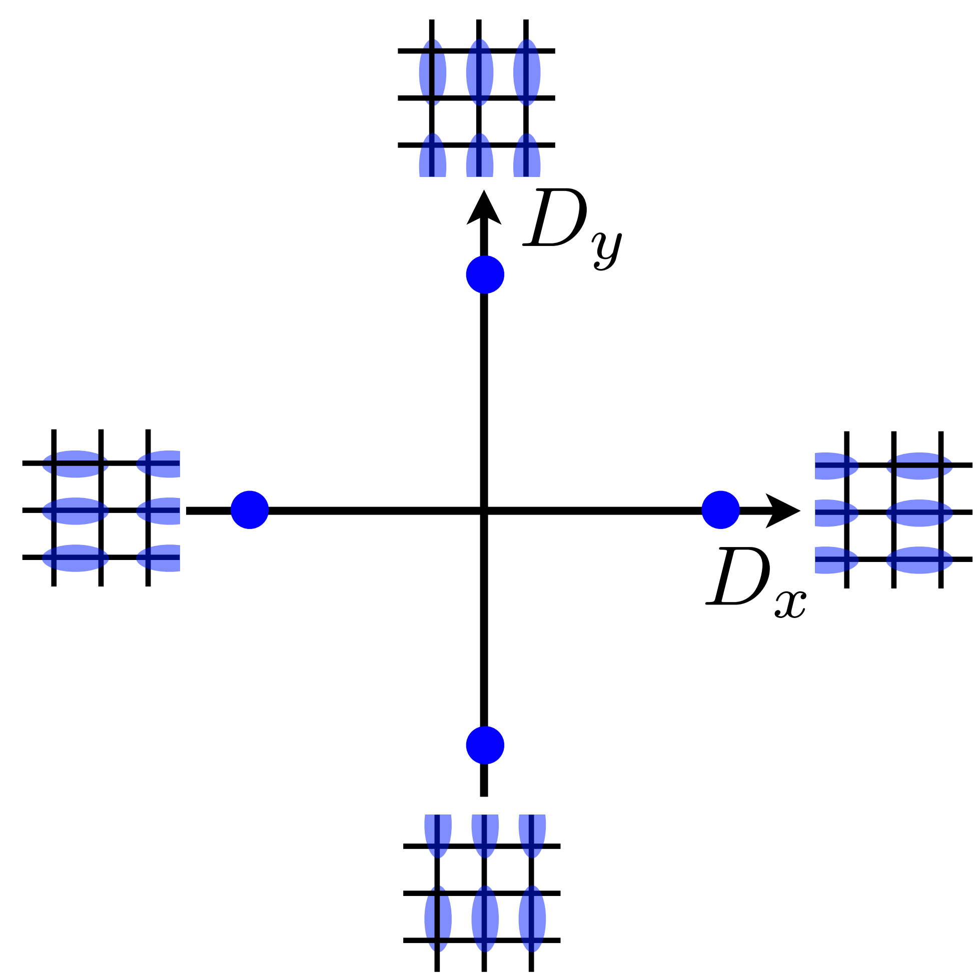

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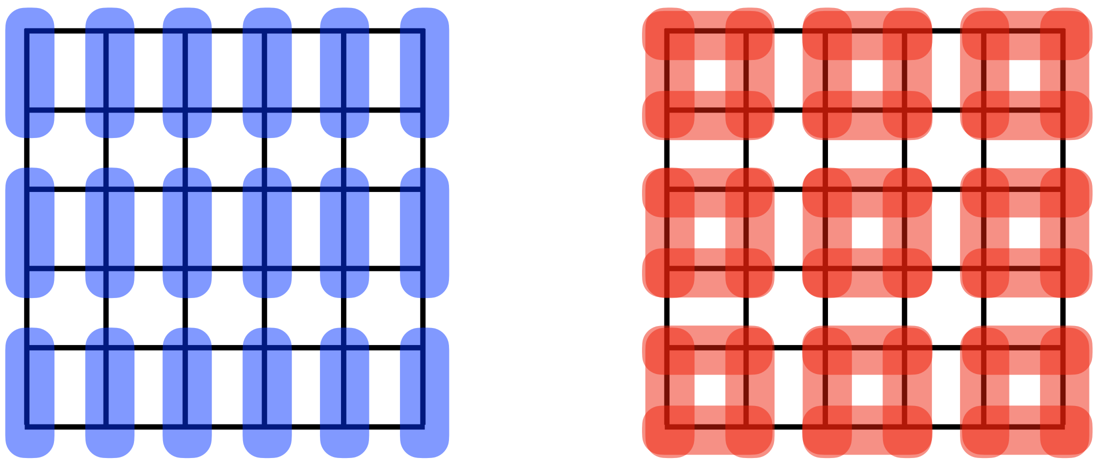

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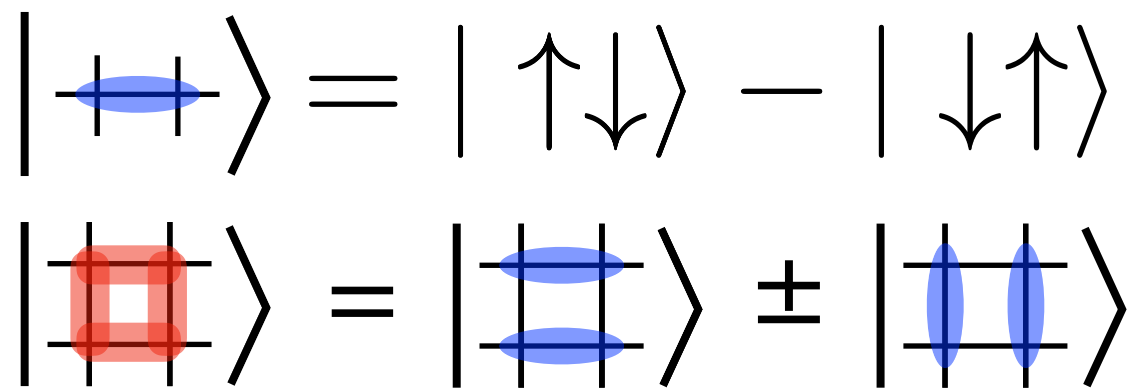

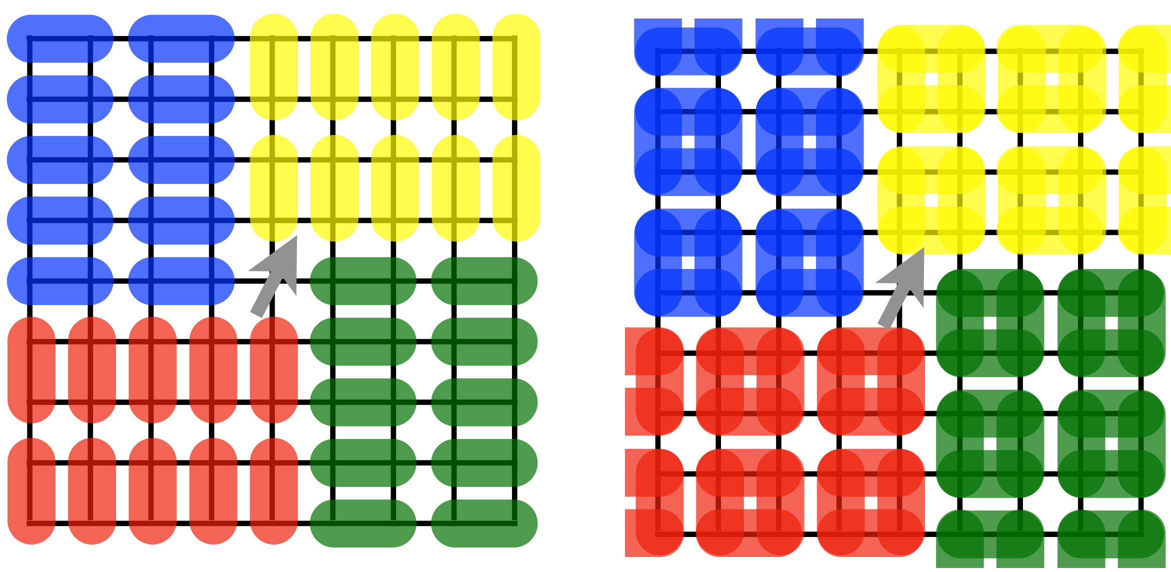

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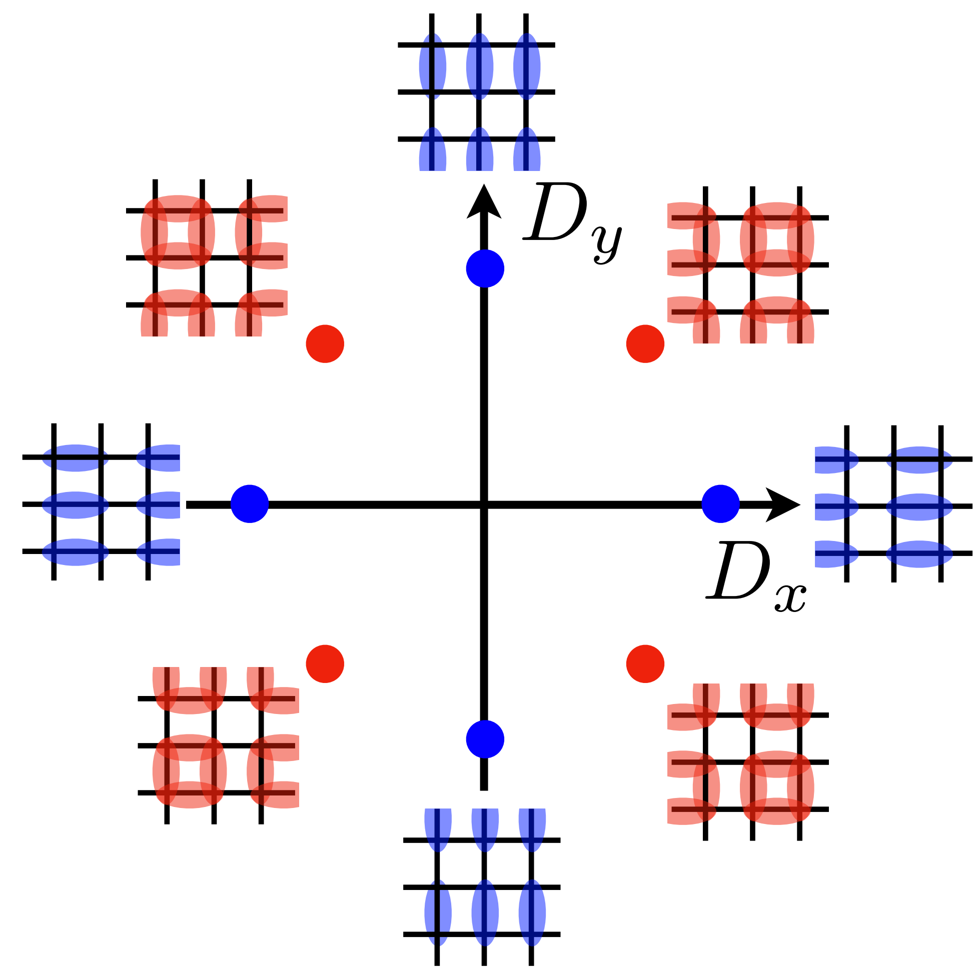

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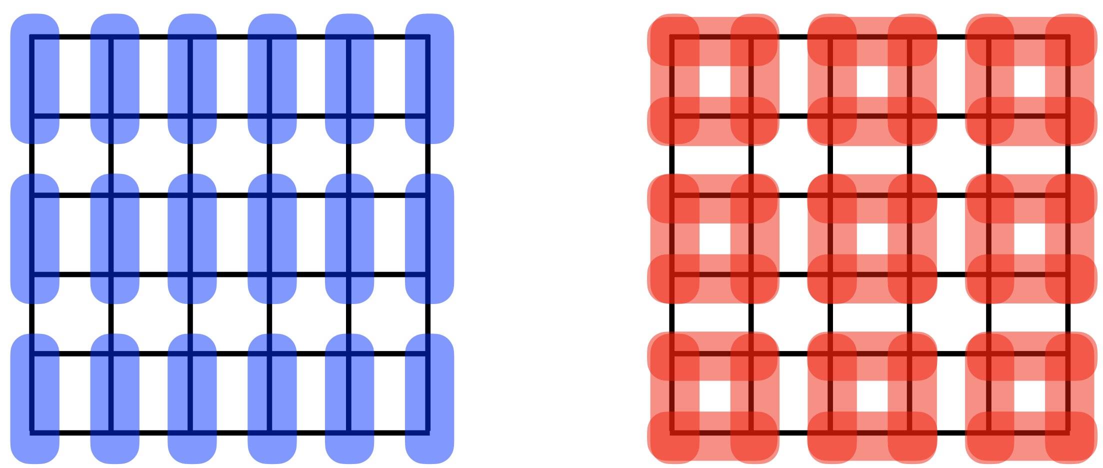

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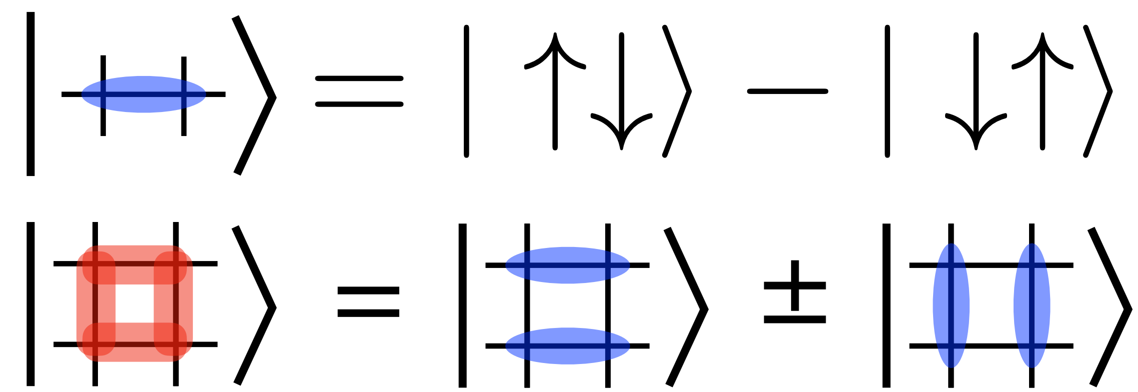

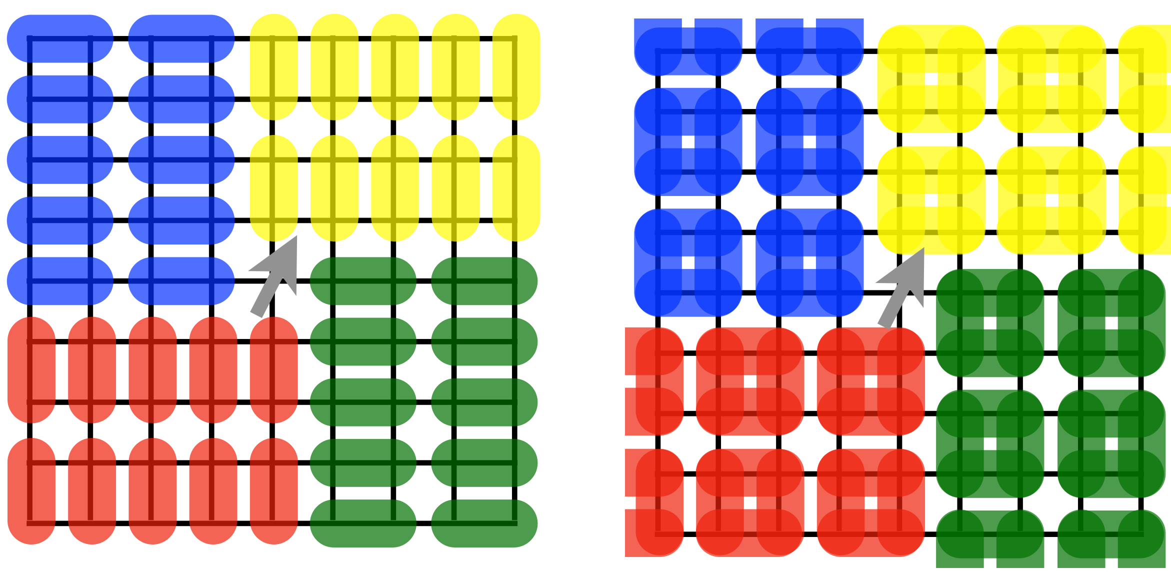

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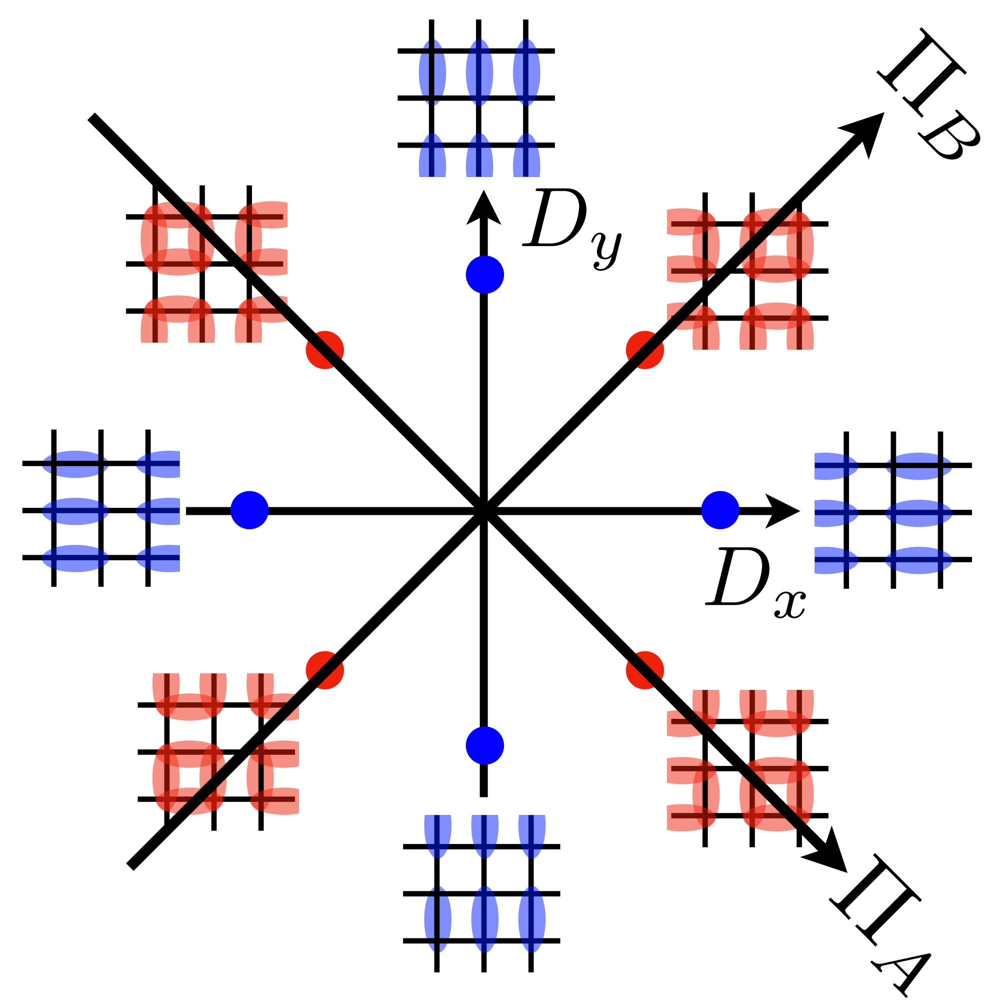

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"Designer" Hamiltonians

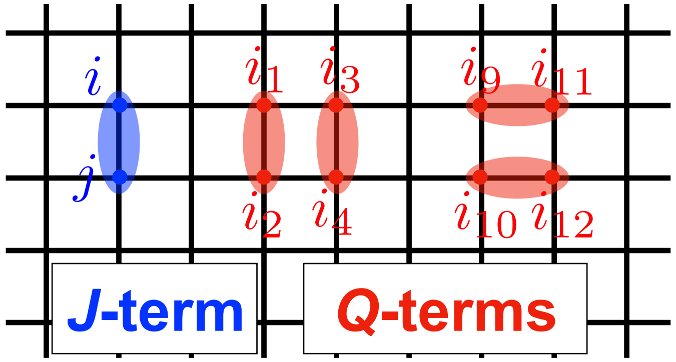
Construct sign-free models for observing quantum many-body physics!

[R. K. Kaul et al., Ann. Rev. CMP (2013)]
[A. Sandvik, PRL (2007)]

The original JQ model

$$H = -J \sum_{(i,j)\in b} \hat{P}_{ij} - Q \sum_{(i,j,k,l)\in p} \left(\hat{P}_{ij}\hat{P}_{kl} + \hat{P}_{il}\hat{P}_{kj} \right)$$

Induces correlated singlets!



