TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Magnetic ground state of the Kitaev material $Na_2Co_2TeO_6$

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Xianghong Jin

Yuan Li

Quantum Critical Matter

JA 2306/4-1

Emmy Noether-Programm

DFG Deutsche Forschungsgemeinschaft

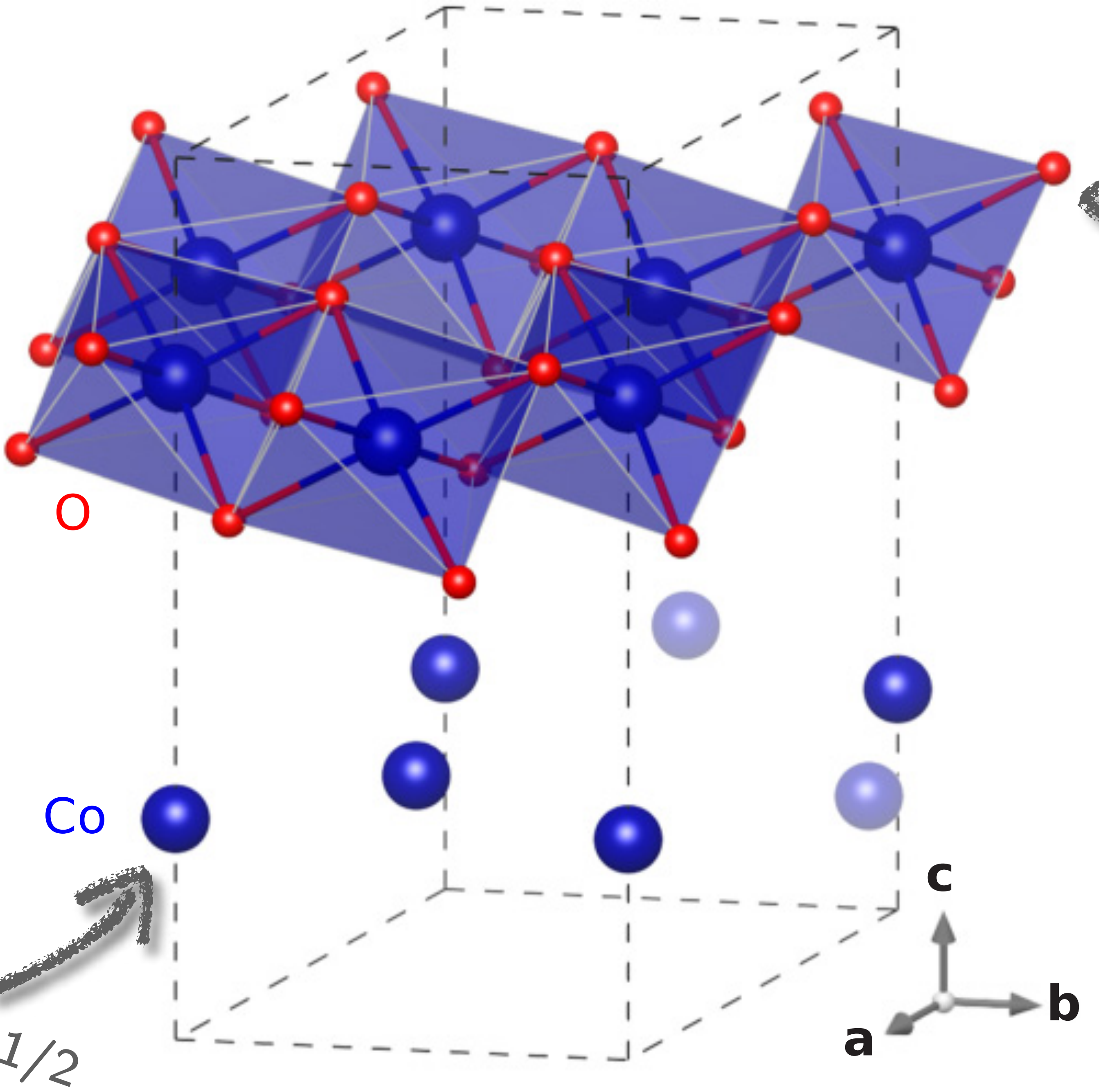
ct.qmat

Complexity and Topology in Quantum Matter

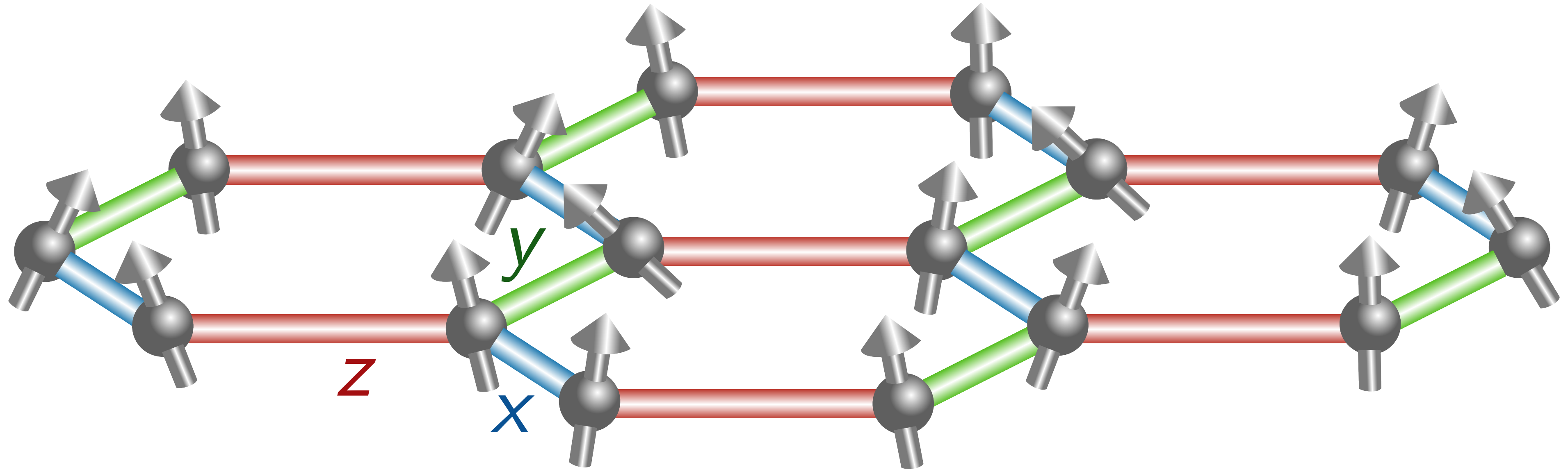
Würzburg-Dresden Cluster of Excellence

SFB 1143

Magnetic Mott insulator $Na_2Co_2TeO_6$



[Chen *et al.*, PRB '21]



Non-Kitaev terms

Effective spin-1/2 model: $$\mathcal{H} = K\left(\sum_{\langle ij\rangle_x} S_i^x S_j^x + \sum_{\langle ij\rangle_y} S_i^y S_j^y + \sum_{\langle ij\rangle_z} S_i^z S_j^z\right) + \ldots$$

Kitaev
exchange

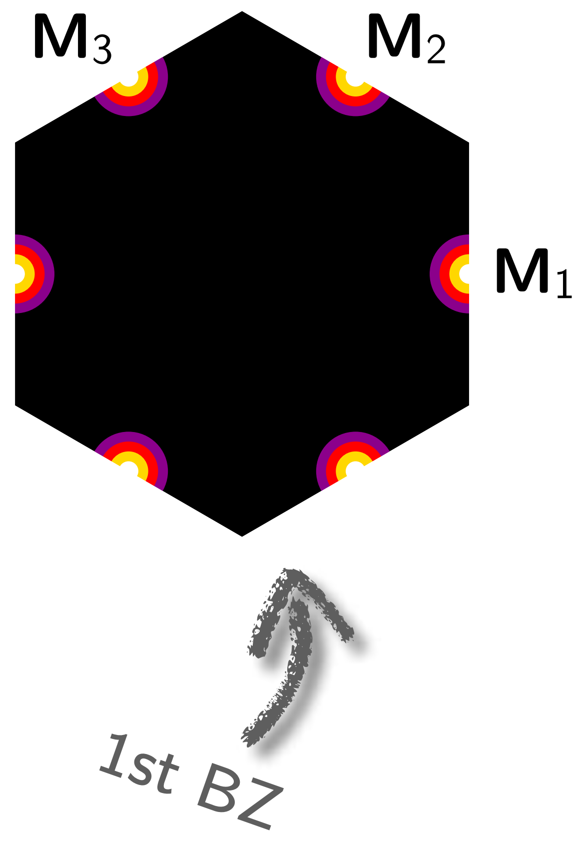
[Liu, Khaliullin, PRB '18]
[Sano, Kato, Motome, PRB '18]

Multi-q vs single-q order: Bragg peaks

Static spin structure factor:

... e.g., from neutron diffraction

[Chen *et al.*, PRB ’21]



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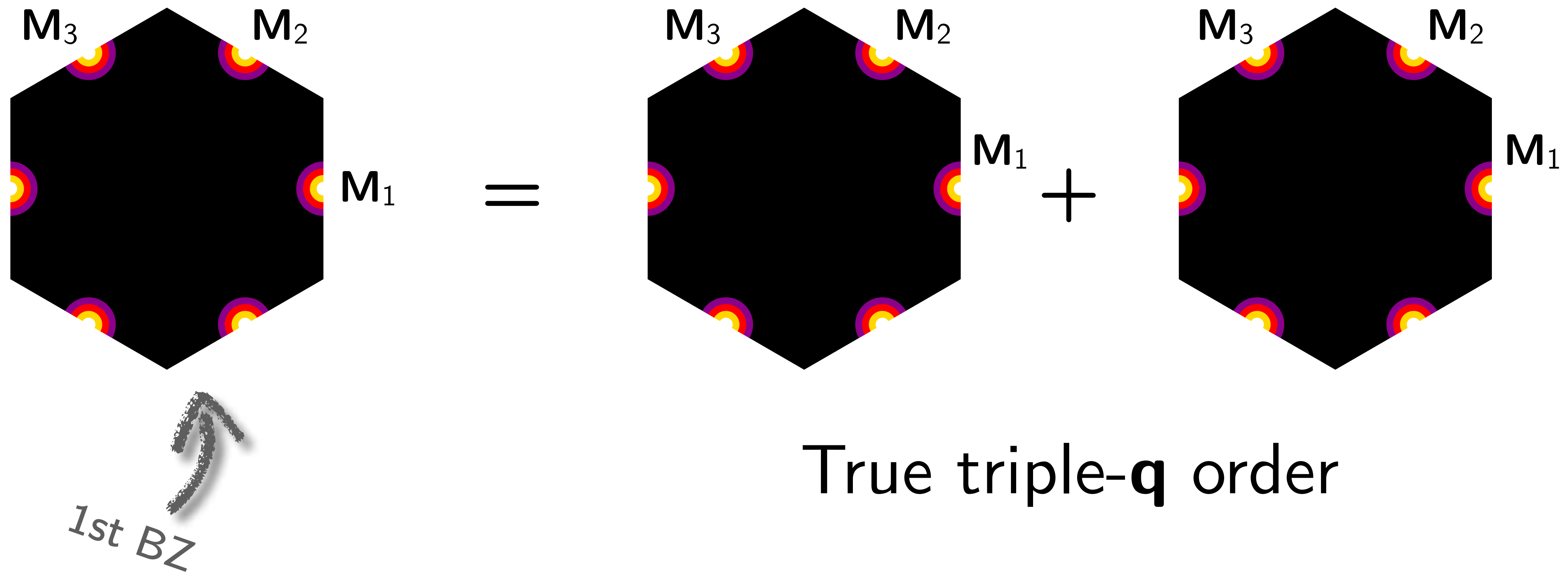

True triple-**q** order

Multi-q vs single-q order: Bragg peaks

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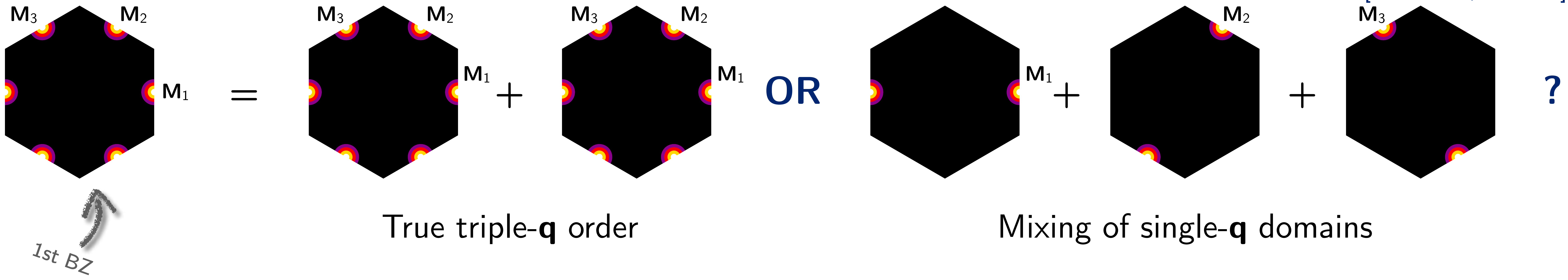

True triple-**q** order

Mixing of single-**q** domains

Multi-q vs single-q order: Bragg peaks

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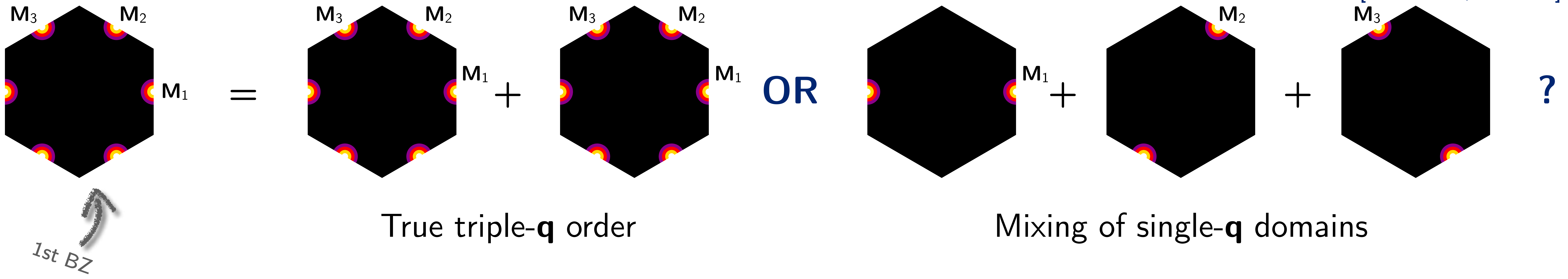
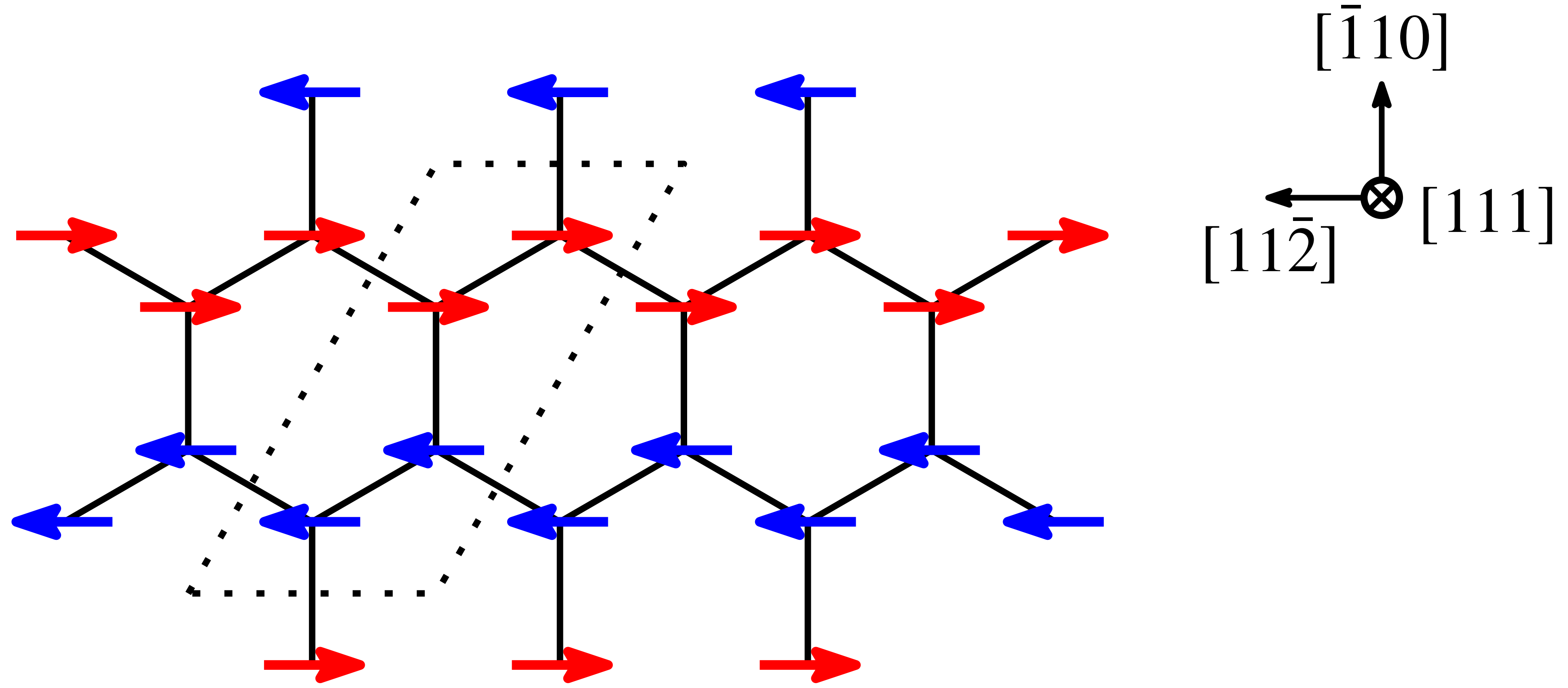


Real space:



α-$RuCl_3$, Na_2IrO_3, ...

[Choi *et al.*, PRL '12]

[Johnson *et al.*, PRB '15]

[Balz *et al.*, PRB '21]

Multi-q vs single-q order: Bragg peaks

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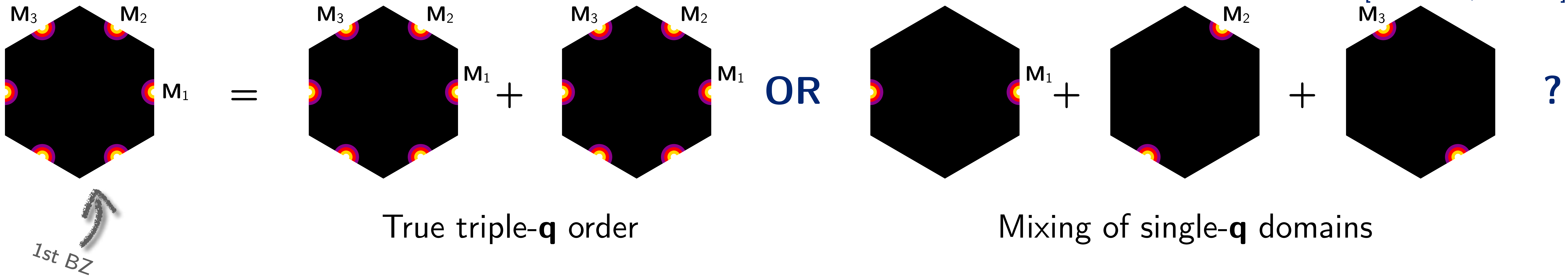

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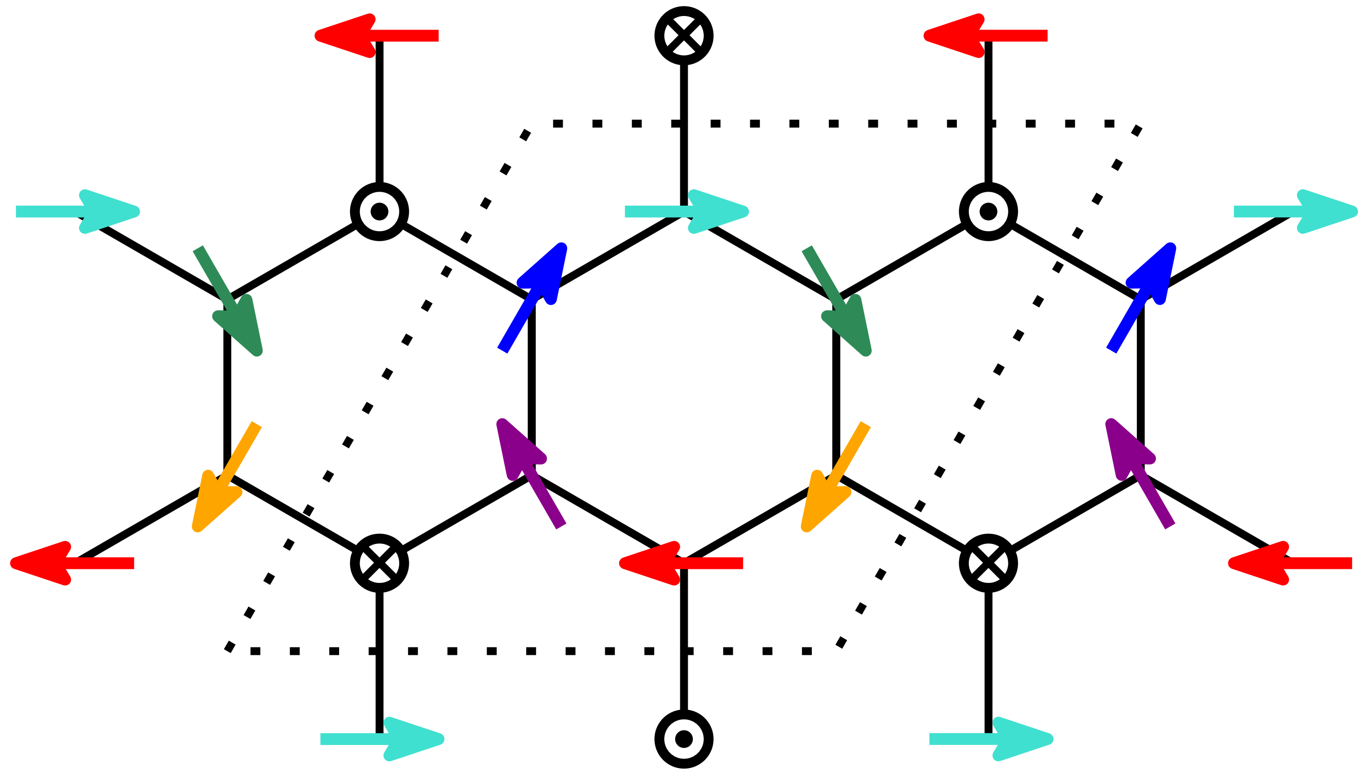
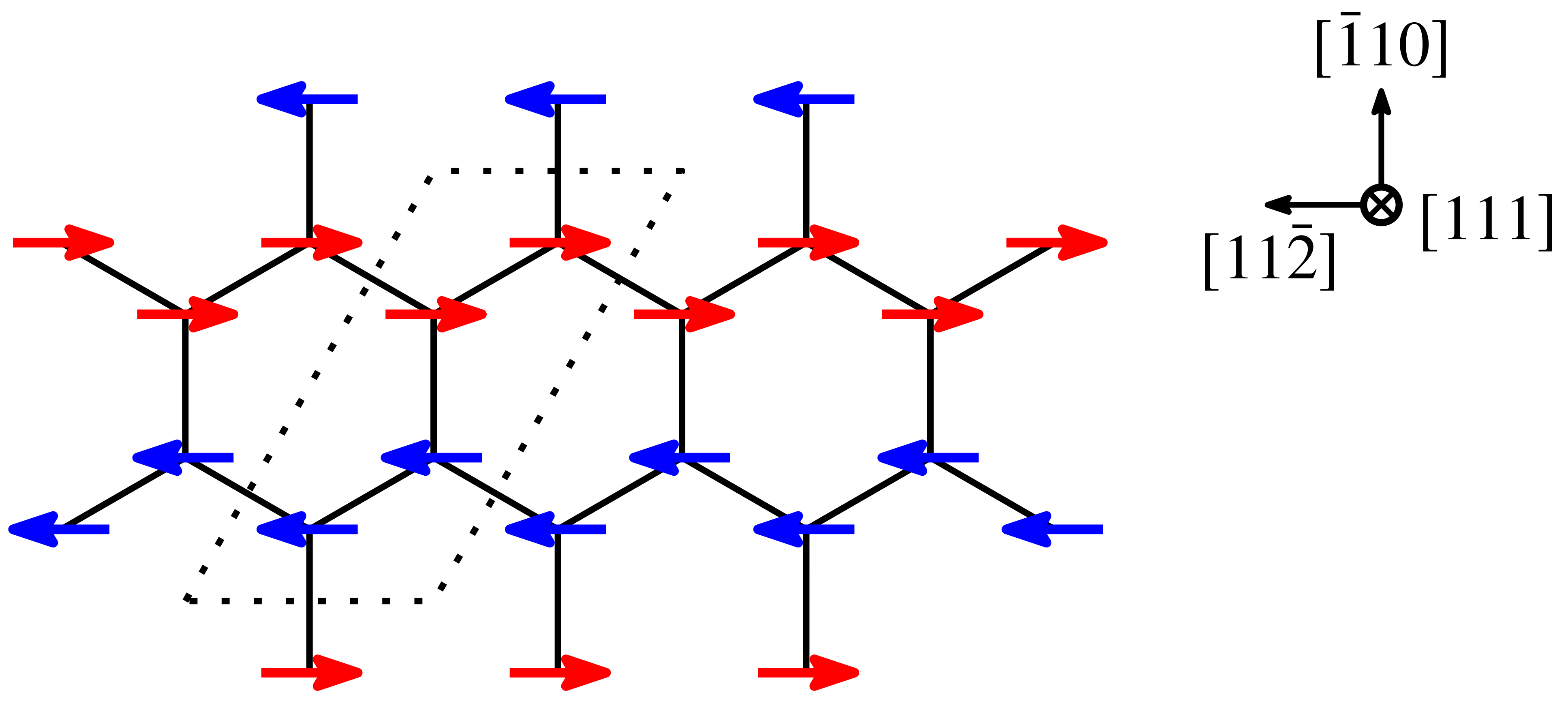




Kitaev-Heisenberg in field: [LJ, Andrade, Vojta, PRL '16]

Bilinear-Biquadratic Kitaev-Heisenberg: [Pohle, Shannon, Motome, PRB '23]

α-$RuCl_3$, Na_2IrO_3, ...

