

Field-Driven $U(1)$ Quantum Spin Liquid in Kitaev's Honeycomb Model

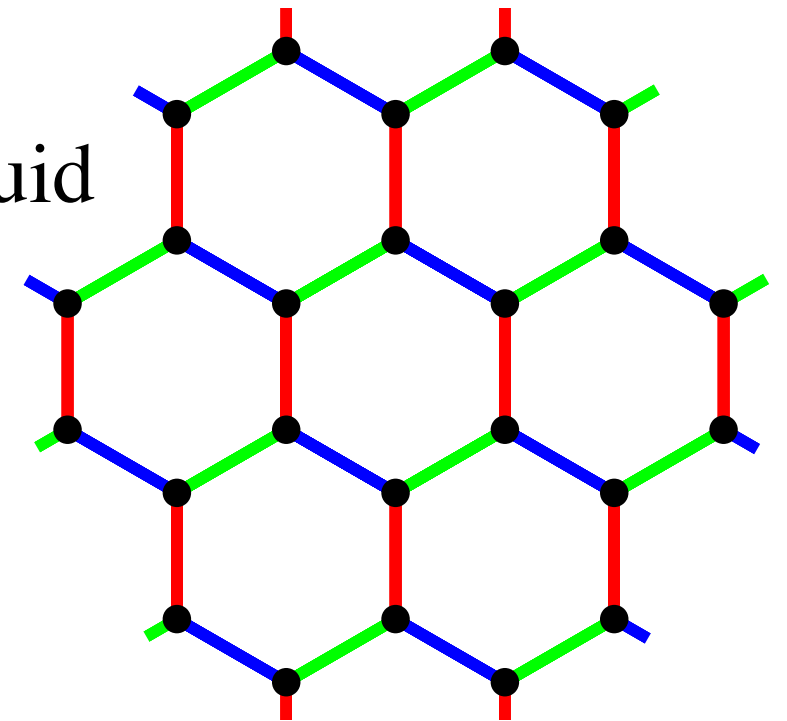
Ciarán Hickey
University of Cologne

Kitaev Model

$$H = \pm K \left(\sum_{\langle i,j \rangle \in x} S_i^x S_j^x + \sum_{\langle i,j \rangle \in y} S_i^y S_j^y + \sum_{\langle i,j \rangle \in z} S_i^z S_j^z \right)$$

- Exactly solvable model of a Z_2 quantum spin liquid

(with only NN two-spin interactions,
which can be realised in materials)



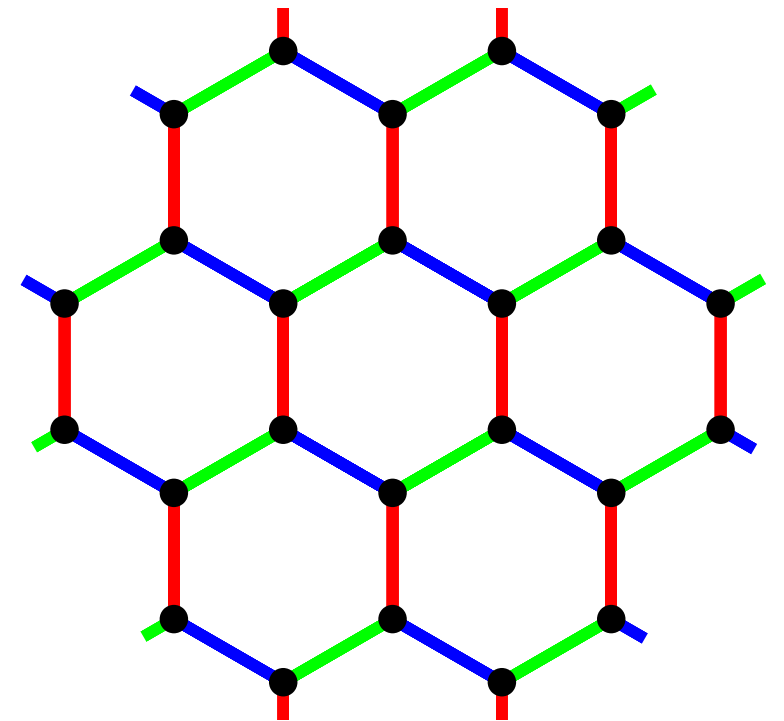
- Rich playground for investigating exact ground state, dynamical and finite temperature properties of Z_2 spin liquids

Kitaev Model

$$H = \pm K \left(\sum_{\langle i,j \rangle \in x} S_i^x S_j^x + \sum_{\langle i,j \rangle \in y} S_i^y S_j^y + \sum_{\langle i,j \rangle \in z} S_i^z S_j^z \right)$$

Kitaev Model
+
Magnetic Field

\approx ???



Outline

- Introduction
- The Kitaev Model in a Magnetic Field
 - Q. Nature of the KSL?
 - Q. Critical Field FM vs AFM?
 - Q. Nature of the GSL?
- Discussion & Conclusion



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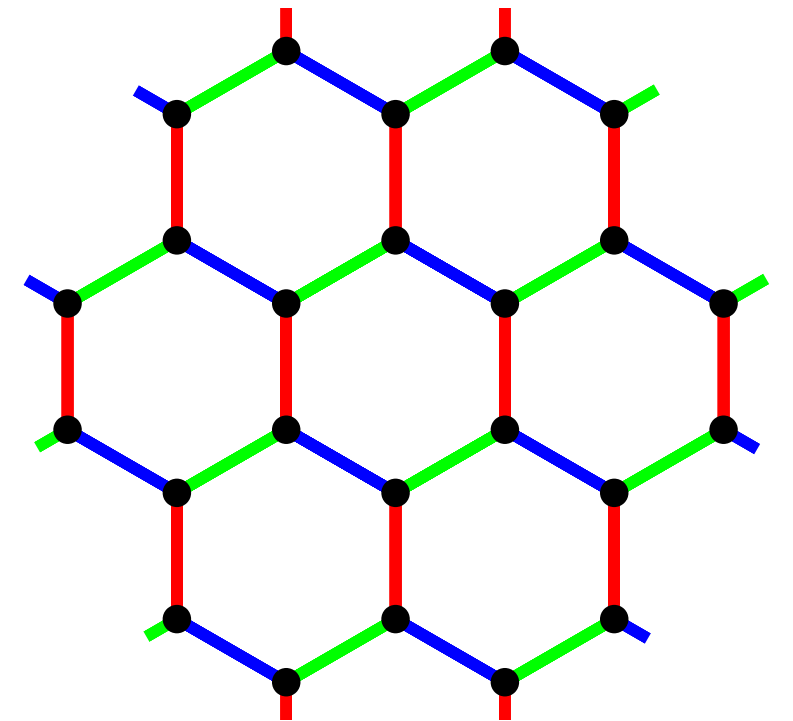
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Kitaev Model

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$$H = \pm K \frac{i}{2} \sum_{\langle i,j \rangle} \hat{u}_{ij} c_i c_j$$



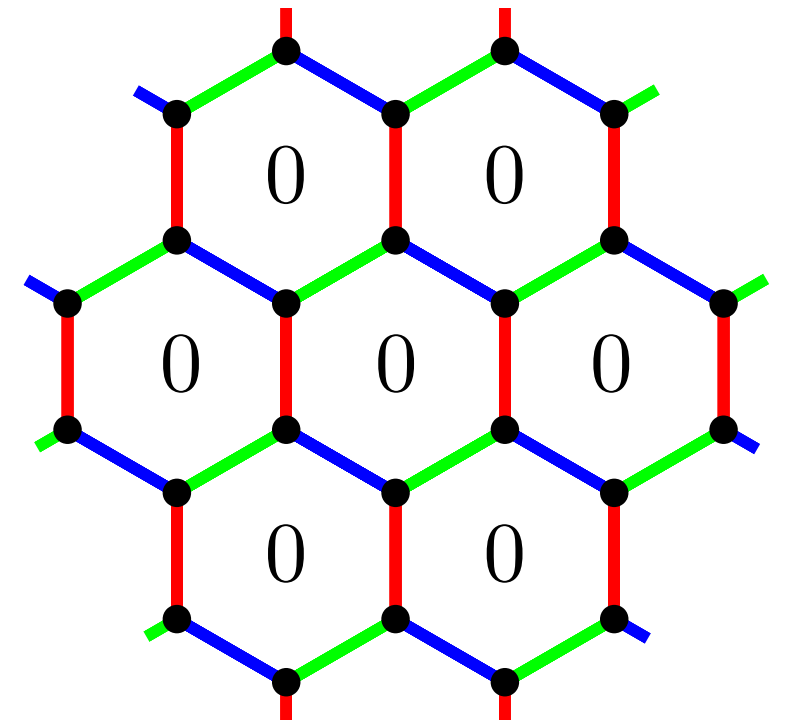
Single, free Majorana fermion
coupled to static Z_2 gauge field!!!

Kitaev Model

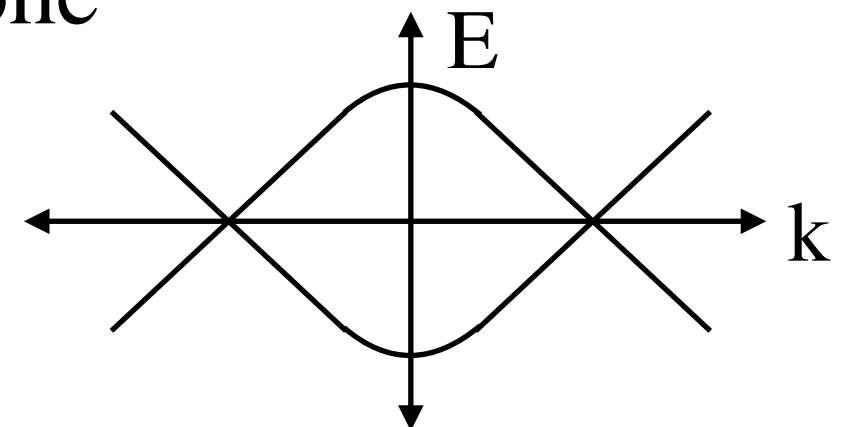
$$H = \pm K \left(\sum_{\langle i,j \rangle \in x} S_i^x S_j^x + \sum_{\langle i,j \rangle \in y} S_i^y S_j^y + \sum_{\langle i,j \rangle \in z} S_i^z S_j^z \right)$$



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- Ground State:
 - Majorana fermions form a Dirac cone
 - All plaquette fluxes = 0

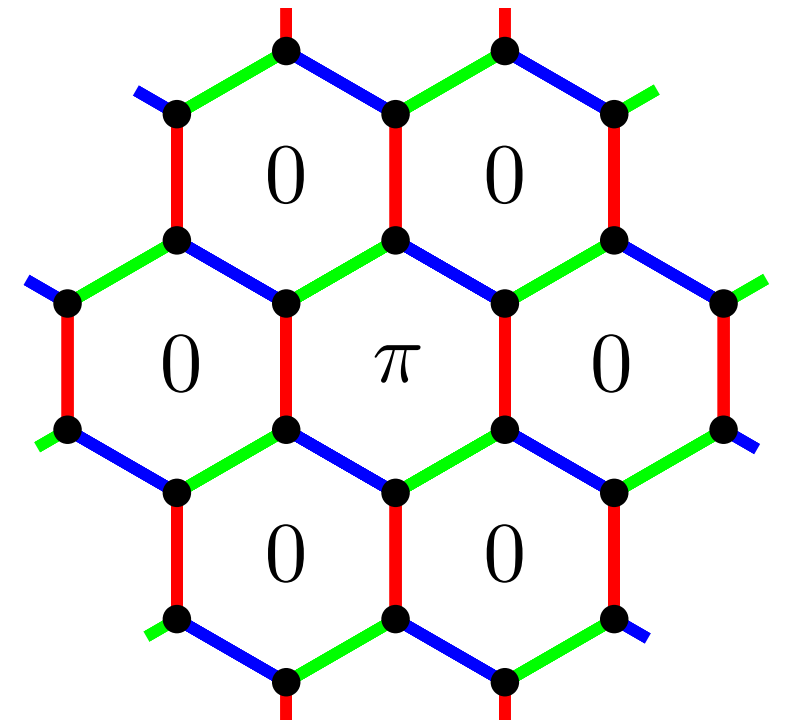


Kitaev Model

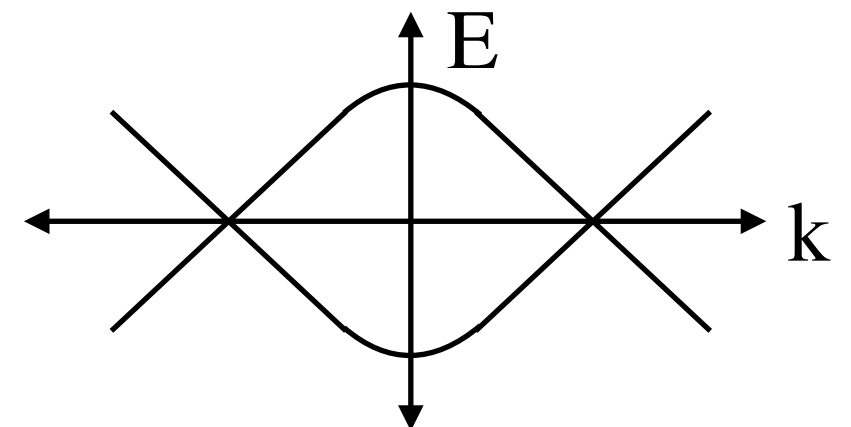
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$$H = \pm K \frac{i}{2} \sum_{\langle i,j \rangle} \hat{u}_{ij} c_i c_j$$



- Two kinds of excitations:
 - Gapless Majorana fermions
 - Gapped flux excitations (visons)



Kitaev Materials

- Kitaev interactions can actually be realized in materials

Ingredients:

d-orbitals
+
Crystal field splitting
+
Spin-orbit coupling
+
Interactions



$$j_{eff} = 1/2$$

$$\begin{array}{l} \text{---} |\uparrow\rangle_{eff} \\ \text{---} |\downarrow\rangle_{eff} \end{array}$$

$$\begin{aligned} |\uparrow\rangle_{eff} &\sim i |zx, \downarrow\rangle + |yz, \downarrow\rangle + |xy, \uparrow\rangle \\ |\downarrow\rangle_{eff} &\sim -i |zx, \uparrow\rangle + |yz, \uparrow\rangle - |xy, \downarrow\rangle \end{aligned}$$

Kitaev Materials

- Kitaev interactions can actually be realized in materials

Ingredients:

d-orbitals
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Interactions



**Spin-orbit entangled
Mott Insulators!**

$$j_{eff} = 1/2$$

$$\begin{array}{l} \text{---} |\uparrow\rangle_{eff} \\ \text{---} |\downarrow\rangle_{eff} \end{array}$$

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Kitaev Materials

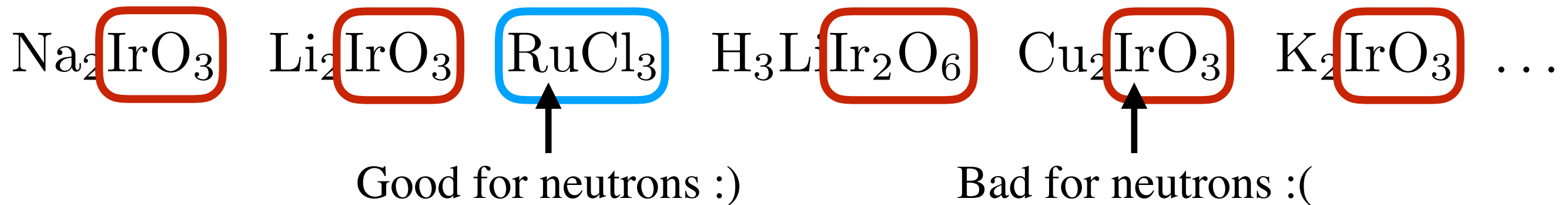
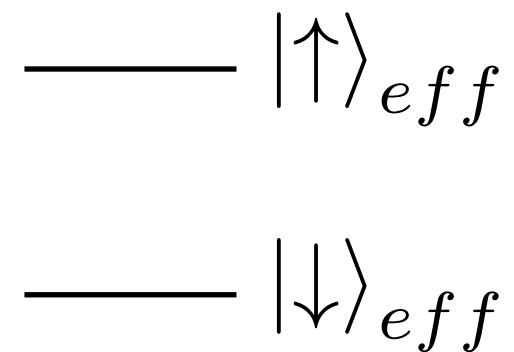
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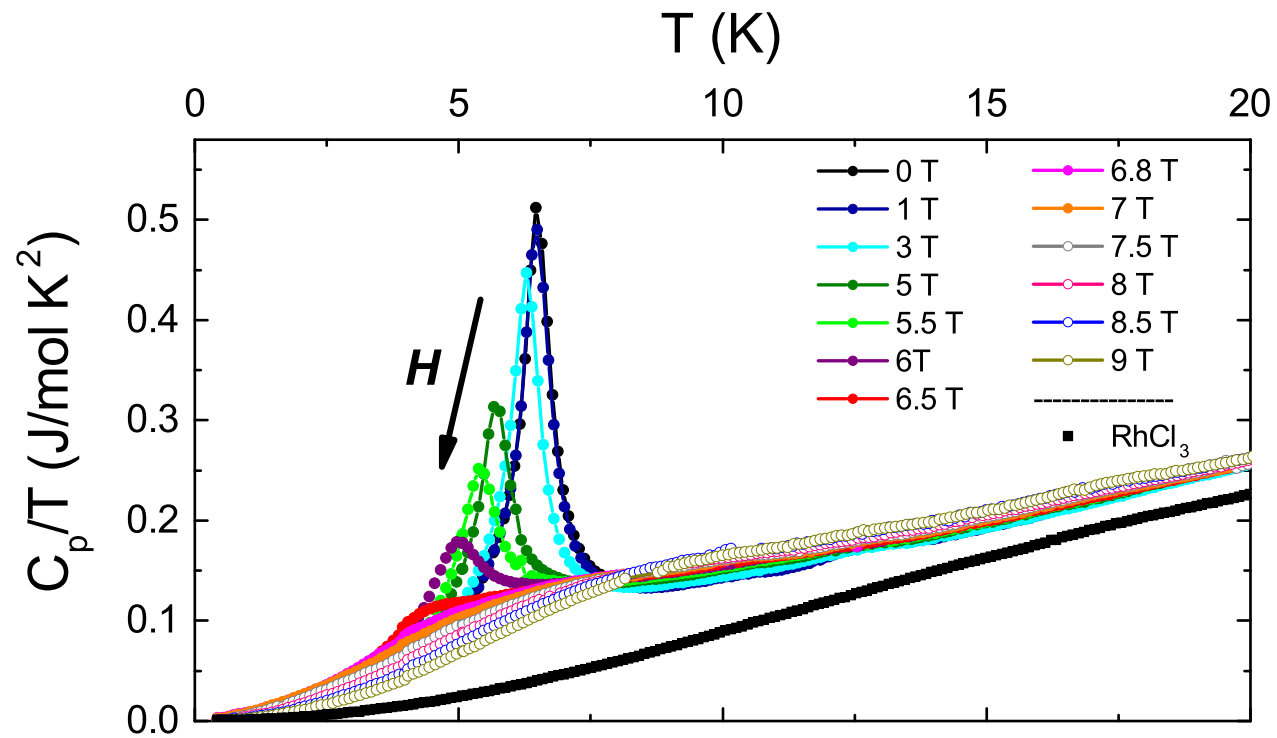
d-orbitals
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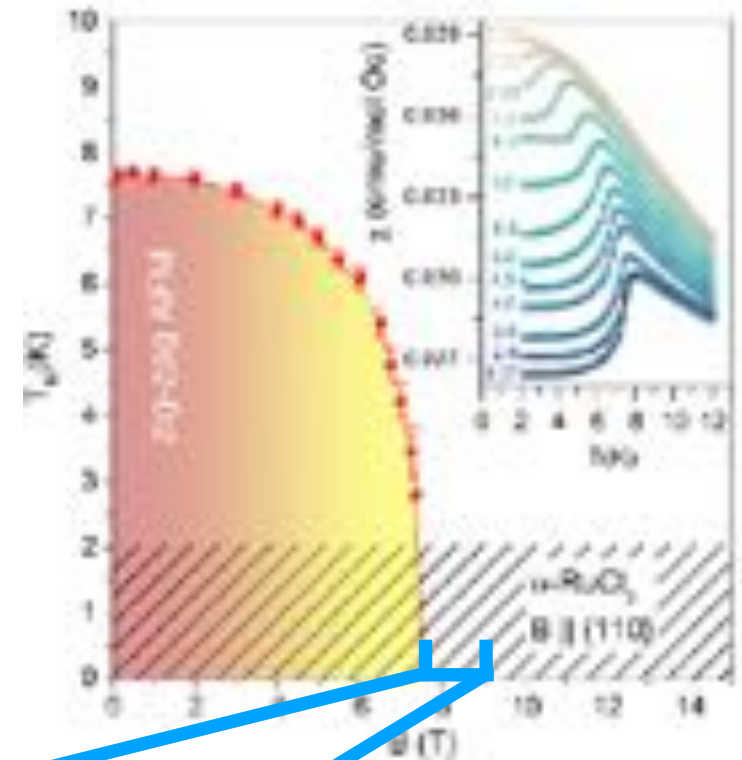
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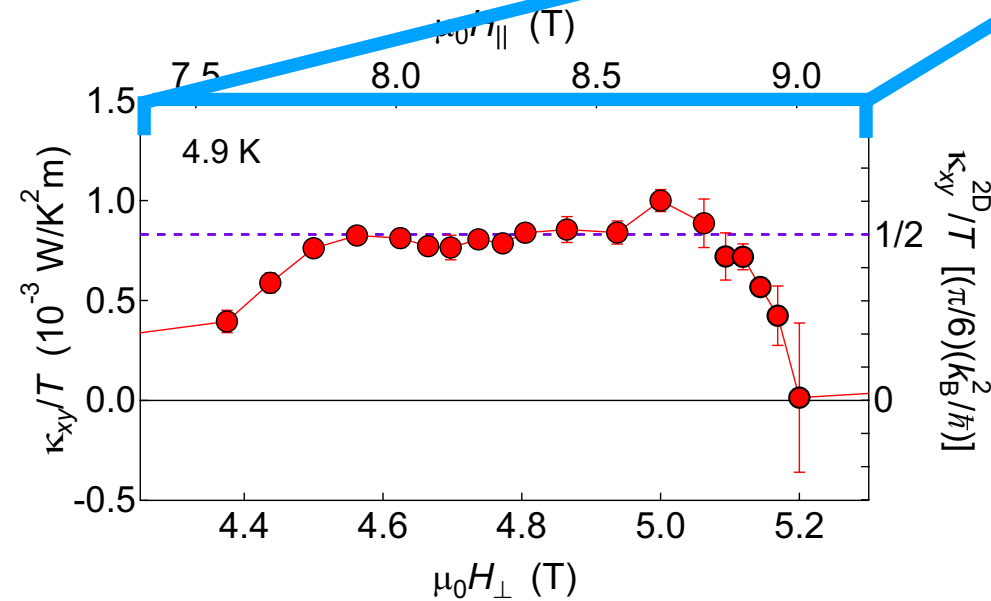
RuCl₃ in Field



A. U. B. Wolter et al., PRB **96**, 041405(R) (2017)



A. Banerjee et al., npj Quantum Mater. **3**, 8 (2018)



Y. Kasahara et al., Nature **559**, 227-231 (2018)

Na₂IrO₃

Li₂IrO₃

RuCl₃

H₃LiIr₂O₆

Cu₂IrO₃

K₂IrO₃ ...

