3D-2D equivalence of ordered states on harmonic honeycomb lattices

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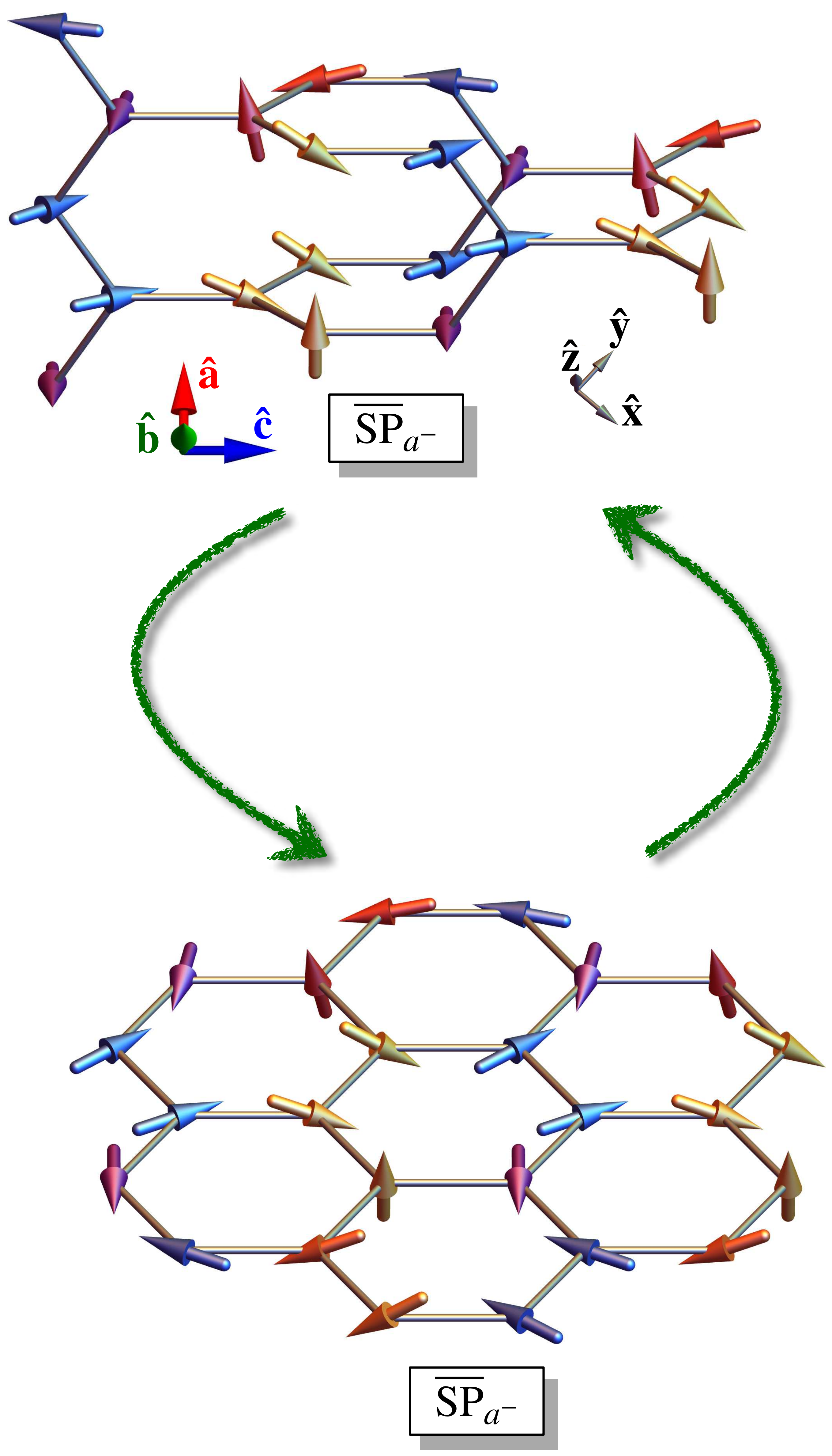
Complexity and Topology in Quantum Matter
Würzburg-Dresden Cluster of Excellence

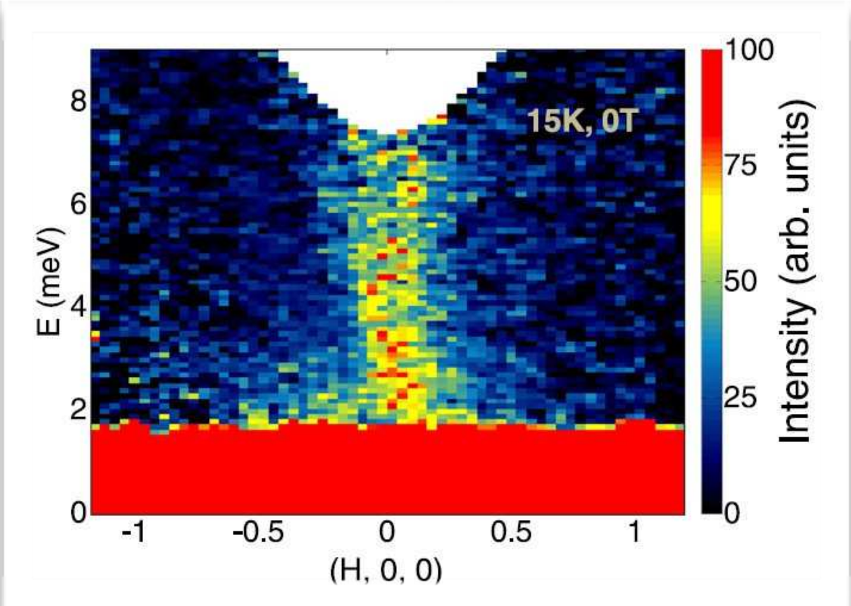
Quantum Critical Matter
JA 2306/4-1
Emmy Noether-Programm
DFG Deutsche Forschungsgemeinschaft

Outline

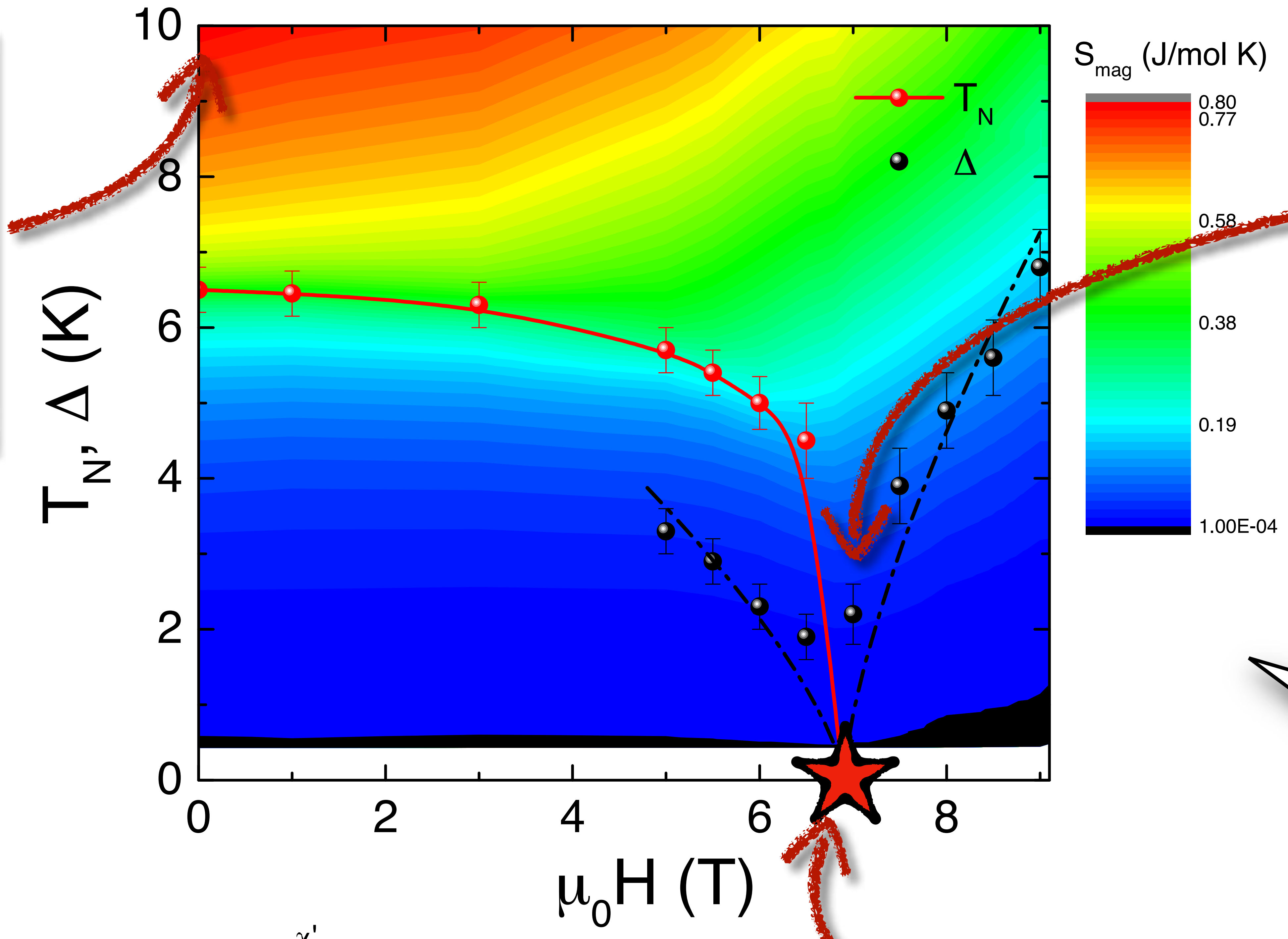
1. Introduction
2. 3D-2D mapping
3. Heisenberg-Kitaev-Γ models on the hyperhoneycomb lattice
4. Quantum effects
5. Conclusions

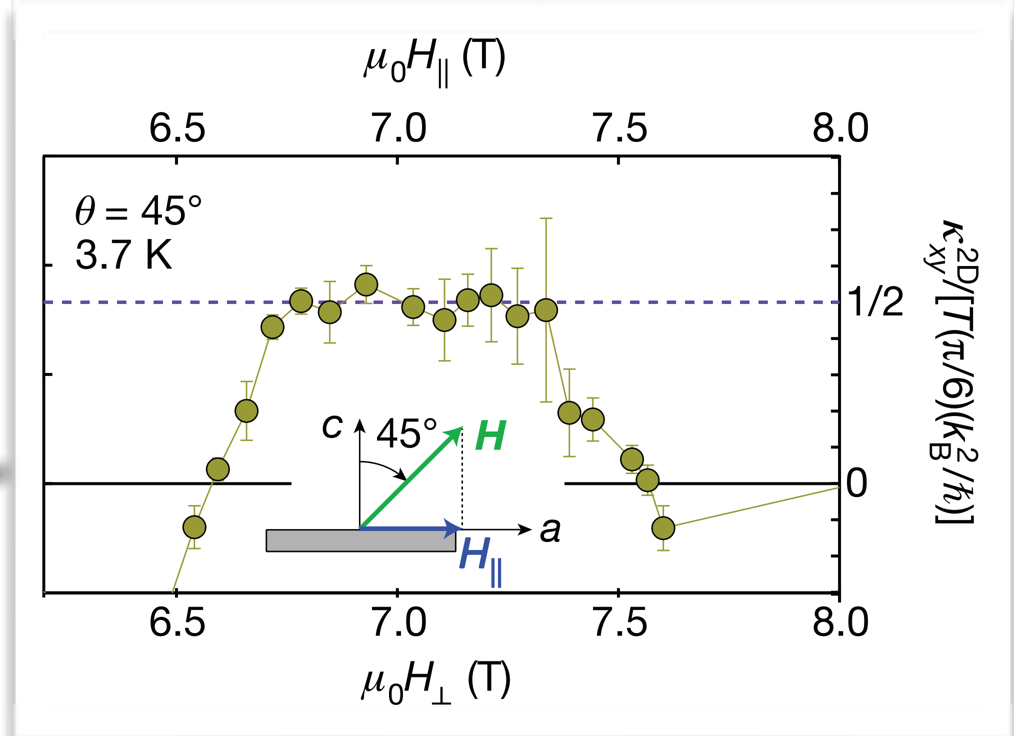


Honeycomb Kitaev materials

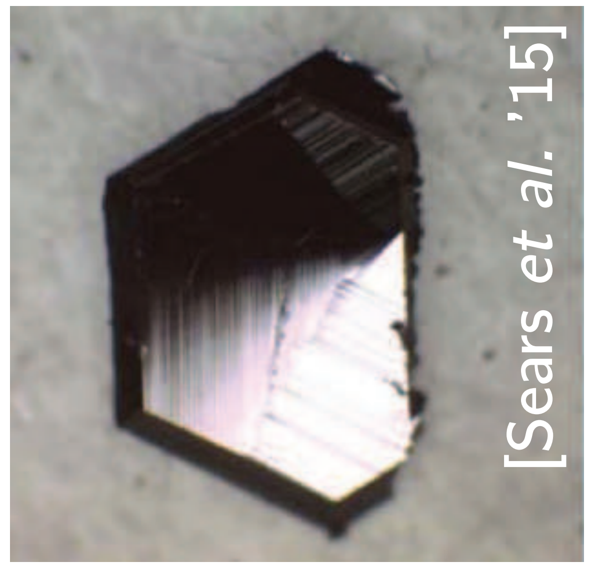


[Banerjee *et al.* '16; '17]

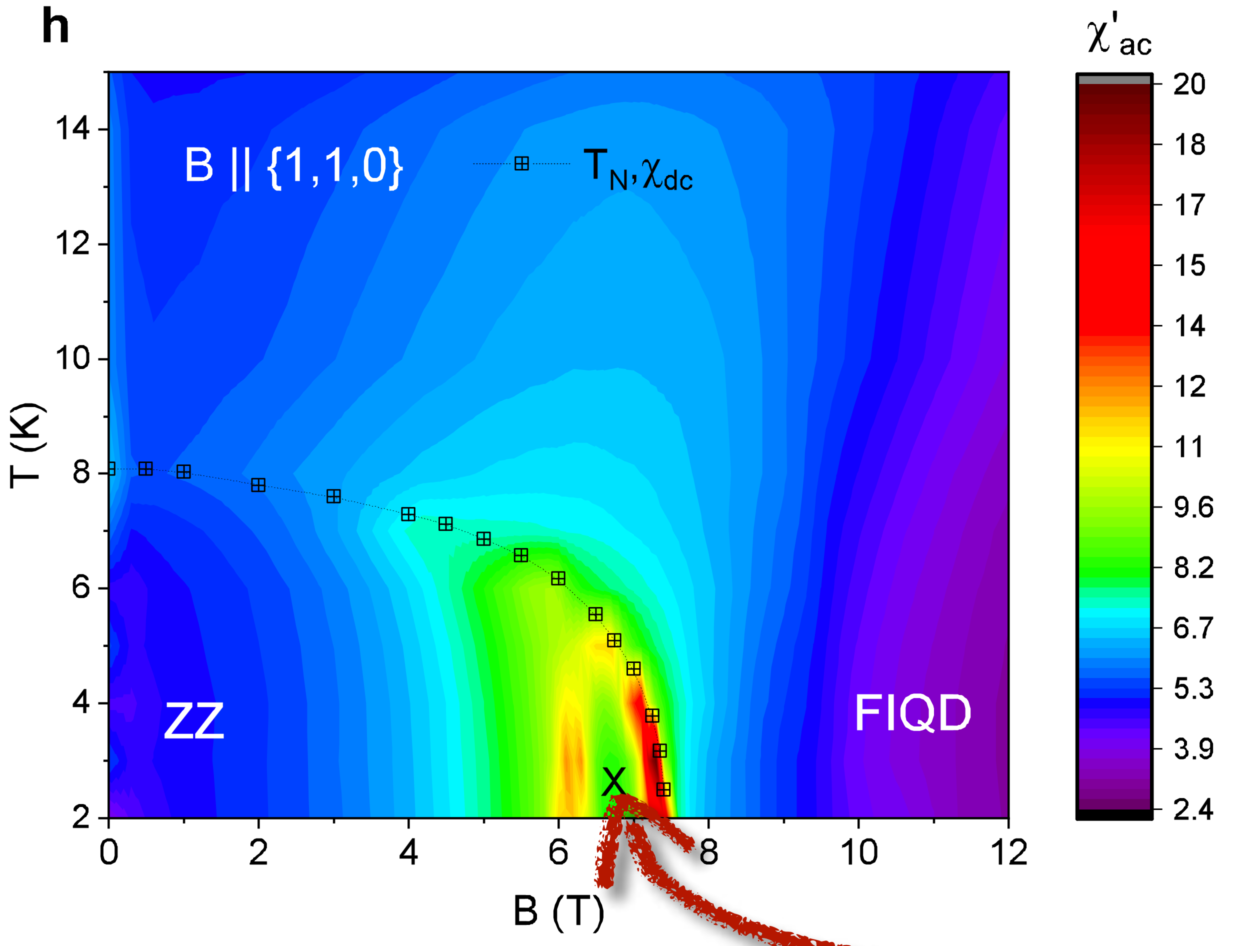




[Kasahara *et al.* '18]



α-$RuCl_3$



[Lampen-Kelley, LJ, *et al.* '18]

QCP

[Wolter, Corredor, LJ, *et al.* '17]

intermediate ordered phase

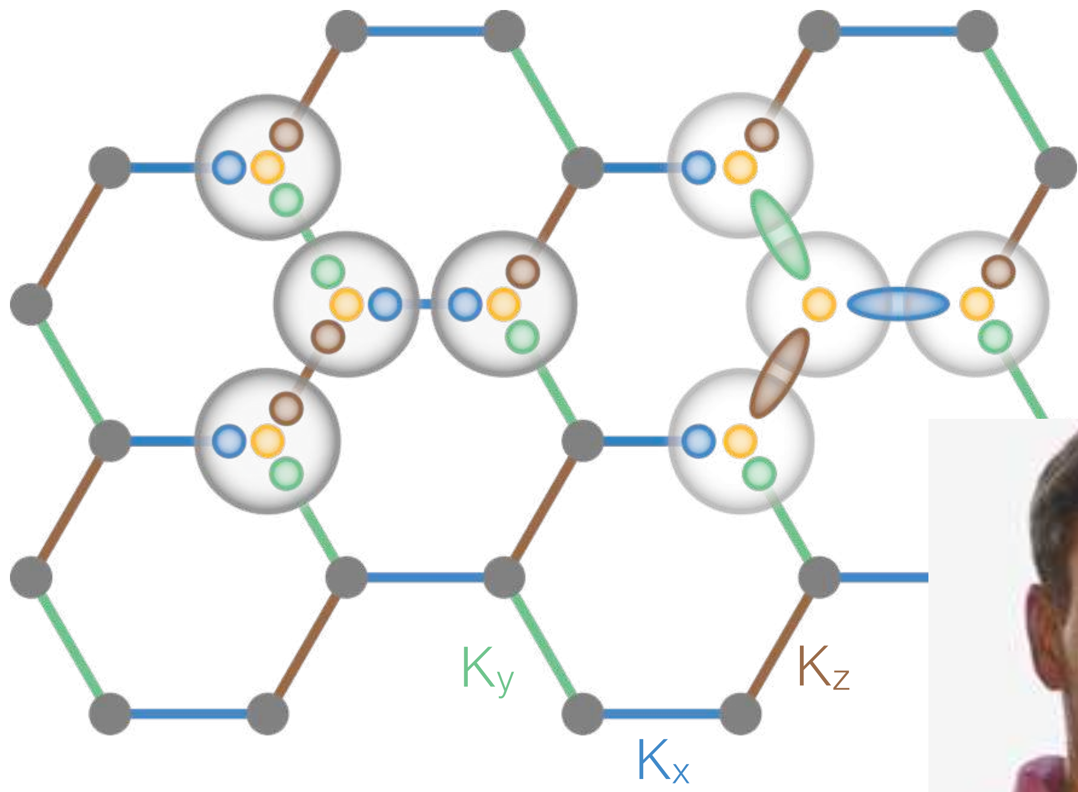
Topical Reviews: [LJ & Vojta, JPCM '19]

[Winter *et al.*, JPCM '17]

→ Talk by S. Winter (11:20 a.m.)

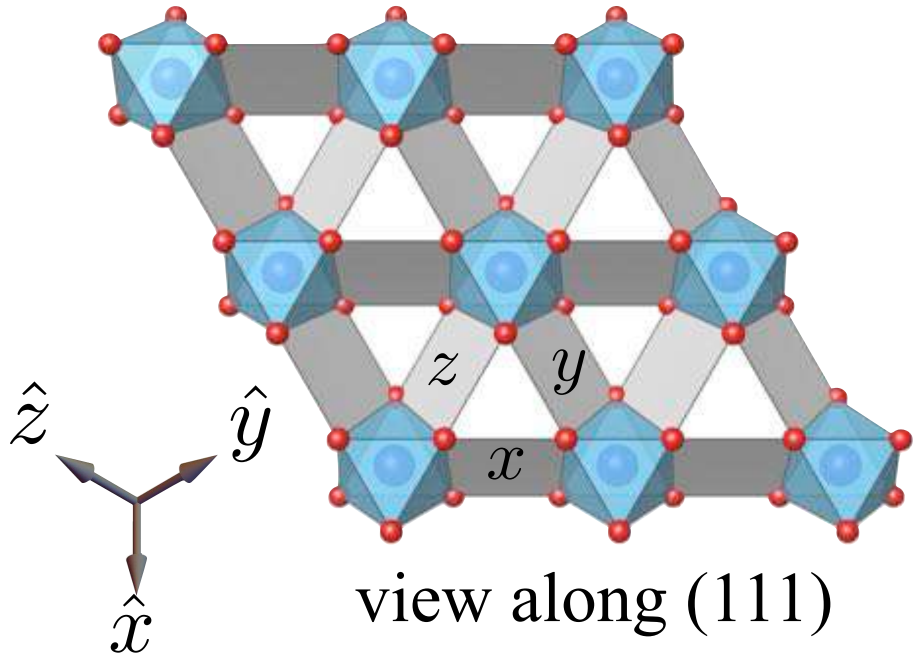
Kitaev honeycomb model?

[Kitaev '06]

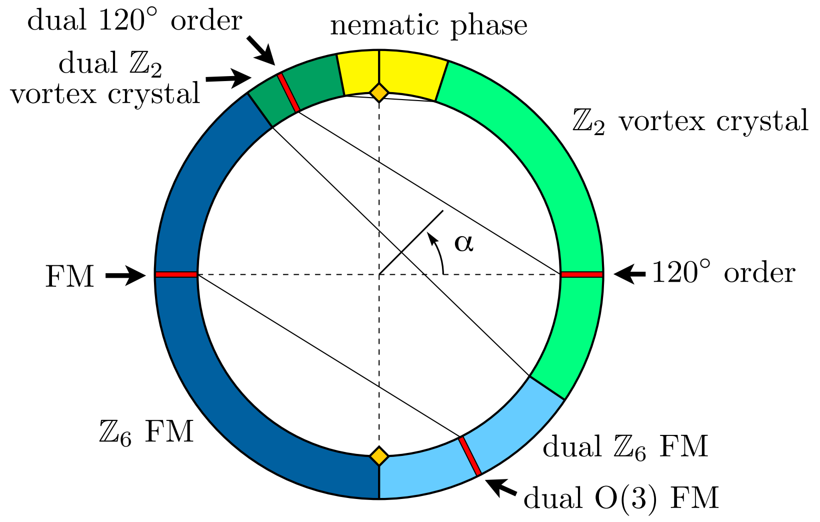


Other lattices?

2D: triangular ($Ba_3Ir_xTi_{3-x}O_9$, ...)



