

Emergent Phenomena in Quantum Materials

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Wilhelm Krüger (Dresden)

David Moser (Dresden)

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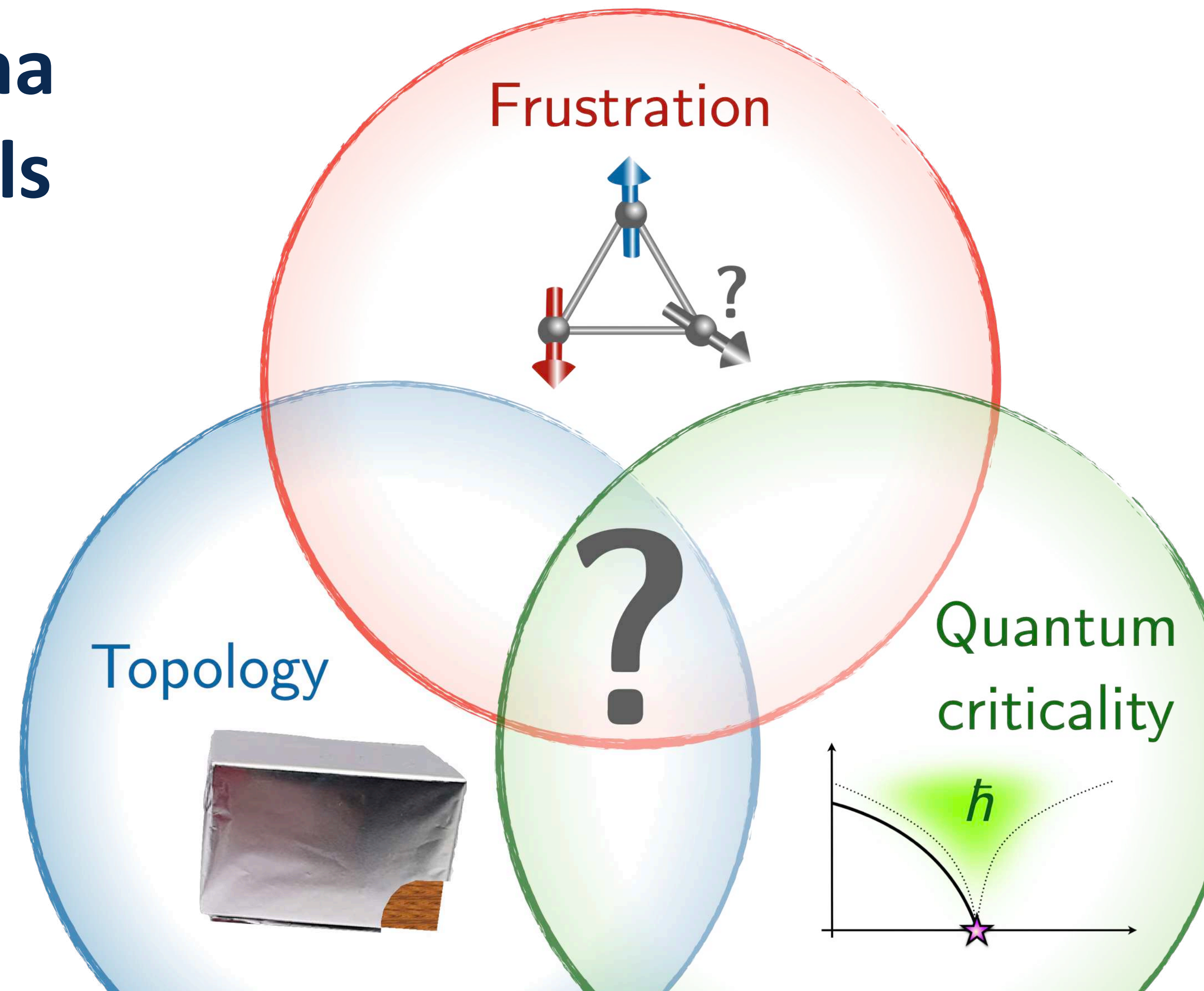
Fakher Assaad (Würzburg)

Zi Yang Meng (Hong Kong)

Zihong Liu (Würzburg → Dresden)

Jonas Schwab (Würzburg)

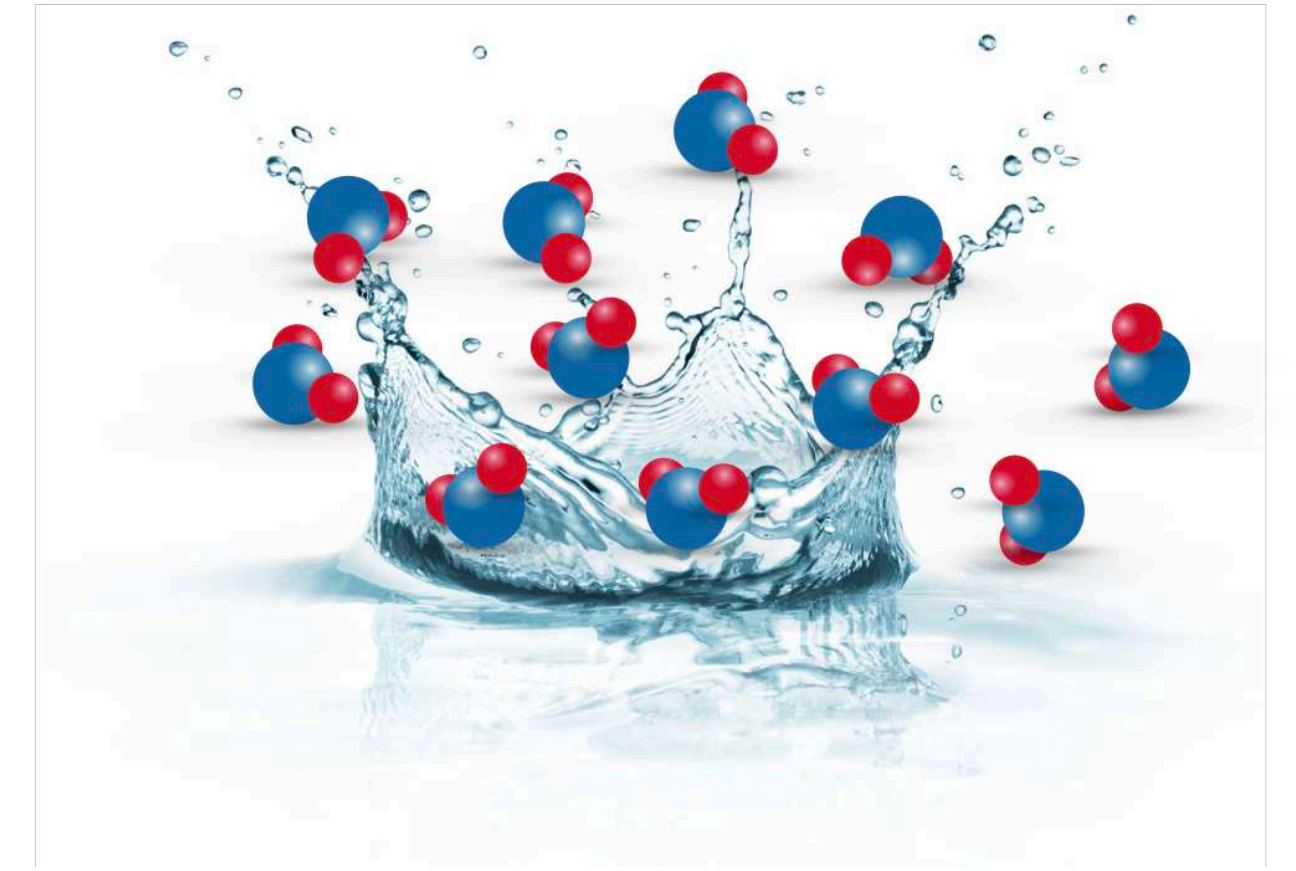
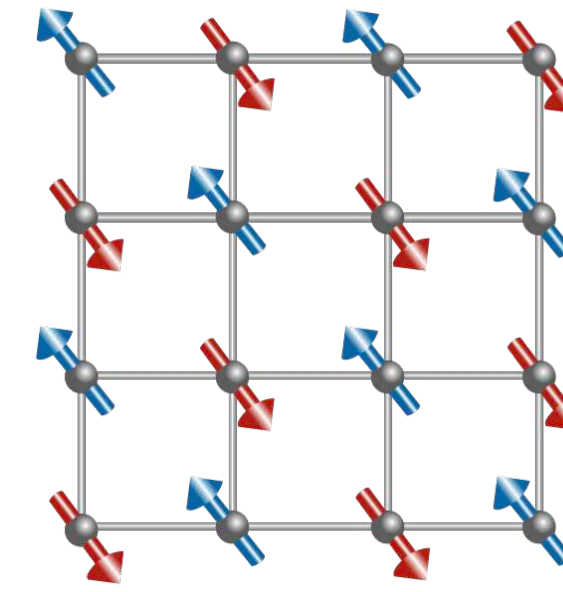
Urban Seifert (Santa Barbara)



Outline

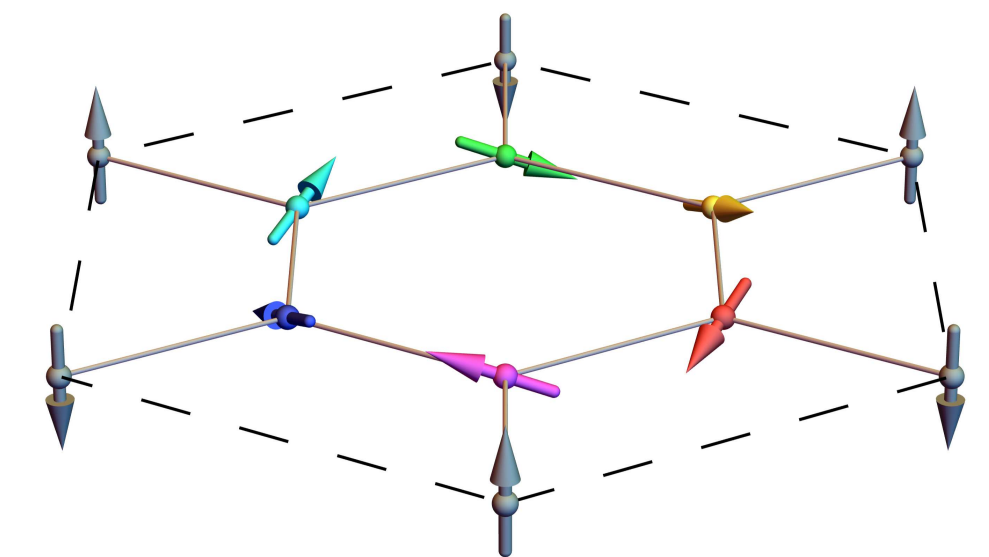
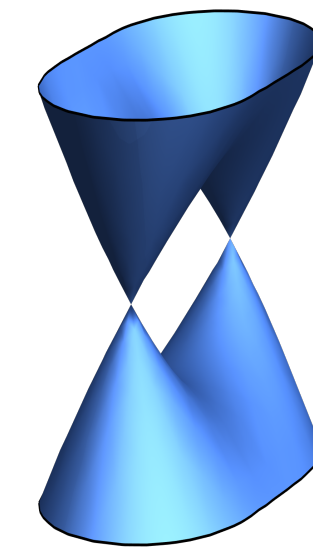
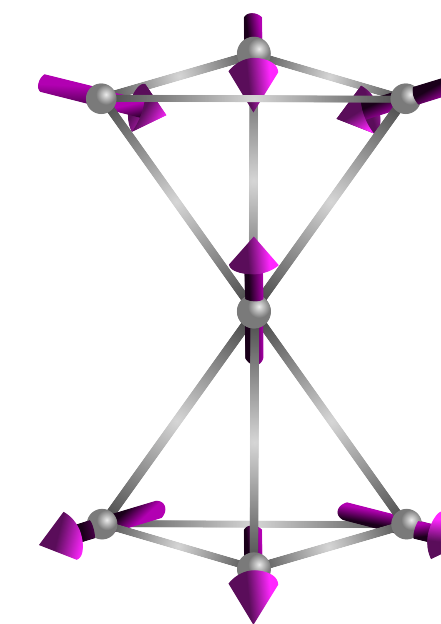
(1) Introduction

- ▶ Research Motivation
- ▶ Research Goals

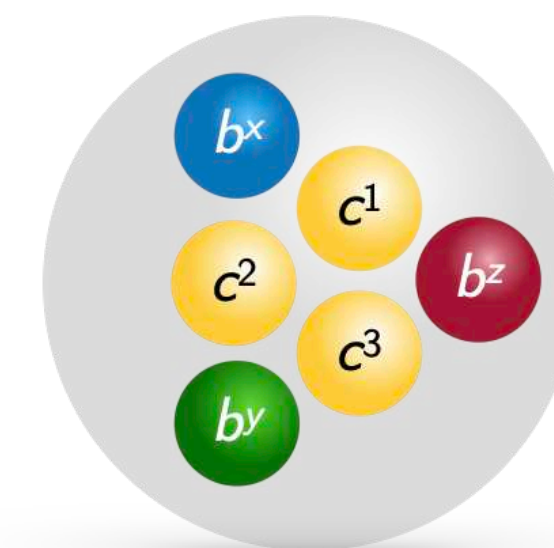


(2) Emergent Phenomena in Quantum Materials

- ▶ Emergent Symmetries
- ▶ Emergent Topology
- ▶ Emergent Orders
- ▶ Emergent Particles



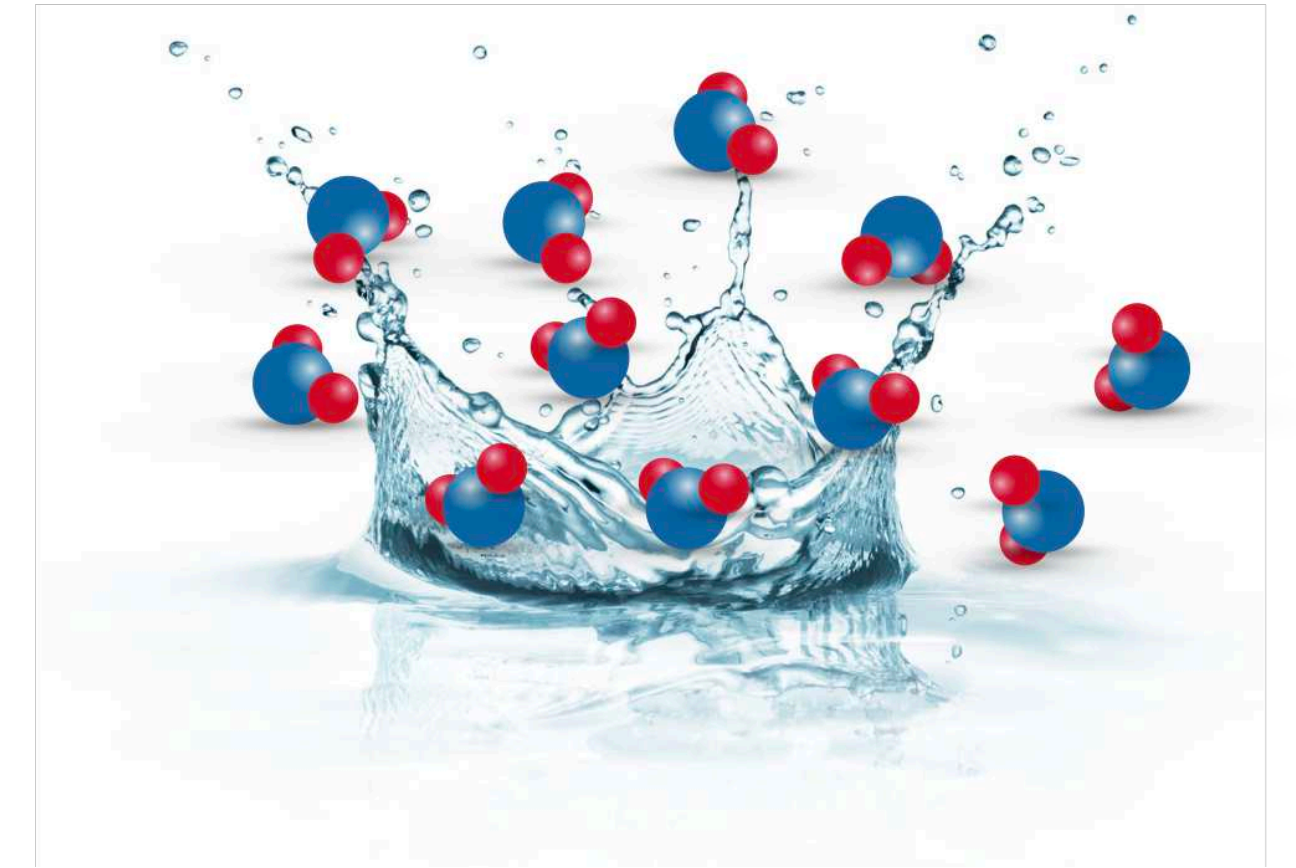
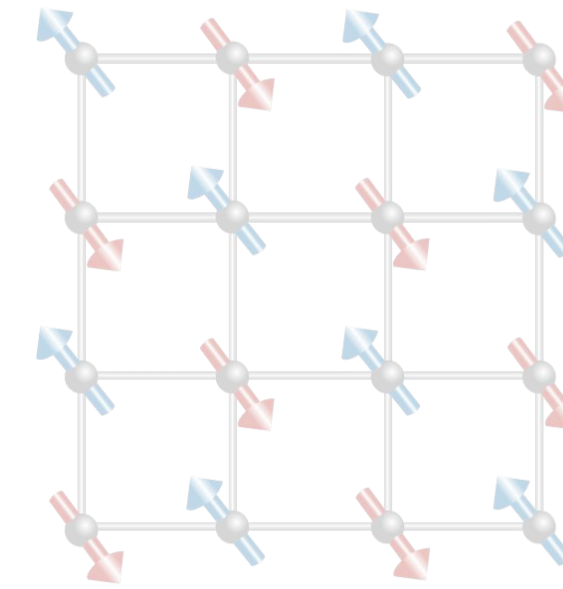
(3) Summary