Motivation

1. Before we try to understand the complicated materials:

First we should try to understand just the
pure Kitaev model in a magnetic field

2. From a theory perspective:

Natural to ask what happens to Kitaev's
quantum spin liquid in a magnetic field

Adding a Magnetic Field

- What happens if we add a magnetic field?

$$H = \pm K \sum_{\langle i,j \rangle \in \gamma} S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

FM - Kitaev
Coupling $-K$



$h \ll K$
???

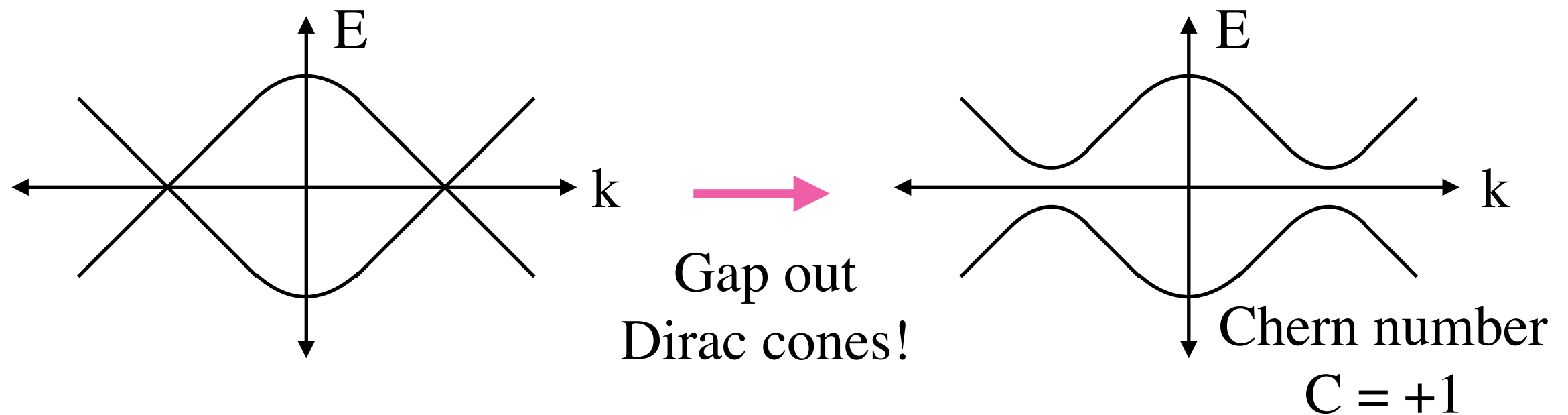
$h \gg K$
Polarised along
field direction

AFM - Kitaev
Coupling $+K$



Kitaev's Gapless QSL in a [111] Field

- Kitaev showed, using perturbation theory, that a [111] magnetic field can:



- We have a gapped insulator of Majorana's with $C = +1$
- Single, chiral Majorana edge mode with half-integer quantised thermal Hall conductance
- In terms of spins we have a gapped quantum spin liquid (KSL)

Adding a Magnetic Field

- What happens if we add a magnetic field?

$$H = \pm K \sum_{\langle i,j \rangle \in \gamma} S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

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$h \ll K$

Gapped Quantum
Spin Liquid

???

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Polarised along
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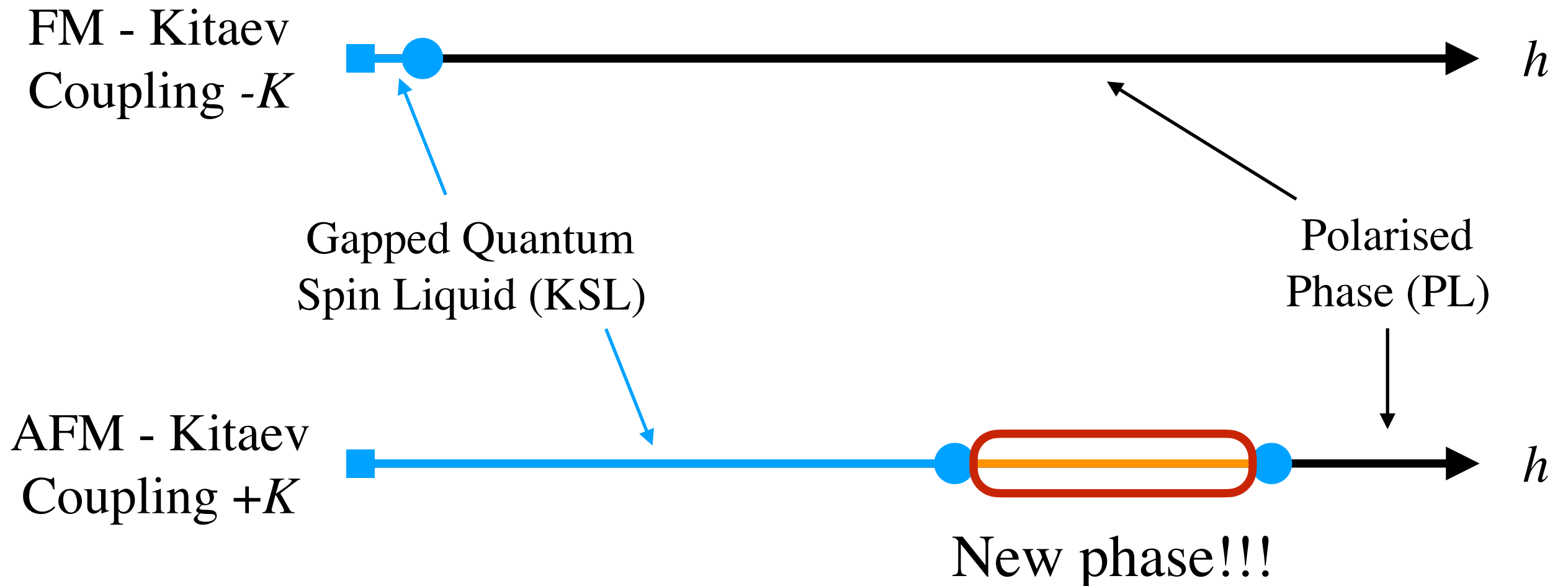
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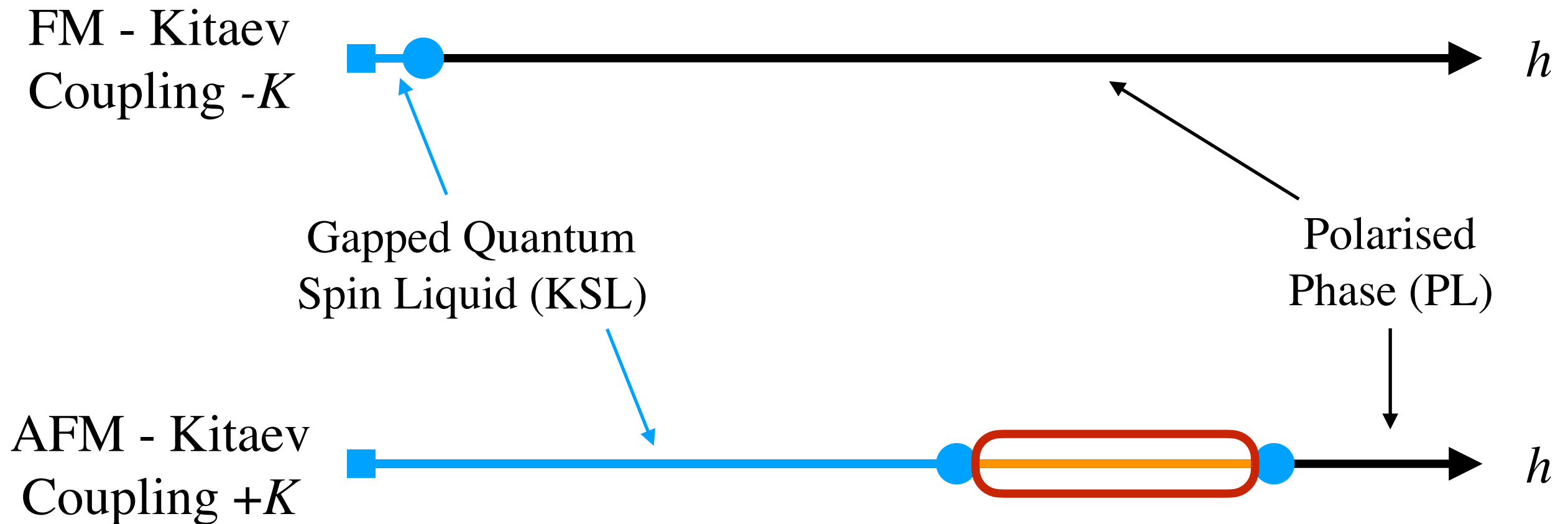
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Adding a Magnetic Field

- What happens if we add a magnetic field?

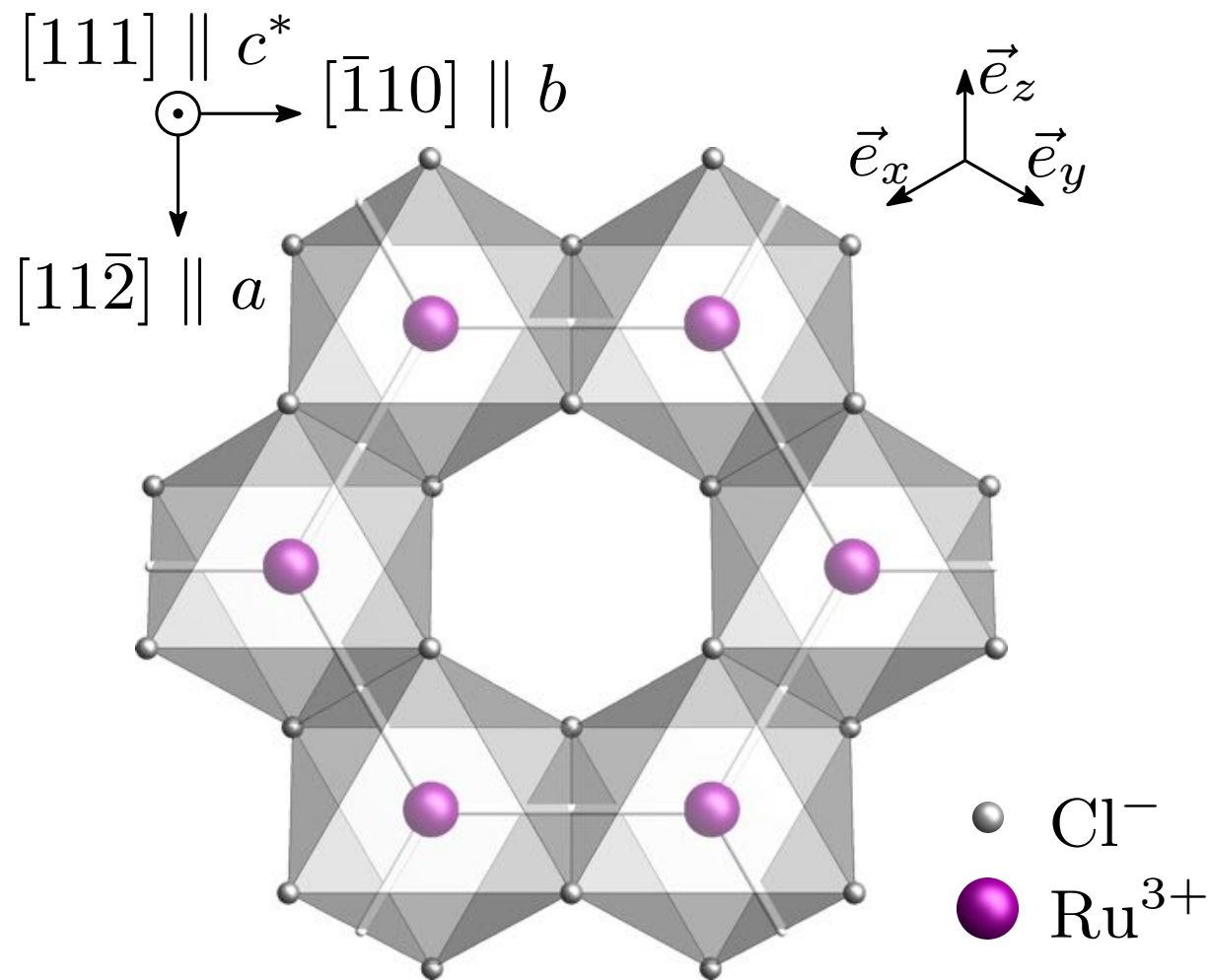
$$H = \pm K \sum_{\langle i,j \rangle \in \gamma} S_i^\gamma S_j^\gamma - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$



$\mathbf{h} \parallel [111]$ Direction:

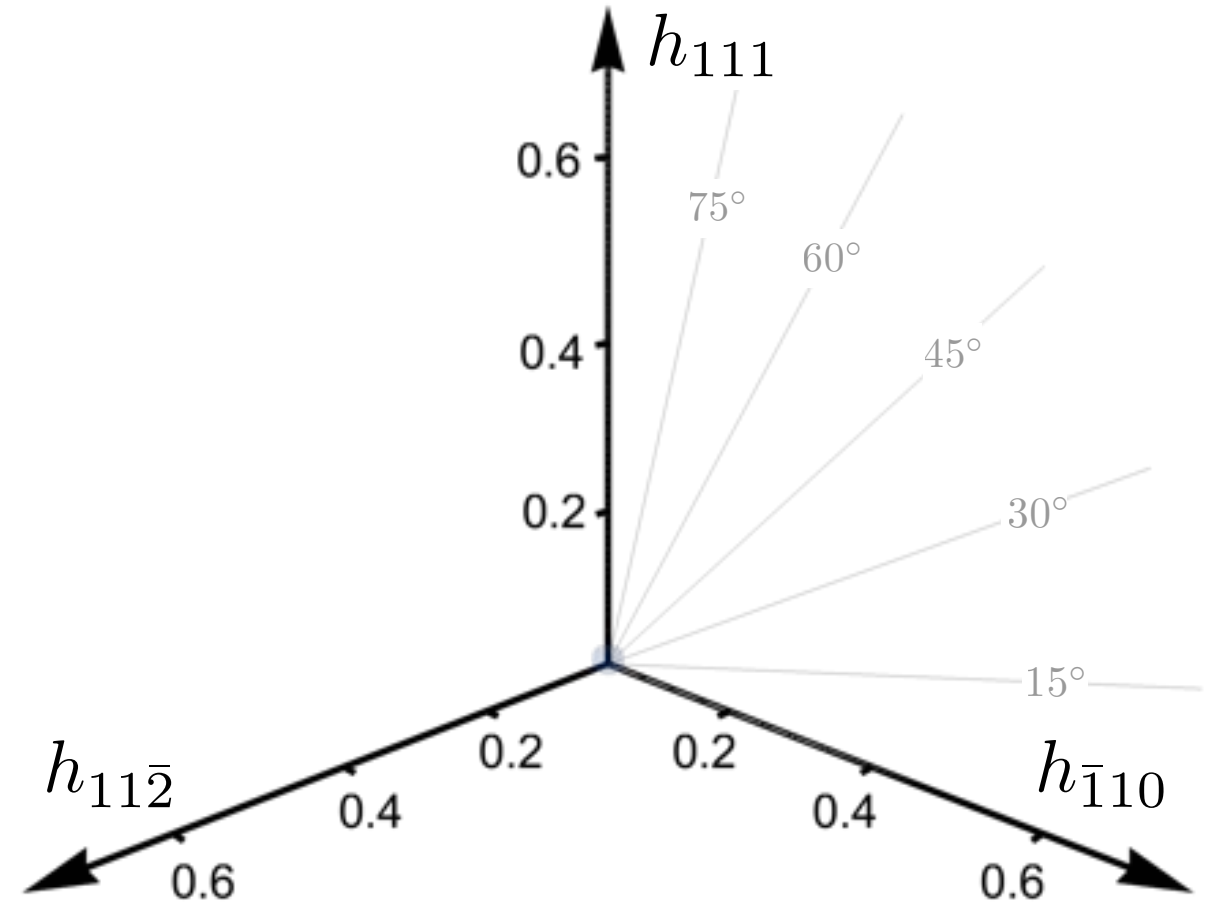
- S. Fey, MSc Thesis (2013)
- Z. Zhu et al., PRB **97**, 241110(R) (2018)
- M. Gohlke et al., PRB **98**, 014418 (2018)

Phase Diagrams in Tilted Magnetic Fields



L. Janssen et al., PRB **96**, 064430 (2017)

Out-of-plane field direction (c axis)

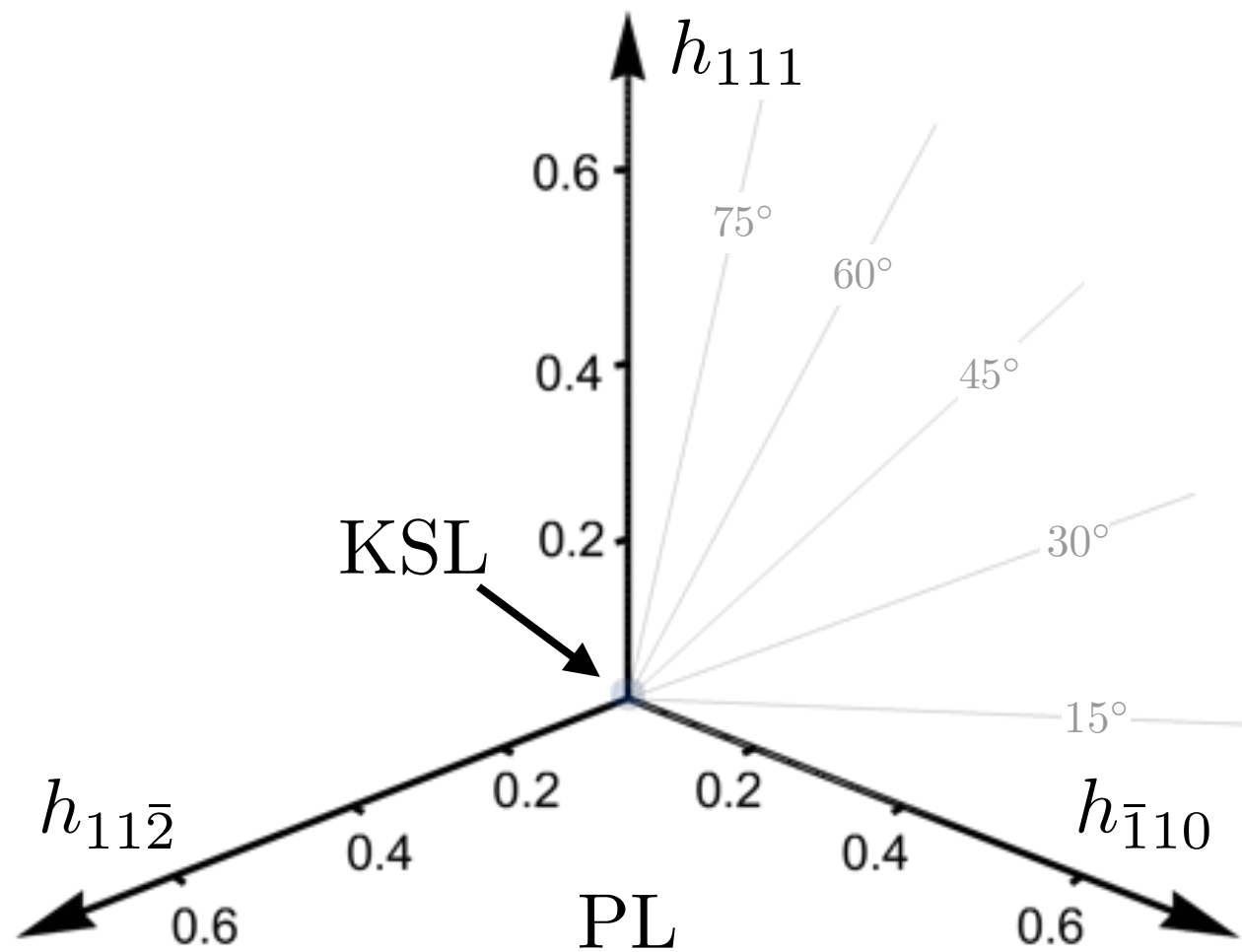


In-plane field directions (a, b axes)