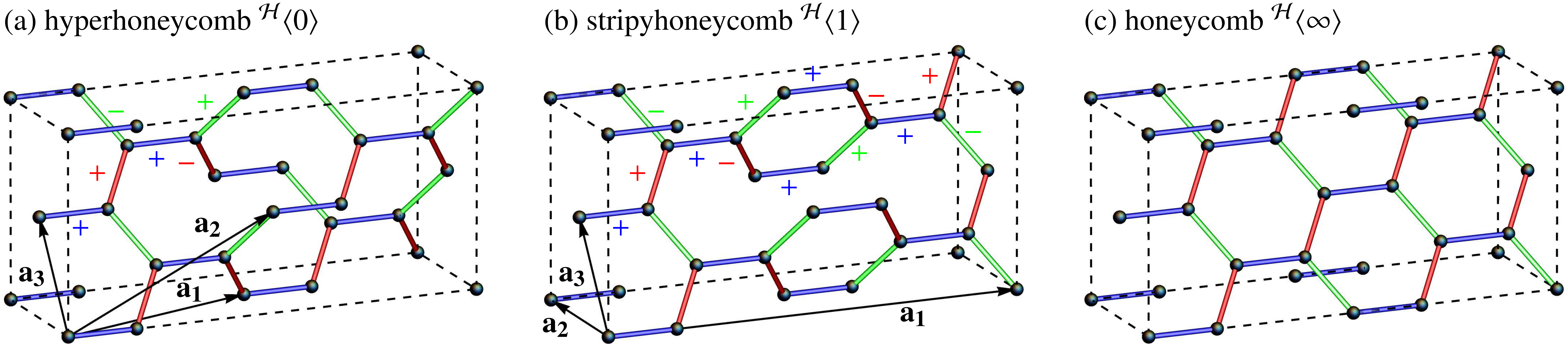
Heisenberg-Kitaev model:



... no (soluble) Kitaev limit

[Becker *et al.* '15]
[Rousochatzakis *et al.* '16]
Review: [Trebst '17]

3D:

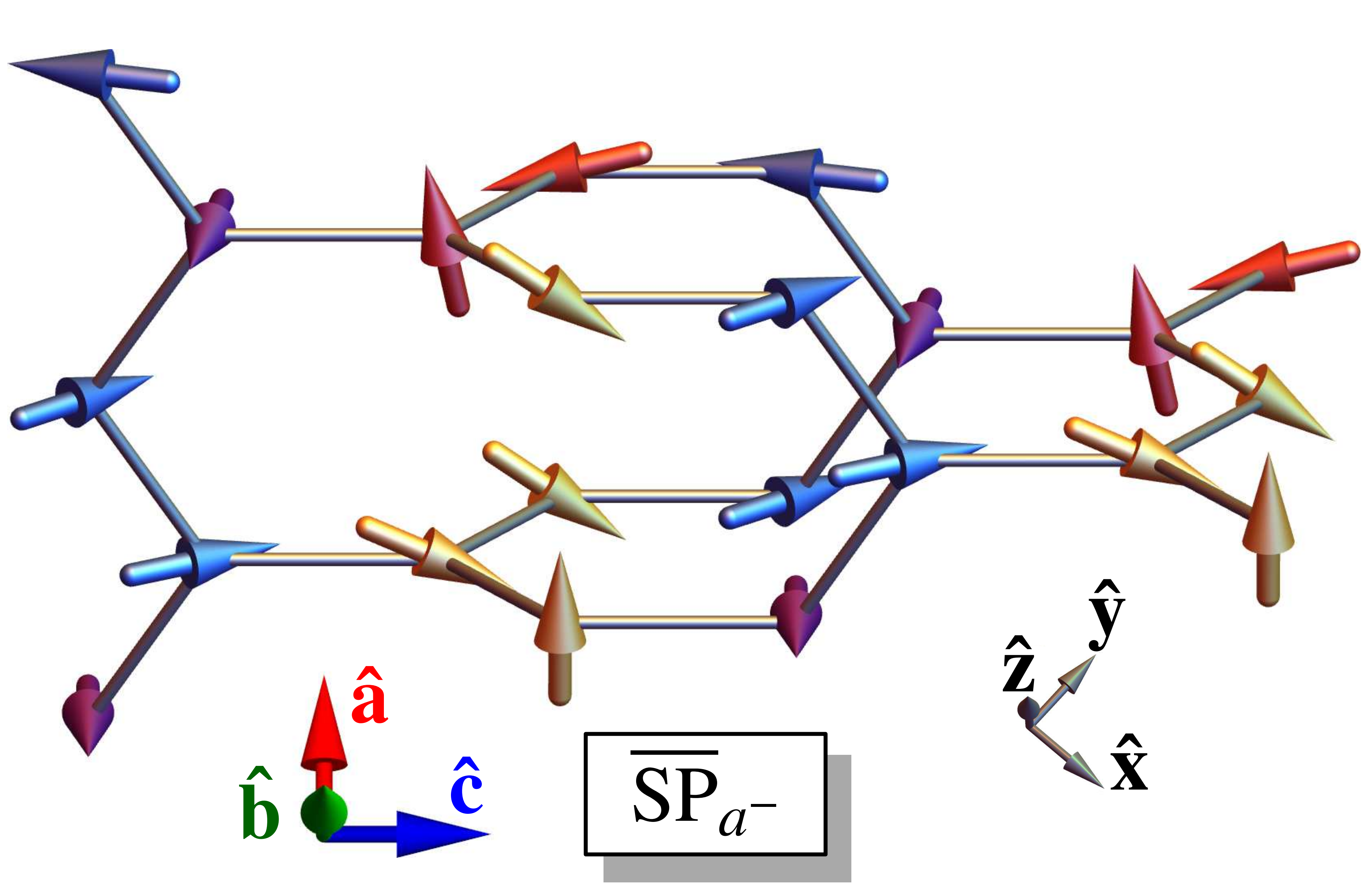


β-Li_2IrO_3, ... γ-Li_2IrO_3, ... α-Li_2IrO_3, α-$RuCl_3$, ...

[Modic *et al.*, '14]
[Kimchi *et al.* '14]

Li_2IrO_3: Magnetic order

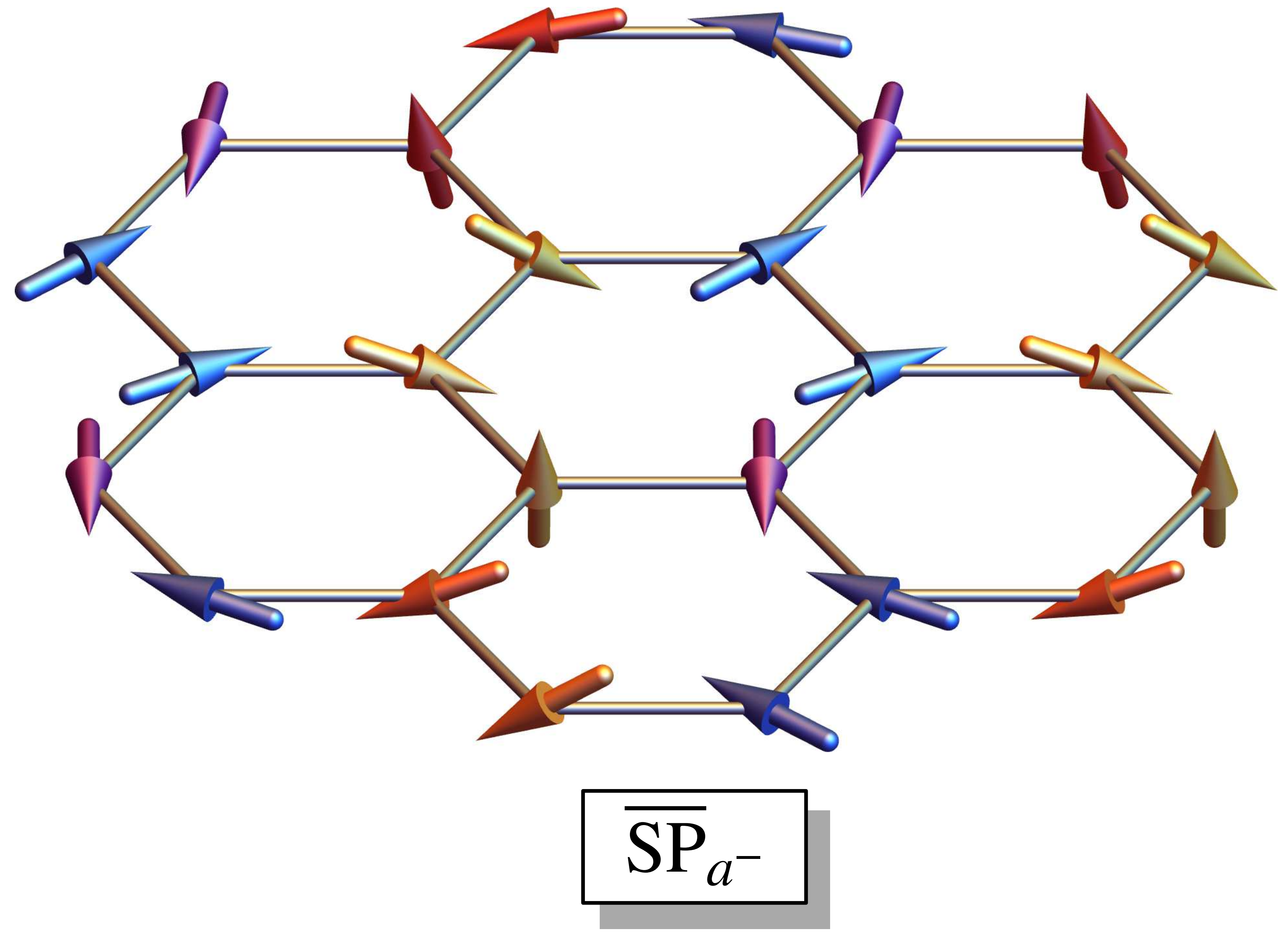
β-Li_2IrO_3



incommensurate spiral

[Biffin *et al.* '14]

α-Li_2IrO_3



incommensurate spiral

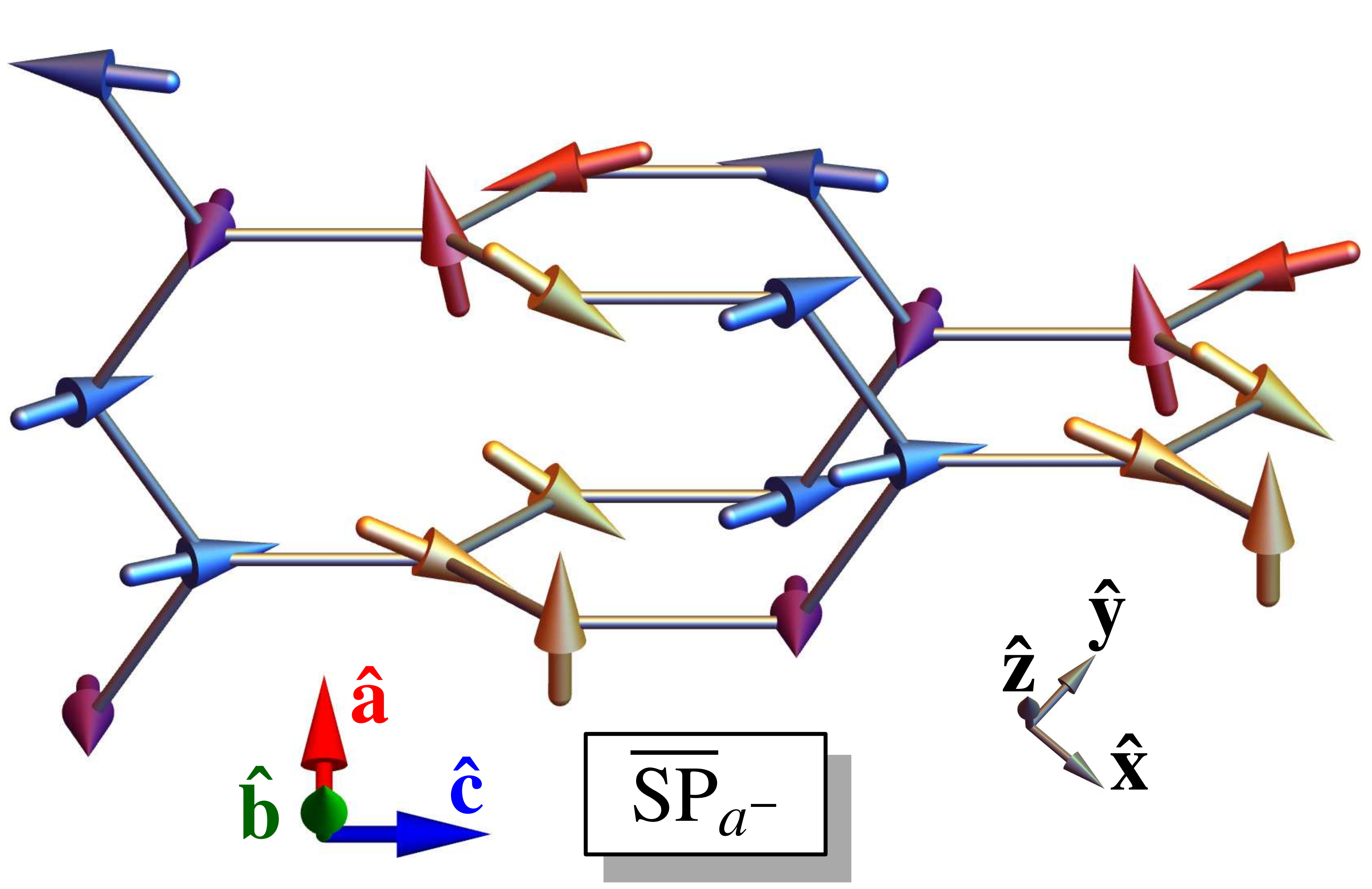
[Williams *et al.* '16]

... and γ-Li_2IrO_3 as well

[Modic *et al.* '14]

Li_2IrO_3: Magnetic order

β-Li_2IrO_3



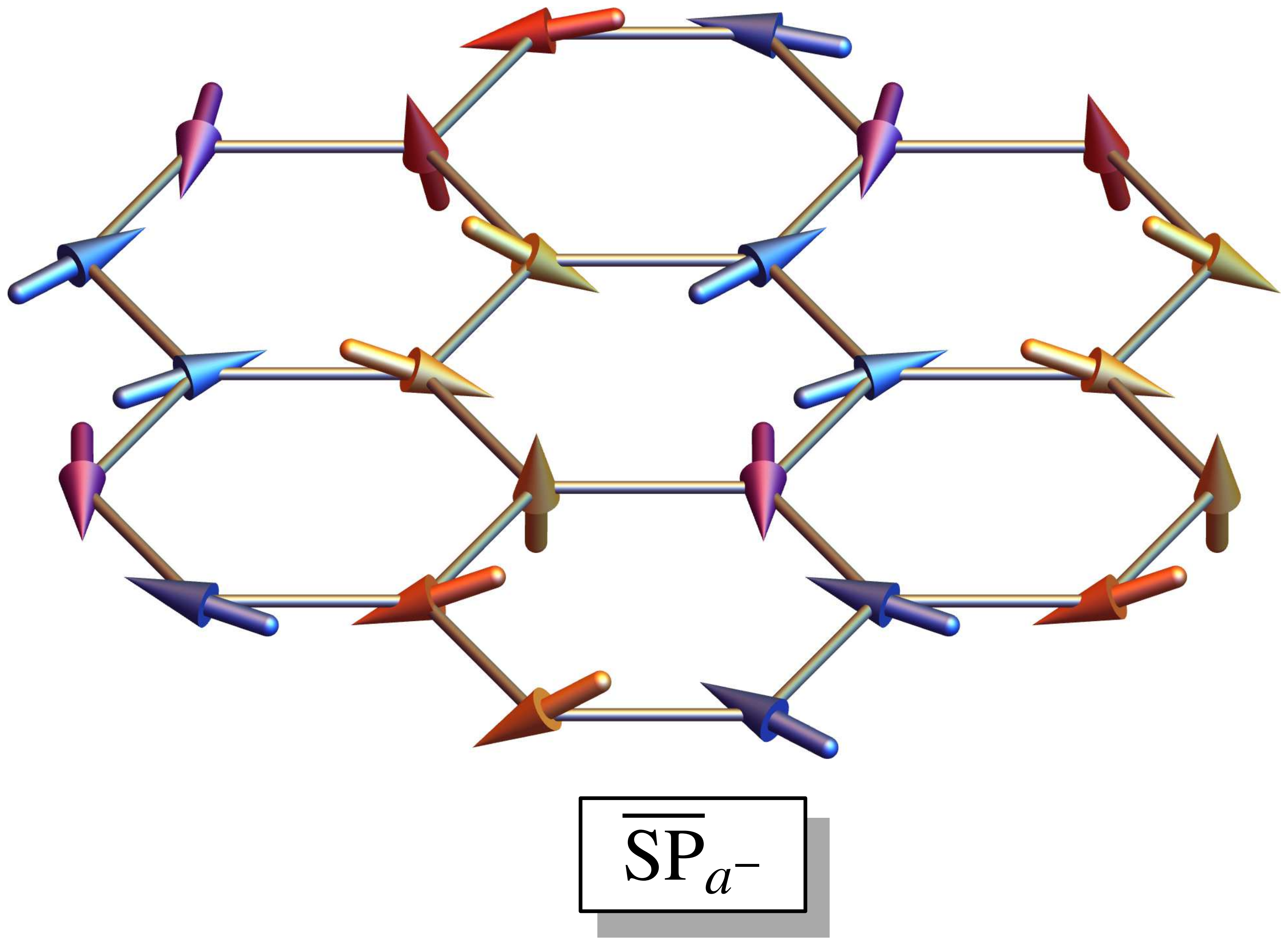
incommensurate spiral

[Biffin *et al.* '14]

3D-2D equivalence

- Classical energies ✓
- Phase diagrams ✓
- Direction of moments ✓
- Magnon bands (✓)
- Quantum effects ✗

α-Li_2IrO_3



incommensurate spiral

[Williams *et al.* '16]

$\boxed{\text{Coordination number: } \mathbf{3}}$

... and γ-Li_2IrO_3 as well

[Modic *et al.* '14]

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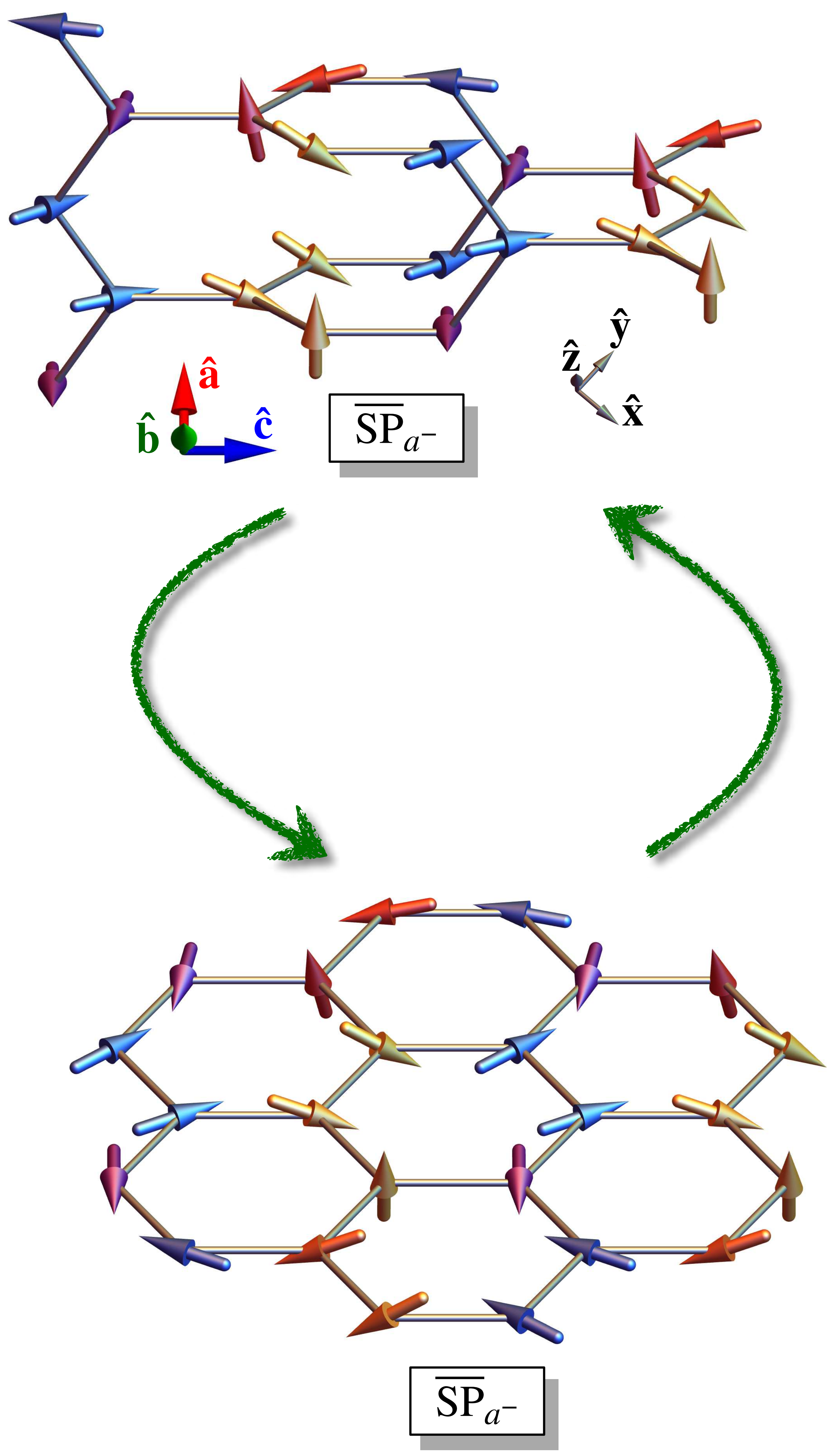
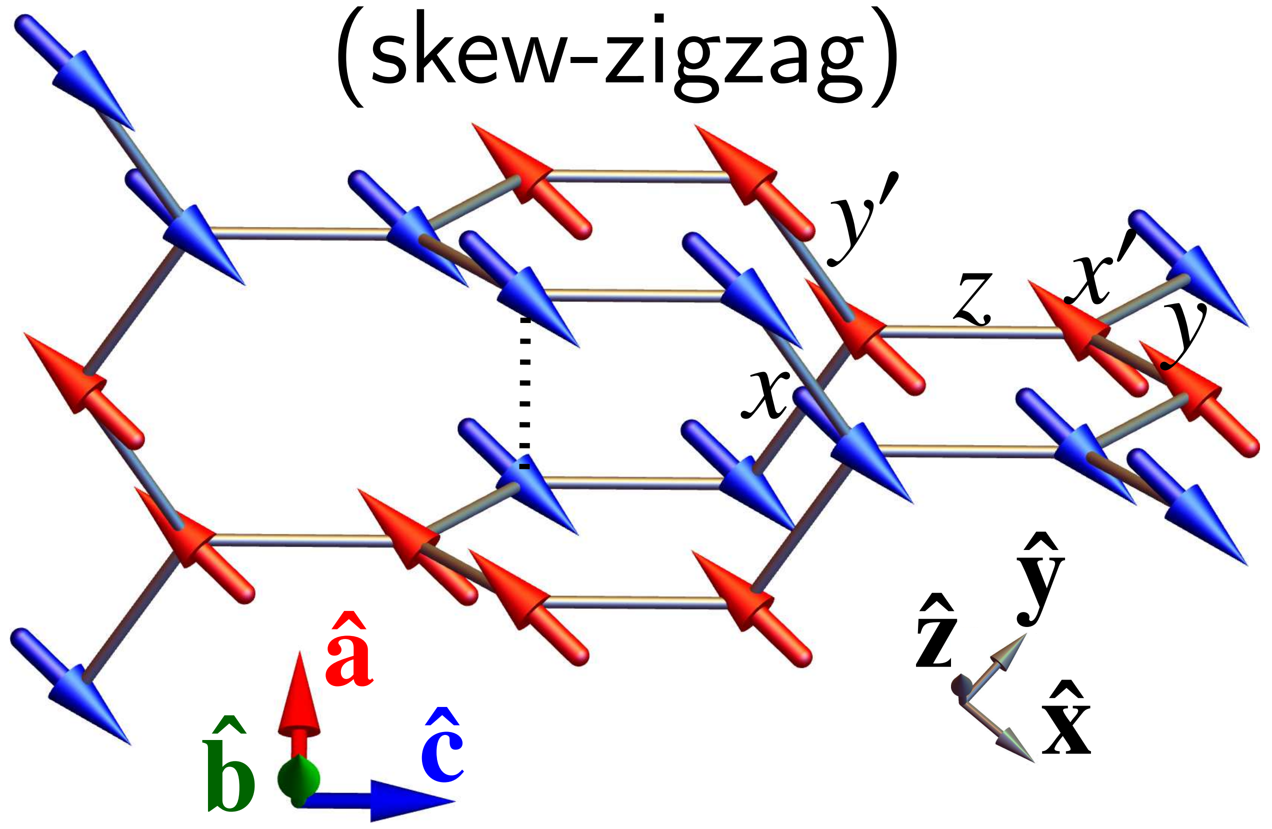


3D-2D mapping: real space

hyperhoneycomb
(skew-zigzag)