Outline

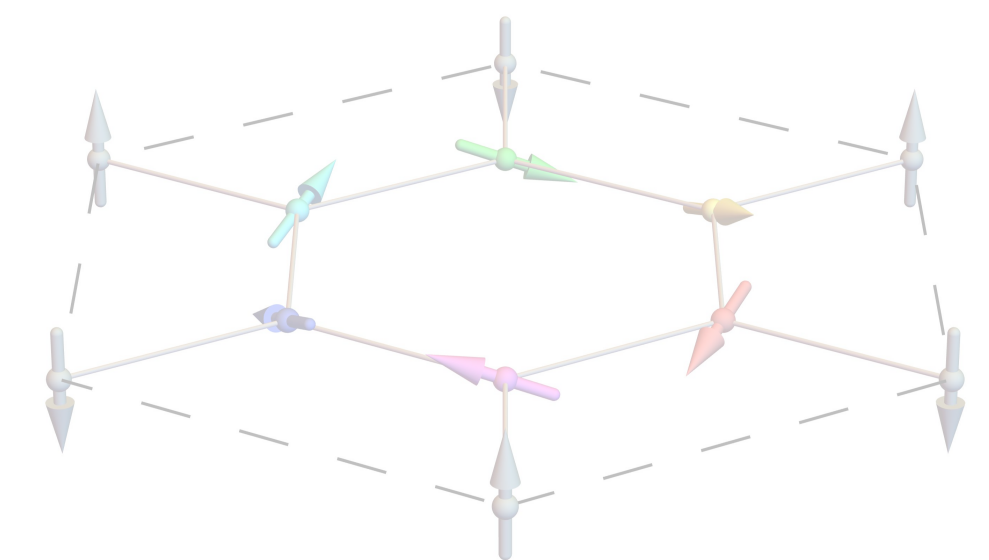
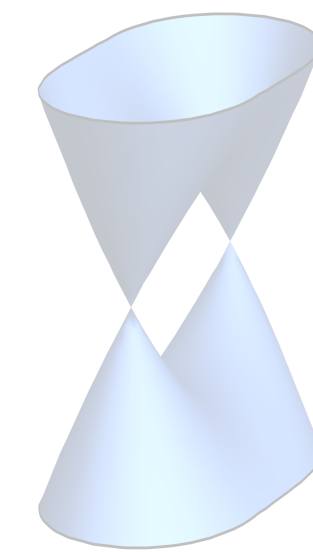
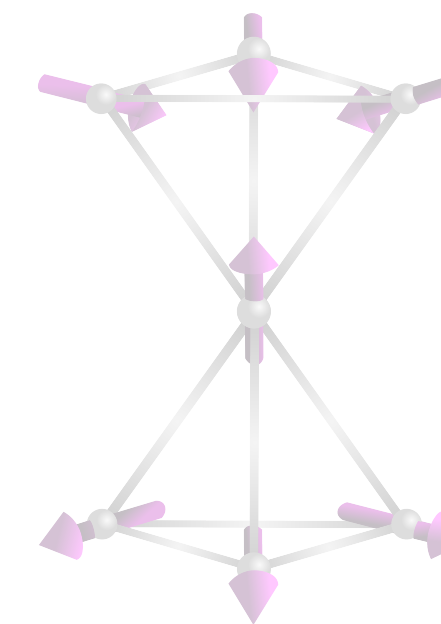
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- ▶ Research Goals

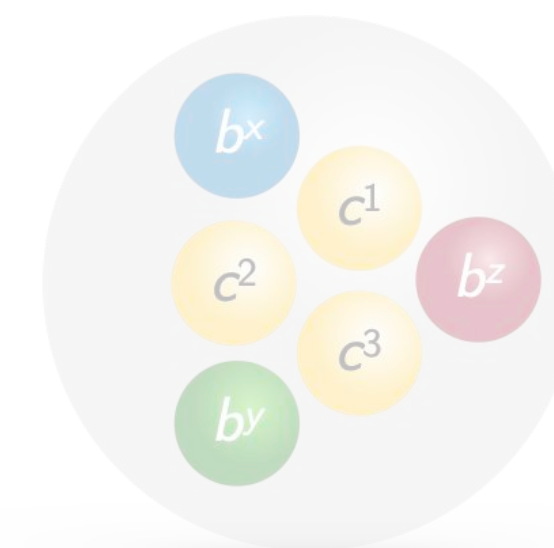


(2) Emergent Phenomena in Quantum Materials

- ▶ Emergent Symmetries
- ▶ Emergent Topology
- ▶ Emergent Orders
- ▶ Emergent Particles



(3) Summary



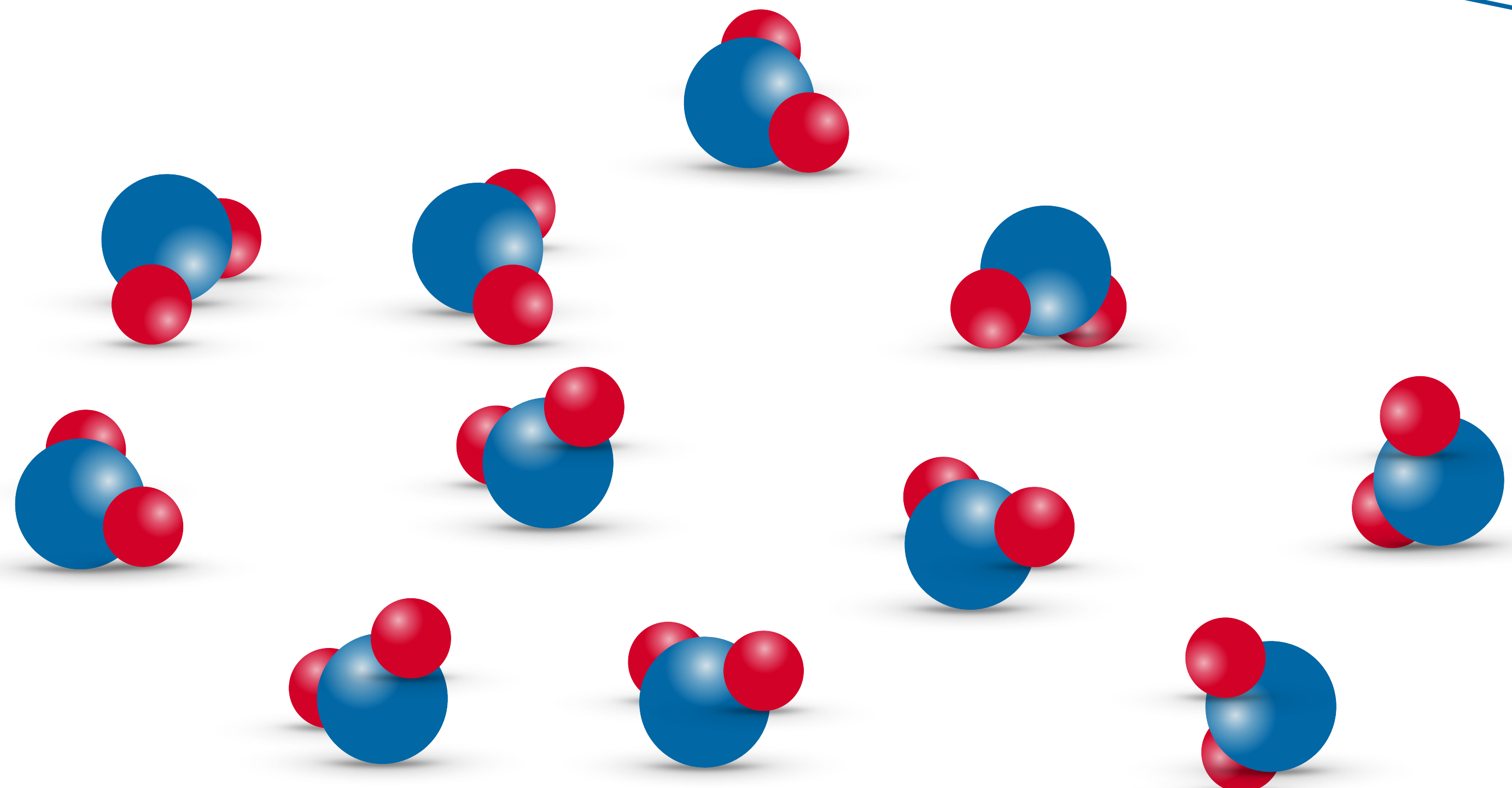
Reductionism



Matter

Reductionism

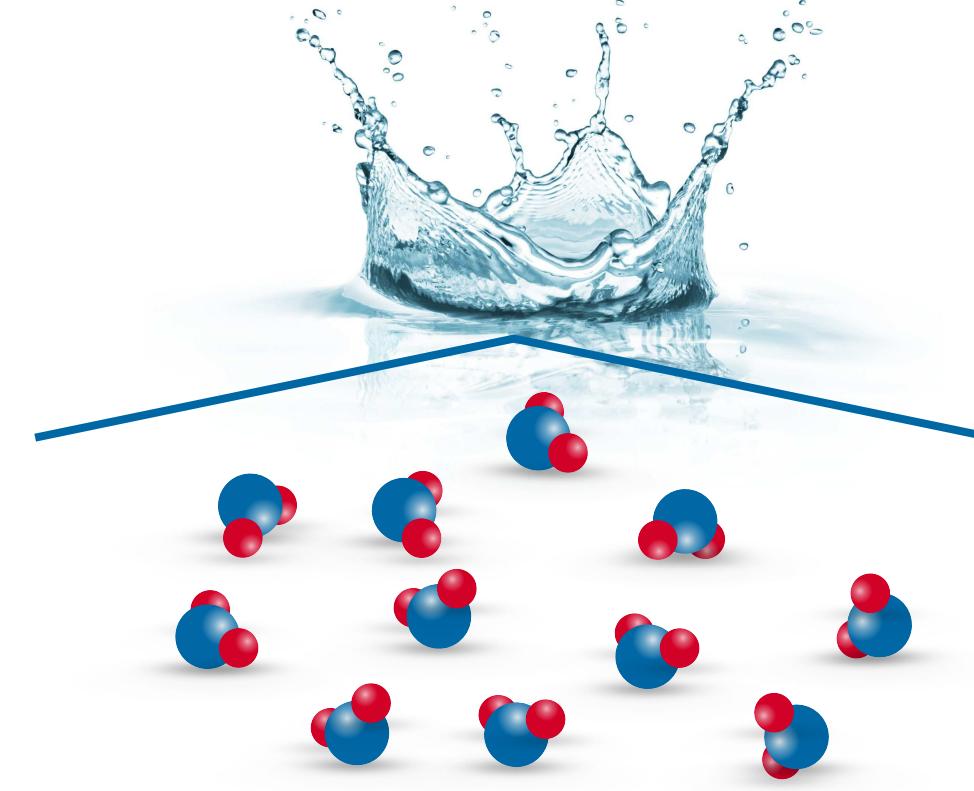
Matter



Molecules

Reductionism

Matter



Molecules

1 H Hydrogen 1.008	2 He Helium 4.002602																
3 Li Lithium 6.94	4 Be Beryllium 9.0121831	5 B Boron 10.81	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998403163	10 Ne Neon 20.1797										
11 Na Sodium 22.98976928	12 Mg Magnesium 24.305	13 Al Aluminium 26.9815385	14 Si Silicon 28.085	15 P Phosphorus 30.973761998	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.948										
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955908	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938044	26 Fe Iron 55.845	27 Co Cobalt 58.933194	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.630	33 As Arsenic 74.921595	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90584	40 Zr Zirconium 91.224	41 Nb Niobium 92.90637	42 Mo Molybdenum 95.95	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.293
55 Cs Caesium 132.90545196	56 Ba Barium 137.327	57 - 71 Lanthanoids	72 Hf Hafnium 178.49	73 Ta Tantalum 180.94788	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.966569	80 Hg Mercury 200.592	81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 208.98040	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 - 103 Actinoids	104 Rf Rutherfordium (261)	105 Db Dubnium (268)	106 Sg Seaborgium (269)	107 Bh Bohrium (270)	108 Hs Hassium (285)	109 Mt Meitnerium (276)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (282)	112 Cn Copernicium (285)	113 Nh Nihonium (286)	114 Fl Flerovium (289)	115 Mc Moscovium (289)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)

Atoms

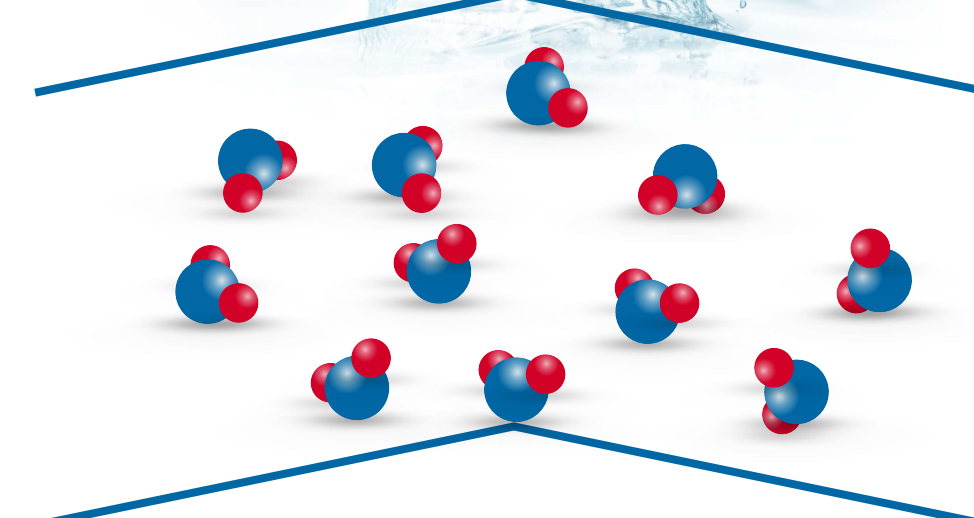
57 La Lanthanum 138.90547	58 Ce Cerium 140.36	59 Pr Praseodymium 140.90766	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92535	66 Dy Dysprosium 162.500	67 Ho Holmium 164.93033	68 Er Erbium 167.259	69 Tm Thulium 168.93422	70 Yb Ytterbium 173.045	71 Lu Lutetium 174.9668
89 Ac Actinium (227)	90 Th Thorium 232.0377	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (261)

Reductionism

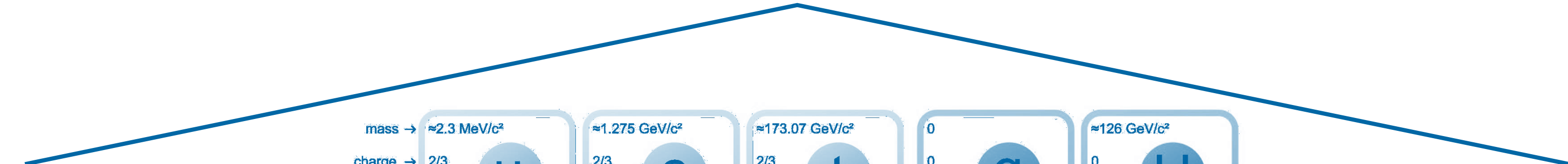
Matter



Molecules



Atoms



mass →	≈2.3 MeV/c ²	≈1.275 GeV/c ²	≈173.07 GeV/c ²	0	≈126 GeV/c ²
charge →	2/3	2/3	2/3	0	0
spin →	1/2	1/2	1/2	1	0
	u up	c charm	t top	g gluon	H Higgs boson
QUARKS	≈4.8 MeV/c ² -1/3 1/2 d down	≈95 MeV/c ² -1/3 1/2 s strange	≈4.18 GeV/c ² -1/3 1/2 b bottom	0 0 1 γ photon	
	0.511 MeV/c ² -1 1/2 e electron	105.7 MeV/c ² -1 1/2 μ muon	1.777 GeV/c ² -1 1/2 τ tau	0 1 Z Z boson	
LEPTONS	<2.2 eV/c ² 0 1/2 ν_e electron neutrino	<0.17 MeV/c ² 0 1/2 ν_μ muon neutrino	<15.5 MeV/c ² 0 1/2 ν_τ tau neutrino	80.4 GeV/c ² ±1 1 W W boson	GAUGE BOSONS

Elementary particles

FIELDS ARRANGED BY PURITY

→
MORE PURE

SOCIOLOGY IS
JUST APPLIED
PSYCHOLOGY

PSYCHOLOGY IS
JUST APPLIED
BIOLOGY

BIOLOGY IS
JUST APPLIED
CHEMISTRY

WHICH IS JUST
APPLIED PHYSICS.
IT'S NICE TO
BE ON TOP.