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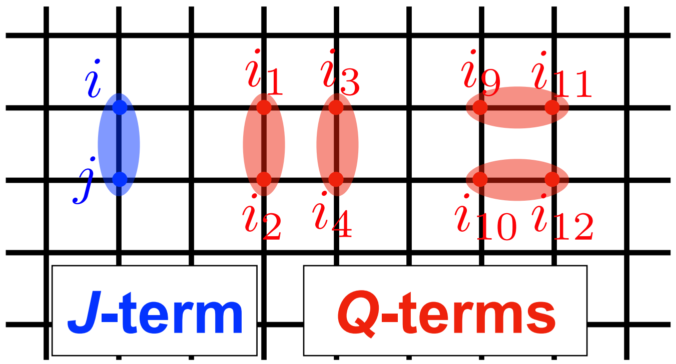
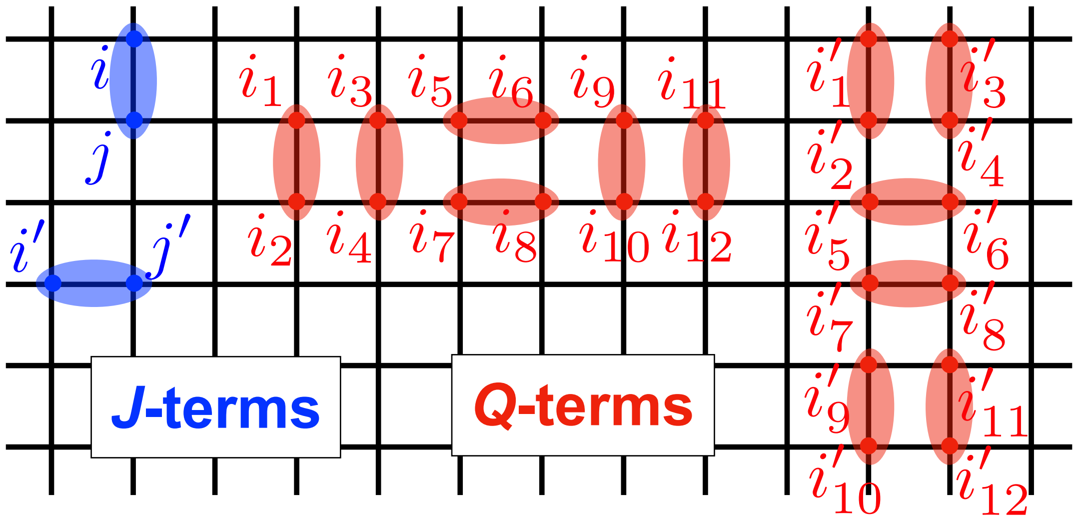


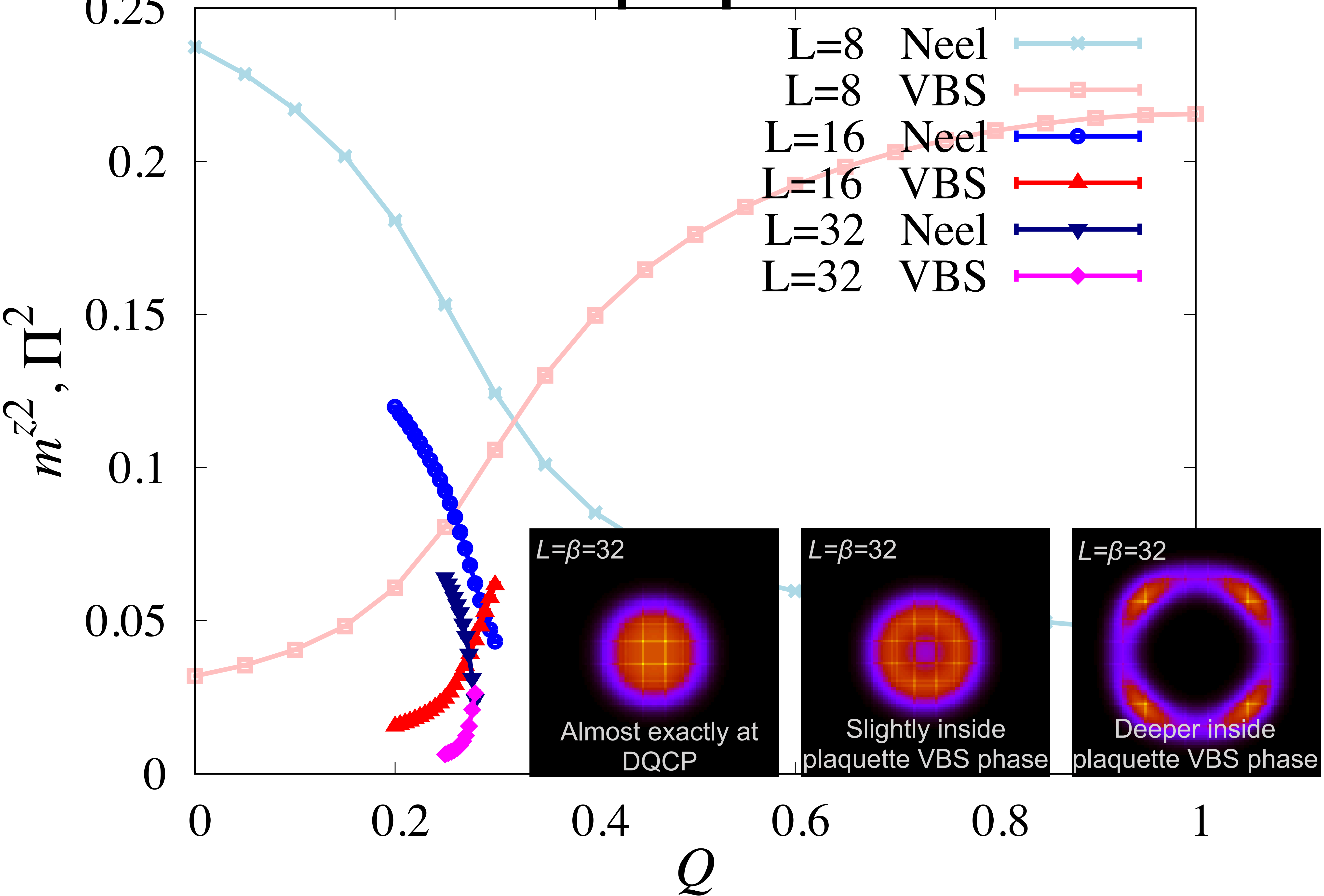
<u>The JQ6 model</u>

$$H = -J \sum_{(i,j)\in b} \hat{P}_{ij} - Q \sum_{\substack{(i,j,k,l)\in p \\ (m,n,o,p)\in p' \\ (q,r,s,t)\in p'' \\ (p,p',p'')\in \text{row,column}}} \left(\hat{P}_{ij}\hat{P}_{kl}\hat{P}_{mp}\hat{P}_{on}\hat{P}_{qr}\hat{P}_{st} + \hat{P}_{il}\hat{P}_{kj}\hat{P}_{mn}\hat{P}_{op}\hat{P}_{qt}\hat{P}_{sr}\right)$$

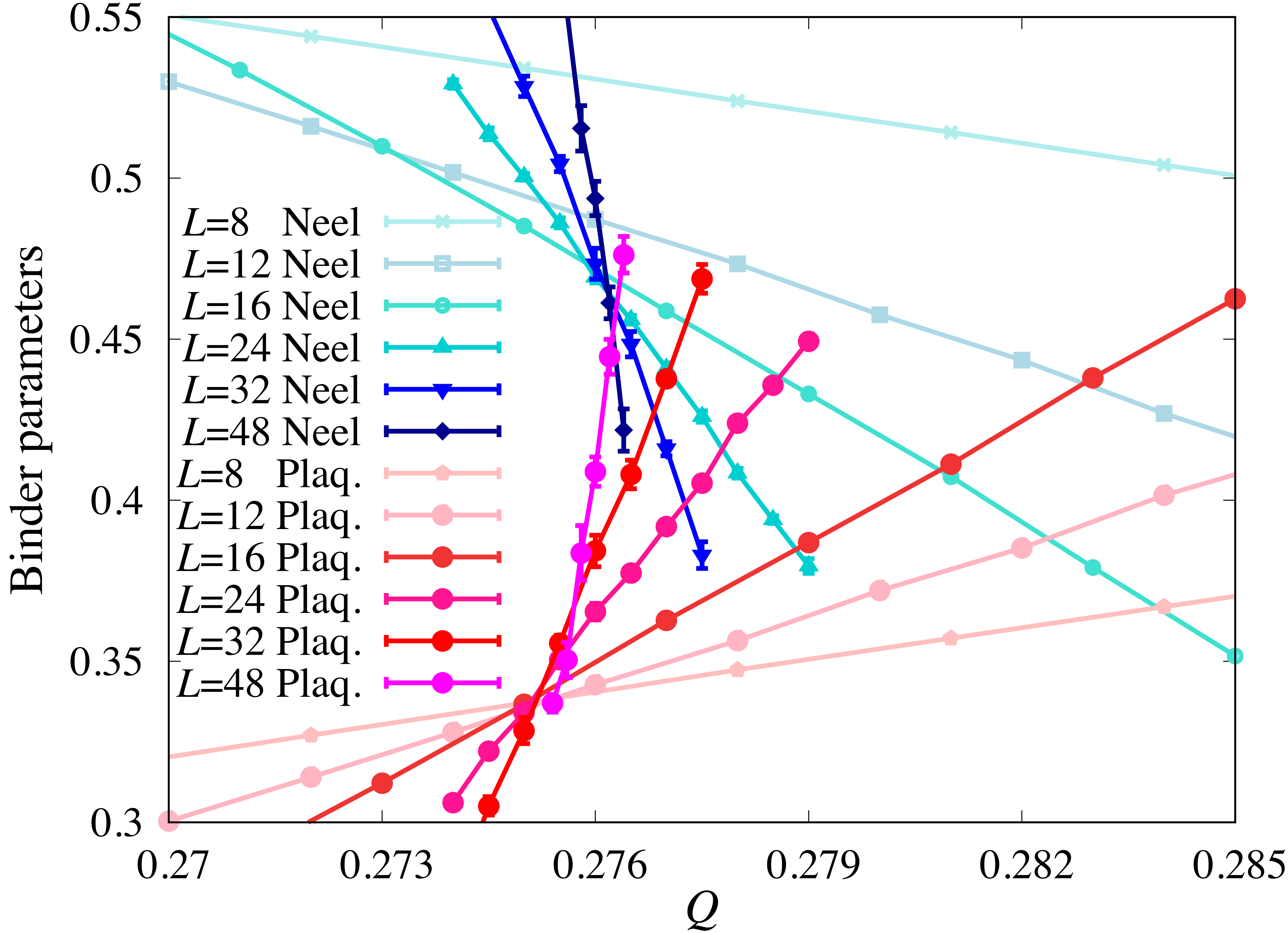


Induces correlated plaquette singlets, while avoiding columnar VBS!

Direct Néel-to-plqVBS transition



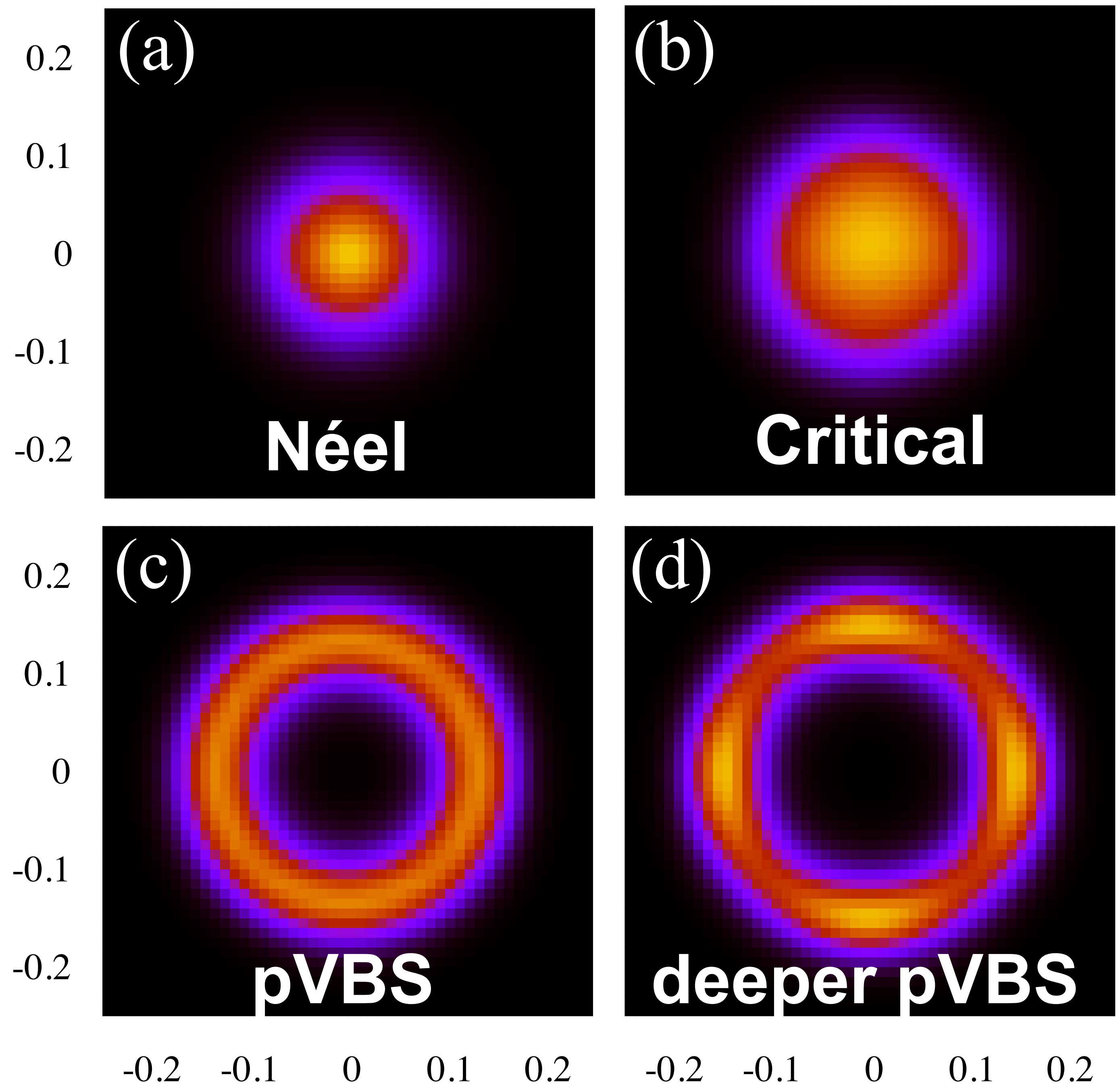
Binder parameter crossings

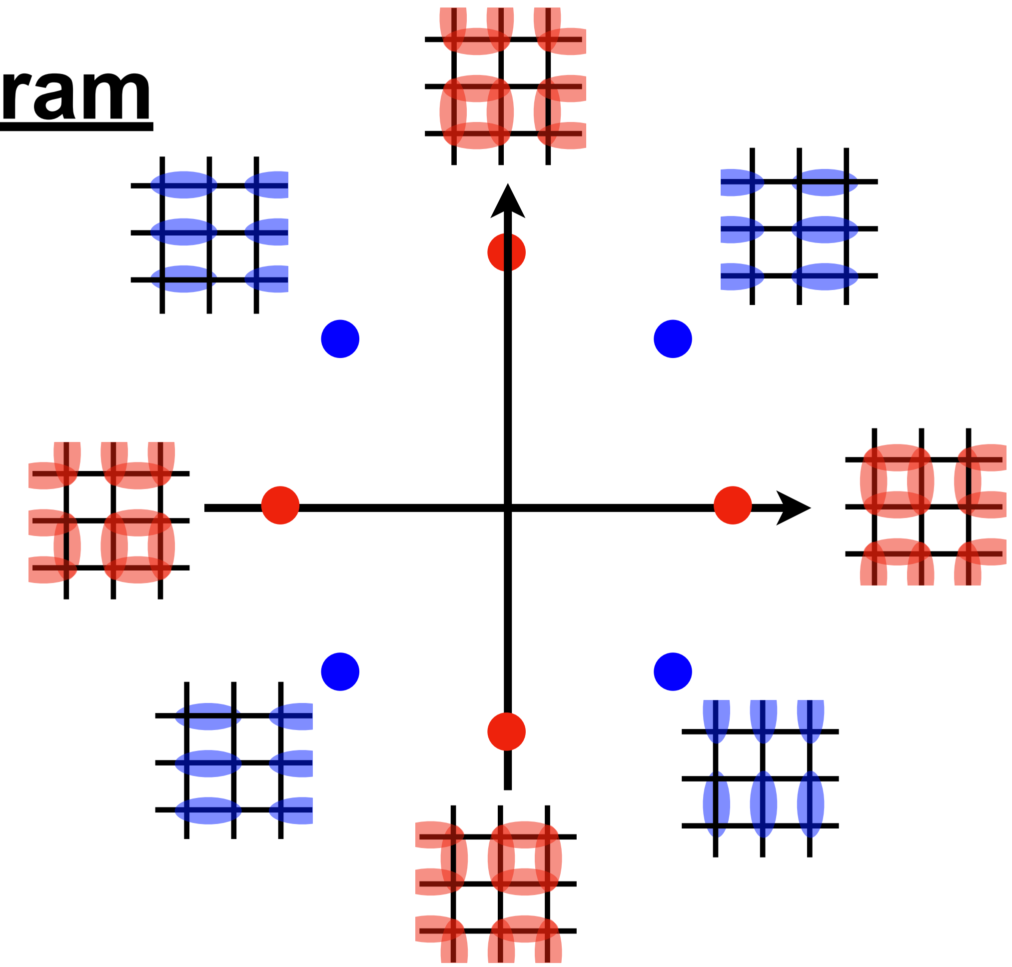


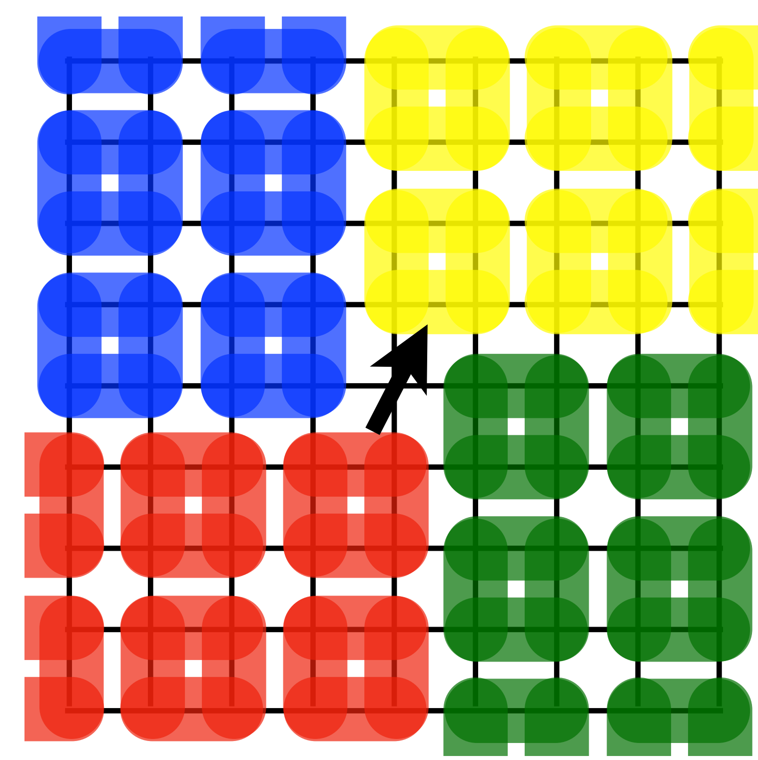
Emergent Symmetries

<u>The plaquette order parameter's histogram shows emergent U(1) symmetry!</u>

$L = 48$







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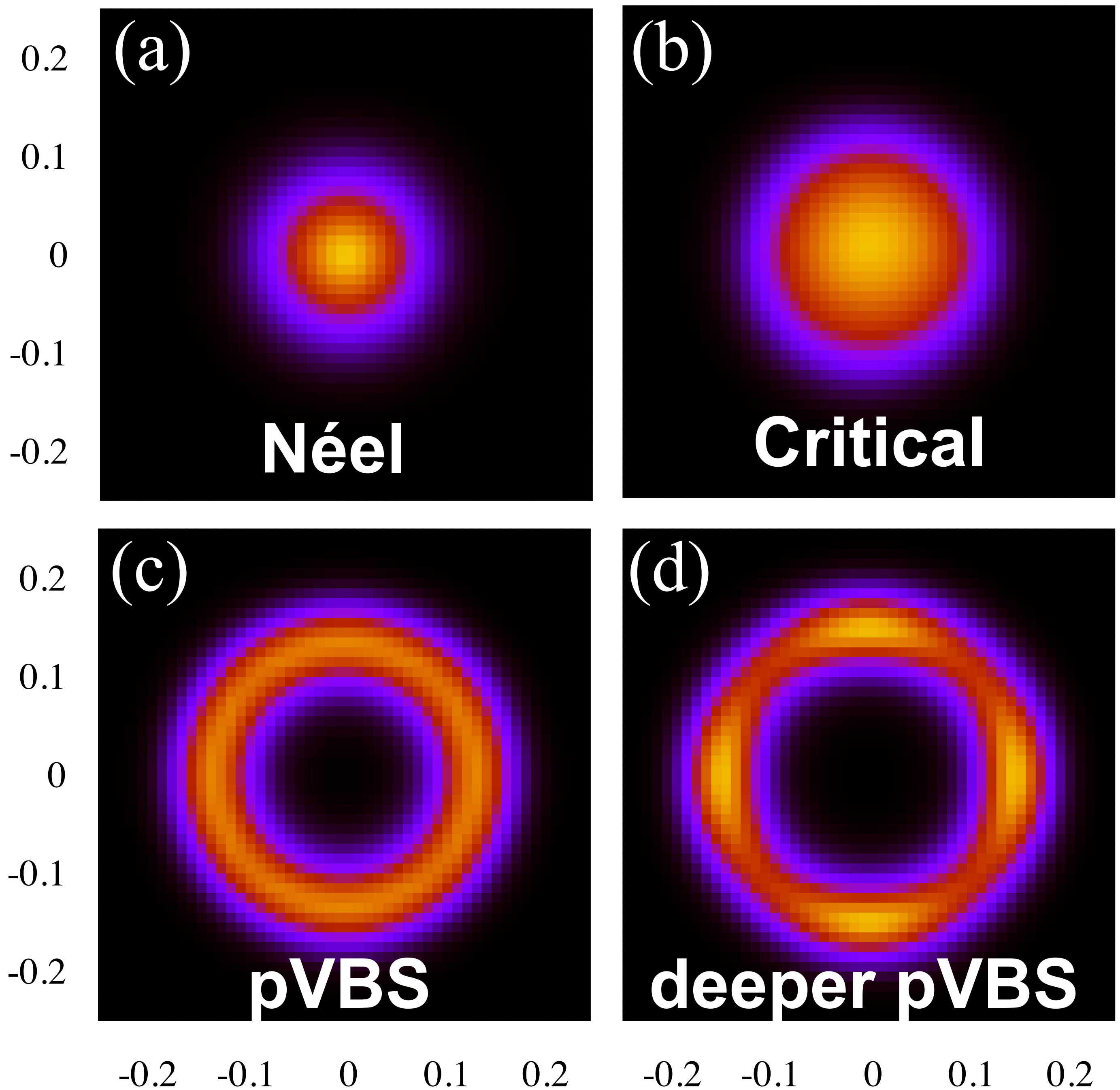

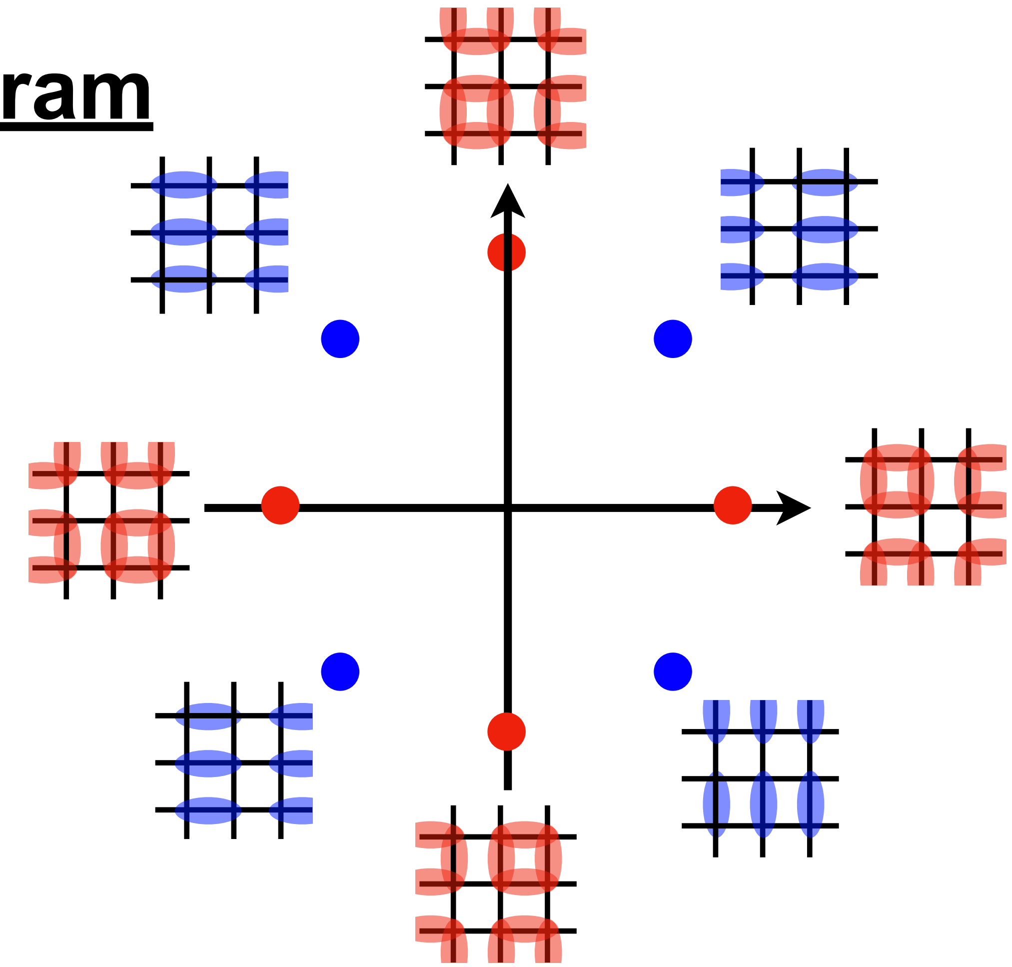

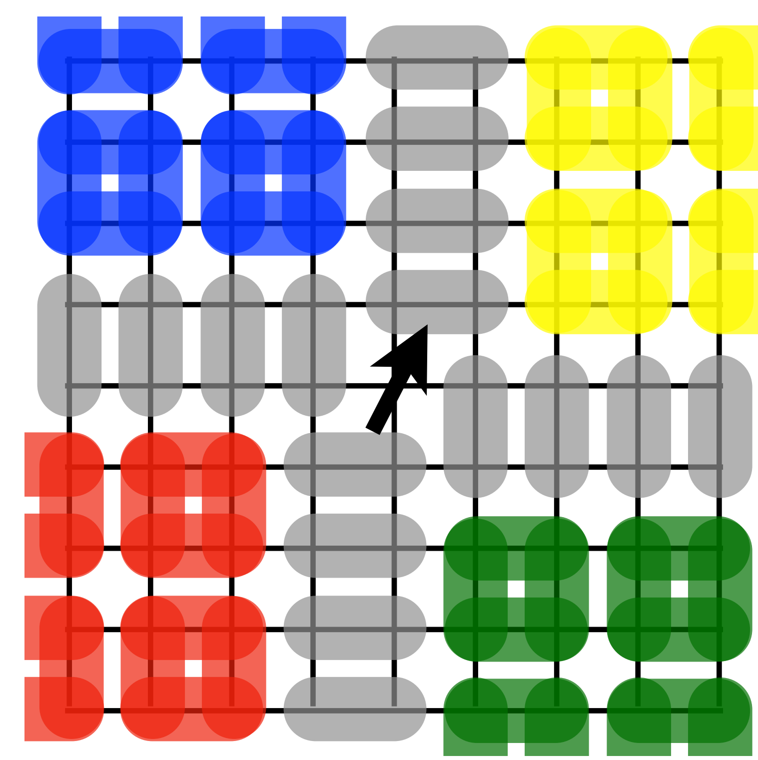

Emergent Symmetries

We further observe possible emergent SO(5) among the Néel and plaquette order parameters