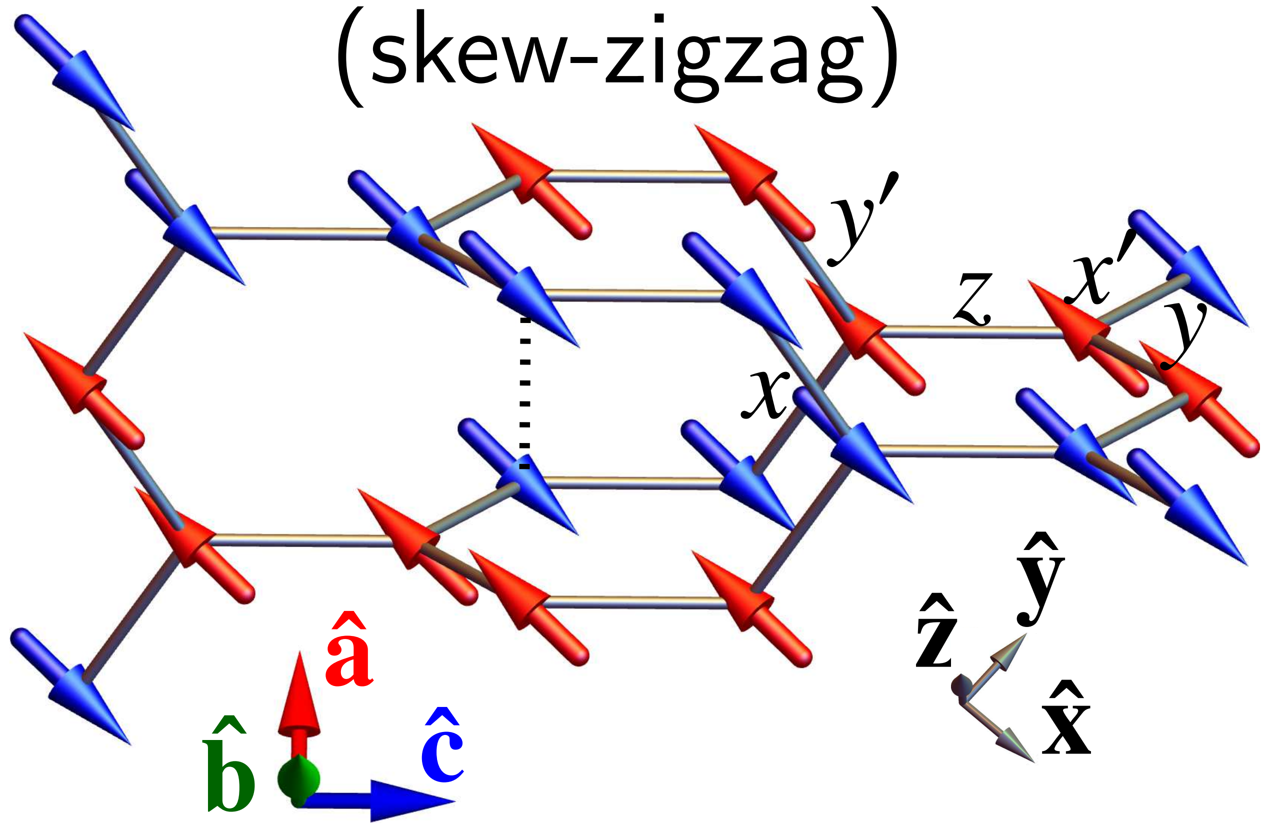


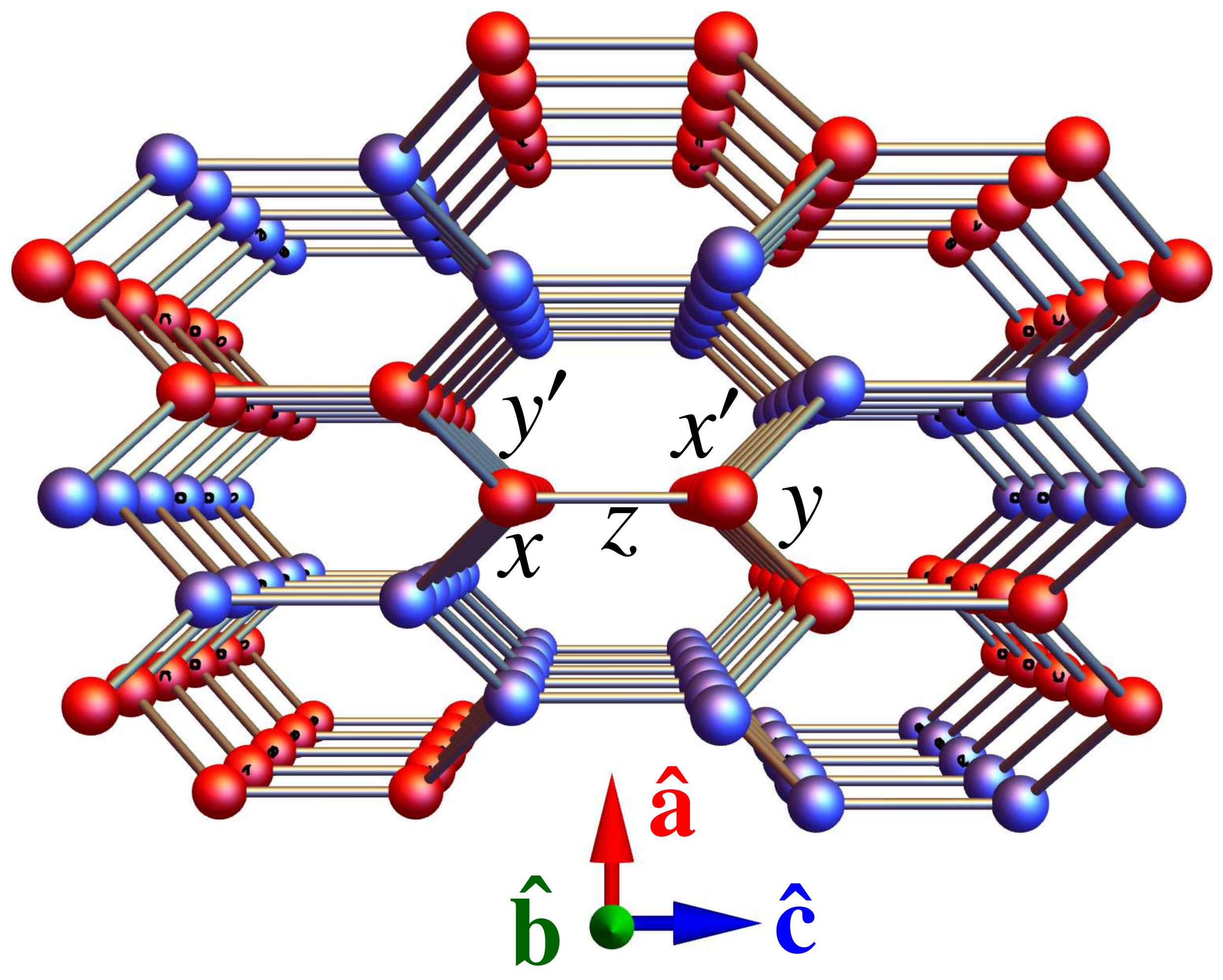
... can be induced in β-Li_2IrO_3 by magnetic field

[Ruiz *et al.* '17]

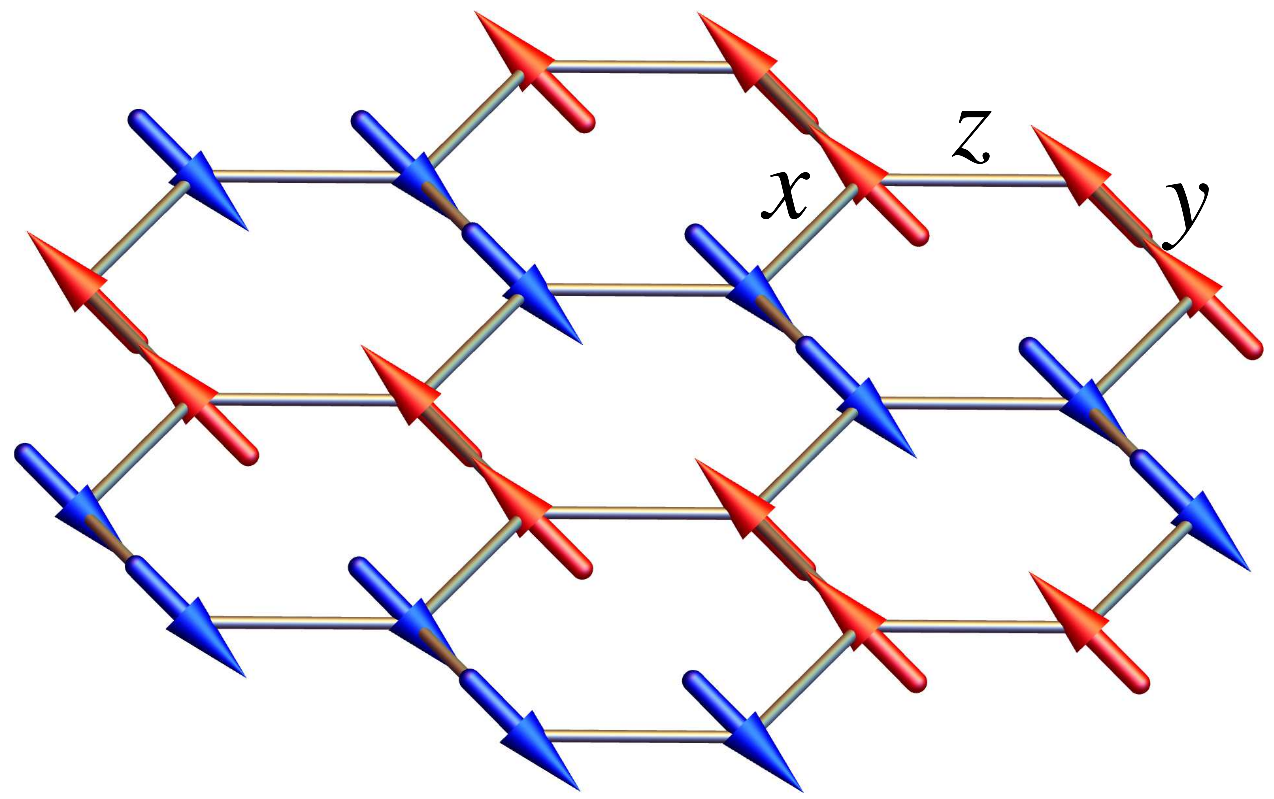
3D-2D mapping: real space

hyperhoneycomb
(skew-zigzag)





honeycomb
(zigzag)



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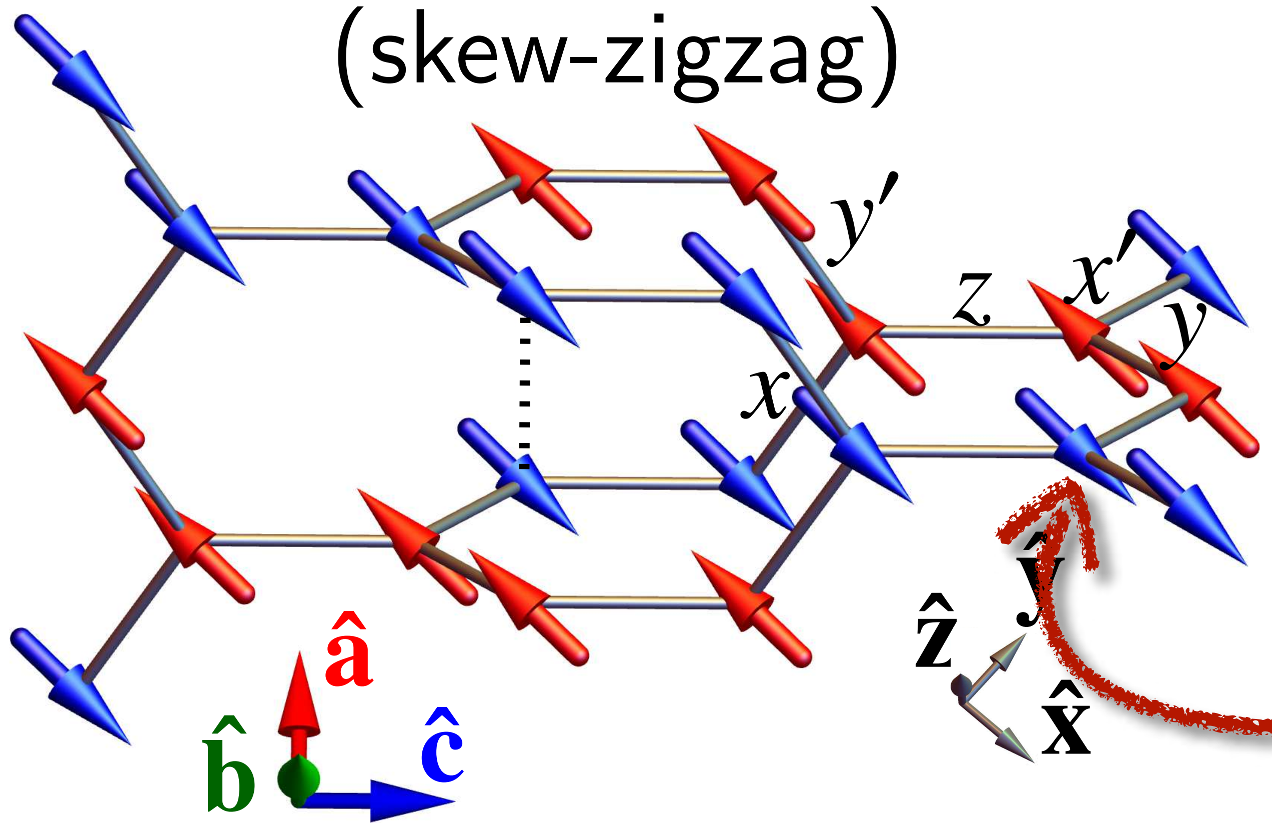
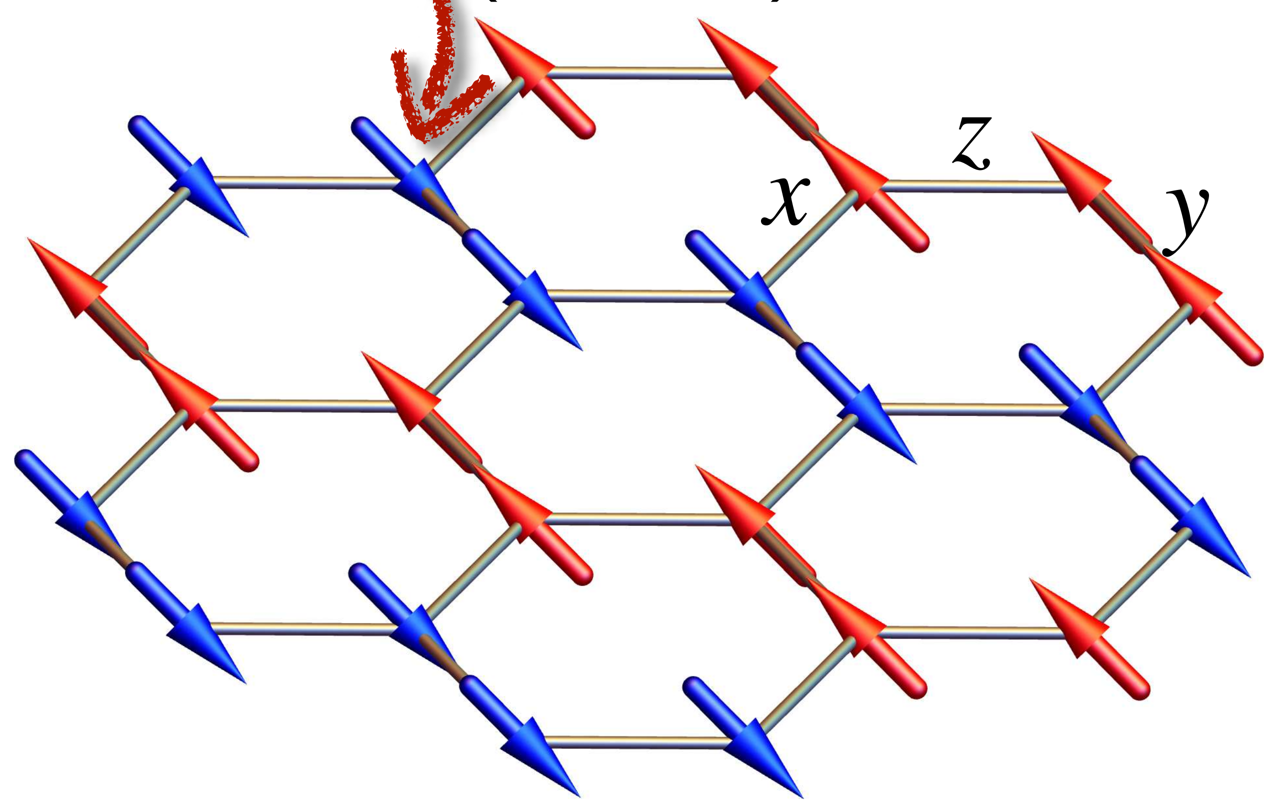
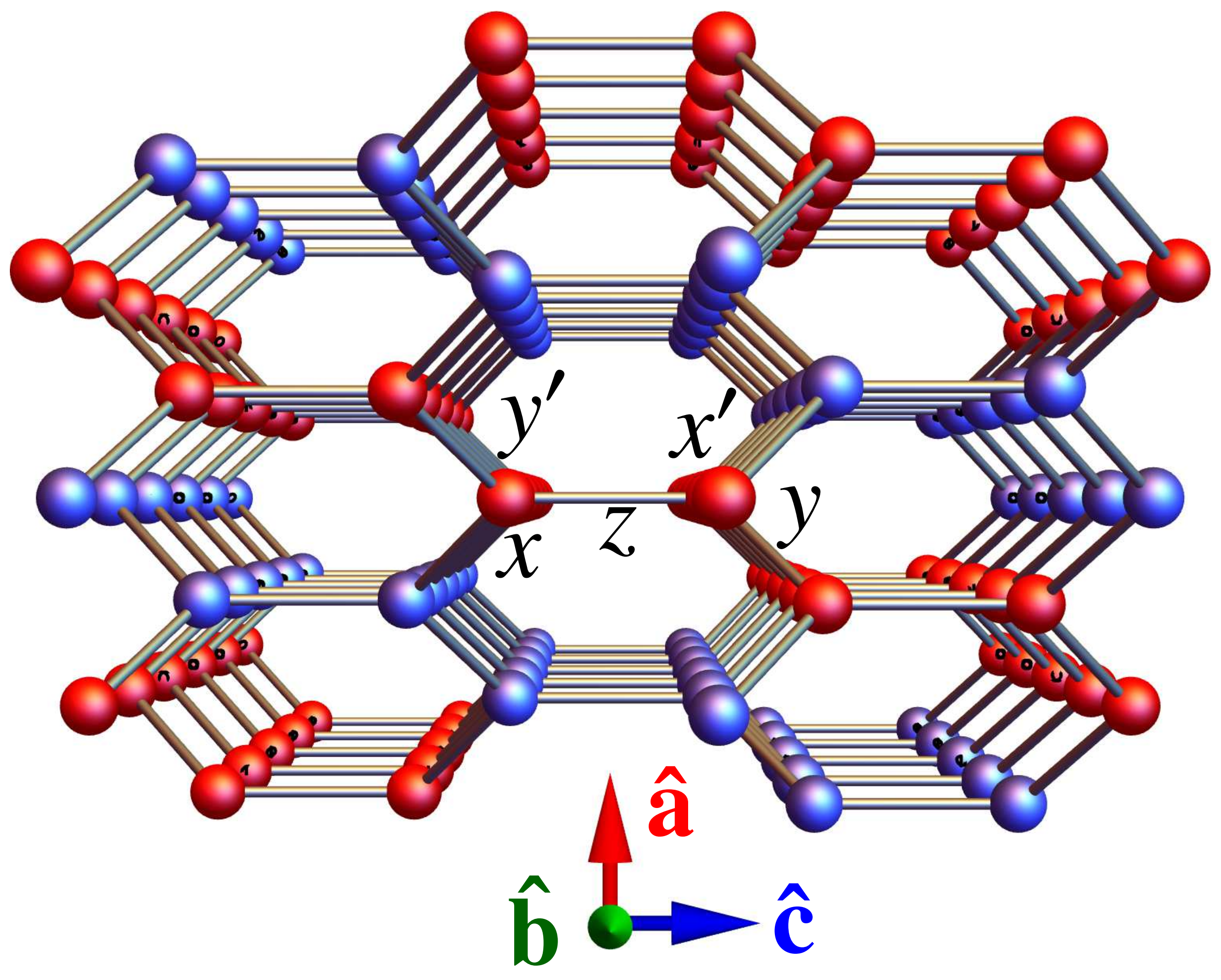


identical neighbors

honeycomb
(zigzag)

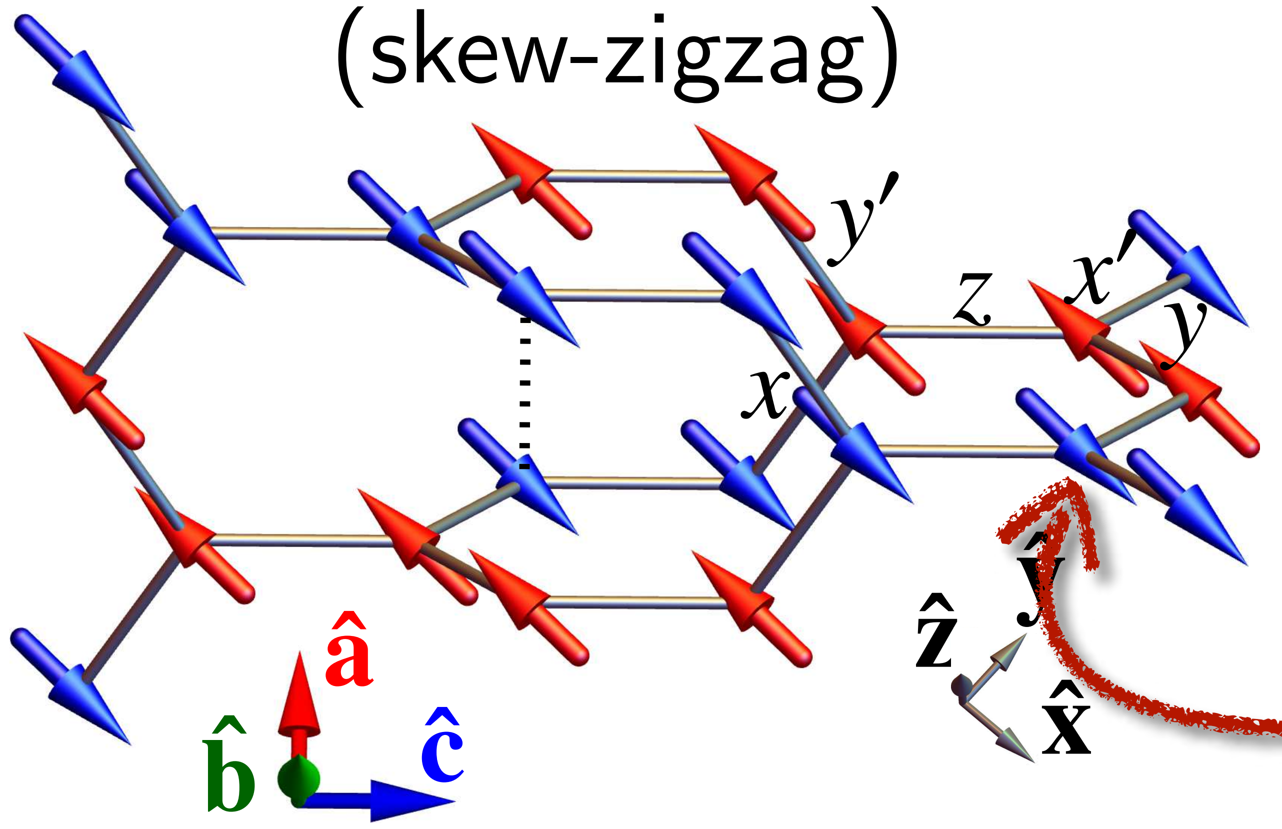


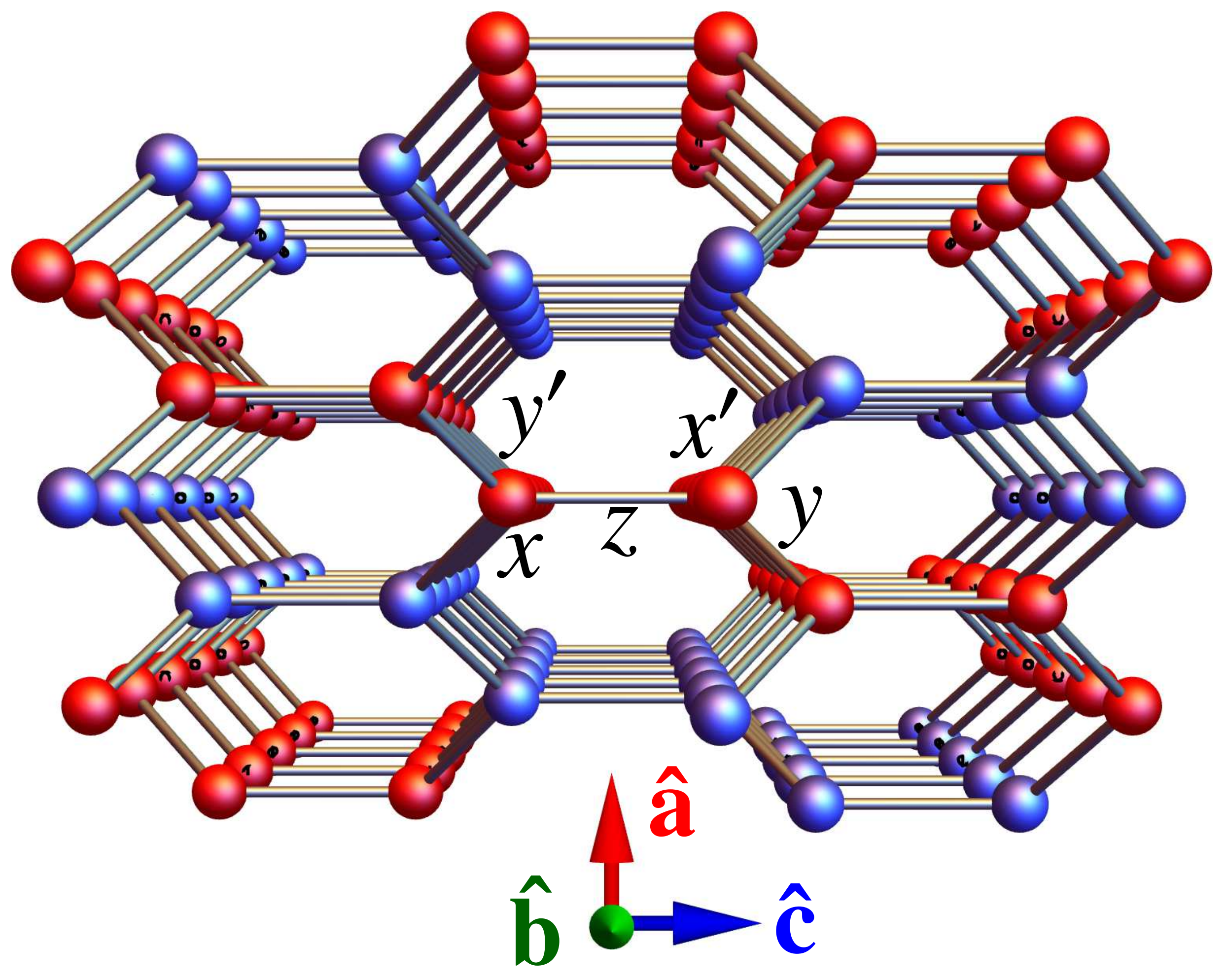
⇒ identical classical energies



3D-2D mapping: real space

hyperhoneycomb
(skew-zigzag)