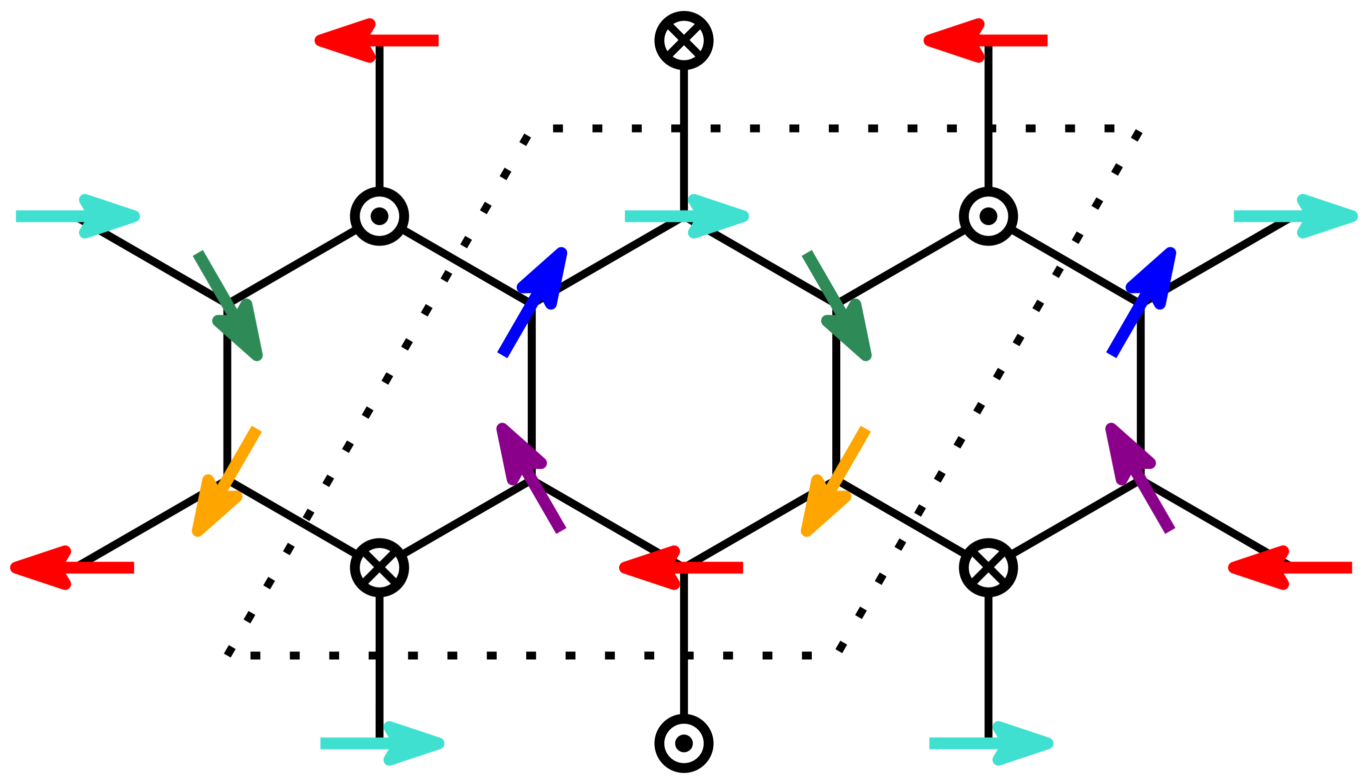
[Choi *et al.*, PRL '12]

[Johnson *et al.*, PRB '15]

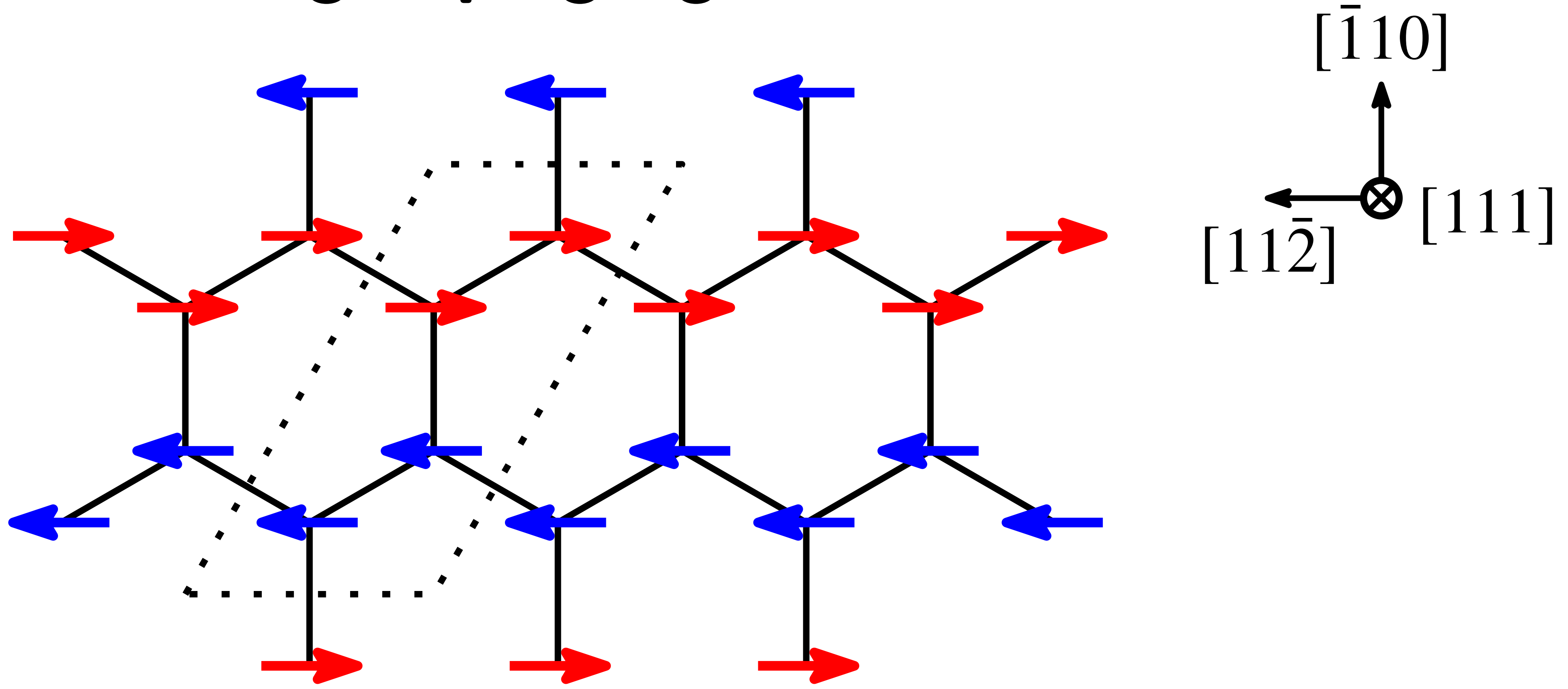
[Balz *et al.*, PRB '21]

Multi-q vs single-q order: Symmetries

Triple-**q** AFM



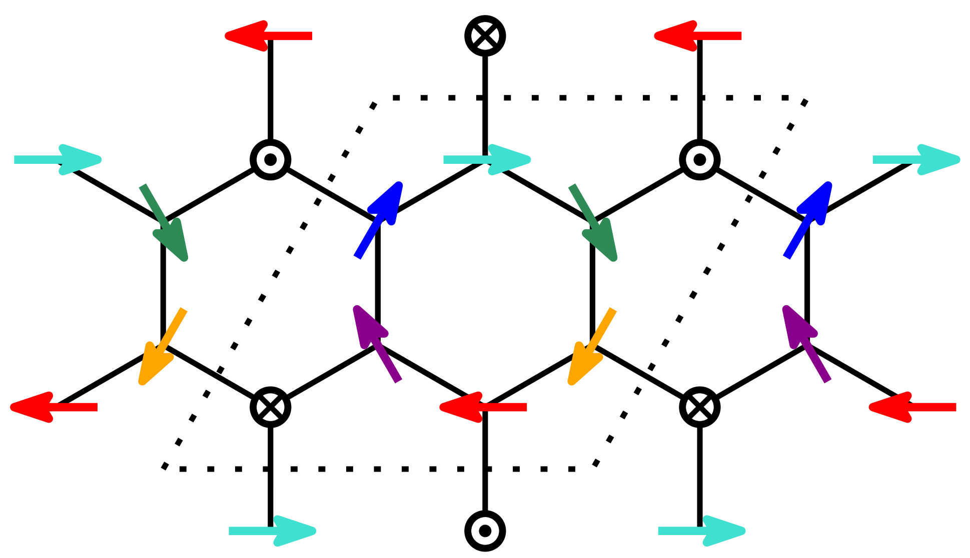
Single-**q** zigzag AFM



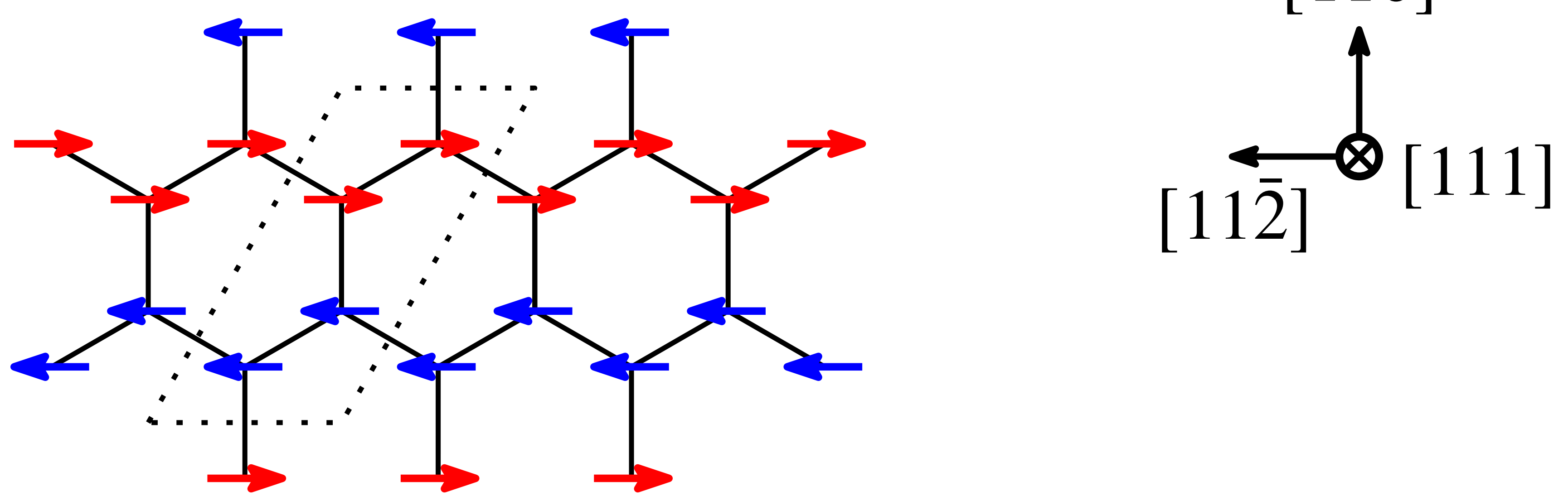
	Triple-**q** AFM	Single-**q** zigzag AFM
Time reversal:	✗	✗
Spin-lattice rotation C_3^*:	✓	✗
Translation $T_{\mathbf{a}_1}$:	✗	✗
Translation $T_{\mathbf{a}_2}$:	✗	✓

Multi-q vs single-q order: Magnetic excitation spectrum

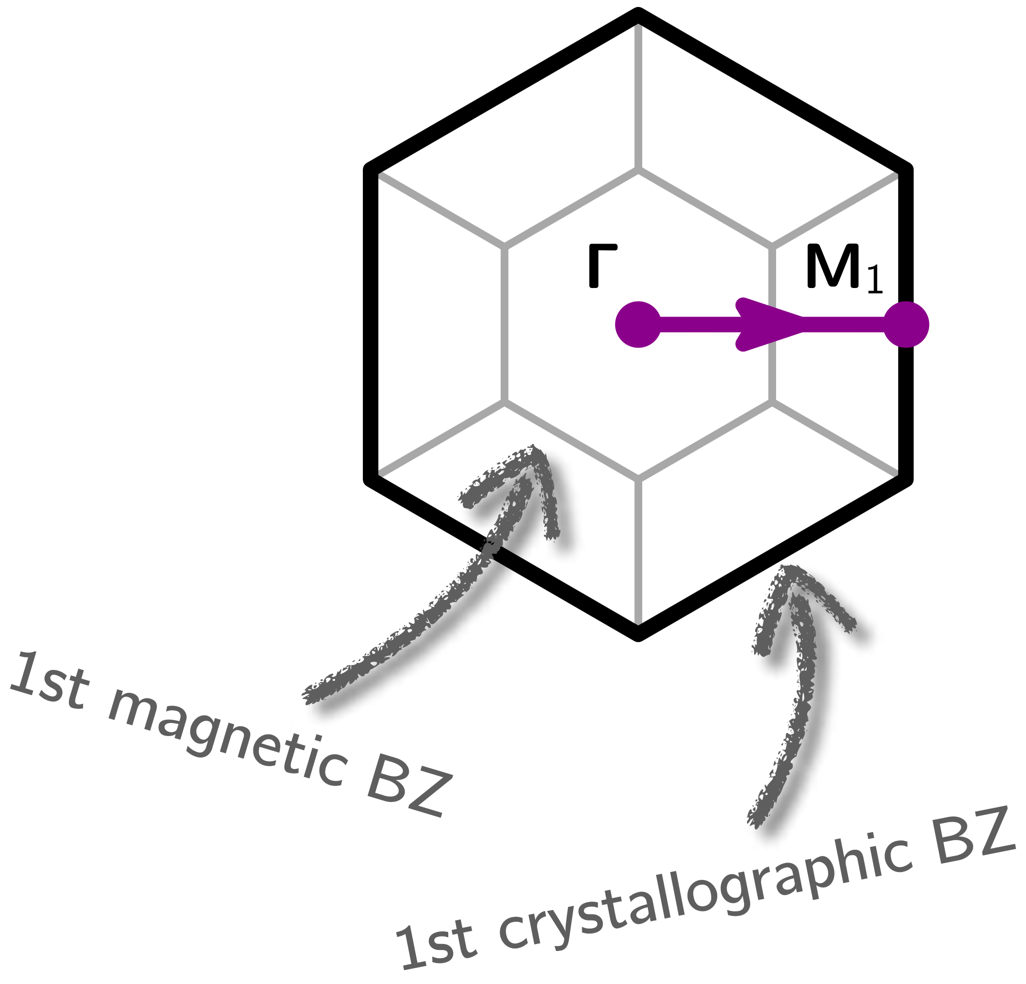
Triple-**q** AFM



Single-**q** zigzag AFM

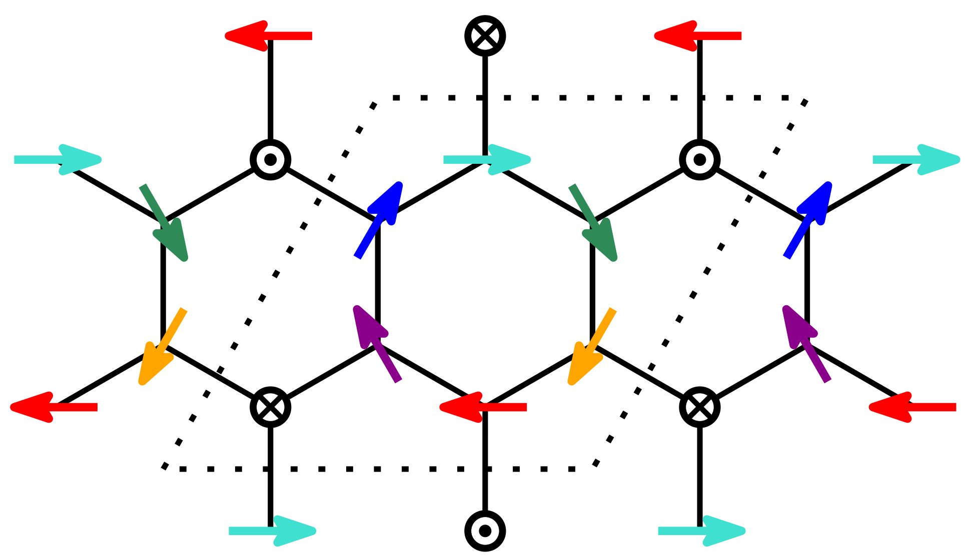


Brillouin zone path:

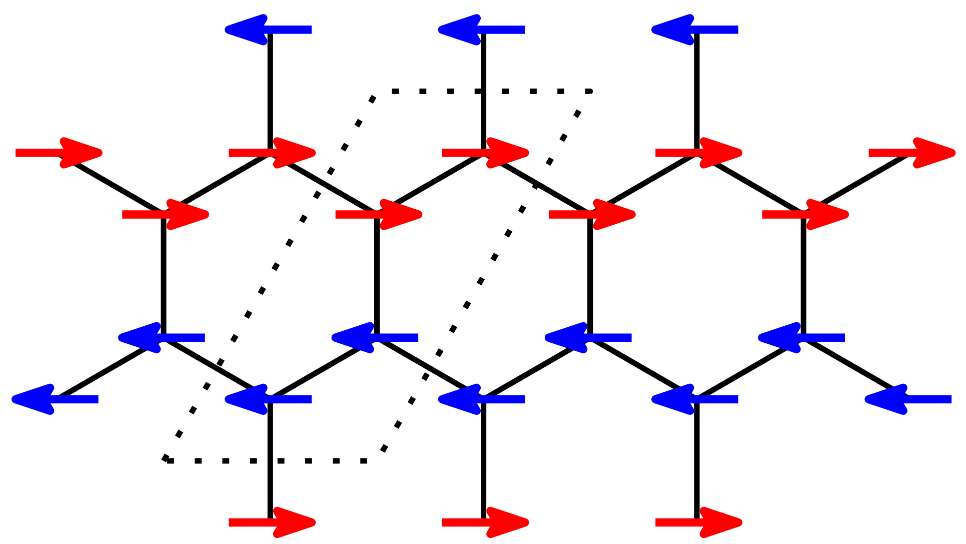


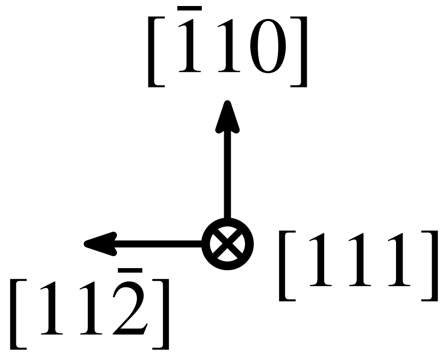
Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM



Single-**q** zigzag AFM





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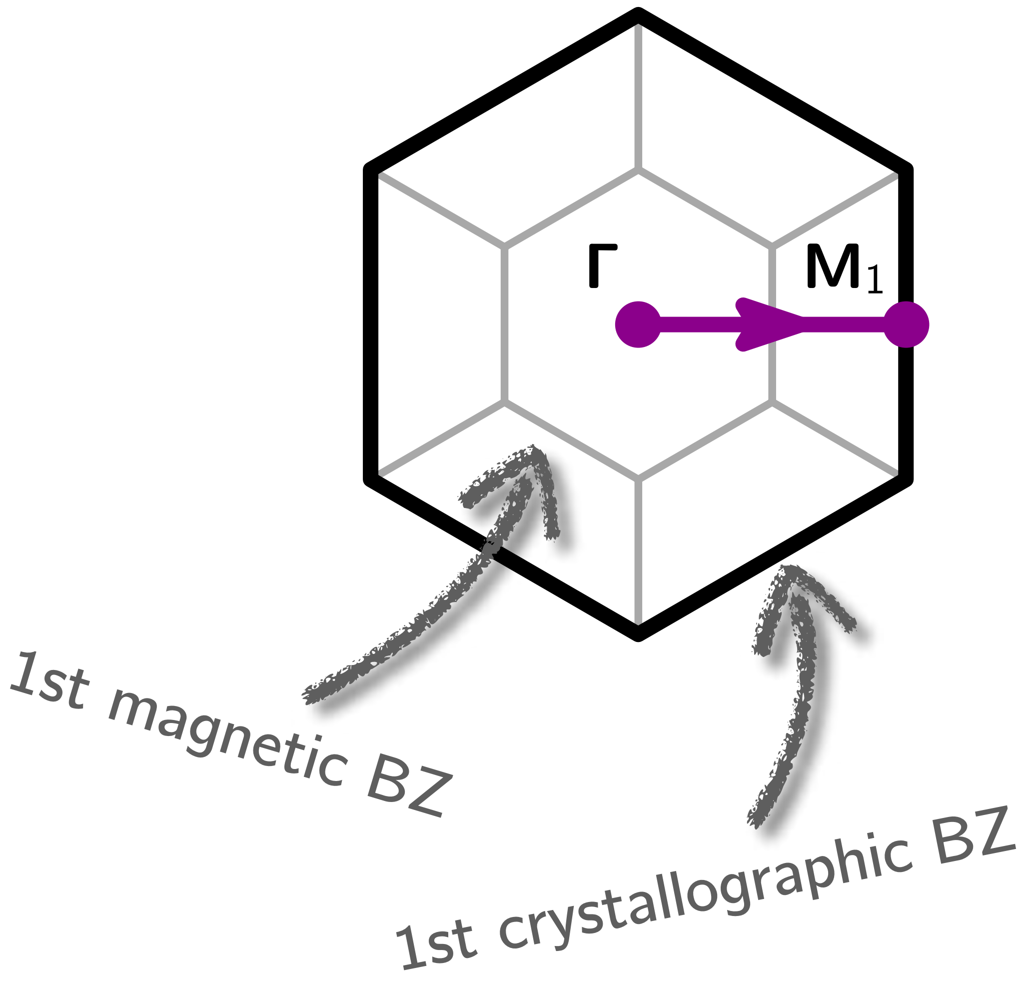
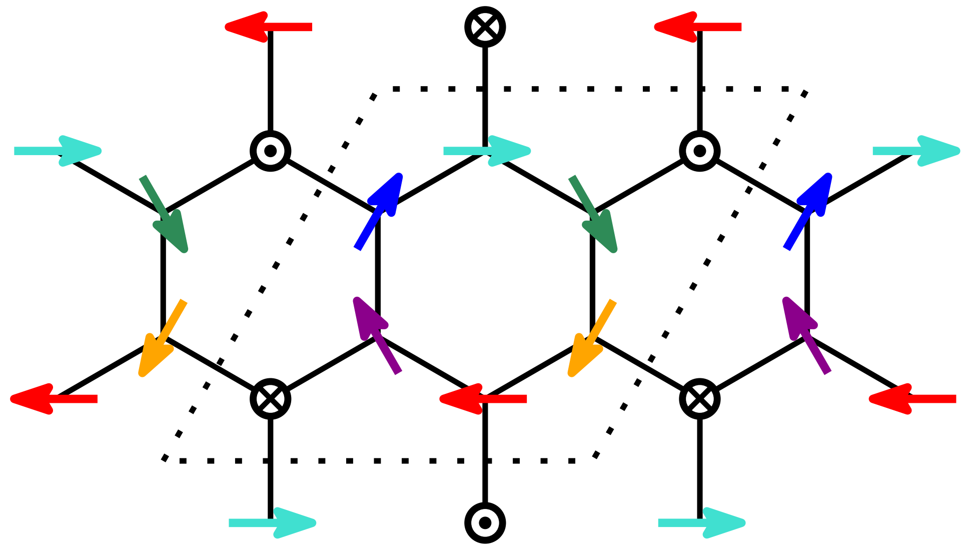


Spectrum necessarily symmetric

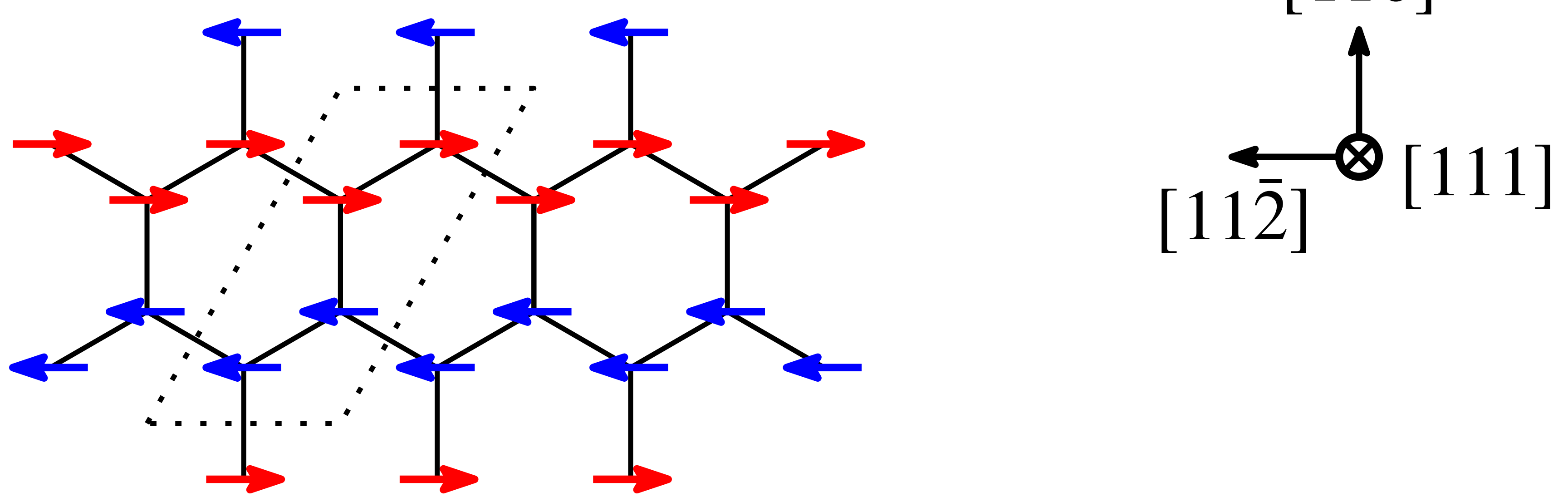
... independent of modeling

Multi-q vs single-q order: Magnetic excitation spectrum

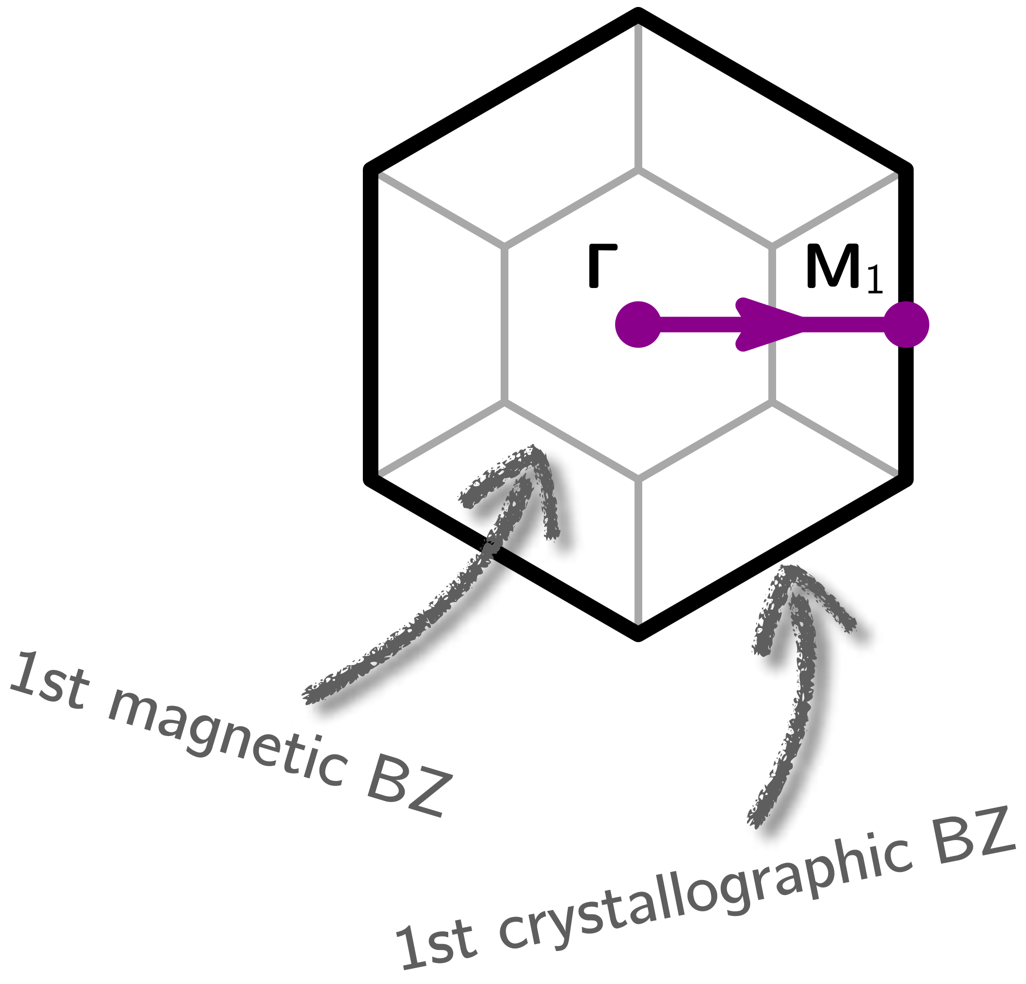
Triple-**q** AFM

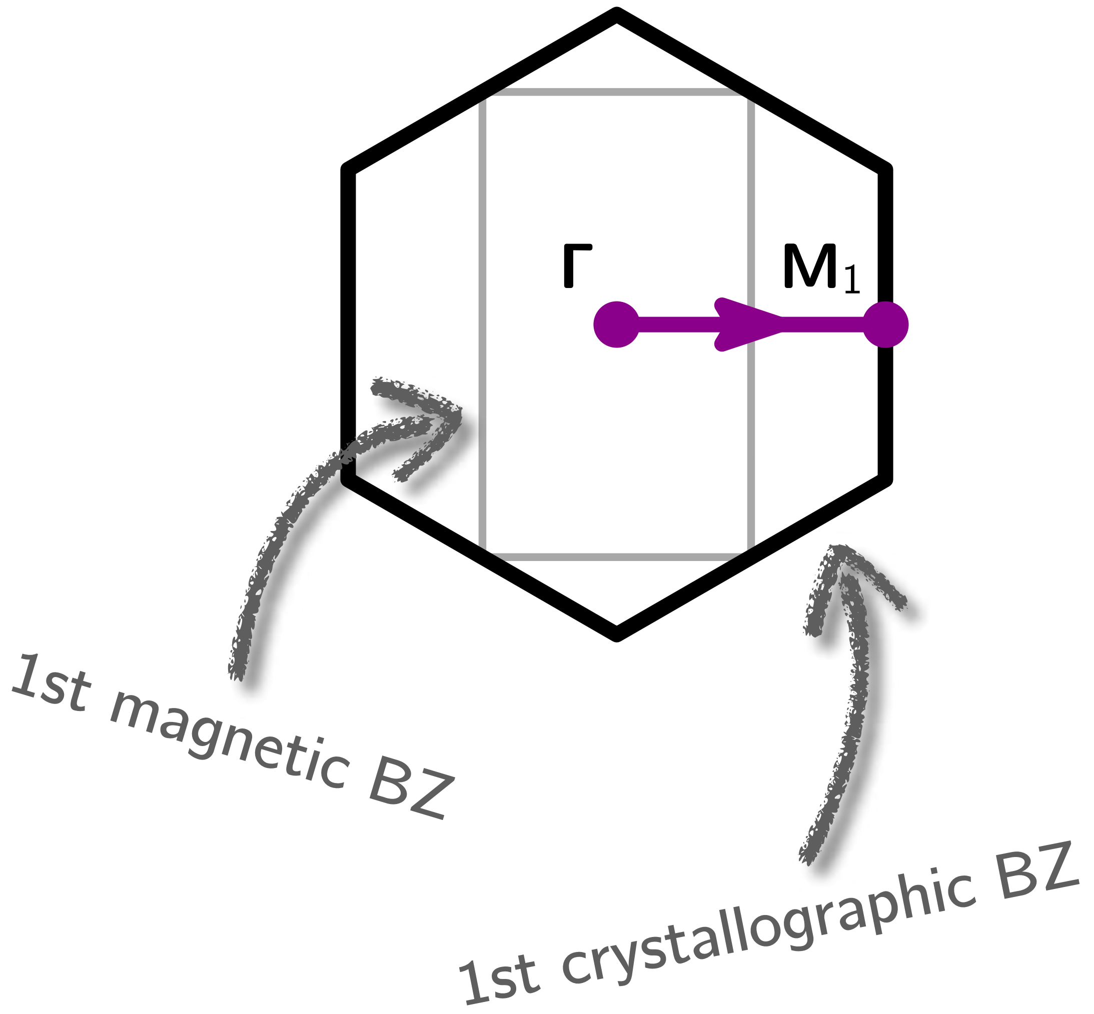


Single-**q** zigzag AFM



Brillouin zone path:





Spectrum necessarily symmetric

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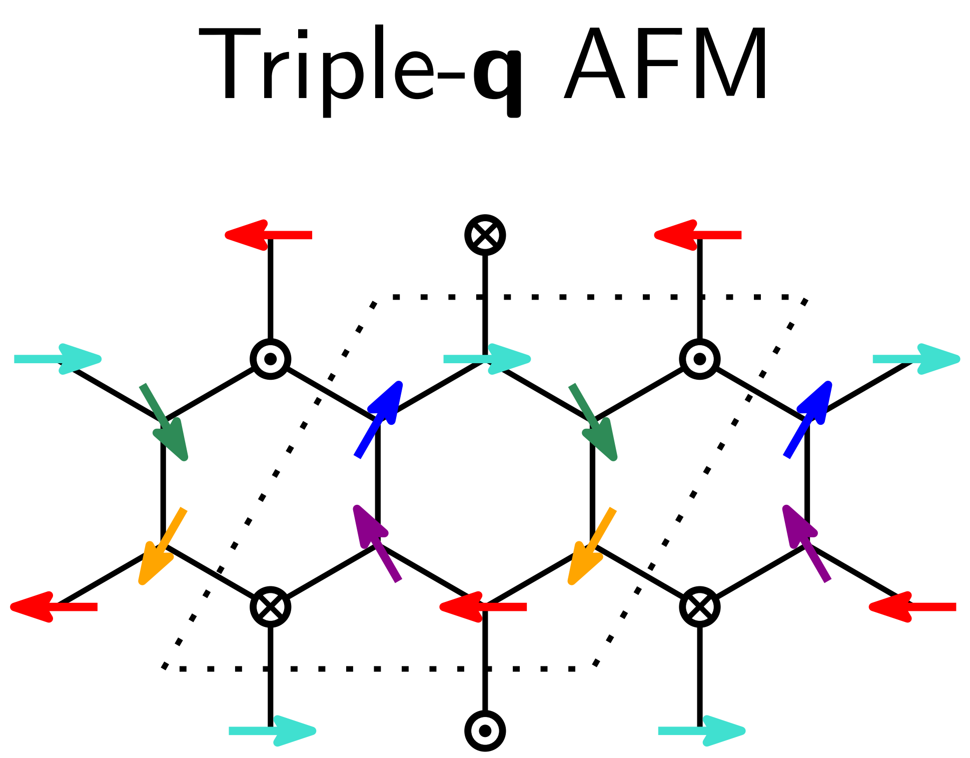
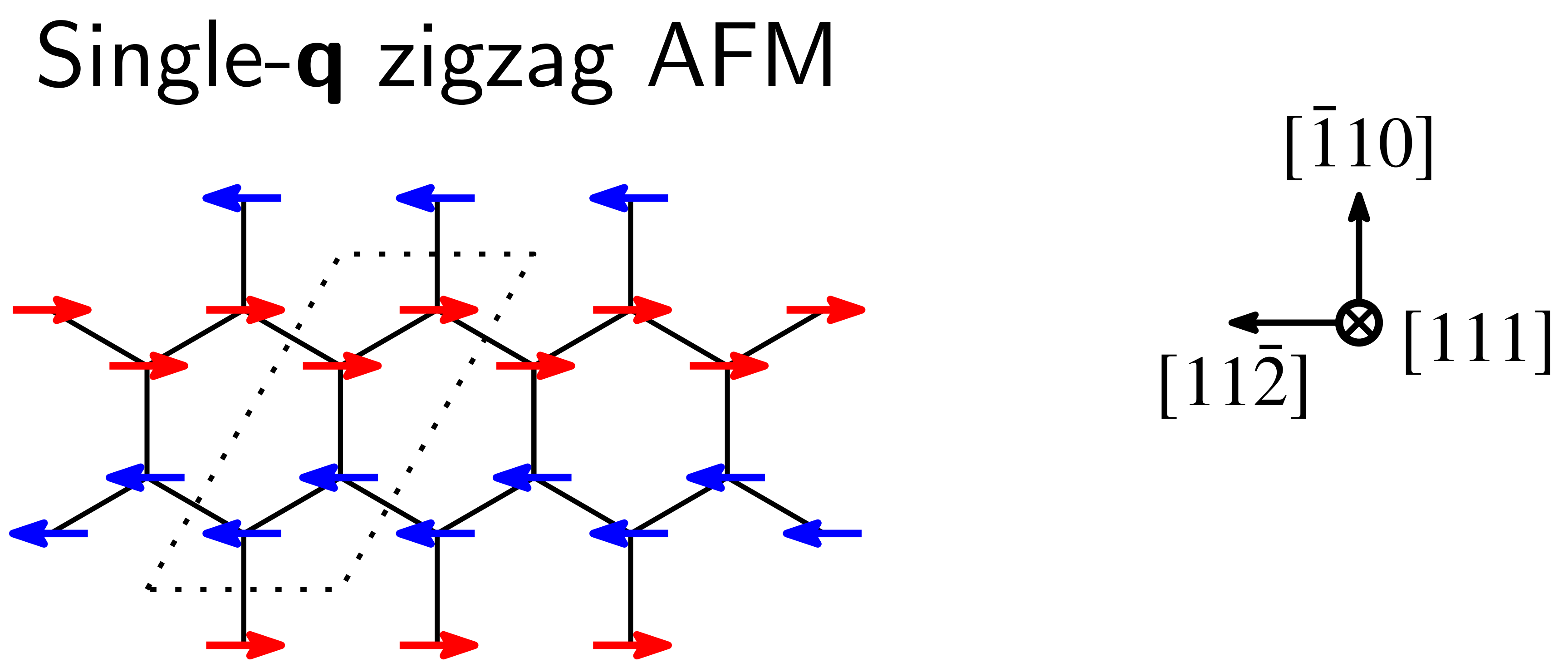
Multi-q vs single-q order: Magnetic excitation spectrum





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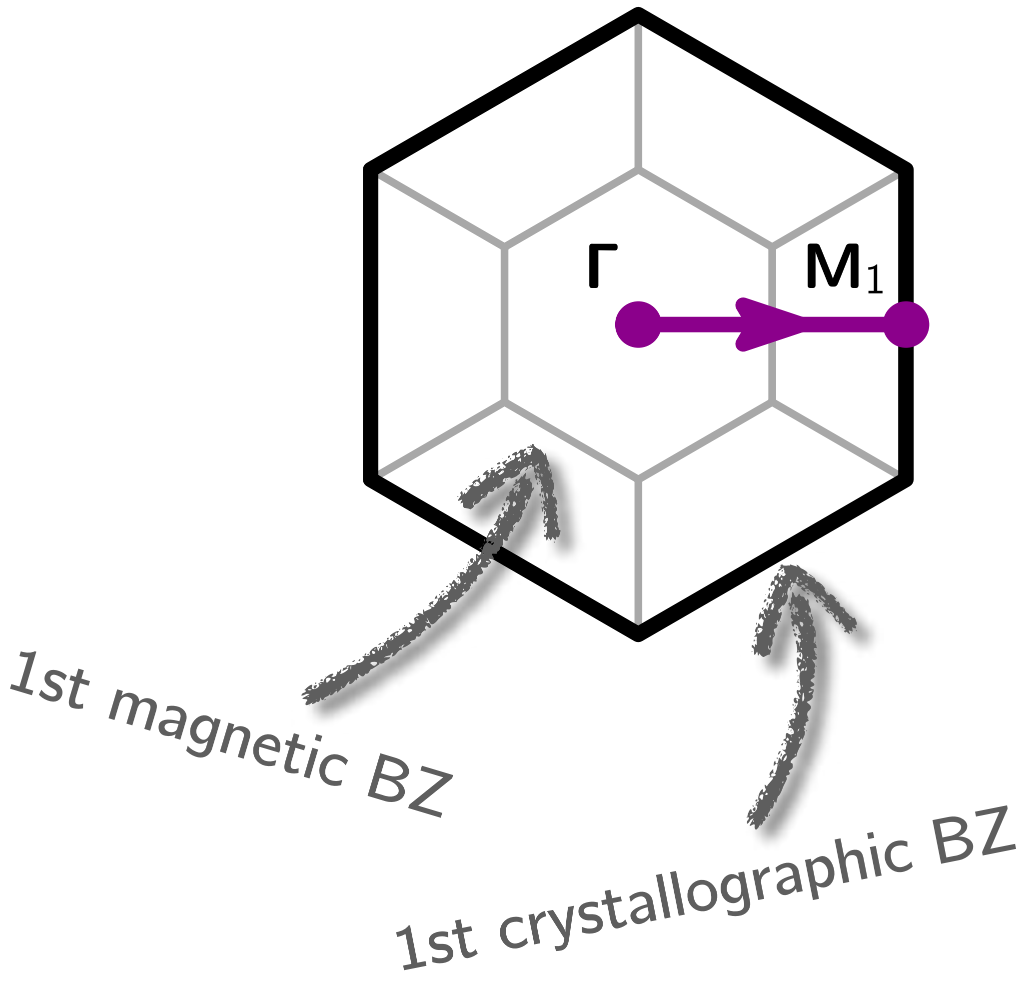