OH, HEY, I DIDN'T
SEE YOU GUYS ALL
THE WAY OVER THERE.



SOCIOLOGISTS

PSYCHOLOGISTS

BIOLOGISTS

CHEMISTS

PHYSICISTS

MATHEMATICIANS

Complexity



Emergence

The whole is
greater than the sum of
its parts!



Aristotle, 385-322 BC

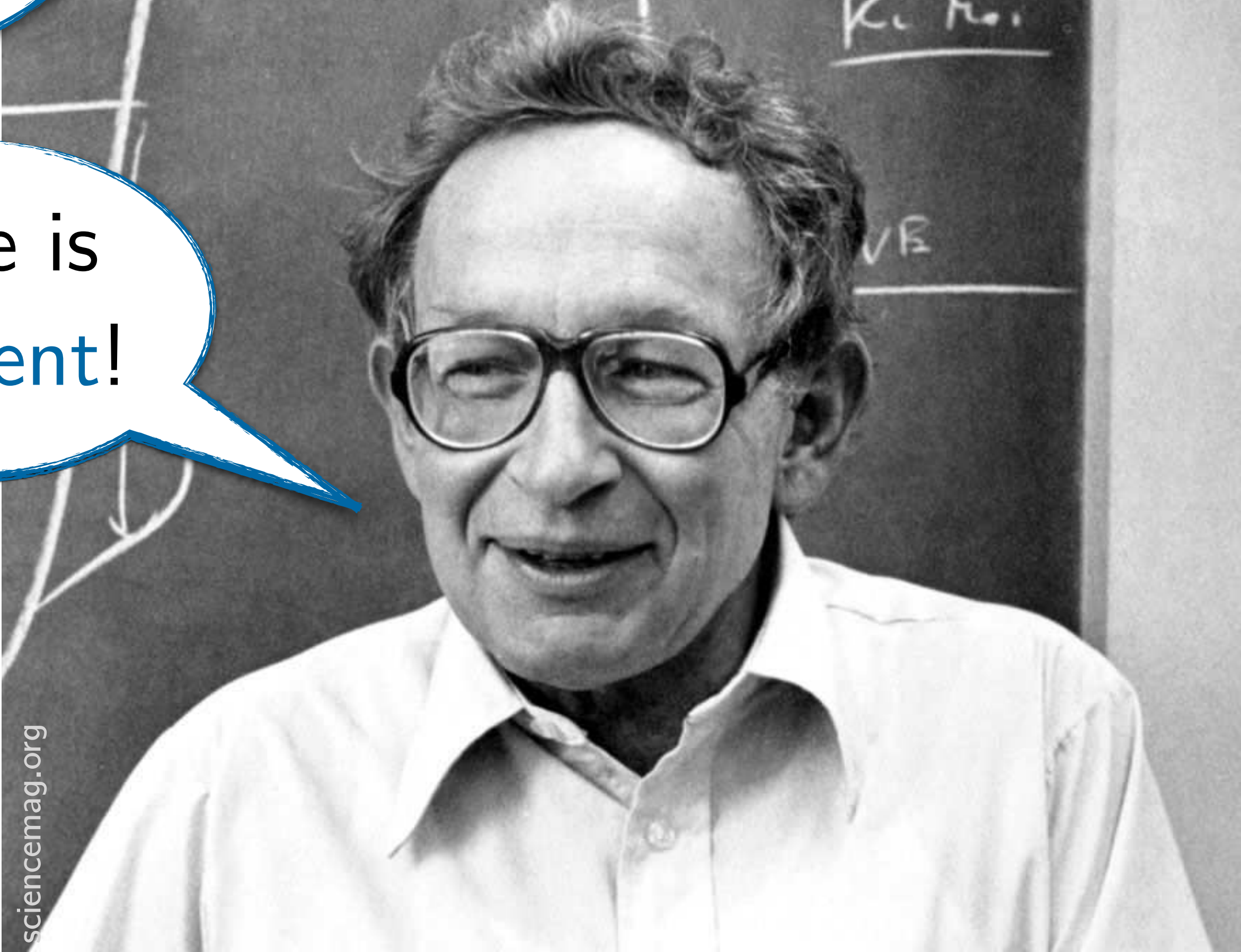
Emergence

The whole is
greater than the sum of
its parts!

More is
different!



Aristotle, 385-322 BC



Anderson, 1923-2020 AD

[Anderson, Science '72]

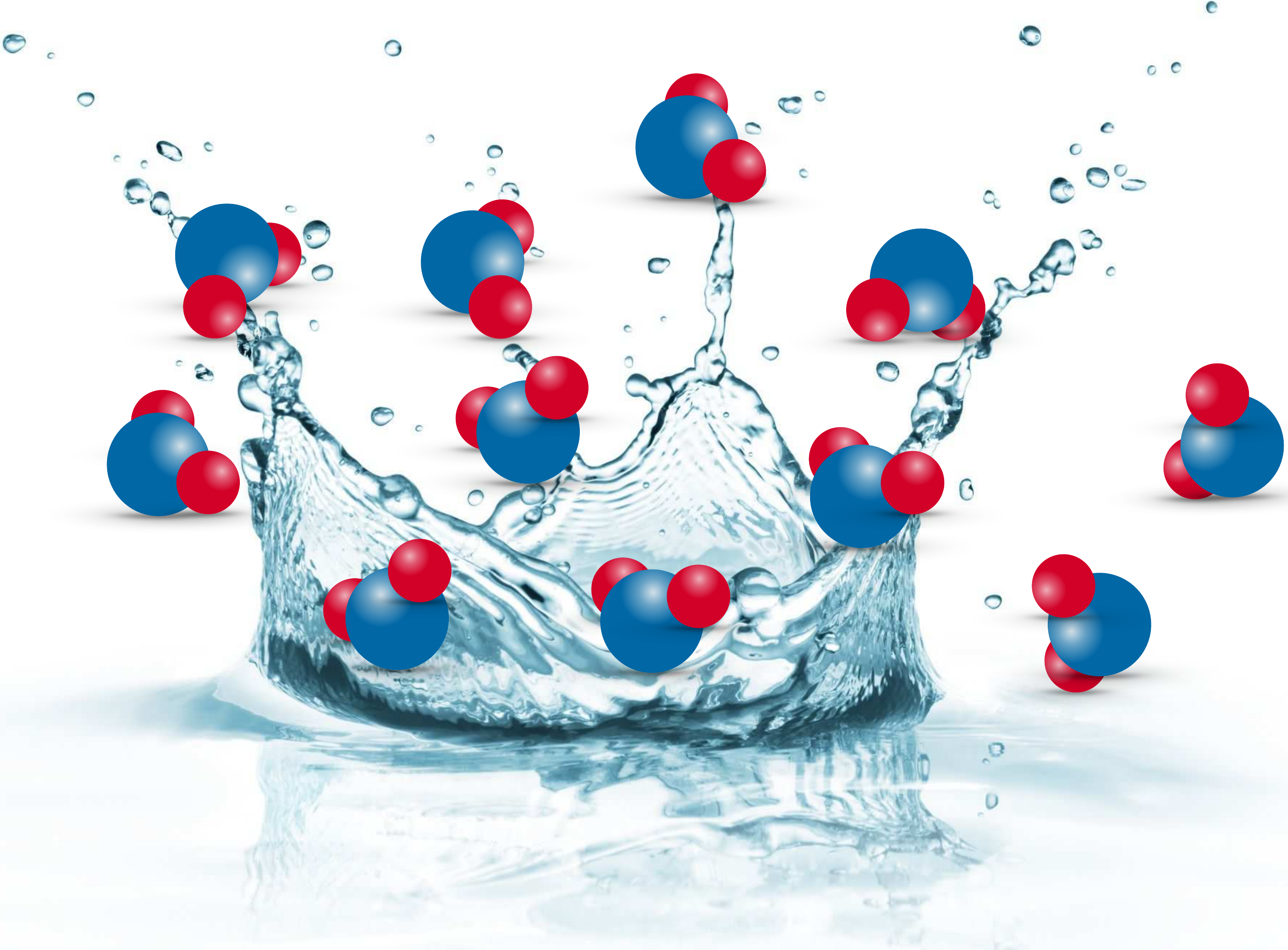
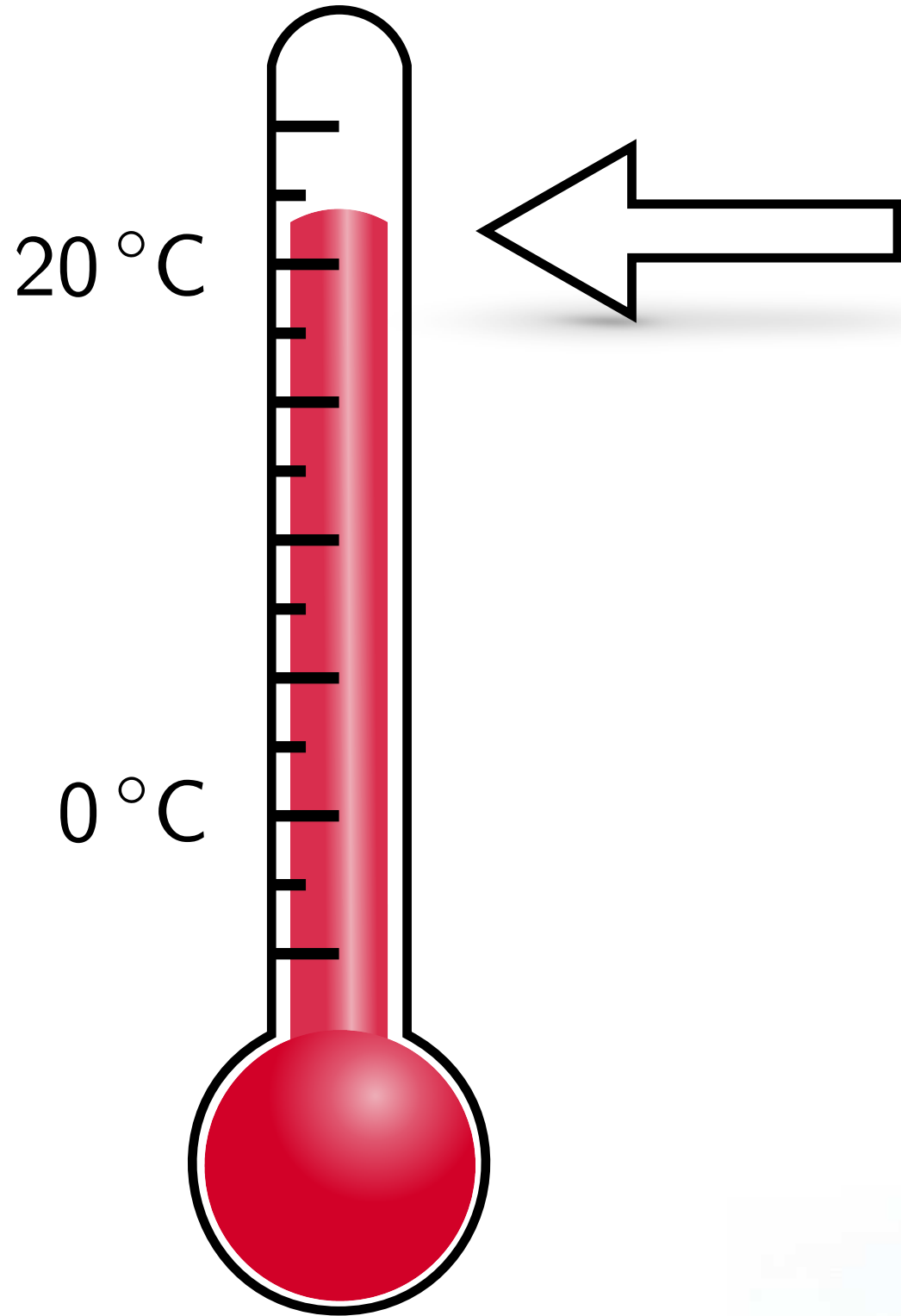
Living Bridges