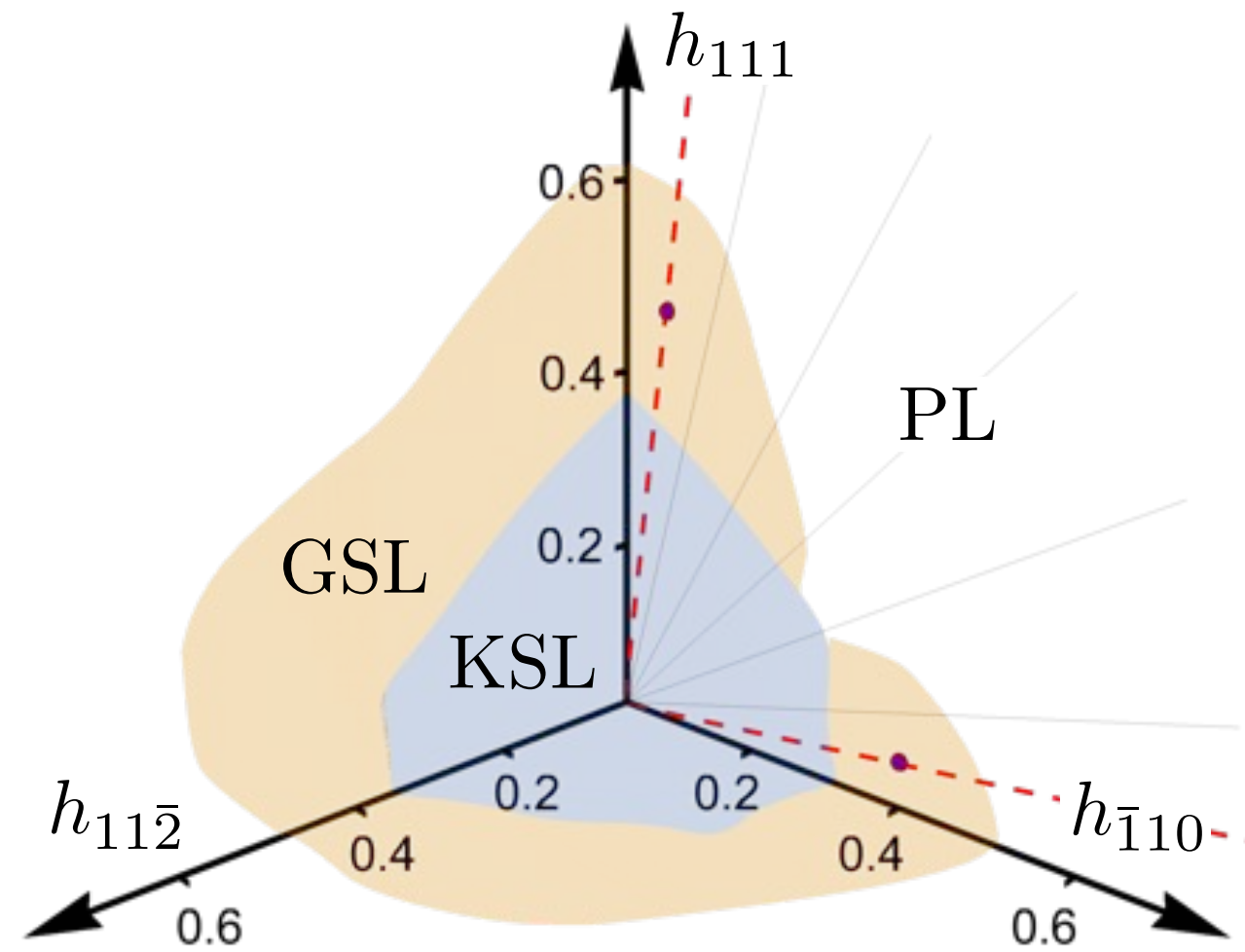
Phase Diagrams in Tilted Magnetic Fields

Uniform \mathbf{h}

FM Kitaev Coupling



AFM Kitaev Coupling



KSL = Kitaev Spin Liquid
PL = Polarised phase (trivial)

GSL = Gapless Spin Liquid

Phase Diagrams in Tilted Magnetic Fields

Uniform h

Q. What is the nature of the KSL phase in a magnetic field?

Q. Why is the critical field so different?

Q. What is the nature of the intermediate “GSL” phase?

KSL = Kitaev Spin Liquid
PL = Polarised phase (trivial)

GSL = Gapless Spin Liquid

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Gapped KSL

- From Kitaev's perturbative arguments we know the phase should exhibit "Ising Anyon Topological Order"
- Can be identified by the modular S -matrix:

$$S_{ab} \sim \langle \text{Diagram} \rangle$$

Info on quantum dimensions

$$S = \begin{pmatrix} 0.50 & 0.71 & 0.50 \\ 0.71 & 0.00 & -0.71 \\ 0.50 & -0.71 & 0.50 \end{pmatrix}$$

Theoretical Result

$$S = \begin{pmatrix} 0.46 & 0.74 & 0.47 \\ 0.71 & 0.04e^{-0.91i} & -0.70 \\ 0.49 & -0.67e^{0.02i} & 0.58e^{-0.13i} \end{pmatrix}$$

Numerical Result

Ising Anyon Topological Order!

Gapped KSL

- From Kitaev's perturbative arguments we know the phase should exhibit "Ising Anyon Topological Order"

- Can be identified by the modular S -matrix:

Q. What is the nature of the KSL phase in a magnetic field?



A. Gapped Quantum Spin Liquid with "Ising Anyons"

$$S = \begin{pmatrix} 0.46 & 0.74 & 0.47 \\ 0.71 & 0.04e^{-0.91i} & -0.70 \\ 0.50 & -0.71 & 0.50 \end{pmatrix} \quad S = \begin{pmatrix} 0.46 & 0.74 & 0.47 \\ 0.71 & 0.04e^{-0.91i} & -0.70 \\ 0.49 & -0.67e^{0.02i} & 0.58e^{-0.13i} \end{pmatrix}$$

Theoretical Result

Numerical Result

Ising Anyon Topological Order!

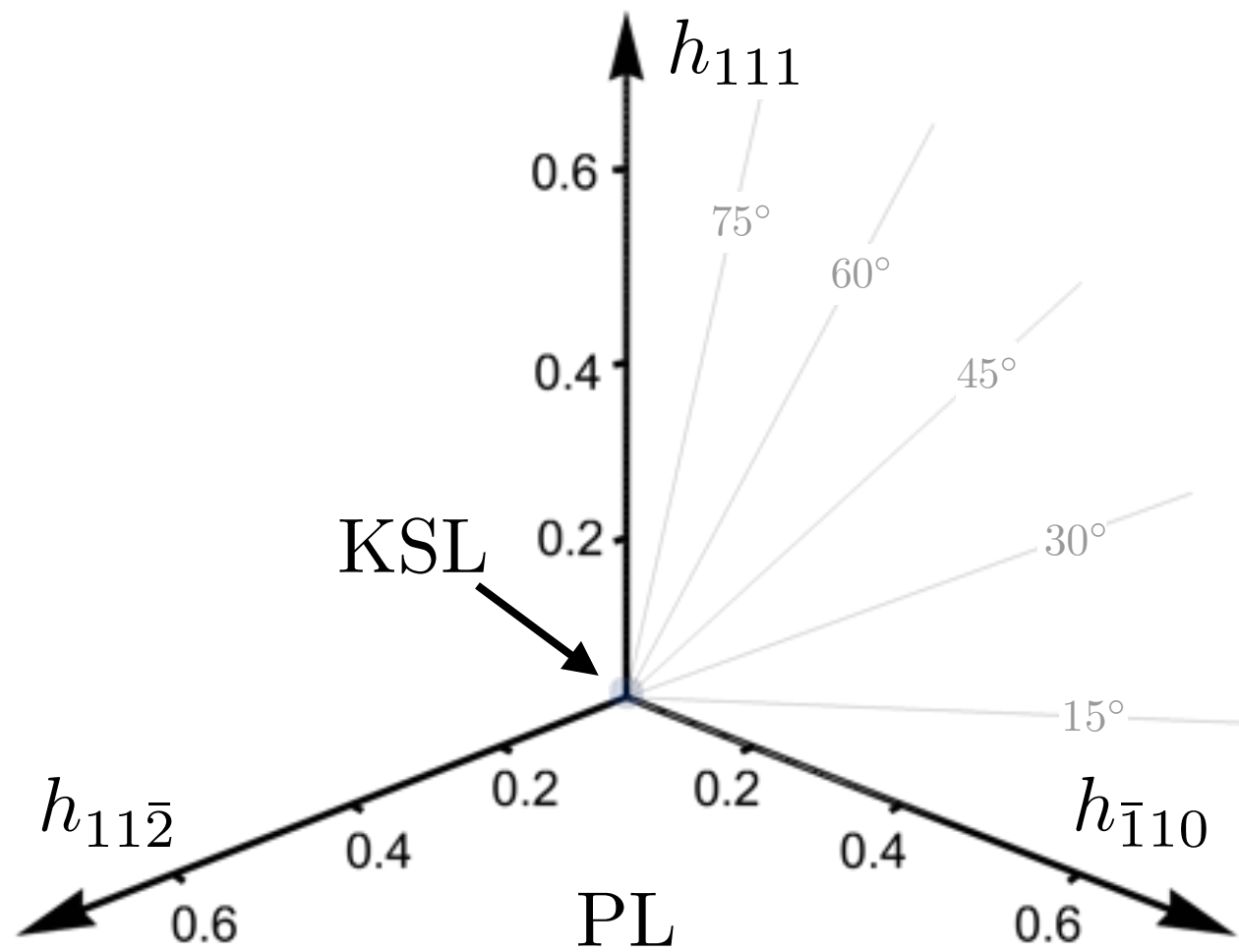
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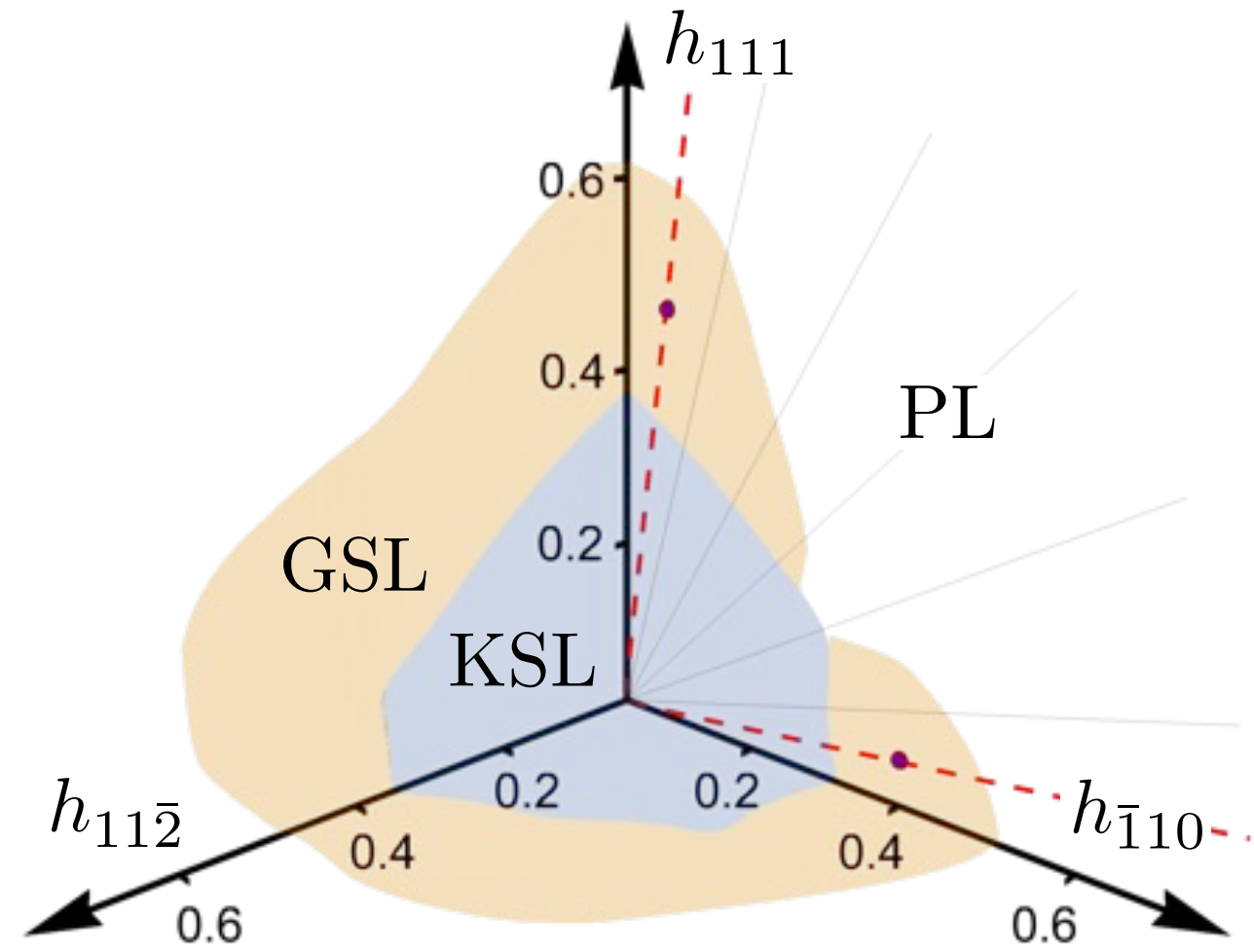
Critical Field for KSL