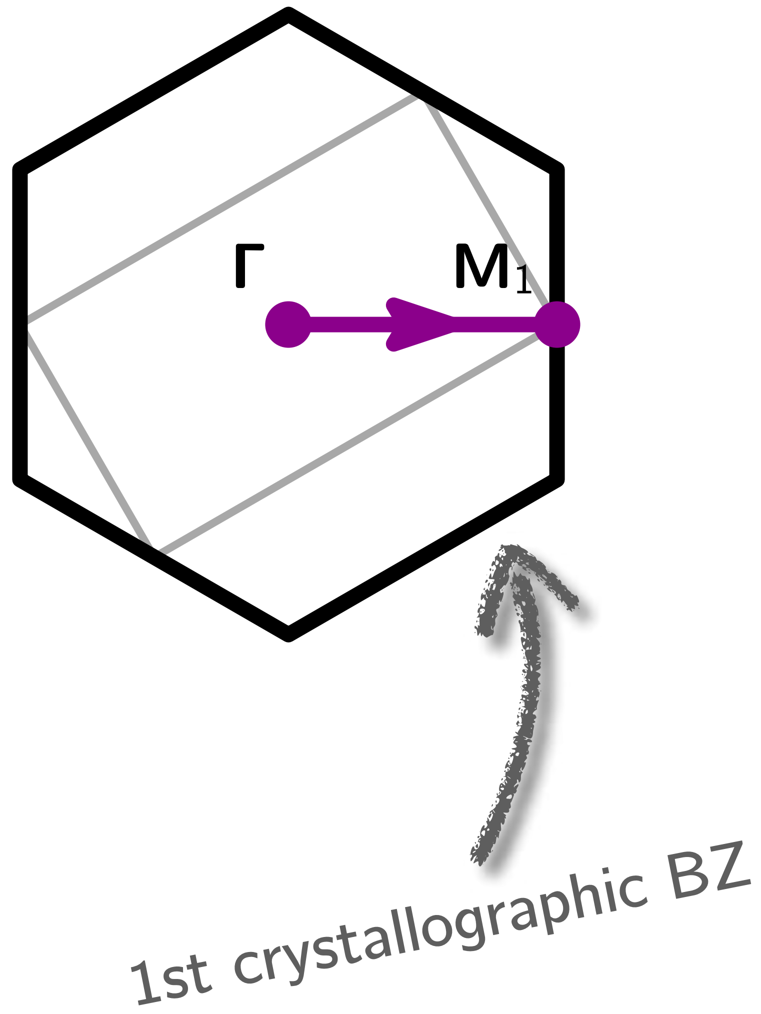

Spectrum necessarily symmetric

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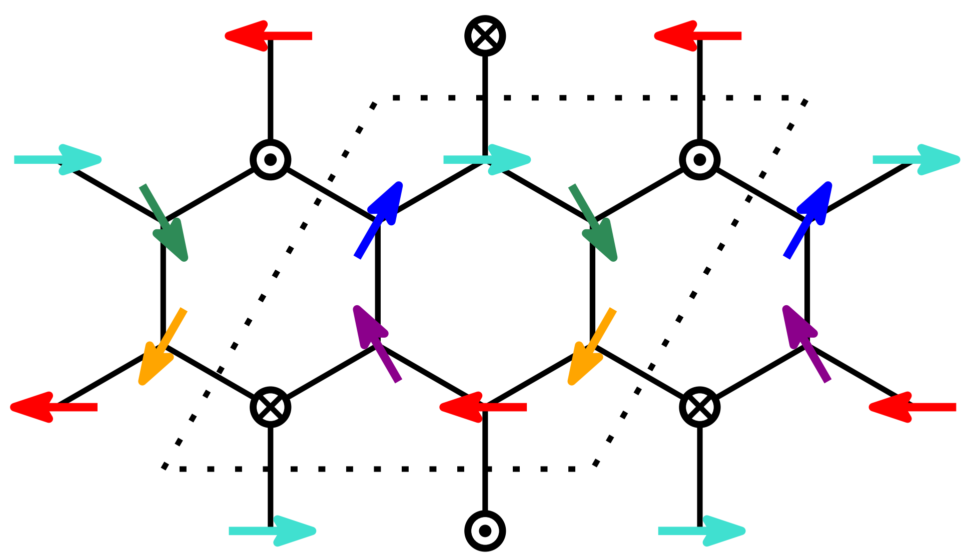
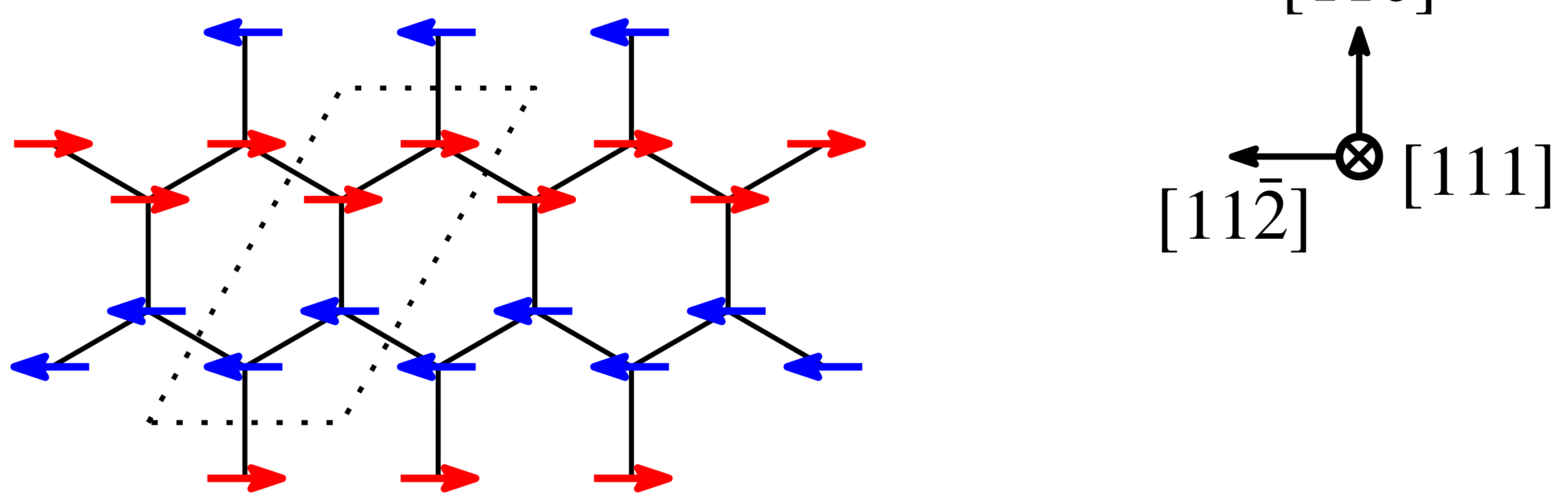
Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM



Single-**q** zigzag AFM



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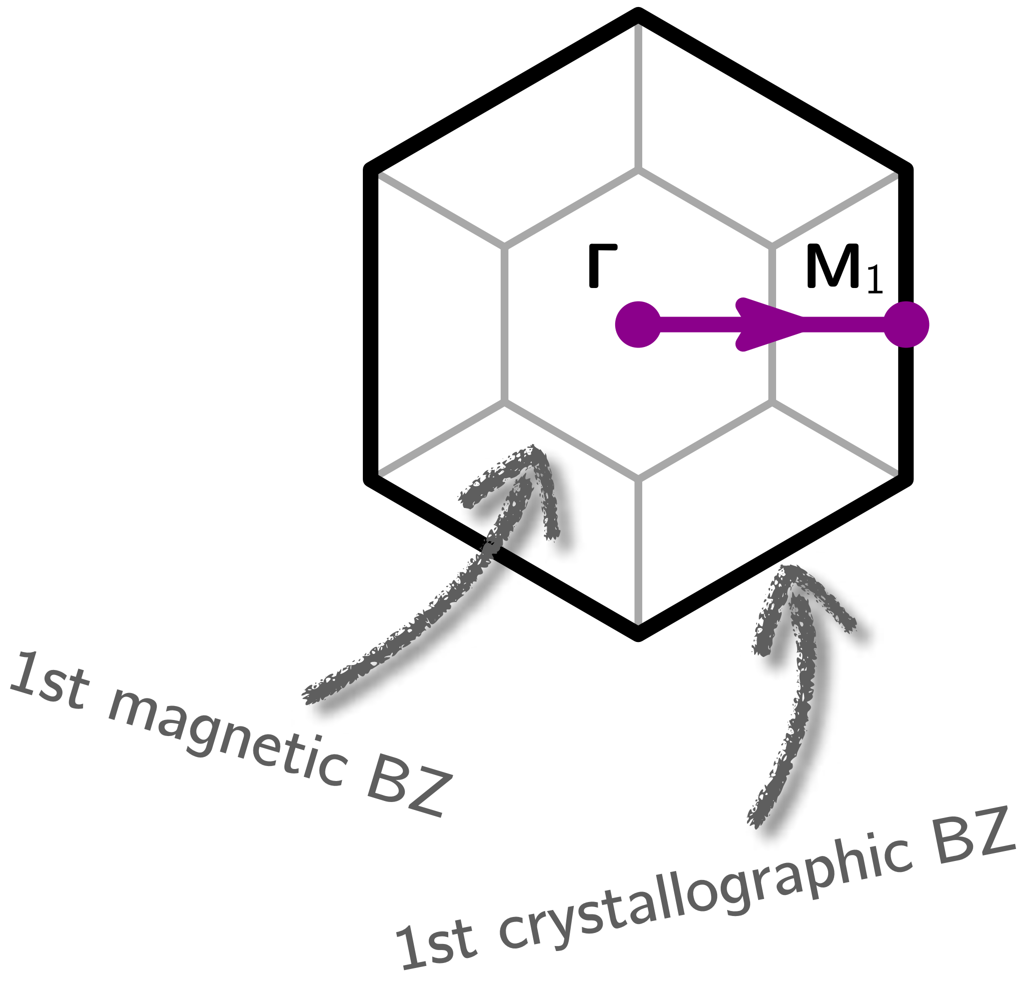

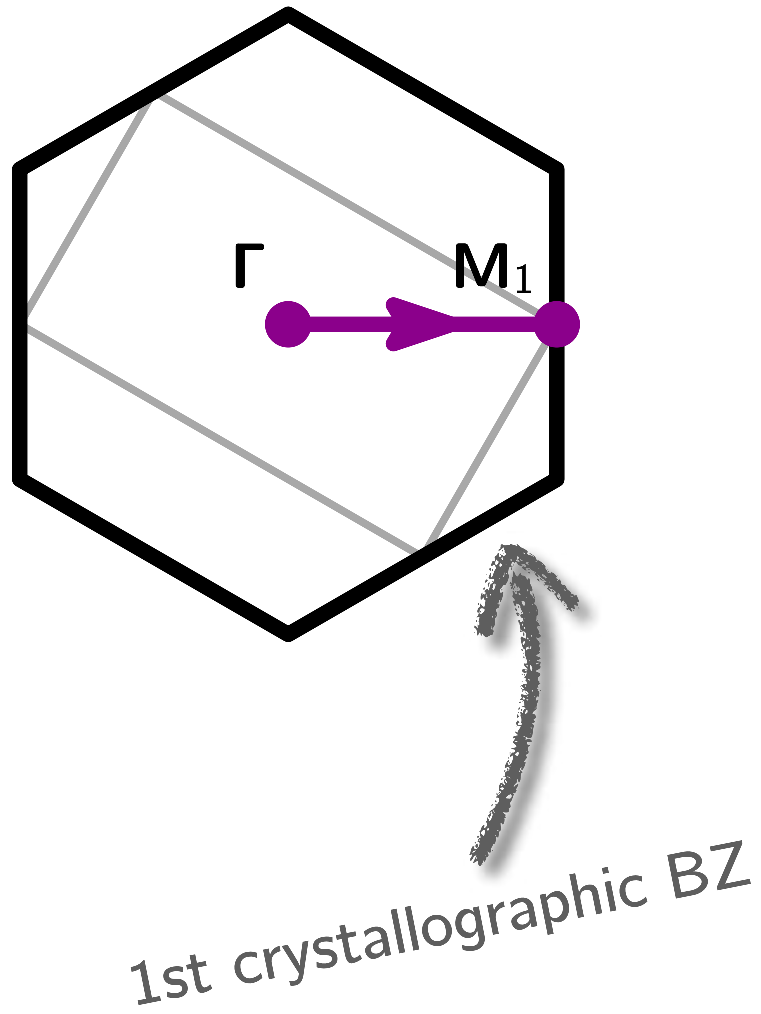

Spectrum necessarily symmetric

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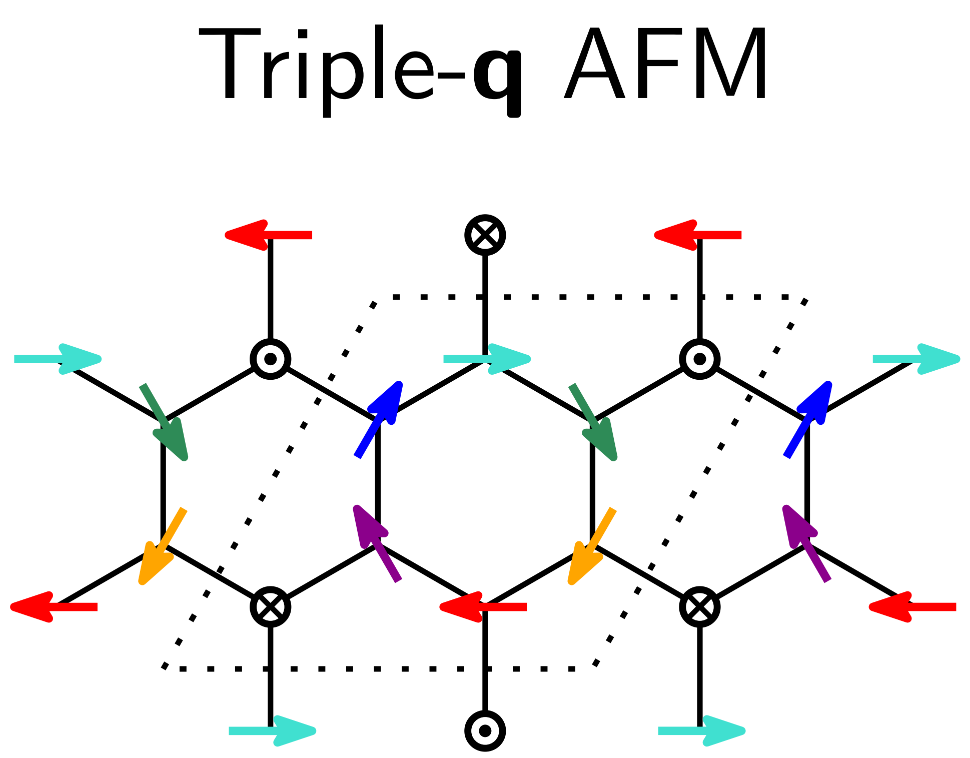
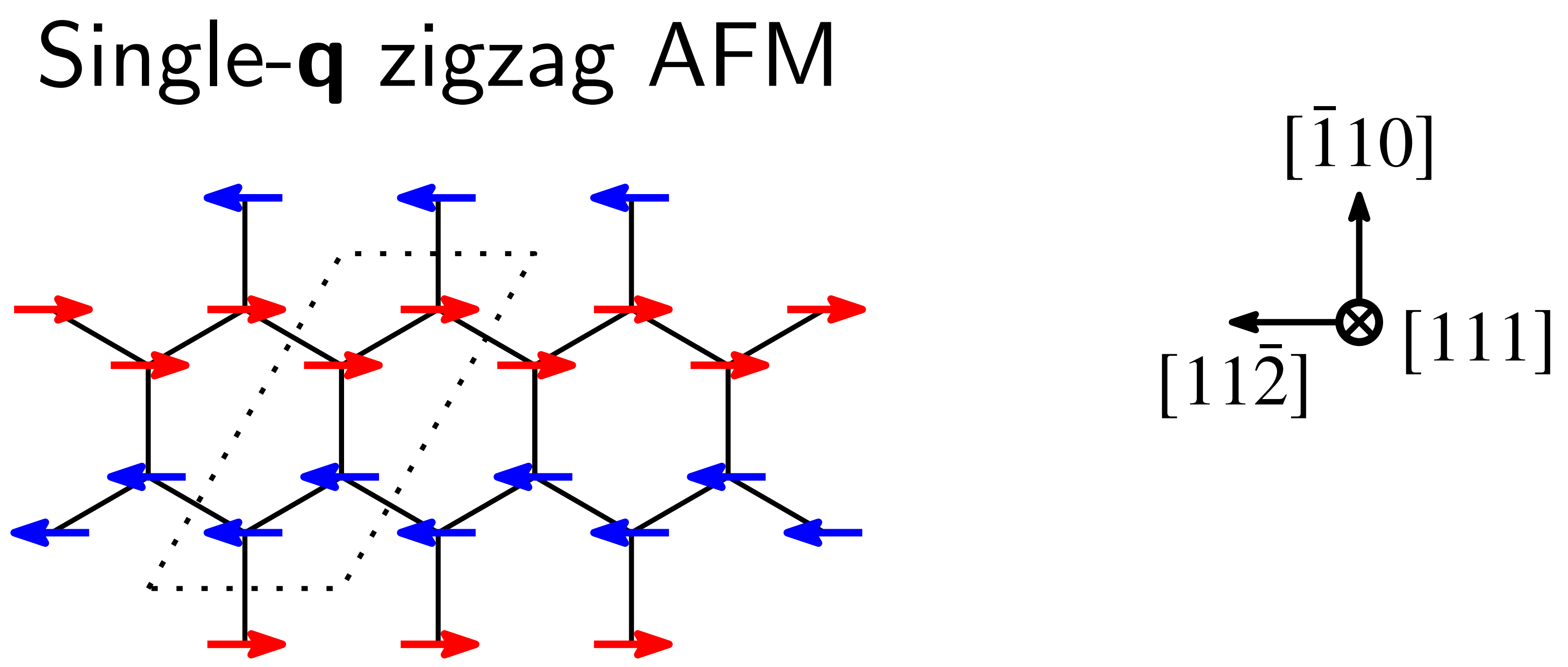
Multi-q vs single-q order: Magnetic excitation spectrum





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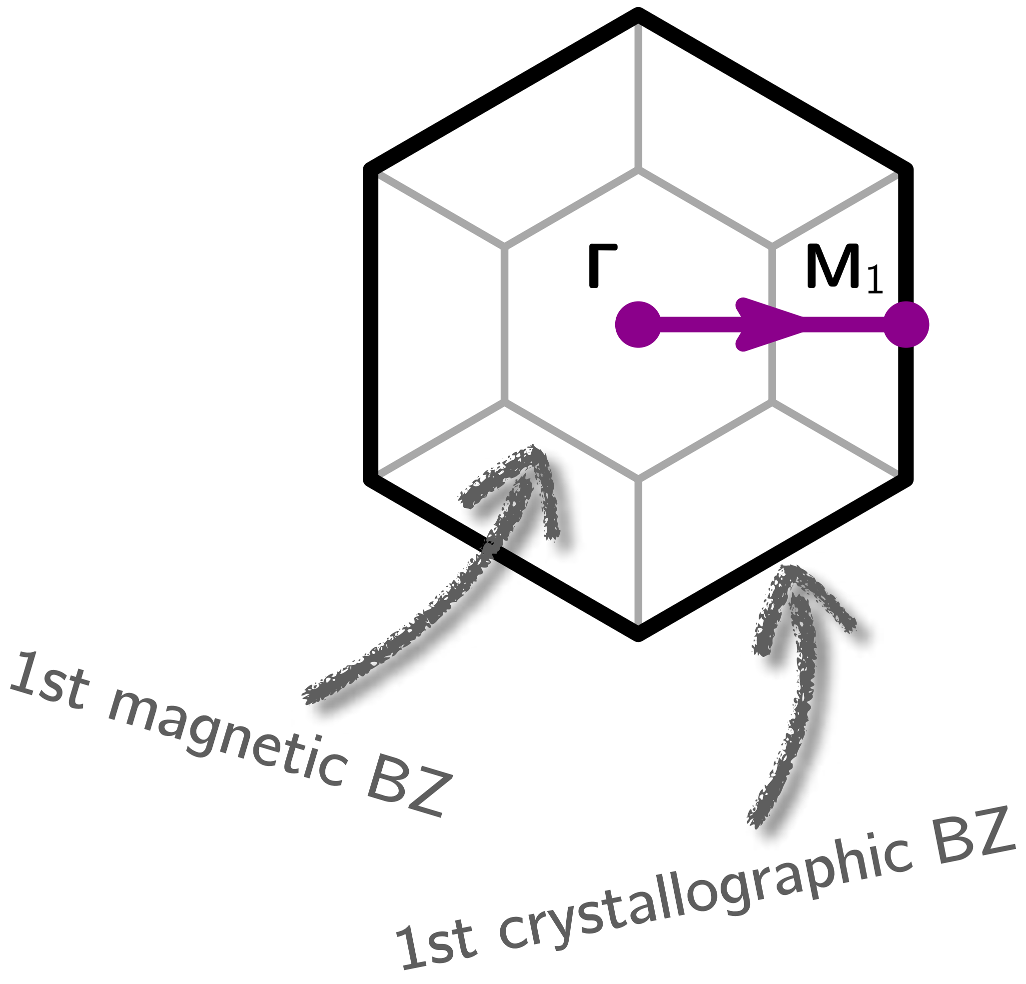
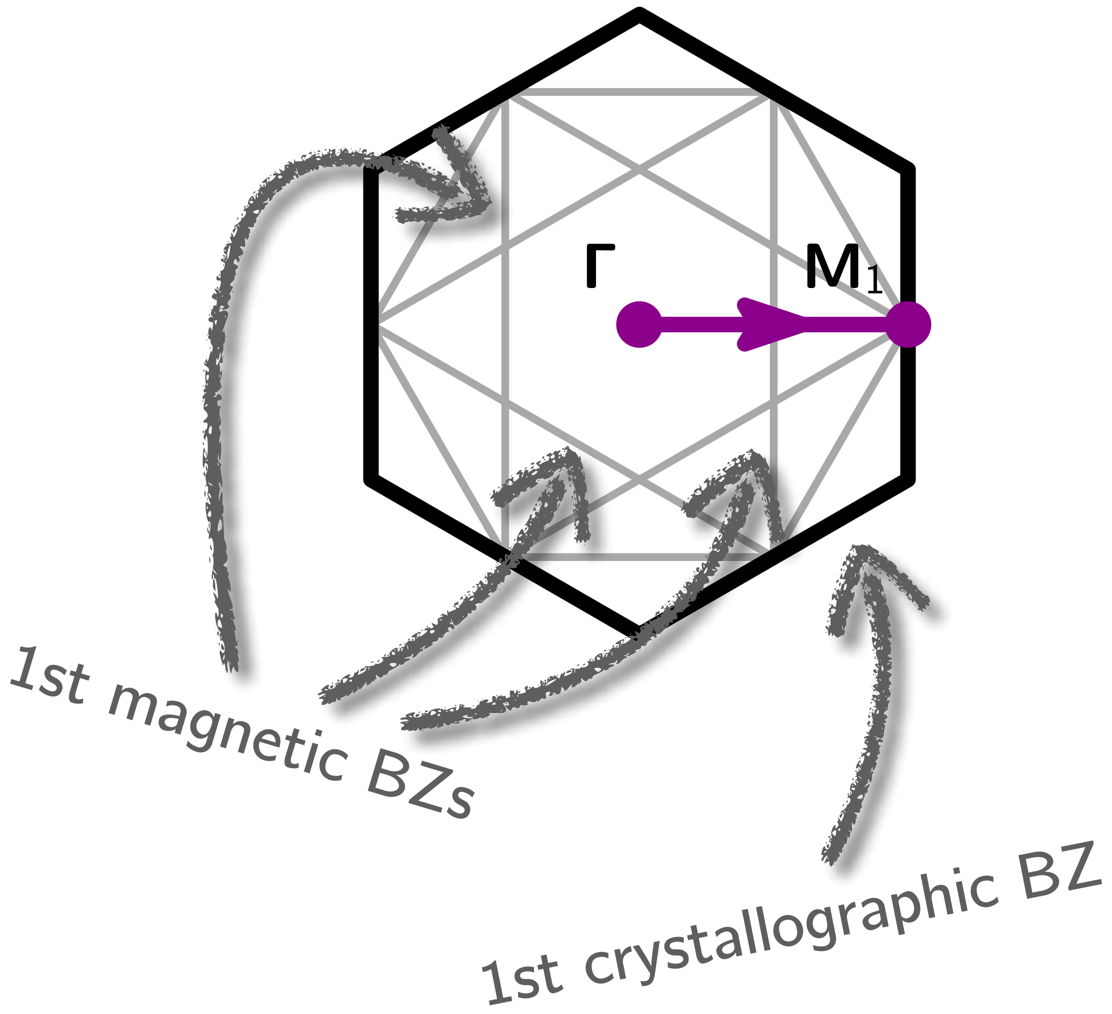