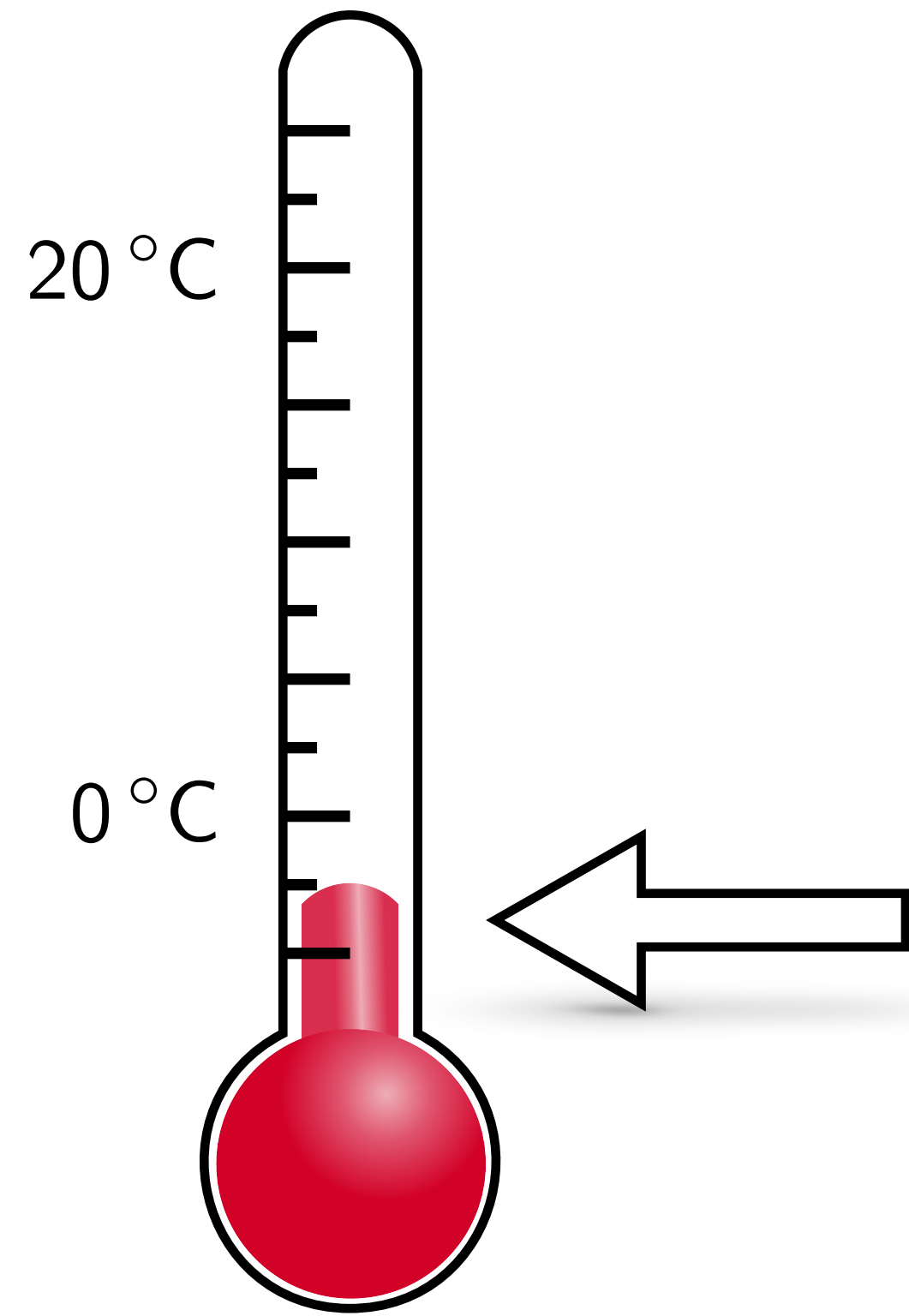
Living Bridges



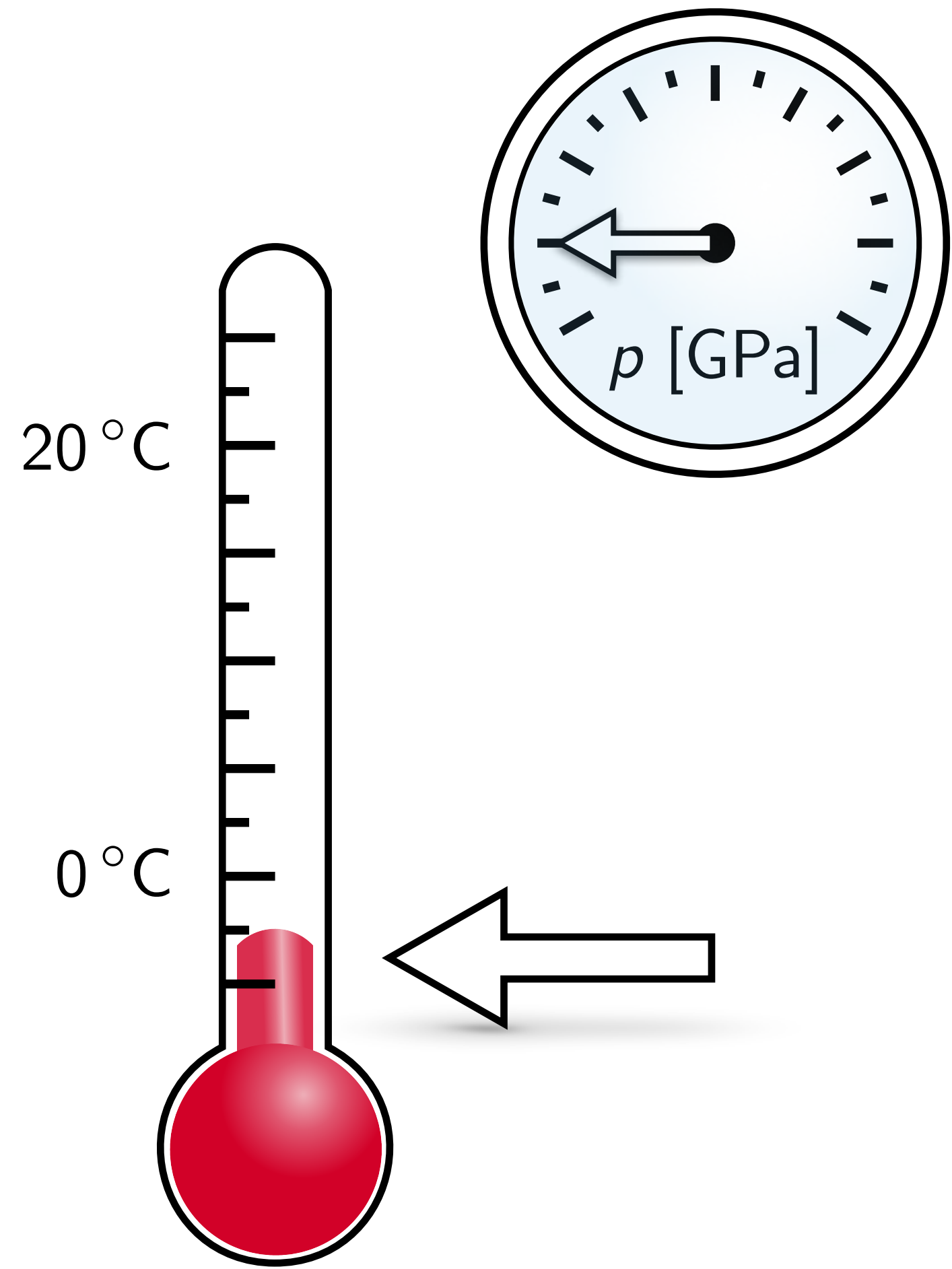
Snowflakes



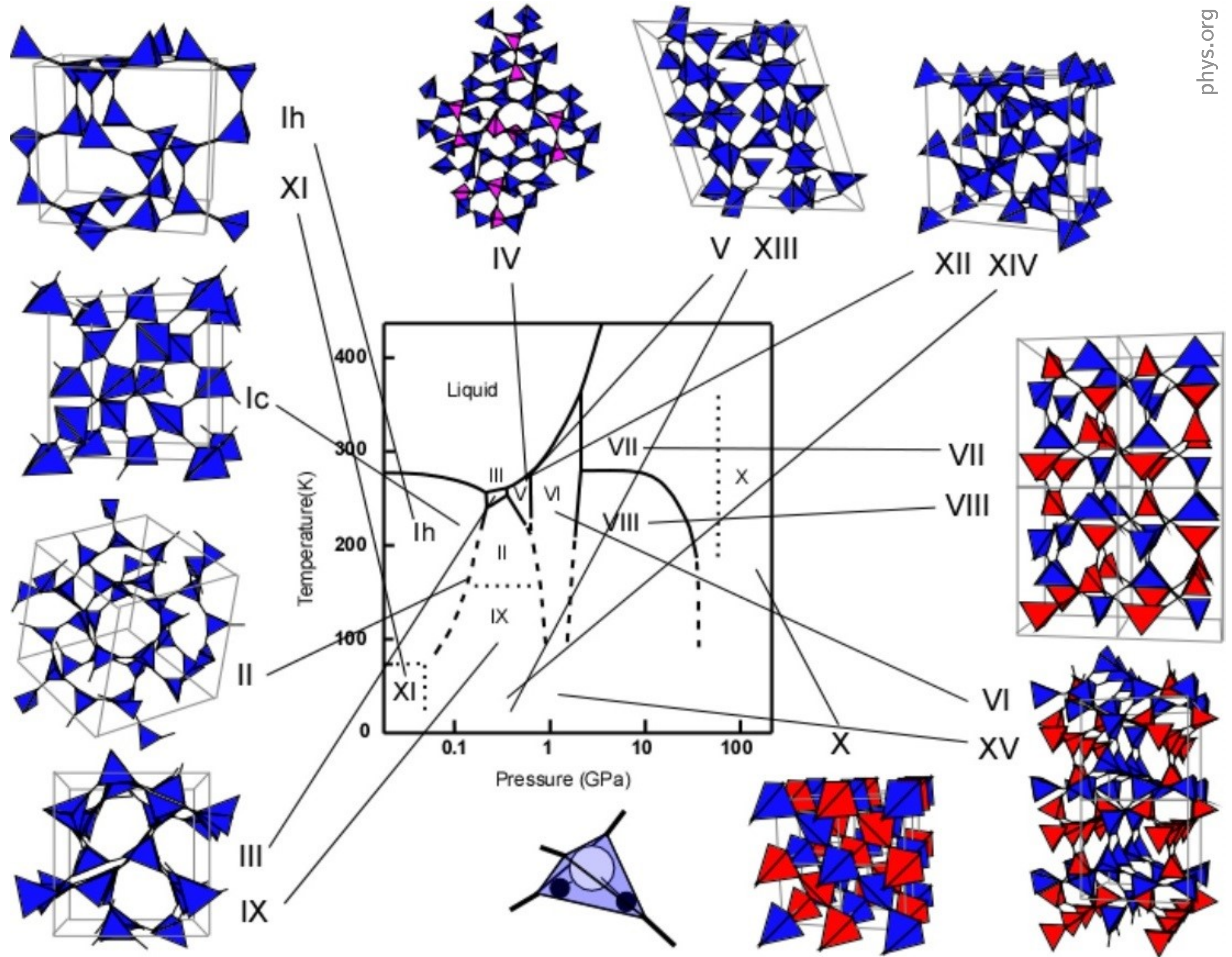
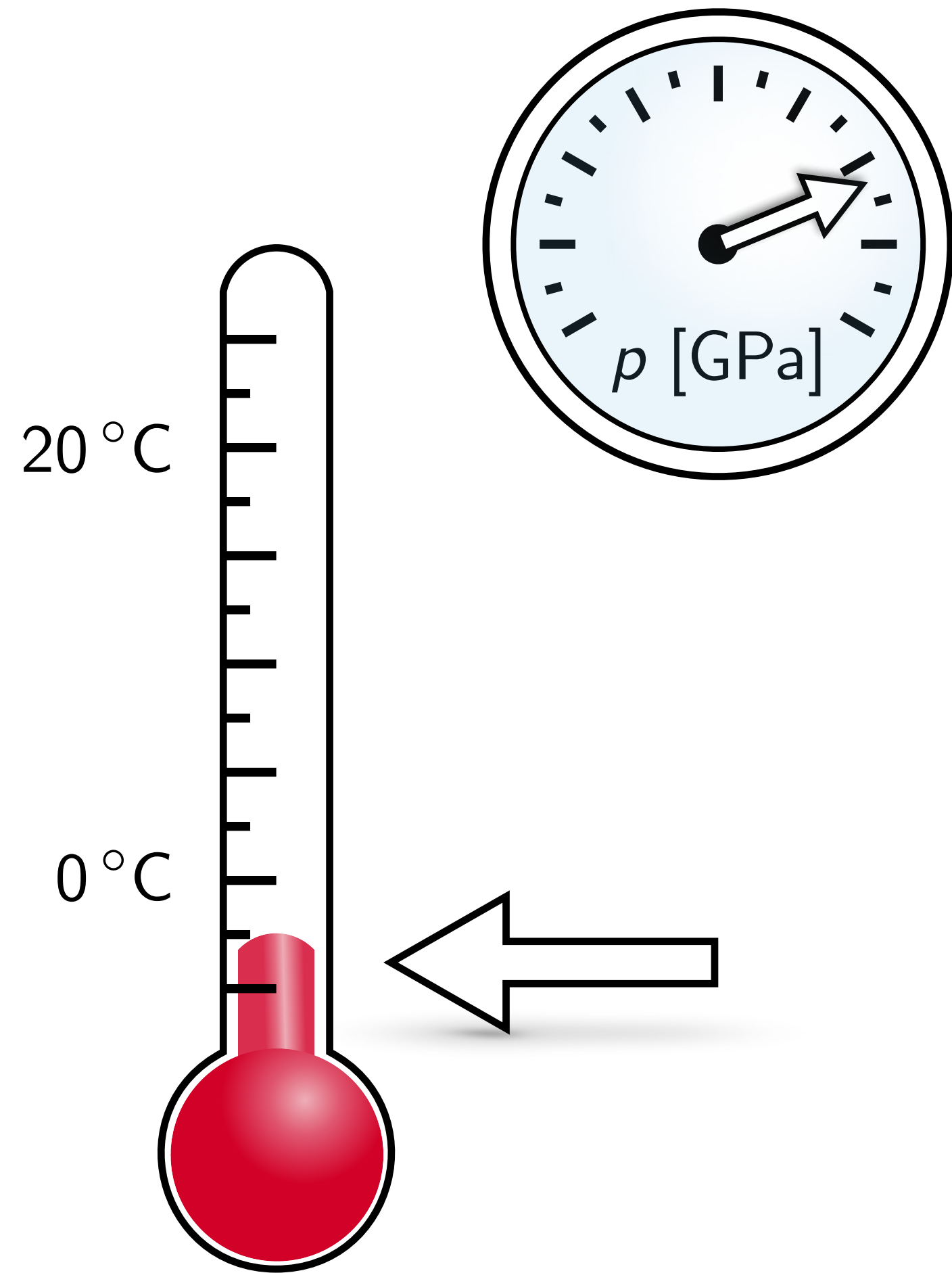
Snowflakes