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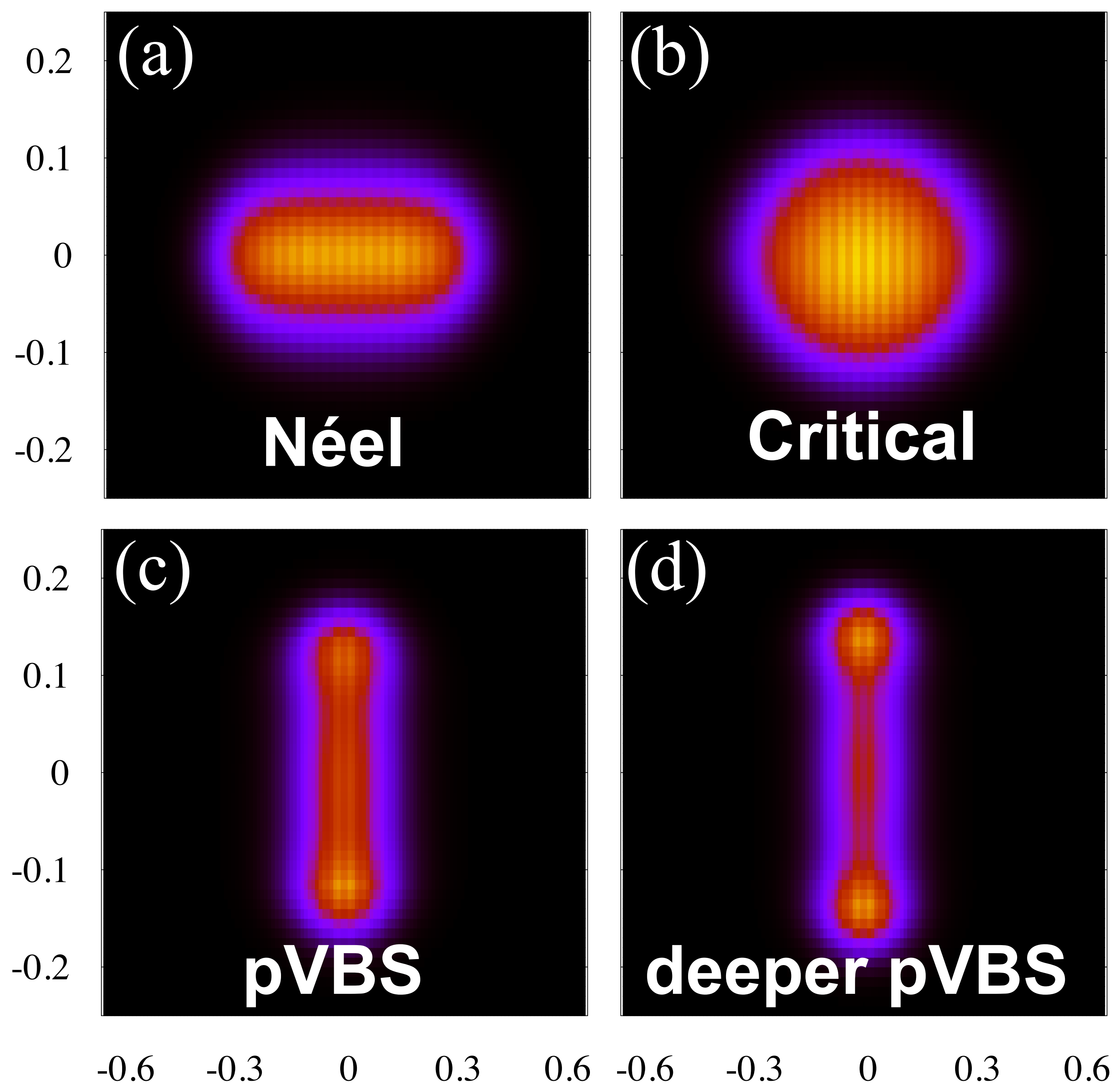


$$\begin{pmatrix} m^x \\ m^y \\ m^z \\ \Pi_A \\ \Pi_B \end{pmatrix}$$

Néel order has 3 components for SO(3)

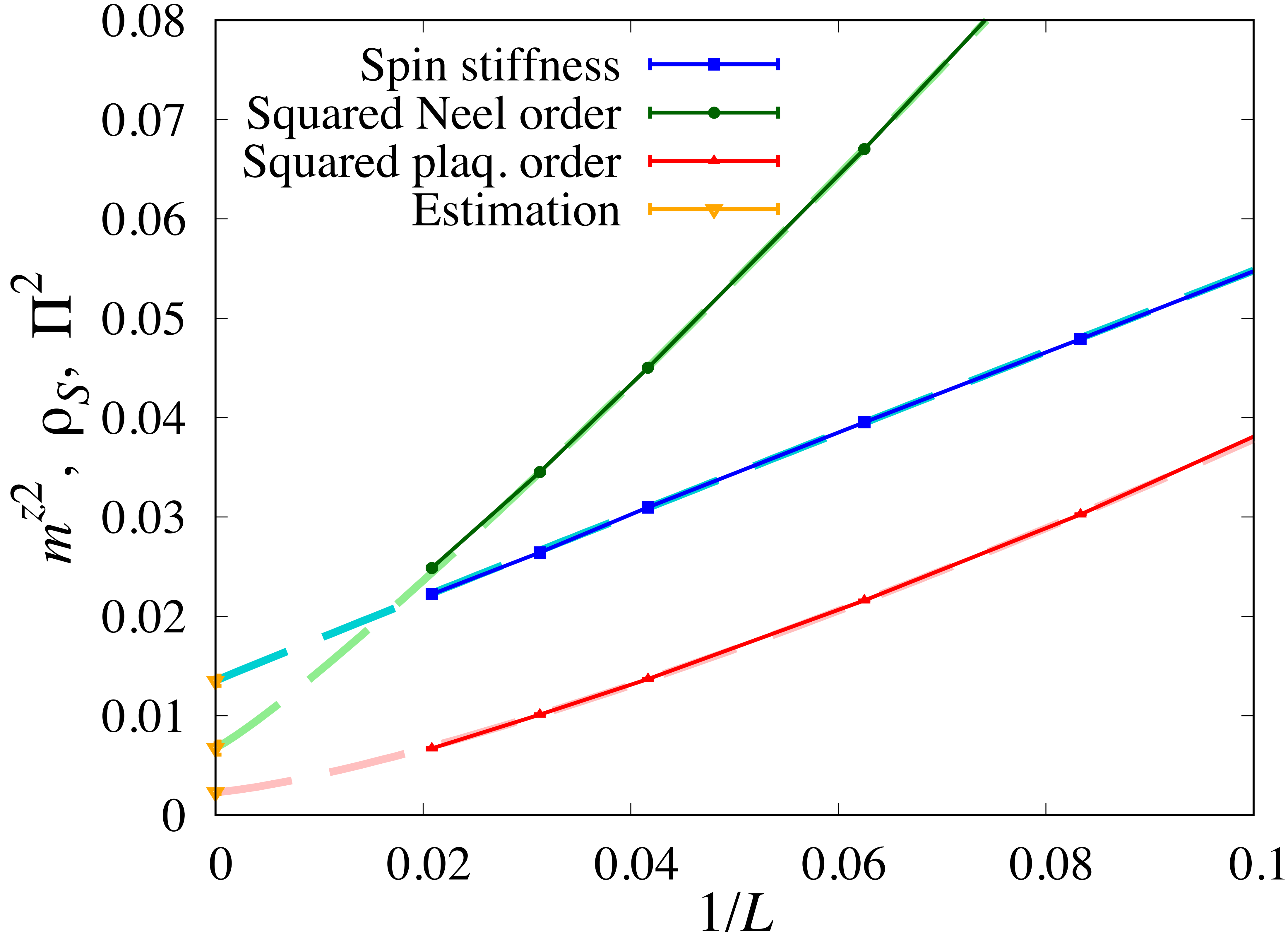
Plaquette order has 2 components forming Z_4

May form a ***5 component*** order parameter **unifying** the Néel & VBS orders!

[A. Nahum et al., PRL (2015)]

[B. Zhao, P. Weinberg & A.W. Sandvik, Nat.Phys. (2018)]

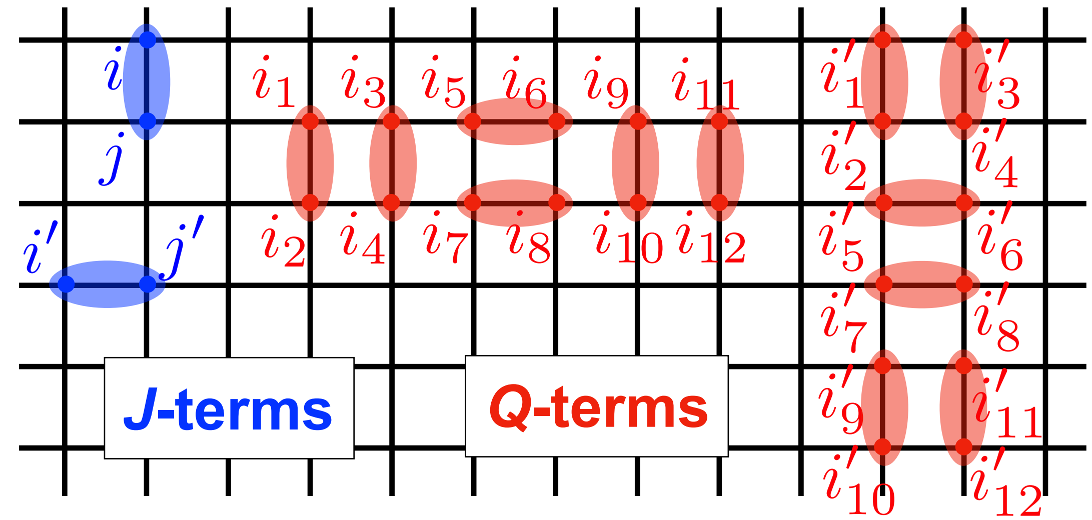
Order parameters show FOT!



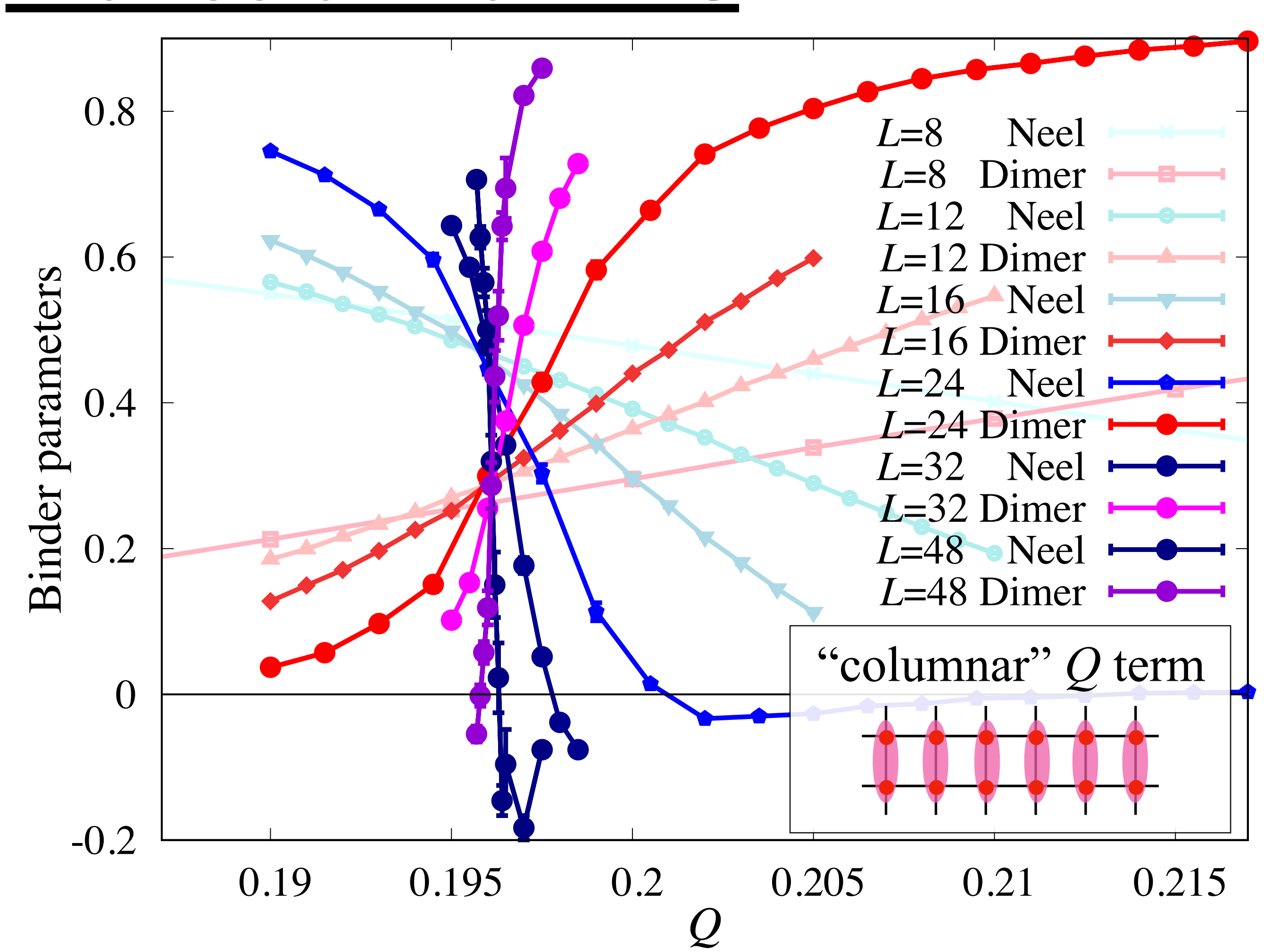
Possible reason for FOT

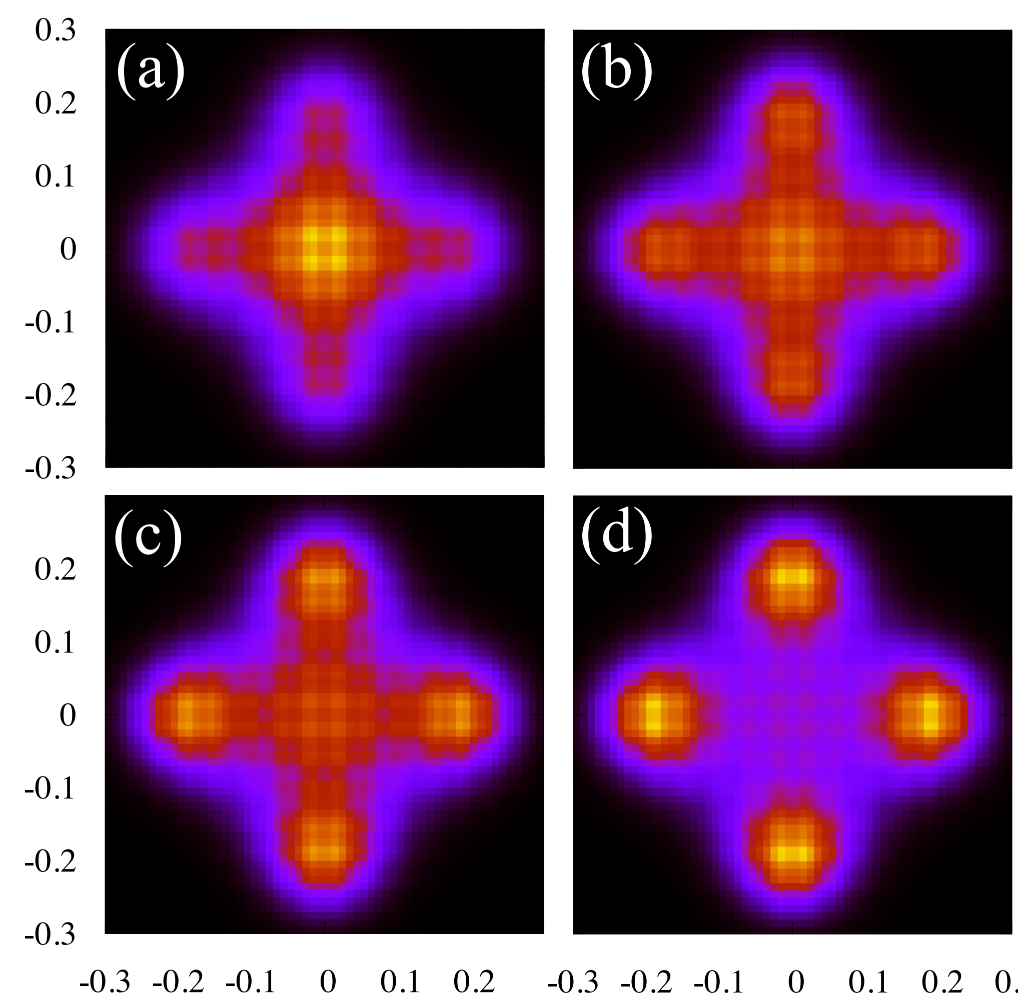
"Blame" the 12-body interaction for the first order transition

When we add many-body interactions to a classical Ising model, the transition becomes first-order due to induced nucleation process.



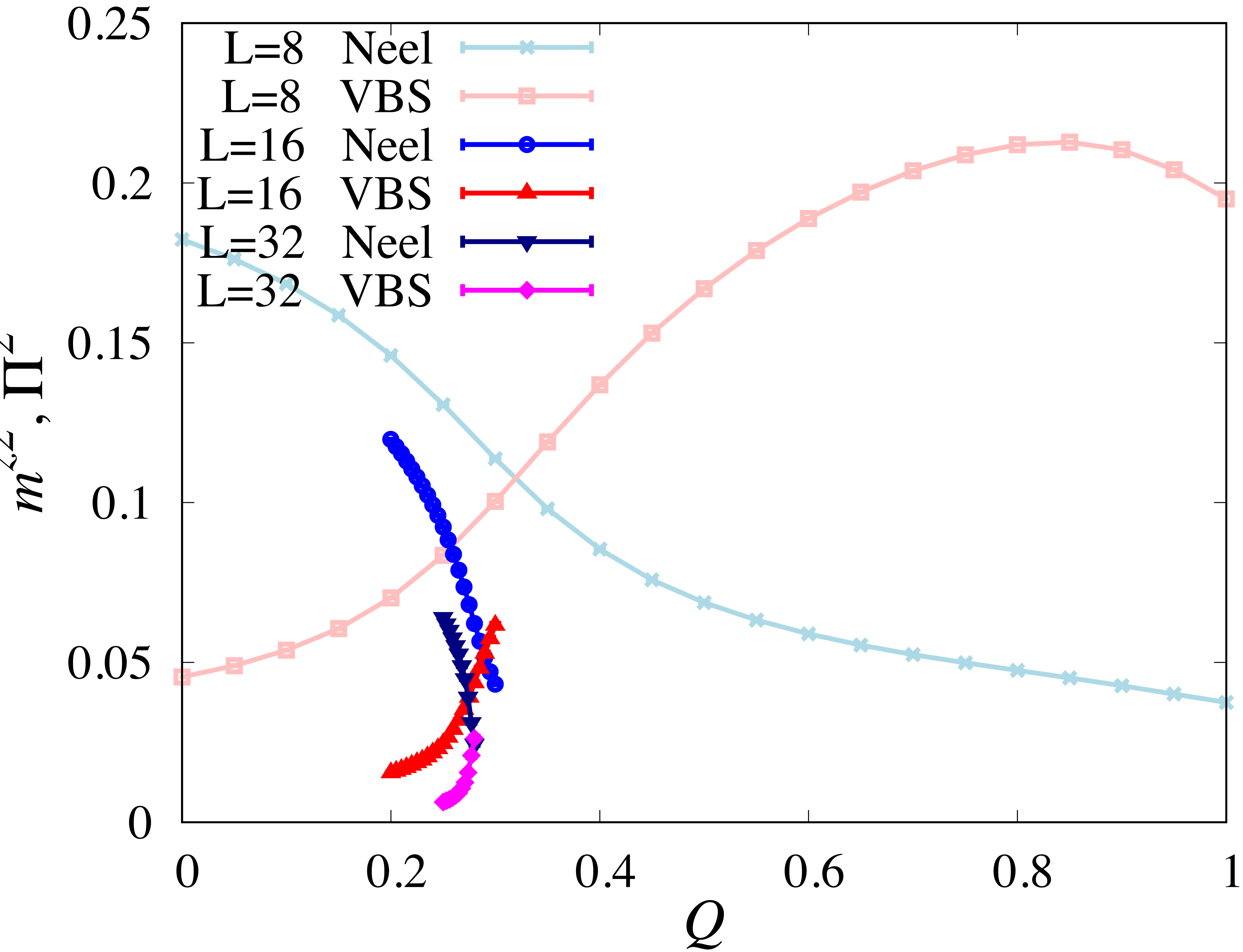
Comparison with a different 12-body interactive system with columnar VBS





Another phase transition!

$$H = -J \sum \hat{P}_{ij} - Q \sum \left(\hat{P}_{ij}\hat{P}_{kl}\hat{P}_{mp}\hat{P}_{on}\hat{P}_{qr}\hat{P}_{st} + \hat{P}_{il}\hat{P}_{kj}\hat{P}_{mn}\hat{P}_{op}\hat{P}_{qt}\hat{P}_{sr} \right)$$



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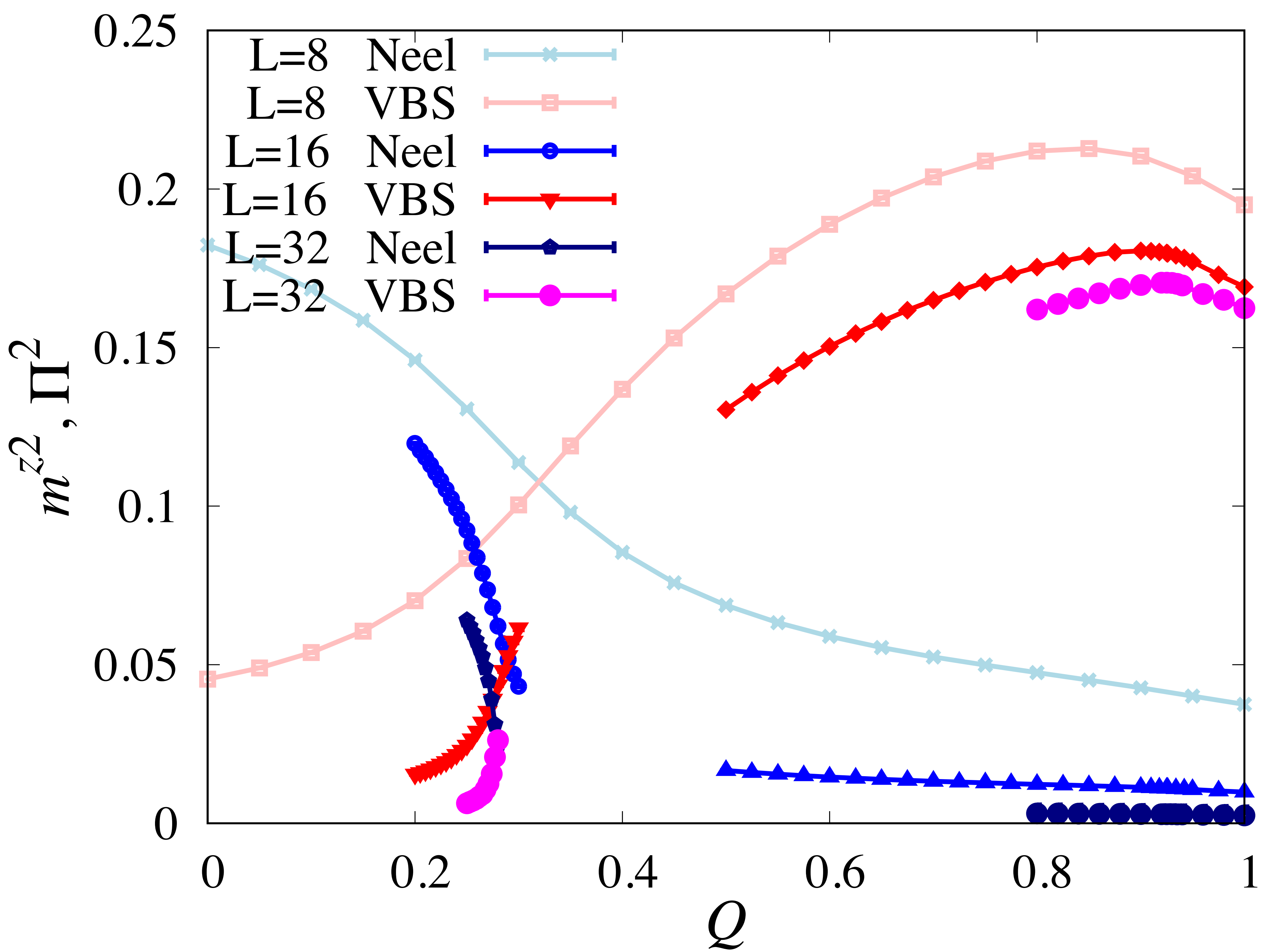