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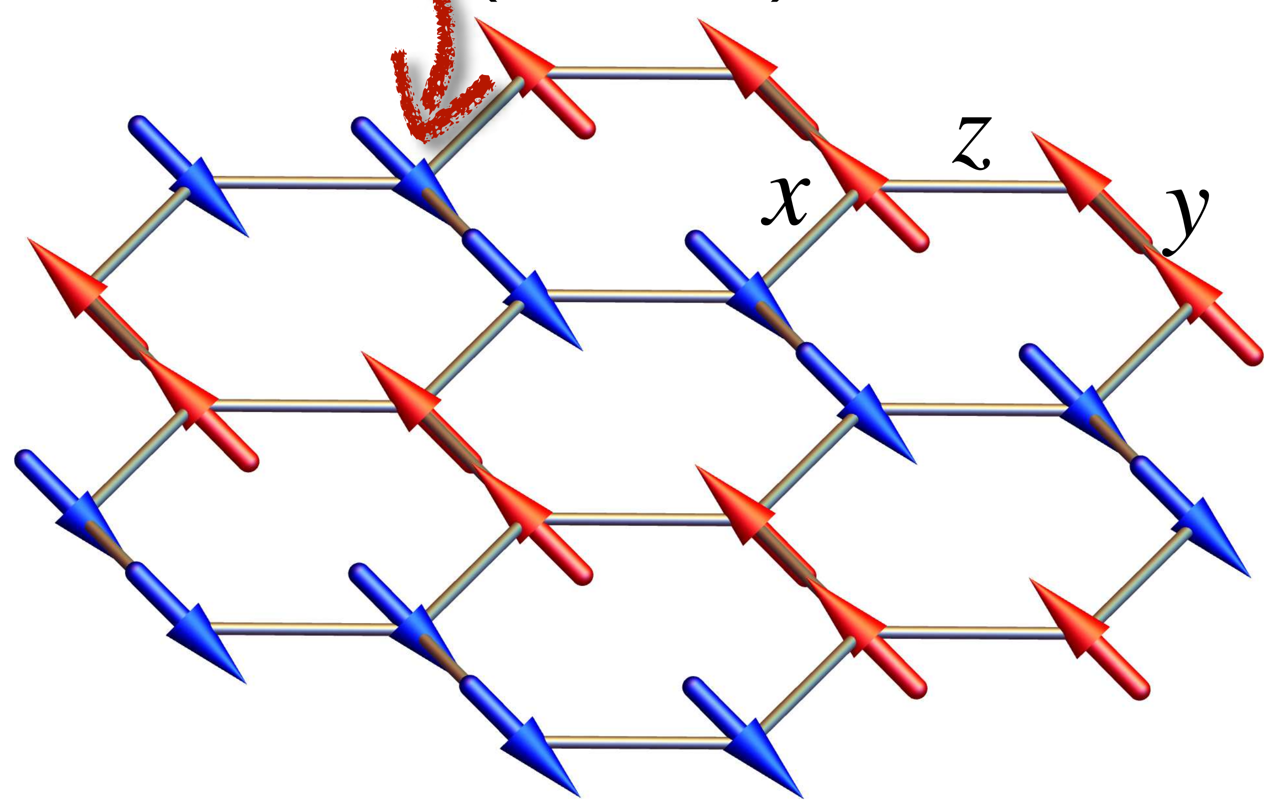
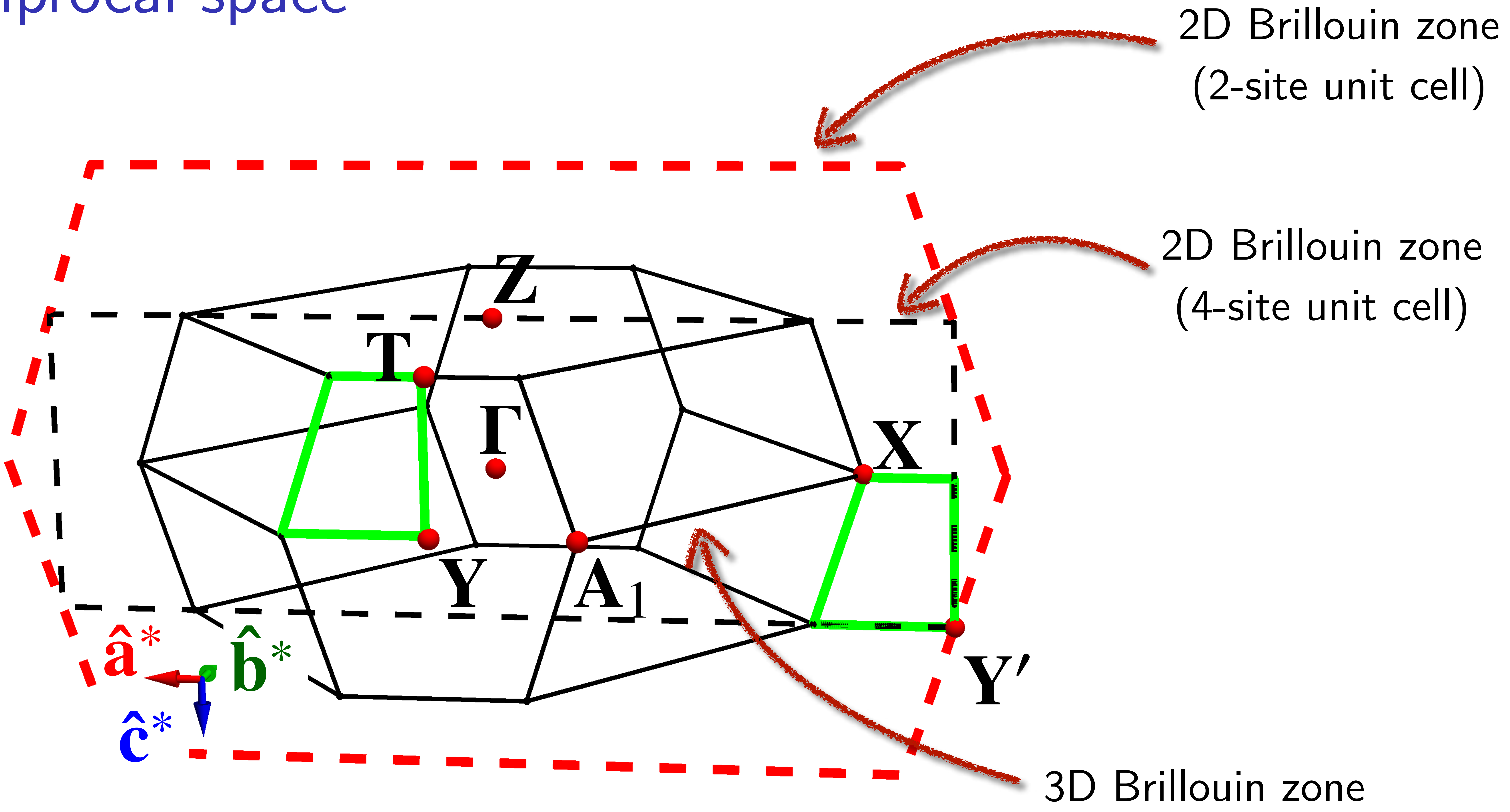


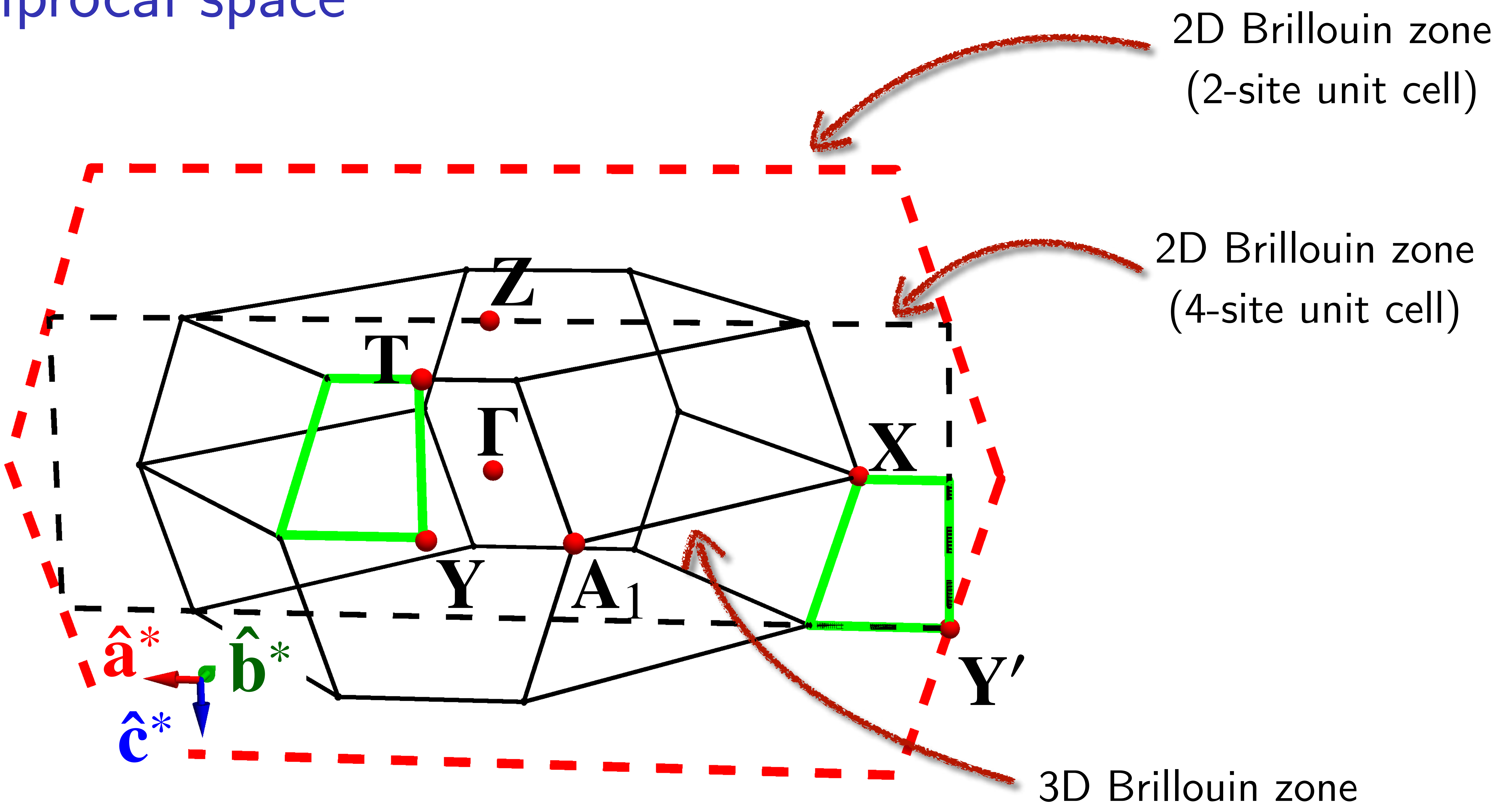
"quasi-2D" states ⟺ sites separated by **b** magnetically equivalent

3D-2D mapping: reciprocal space



... applies to *all* high-symmetry points

3D-2D mapping: reciprocal space



“quasi-2D” states $\Longleftrightarrow$ ordering wavevector in *ac* plane

(modulo reciprocal lattice translations)

... applies to *all* high-symmetry points

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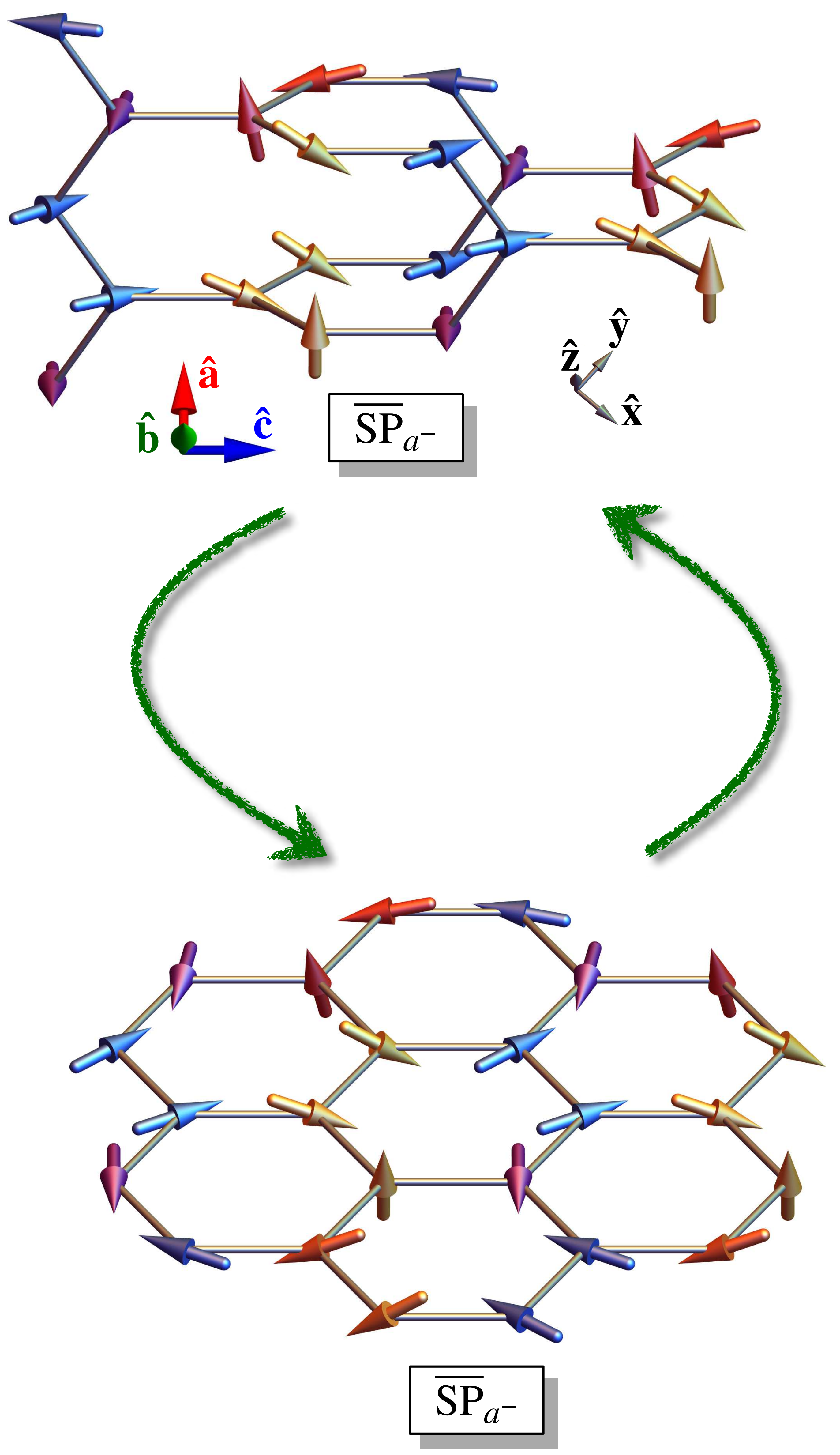
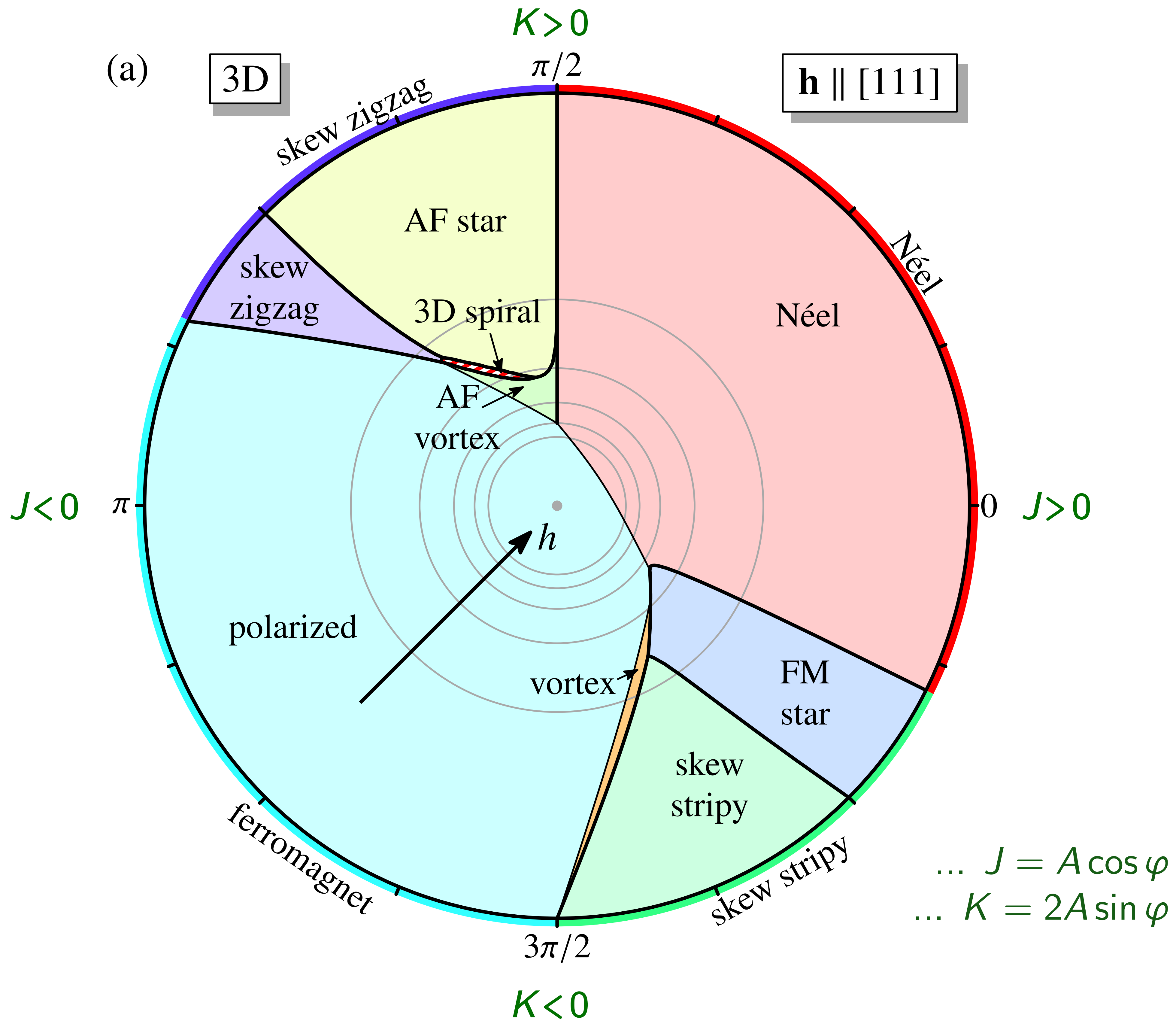


Example #1: Heisenberg-Kitaev model in a magnetic field

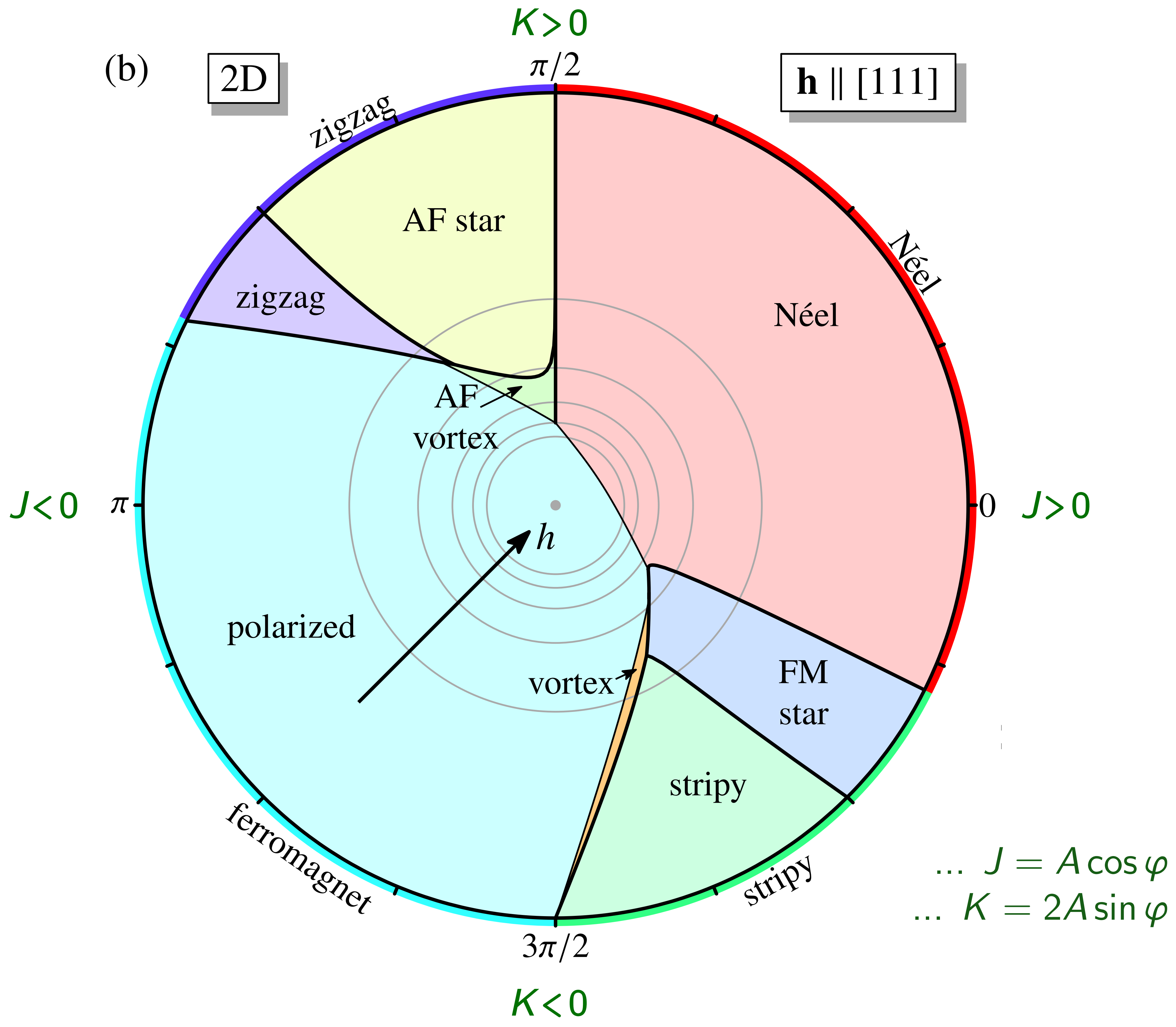
$$\mathcal{H}_{\rm HK} = J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j + K\sum_{\langle ij\rangle_\gamma} S_i^\gamma S_j^\gamma - \mathbf{h}\cdot\sum_i \mathbf{S}_i$$

hyperhoneycomb



[Krüger, Vojta, LJ, arXiv:1907.05423]

honeycomb



[LJ, Andrade, Vojta, PRL '16]

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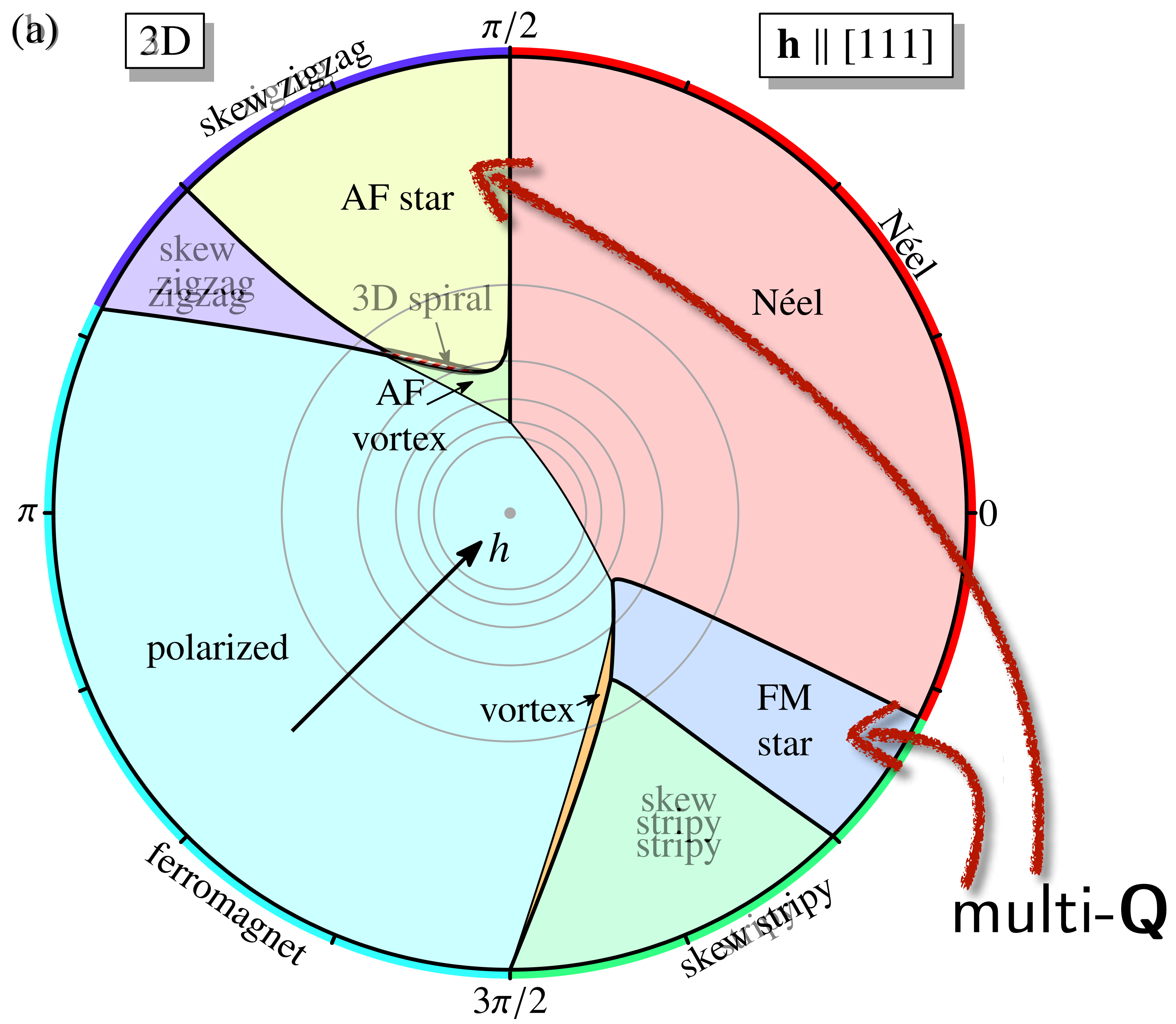
hyperhoneycomb+honeycomb