Phases of Ice



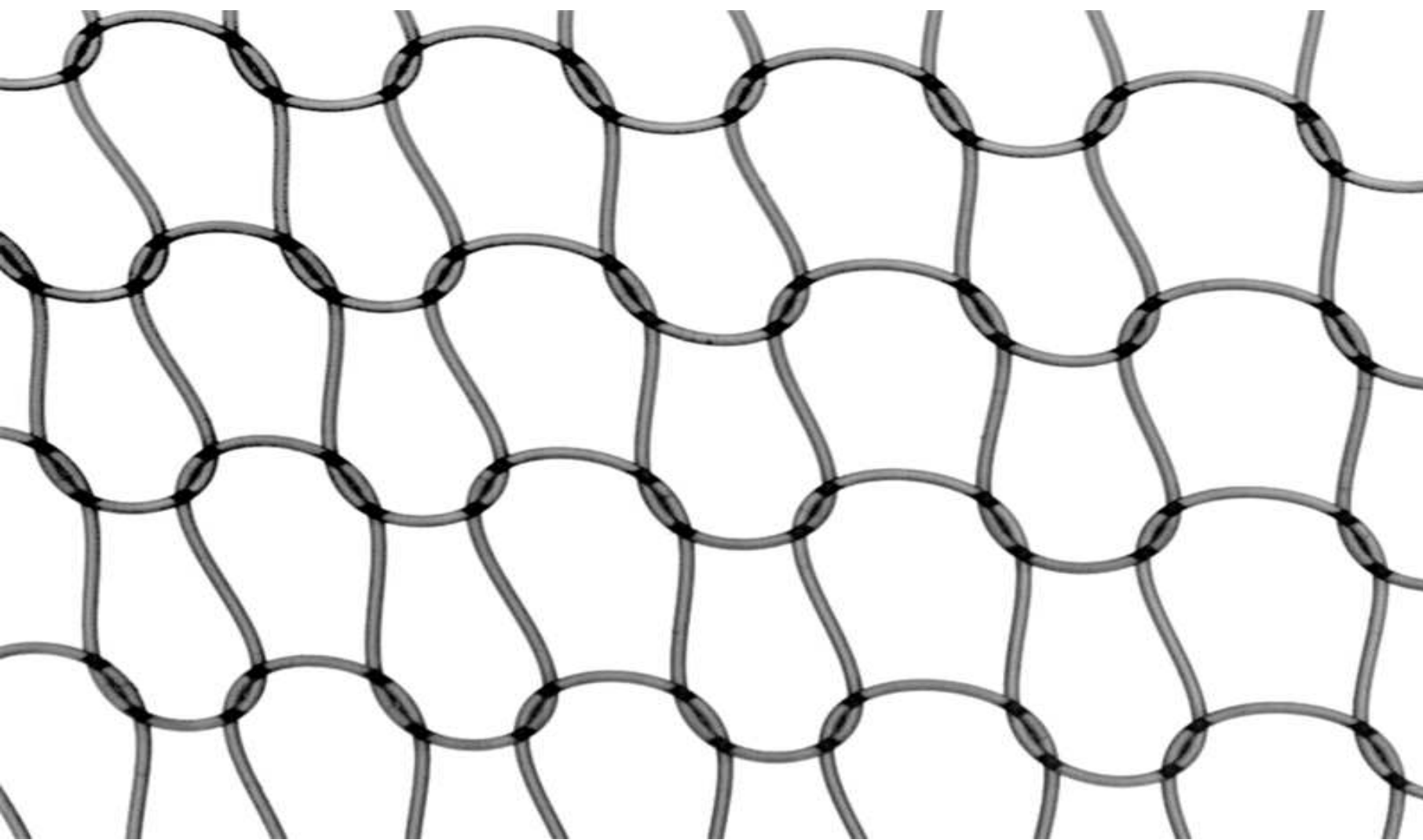
Phases of Ice



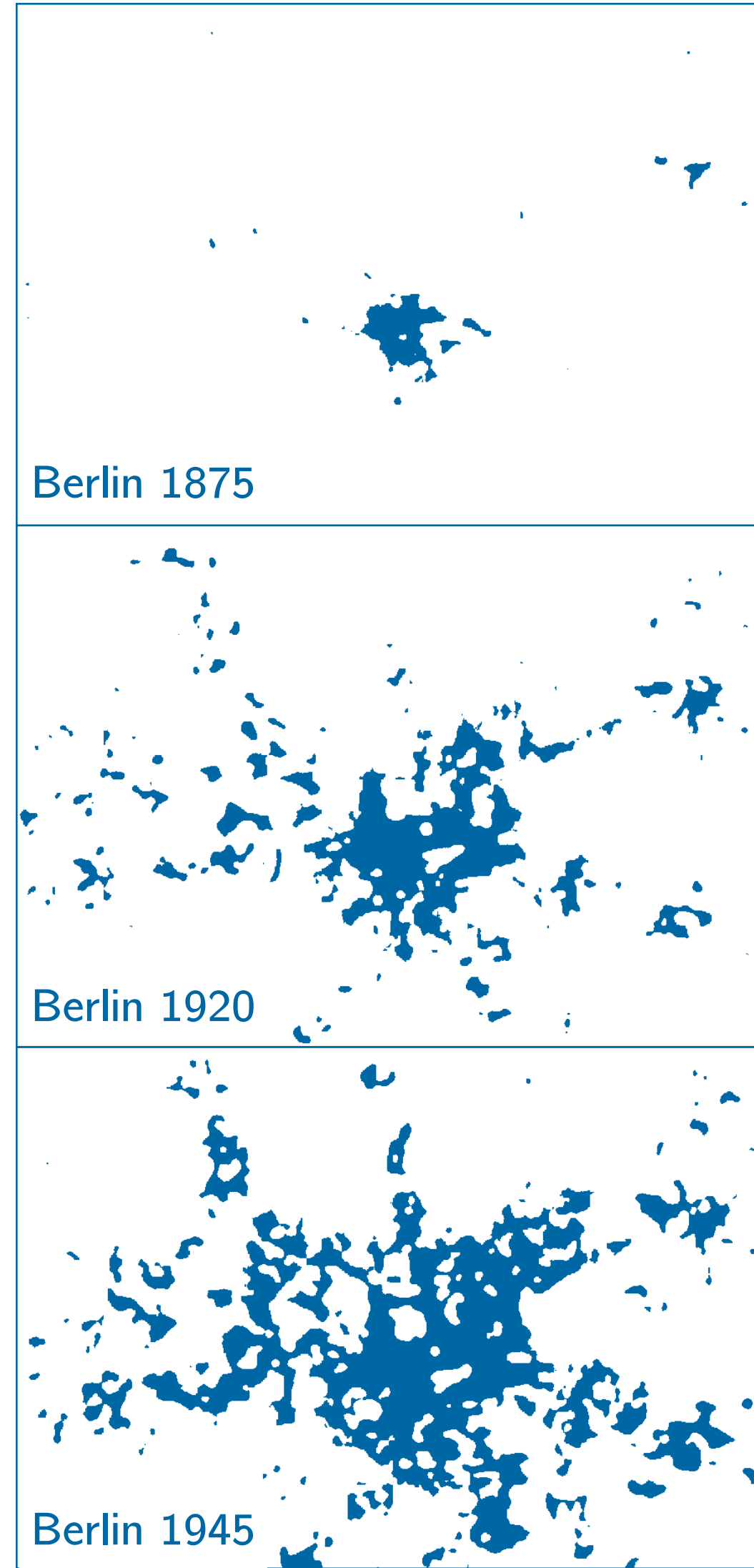
Emergent Phenomena



[Portugal *et al.*, Nature '14]



[Poincloux *et al.*, PRX '18]

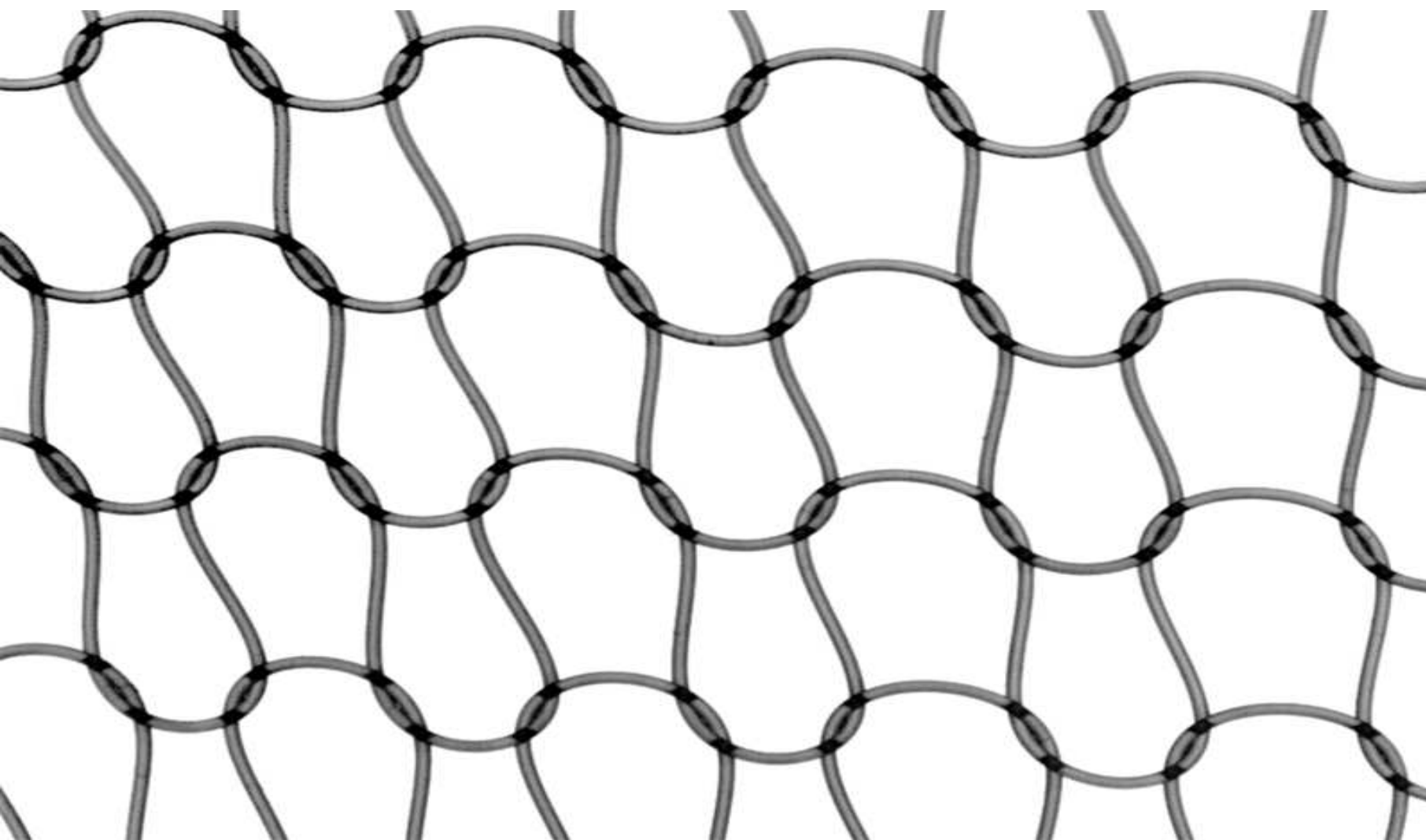


[Makse *et al.*, Nature '95]

Emergent Phenomena



[Portugal *et al.*, Nature '14]

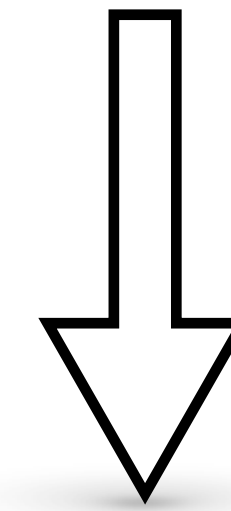


[Poincloux *et al.*, PRX '18]



[Makse *et al.*, Nature '95]

Many constituents
with simple rules

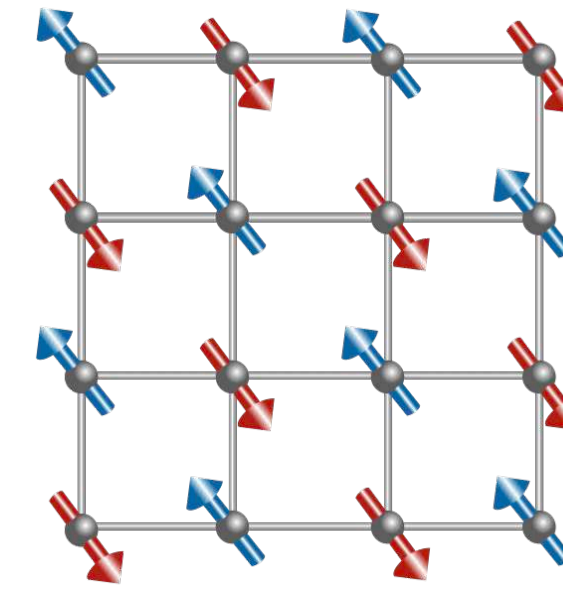


Complex structures
with new properties

Outline

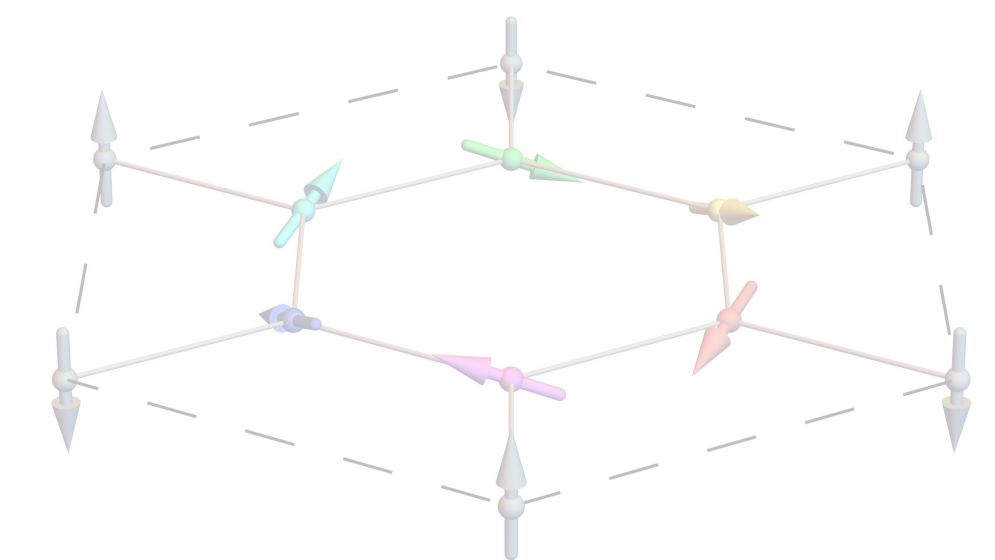
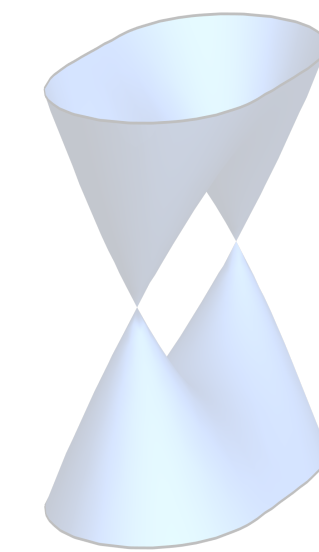
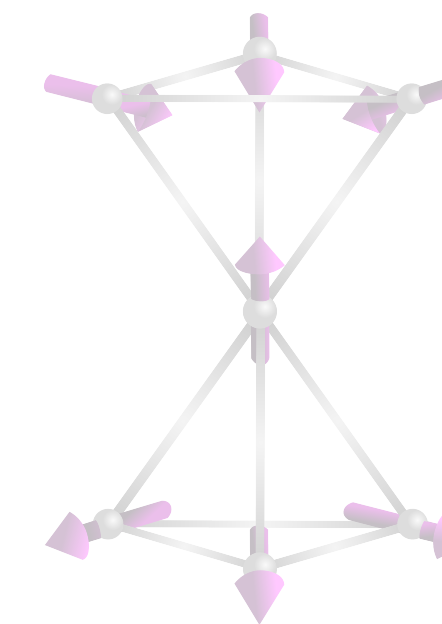
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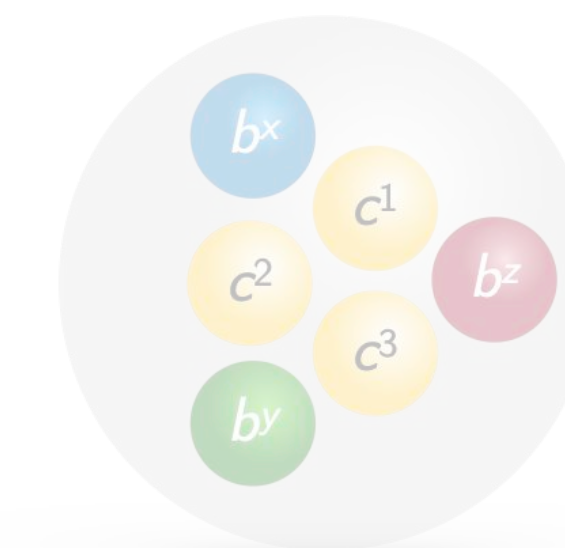


(2) Emergent Phenomena in Quantum Materials

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- ▶ Emergent Topology
- ▶ Emergent Orders
- ▶ Emergent Particles

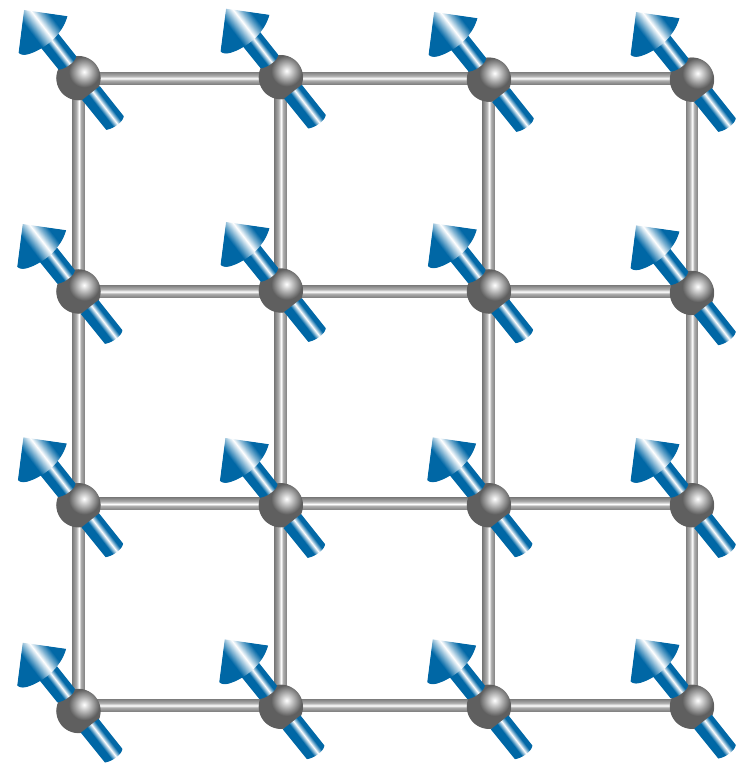


(3) Summary



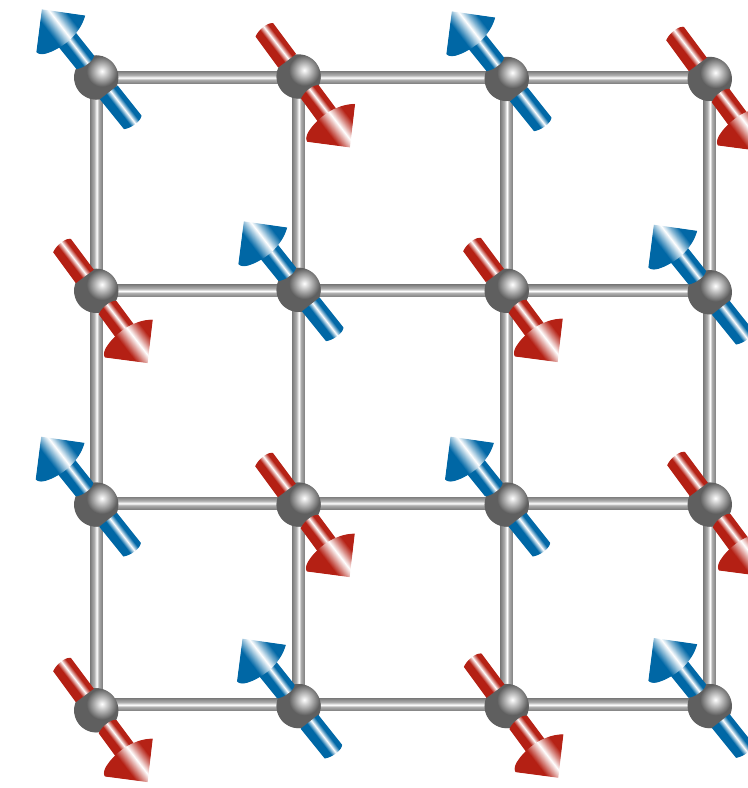
Possible States of Matter?