Spectrum necessarily symmetric

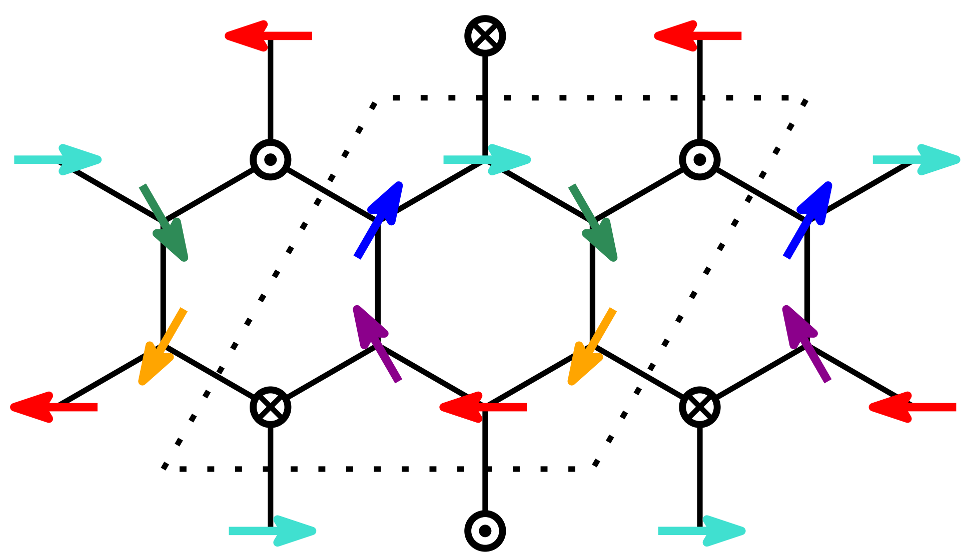
... independent of modeling

Spectrum generically asymmetric

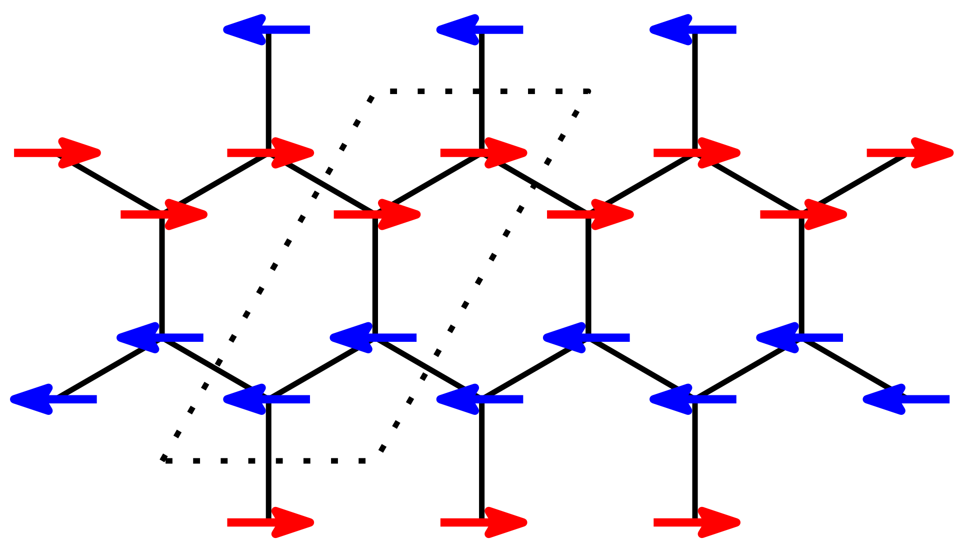
... unless fine-tuned

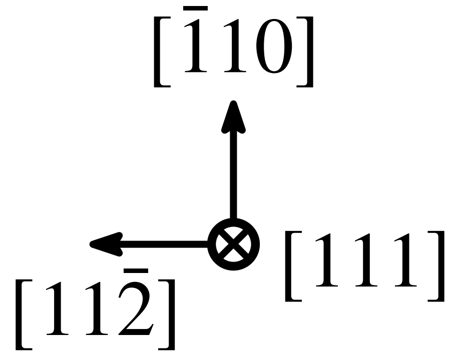
Multi-q vs single-q order: Magnetic excitation spectrum

Triple-**q** AFM

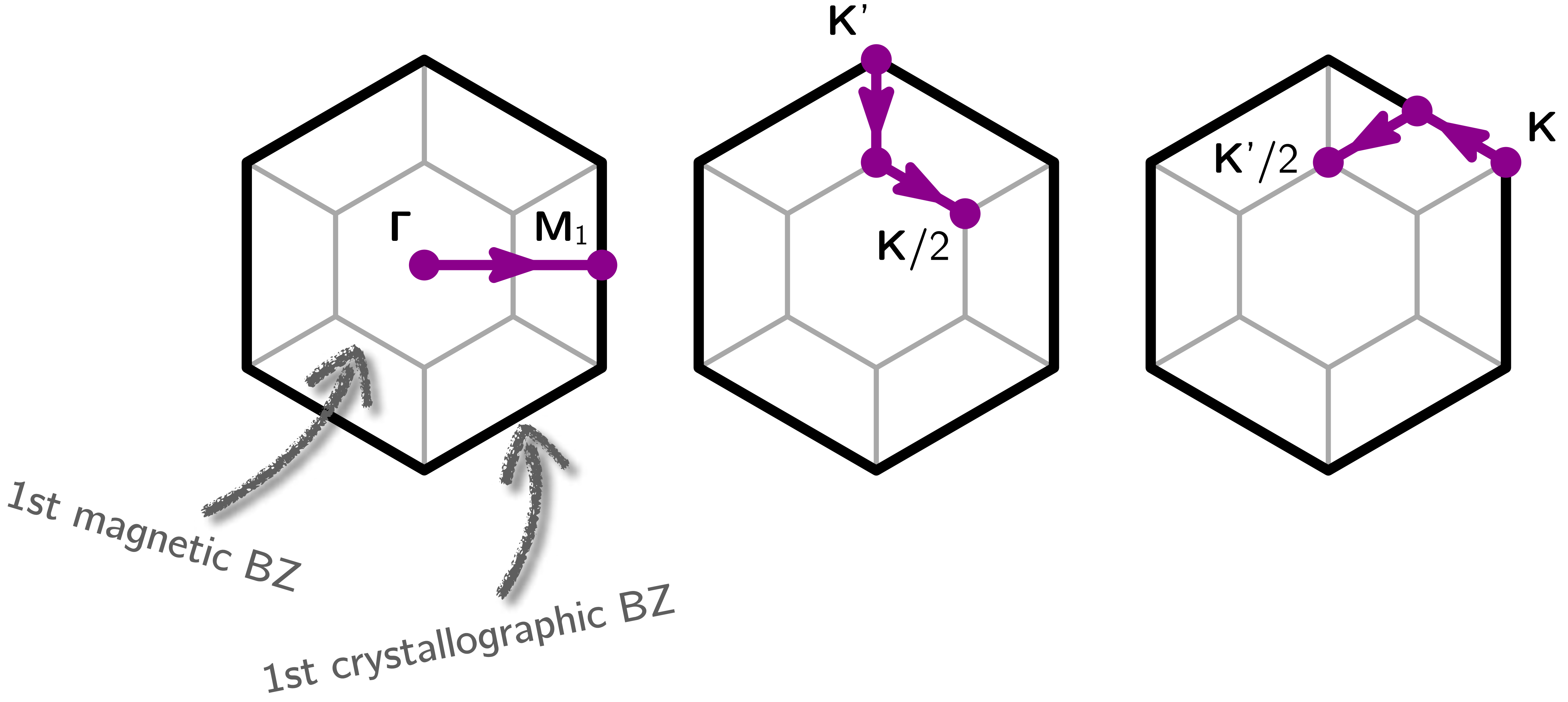


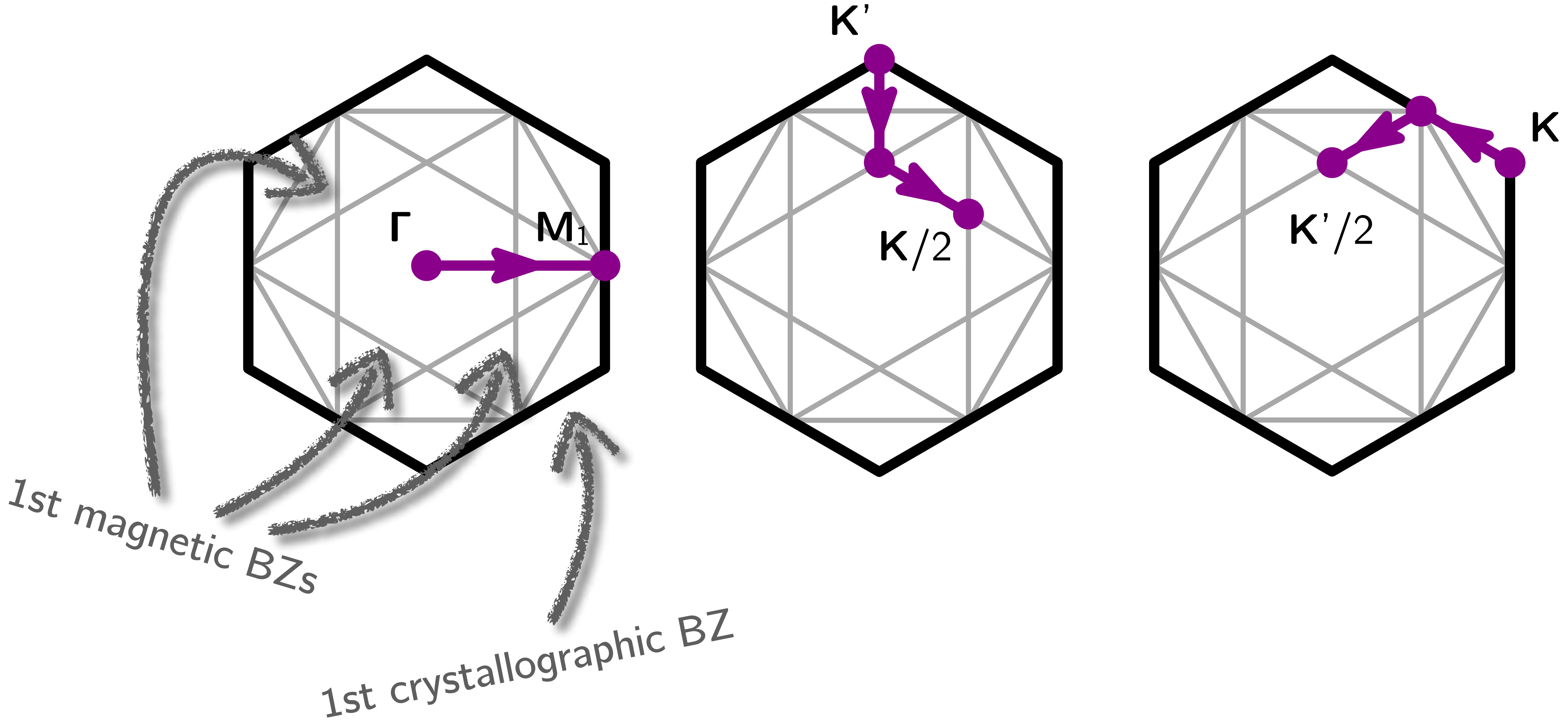
Single-**q** zigzag AFM





Brillouin zone path:





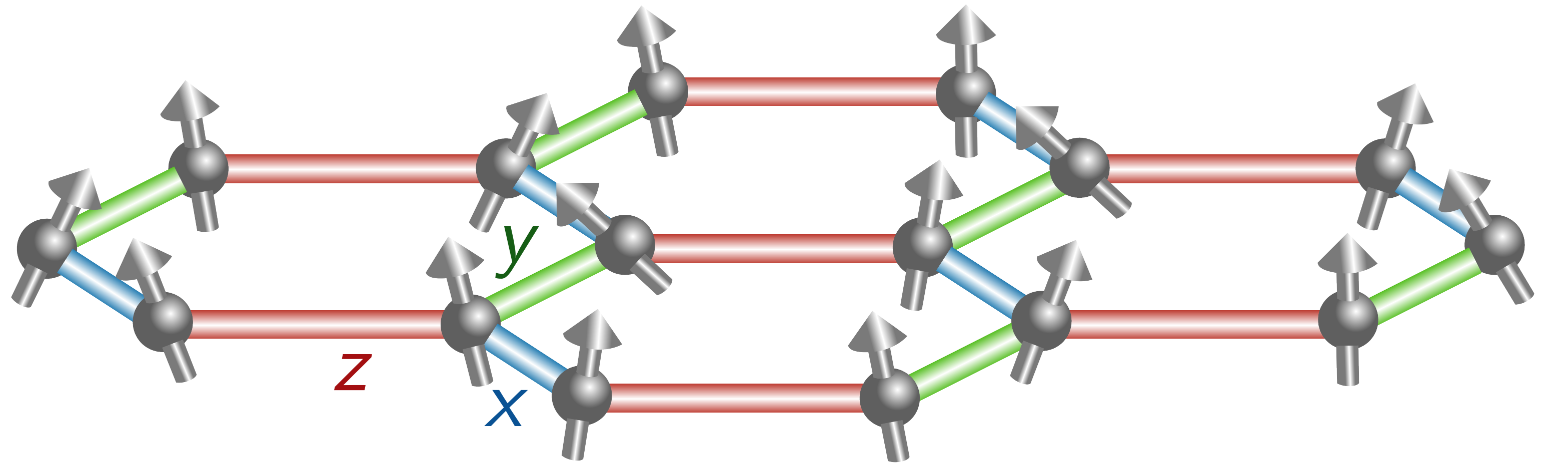
Spectrum necessarily symmetric

... independent of modeling

Spectrum generically asymmetric

... unless fine-tuned

Example: HKΓΓ’ model @ hidden SU(2) point



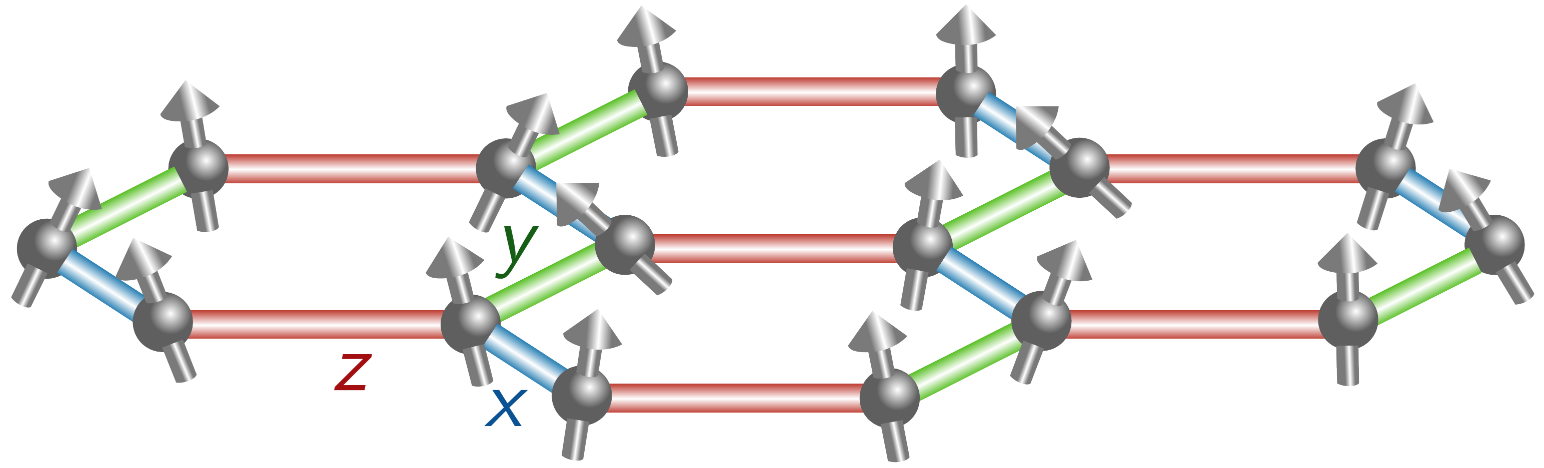
Hamiltonian:

$$\mathcal{H}_0 = \sum_{\langle ij \rangle_\gamma} \Big[J_1 \mathbf{S}_i \cdot \mathbf{S}_j + K_1 S_i^\gamma S_j^\gamma + \Gamma_1 (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma_1' (S_i^\gamma S_j^\alpha + S_i^\alpha S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\beta S_j^\gamma) \Big]$$

... with (J_1, K_1, Γ_1, Γ'_1) = (-1/9, -2/3, 8/9, -4/9) A

[Chaloupka, Khaliullin, PRB ’15]

Example: HKΓΓ' model @ hidden SU(2) point



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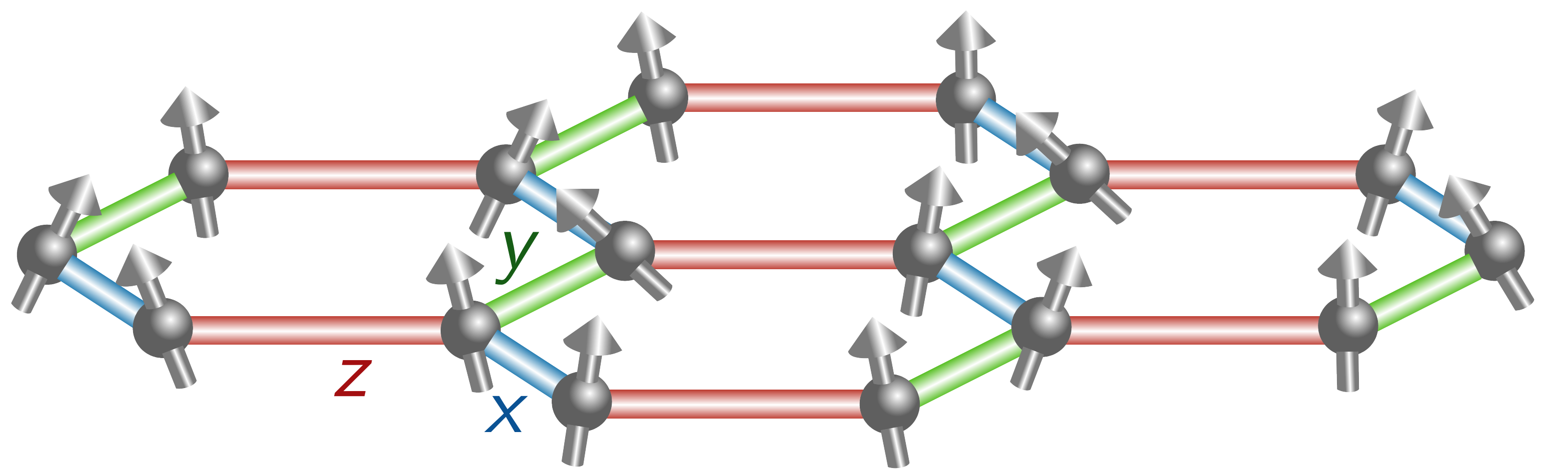
[Chaloupka, Khaliullin, PRB '15]

Hidden SU(2) symmetry: $\mathbf{S}_i \mapsto \tilde{\mathbf{S}}_i = T_{14} \mathbf{S}_i$: $\mathcal{H}_0 \mapsto \tilde{\mathcal{H}}_0 = A \sum_{\langle ij \rangle} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_j$

Local rotation

Example: HKΓΓ’ model @ hidden SU(2) point



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[Chaloupka, Khaliullin, PRB '15]

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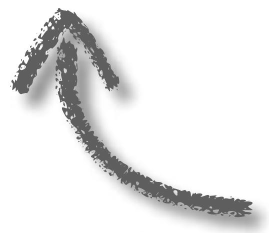
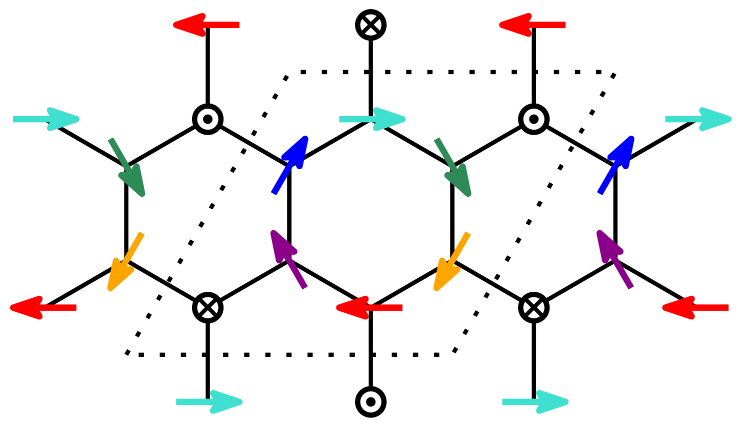
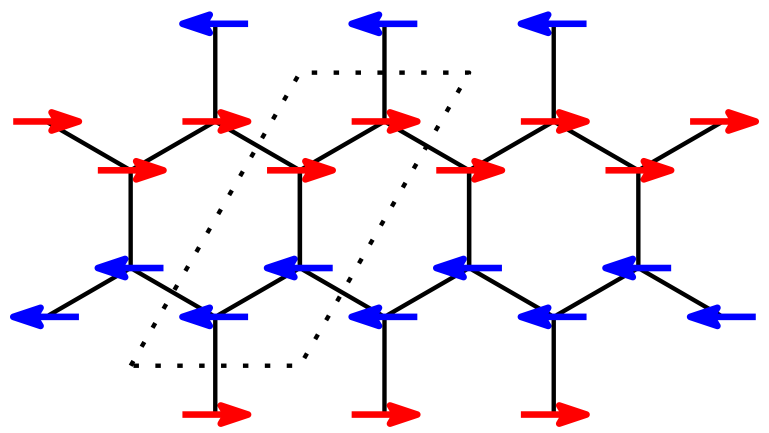


Ground state manifold:

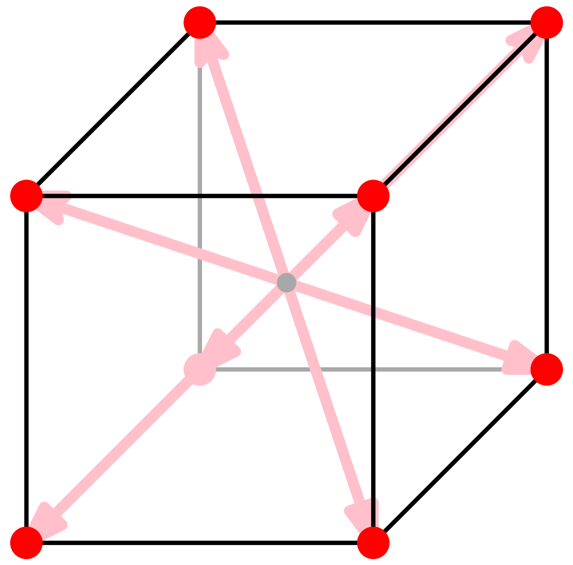
$\mathbf{S}_i$:



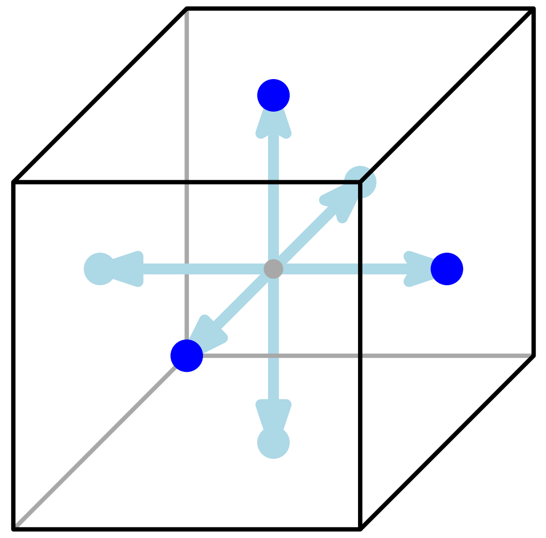


$\updownarrow$ $\updownarrow$

$\tilde{\mathbf{S}}_i$:

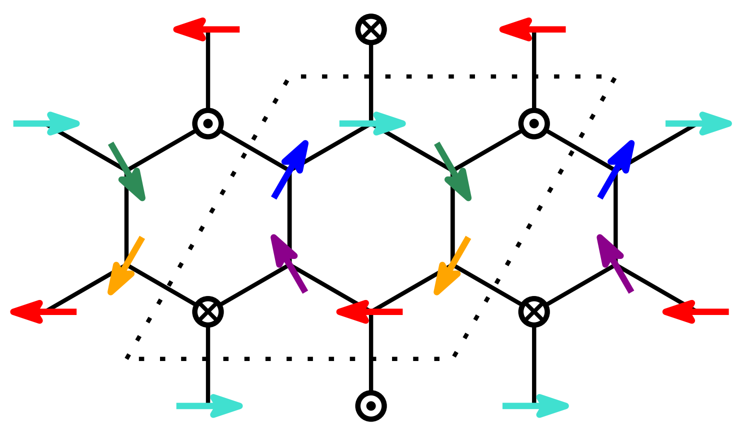


4 diagonals

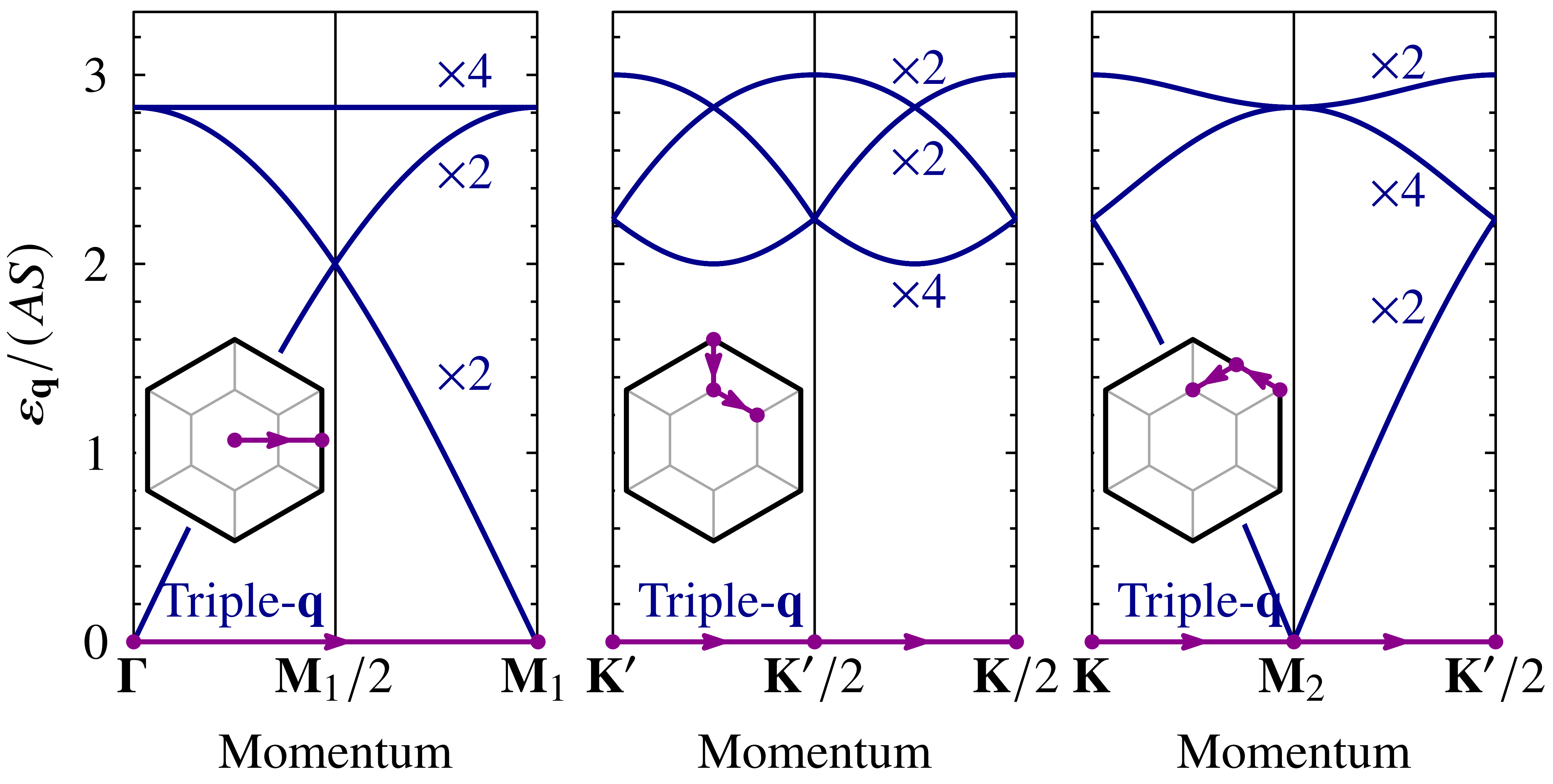


3 cubic axes

Magnon spectrum @ hidden SU(2) point

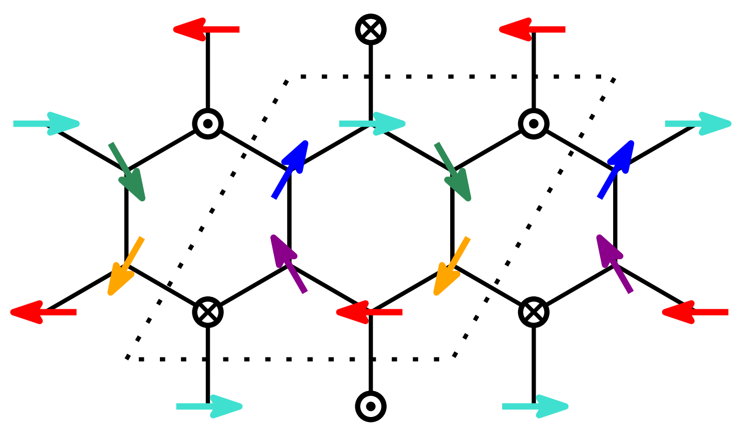


Triple-**q** AFM

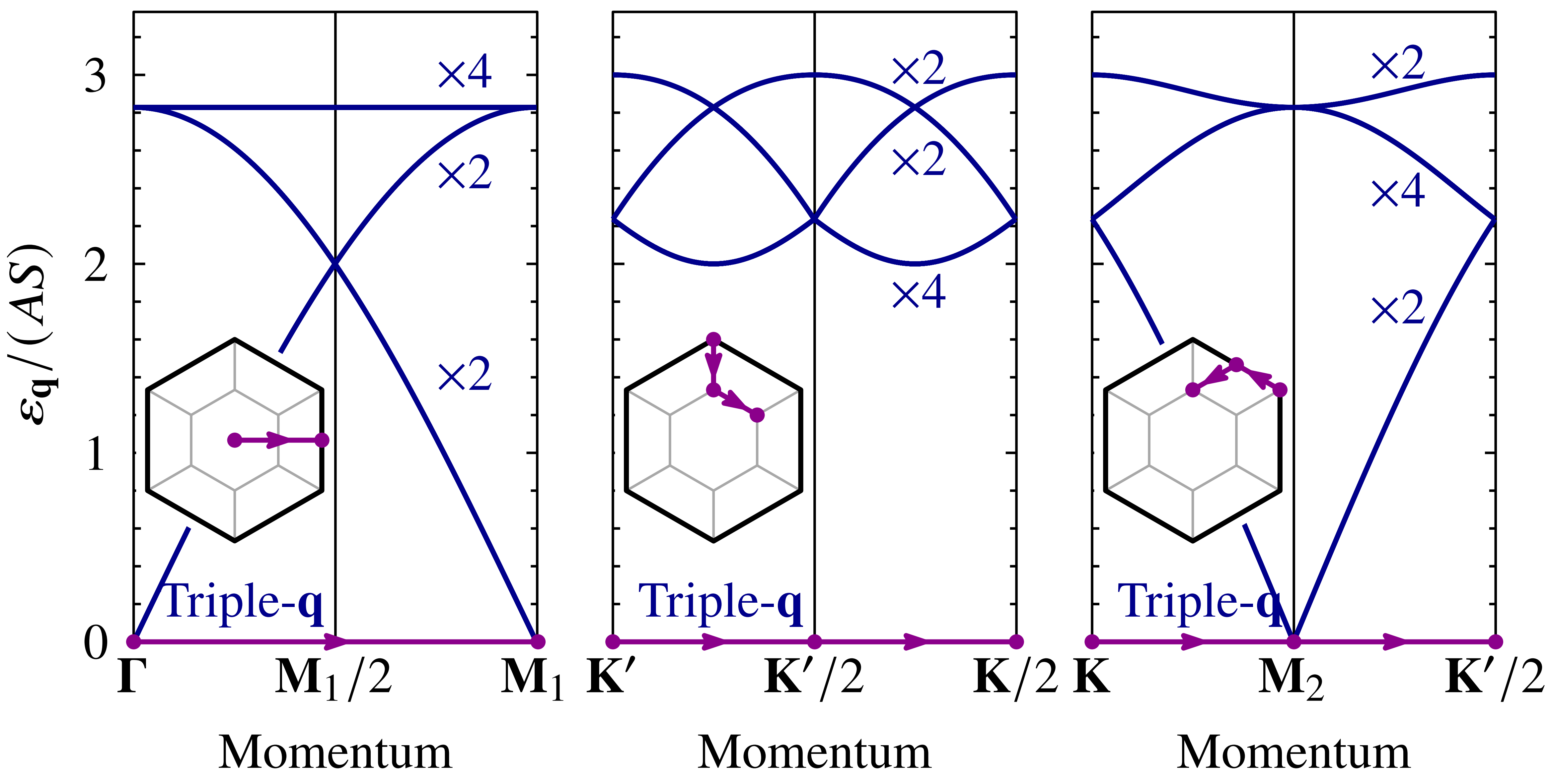


... fully symmetric

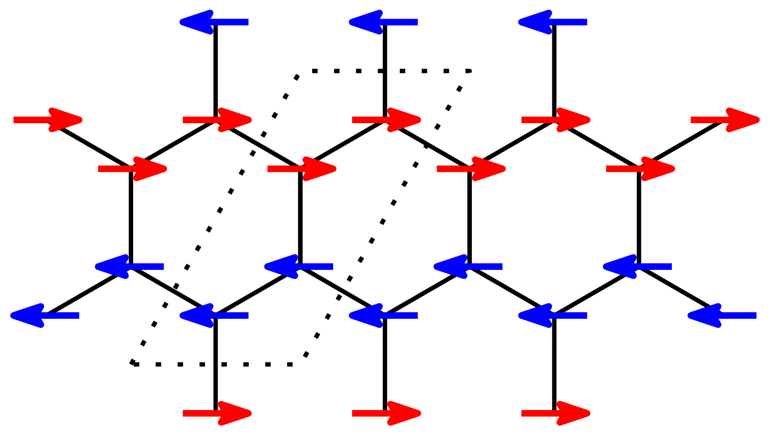
Magnon spectrum @ hidden SU(2) point



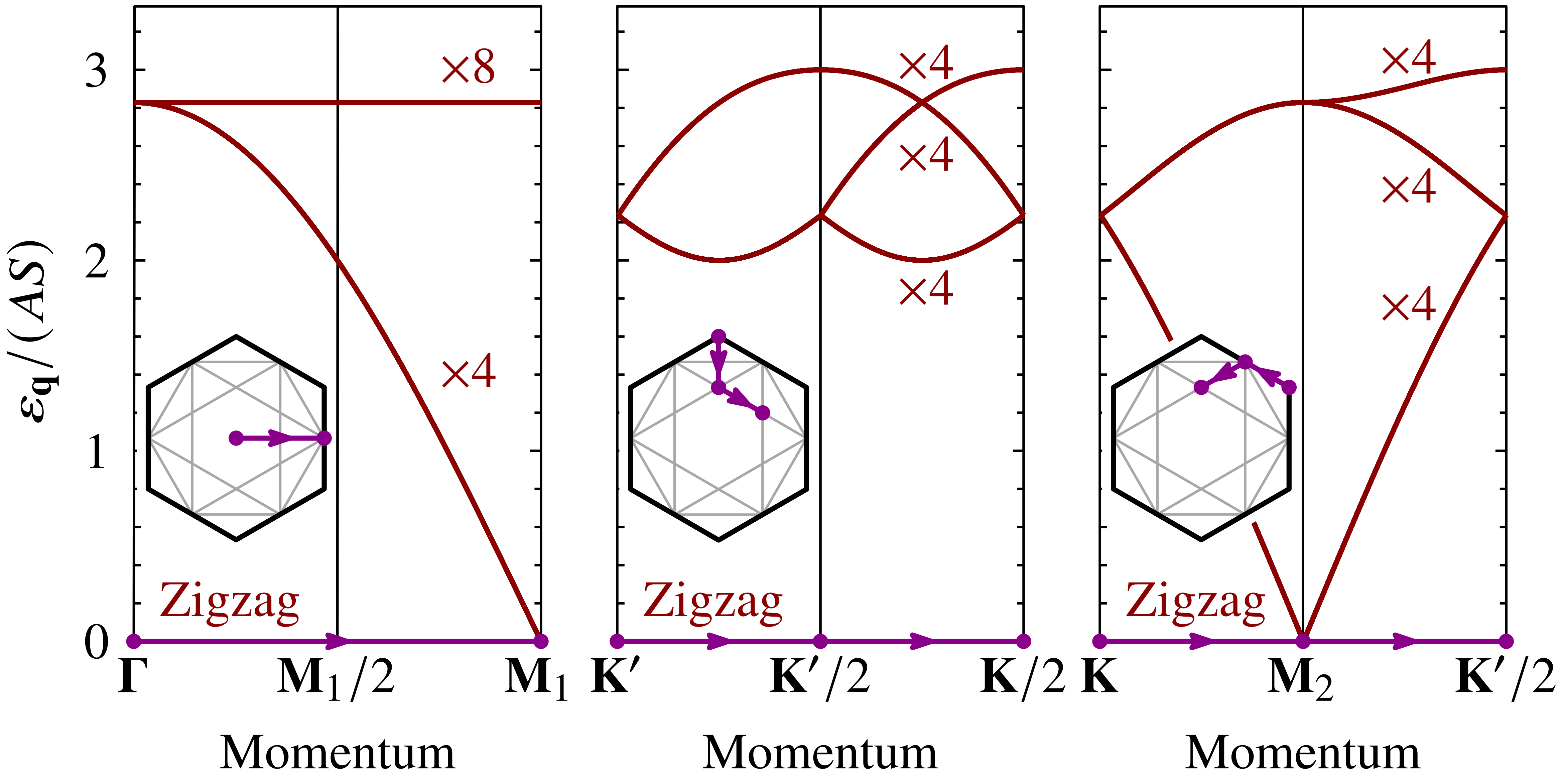
Triple-**q** AFM



... fully symmetric

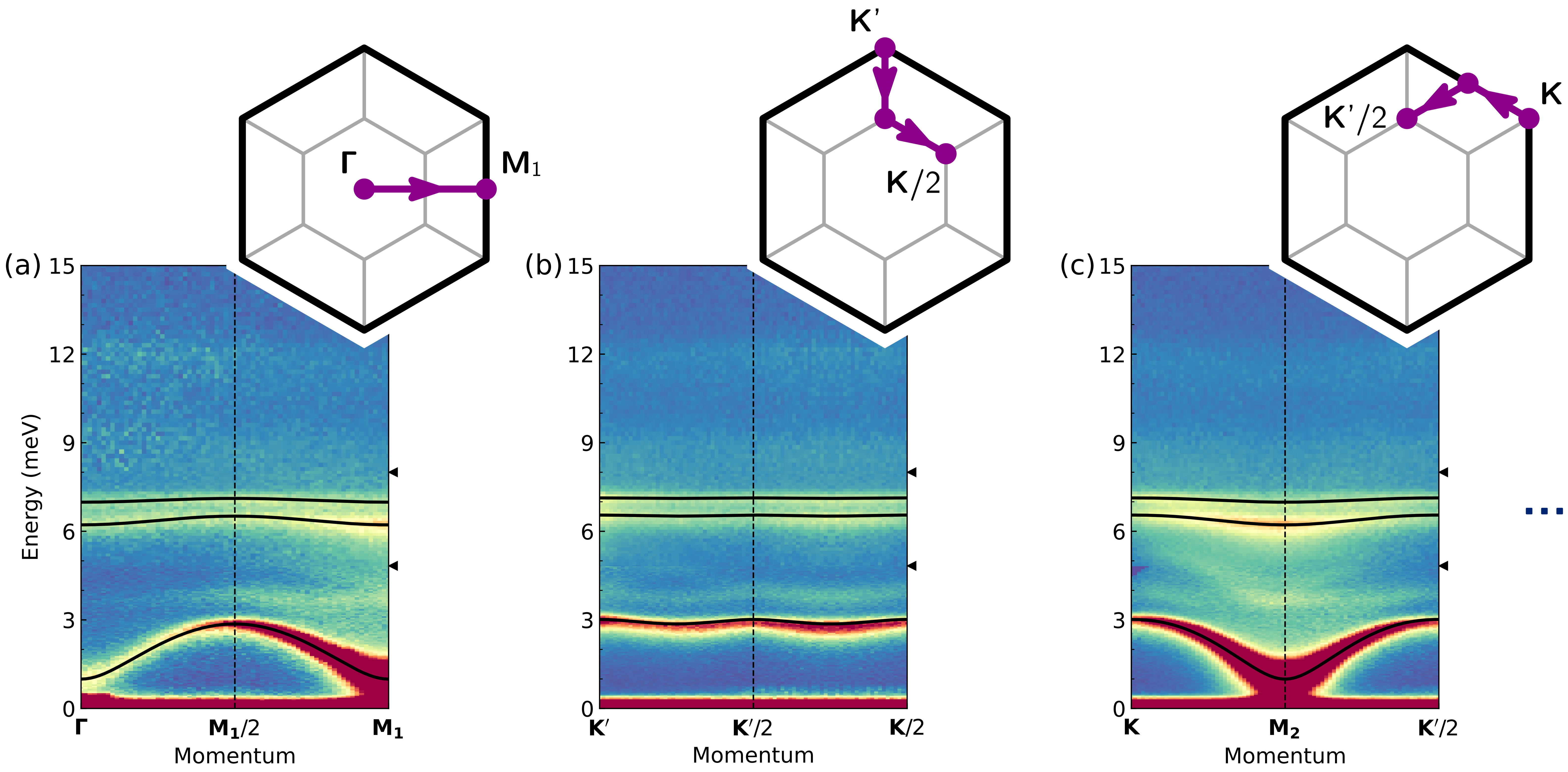


Zigzag AFM



... at least some bands asymmetric

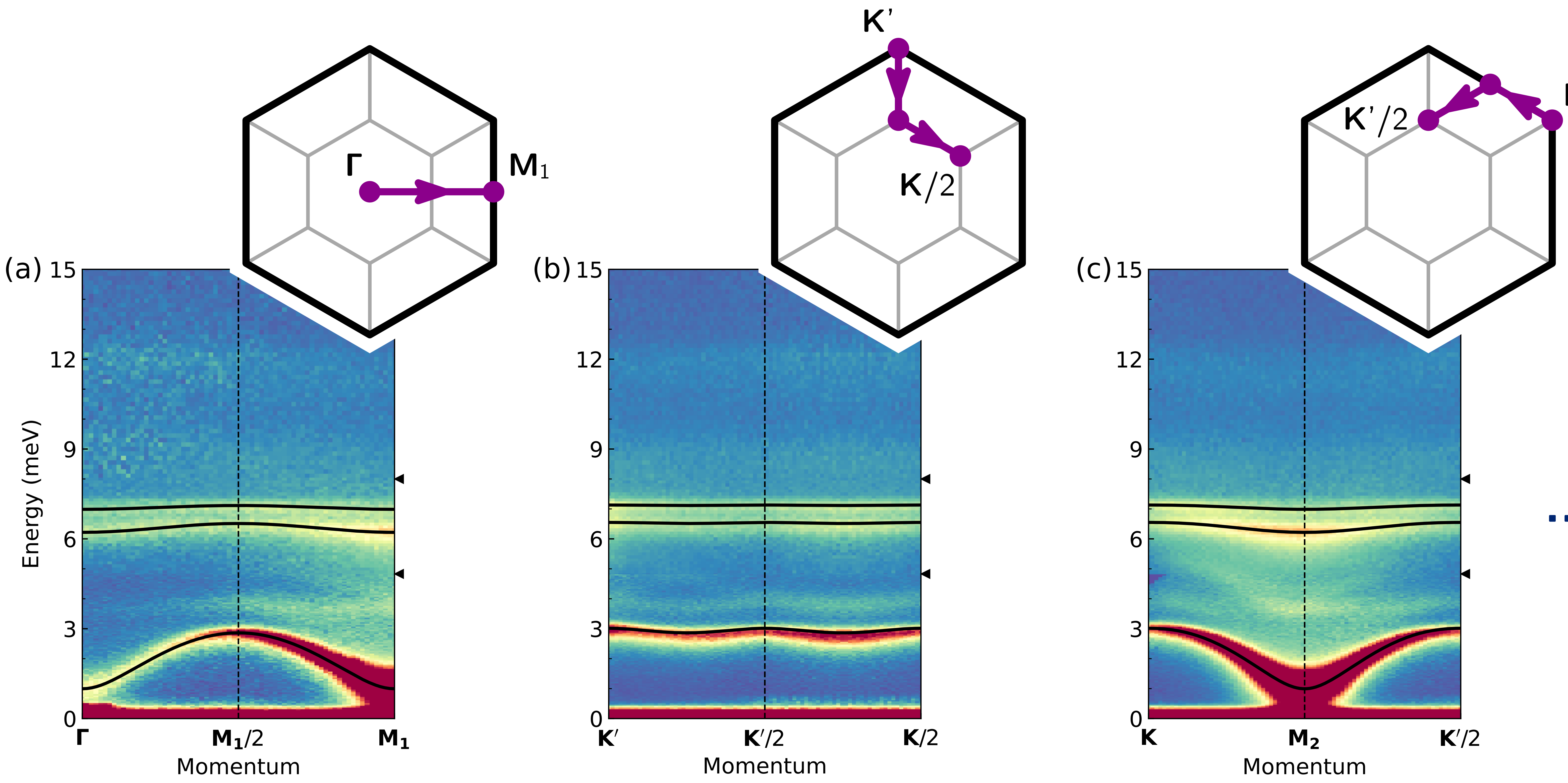
$Na_2Co_2TeO_6$: Inelastic neutron scattering