Uniform \mathbf{h}

FM Kitaev Coupling



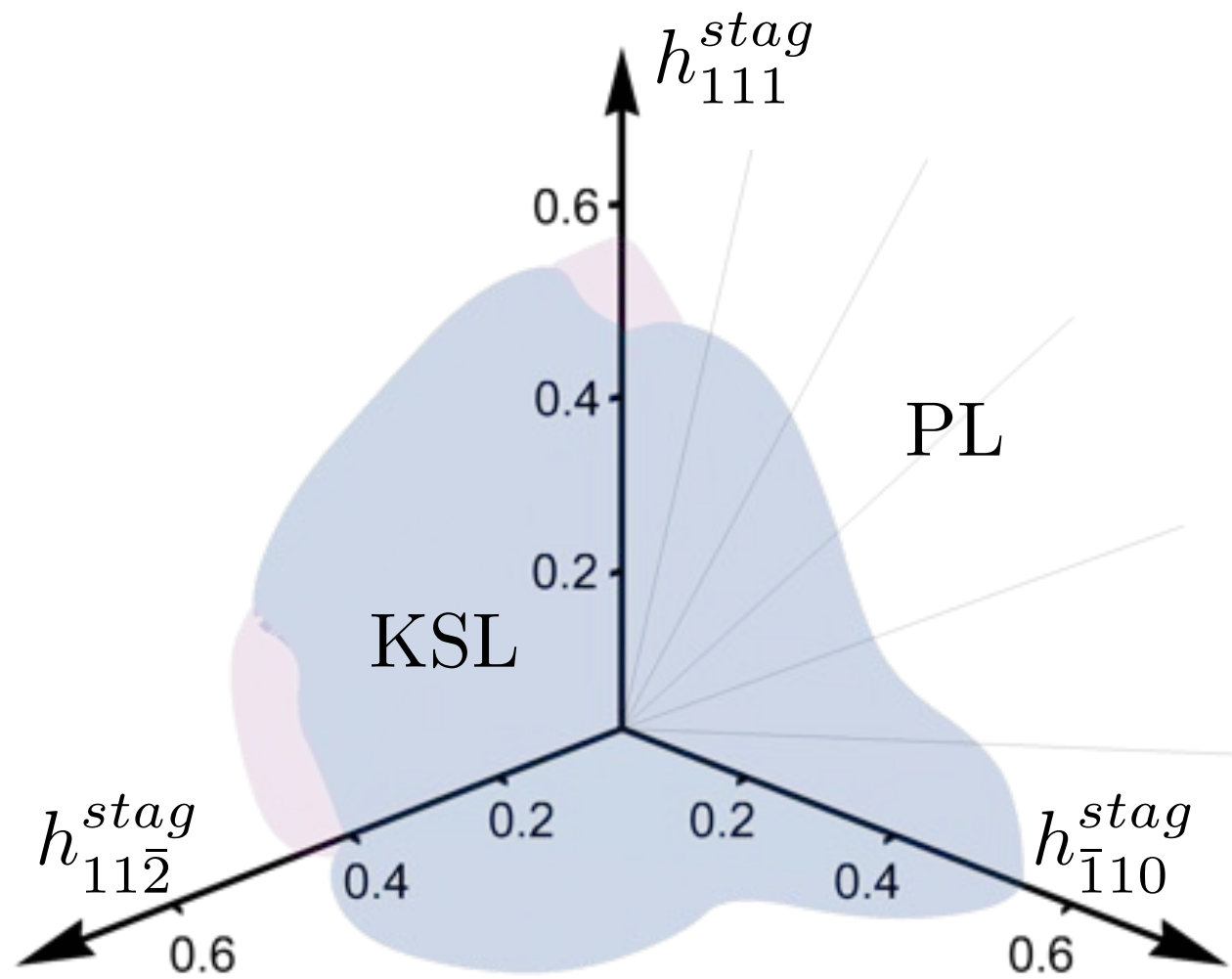
AFM Kitaev Coupling



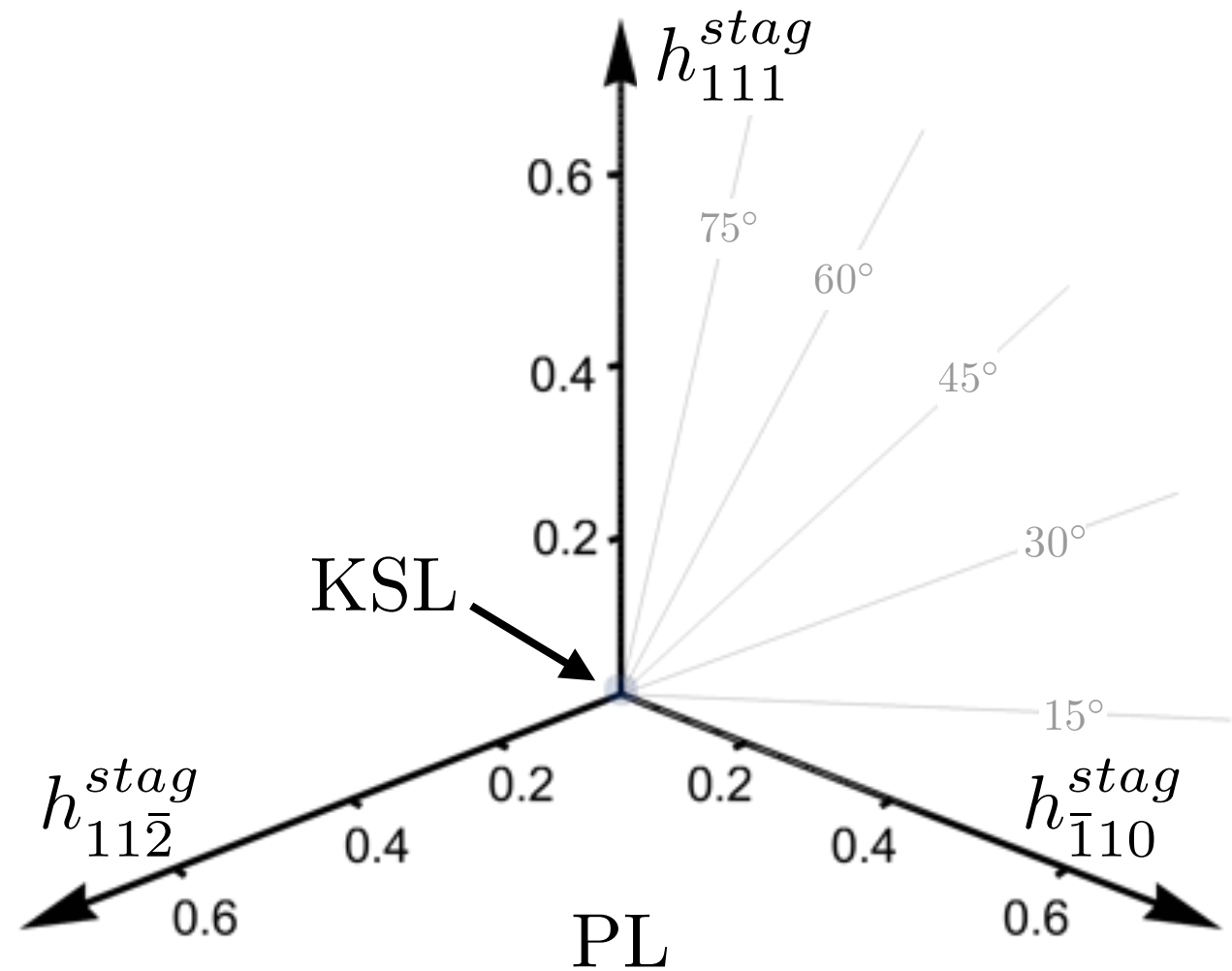
Critical Field for KSL

Staggered \mathbf{h}

FM Kitaev Coupling



AFM Kitaev Coupling



Critical Field for KSL

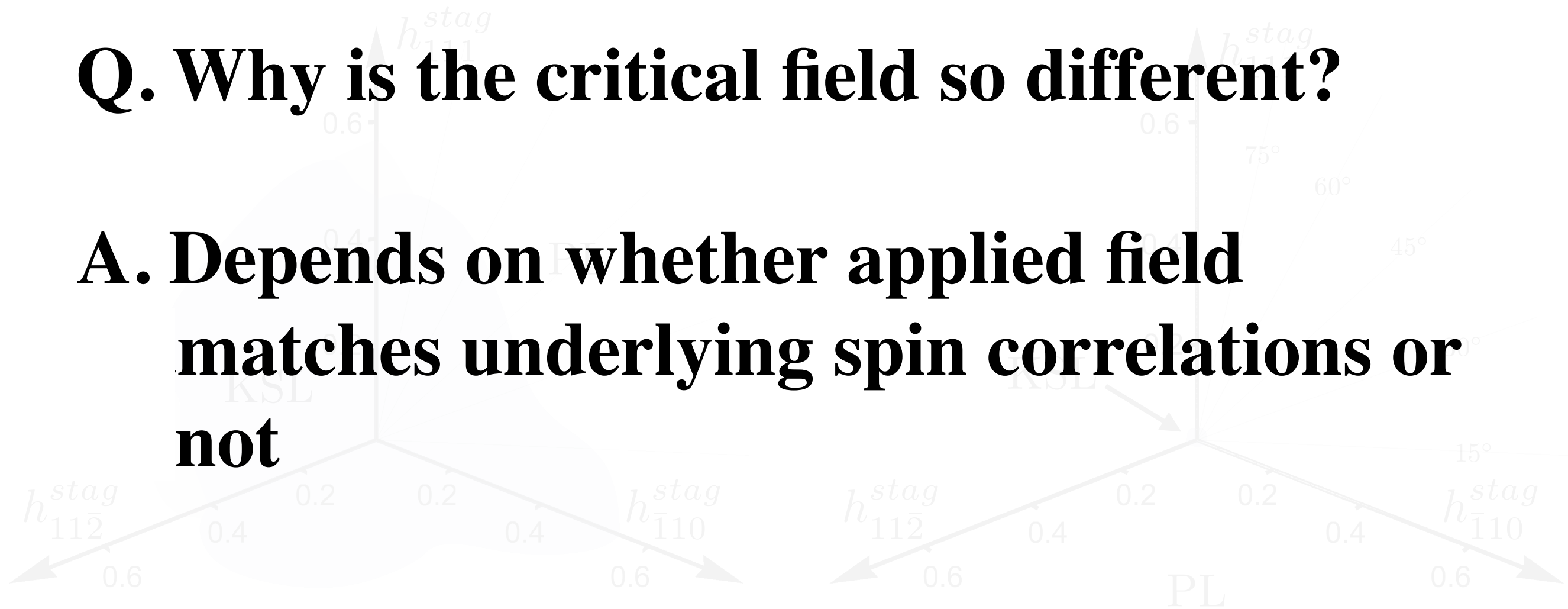
Staggered h

FM Kitaev Coupling

AFM Kitaev Coupling

Q. Why is the critical field so different?

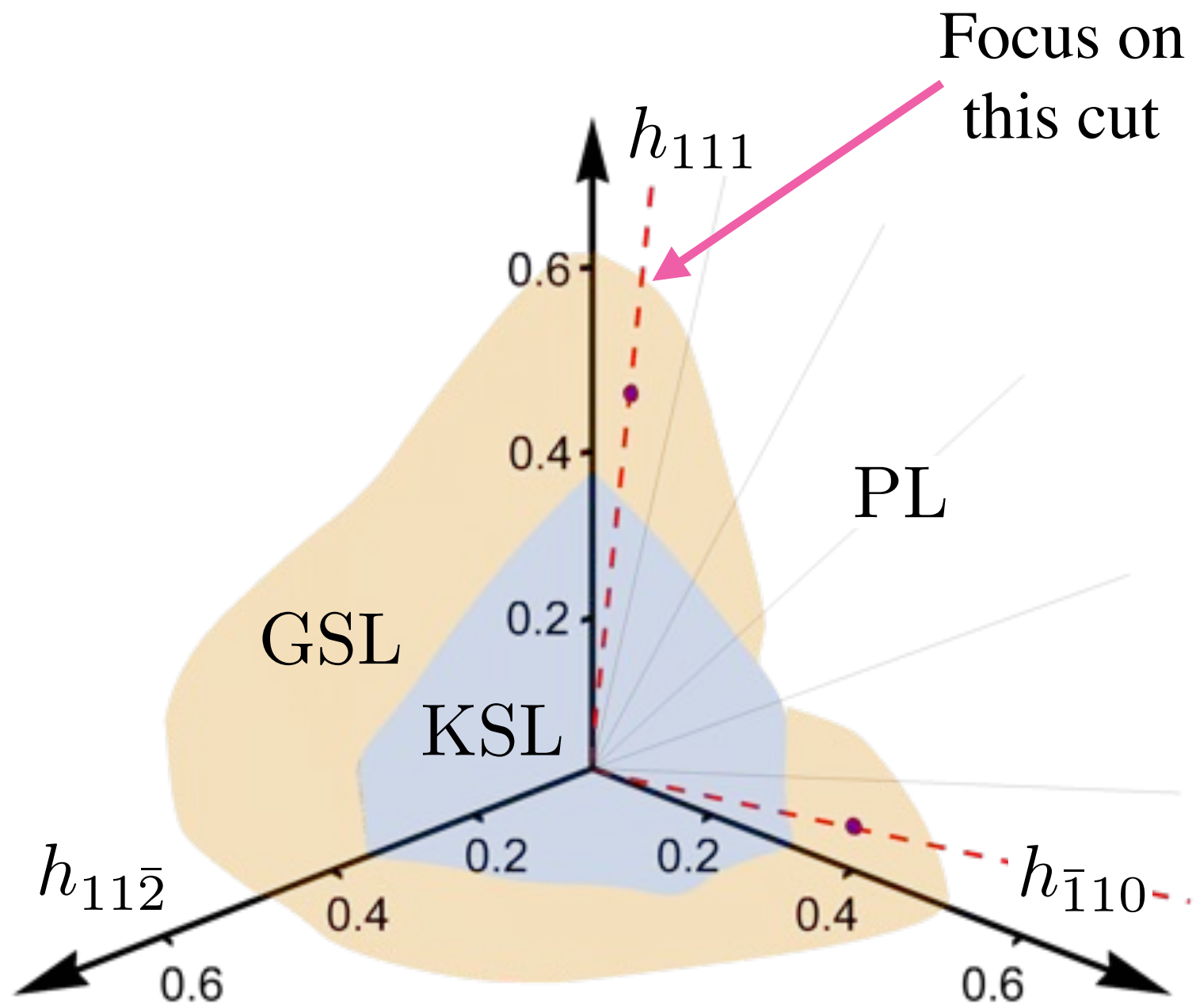
A. Depends on whether applied field matches underlying spin correlations or not



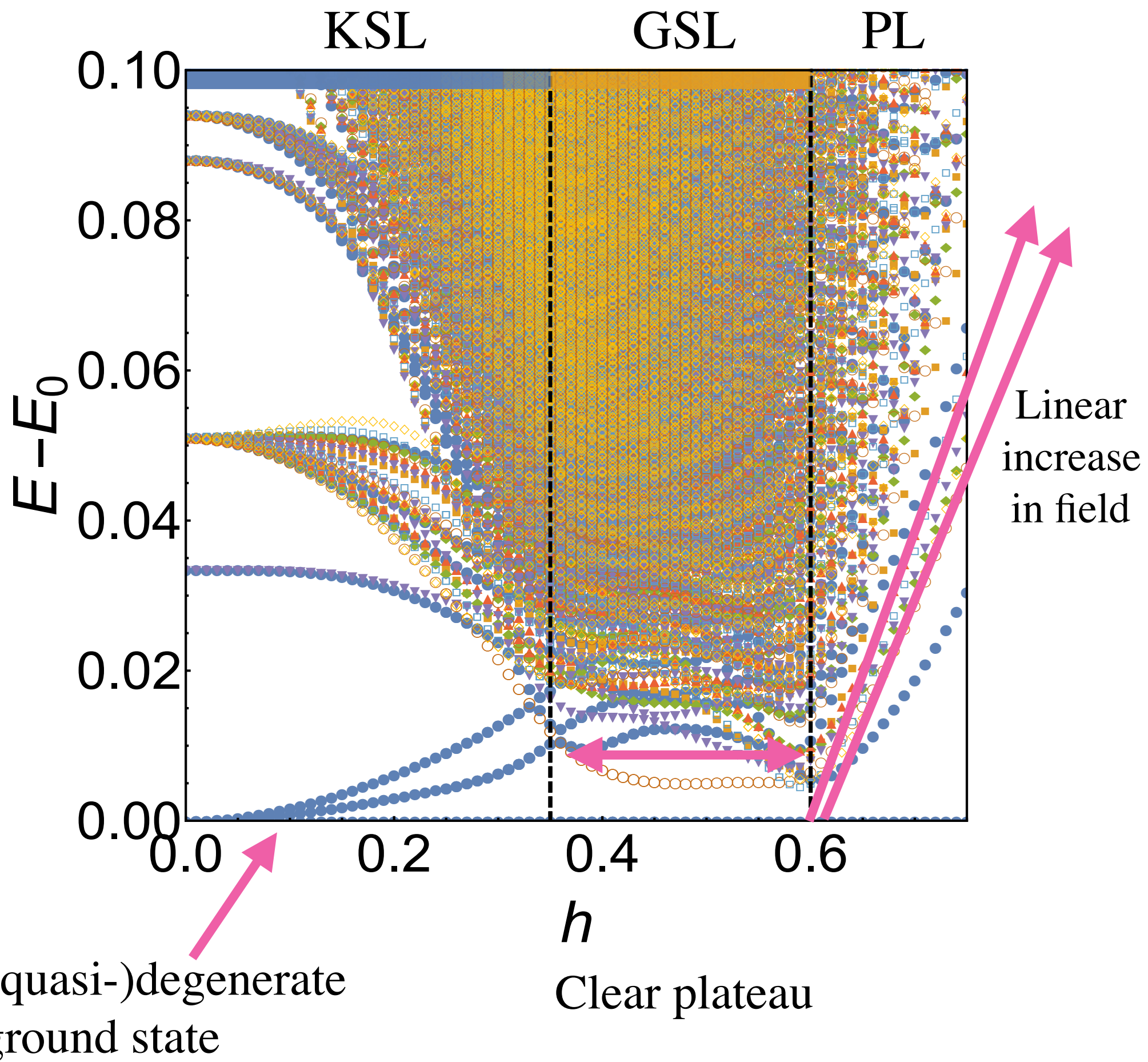
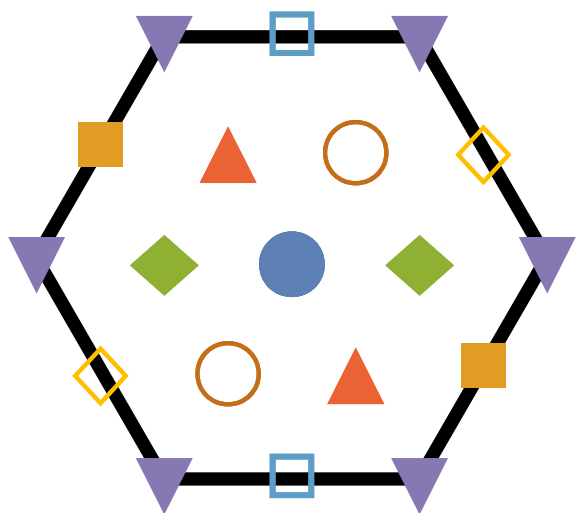
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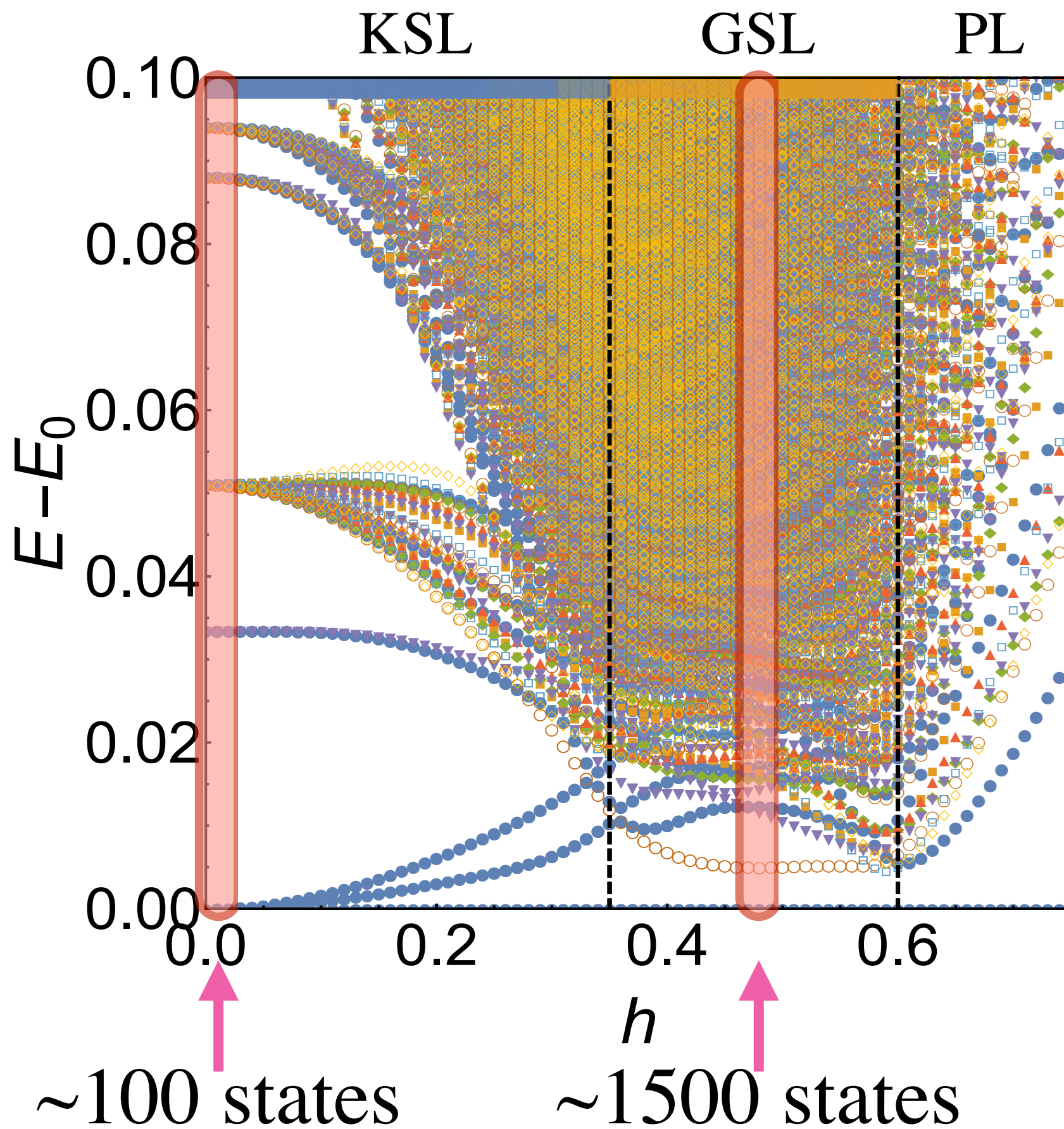
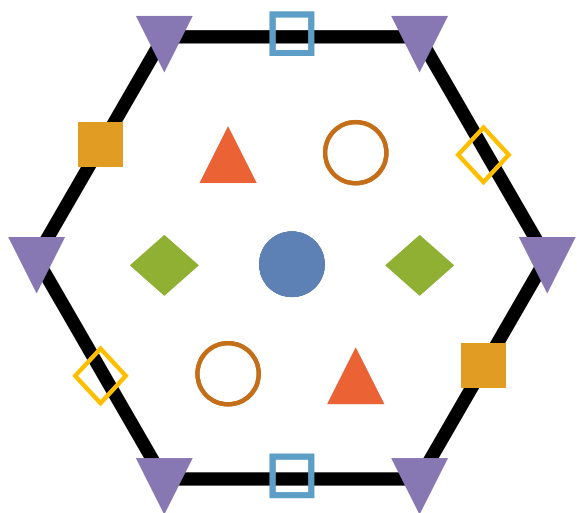
Nature of the GSL?