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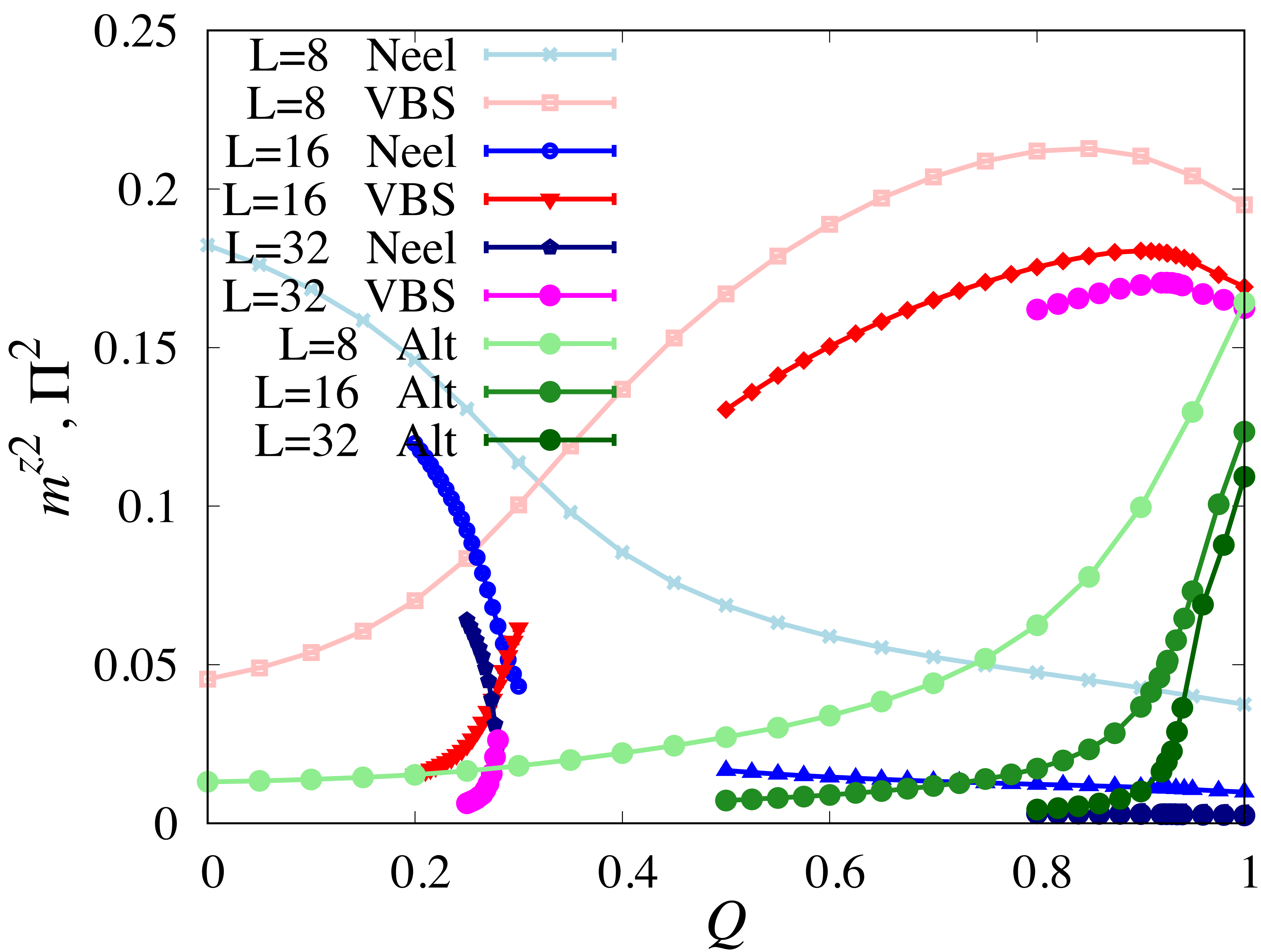

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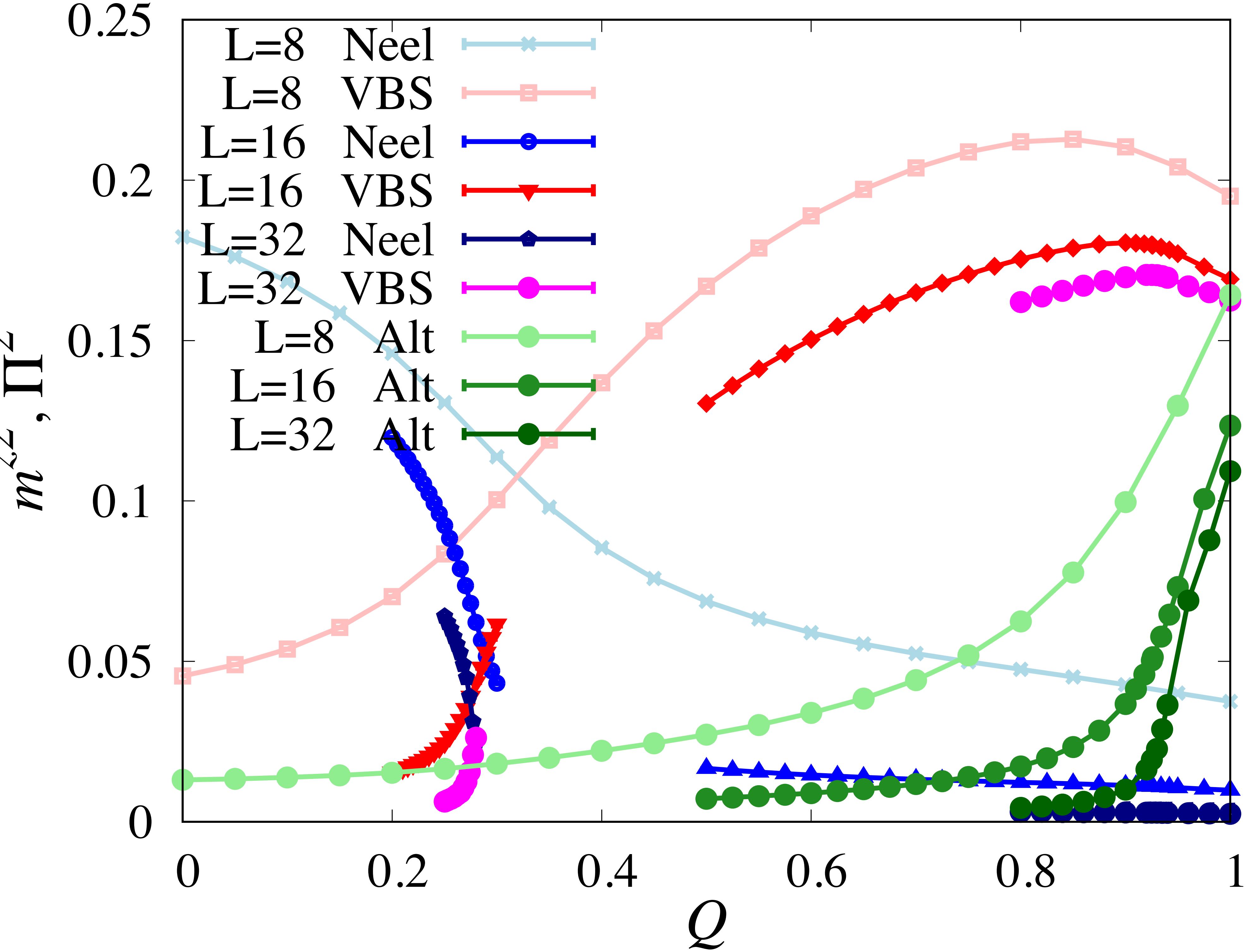

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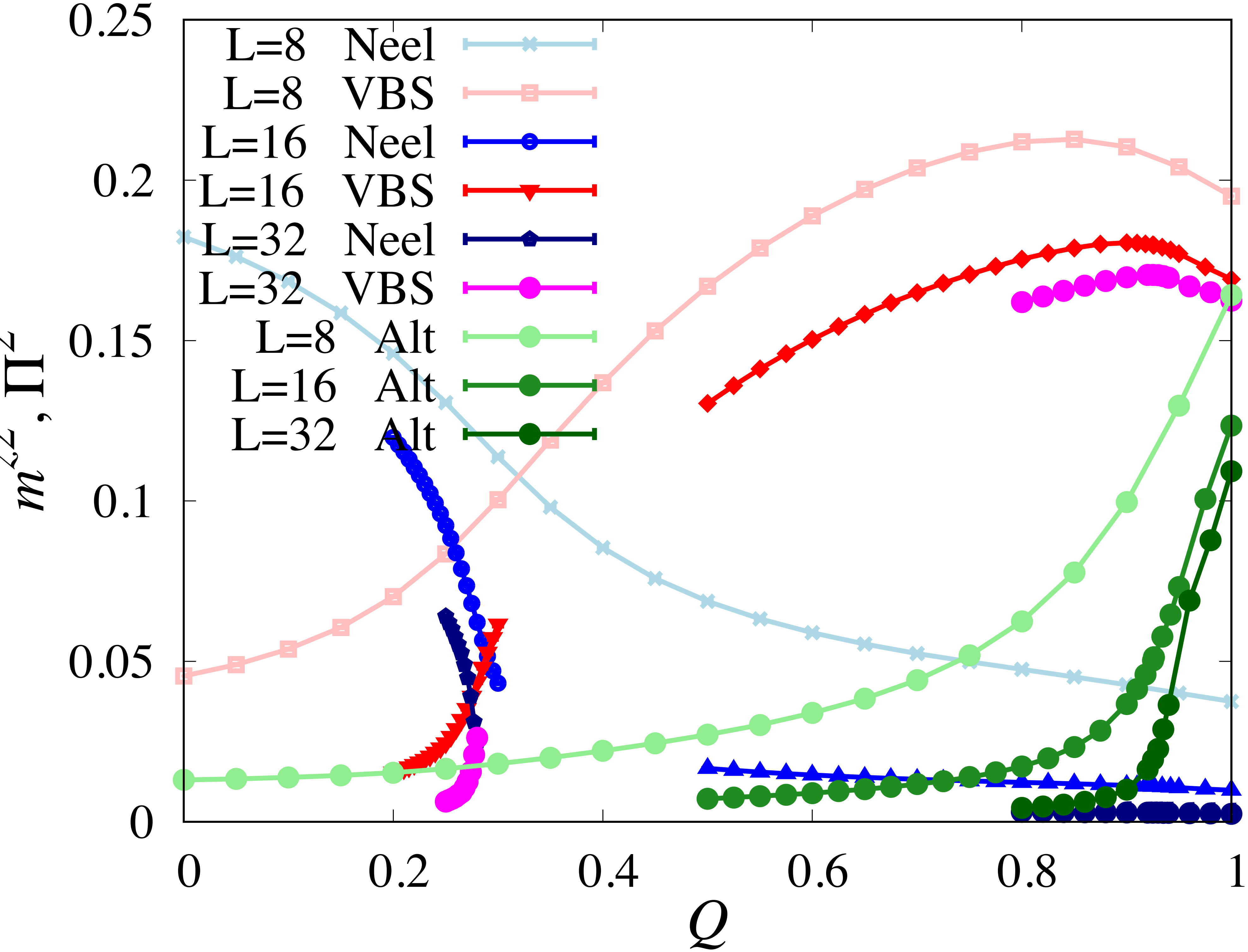

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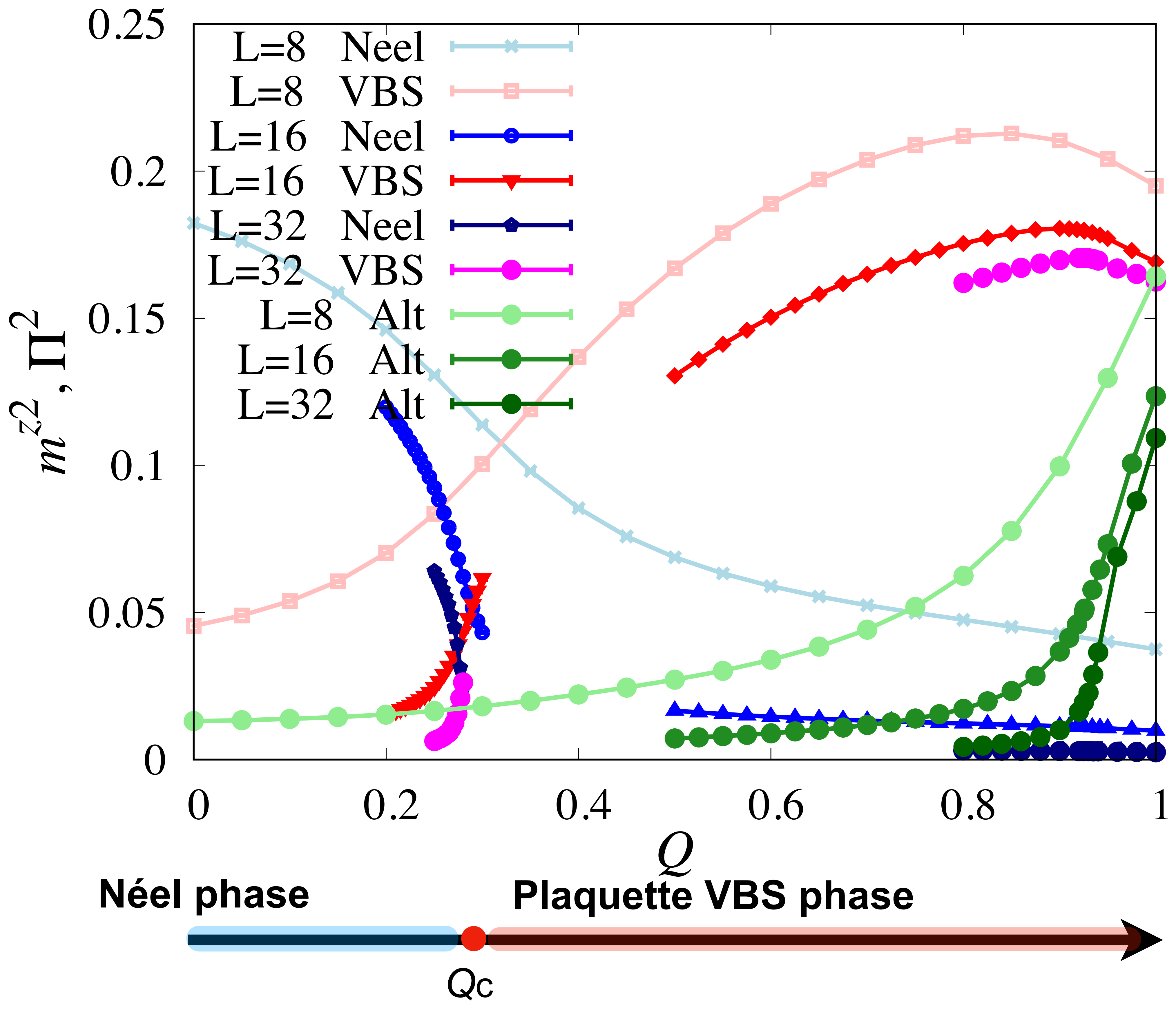

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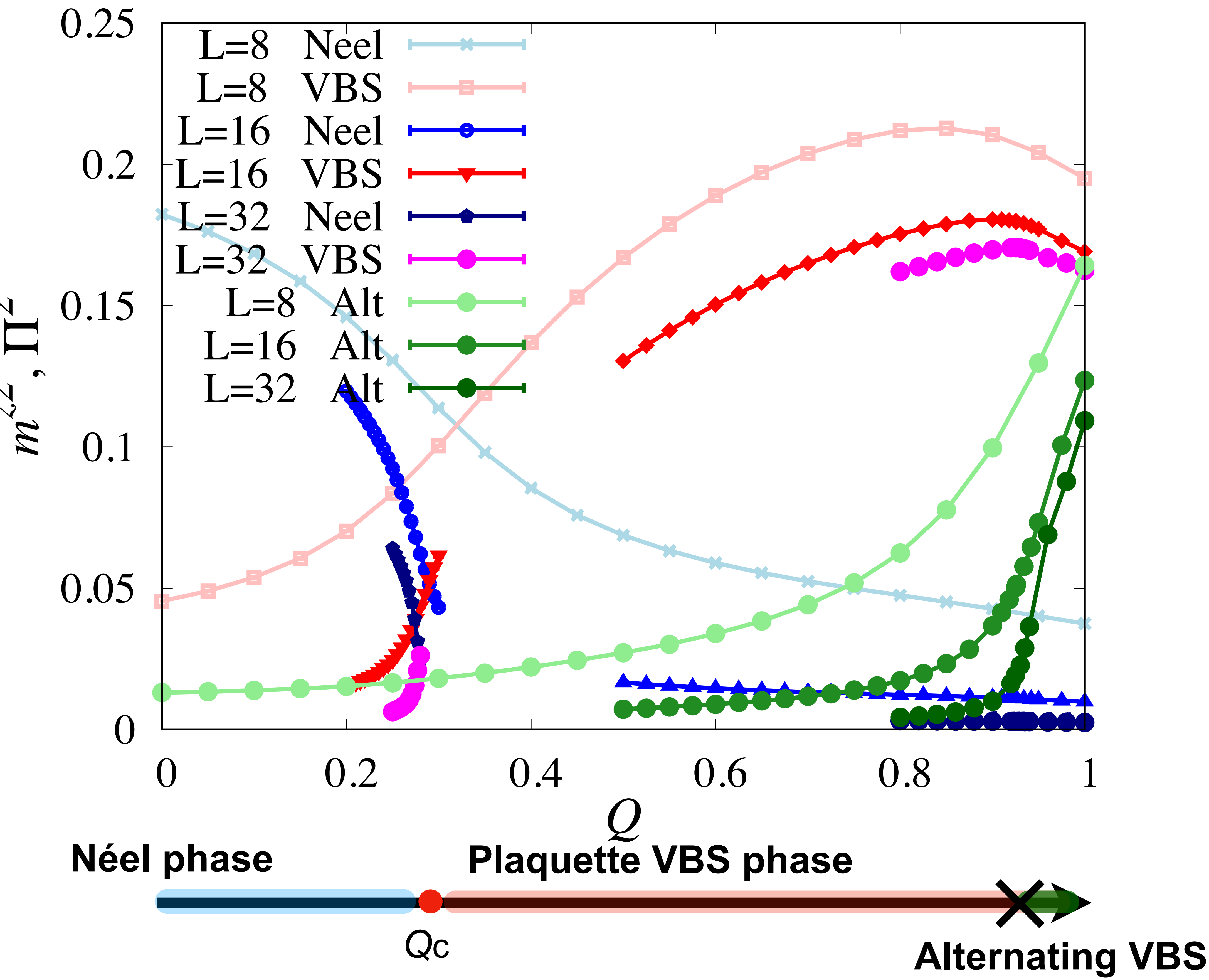

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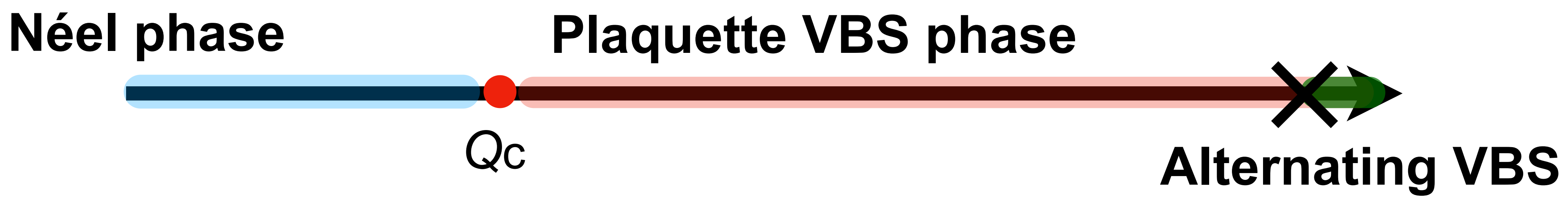

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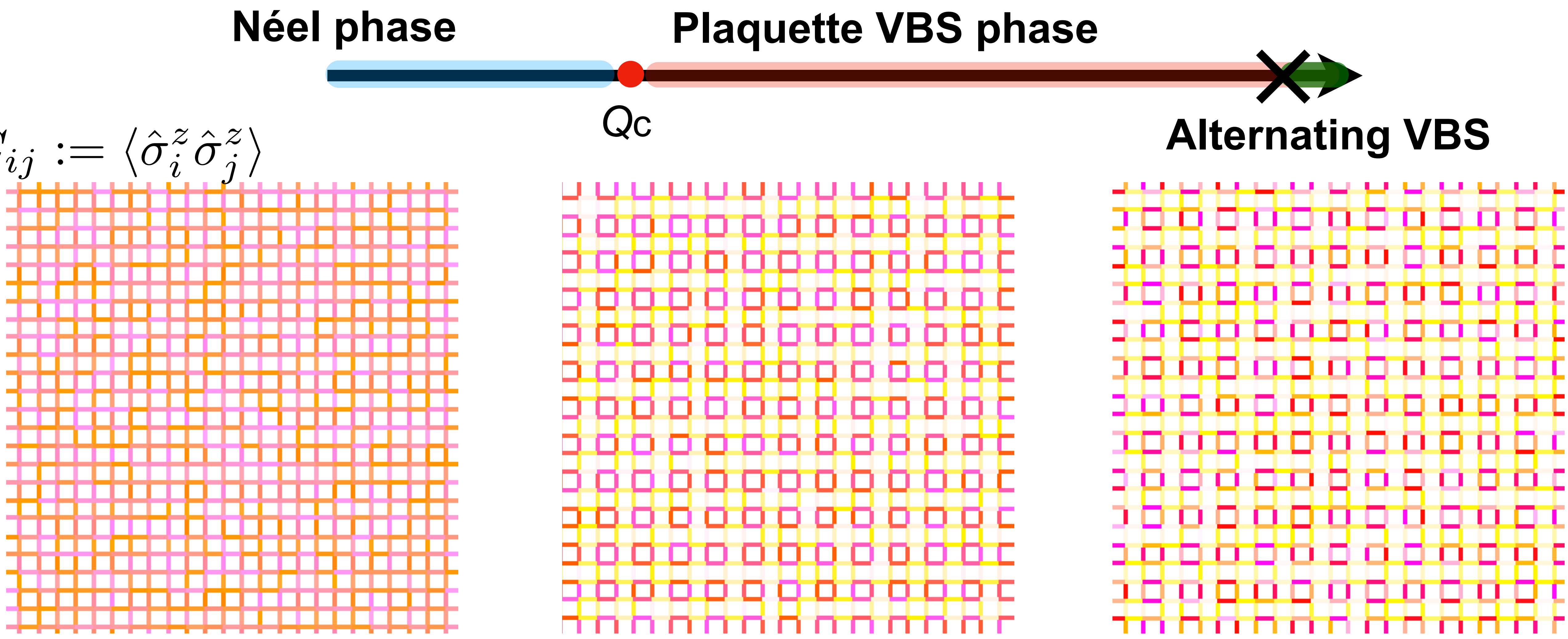