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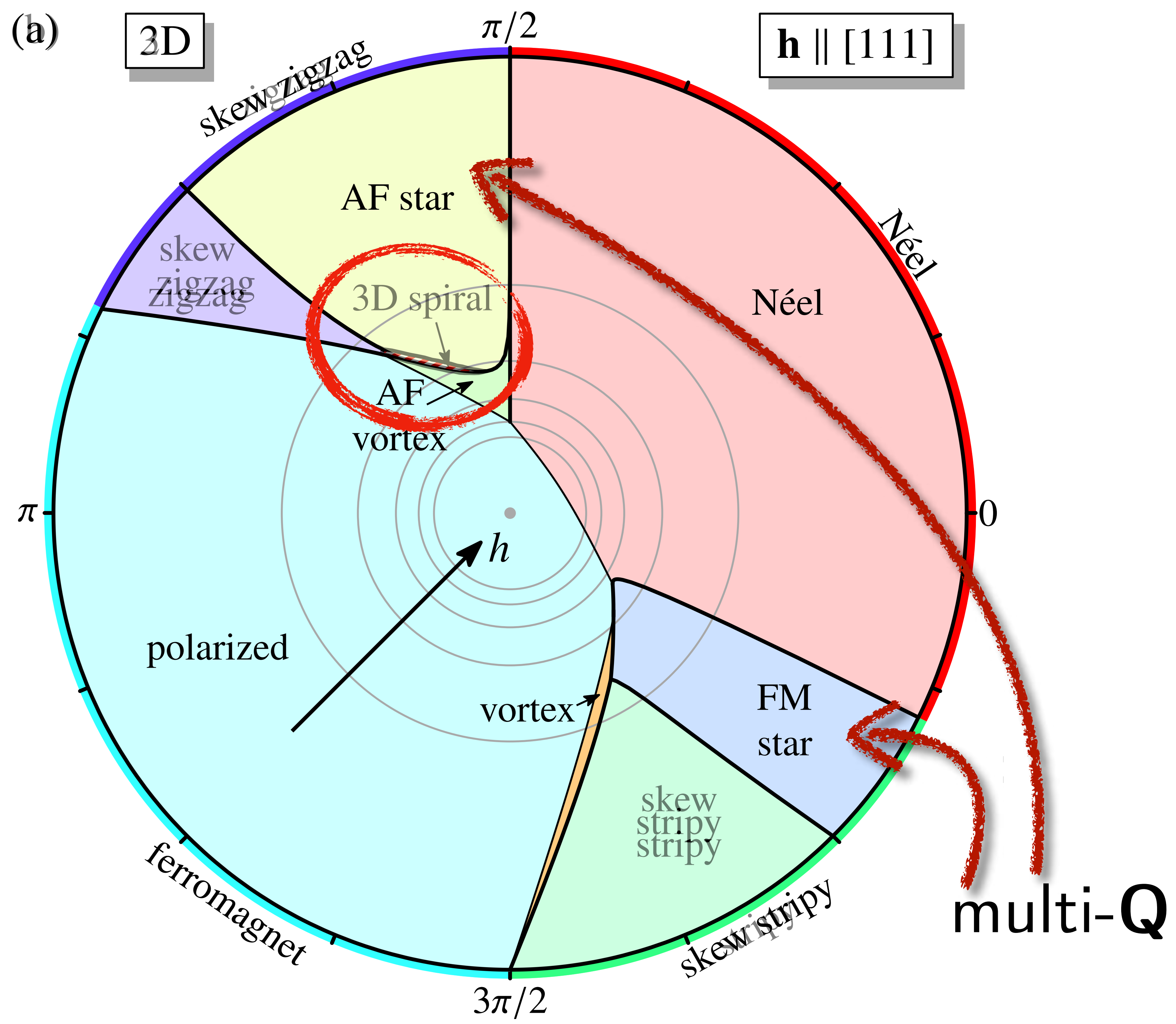
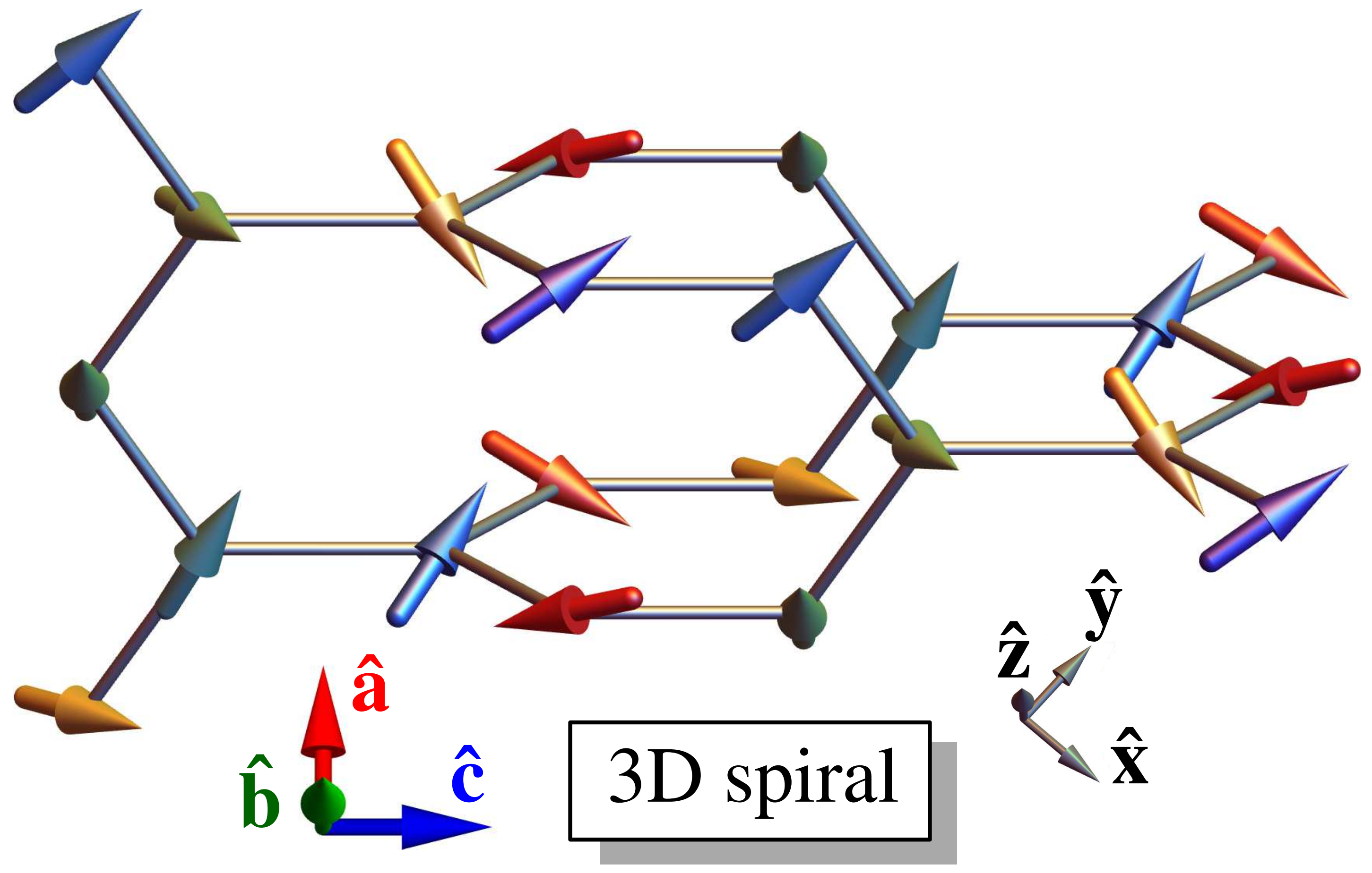
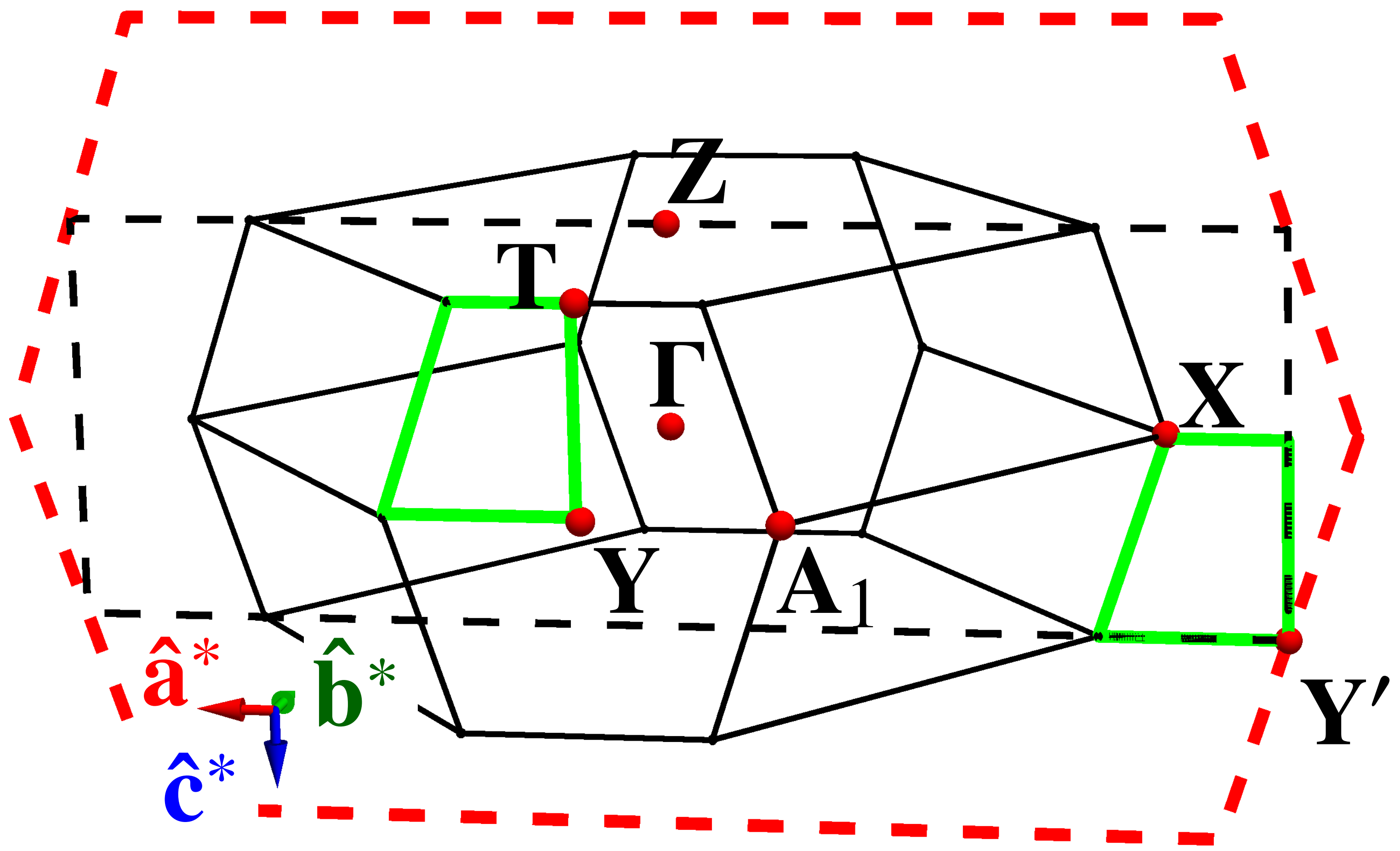


3D spiral state



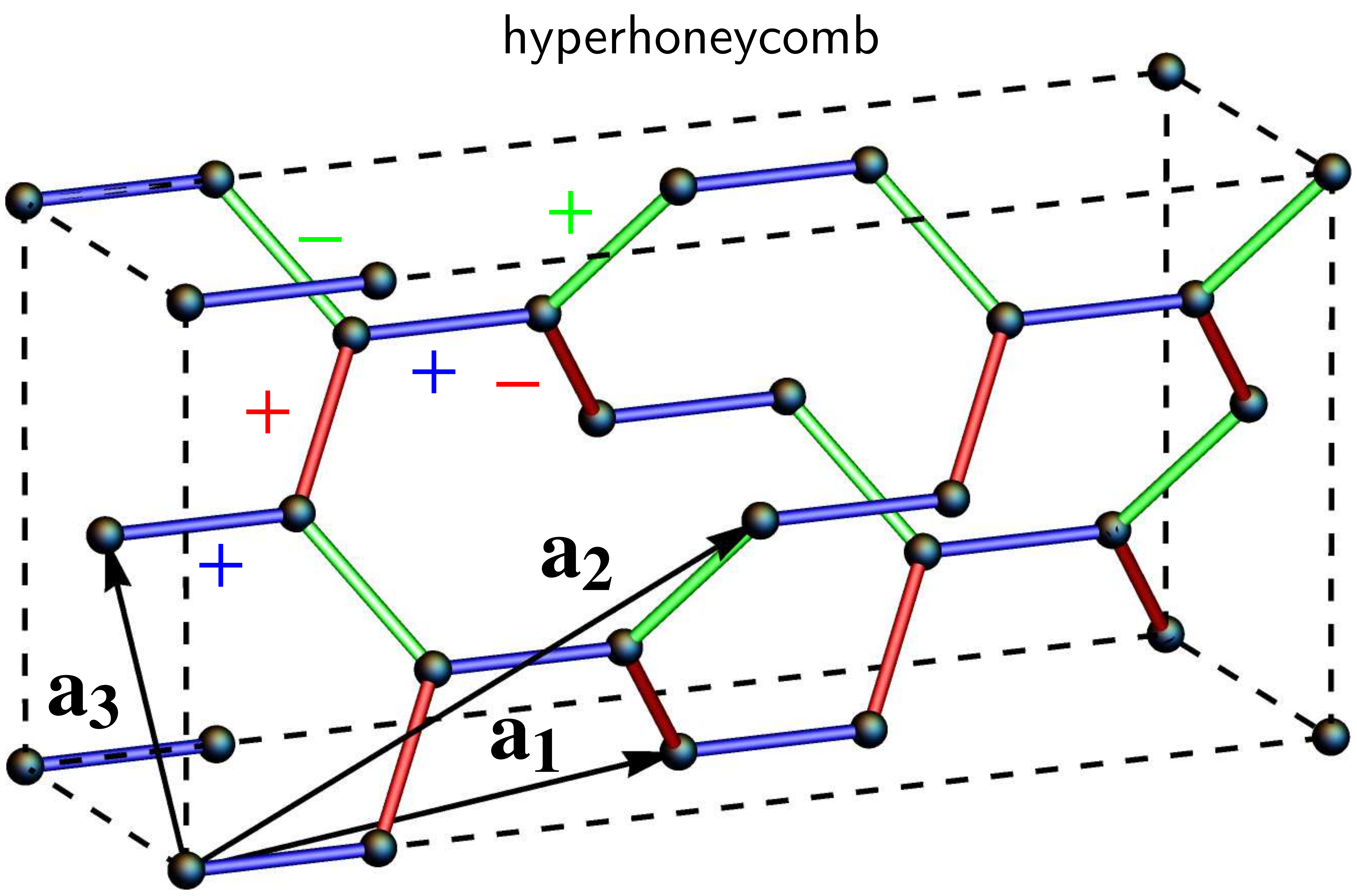


magnetically inequivalent sites along **b**!

$$\mathbf{Q} = \frac{2}{3}\mathbf{Y} \notin \ ac \text{ plane!}$$

$\Rightarrow$ “true-3D” state

Example #2: Γ interactions



2 different types of x and y bonds

... but same local environment

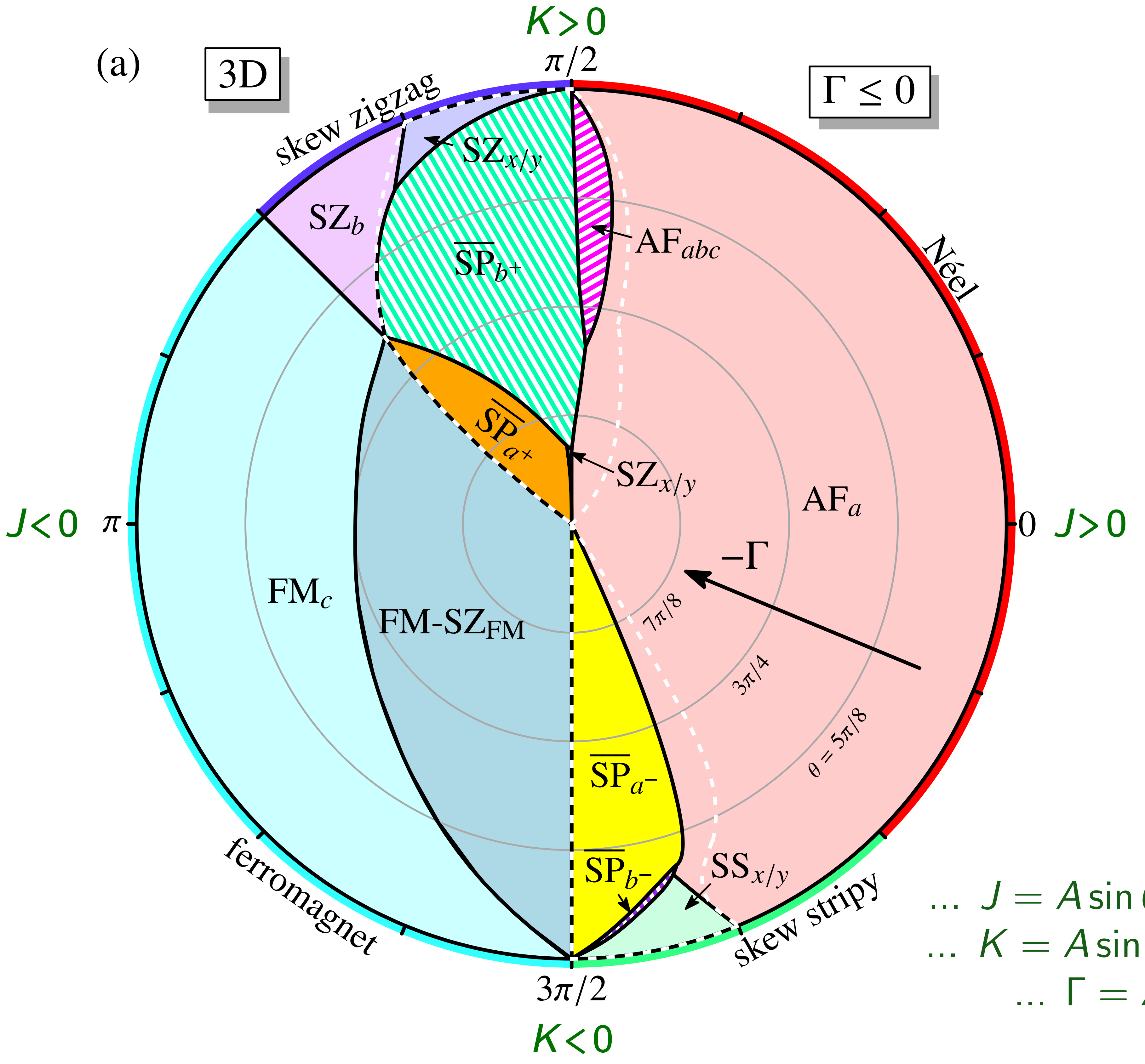
... choose interactions accordingly

[Lee & Kim, PRB '15]

Example #2: HK±Γ model

$$\mathcal{H}_{\mathrm{HK\Gamma}} = \sum_{\langle ij \rangle_\gamma} \left[J\mathbf{S}_i \cdot \mathbf{S}_j + K S_i^\gamma S_j^\gamma \pm \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \right]$$

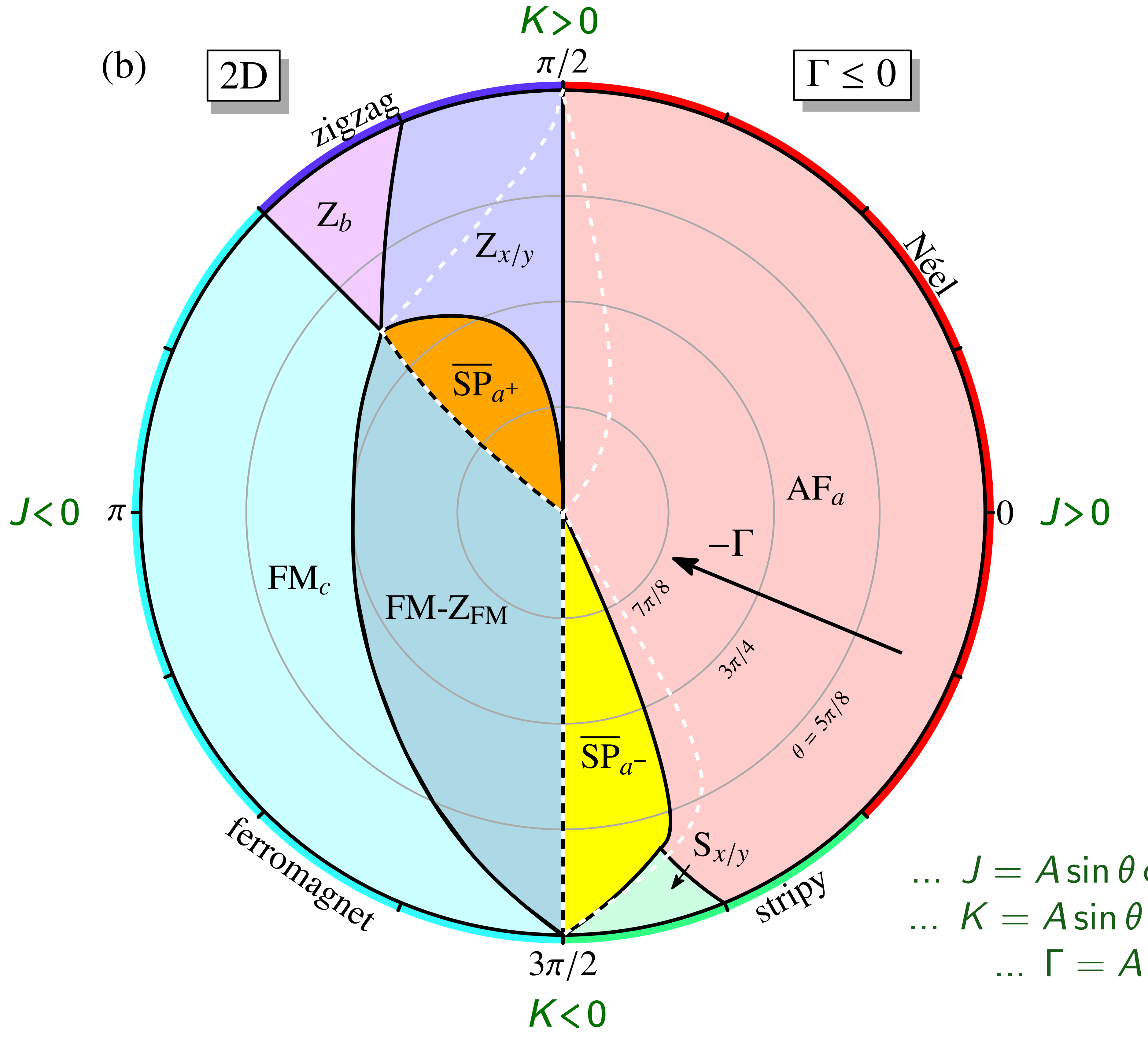
hyperhoneycomb



... $J = A \sin\theta \cos\varphi$
... $K = A \sin\theta \sin\varphi$
... $\Gamma = A \cos\theta$

[Lee & Kim, PRB '15]

honeycomb



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[Krüger, Vojta, LJ, arXiv:1907.05423]