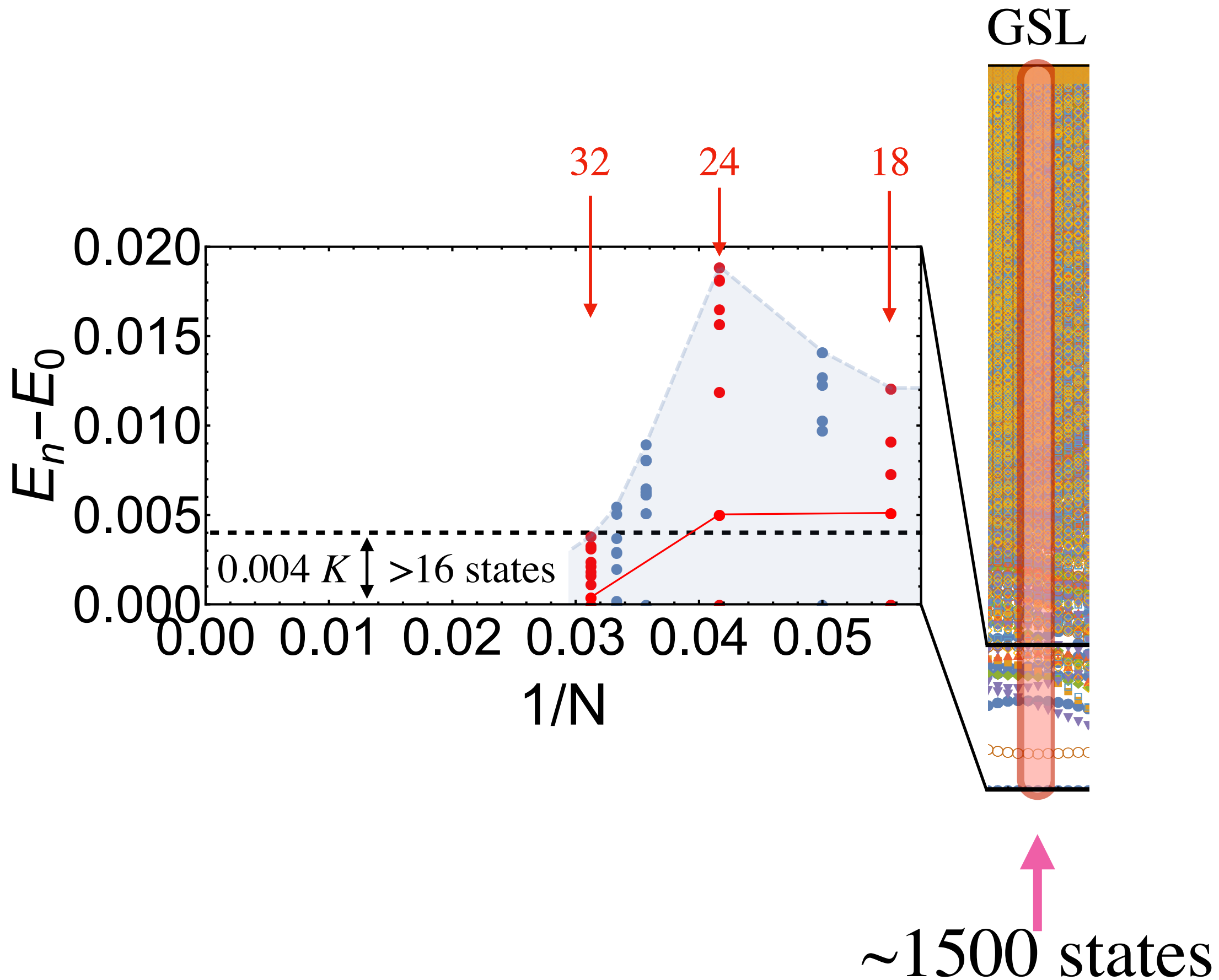
Low-Energy Spectrum



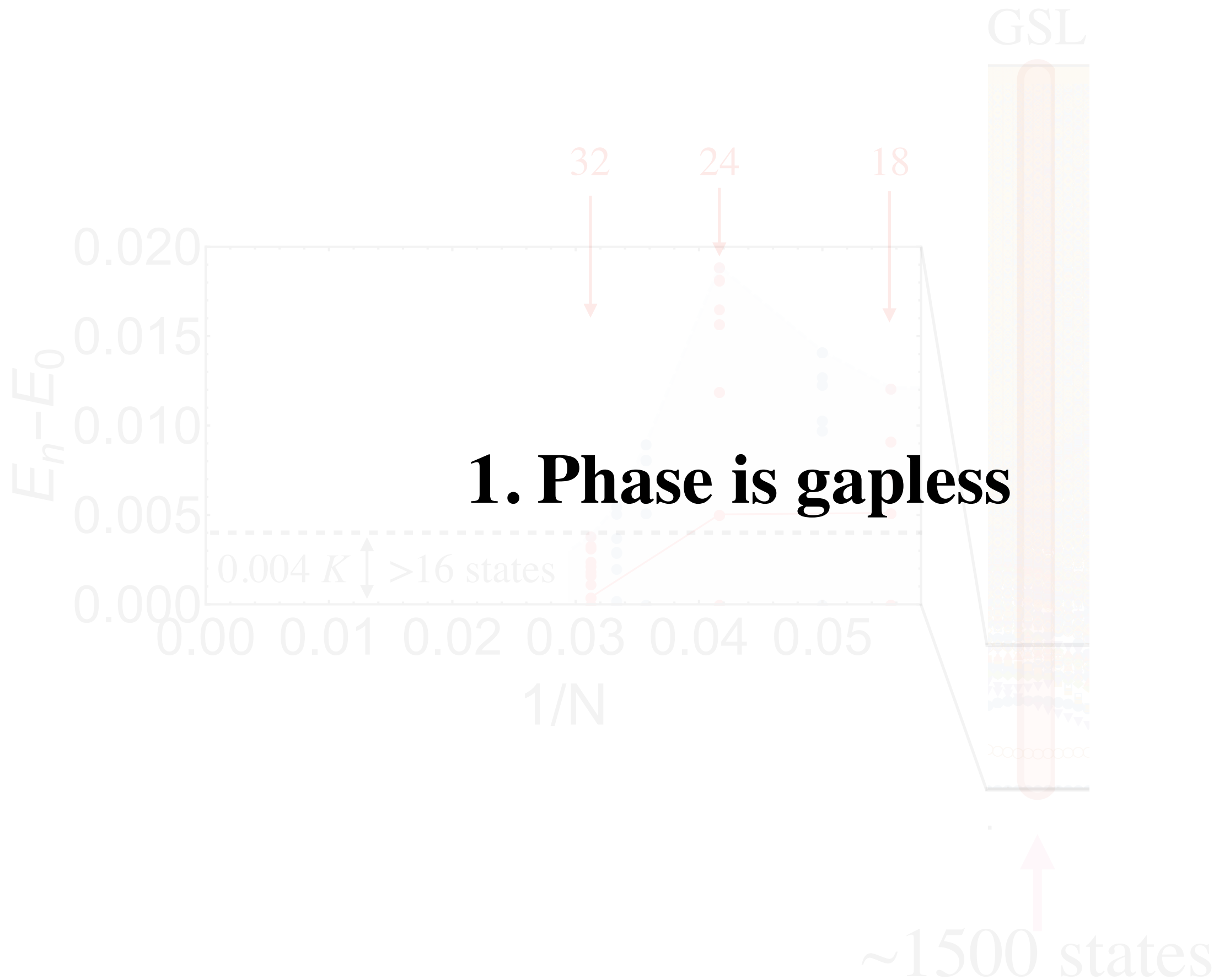
Low-Energy Spectrum



Low-Energy Spectrum



Low-Energy Spectrum

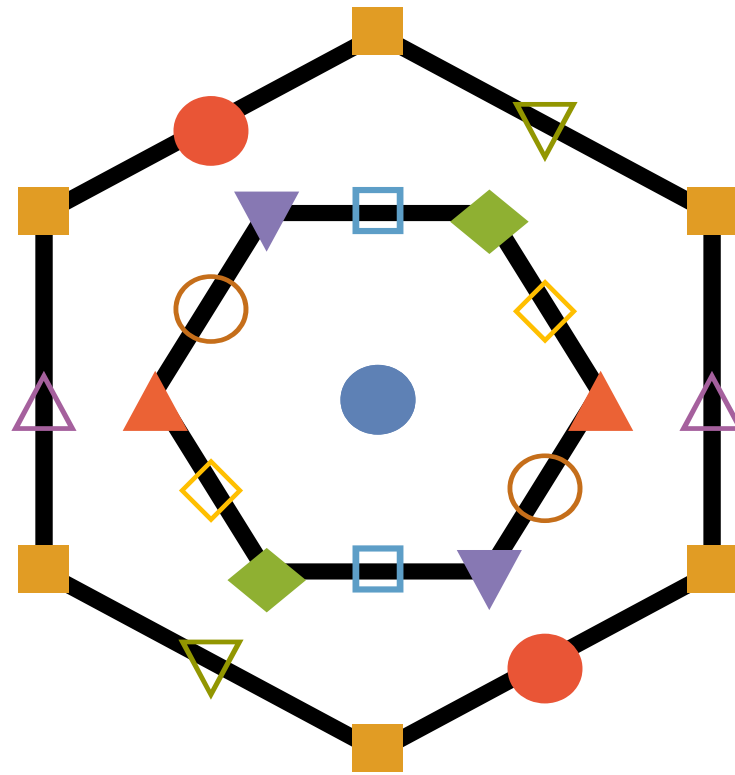


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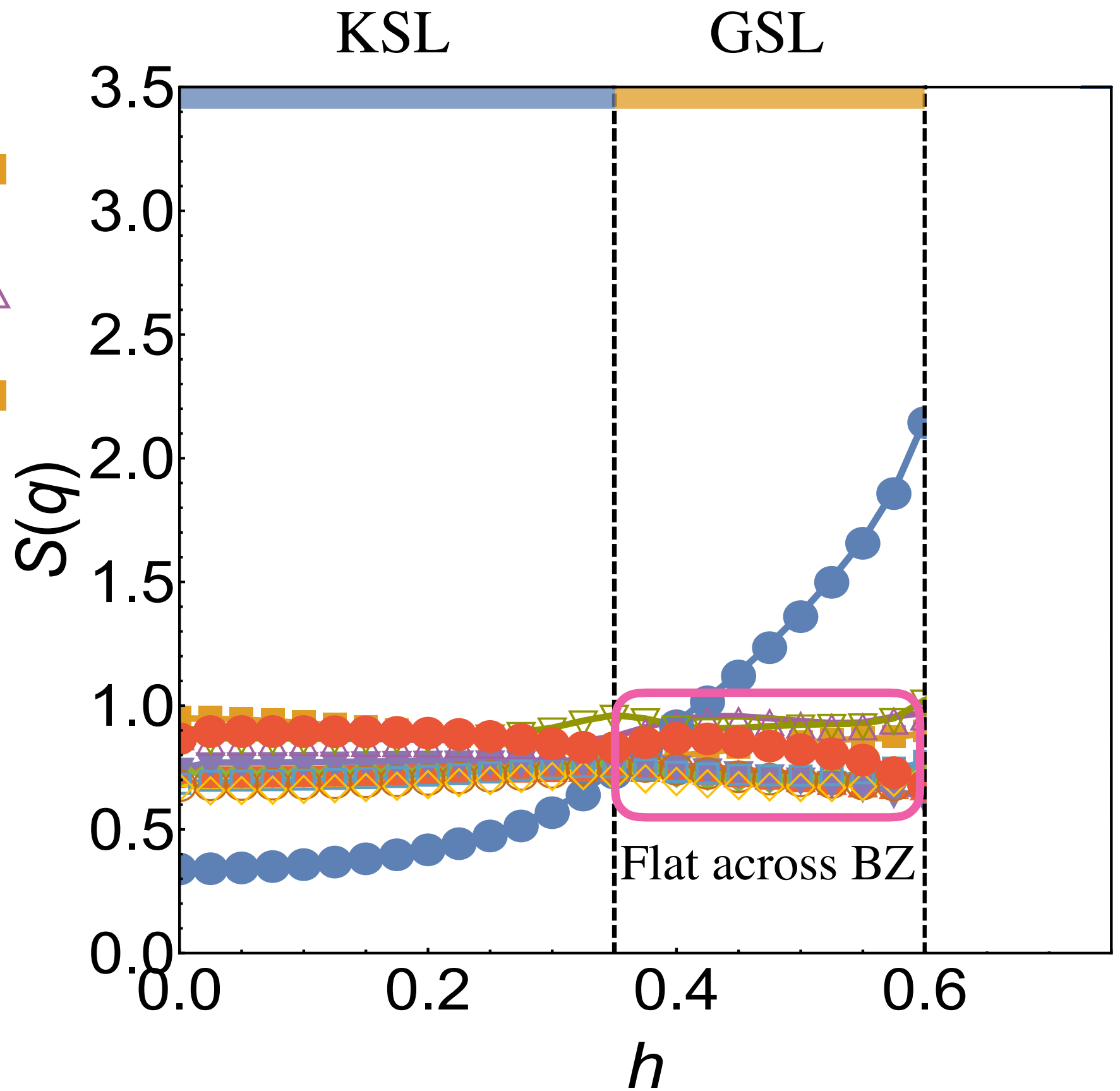
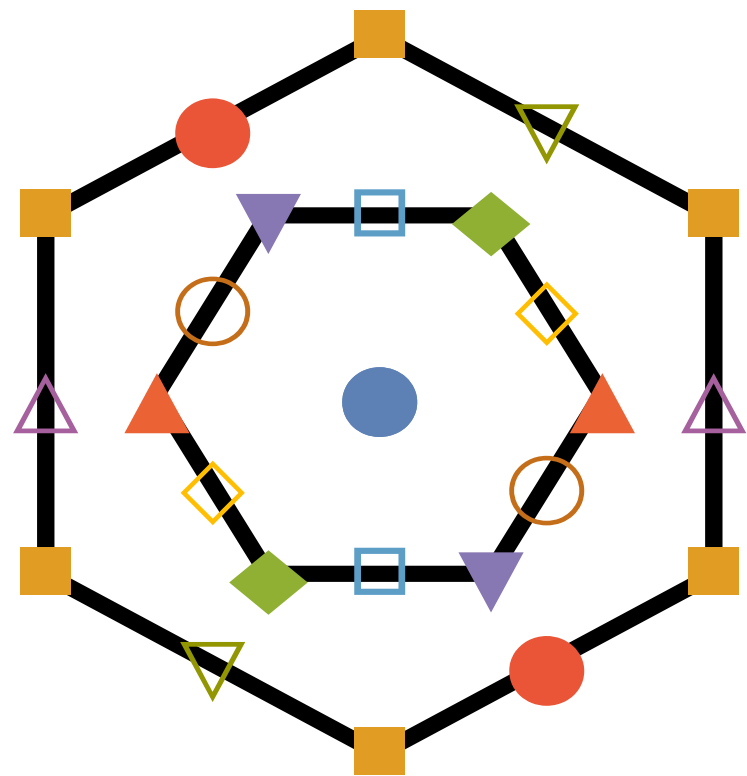
Static Spin Structure Factor

$$S(\mathbf{q}) = \left\langle \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j e^{i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \right\rangle$$

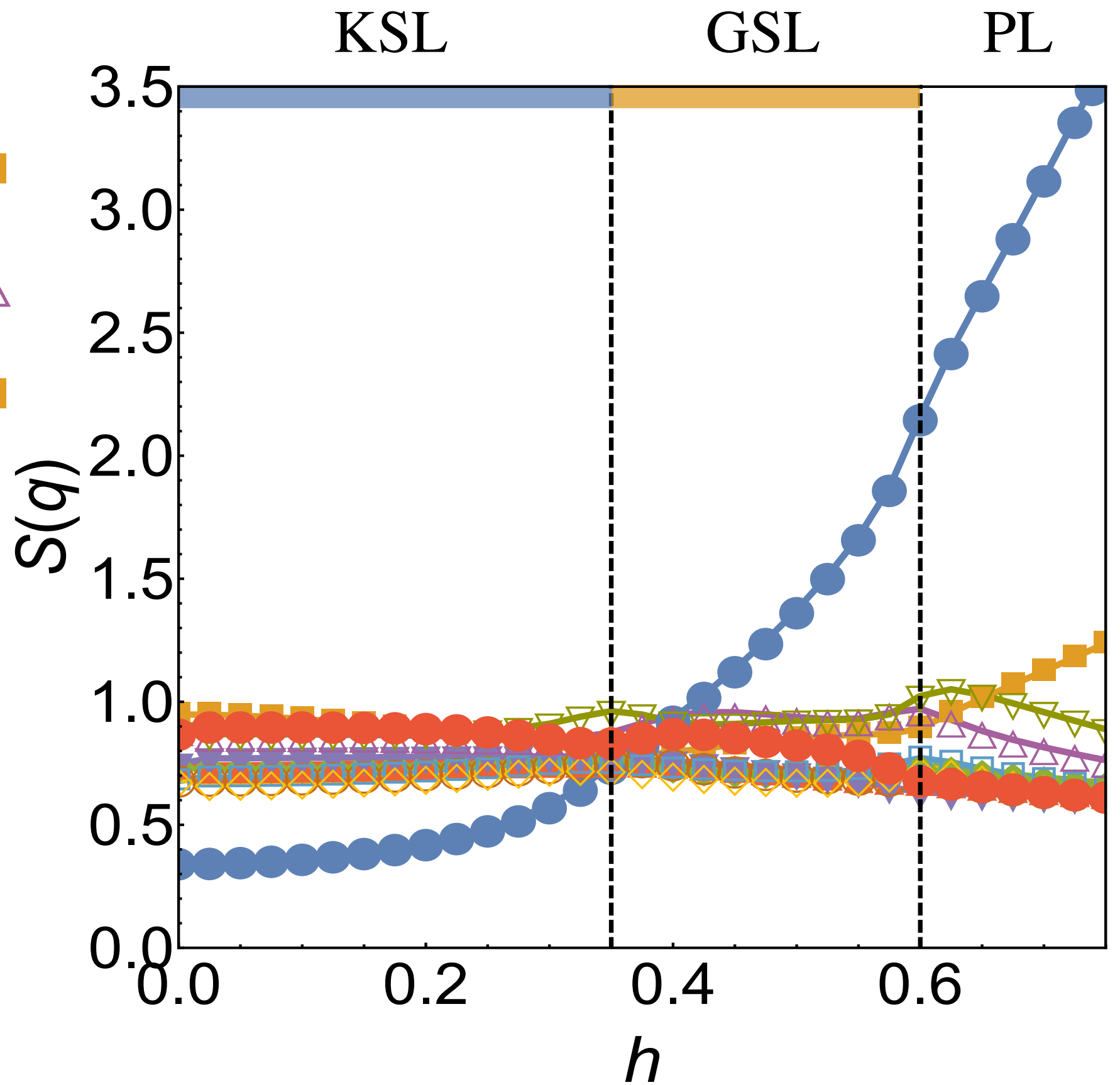
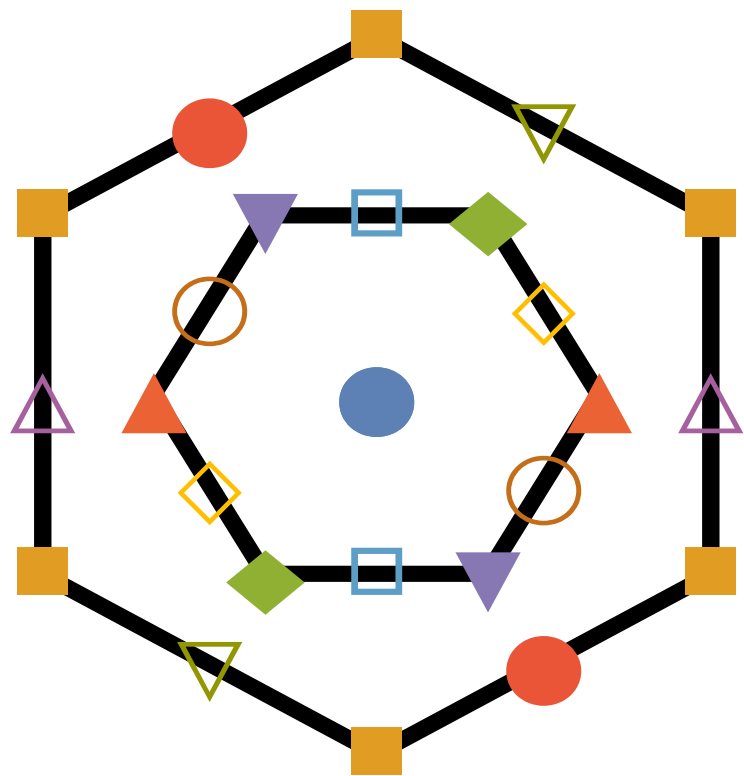


- FT of spin-spin correlation function
- Peaks in the static structure factor indicate magnetic ordering

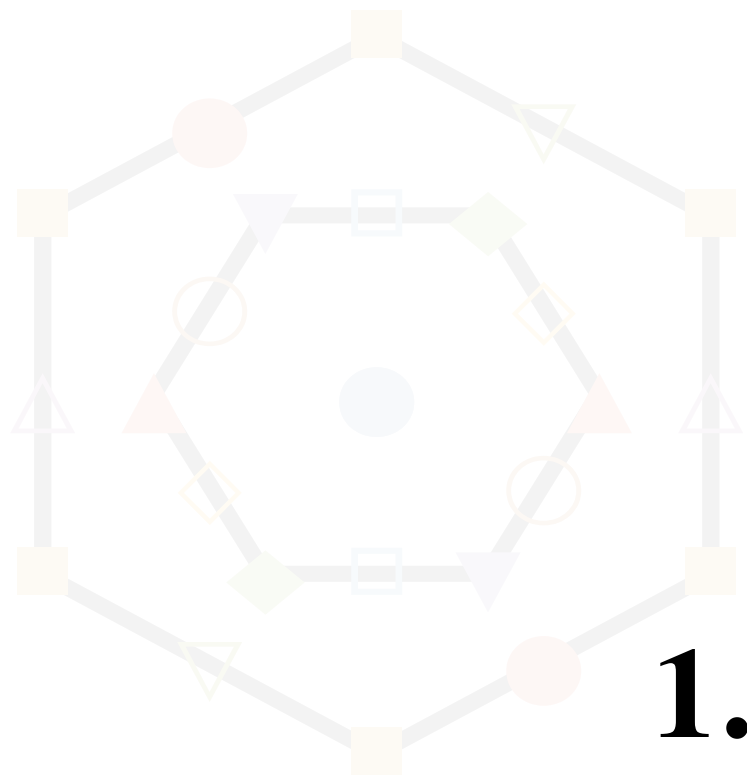
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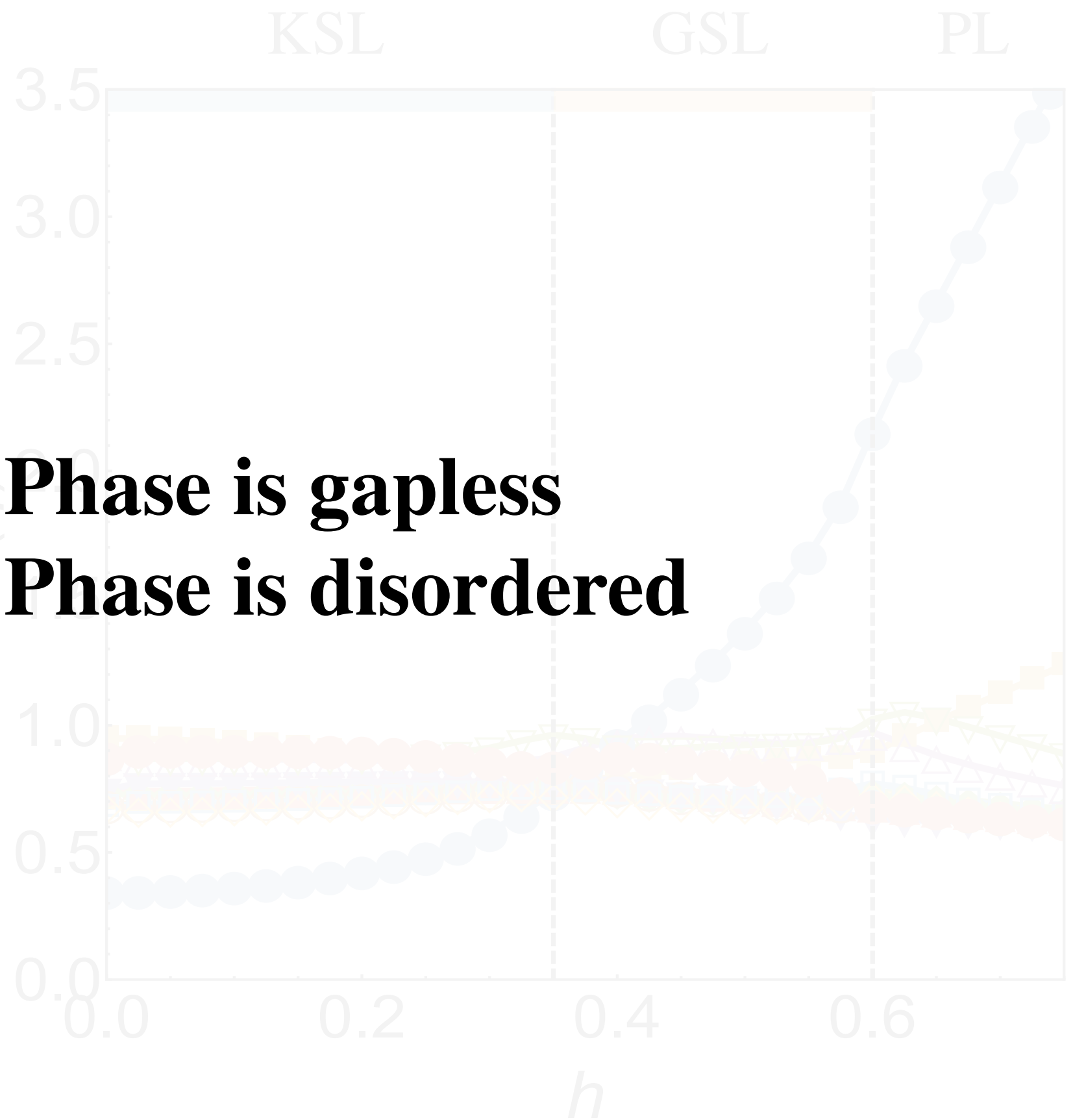
Static Spin Structure Factor