Symmetry classification:



Ferromagnet

Spin: $SU(2) \rightarrow U(1)$



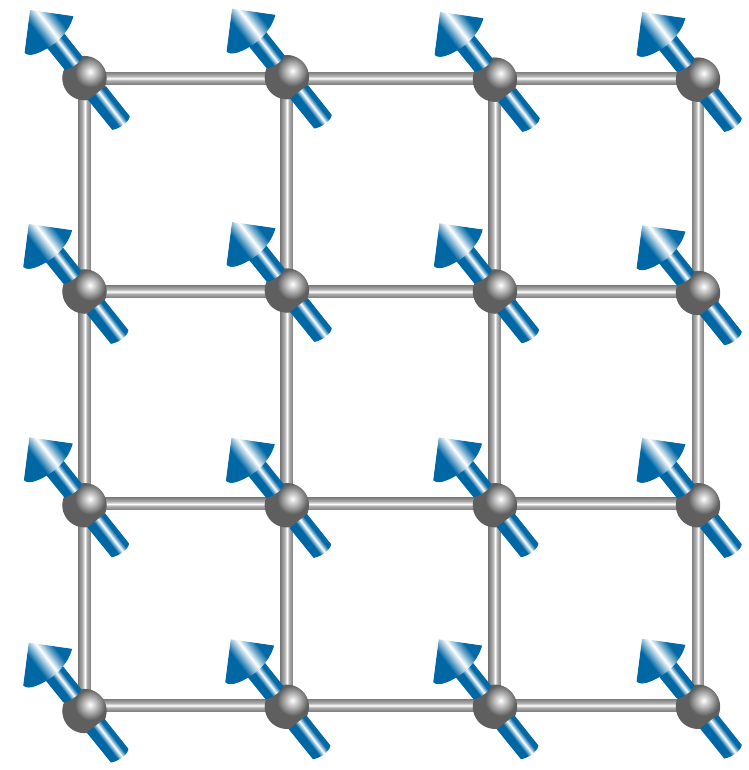
Antiferromagnet

Spin: $SU(2) \rightarrow U(1)$

Lattice: $T_a \rightarrow T_{2a}$

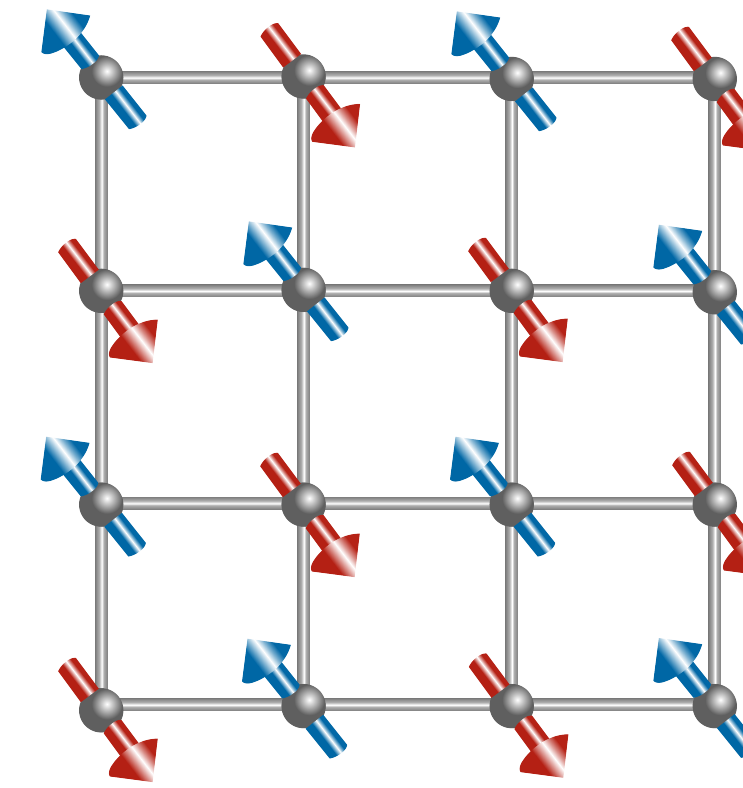
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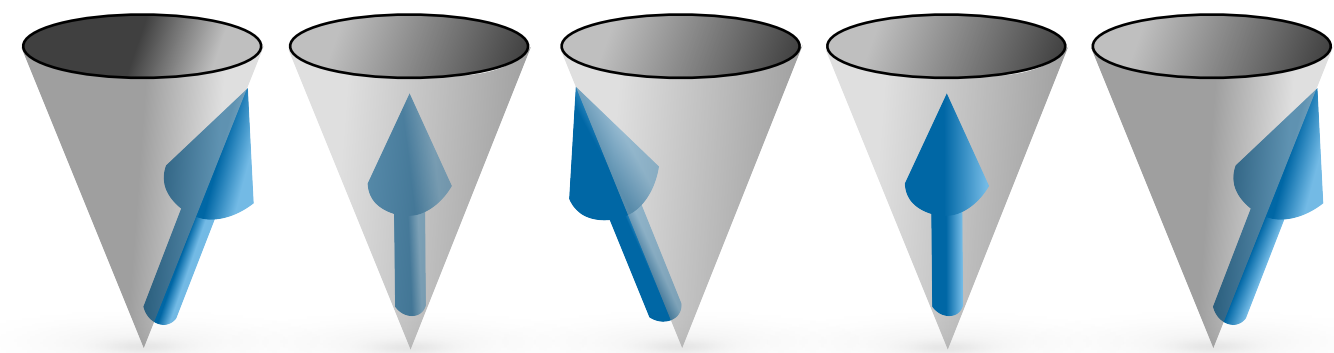


Antiferromagnet

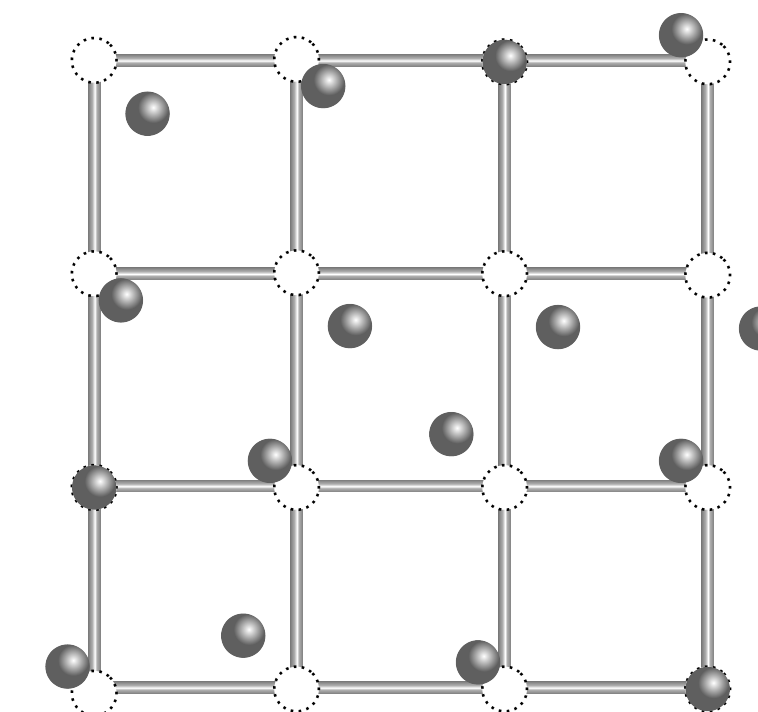
Spin: $SU(2) \rightarrow U(1)$

Lattice: $T_a \rightarrow T_{2a}$

Effective excitations: Quasiparticles



Spin: Magnons



Lattice: Phonons

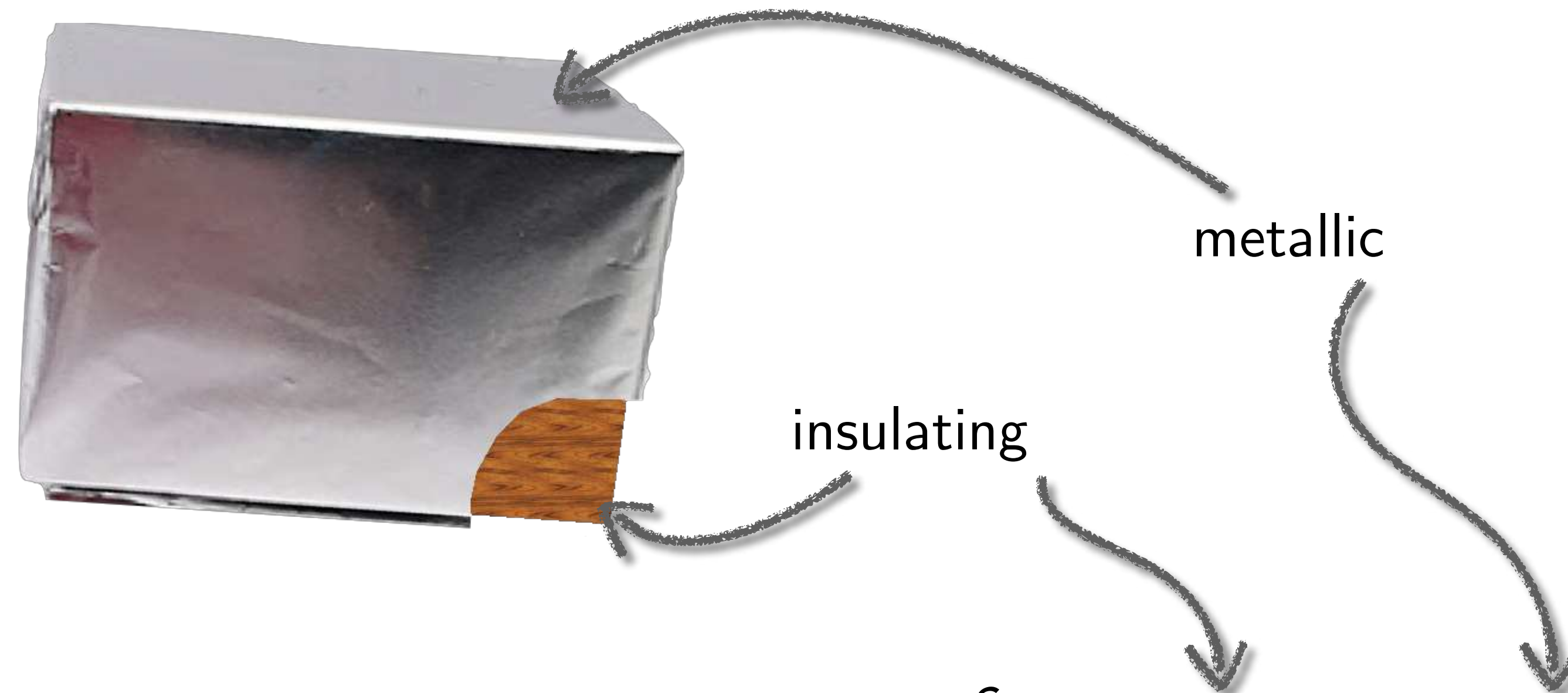
Ingredient #1: Topology

Topological insulator:

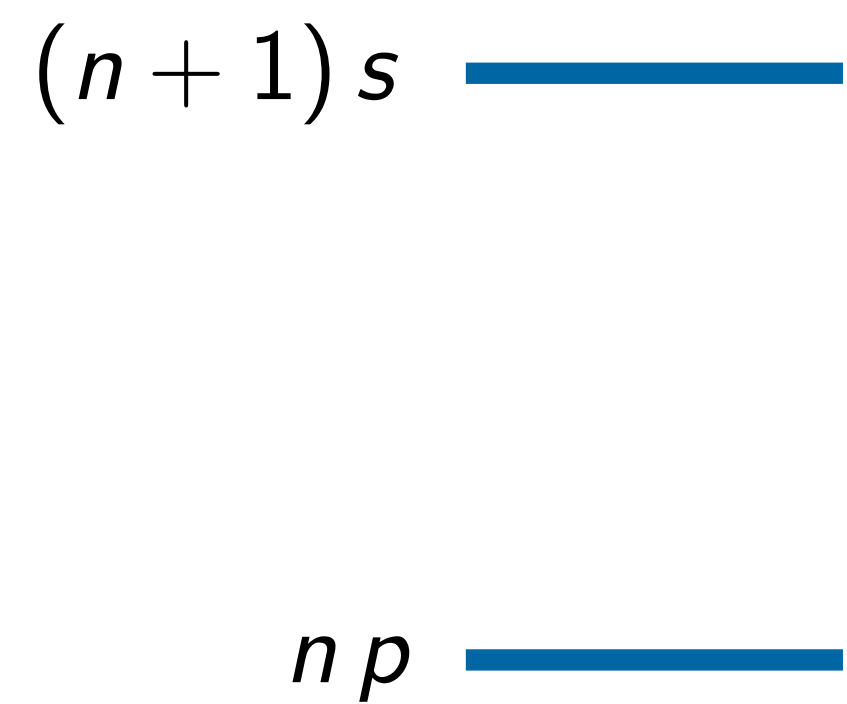


Ingredient #1: Topology

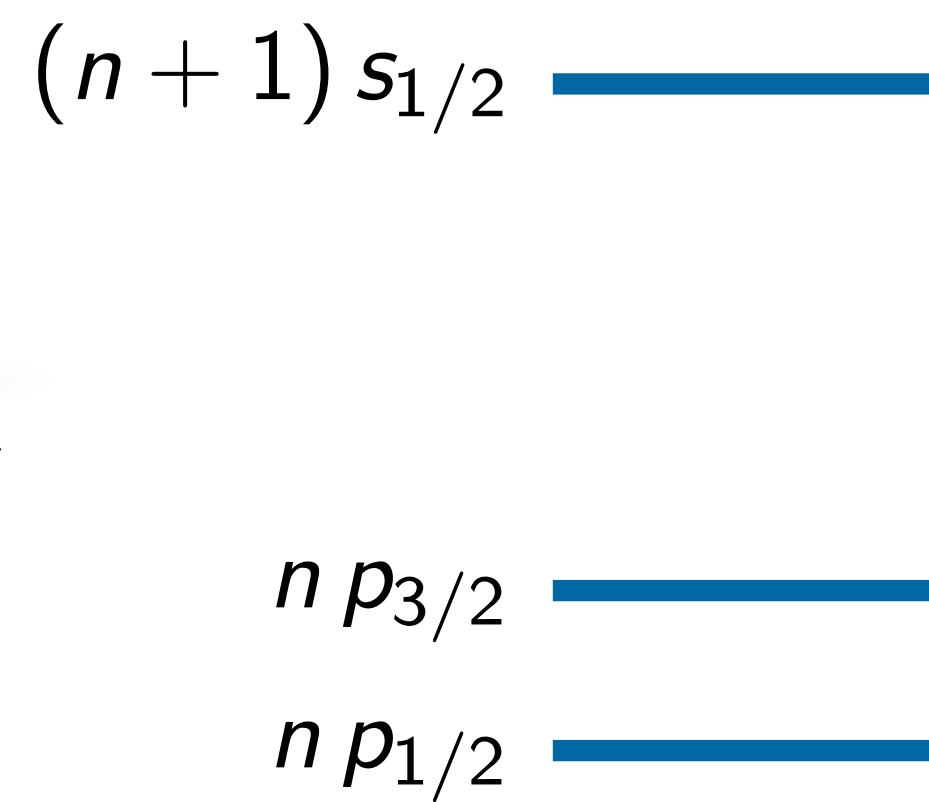
Topological insulator:



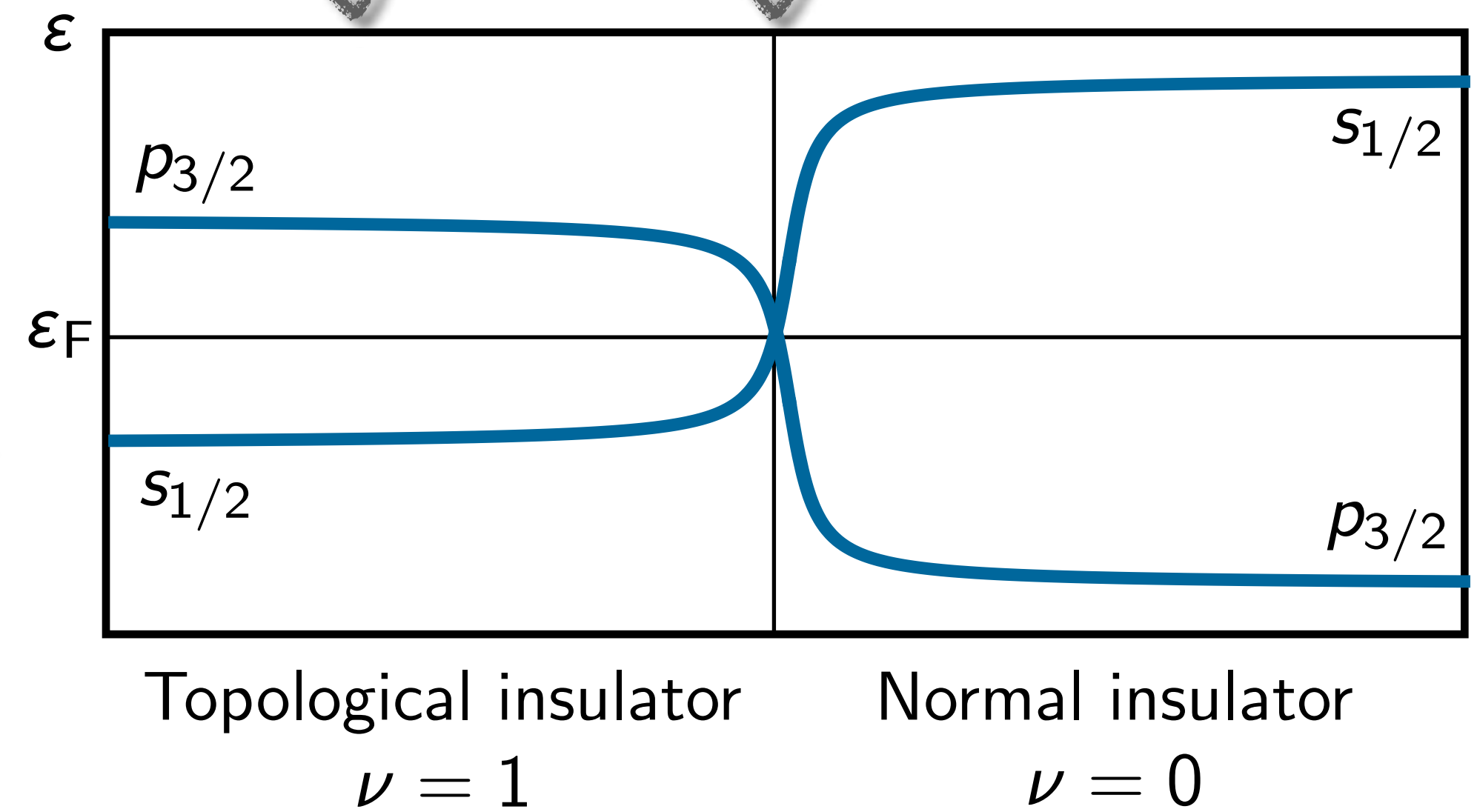
Band inversion:



small $\vec{L} \cdot \vec{\sigma}$



large $\vec{L} \cdot \vec{\sigma}$

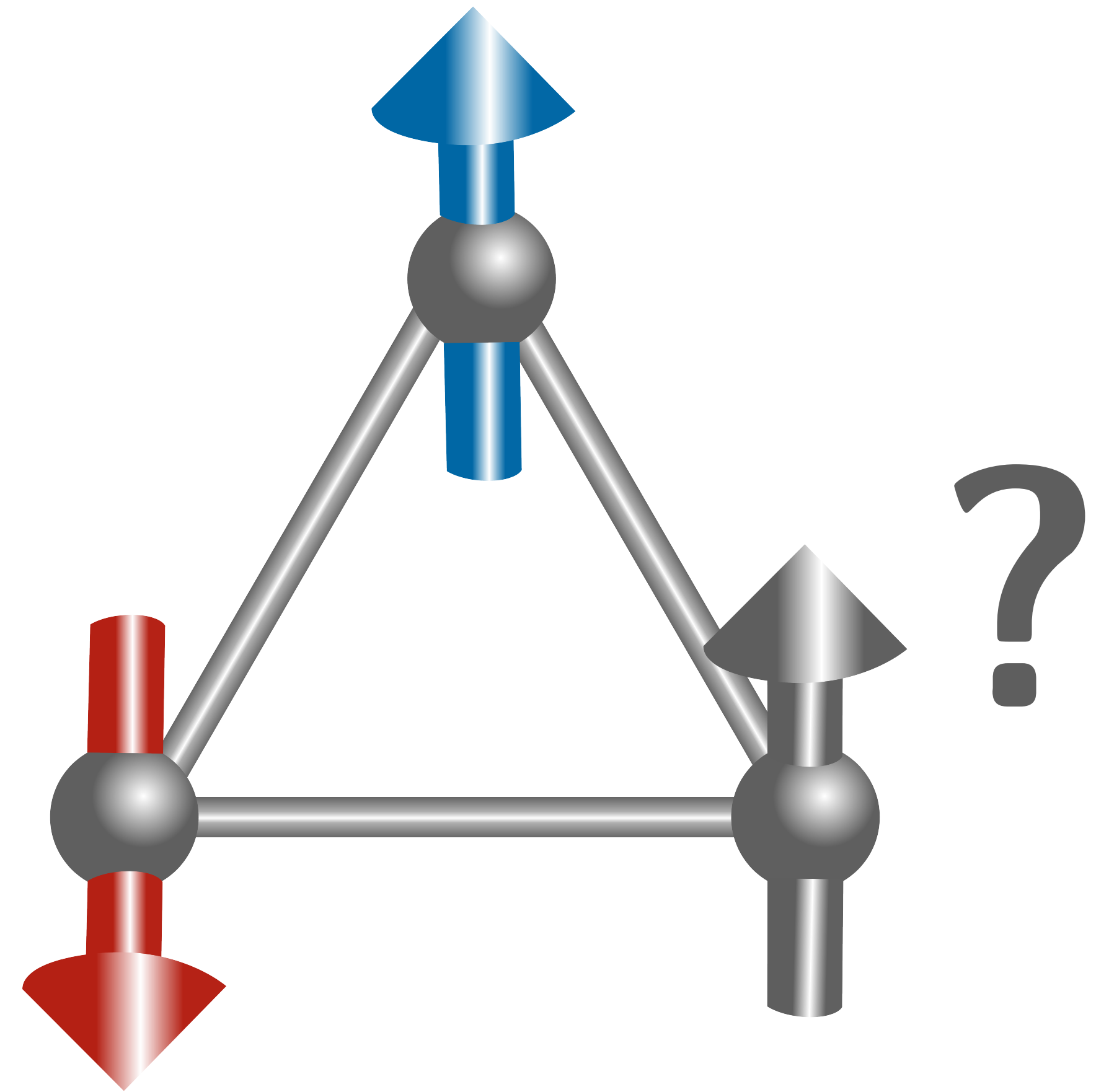


[Kane & Mele, PRL '05]
[König *et al.*, Science '07]

Ingredient #2: Frustration

Antiferromagnetic interaction:

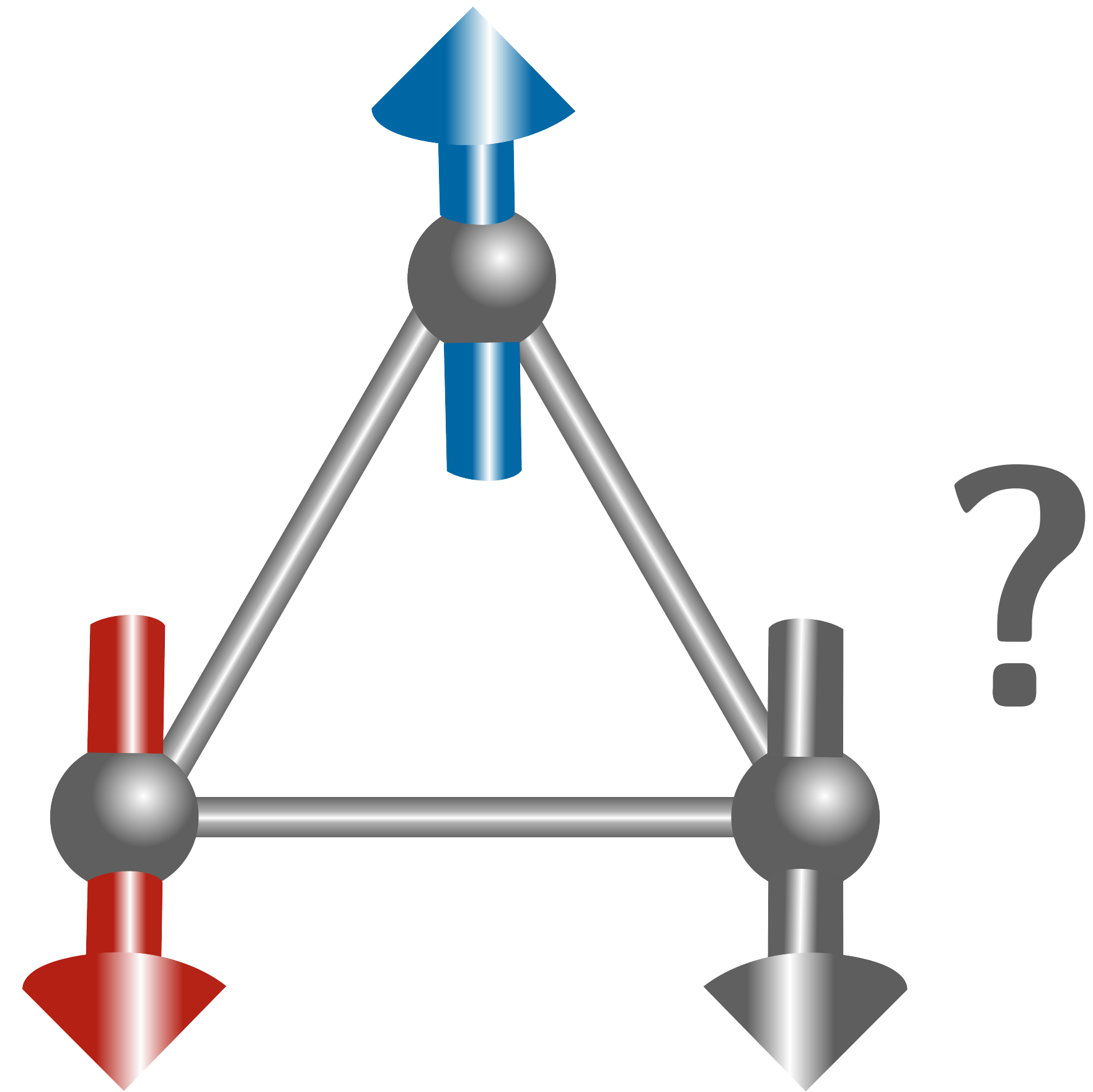
$$\mathcal{H}_{ij} = JS_i^z S_j^z \quad J > 0$$



Ingredient #2: Frustration

Antiferromagnetic interaction:

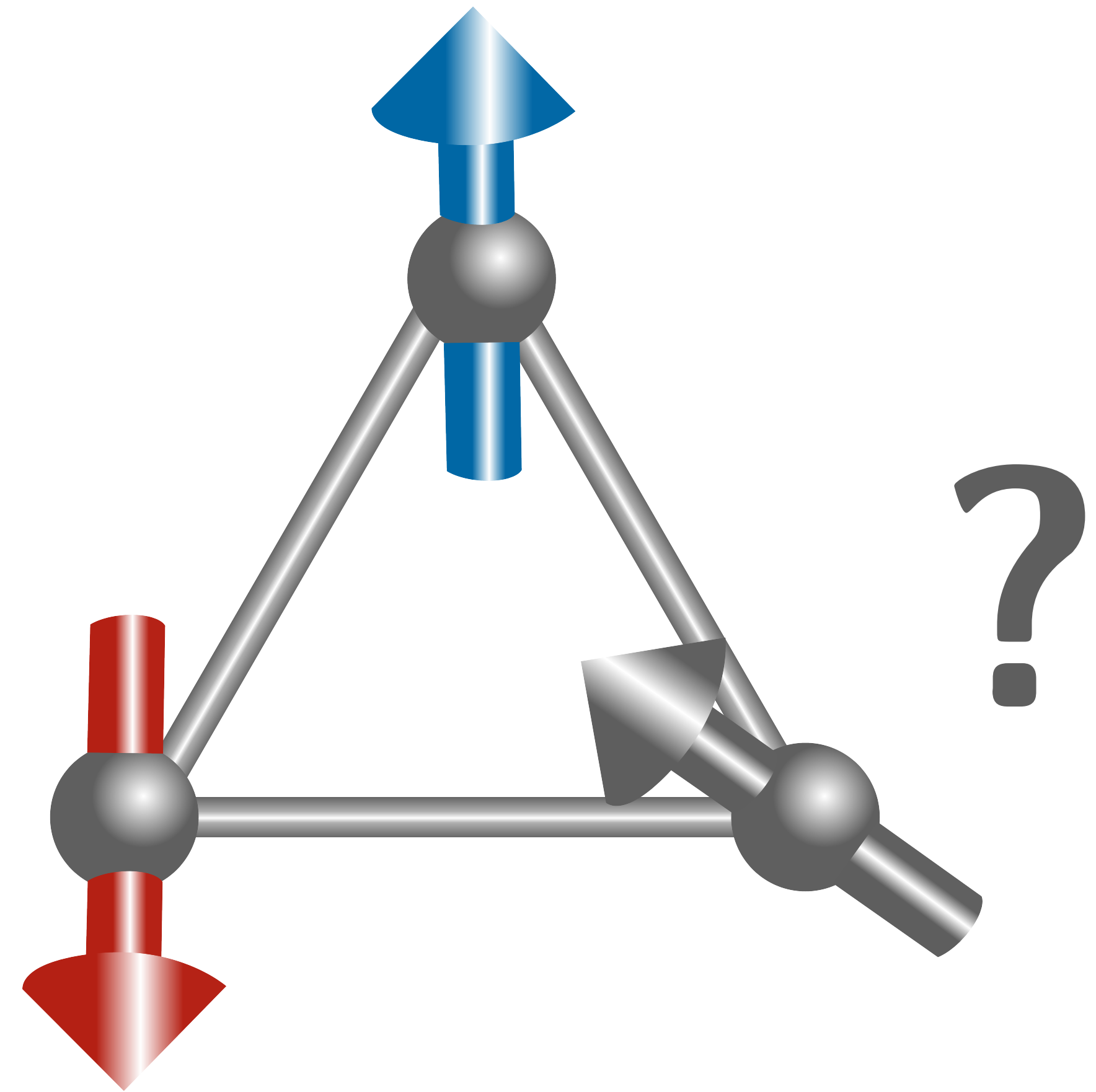
$$\mathcal{H}_{ij} = JS_i^z S_j^z \quad J > 0$$