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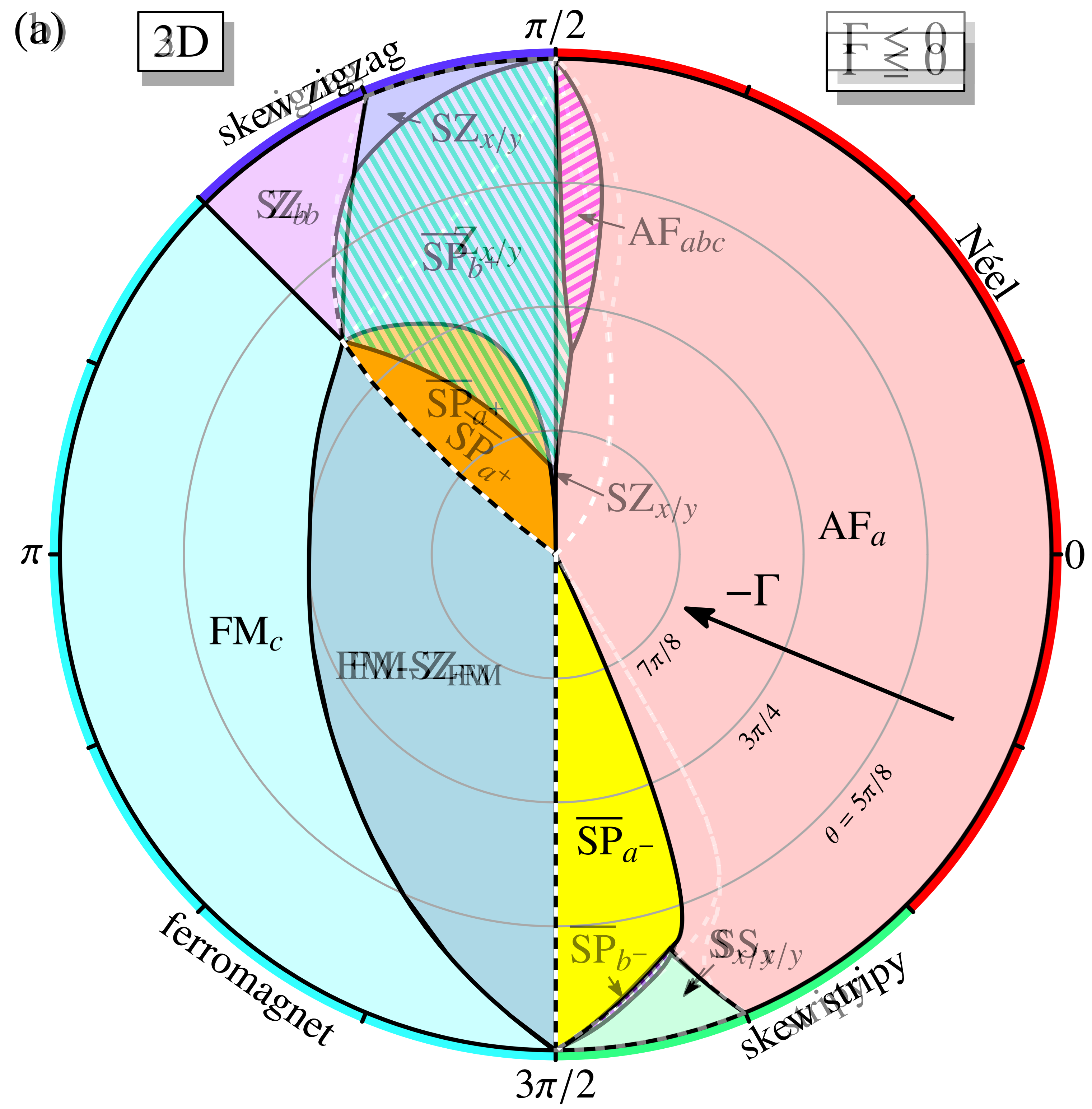
hyperhoneycomb+honeycomb



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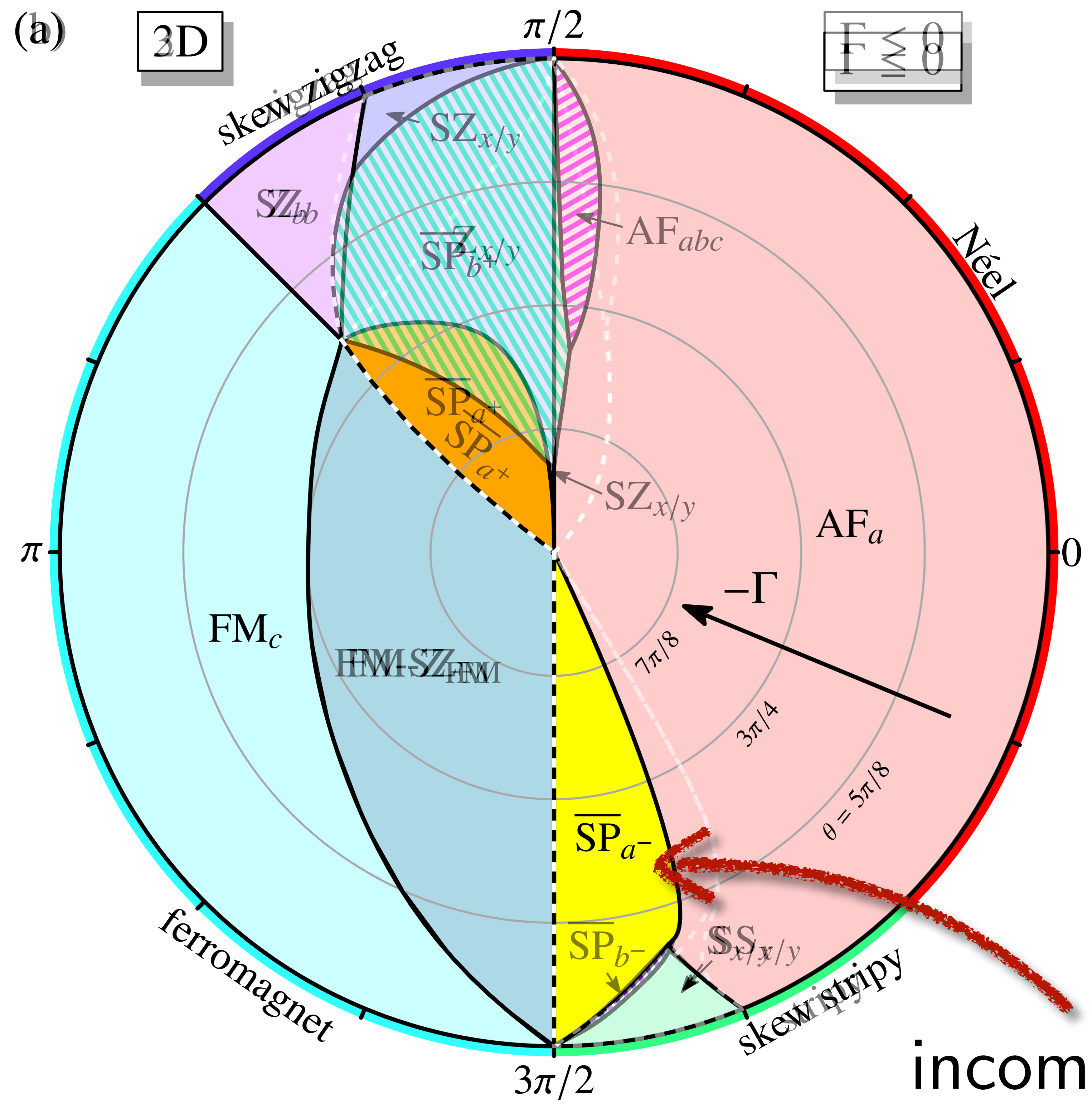
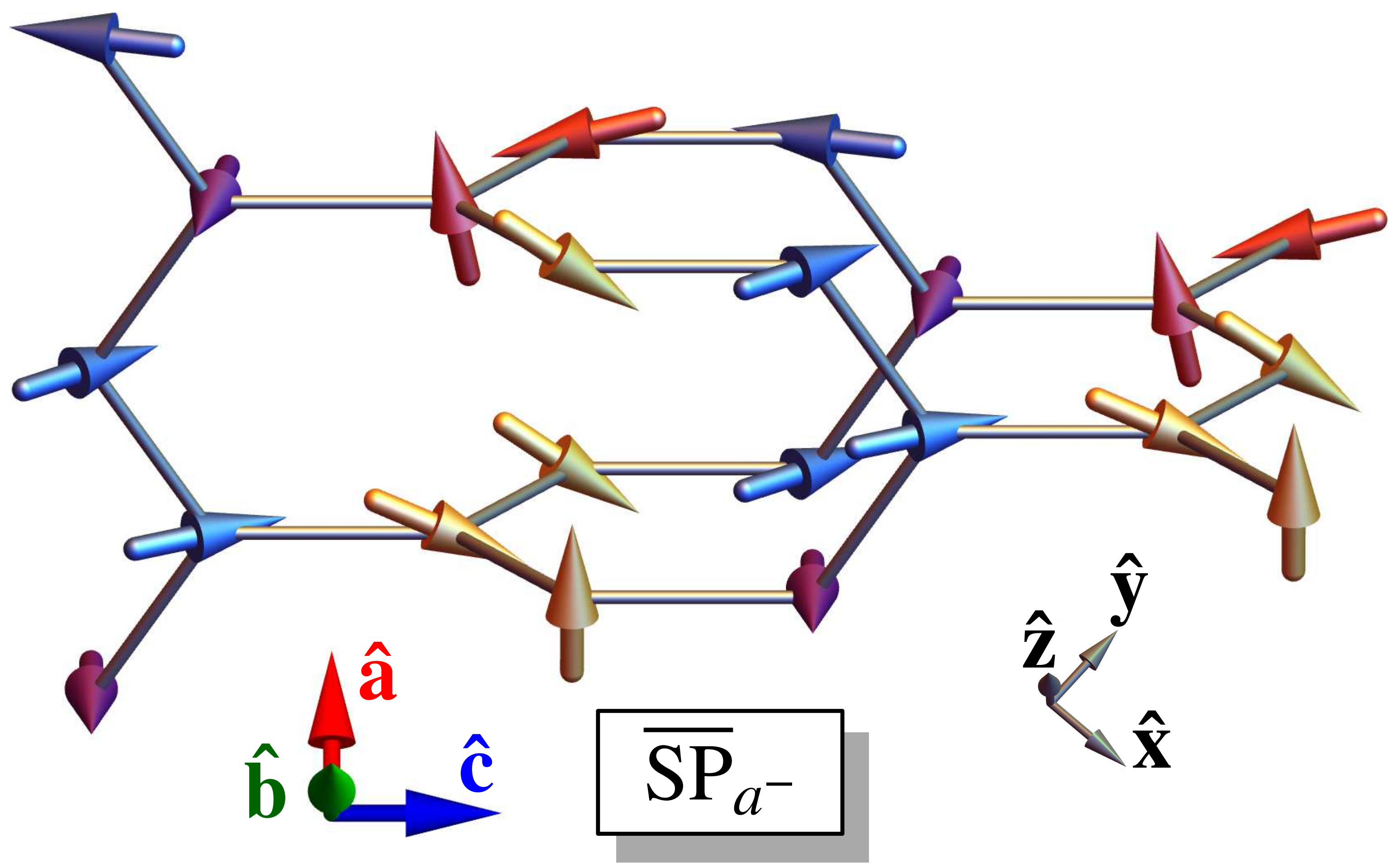
hyperhoneycomb+honeycomb

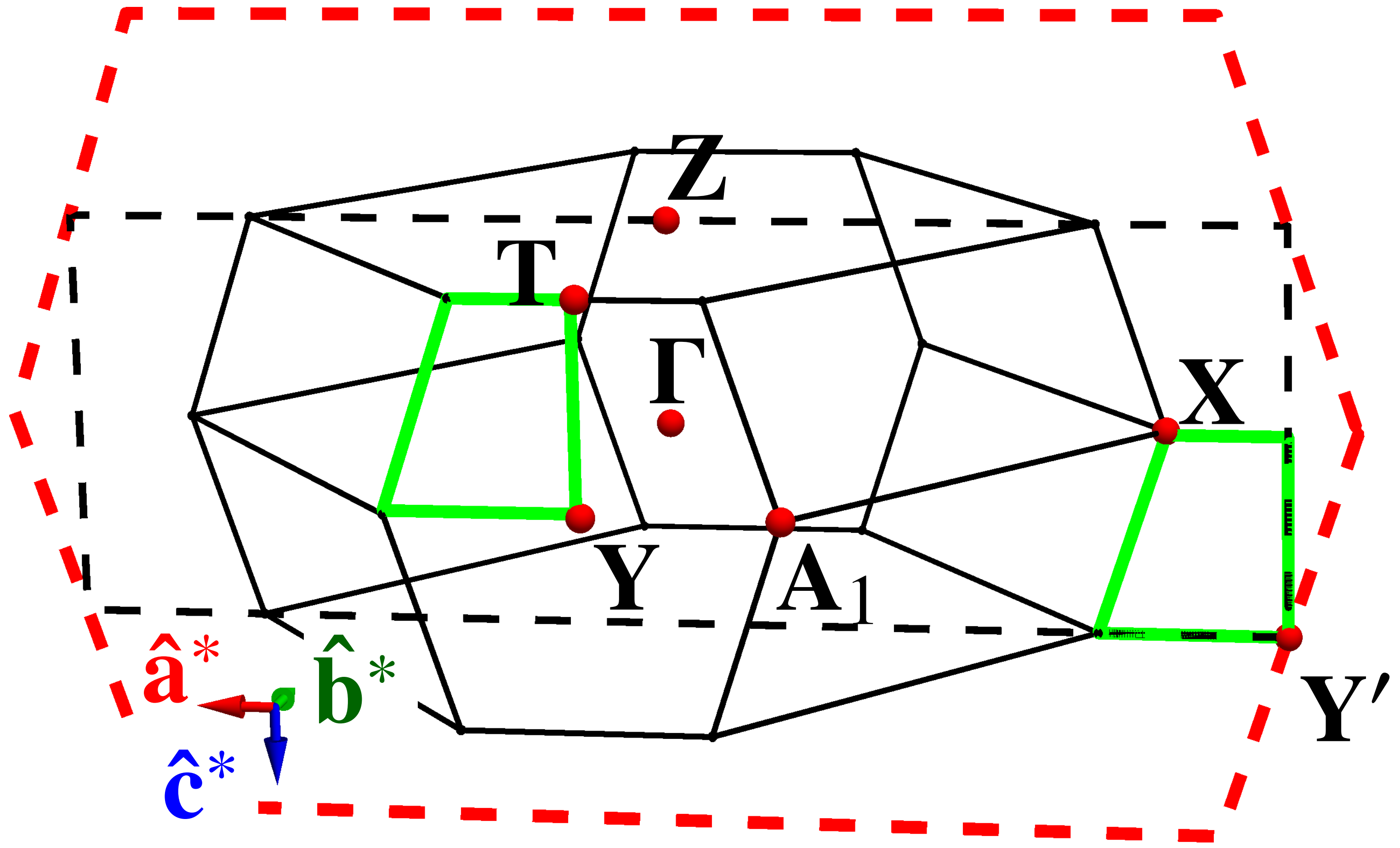


incommensurate spiral (Li_2IrO_3)

Incommensurate spiral



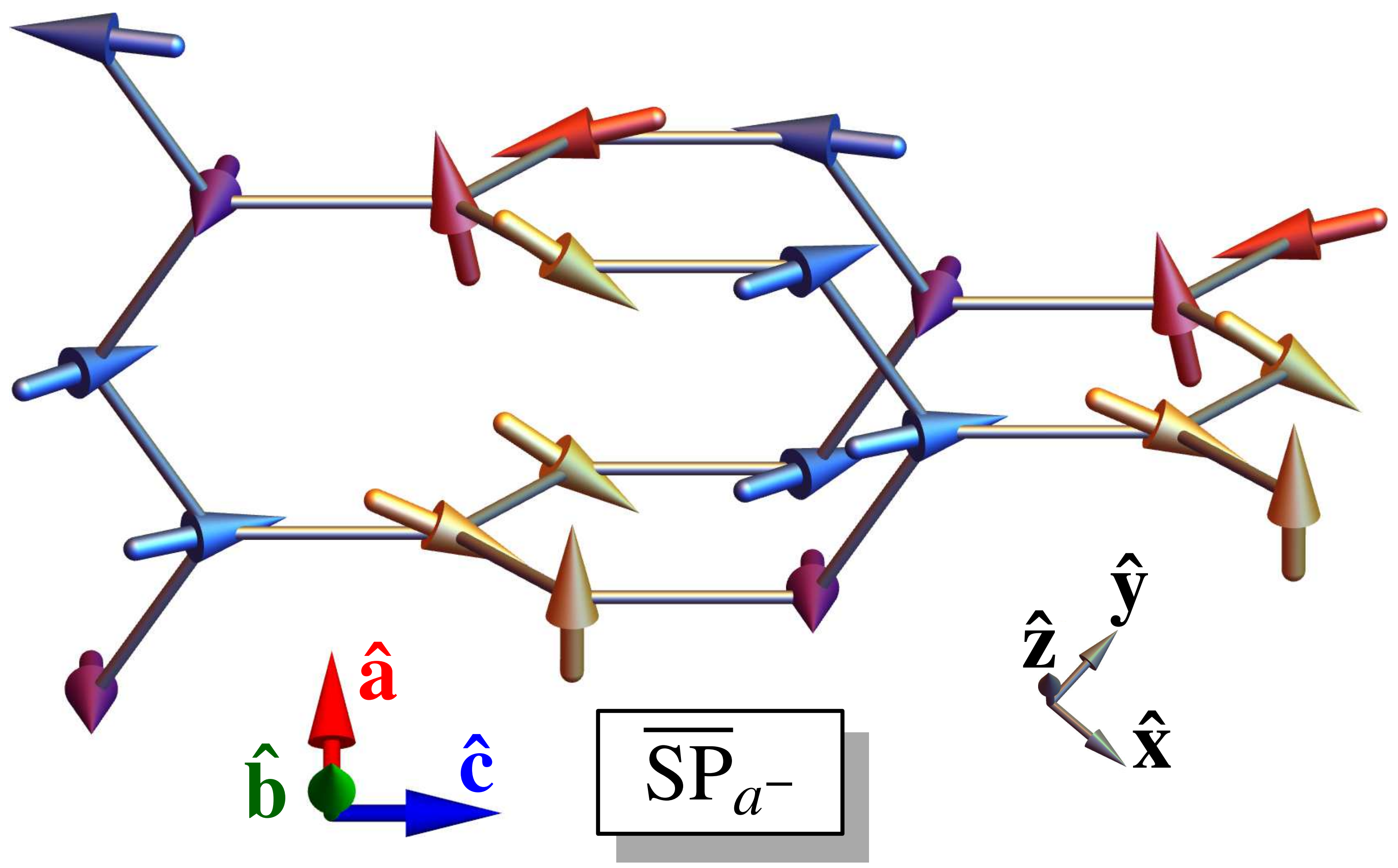
magnetically equivalent sites along **b**!



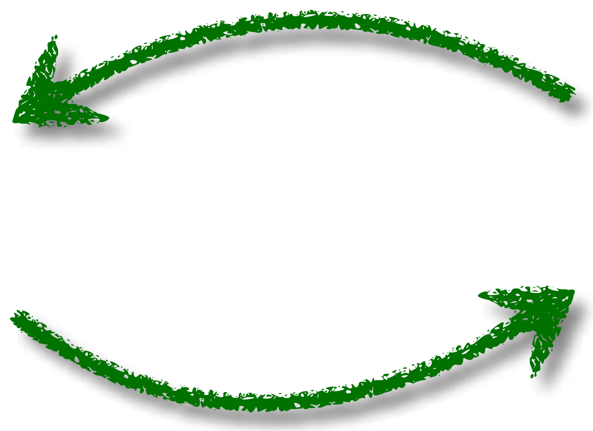
$\mathbf{Q} \parallel \mathbf{a}^* \in$ *ac* plane!