Static Spin Structure Factor



- 1. Phase is gapless**
- 2. Phase is disordered**



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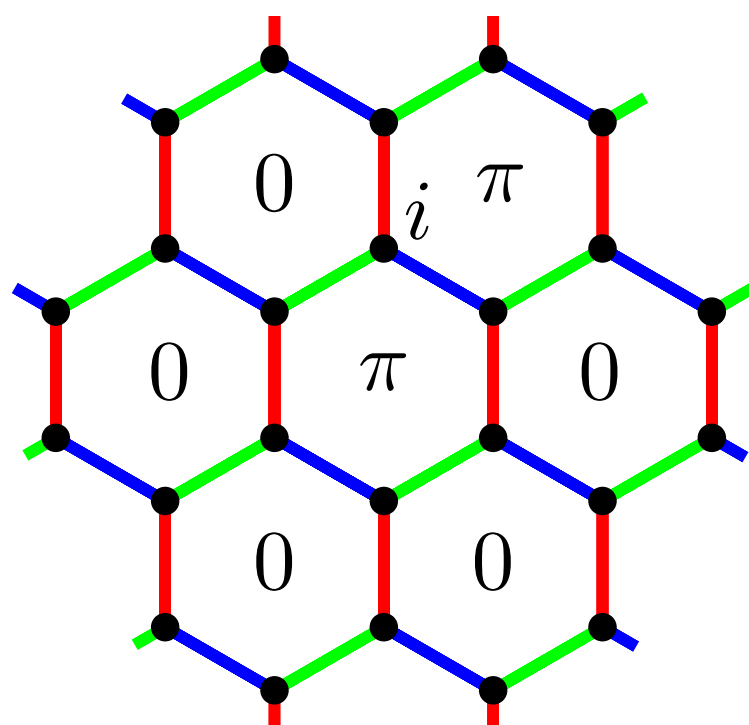
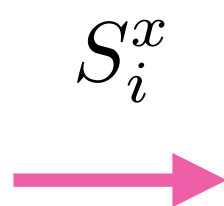
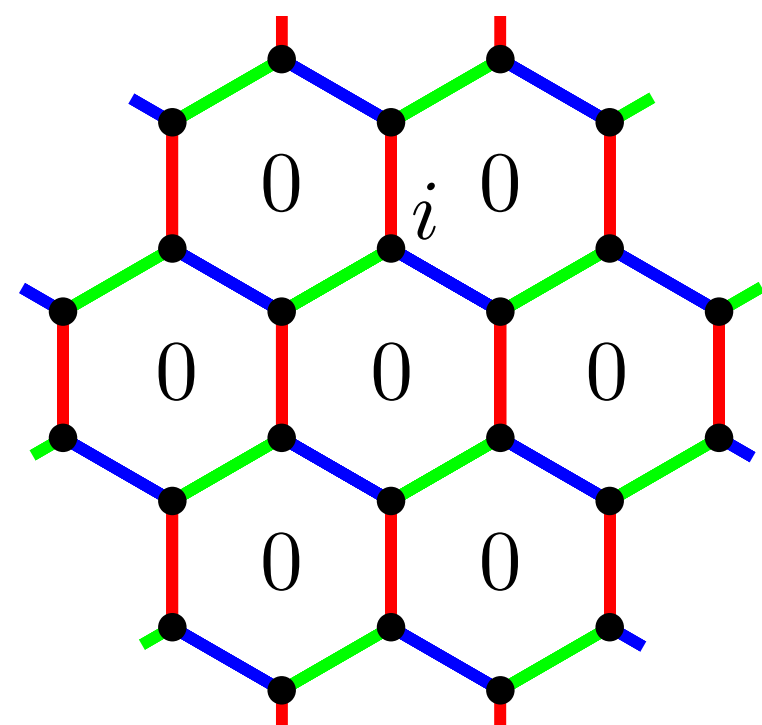
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Dynamical Spin Structure Factor

$$S^{\alpha\alpha}(\mathbf{Q}, \omega) = \sum_n |\langle n | S_{\mathbf{Q}}^{\alpha} | 0 \rangle|^2 \delta(\omega - (E_n - E_0))$$

$$\sum_i S_i^{\alpha} e^{i\mathbf{Q} \cdot \mathbf{r}_i} | 0 \rangle$$

$$S_i^{\alpha} | 0 \rangle$$



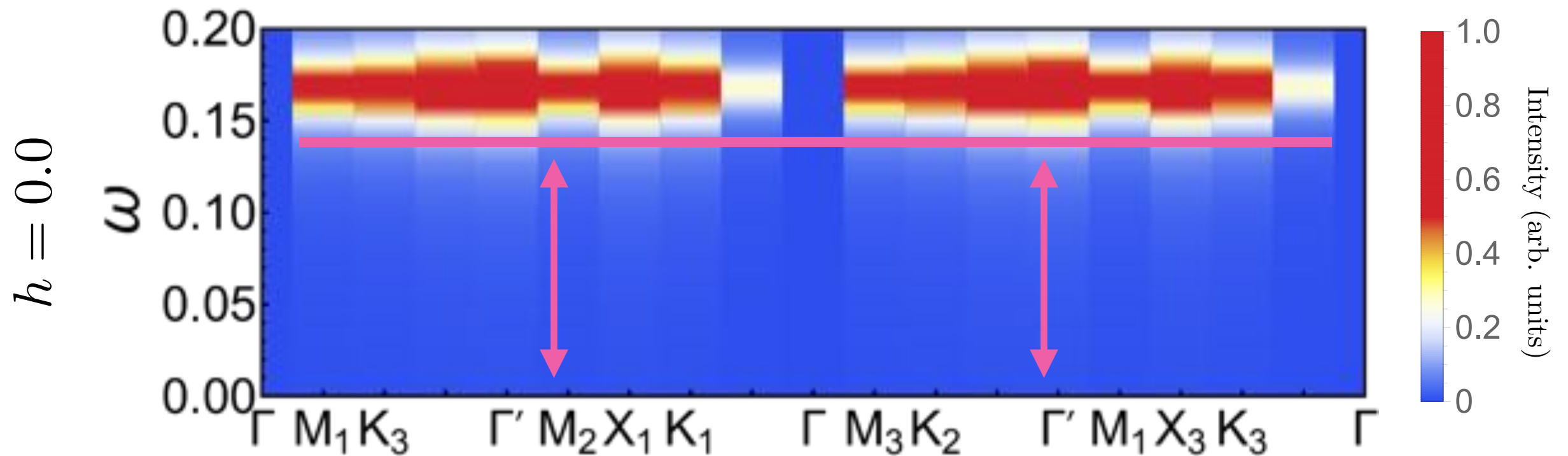
+ c Majorana fermion excitation

Dynamical Spin Structure Factor

$$S^{\alpha\alpha}(\mathbf{Q}, \omega) = \sum_n |\langle n | S_{\mathbf{Q}}^{\alpha} | 0 \rangle|^2 \delta(\omega - (E_n - E_0))$$
$$\sum_i S_i^{\alpha} e^{i\mathbf{Q}\cdot\mathbf{r}_i} | 0 \rangle$$
$$S_i^{\alpha} | 0 \rangle$$

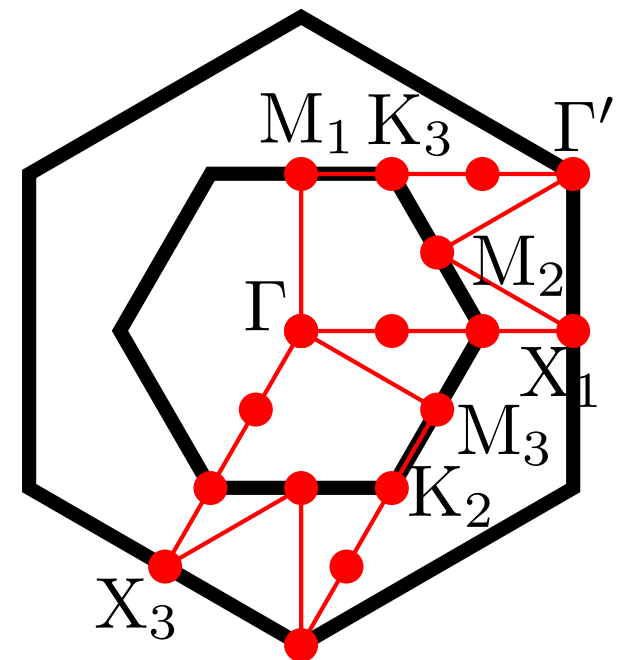
Even though the system is gapless,
the dynamical spin structure factor is gapped!

Dynamical Spin Structure Factor

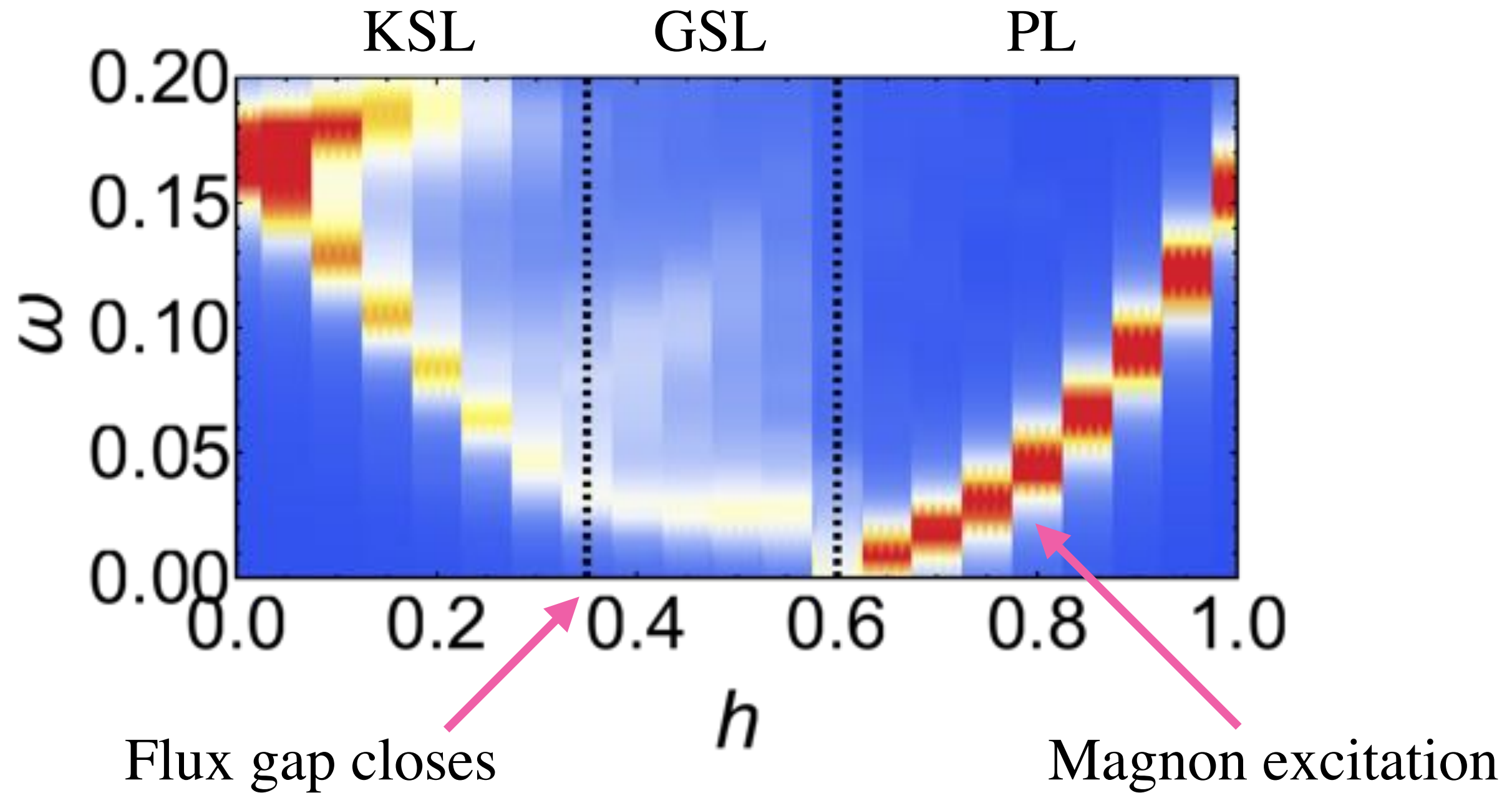


Clear flux gap! (across all momenta)

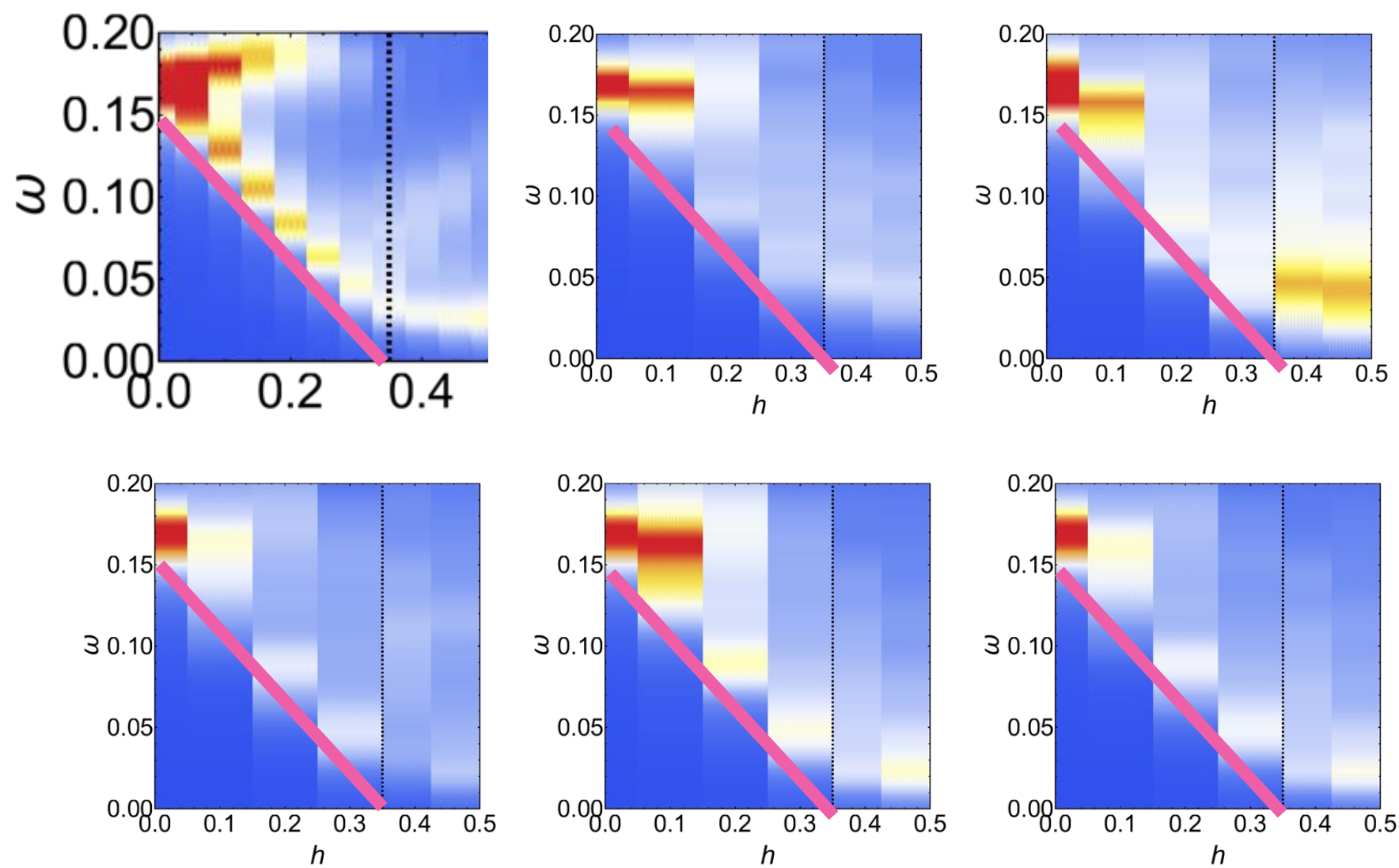
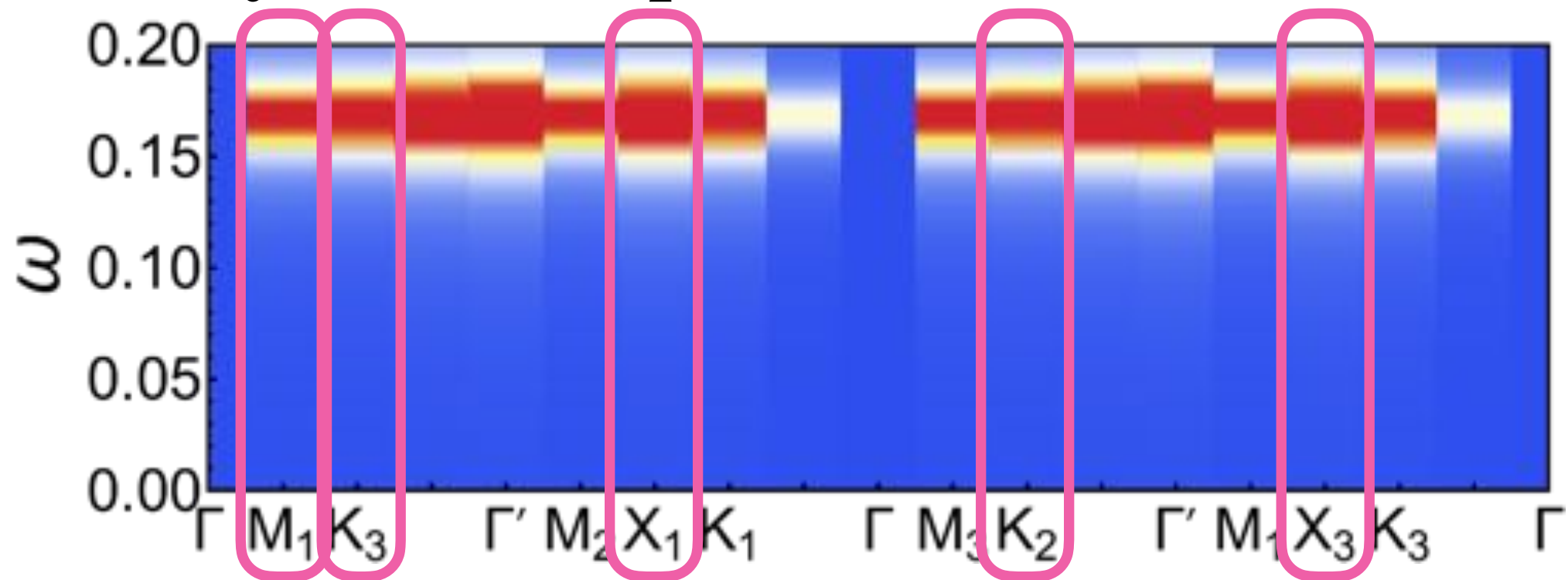
What happens as we increase field?