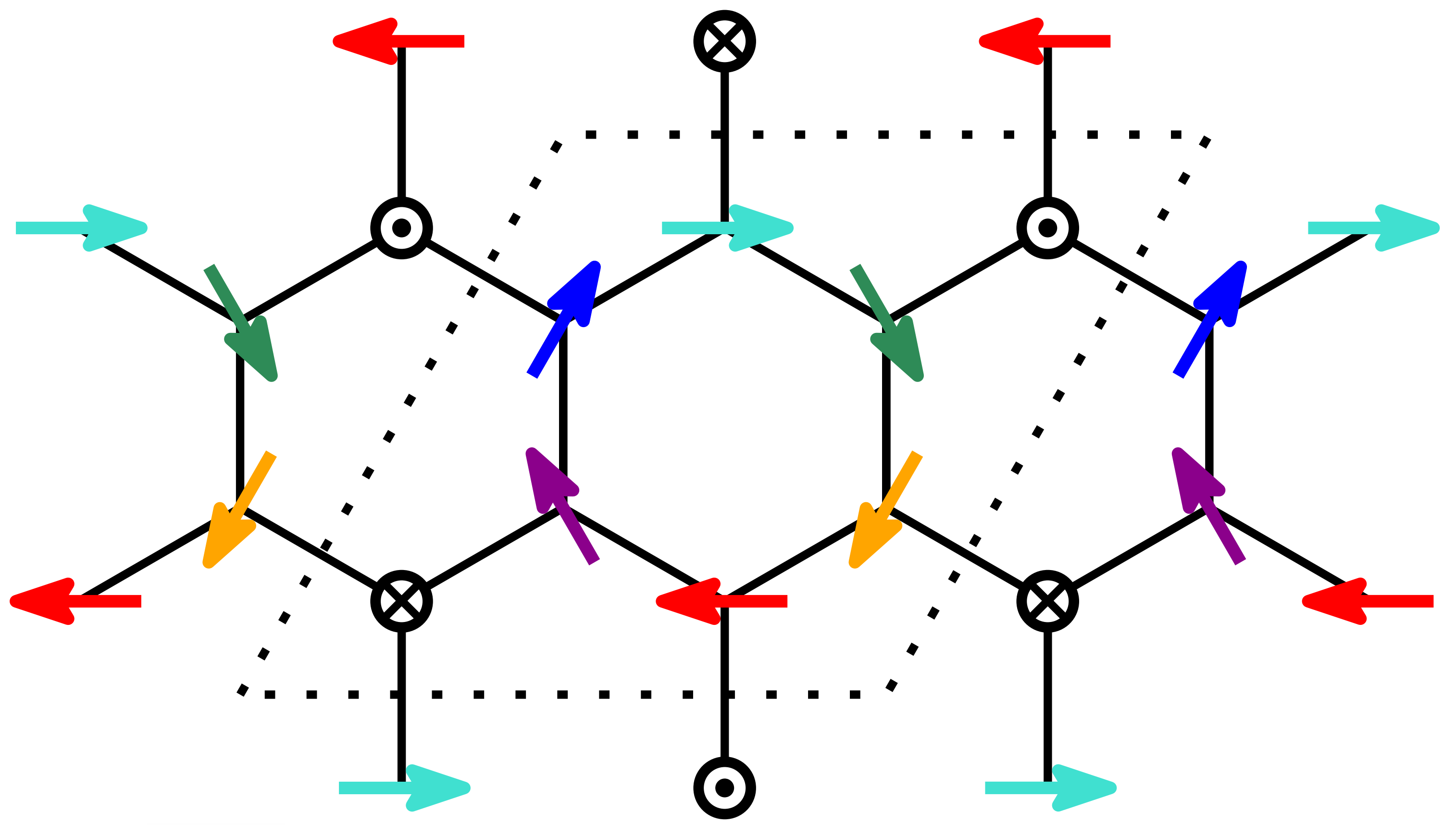
… perfectly symmetric magnon bands

[Krüger, Chen, Jin, Li, LJ, PRL '23]

$Na_2Co_2TeO_6$: Inelastic neutron scattering



… perfectly symmetric magnon bands

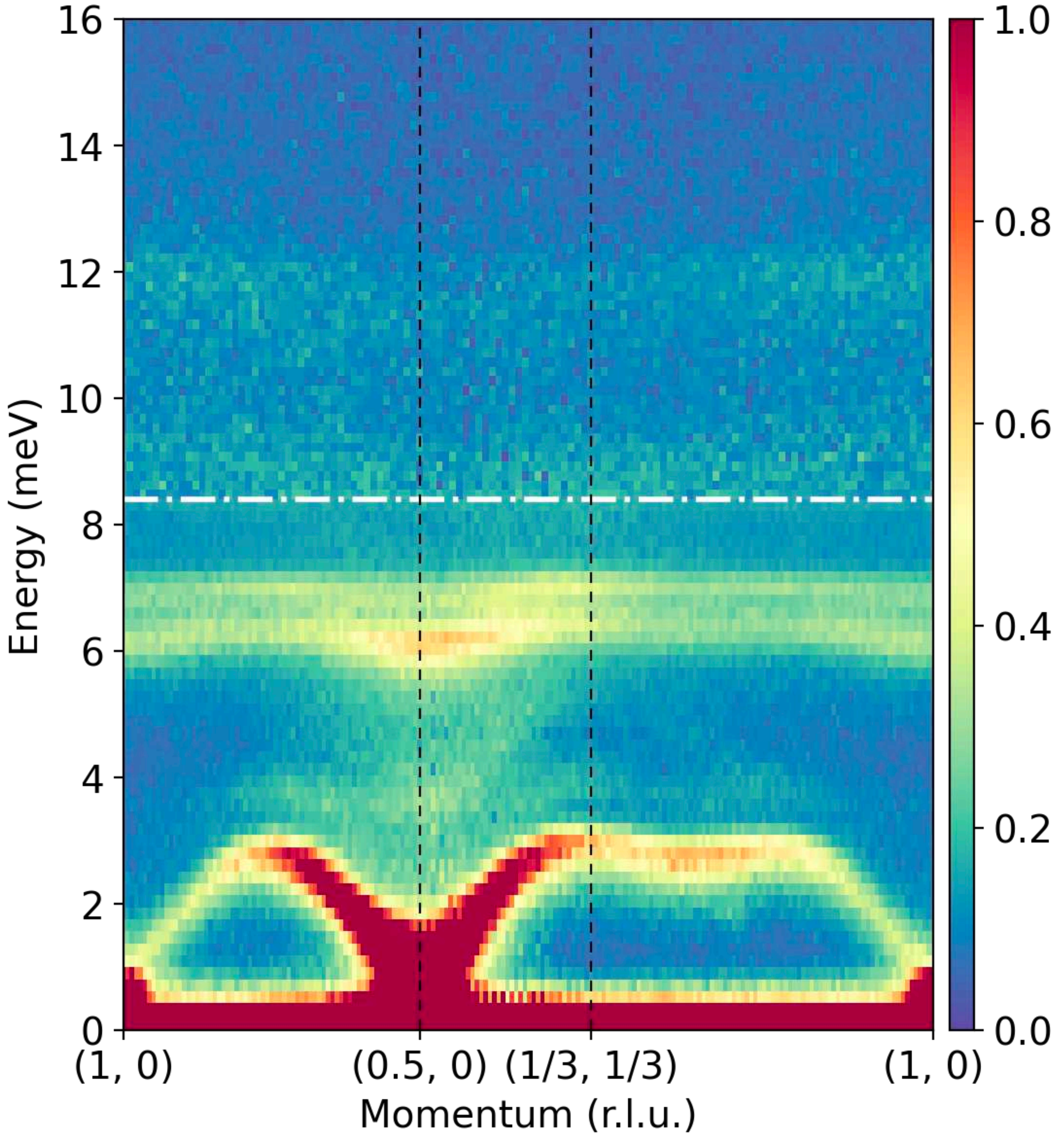


$Na_2Co_2TeO_6$ features triple-**q** AFM order at low temperatures

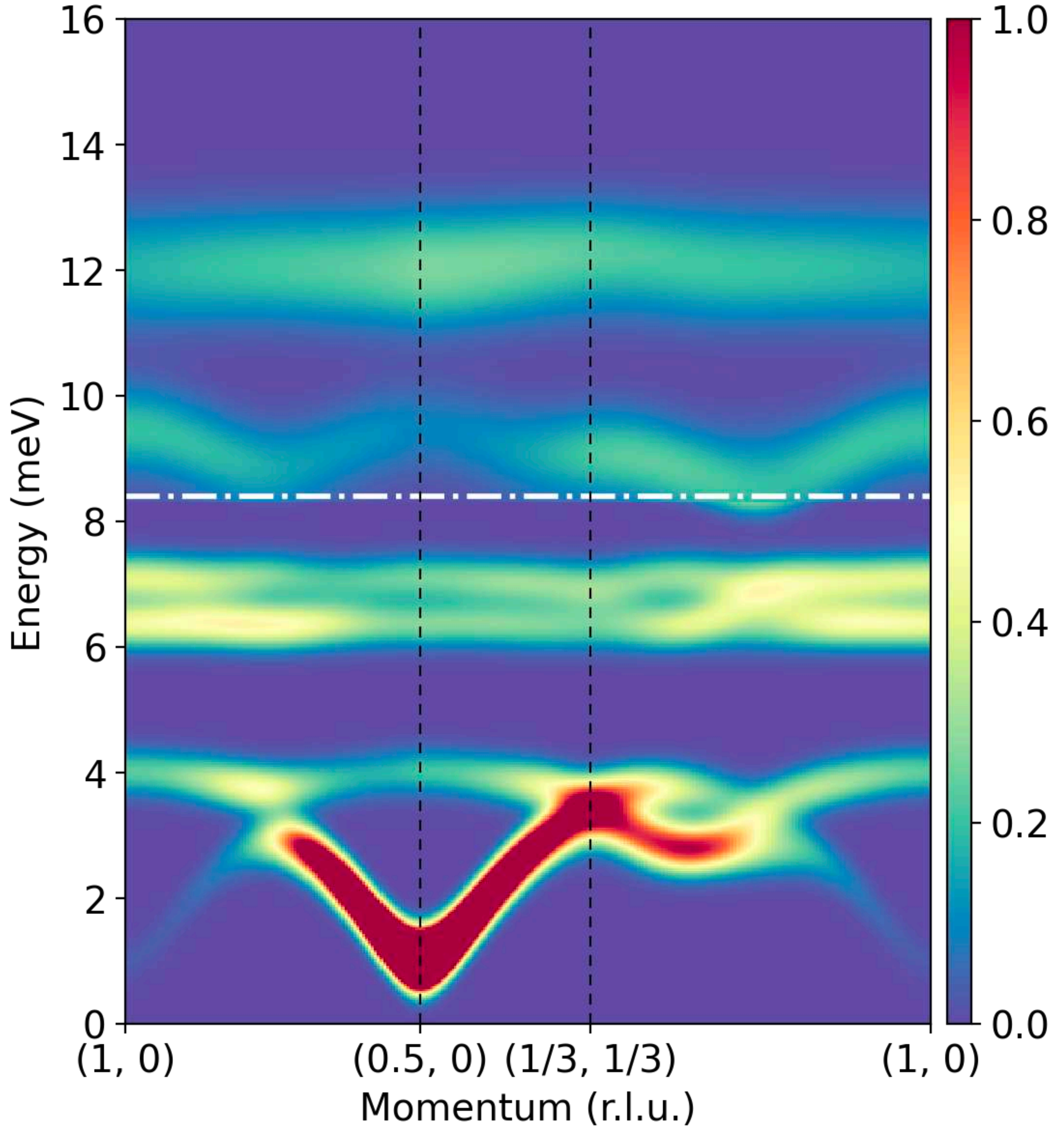
[Krüger, Chen, Jin, Li, LJ, PRL '23]

$Na_2Co_2TeO_6$: Experiment vs. theory

Inelastic neutron scattering



Linear spin wave model



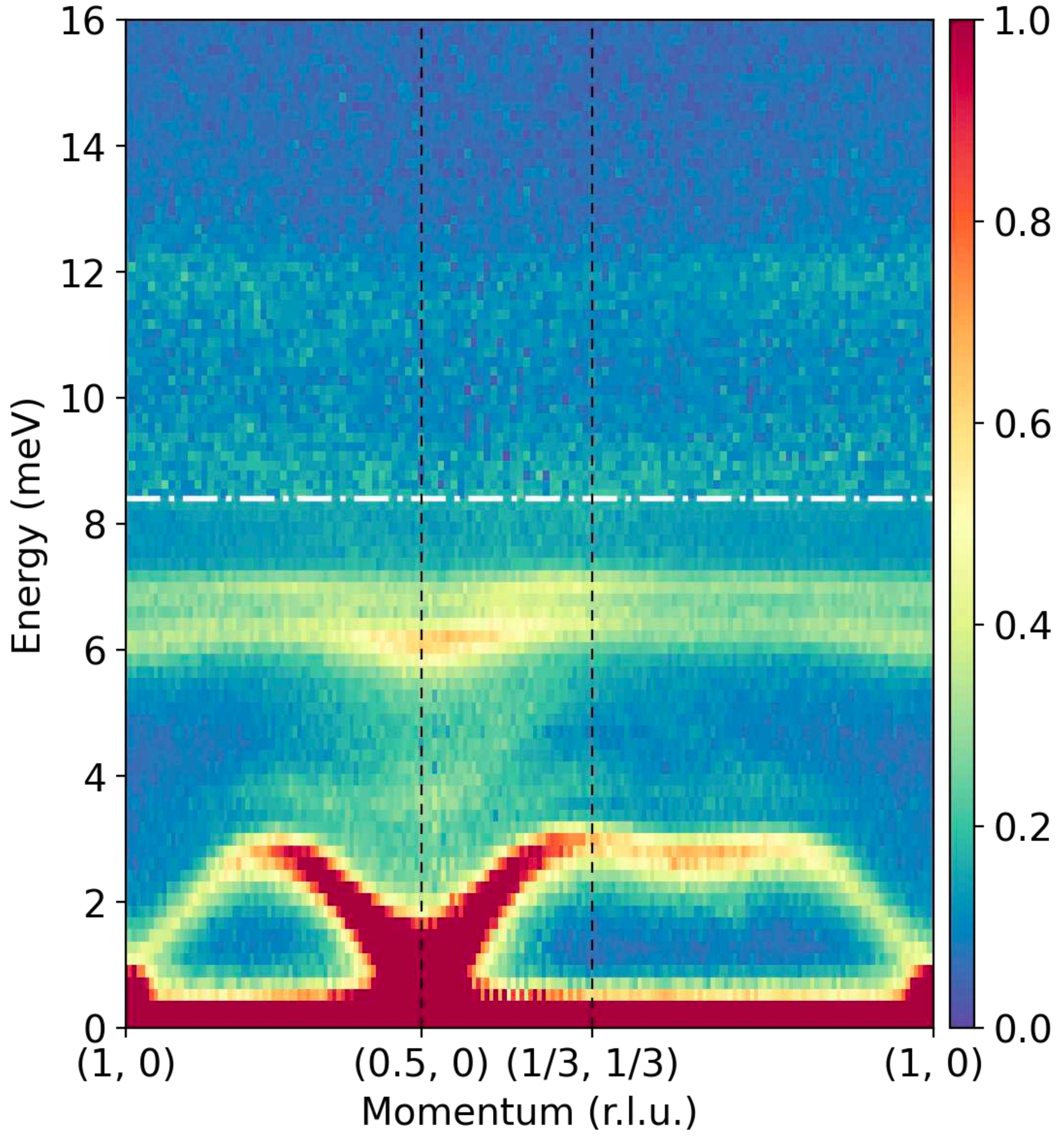
Effective spin model:

Material	Reference	$\mathcal{H}_{\text{Kitaev}}$	$\mathcal{H}_{\text{H}\Gamma\Gamma'}$					
		K_1 (meV)	J_1 (meV)	Γ_1 (meV)	Γ'_1 (meV)	J_2^A (meV)	J_2^B (meV)	J_3 (meV)
$Na_2Co_2TeO_6$	this work	-8.29	1.23	1.86	-2.27	0.32	-0.24	0.47

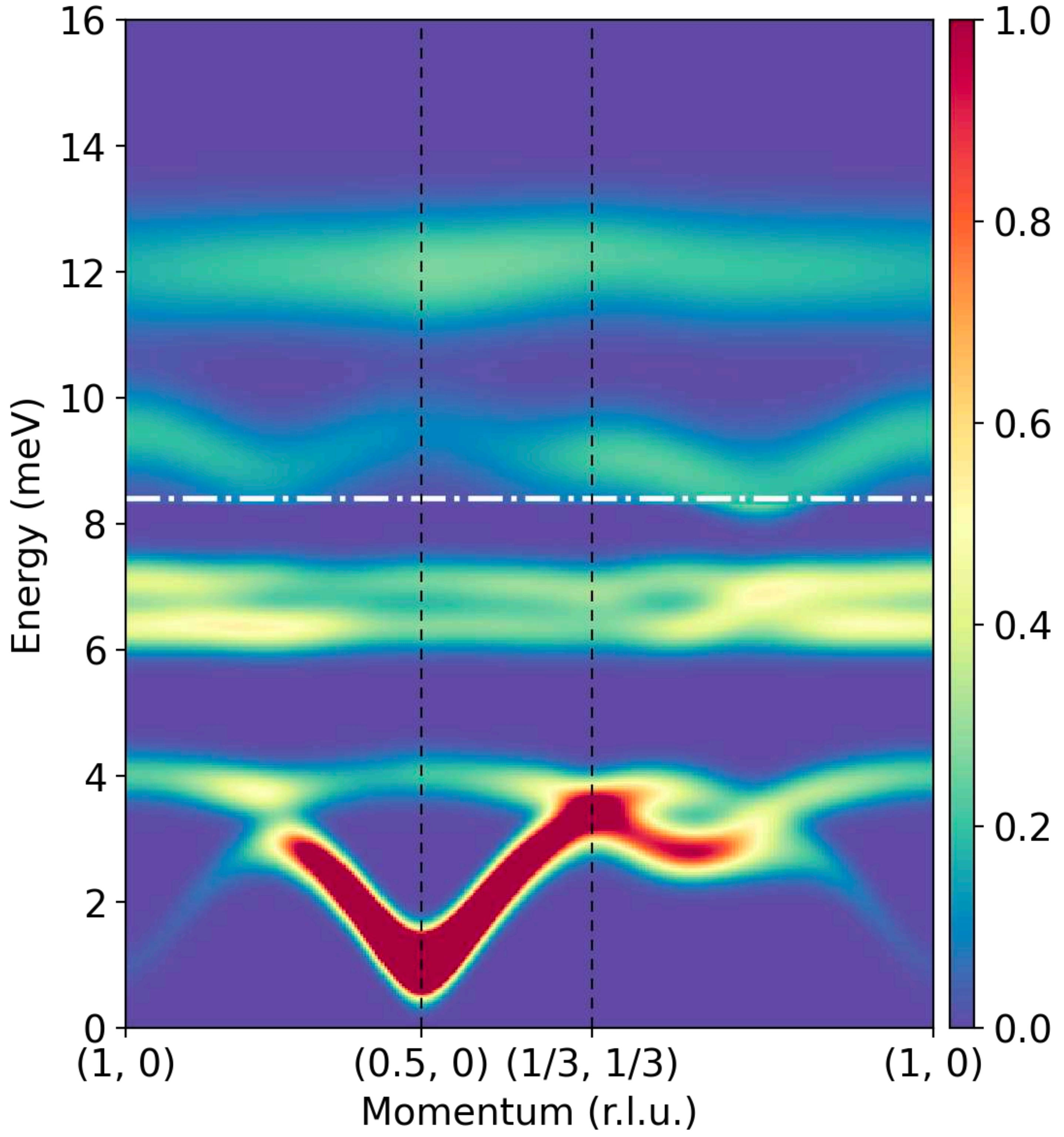
+ nonbilinear exchange

$Na_2Co_2TeO_6$: Experiment vs. theory

Inelastic neutron scattering



Linear spin wave model



Effective spin model:

Material	Reference	$\mathcal{H}_{\text{Kitaev}}$ K_1 (meV)	$\mathcal{H}_{\text{H}\Gamma\Gamma'}$ J_1 (meV)	Γ_1 (meV)	Γ'_1 (meV)	J_2^A (meV)	J_2^B (meV)	J_3 (meV)
$Na_2Co_2TeO_6$	this work	-8.29	1.23	1.86	-2.27	0.32	-0.24	0.47
Na_2IrO_3	[Winter *et al.* '16]	-17.00	–	–	–	–	–	6.80
α-$RuCl_3$	[Winter *et al.* '17]	-5.00	-0.50	2.50	–	–	–	0.50

+ nonbilinear exchange

Candidate Kitaev magnets: Proximity to quantum spin liquid

1-parameter family of Hamiltonians: $\mathcal{H}(\alpha) = \mathcal{H}_{\mathsf{Kitaev}} + \alpha \mathcal{H}_{\mathsf{H\Gamma\Gamma'}}$

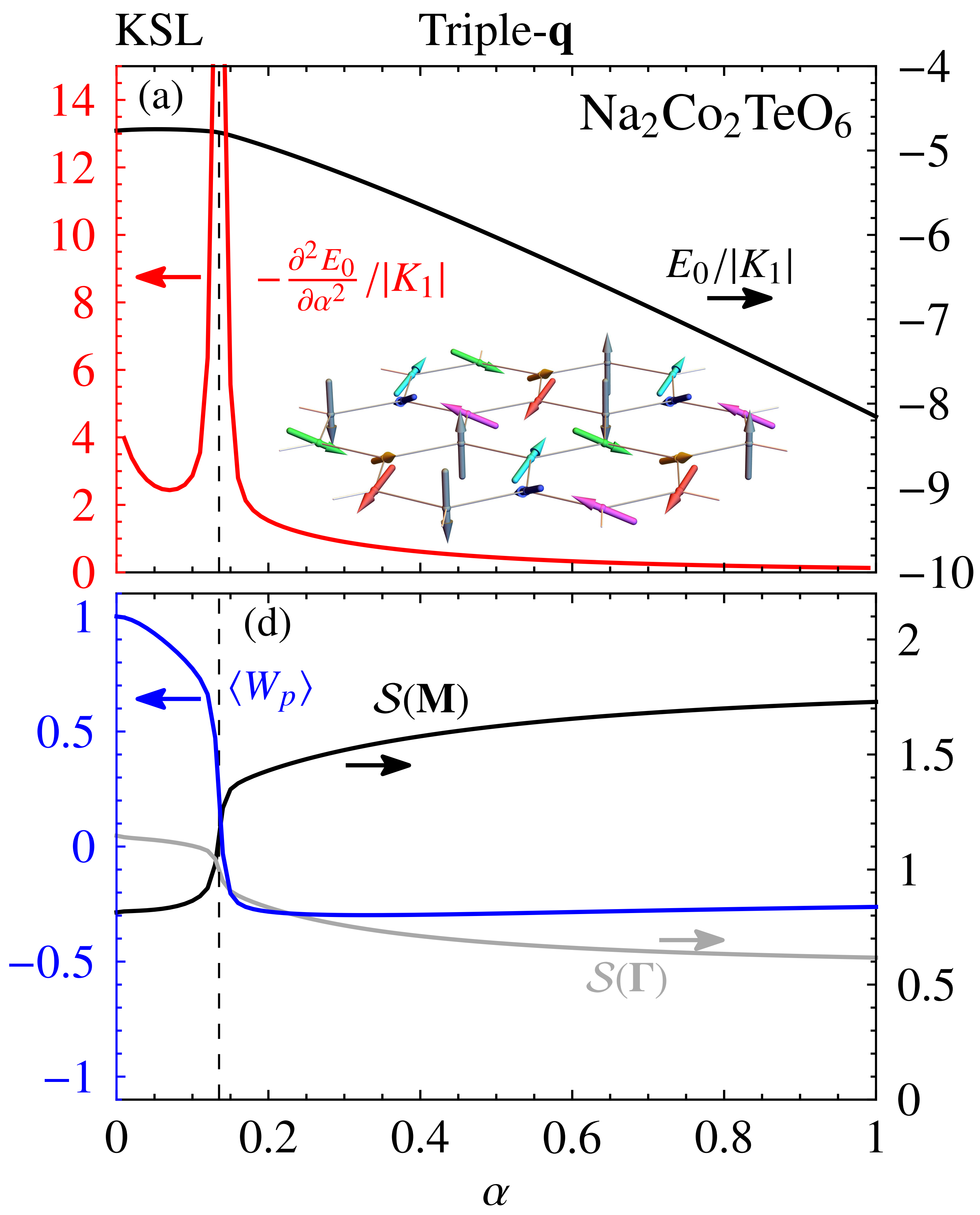
[Krüger, Chen, Jin, Li, LJ, PRL '23]