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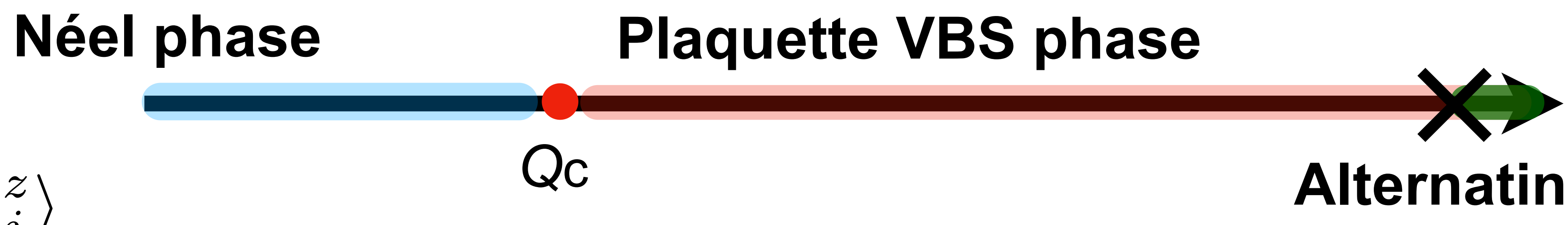

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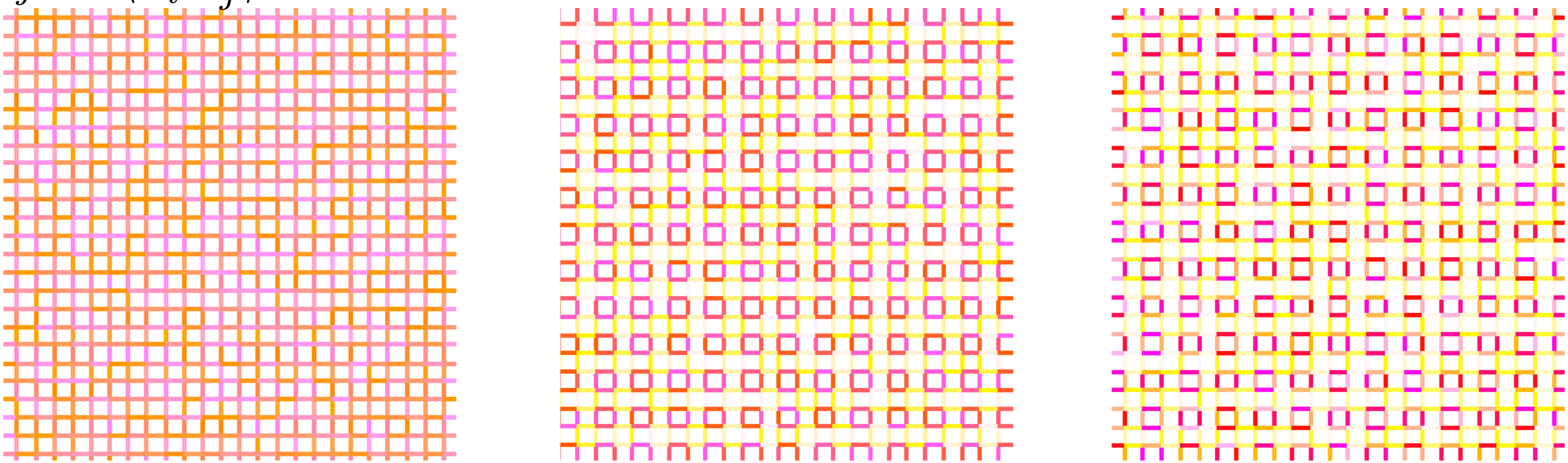
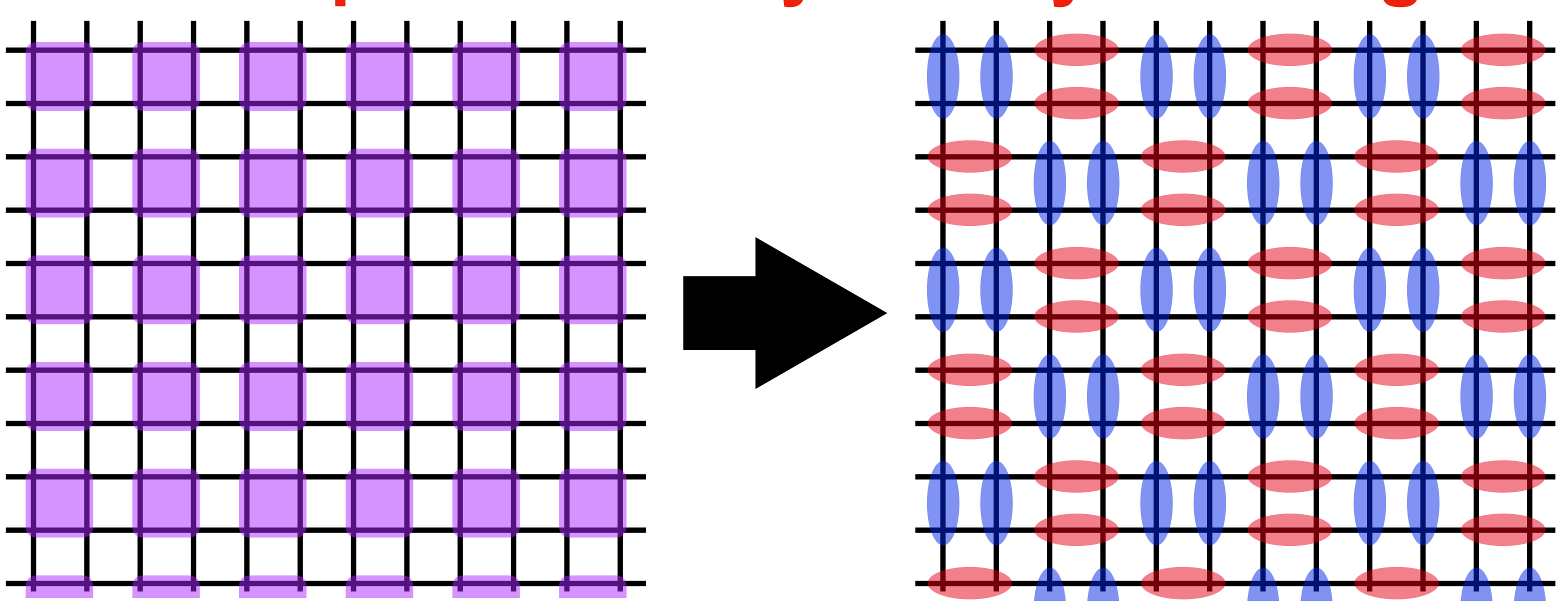


A new phase & Z_2 symmetry breaking!



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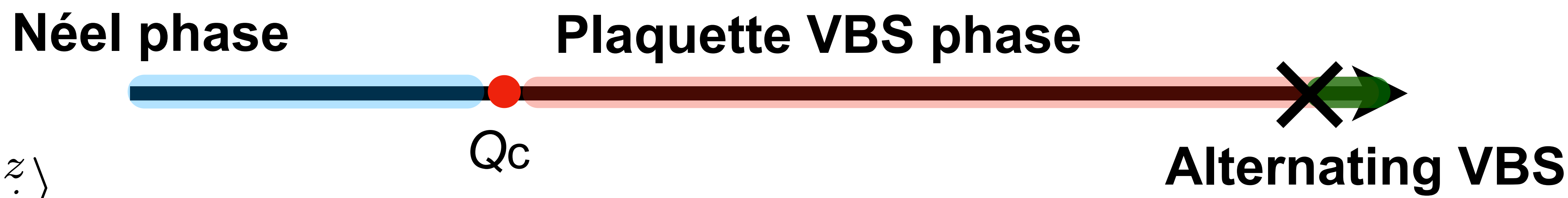

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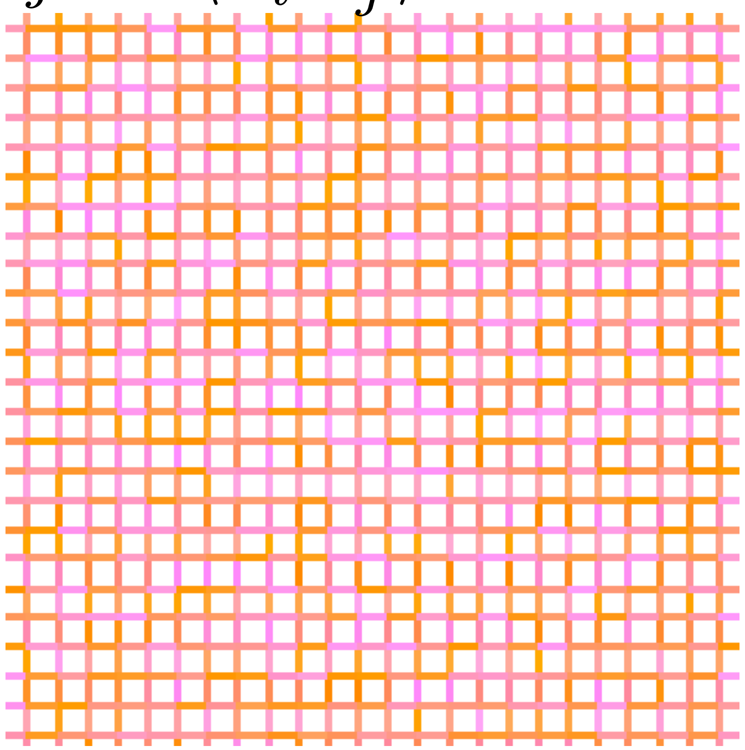

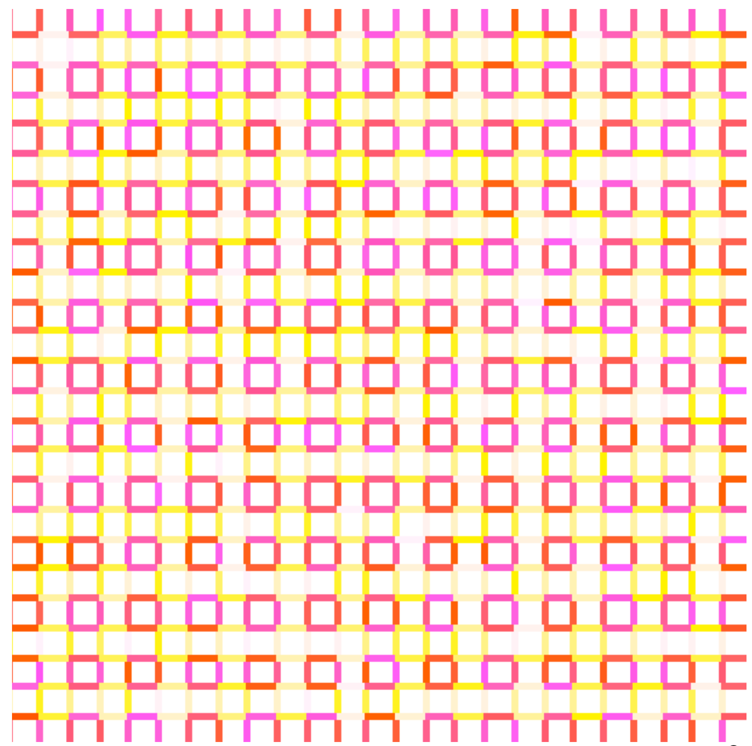

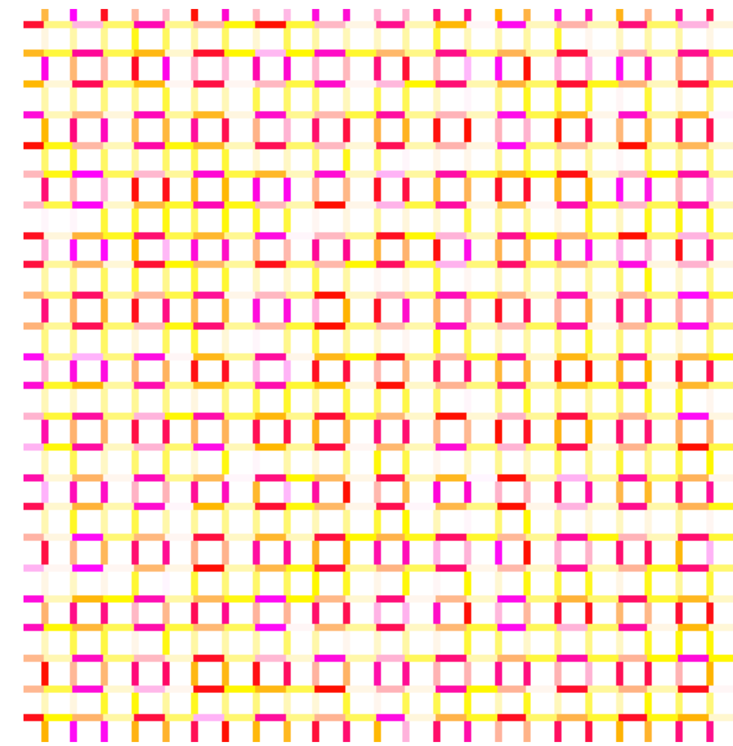

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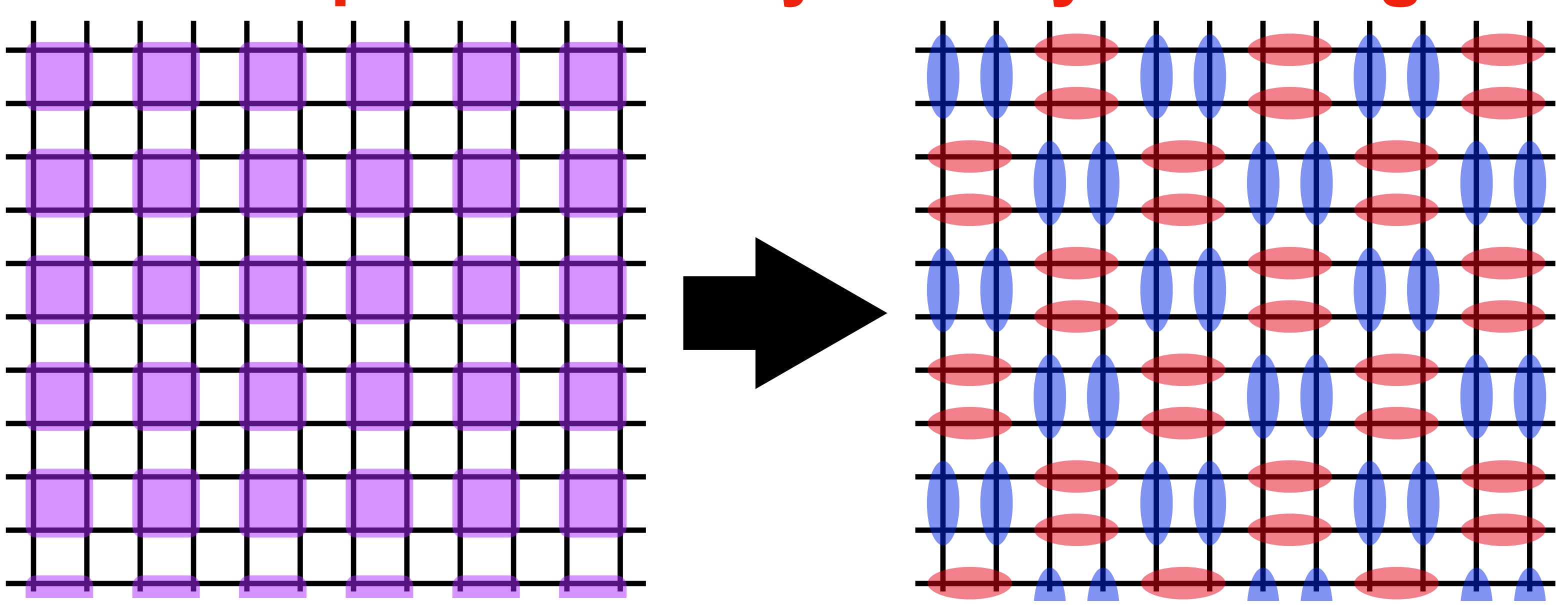

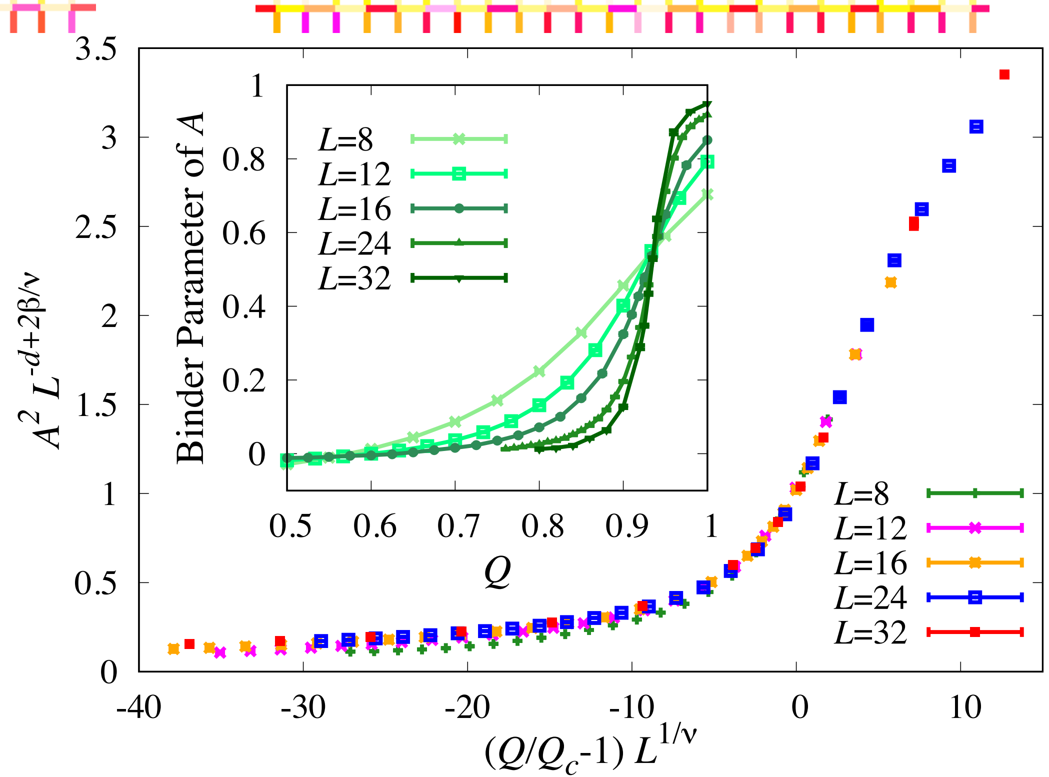

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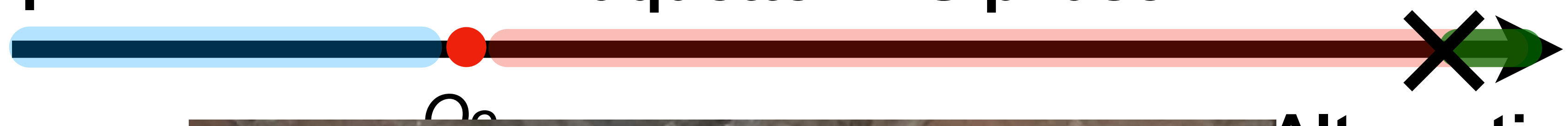
Néel phase **Plaquette VBS phase**



Alternating VBS

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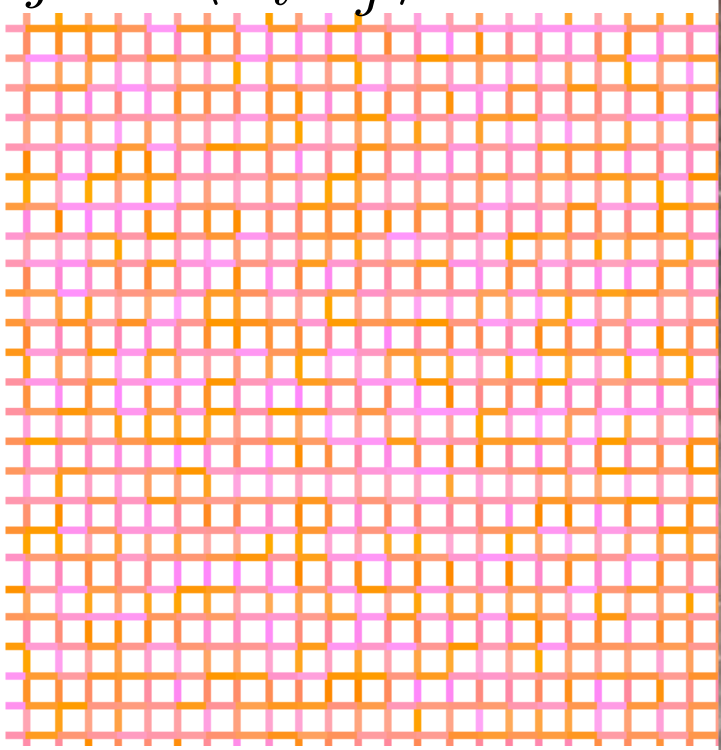