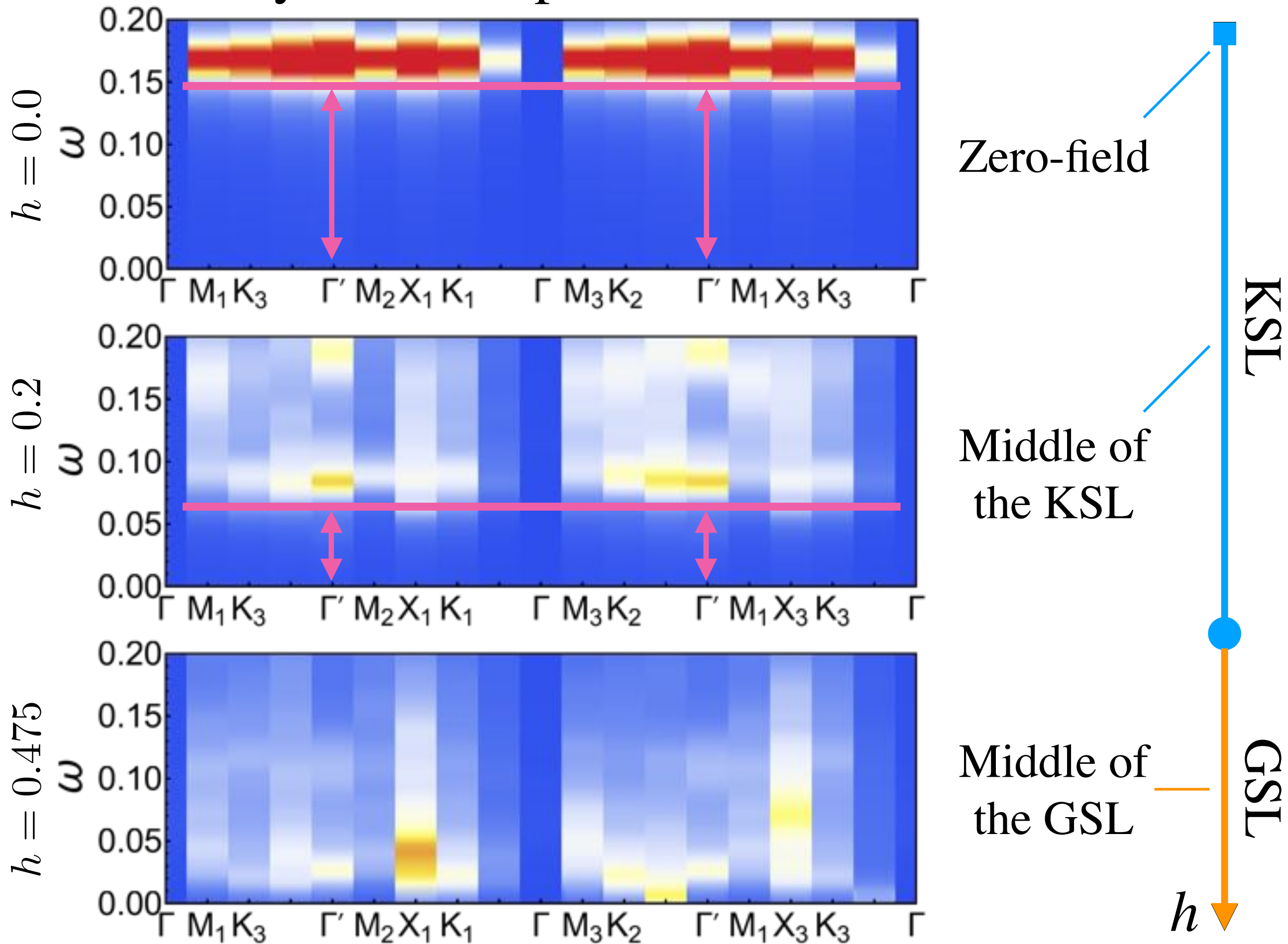
Dynamical Spin Structure Factor



Dynamical Spin Structure Factor

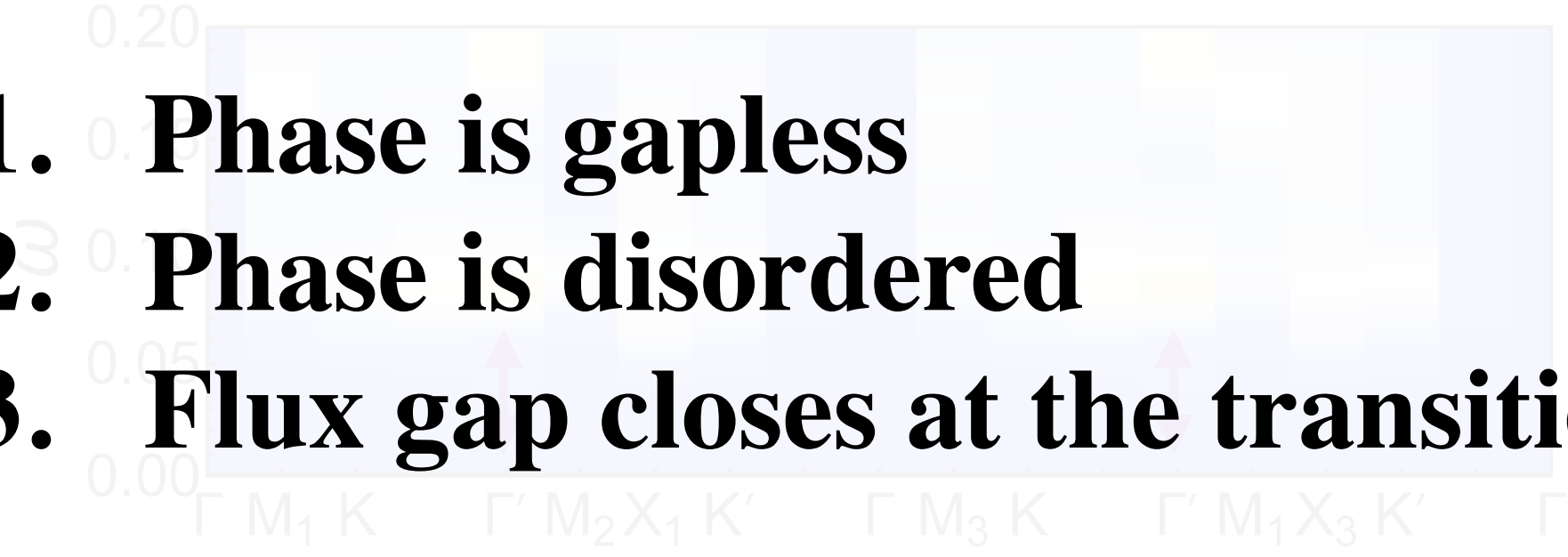


Dynamical Spin Structure Factor





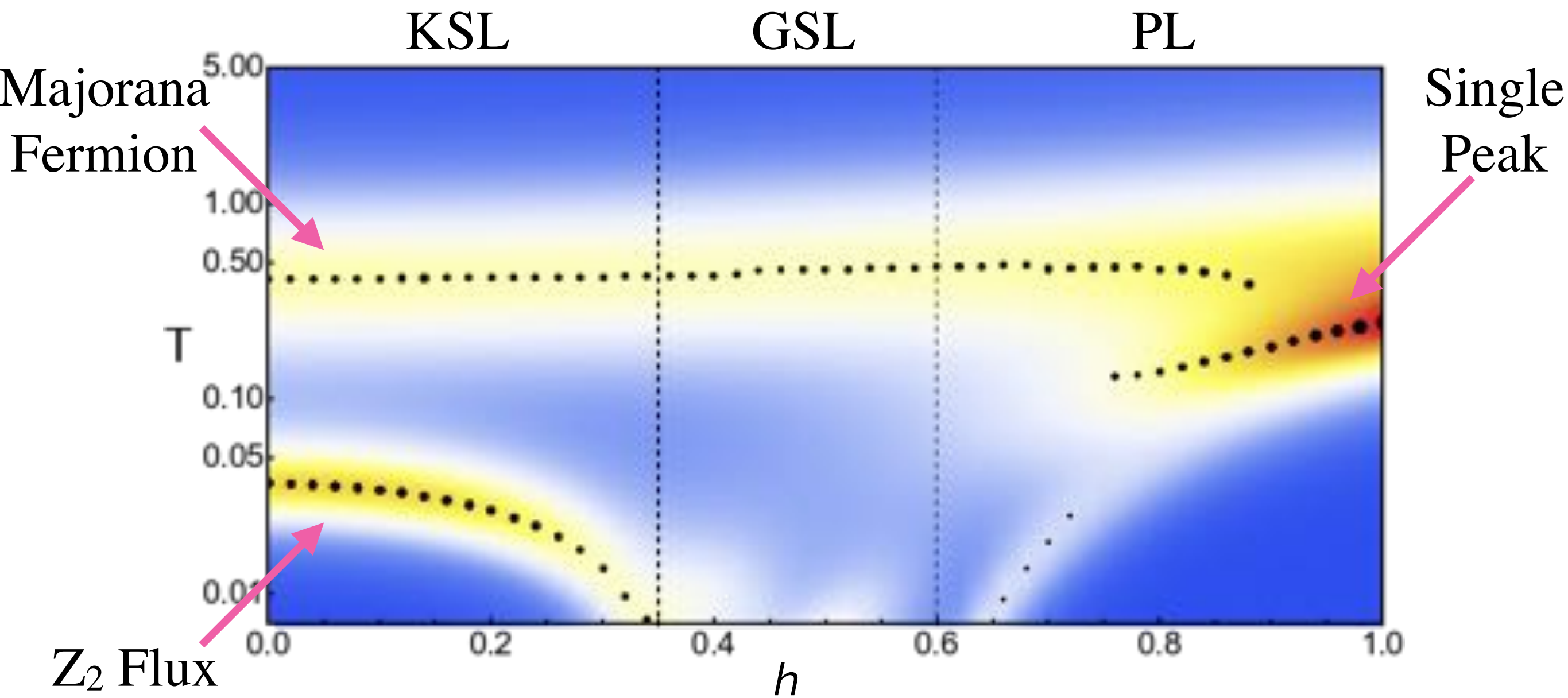
- 1. Phase is gapless**
- 2. Phase is disordered**
- 3. Flux gap closes at the transition**



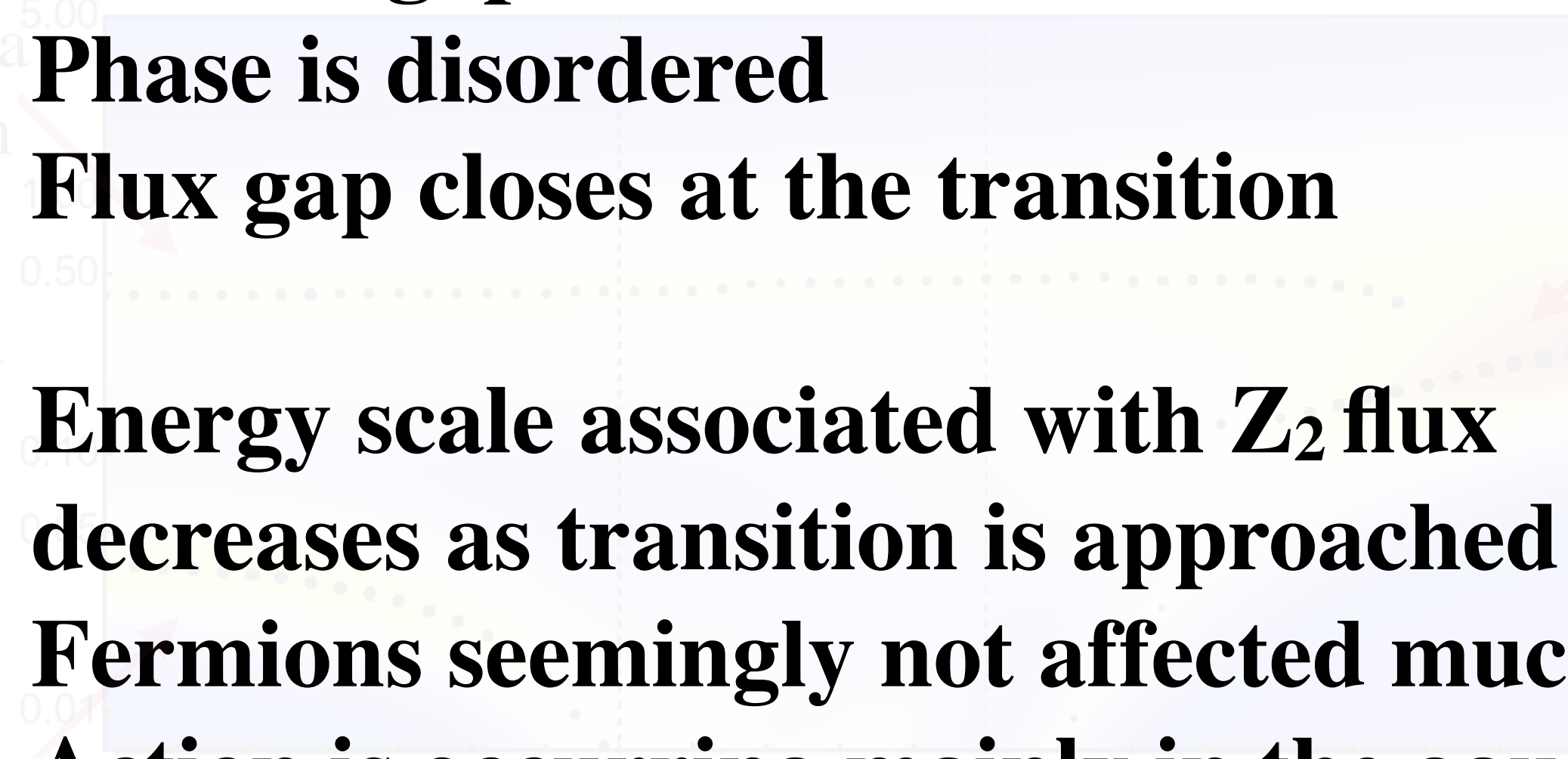
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Specific Heat



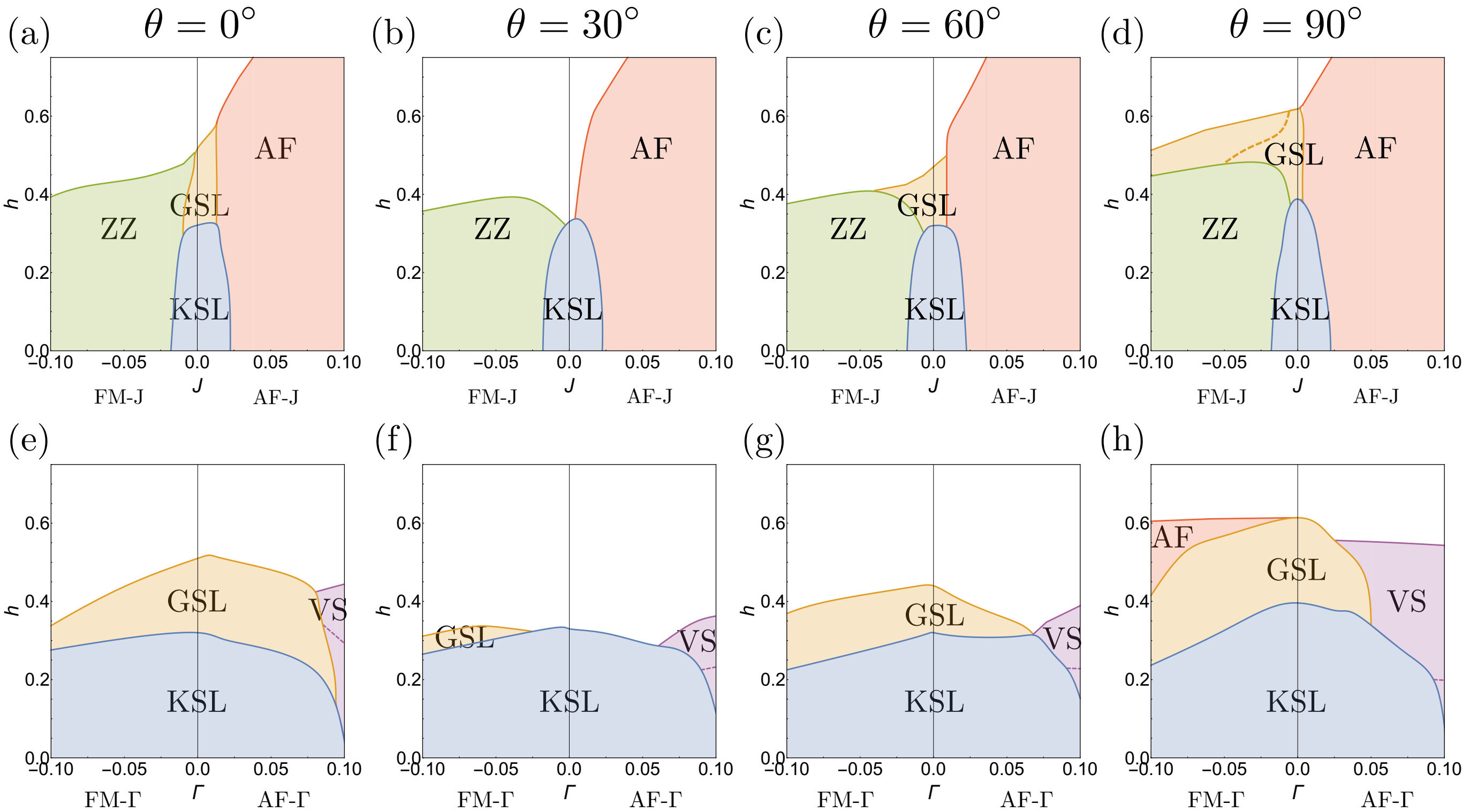
Specific Heat

- 1. Phase is gapless**
 - 2. Phase is disordered**
 - 3. Flux gap closes at the transition**
 - 4. Energy scale associated with Z_2 flux decreases as transition is approached**
 - 5. Fermions seemingly not affected much. Action is occurring mainly in the gauge sector**
- 
- A background plot showing Specific Heat (y-axis, 0.01 to 5.00) versus
- Z_2
- Flux (x-axis, 0 to
- π
-). The plot is divided into regions labeled 'GSL' and 'PL'. A dotted line shows a peak that narrows and shifts as the flux approaches
- π
- . A red arrow points to a 'Single Peak' at the transition point.

Outline

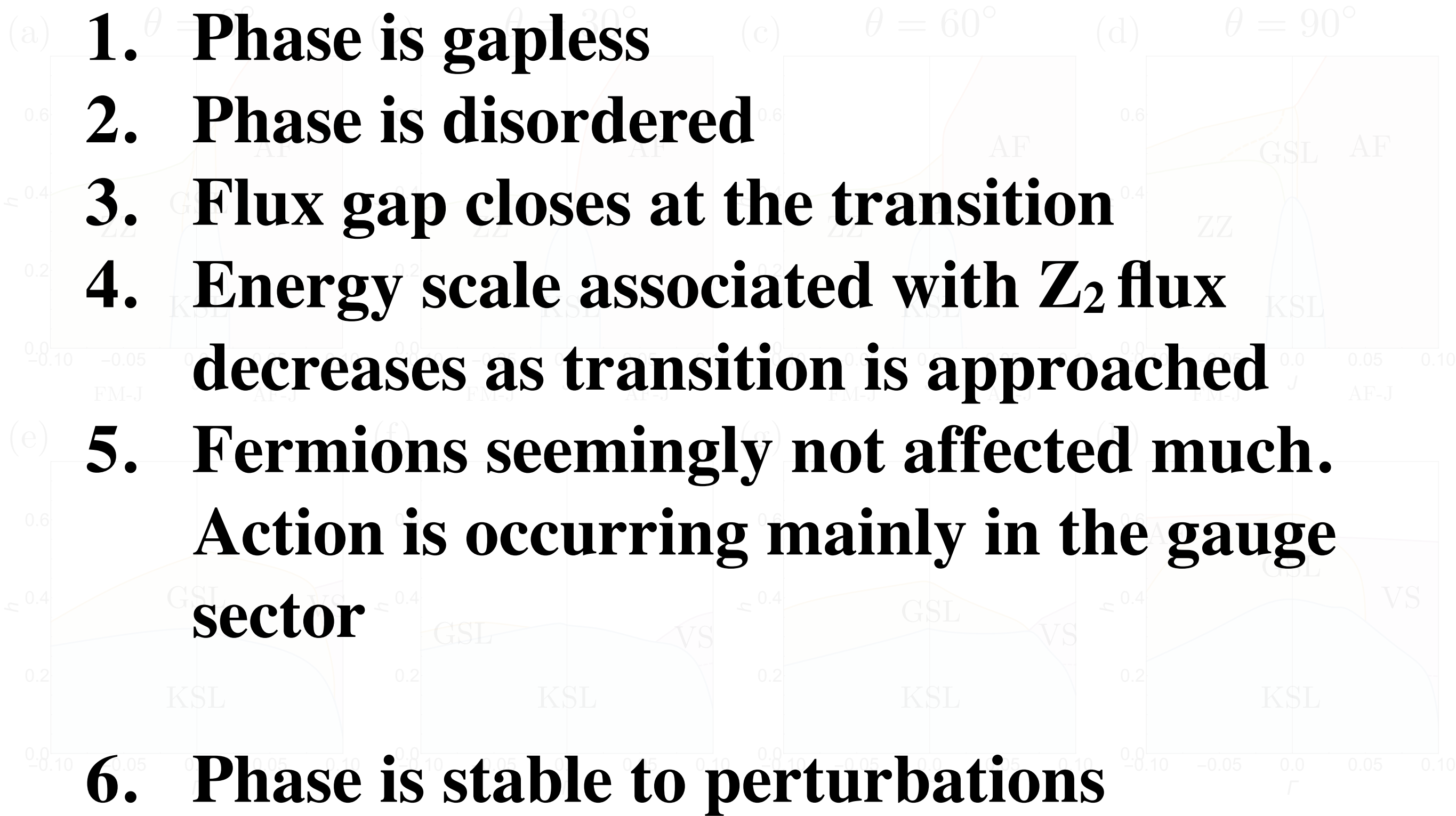
- Introduction
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Relevant Perturbations



Relevant Perturbations

- 1. Phase is gapless**
- 2. Phase is disordered**
- 3. Flux gap closes at the transition**
- 4. Energy scale associated with Z_2 flux decreases as transition is approached**
- 5. Fermions seemingly not affected much. Action is occurring mainly in the gauge sector**
- 6. Phase is stable to perturbations**



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Summary of GSL

1. Phase is gapless
2. Phase is disordered
3. Flux gap closes at the transition
4. Energy scale associated with Z_2 flux decreases as transition is approached
5. Fermions seemingly not affected much. Action is occurring mainly in the gauge sector
6. Phase is stable to perturbations

What's going on?

- Rewrite spins in terms of usual (complex) fermions:

$$S_i^\alpha = f_{i,\mu}^\dagger \sigma_{\mu\nu}^\alpha f_{i,\nu}$$

$$\begin{aligned} f_{i,\mu}^\dagger &\rightarrow e^{-i\phi_i} f_{i,\mu}^\dagger \\ f_{i,\nu} &\rightarrow e^{i\phi_i} f_{i,\nu} \end{aligned} \quad S_i^\alpha \rightarrow S_i^\alpha \quad \text{U(1) (phase) redundancy!}$$

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Gauge Field: \mathbb{Z}_2 (Higgsed)

Fermions: Gapped
Topological SC



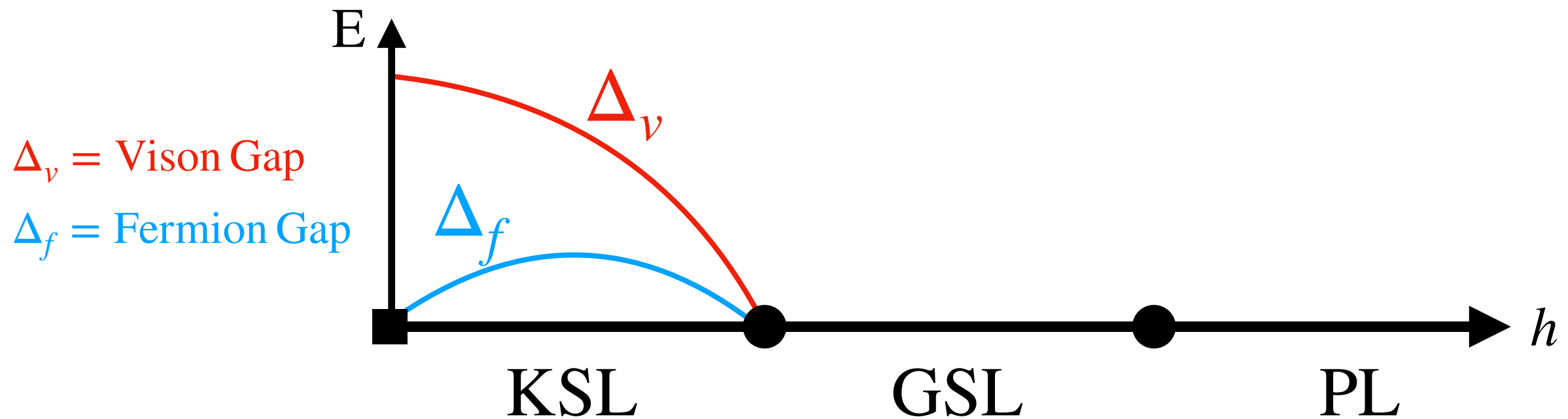
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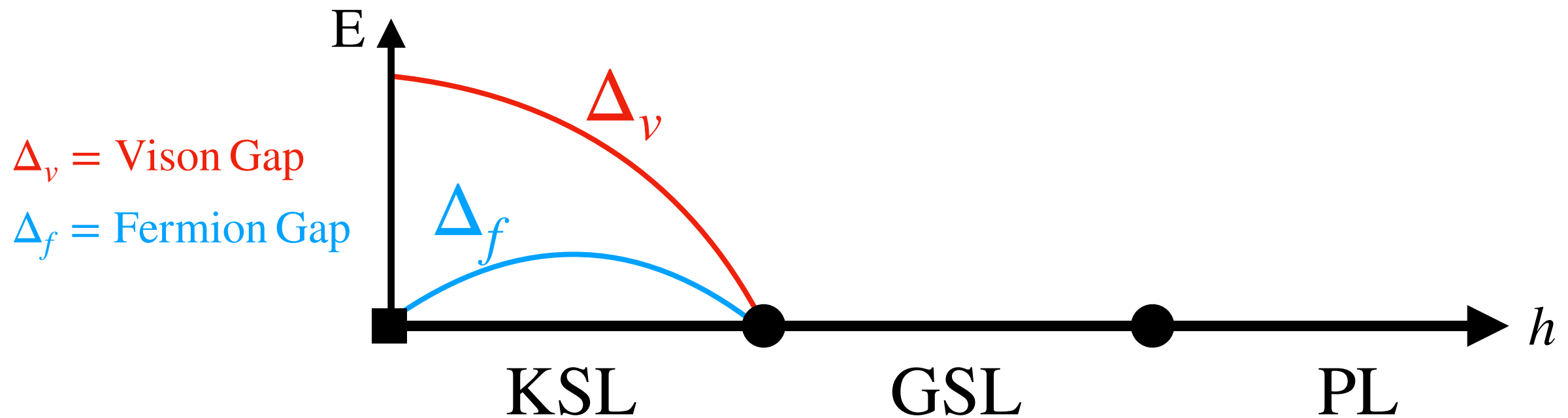
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Fermions: Gapped Topological SC Gapless FS