Candidate Kitaev magnets: Proximity to quantum spin liquid

1-parameter family of Hamiltonians: $\mathcal{H}(\alpha) = \mathcal{H}_{\mathrm{Kitaev}} + \alpha \mathcal{H}_{\mathrm{H}\Gamma\Gamma'}$

Phase diagrams:

... from 24-site exact diagonalization



$\alpha_c = 0.14$

[Krüger, Chen, Jin, Li, LJ, PRL '23]

Candidate Kitaev magnets: Proximity to quantum spin liquid

1-parameter family of Hamiltonians: $\mathcal{H}(\alpha) = \mathcal{H}_{\text{Kitaev}} + \alpha \mathcal{H}_{\text{H}\Gamma\Gamma'}$

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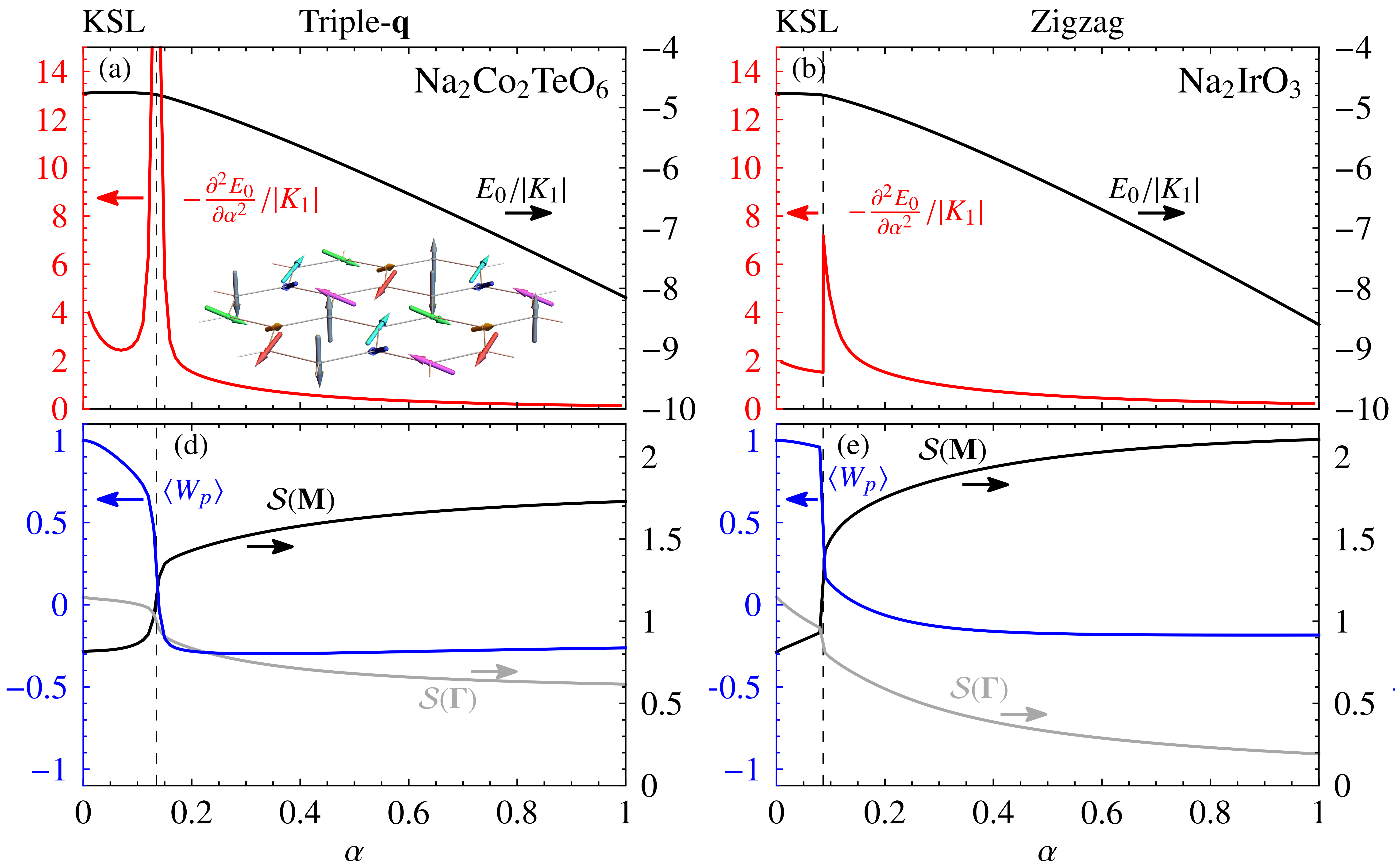

$\alpha_c = 0.14$ $\alpha_c = 0.09$

[Krüger, Chen, Jin, Li, LJ, PRL '23]

Candidate Kitaev magnets: Proximity to quantum spin liquid

1-parameter family of Hamiltonians: $\mathcal{H}(\alpha) = \mathcal{H}_{\mathsf{Kitaev}} + \alpha \mathcal{H}_{\mathsf{H\Gamma\Gamma'}}$

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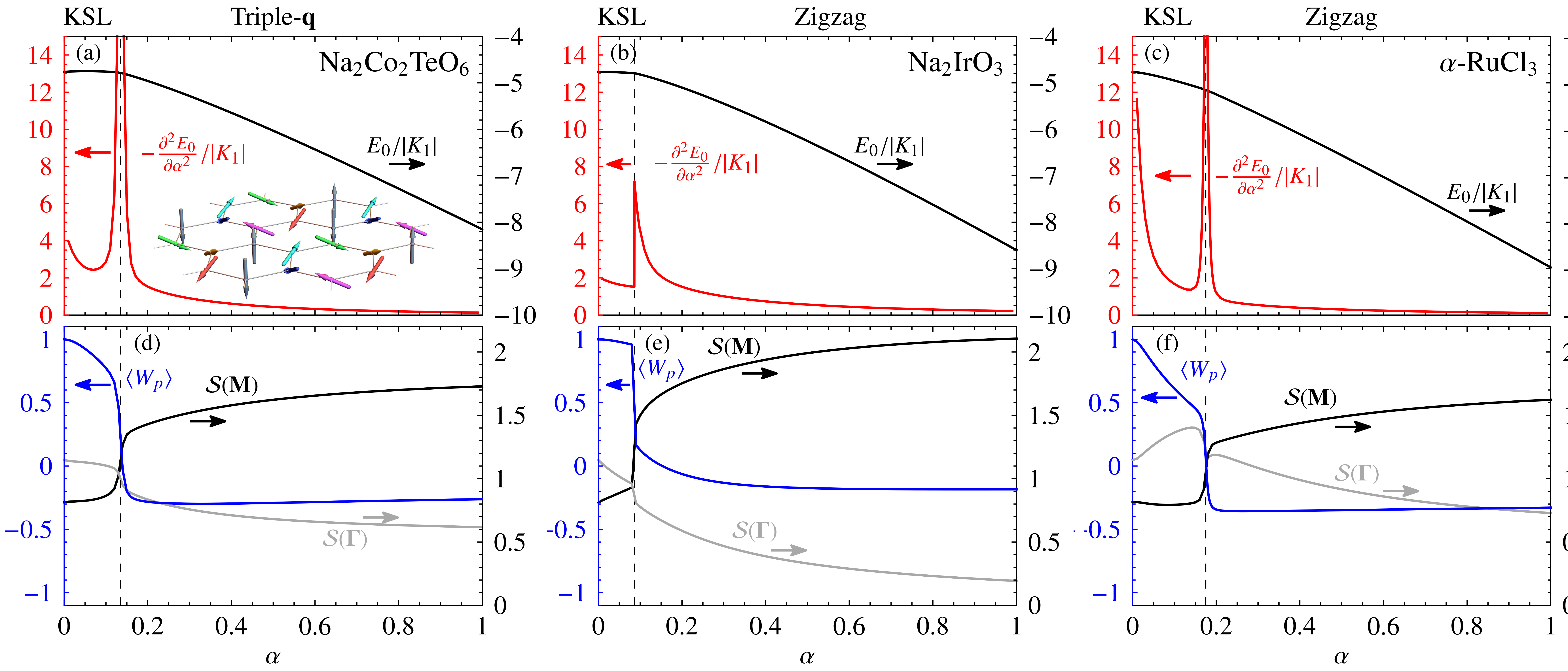


$\alpha_c = 0.14$ $\alpha_c = 0.09$ $\alpha_c = 0.18$

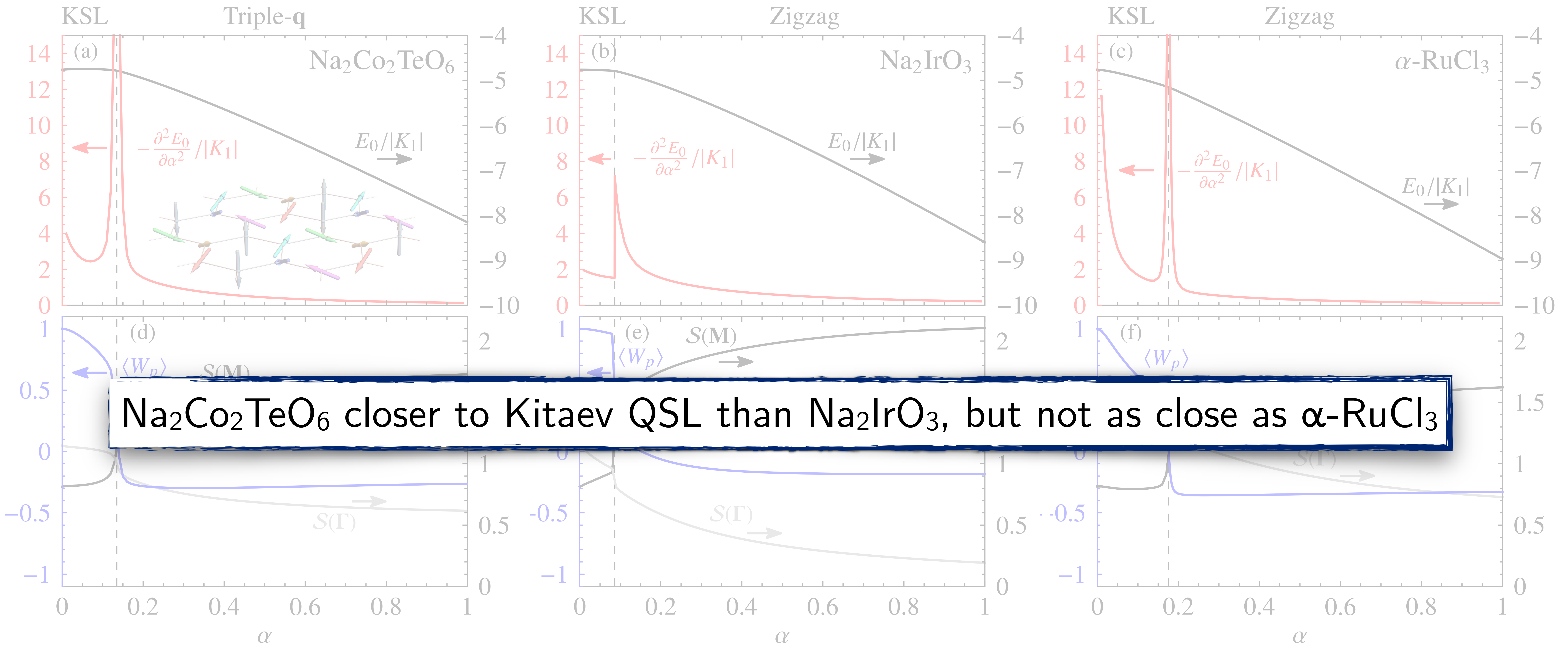
[Krüger, Chen, Jin, Li, LJ, PRL ’23]

Candidate Kitaev magnets: Proximity to quantum spin liquid

1-parameter family of Hamiltonians: $\mathcal{H}(\alpha) = \mathcal{H}_{\text{Kitaev}} + \alpha \mathcal{H}_{\text{H}\Gamma\Gamma'}$

Phase diagrams:

… from 24-site exact diagonalization



$Na_2Co_2TeO_6$ closer to Kitaev QSL than Na_2IrO_3, but not as close as α-$RuCl_3$

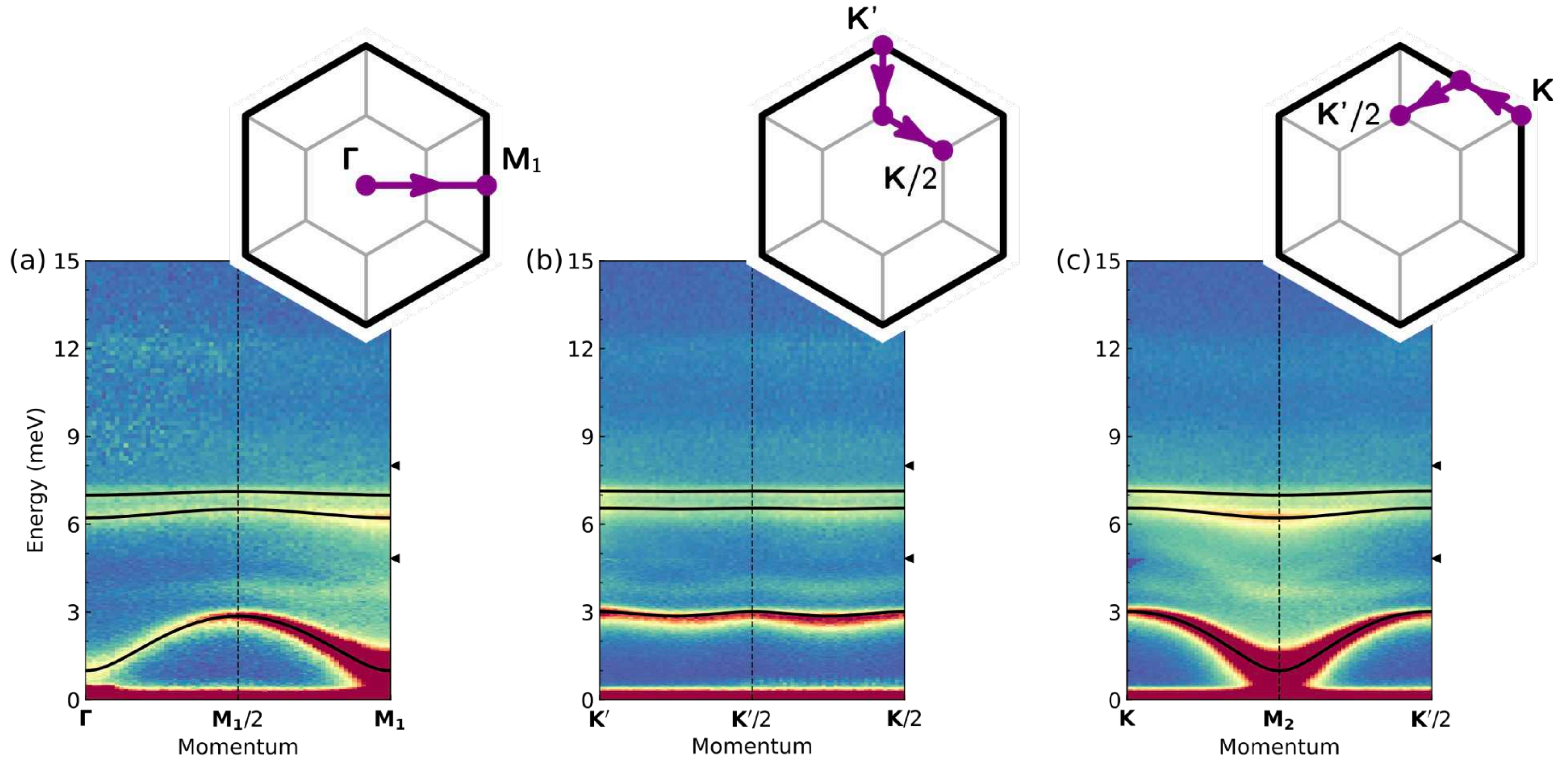
$\alpha_c = 0.14$ $\alpha_c = 0.09$ $\alpha_c = 0.18$

[Krüger, Chen, Jin, Li, LJ, PRL '23]

Conclusions

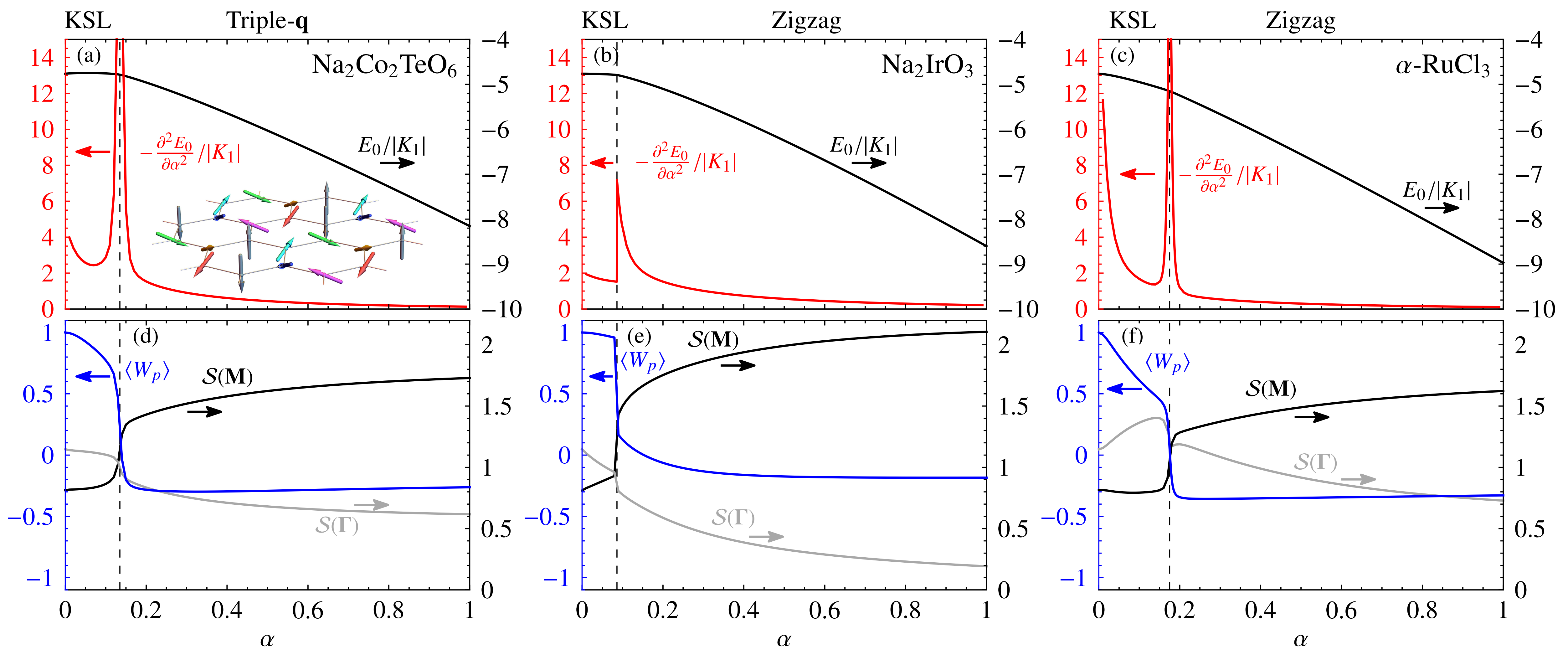
- $Na_2Co_2TeO_6$ features triple-**q** AFM order at low temperatures

... from symmetry of magnon bands



- $Na_2Co_2TeO_6$ closer to Kitaev QSL than Na_2IrO_3, but not as close as α-$RuCl_3$

... from 24-site ED of best-fit model



High-spin d^7 Mott insulators

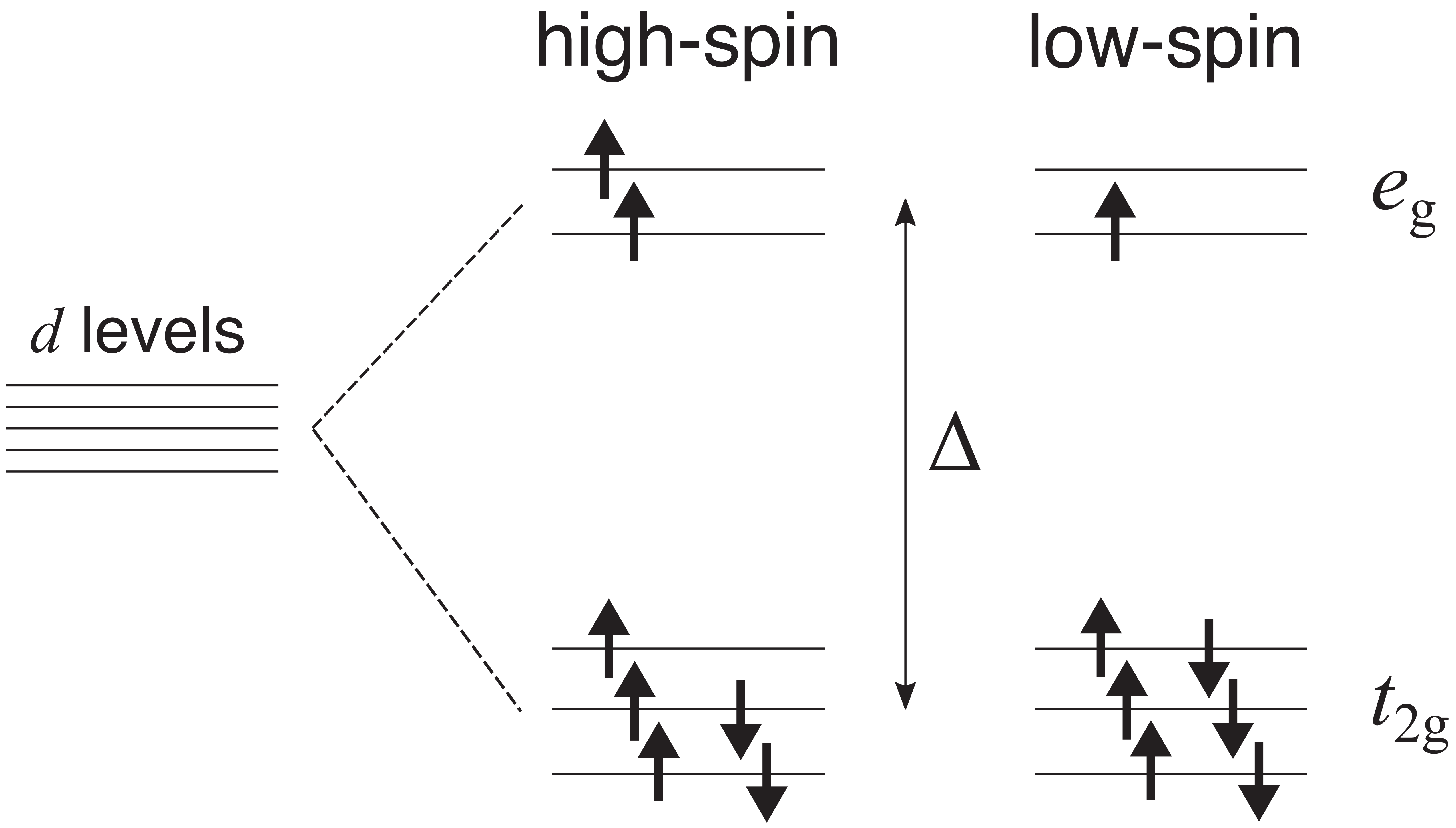


FIG. 1. Atomic d levels splitting into two groups under the octahedral CEF Δ: e_g levels at a higher energy and t_{2g} levels at a lower energy. The d^7 electron configuration can take either high-spin (middle) or low-spin state (right), depending on the strength of Coulomb interactions and Δ.

[Sano, Kato, Motome, PRB '18]