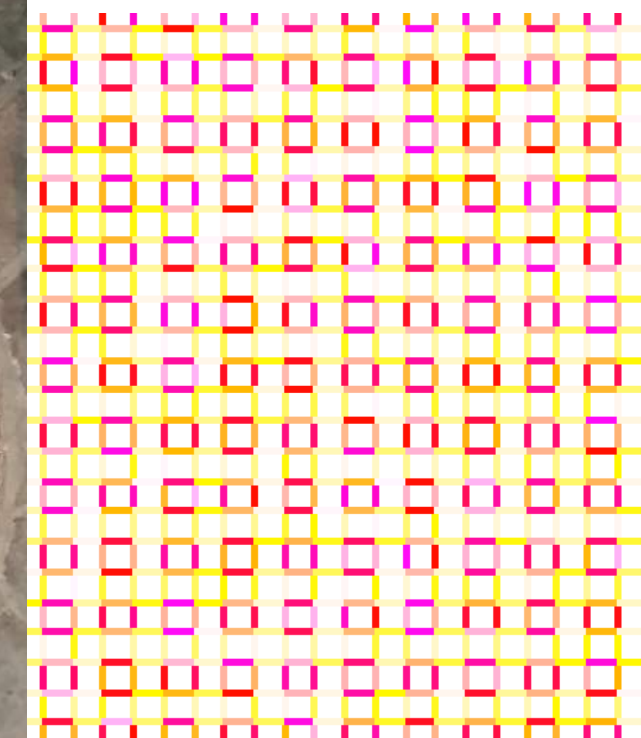

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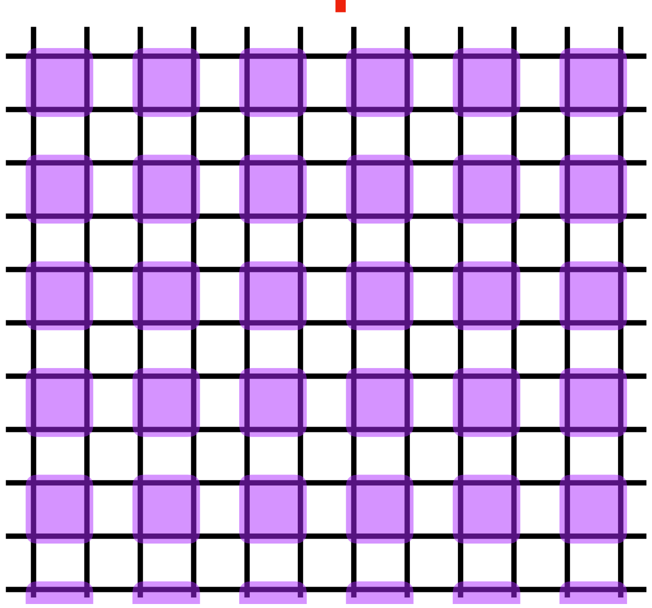
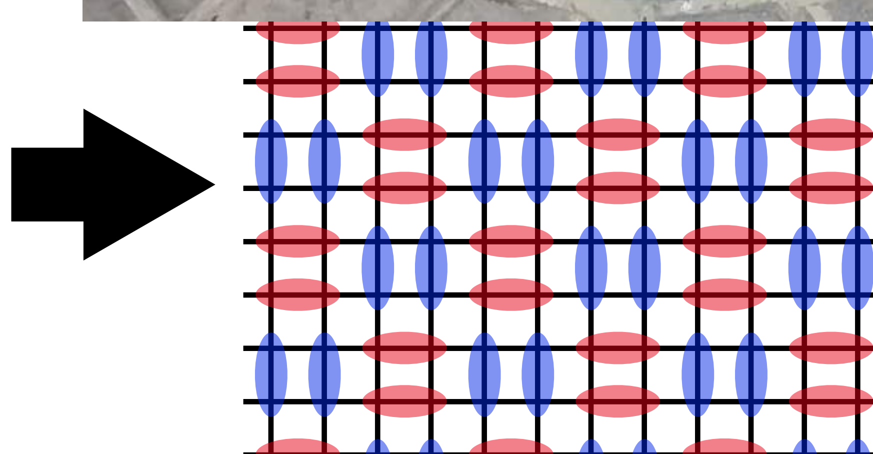
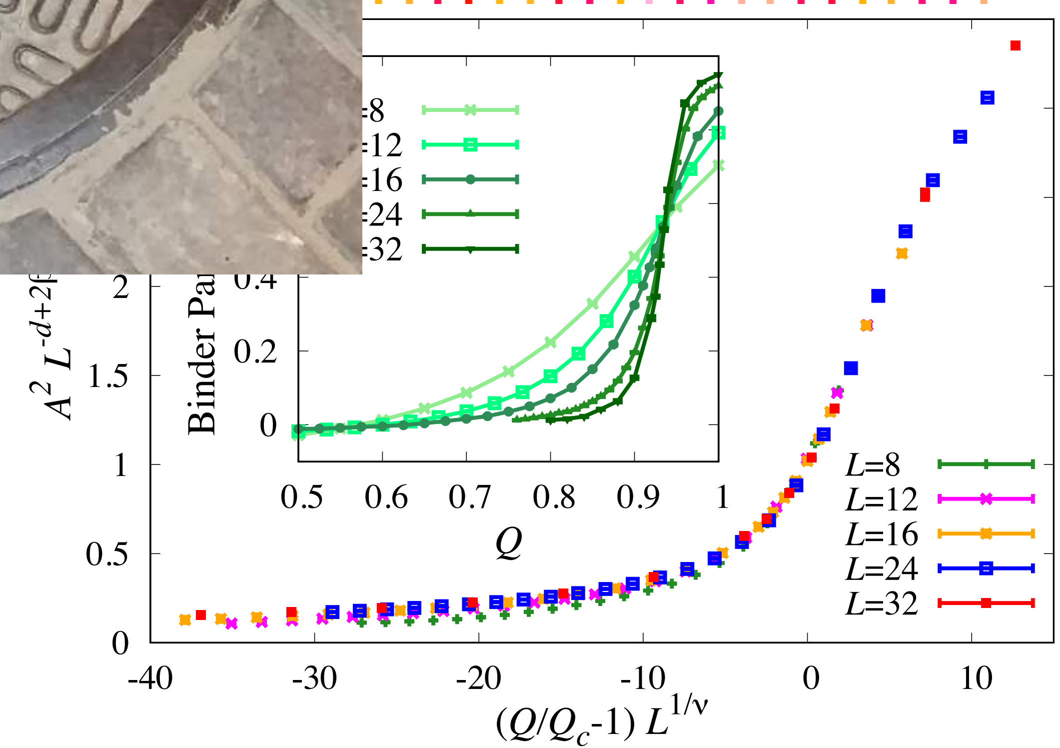






Outline

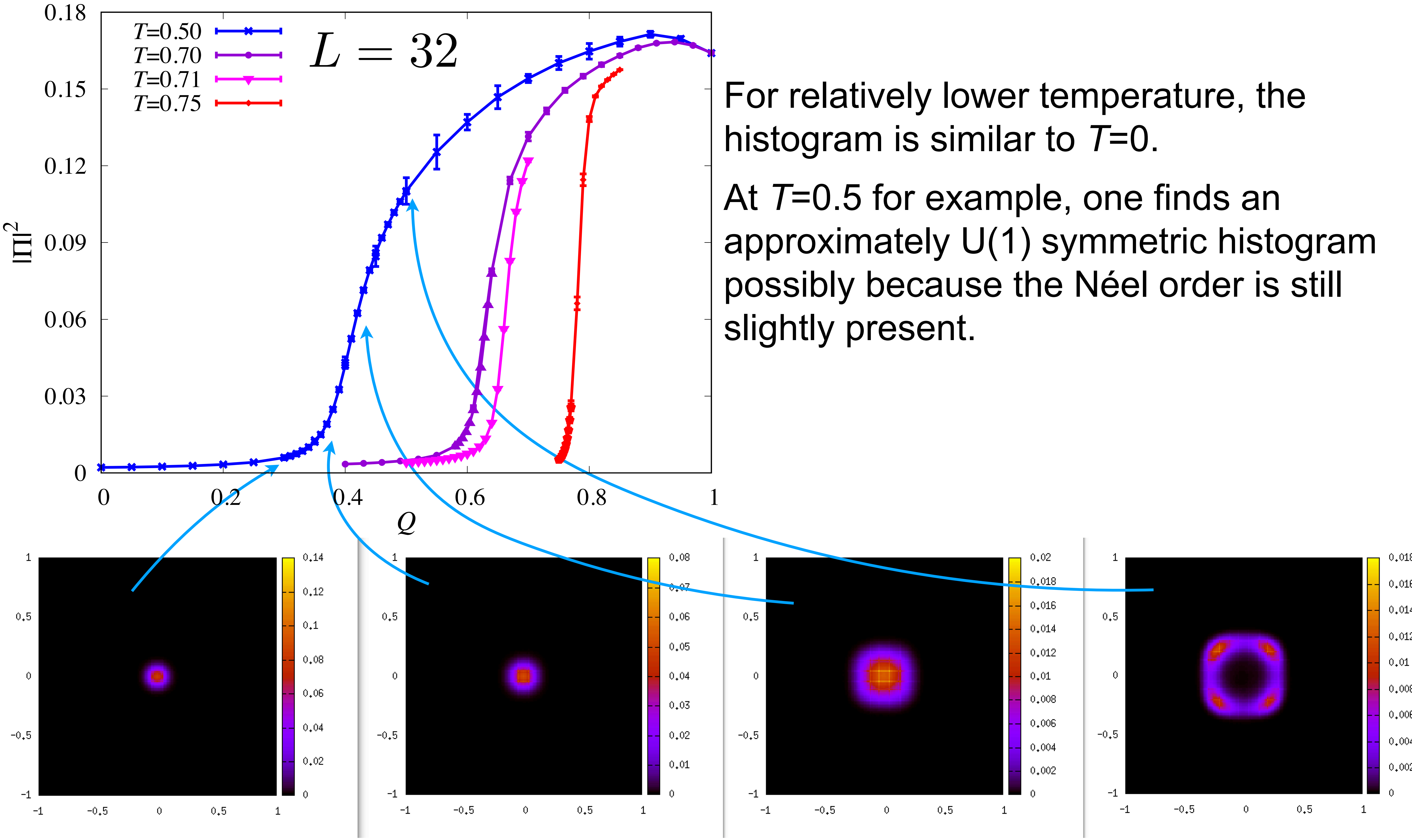
1. Background: Deconfined Quantum Criticality

2. Construction of our model and DQC

3. Finite temperature “vestigial order”

4. Conclusion and discussions

Low T, not so different

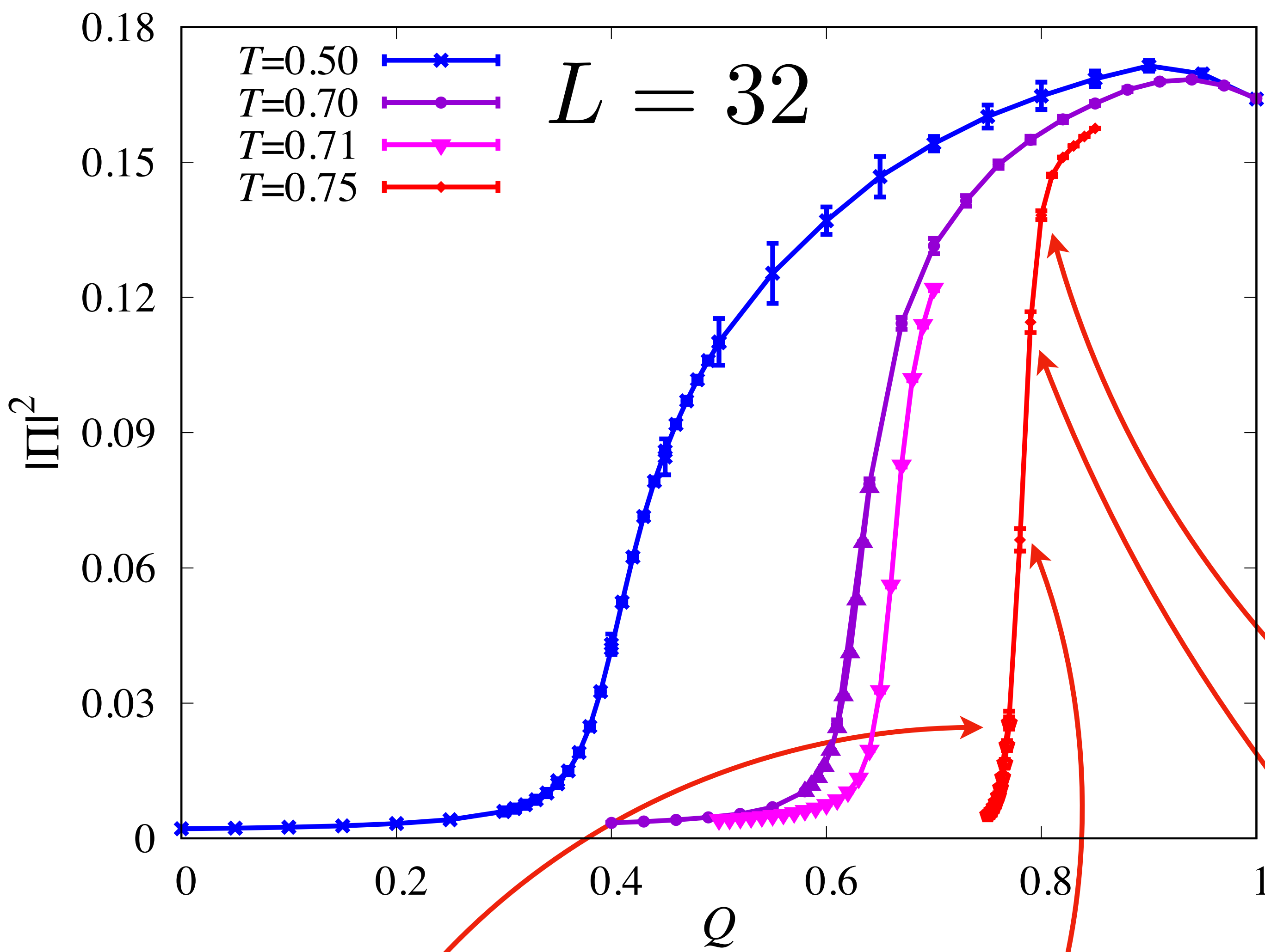


For relatively lower temperature, the histogram is similar to T=0.

At T=0.5 for example, one finds an approximately U(1) symmetric histogram possibly because the Néel order is still slightly present.

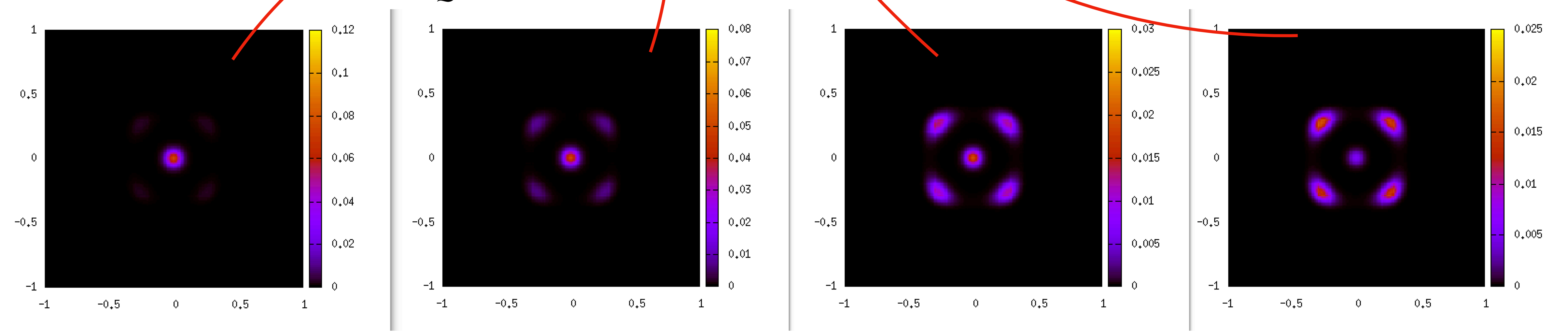
There seems to be NO coexistence, and a little bit of a remainder of U(1) symmetry

Strongly first-order for high *T*



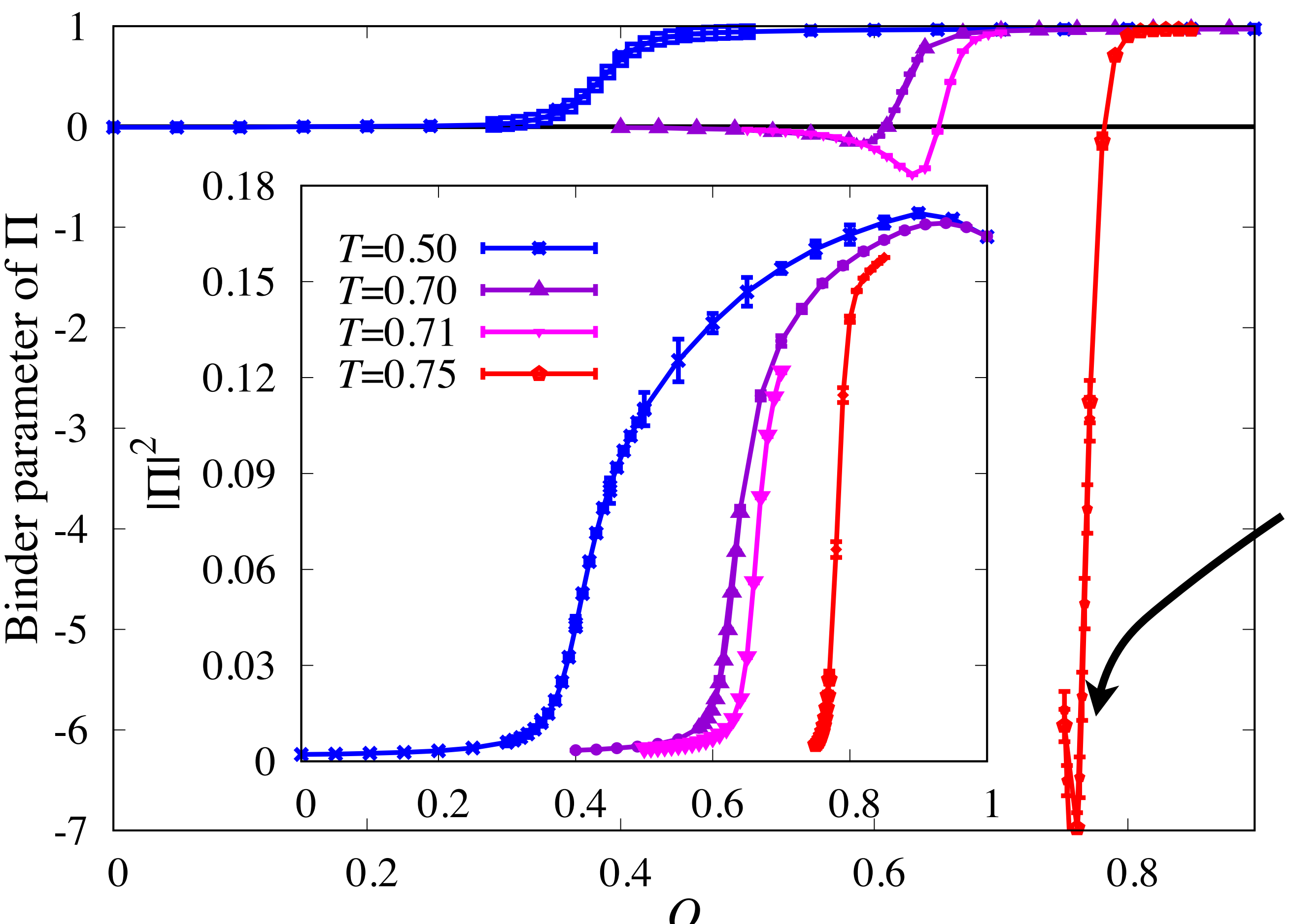
As we go to higher temperature, the rising of the VBS order parameter at the transition becomes sharper and transition becomes more **strongly first-order!**

Possibly explained by either…
(1) “Fluctuation-induced first-order transition”
(2) Vestigial phase



We see a very clear coexistence at the transition points strongly suggesting FOT

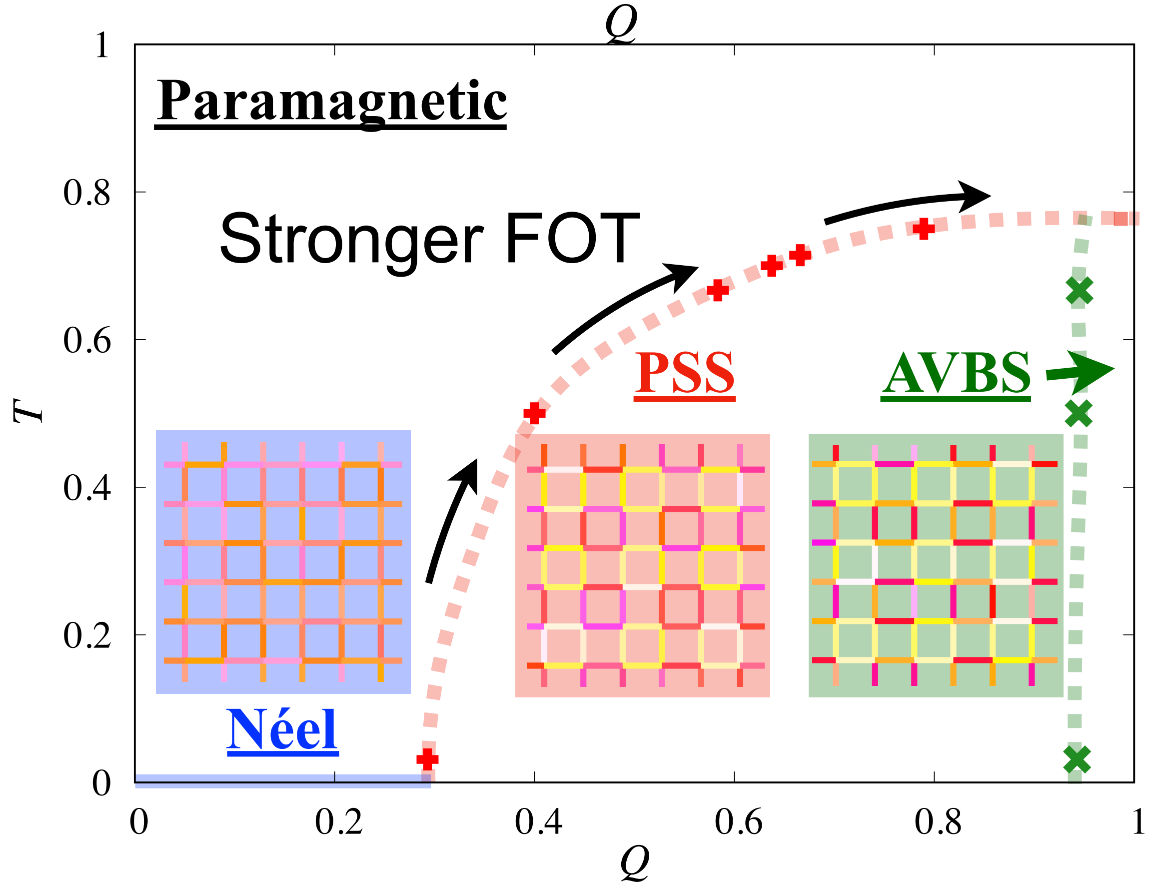
Binder and the phase diagram

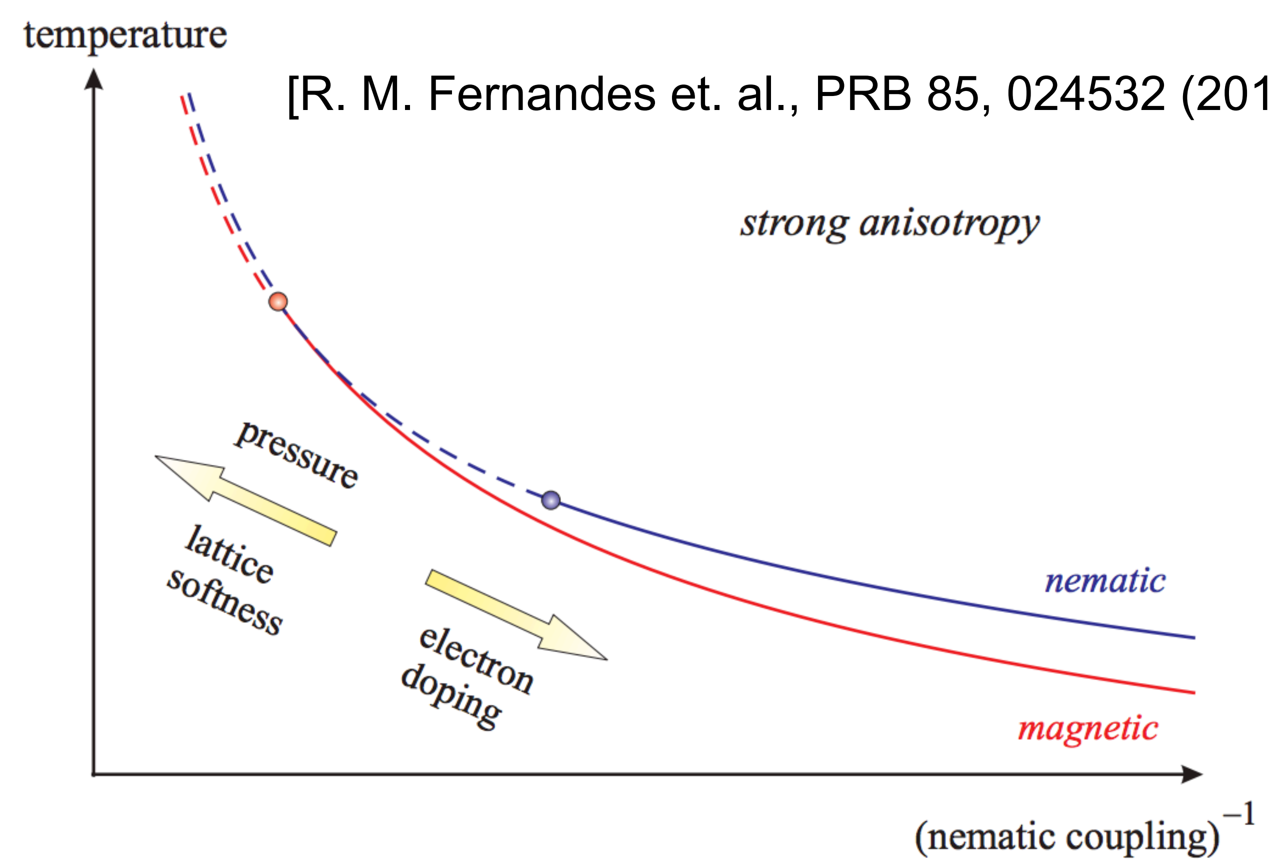


We can see that the **dip of the Binder parameter** (= clear sign of FOT) becomes stronger as we go to higher temperature.