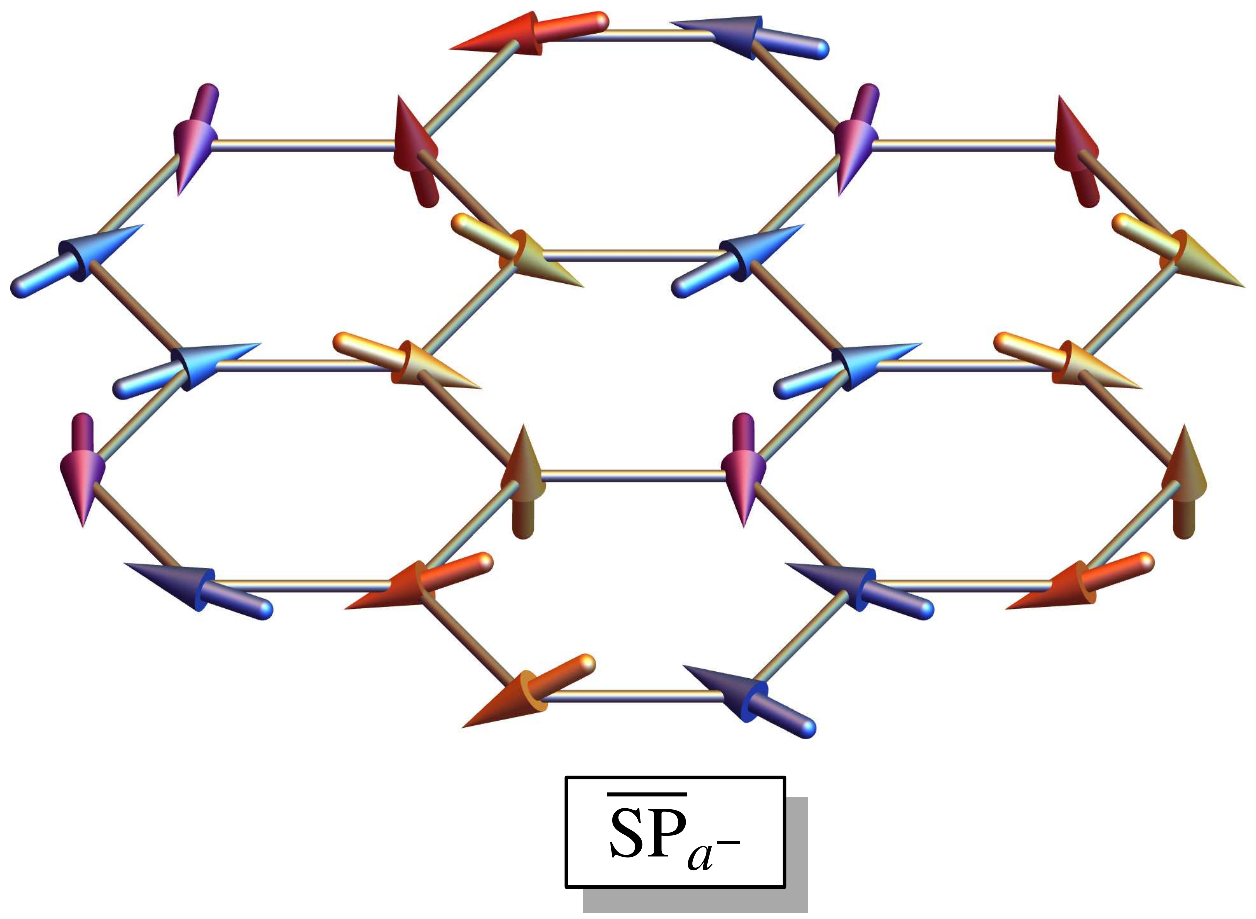
⇒ "quasi-2D" state

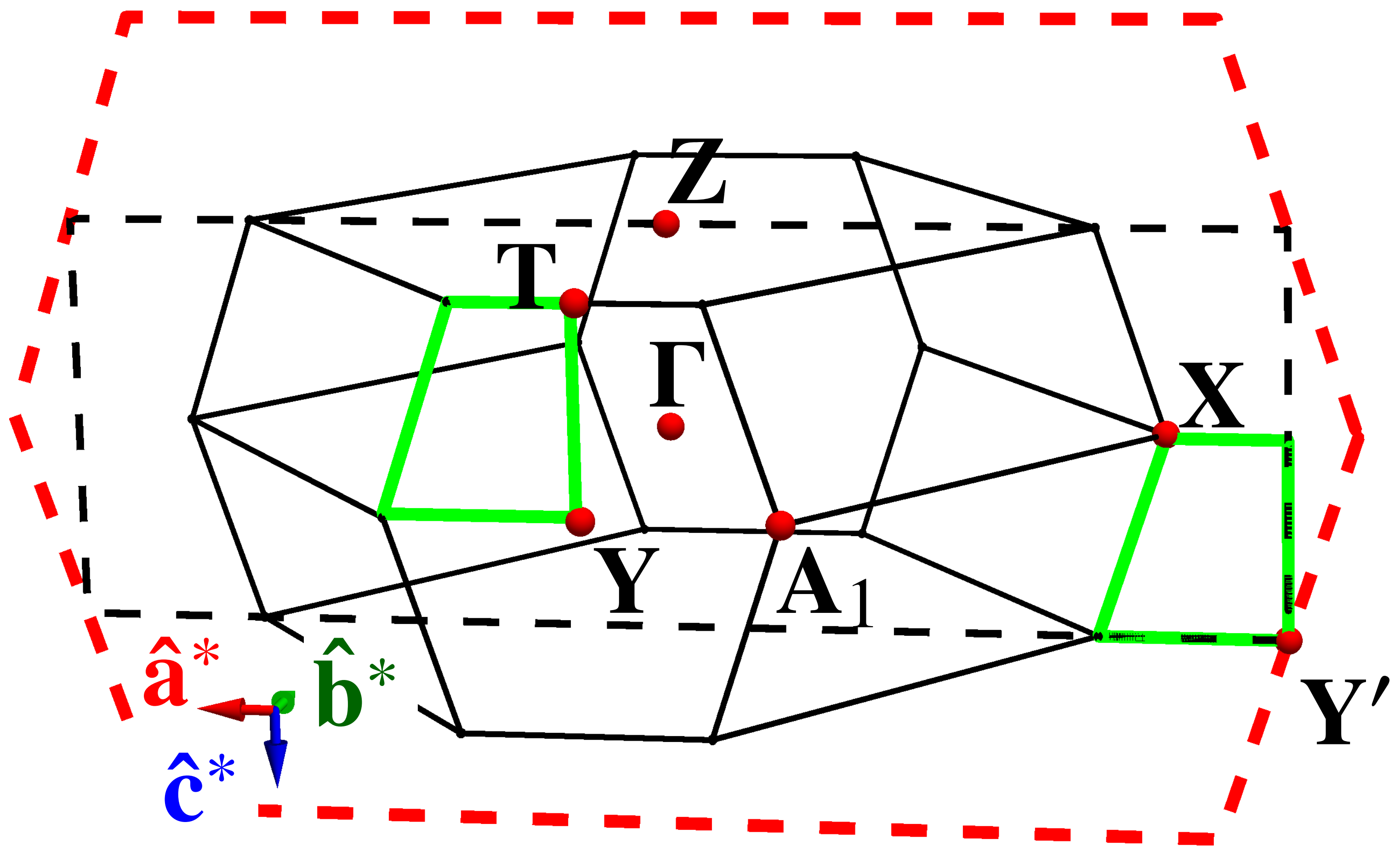
Incommensurate spiral



3D-2D equivalence



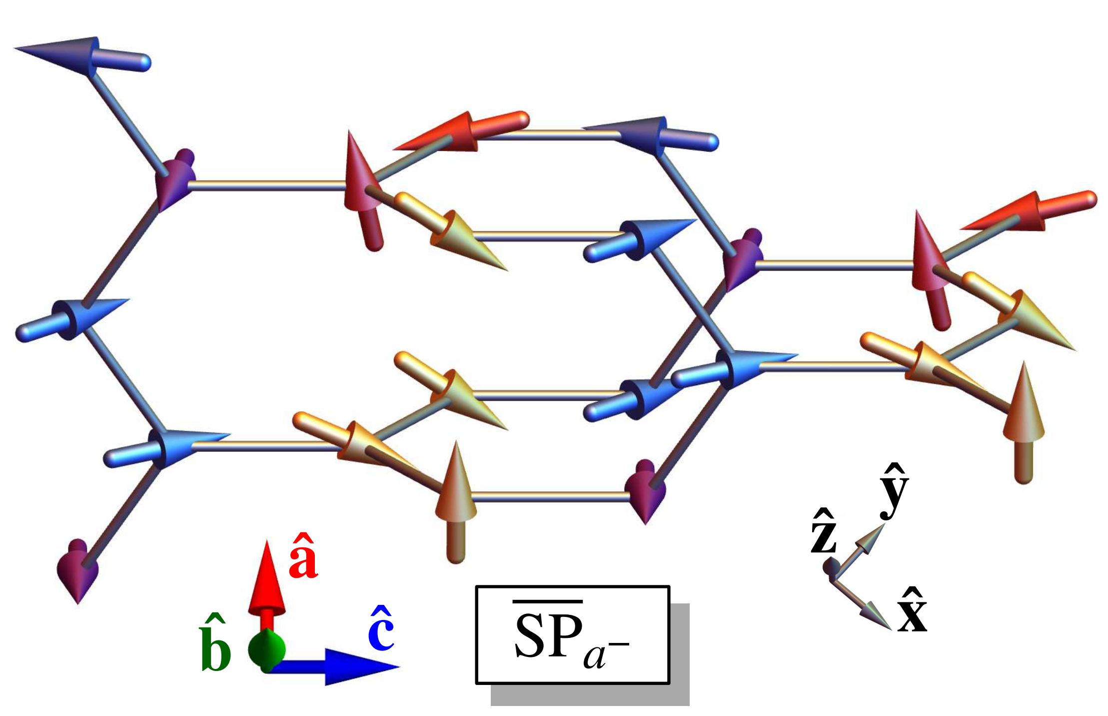




$\mathbf{Q} \parallel \mathbf{a}^* \in$ *ac* plane!

$\boxed{\Rightarrow \text{“quasi-2D” state}}$

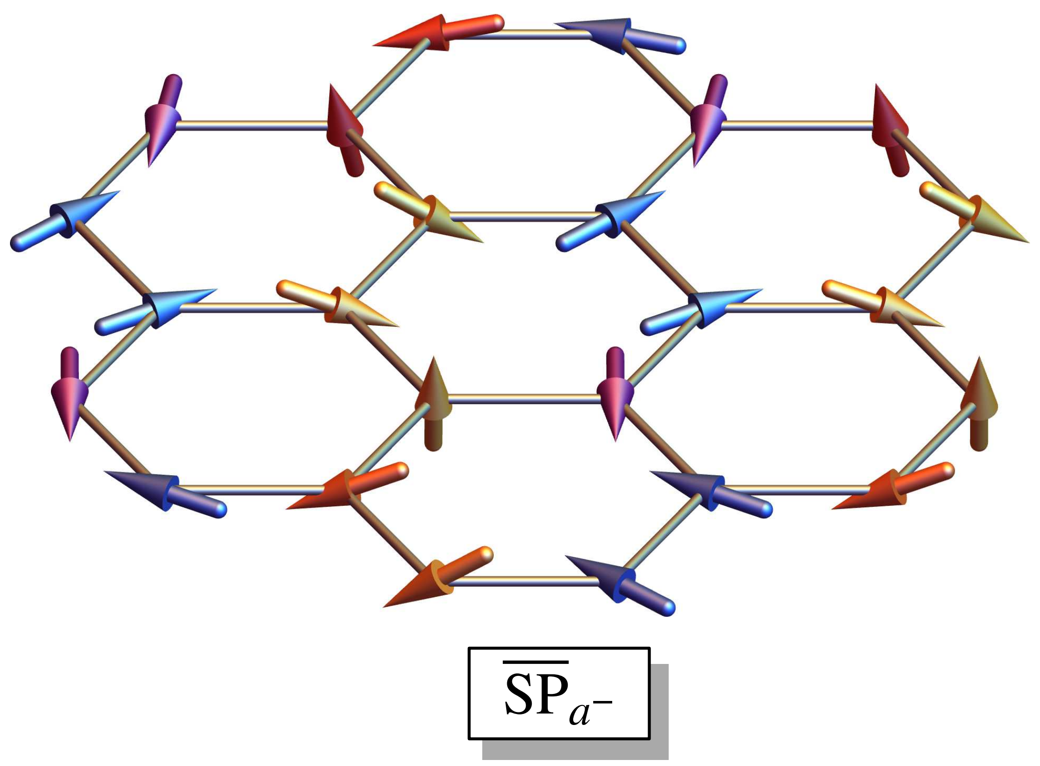
Commensurate period-3 state ($J \ll |K|, |\Gamma|$)



Period-3 state
3D HK±Γ

"*K* state"
[Ducatman *et al.*, PRB '18]

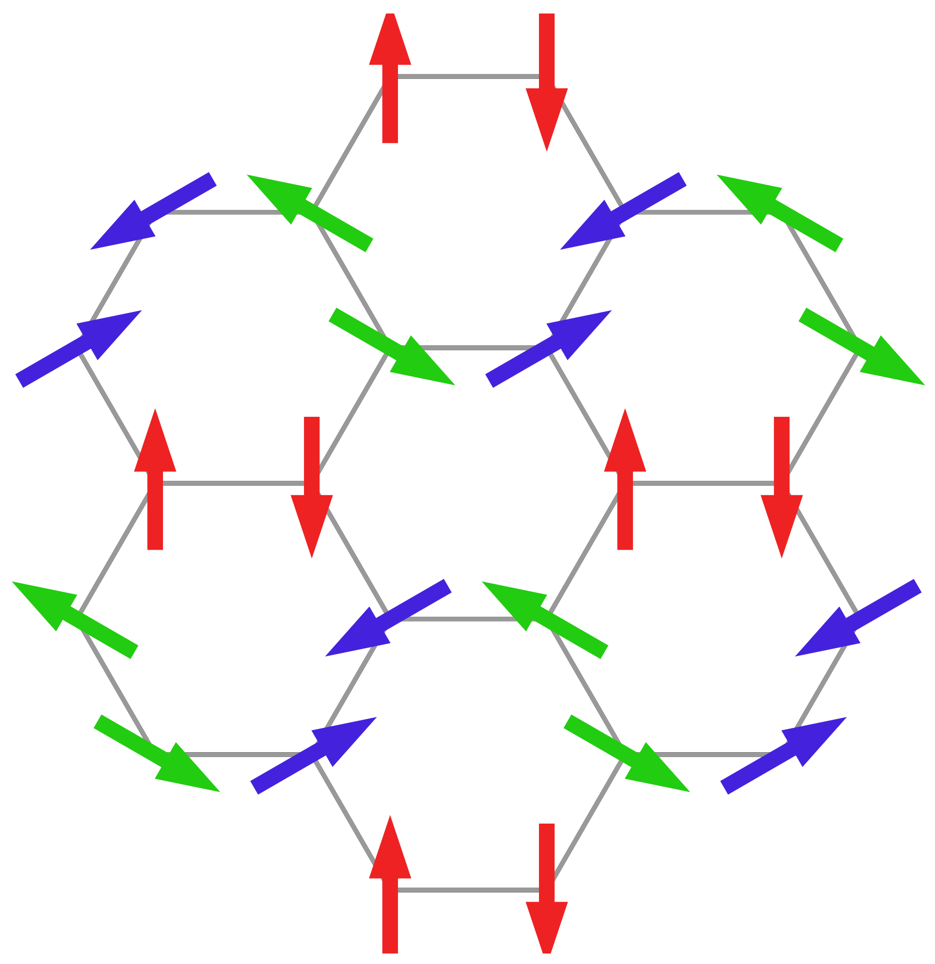
3D-2D equivalence



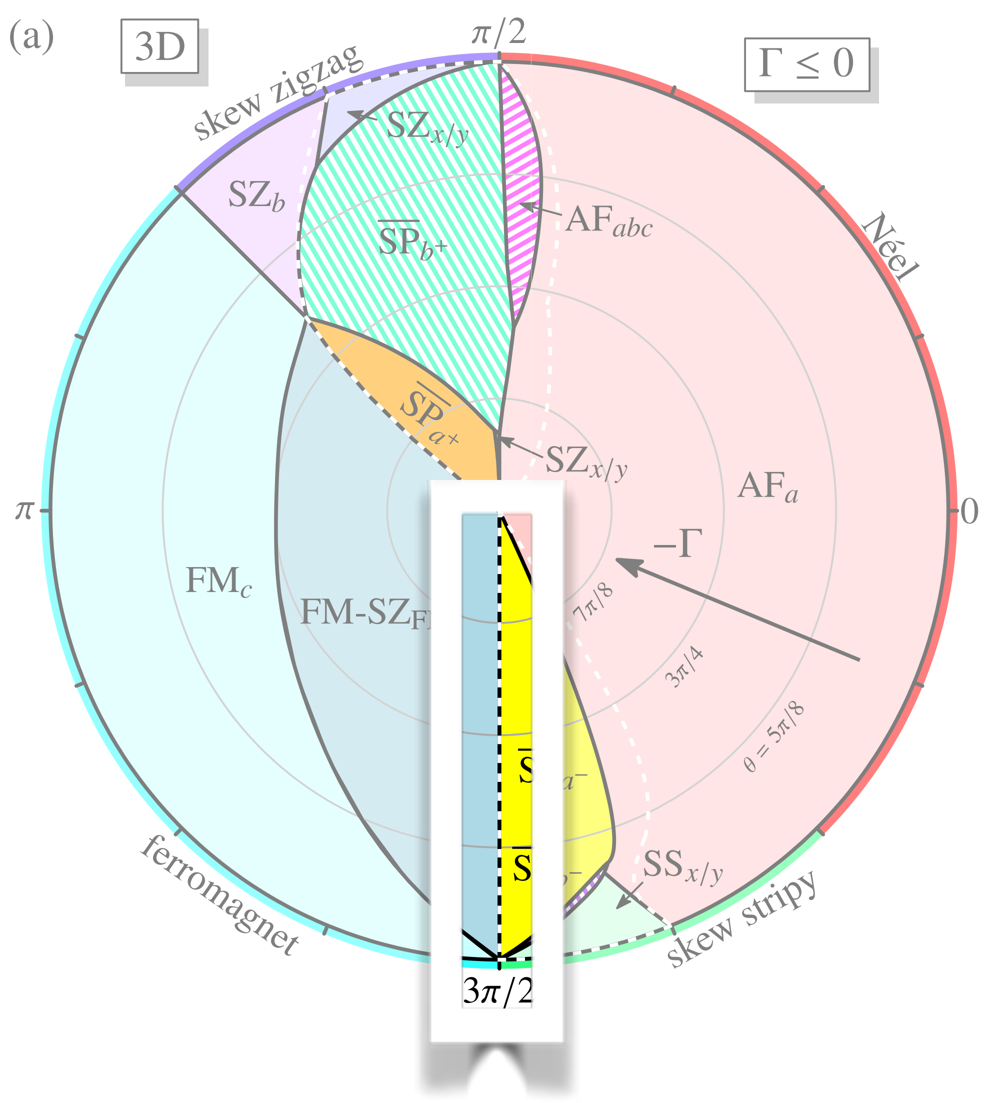
Period-3 state
2D HK±Γ

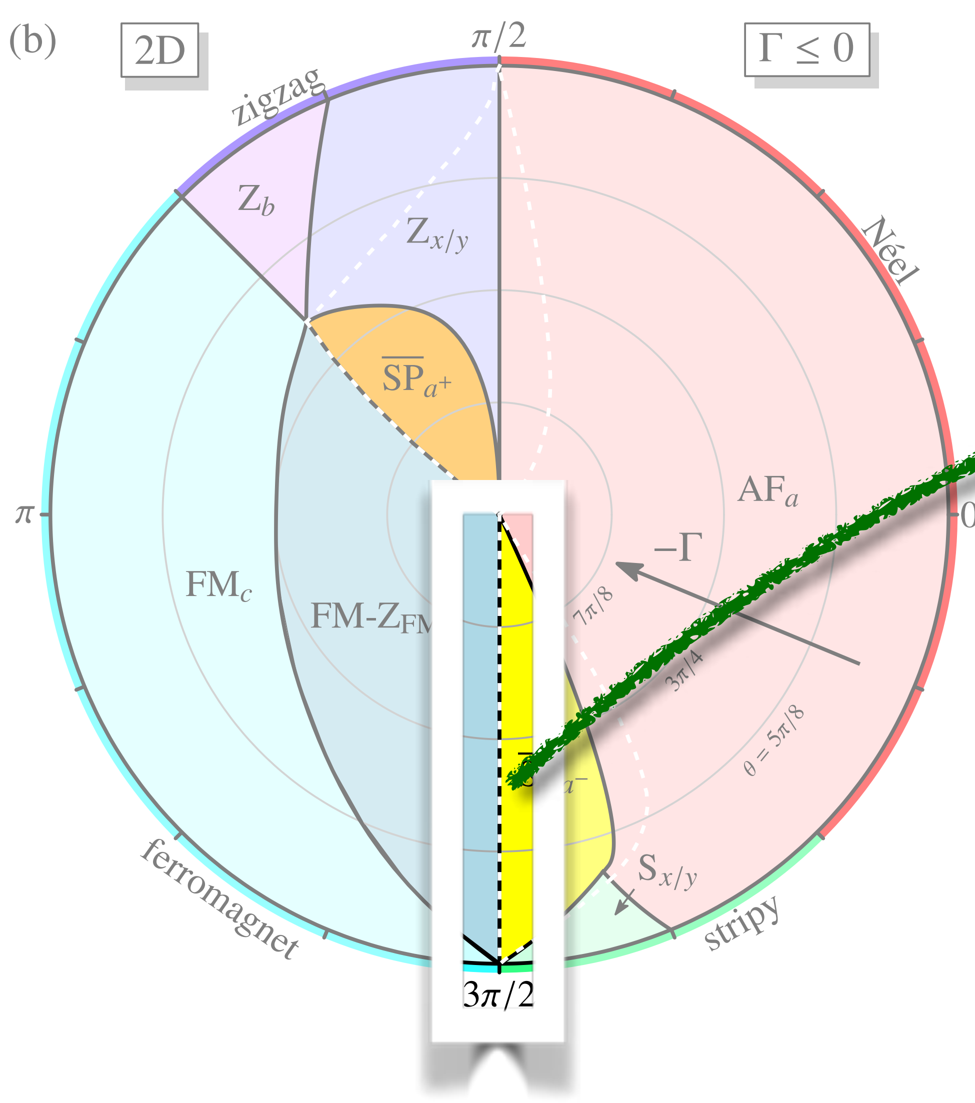
Duality transformation

... that rotates spins by $\pi/2$ ($3\pi/2$) about z axis

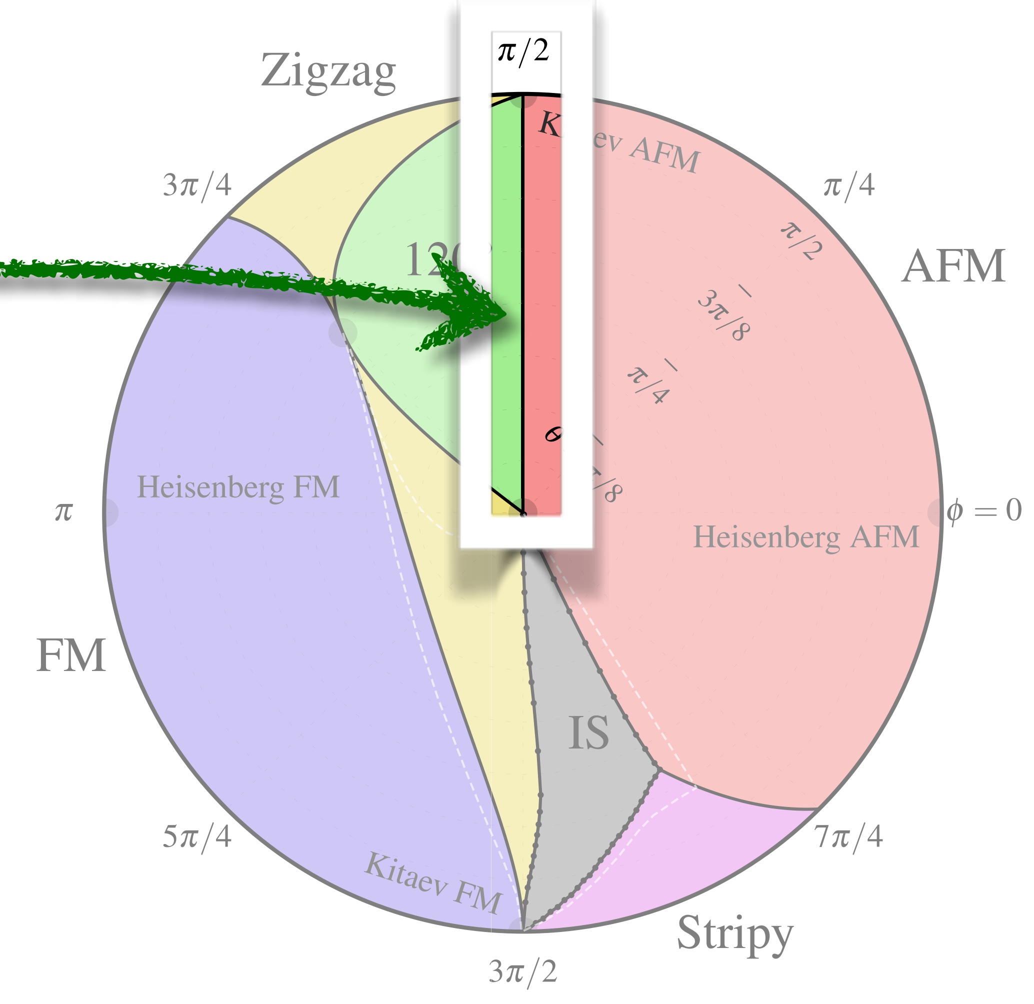


120° state
2D HKΓ





$K \to -K$
$\Gamma \to -\Gamma$



→ Talk by N. Perkins (2:40 p.m.)

[Rau, Lee, Kee, PRL '14]

β-Li_2IrO_3 order: Dual of 120°-state

Duality explains key features of β-Li_2IrO_3:

(i) Zigzag chains of coplanar spins

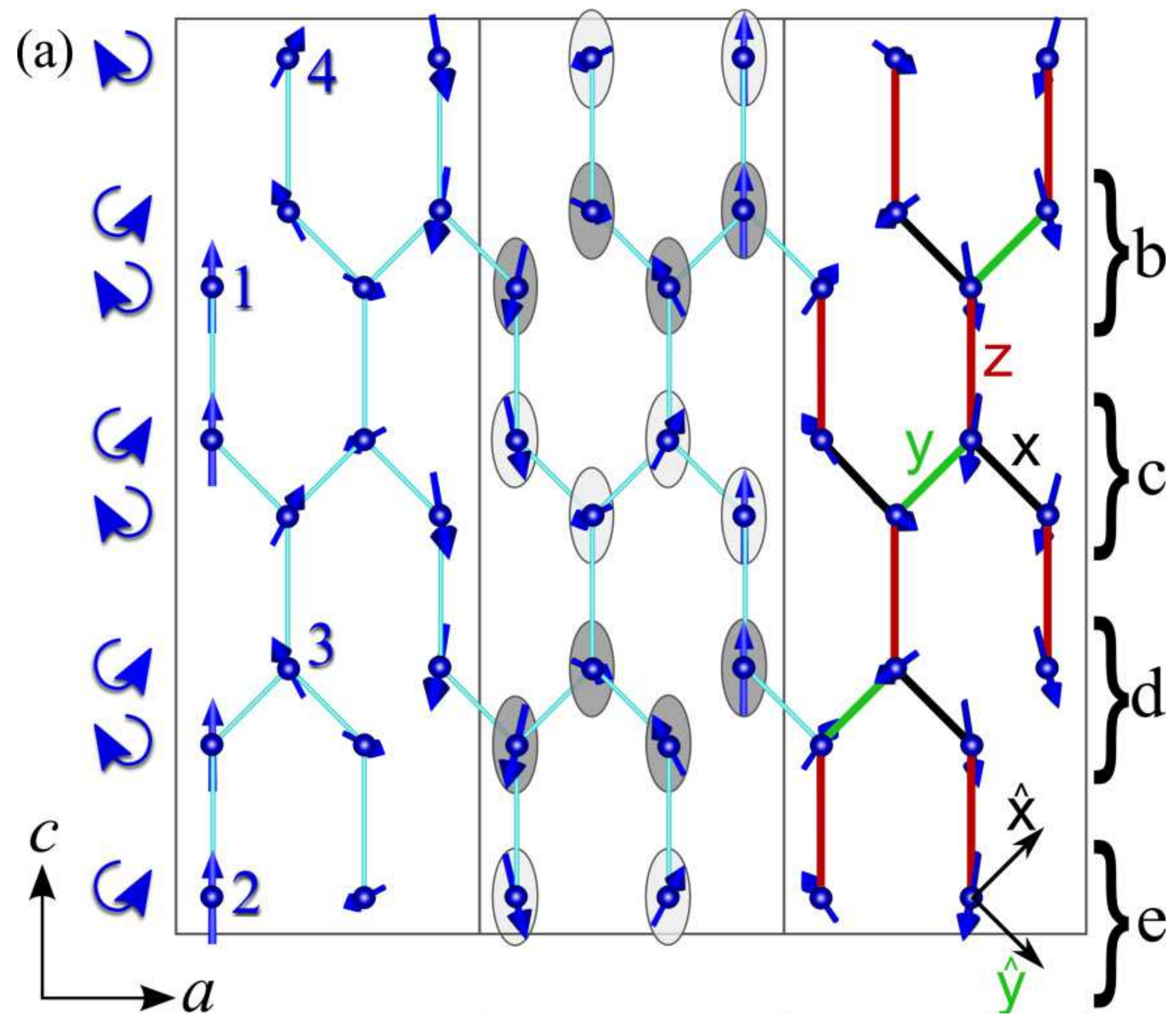
... as duality transformation preserves coplanarity along zigzag chains