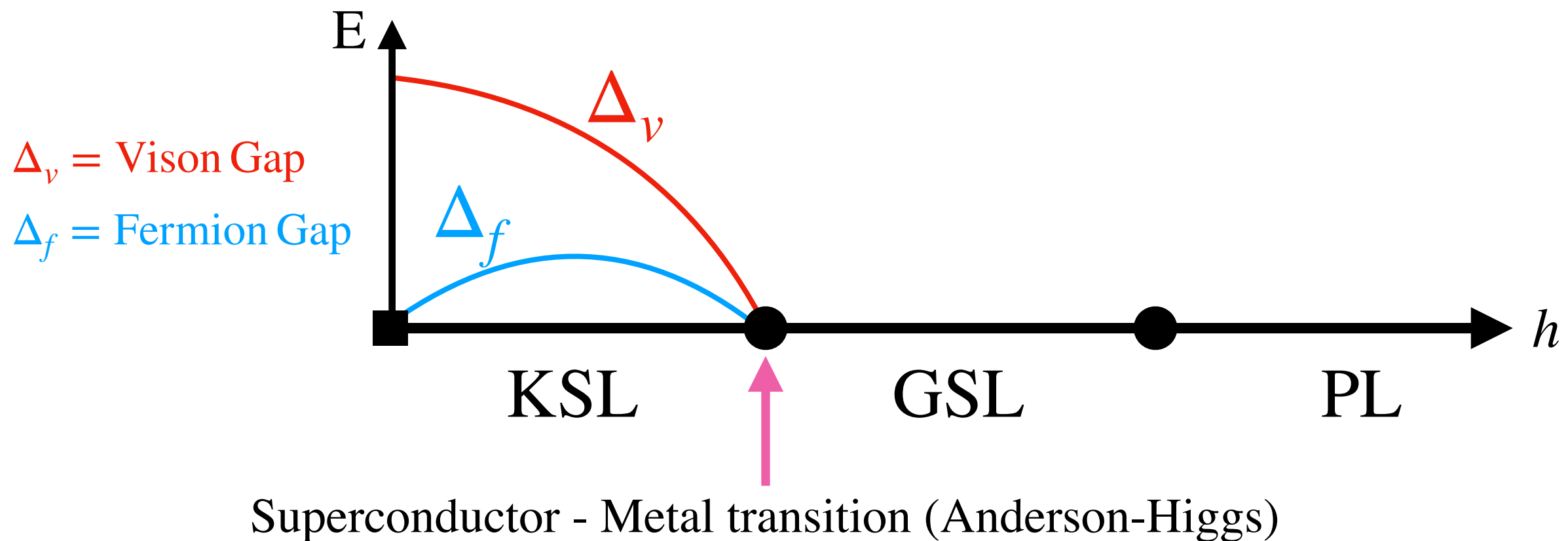
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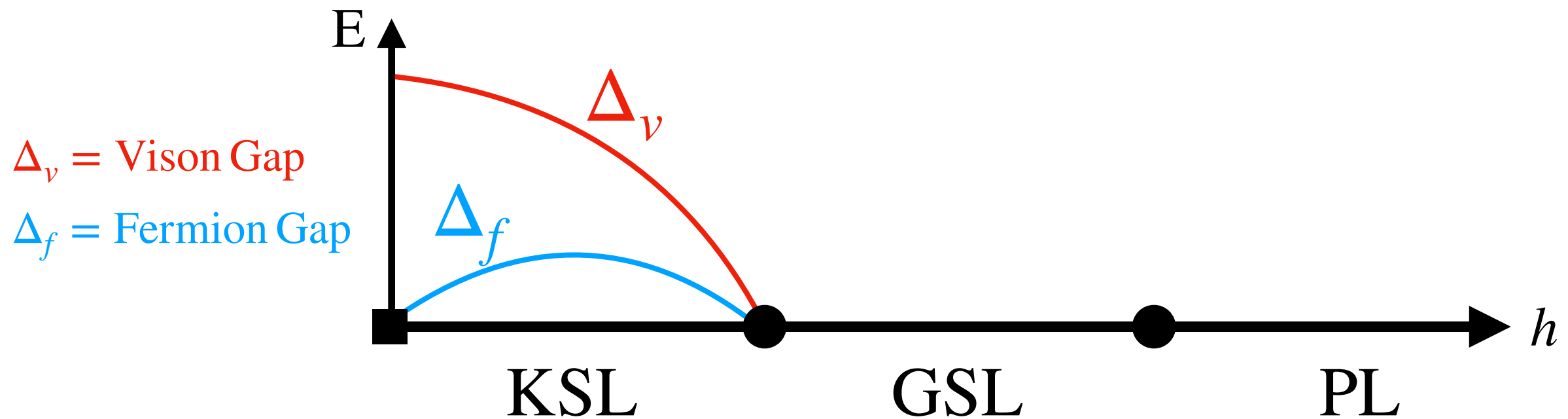
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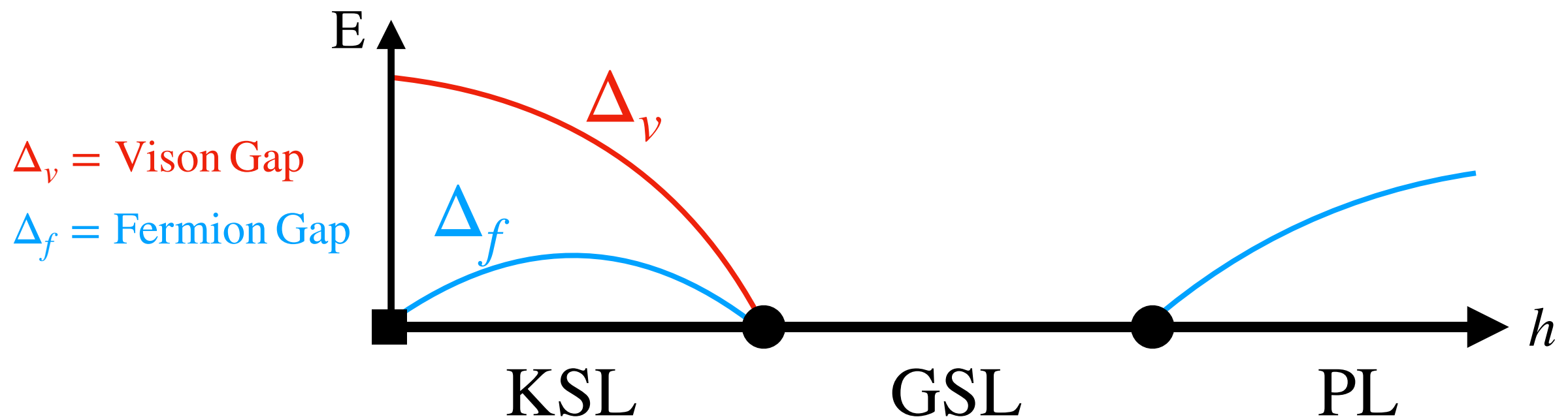
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Gauge Field: \mathbb{Z}_2 (Higgsed) $U(1)$ $U(1)$ (confined)

Fermions: Gapped Topological SC Gapless FS Gapped Trivial Insulator



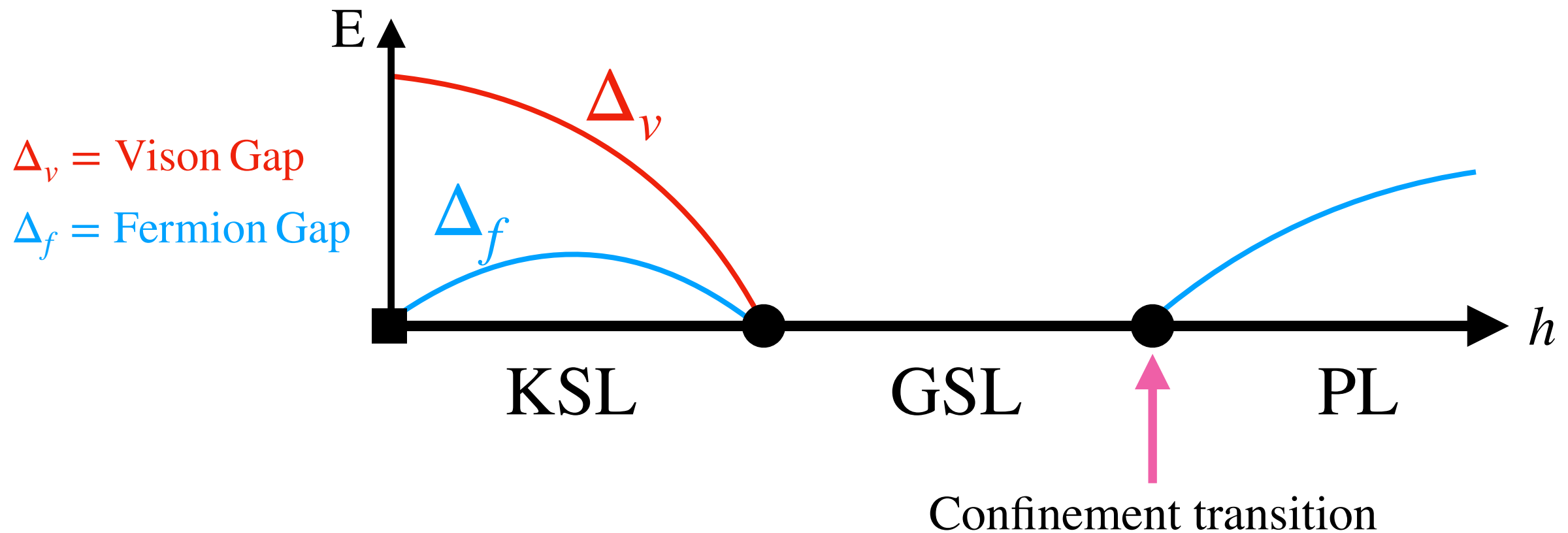
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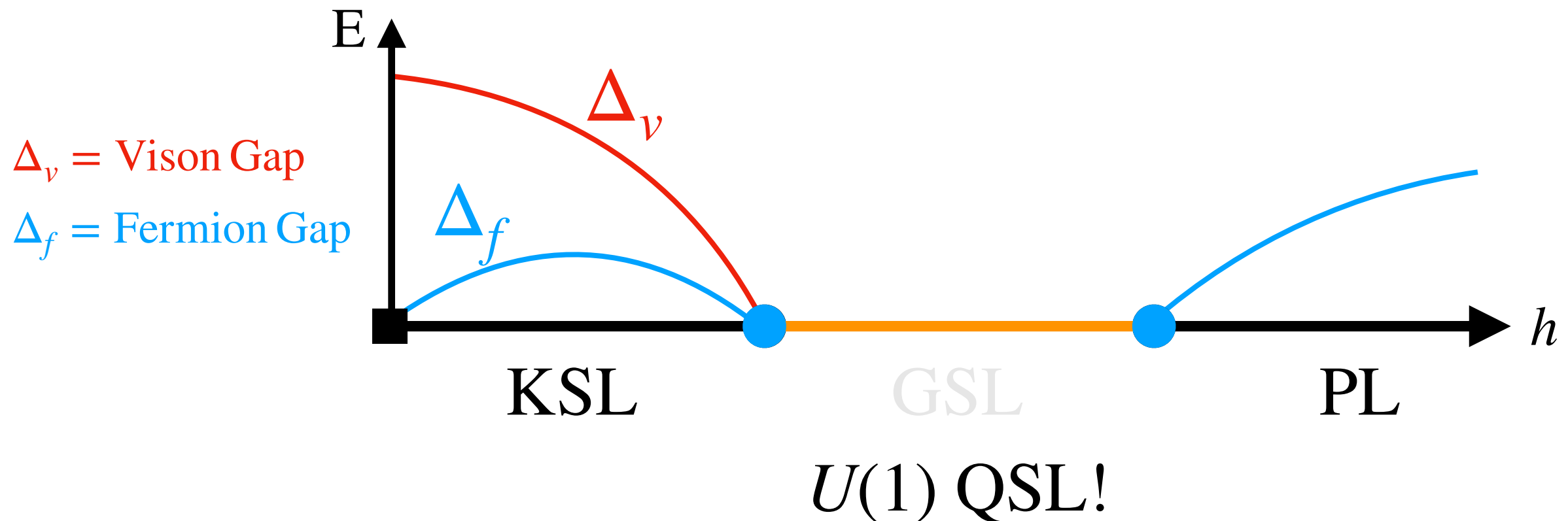
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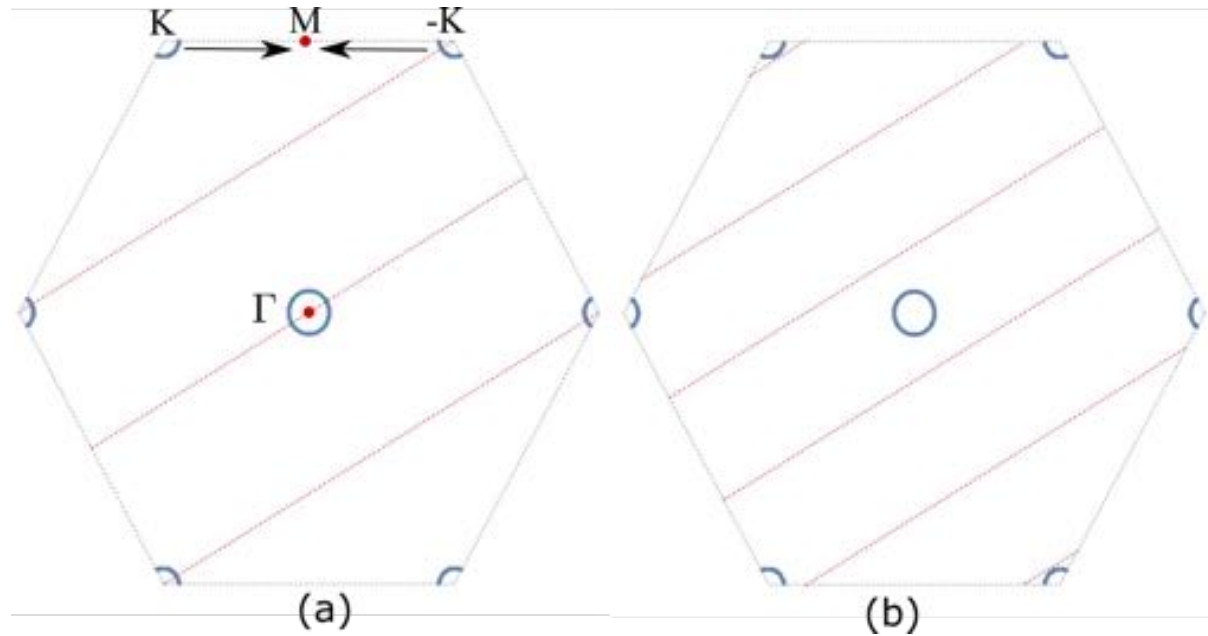
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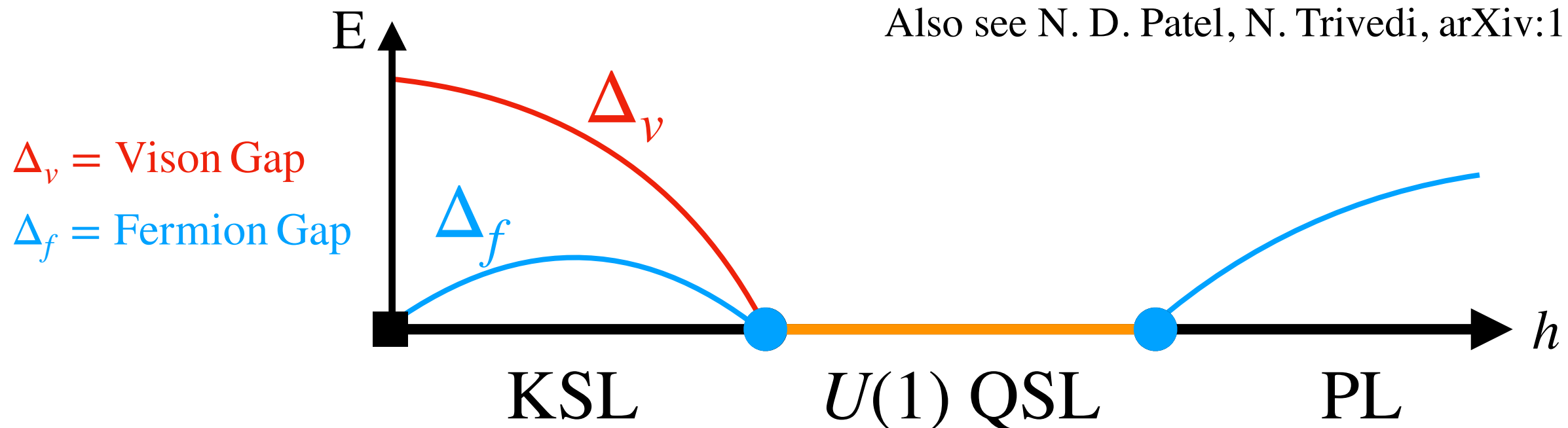
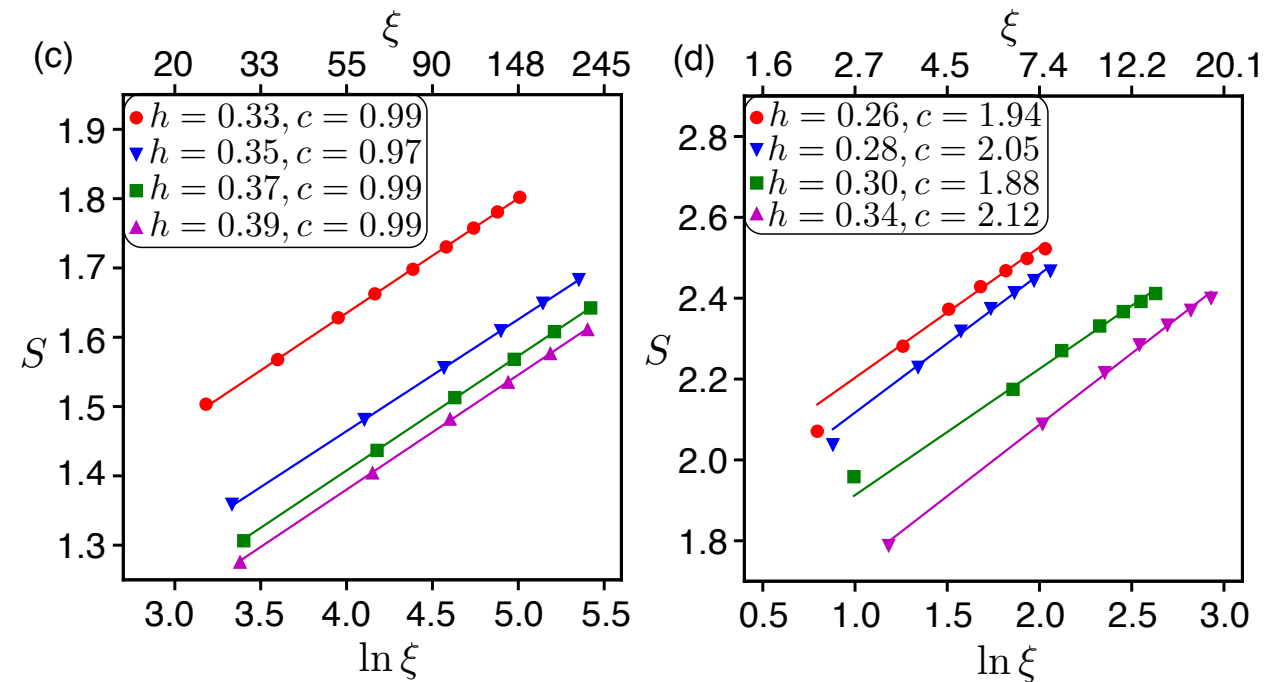
What's going on?

- Central charge consistent with Fermi surface predicted by PSG analysis

H.-C. Jiang et al., arXiv:1809.08247



L. Zou, Y.-C. He, arXiv:1809.09091



Also see N. D. Patel, N. Trivedi, arXiv:1812.06105

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	Fermions	Gauge Field
Known “textbook” Kitaev spin liquids	Gapless SC	Gapped Z_2
	Gapped topological SC	Gapped Z_2
	Gapped trivial SC	Gapped Z_2

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Fermions

Gauge Field

Gapless SC

Gapped Z_2

Gapped topological SC

Gapped Z_2

Gapped trivial SC

Gapped Z_2

New phase!!!

Gapless Metal

Gapless $U(1)$

Thank you!