E.g. the dip for T=0.75 is **HUGE** compared to others.

The expected phase diagram is topologically the same with that of the "strongly 2D" case of vestigial phase analysis

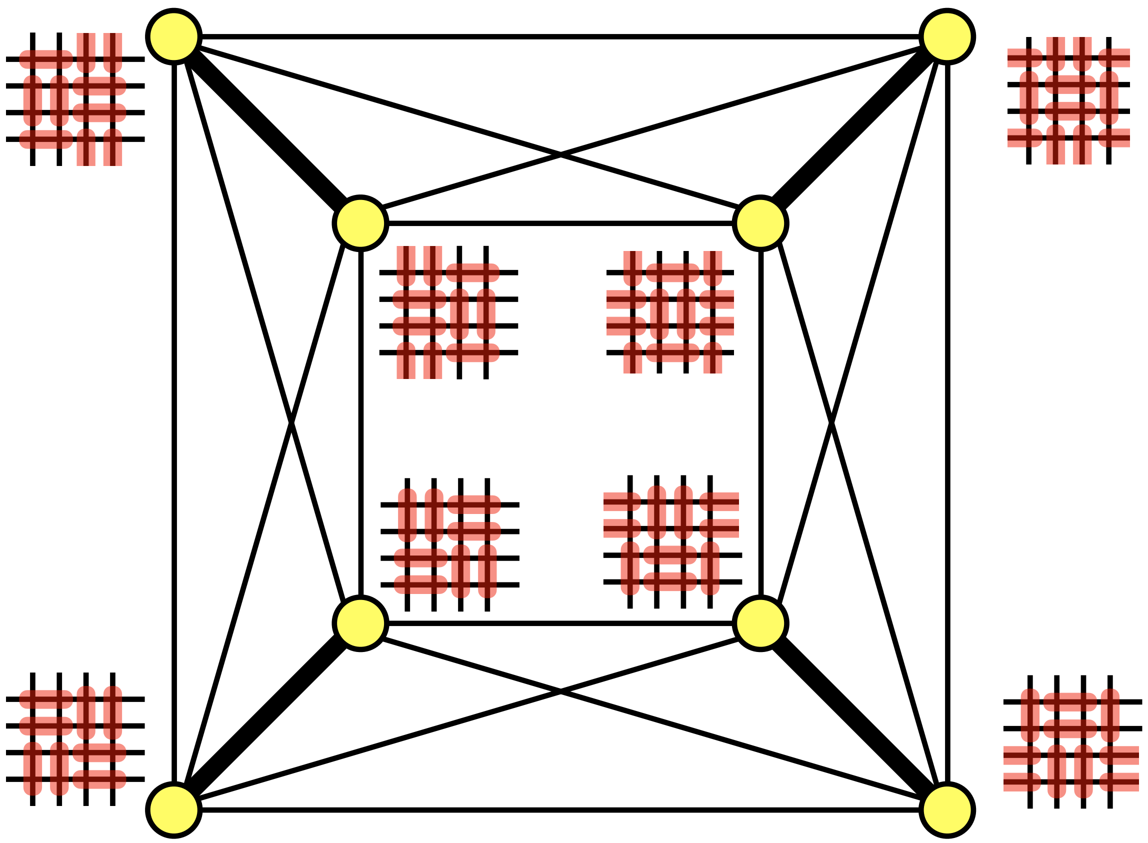




[R. M. Fernandes et. al., PRB 85, 024532 (2012)]

2-step symmetry breaking

Structure and relation of the eight degenerate states

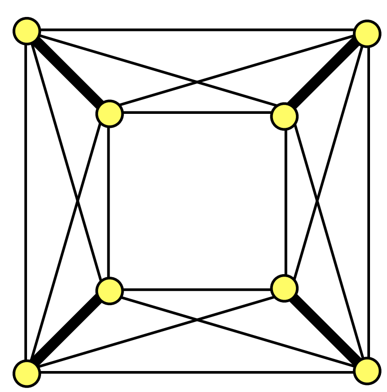
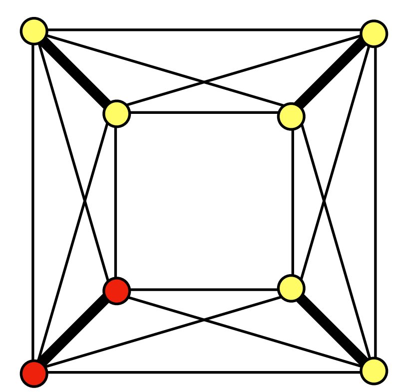
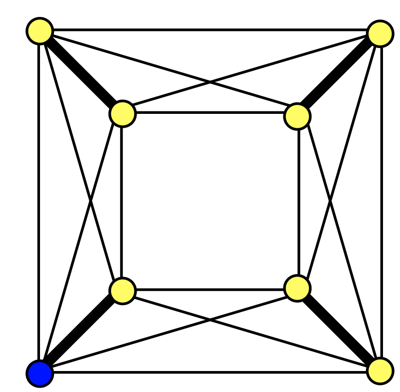


Thick bonds represent fluctuation around the plaquette (or equivalently, 2-step shifts)

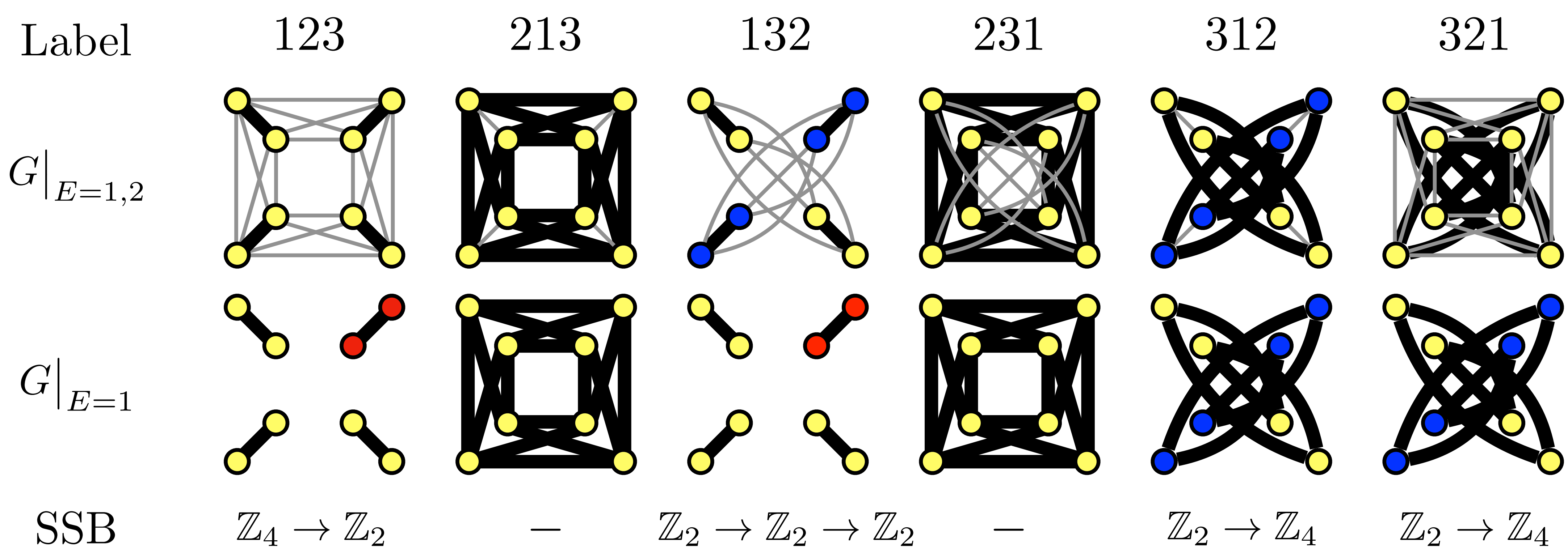
All thin bonds represent 1-step shifting in the *x* or *y* direction

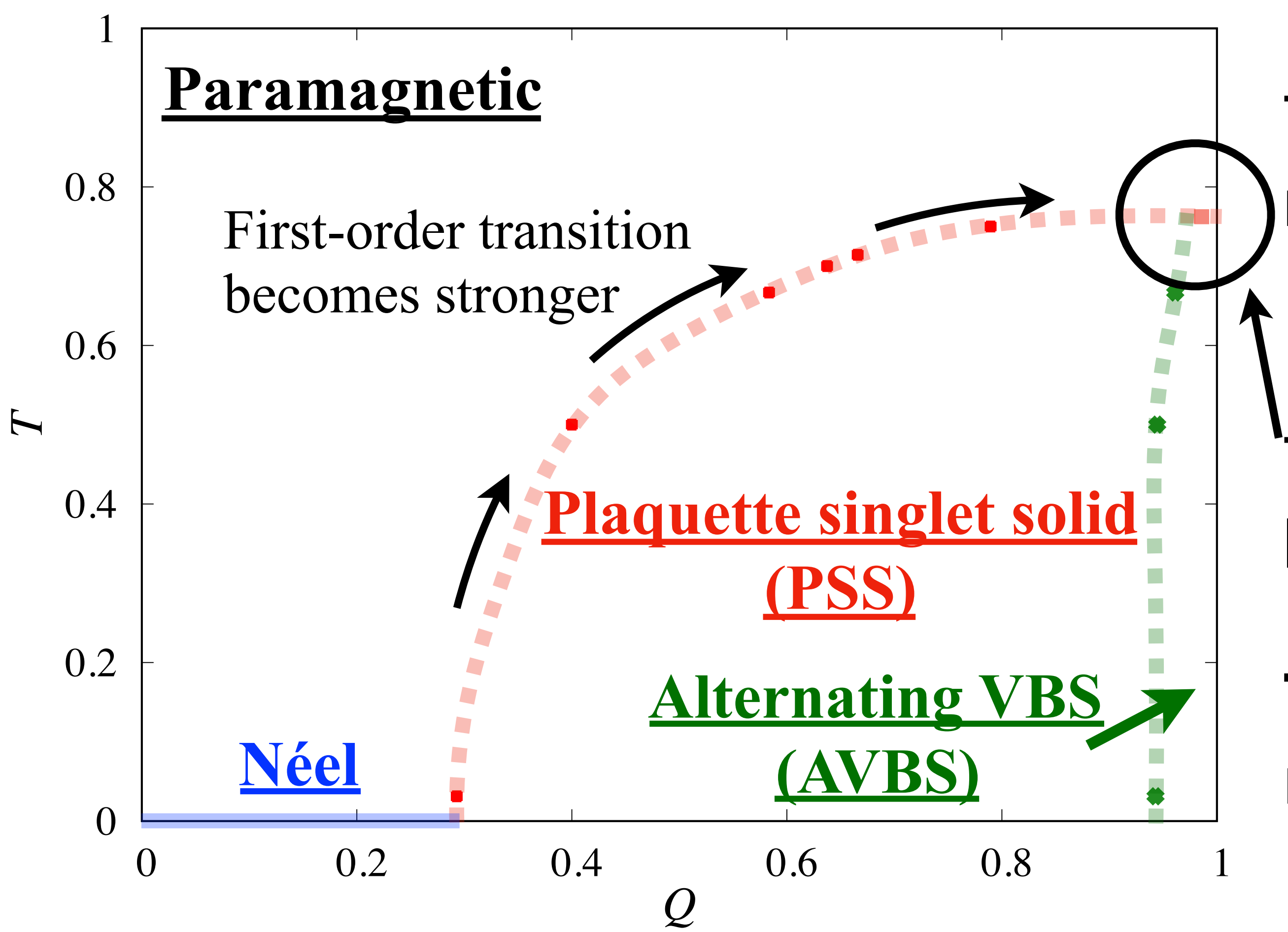
Any two states without bonds have physically the same relations to each other

Automorphism group of the graph is $D_4 \otimes \mathbb{Z}_2^4$

Phases:	Disordered	Plaquette VBS	Alternating VBS
Macro-state graph:			
Automorphism group:	$D_4 \otimes \mathbb{Z}_2^4$	$\mathbb{Z}_2 \otimes \mathbb{Z}_2^4$	$\mathbb{Z}_2 \otimes \mathbb{Z}_2^3$
Broken symmetry:	1 (none)	$D_4/\mathbb{Z}_2$	D_4

Other paths to alternating VBS





The phase diagram cannot have adjacent regions breaking Z_2 before Z_4.

Thus, the phase diagram simply has two lines clashing, forming a FOT line segment.

Then, the increase of "first-orderness" is naturally explained to connect 2 edges.

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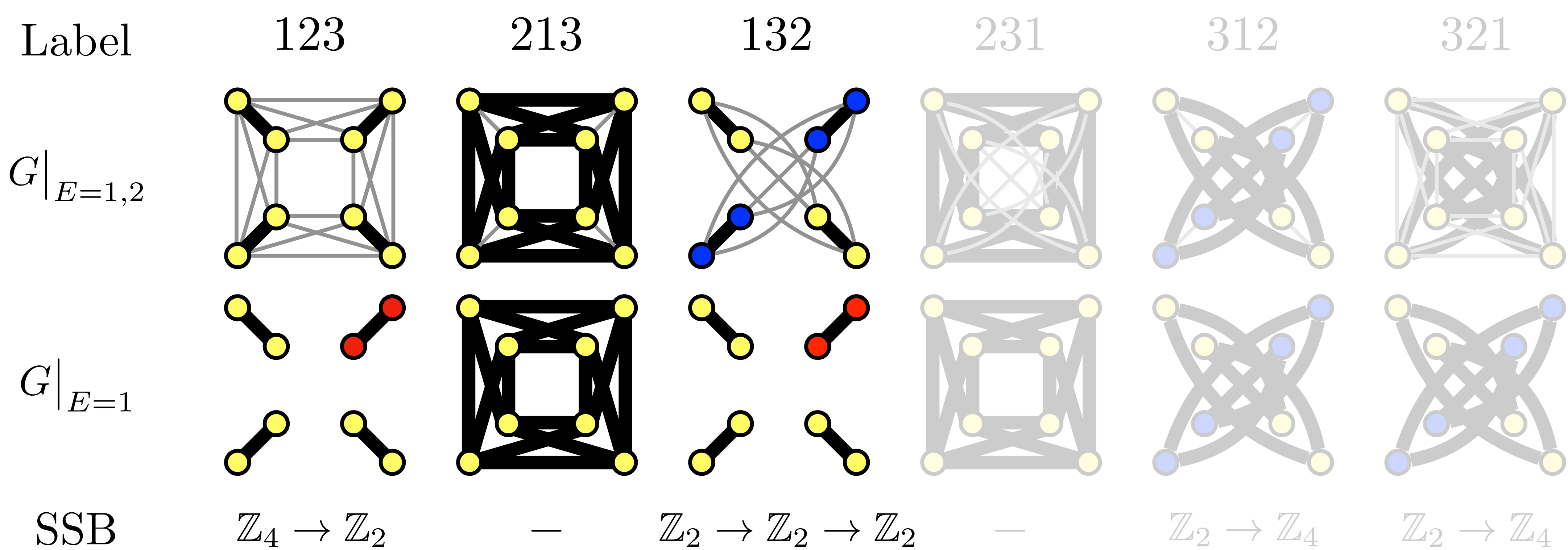

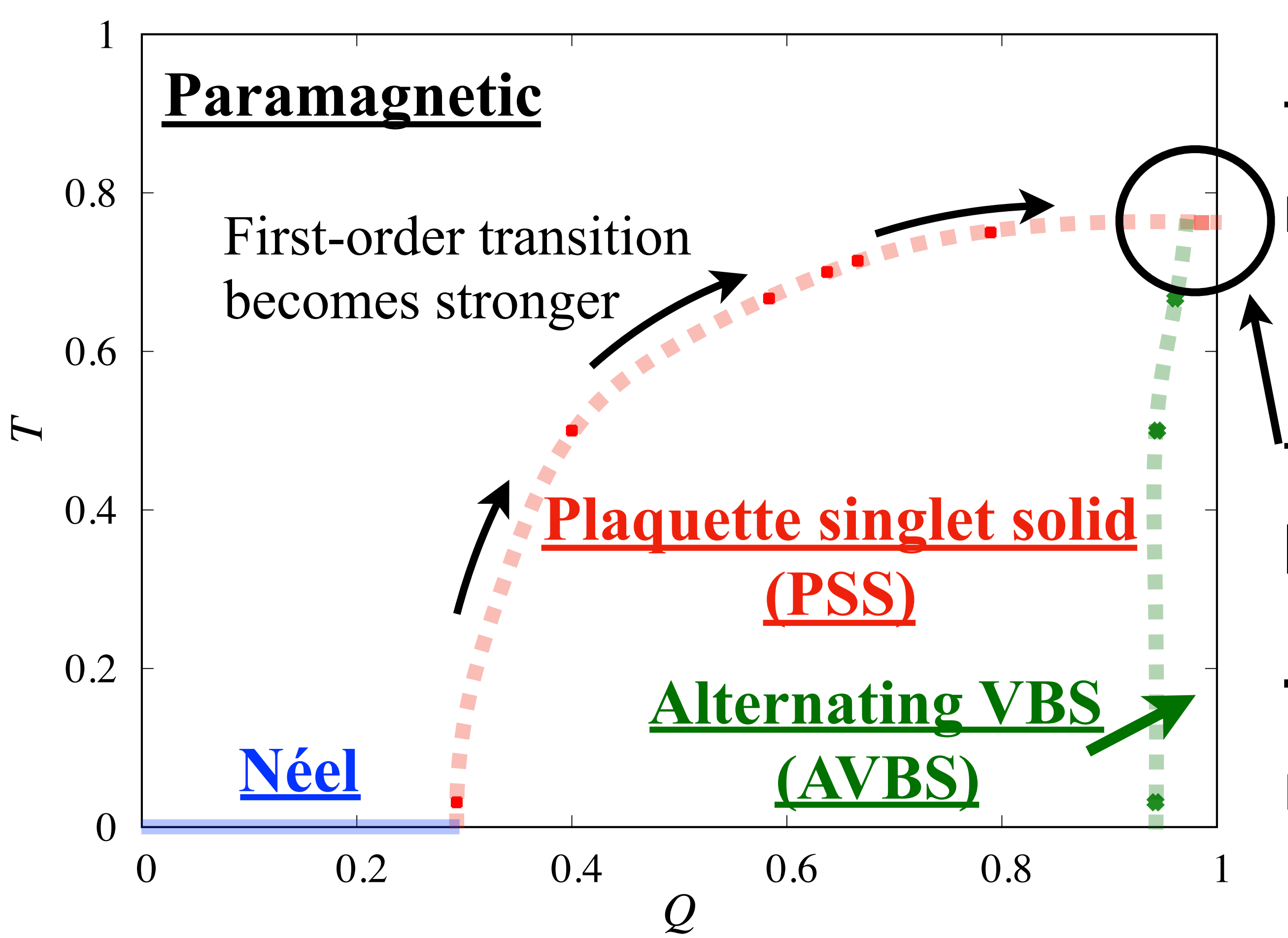

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Conclusions + Overview

Néel-to-plaqVBS quantum phase transition

- ✔ We constructed the first explicit model that clearly has this direct QPT!
- ✔ The QPT is a very weak FOT with possible emergent U(1) and SO(5) symmetry.
- ✔ Similar FOT with emergent SO(4) symmetry has been observed before.
  Is this UNIVERSAL?? [B. Zhao, P. Weinberg & A.W. Sandvik, Nat. Phys. (2019)]
- ✔ Possibly, in plaqVBS, spinons are actually fractons?? [Y. You, et al., 1908.08540 (2019)]

New phase transition with additional Z2 symmetry breaking

- ✔ The alternating VBS phase breaks additional Z_2 symmetry, and is eight-fold.
- ✔ This suggests that the plaquette VBS phase can be understood as an intermediate phase when we add quantum fluctuation to the alternating VBS phase.
- ✔ We observe "fluctuation-induced" strong first-order transitions, which is explained compactly using graph-theoretic analysis

Thank you!

Takahashi & Sandvik [arXiv:19**.*****] in preparation…

Variety of possible “DQC” (補足)

In 2+1d Honeycomb lattice

[K. Harada, T. Okubo, N. Kawashima, S. Todo, et al., PRB (2013)]
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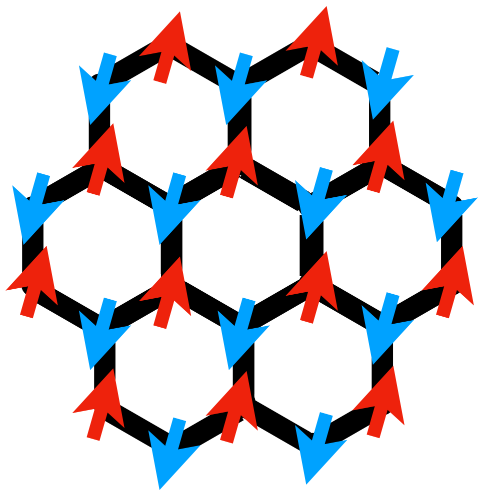
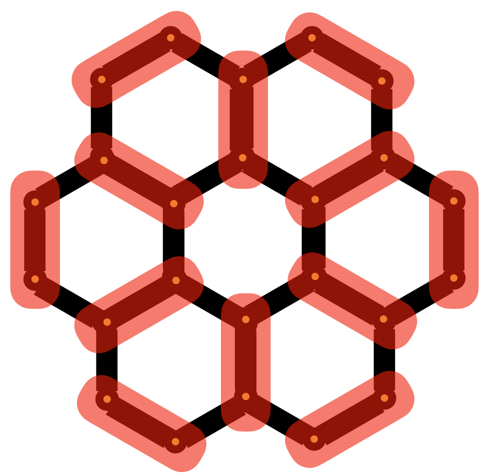


Néel



VBS

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- ✔ **However, this VBS is 3-fold degenerate:**

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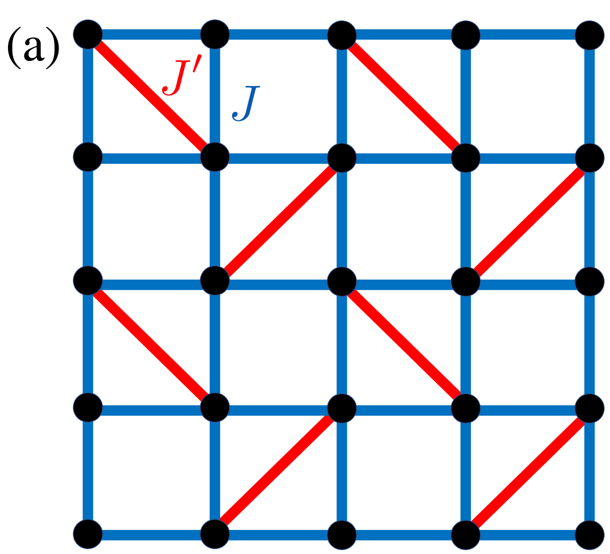
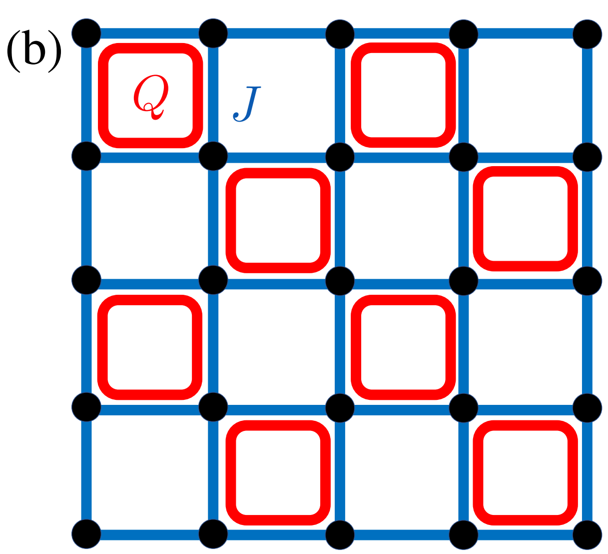
- ✔ **For SU(N) with higher N, continuous!**

Plaquette singlet phase breaking Z2 symmetry

[B. Zhao et al., Nat. Phys. (2019)]
[J. Y. Lee et al., arXiv:1904.07266]