(ii) Counterrotating spirals

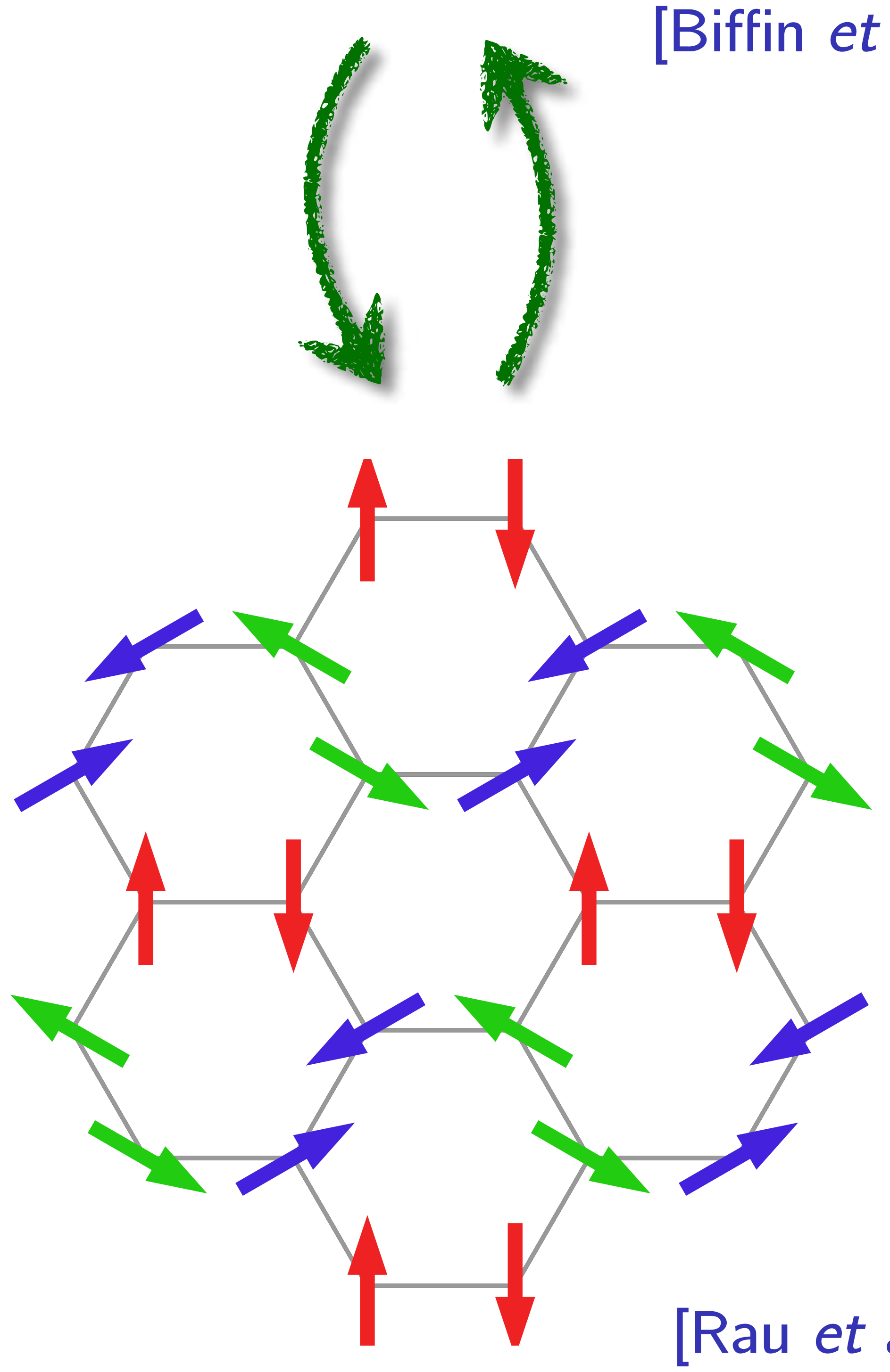
... spins on two sublattices rotate in opposite directions

(iii) Angle between next-nearest neighbors ≈ 120°

... with ordering wavevector $\mathbf{q} = 0.57(1)\mathbf{a}^* \approx 2/3\,\mathbf{a}^*$



[Biffin *et al.* '14]



[Rau *et al.*, '14]

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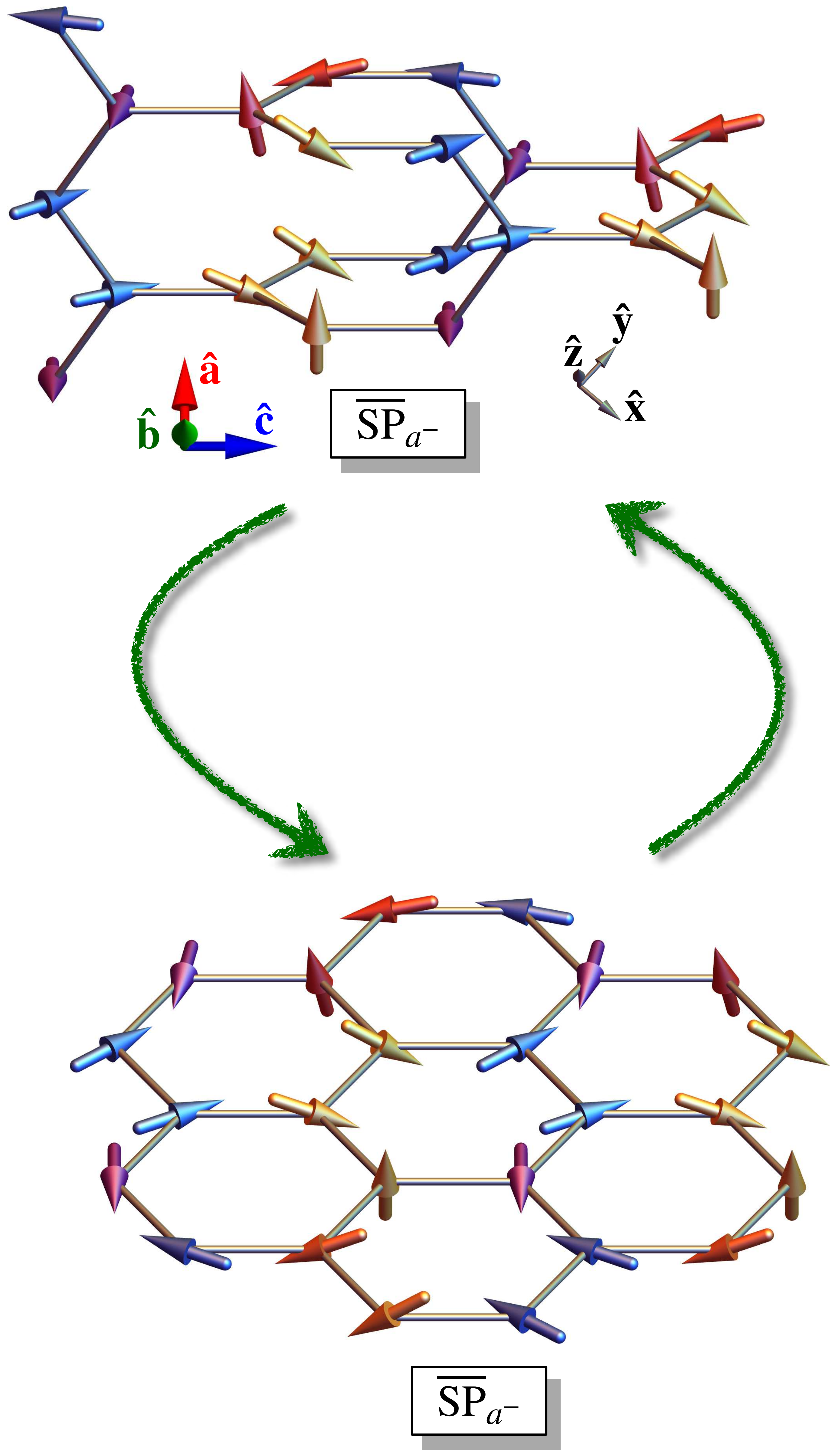
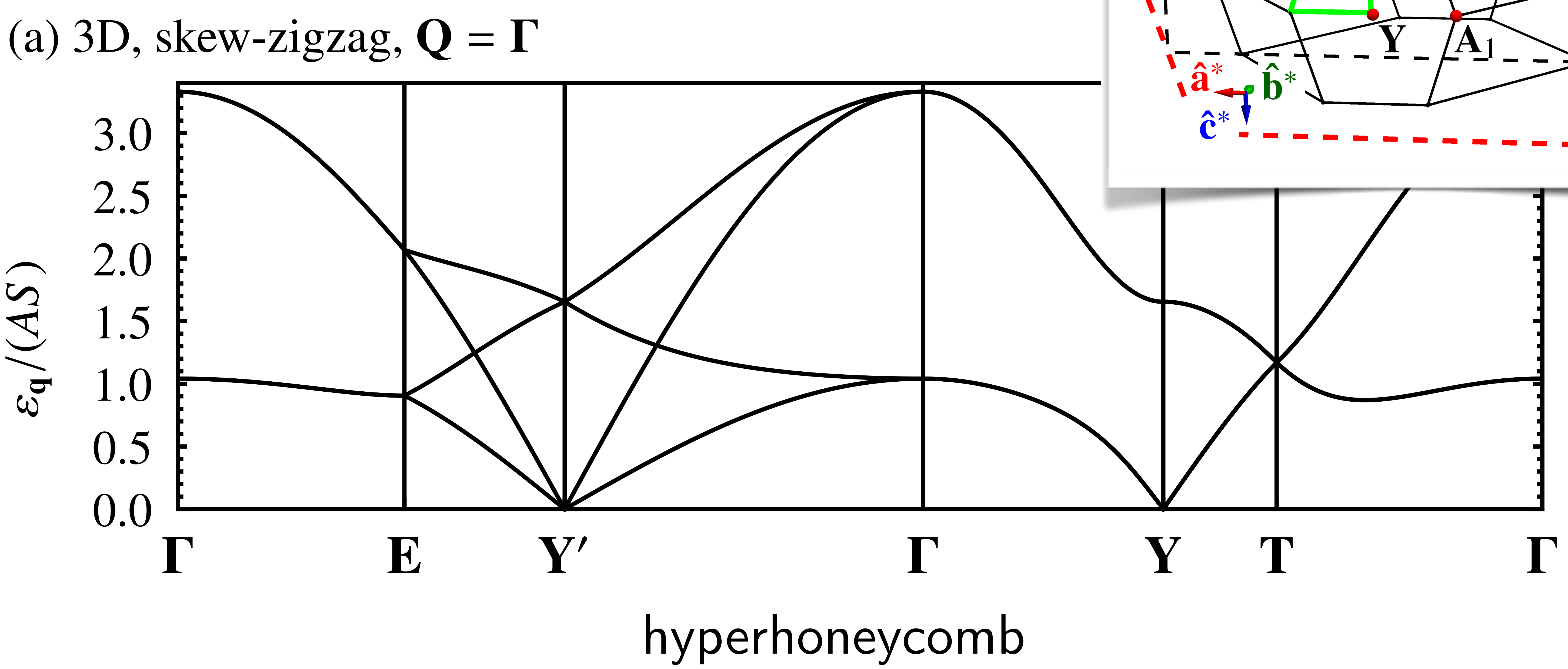
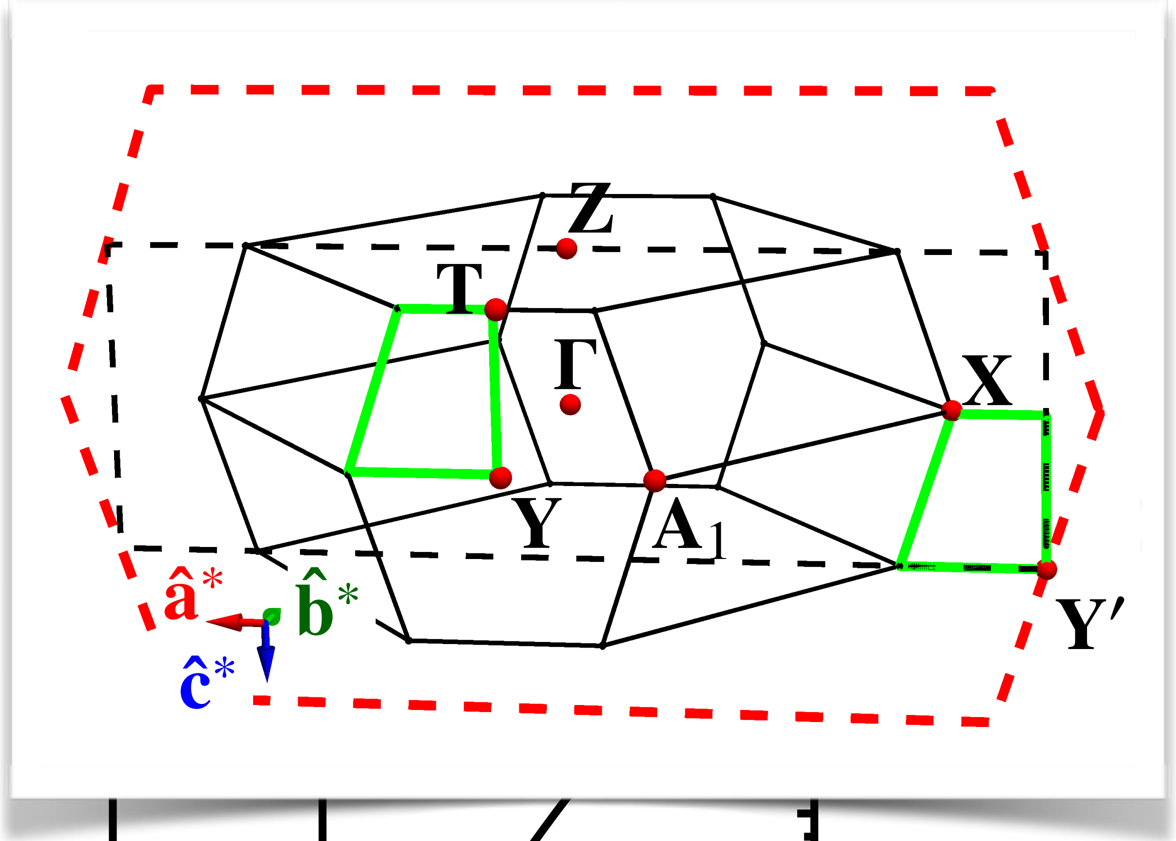
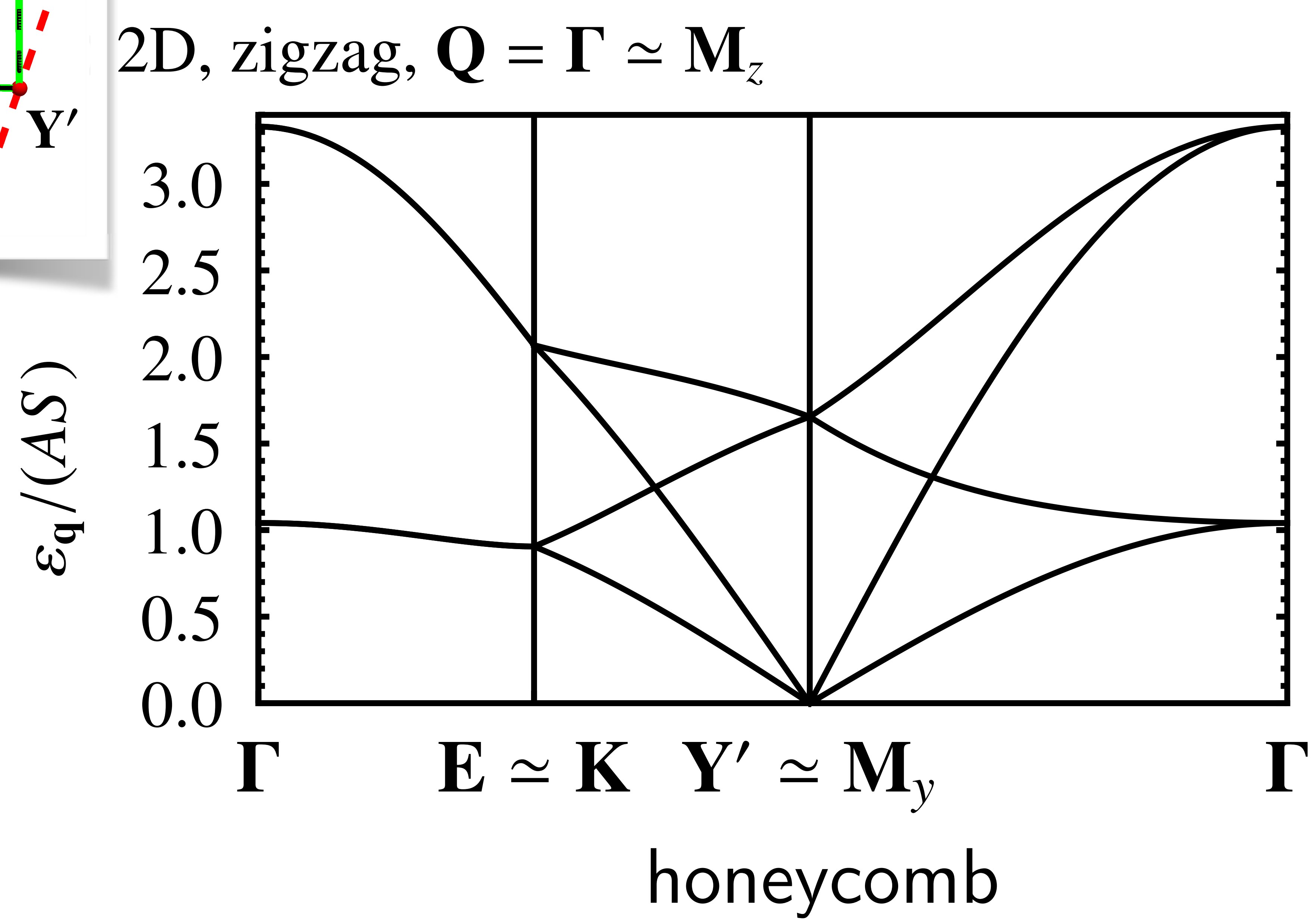


Magnon bands

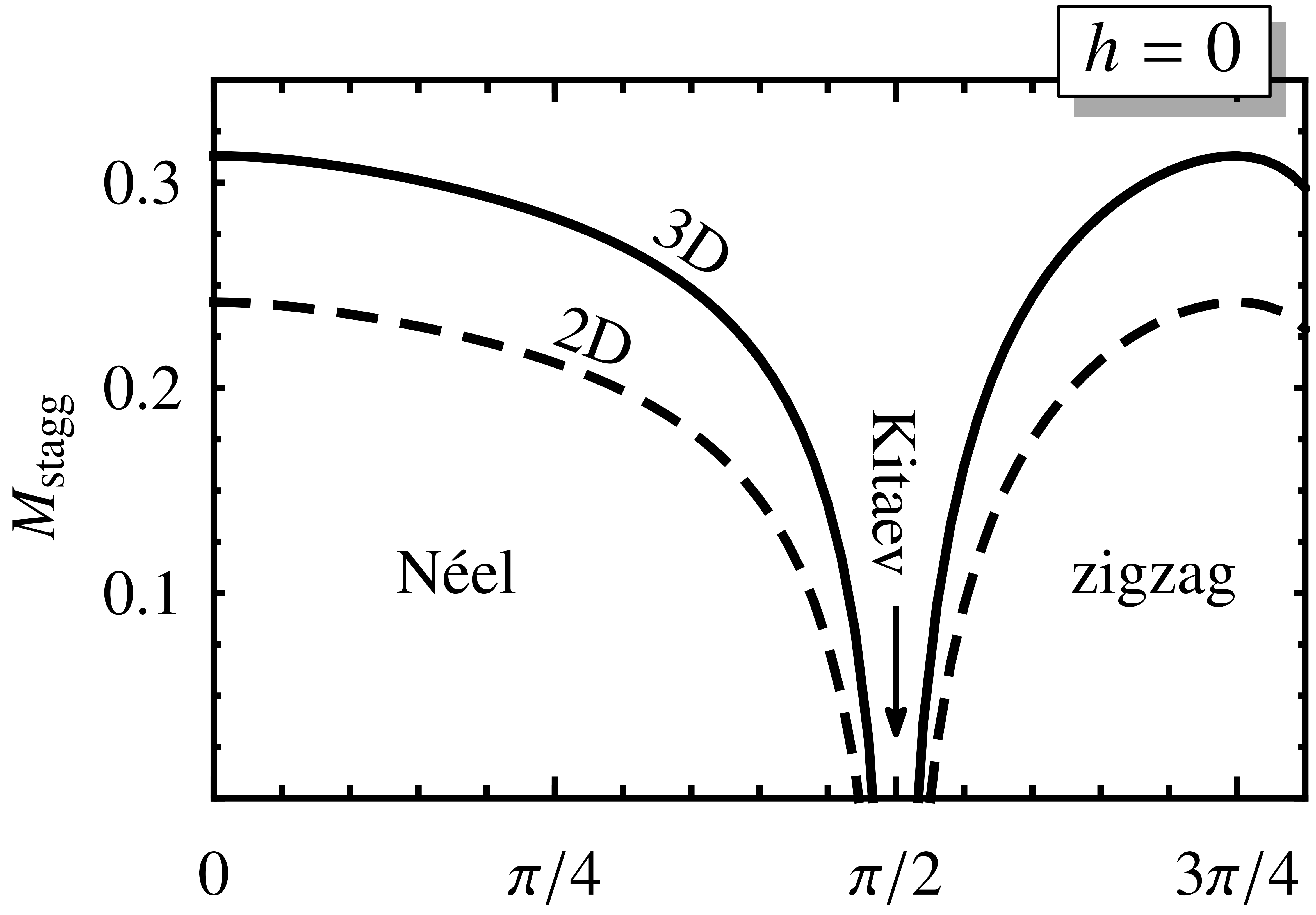






$$\boxed{\varepsilon_{\mathbf{q}}(\text{hyperhoneycomb}) = \varepsilon_{\mathbf{q}}(\text{honeycomb}) \text{ for all } \mathbf{q} \in ac \text{ plane}}$$

Staggered magnetization near Kitaev limit



$\varphi = \arg(2J + \mathrm{i}K)$

... for S = 1/2 Heisenberg-Kitaev model

Conclusions

3D-2D equivalence of ordered states ...

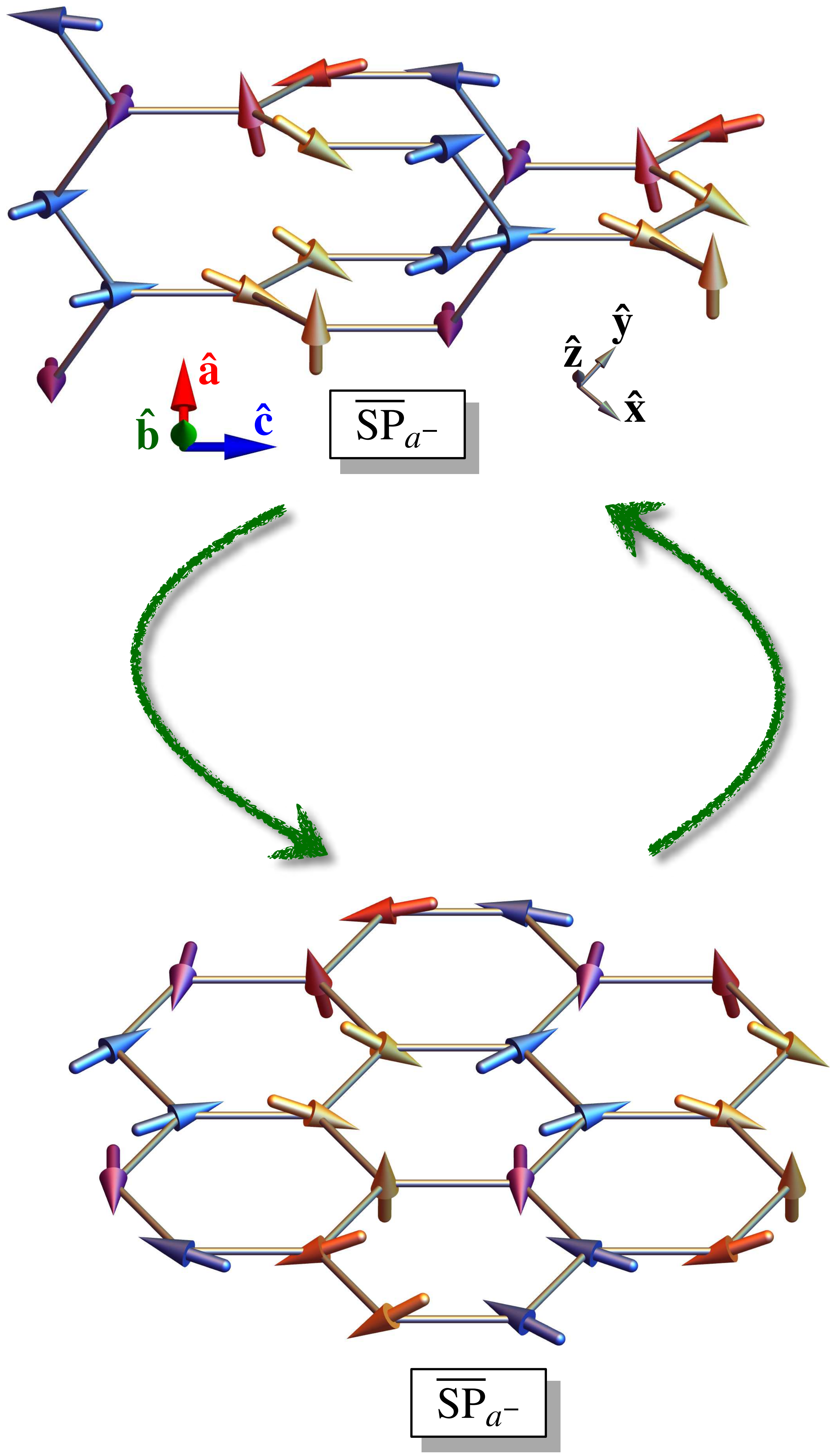
... applies to all ordered states with $\mathbf{Q} \in ac$ plane

... leads to (largely) identical phase diagrams

... can be extended to full harmonic series $^{\mathcal{H}}\langle n \rangle$

... independent of model

... establishes equivalence of magnetic order in α-Li_2IrO_3, β-Li_2IrO_3, and γ-Li_2IrO_3



[Krüger, Vojta, LJ, arXiv:1907.05423]