Shastry-Sutherland



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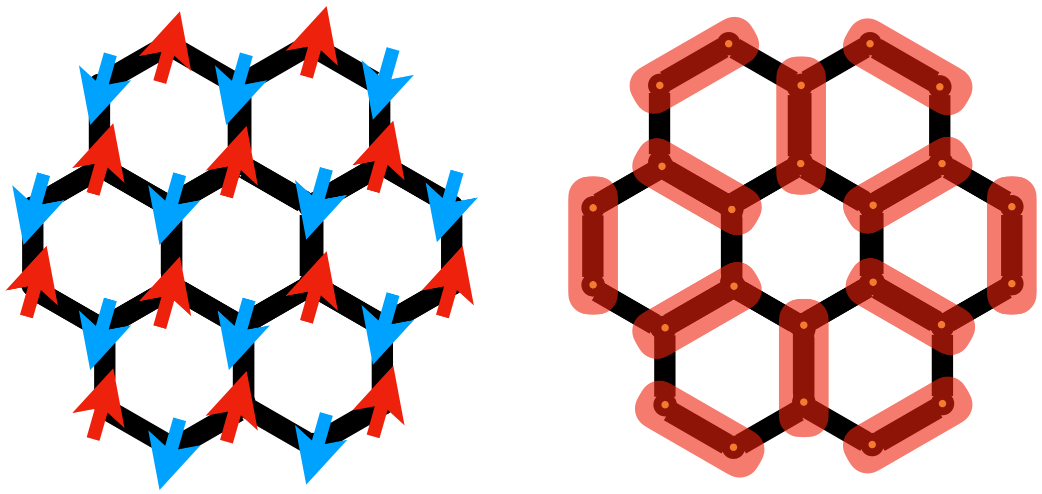

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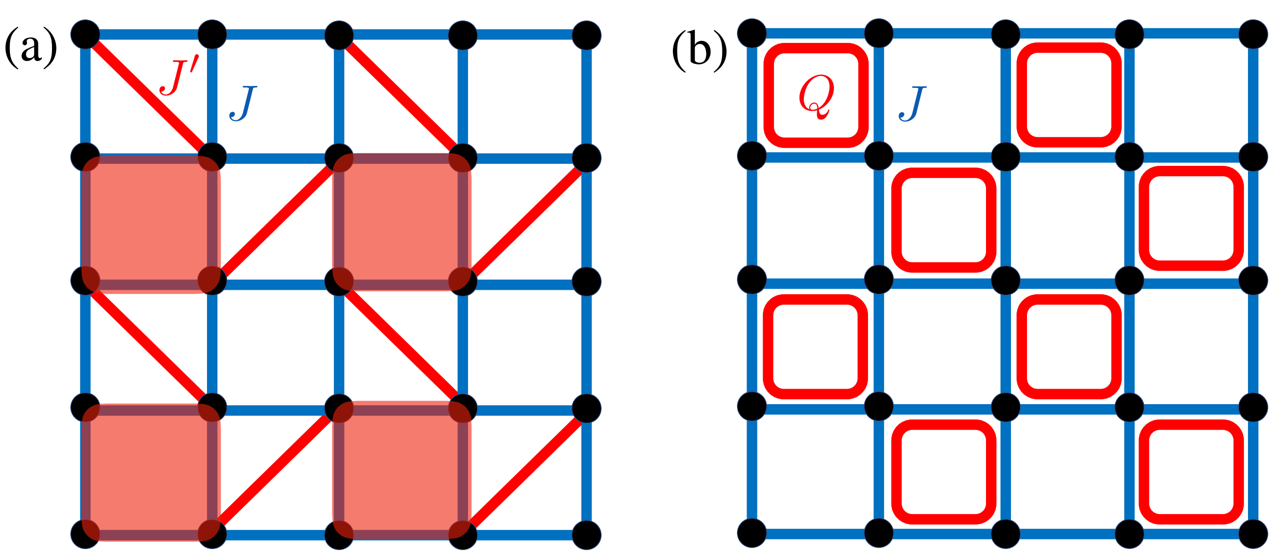

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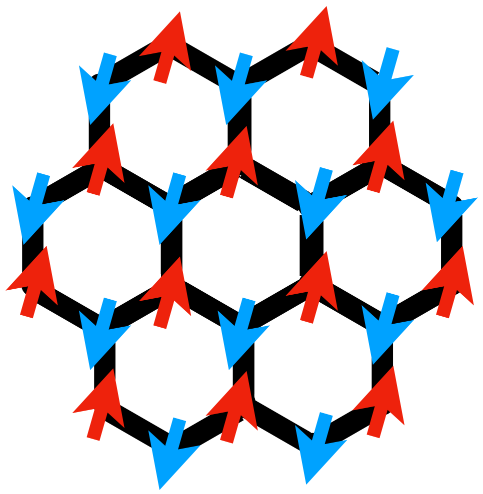

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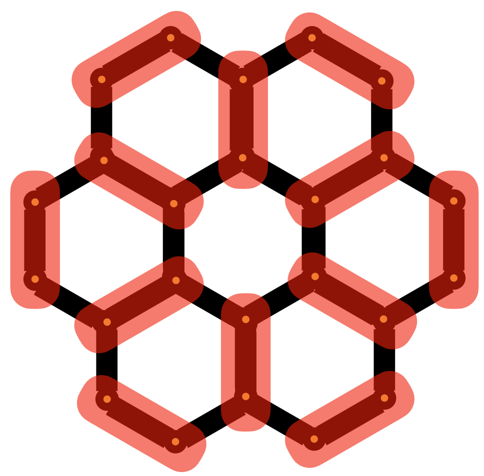

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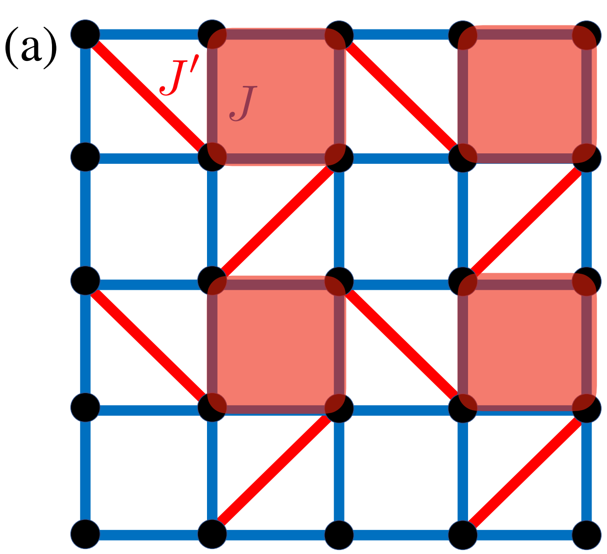

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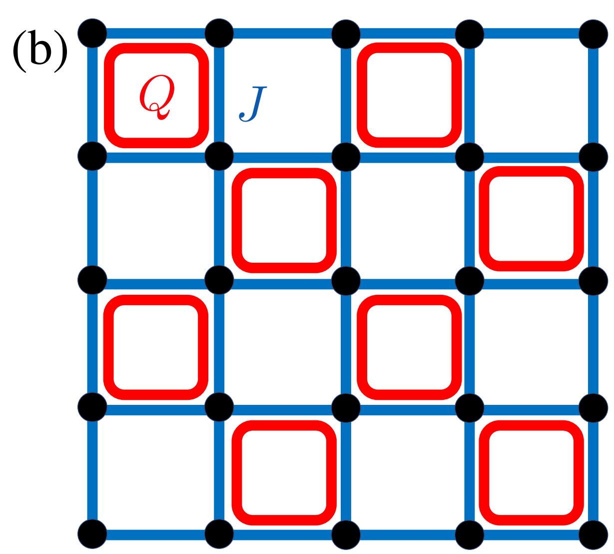

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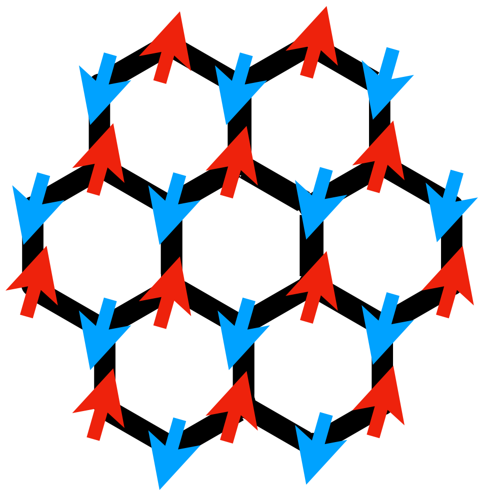

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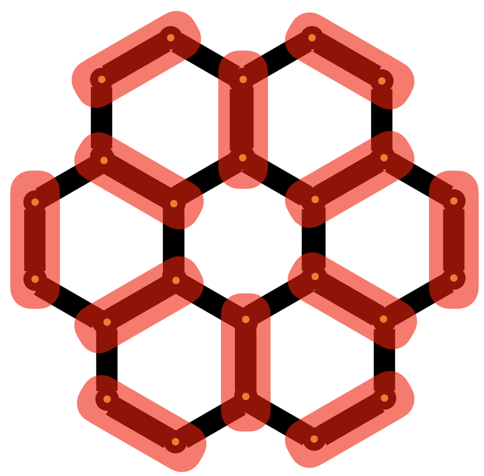

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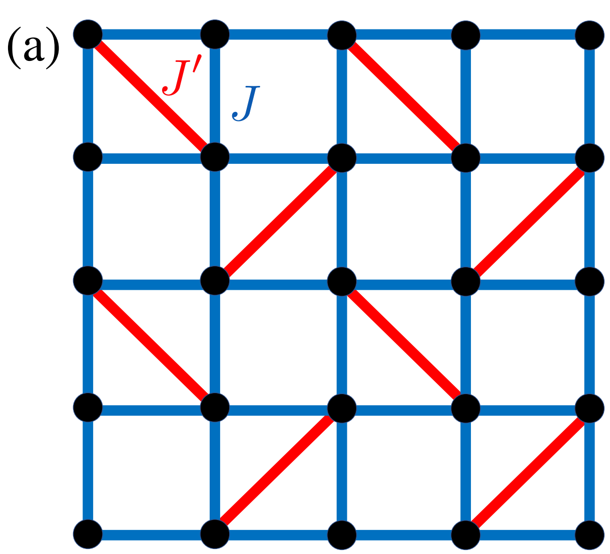

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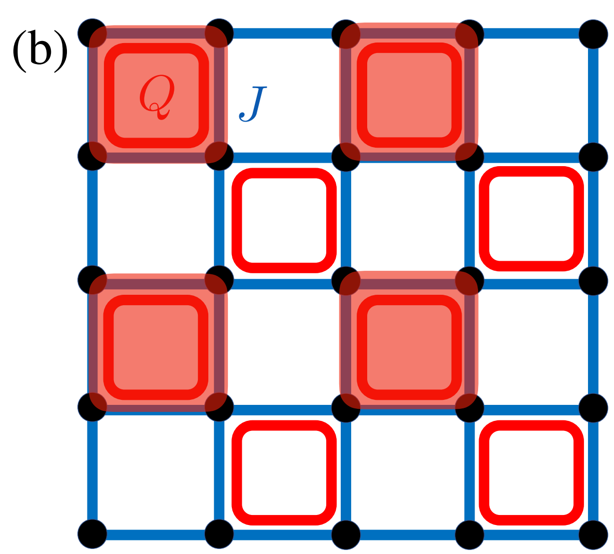

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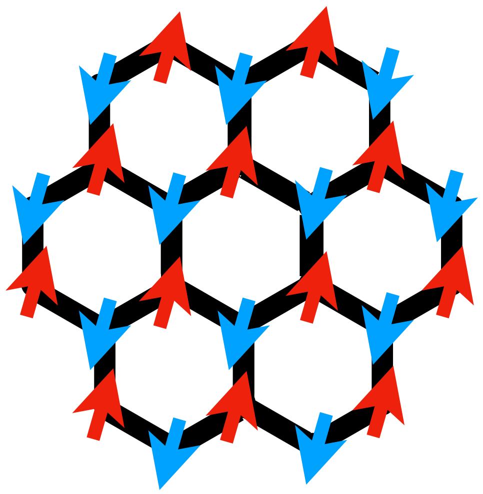

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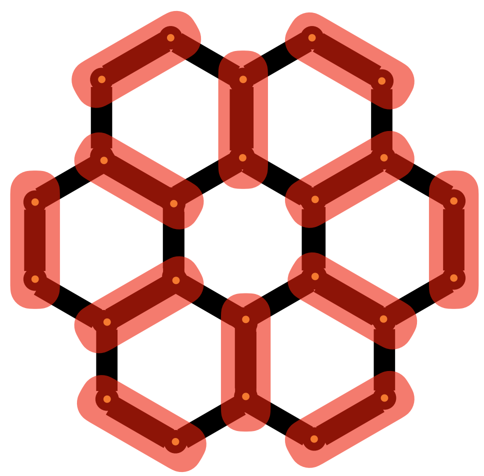

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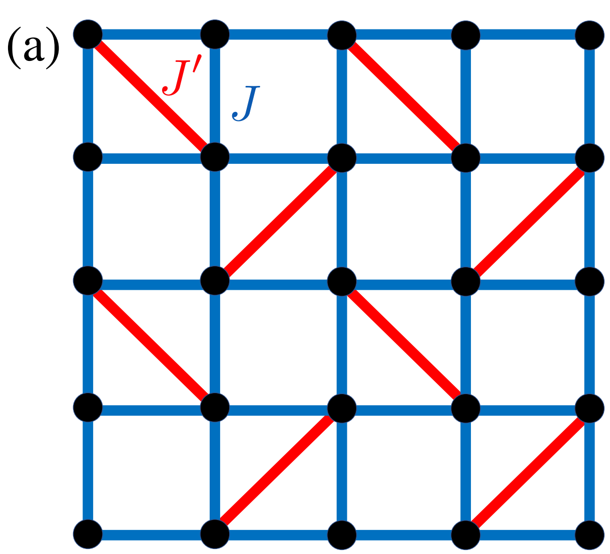

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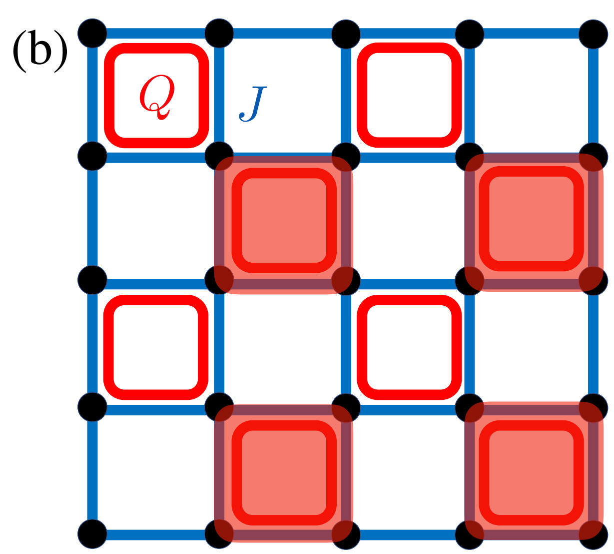

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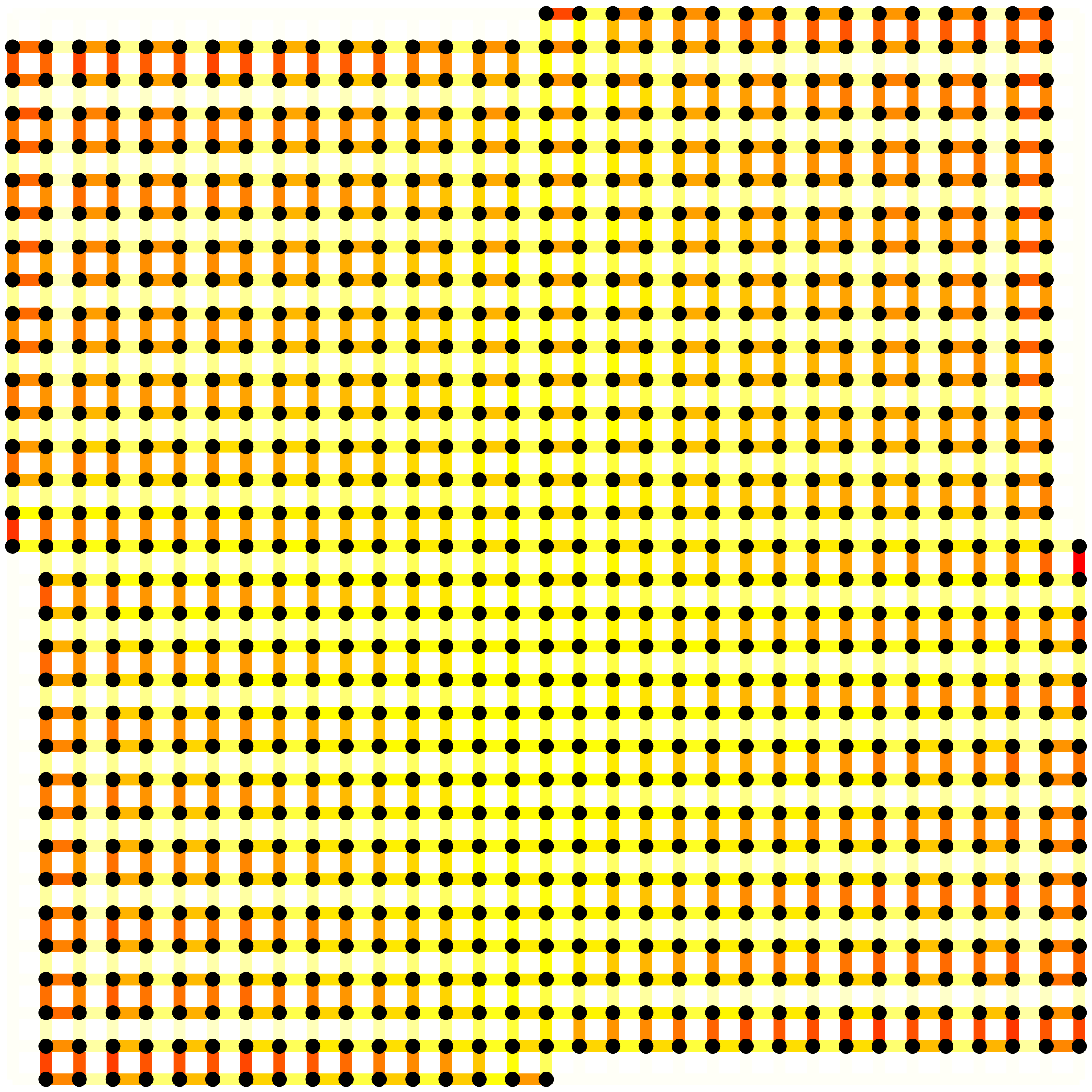
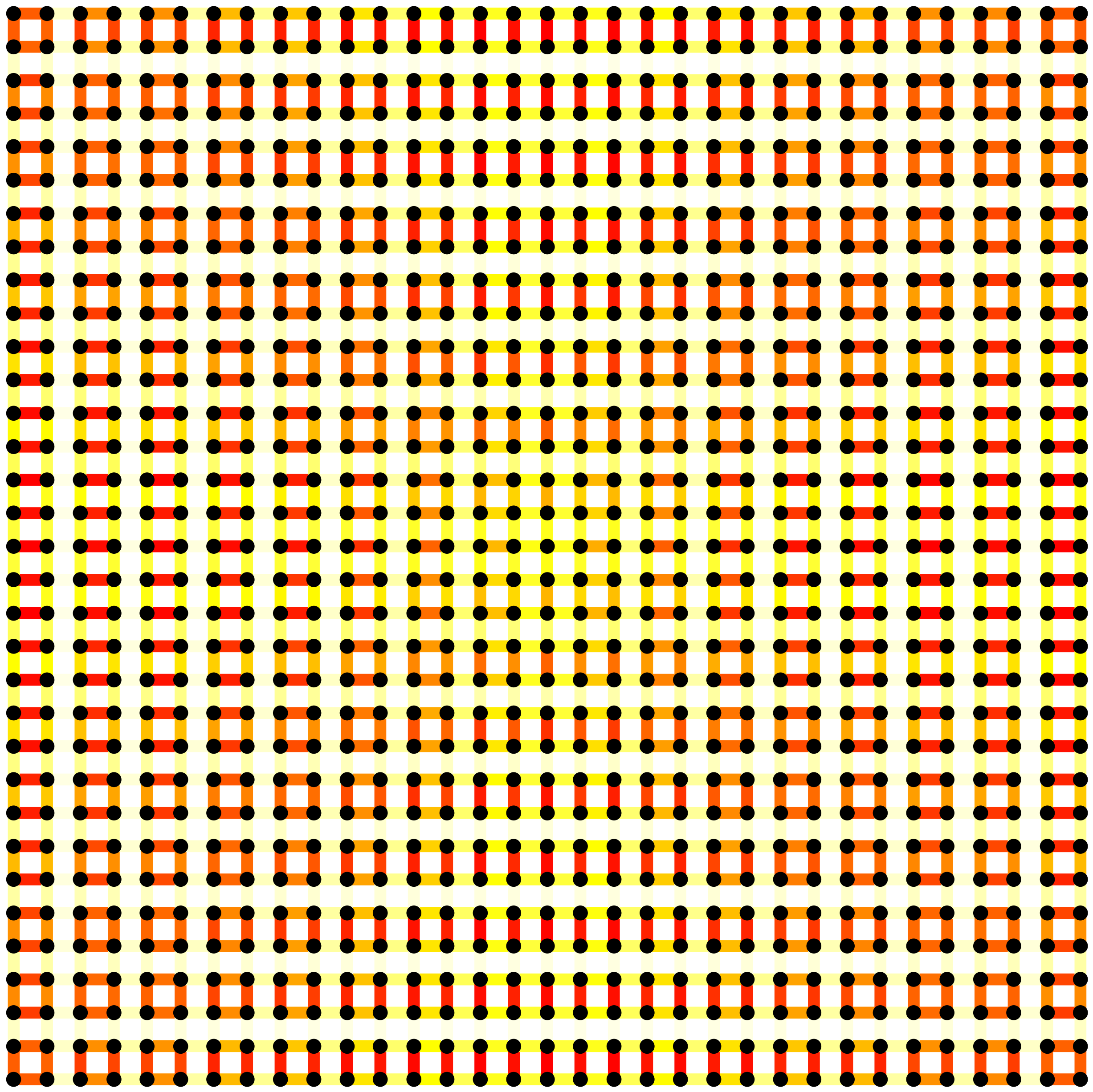
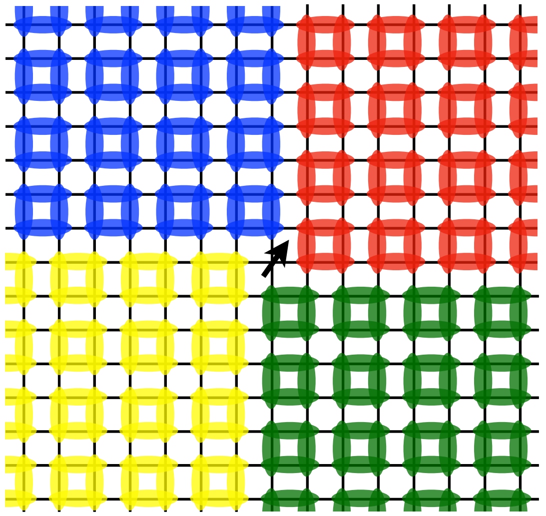
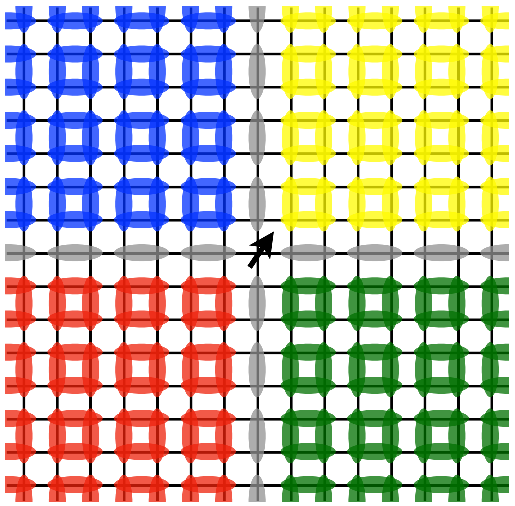
2 types of domain walls (補足)









2 types of domain walls (補足)