Ingredient #2: Frustration

Antiferromagnetic interaction:

$$\mathcal{H}_{ij} = JS_i^z S_j^z \quad J > 0$$



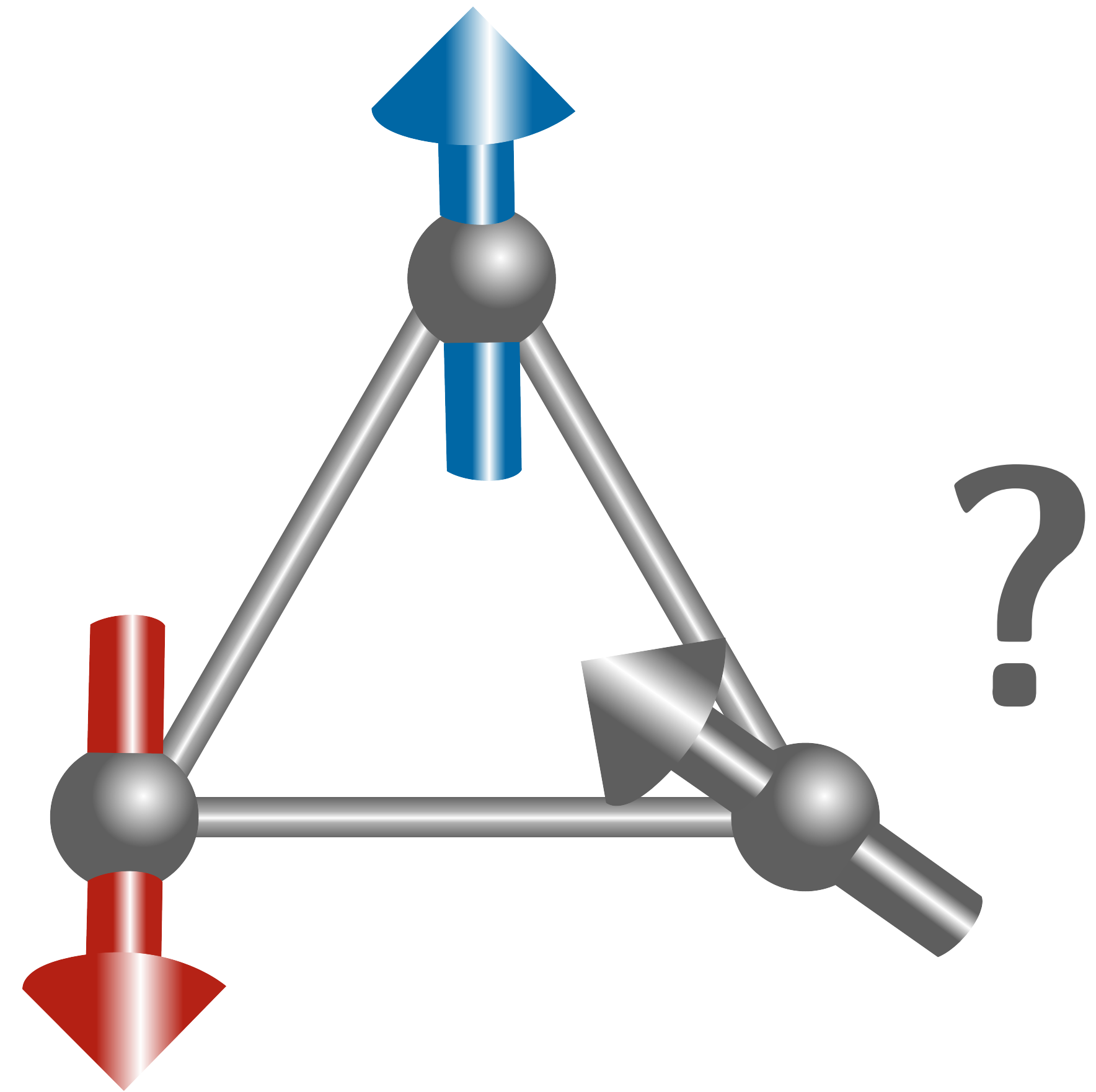
Ingredient #2: Frustration

Antiferromagnetic interaction:

$$\mathcal{H}_{ij} = JS_i^z S_j^z \quad J > 0$$

Frustration:

Incompatible interactions



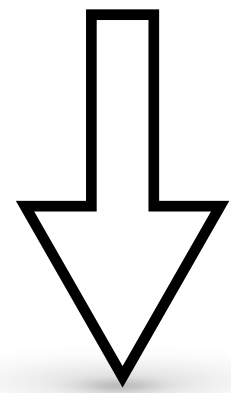
Ingredient #2: Frustration

Antiferromagnetic interaction:

$$\mathcal{H}_{ij} = JS_i^z S_j^z \quad J > 0$$

Frustration:

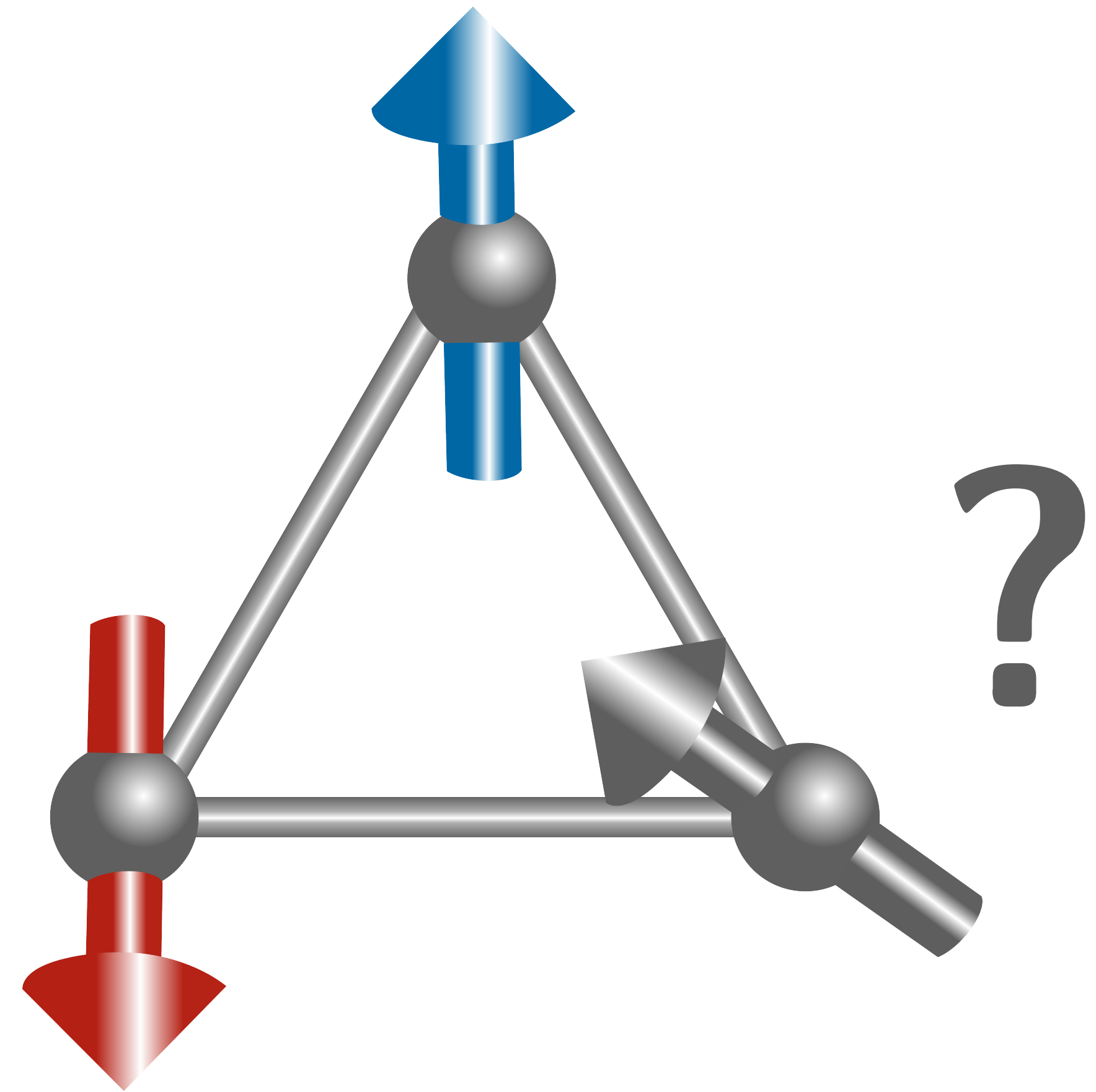
Incompatible interactions



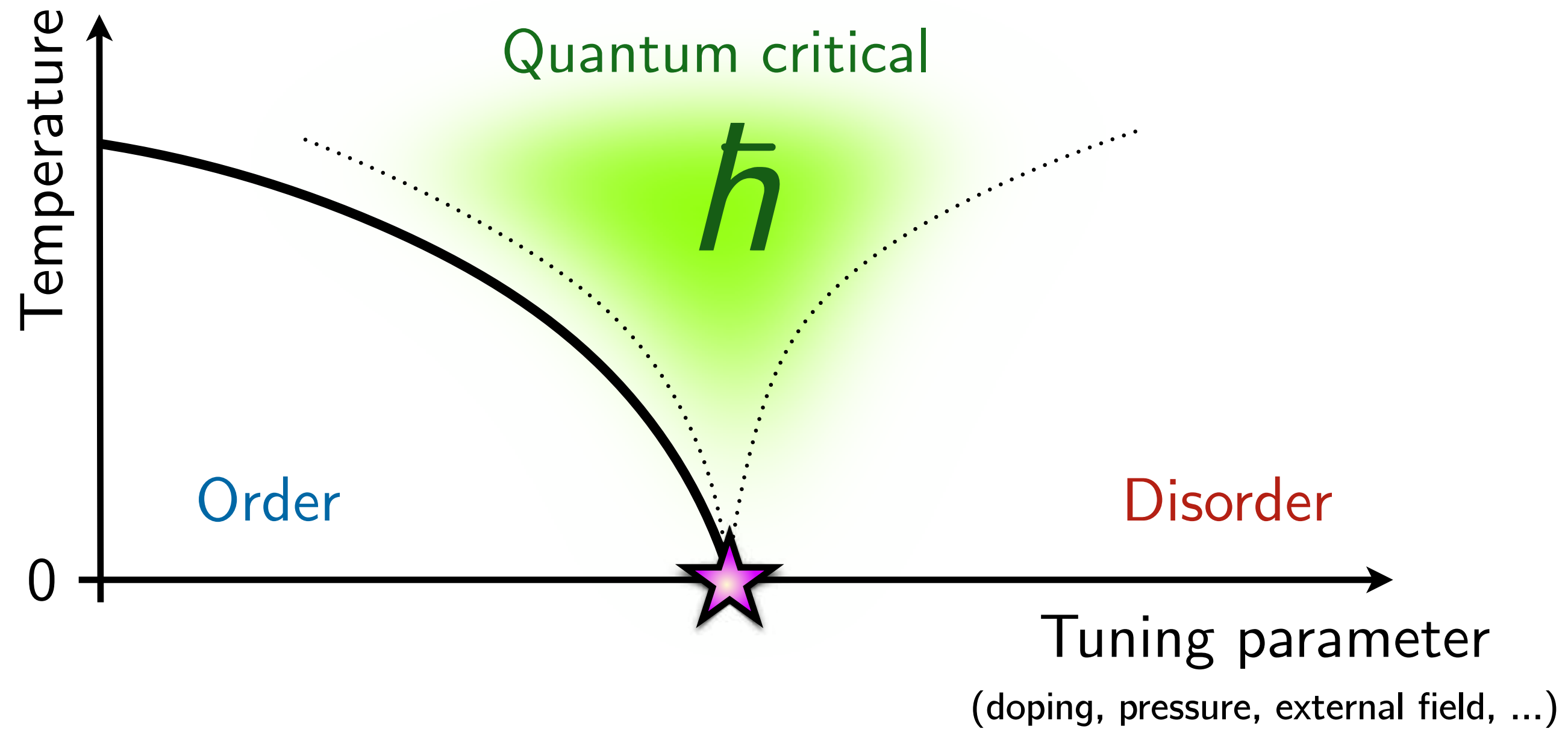
New states of matter
with exotic excitations?



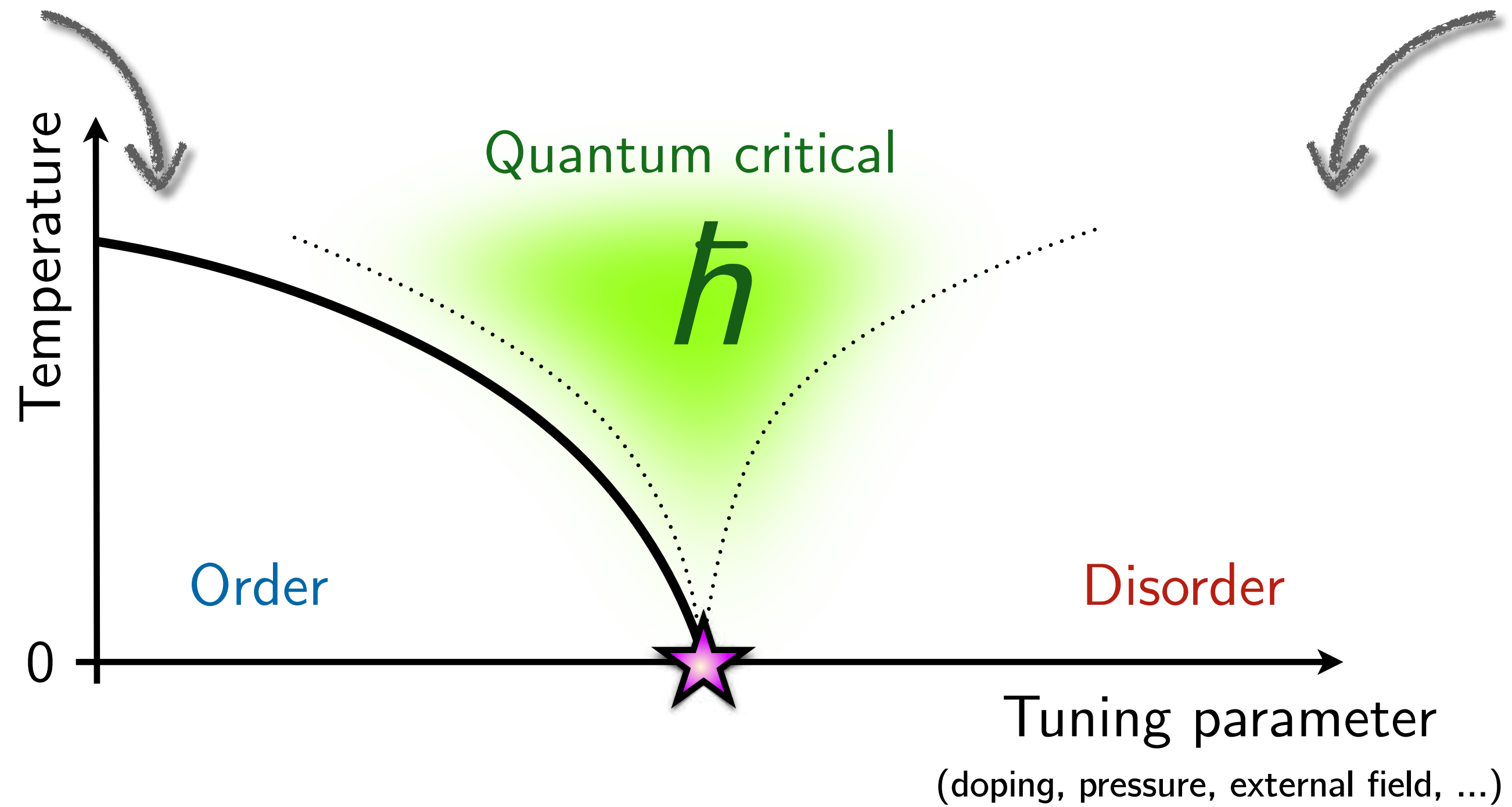
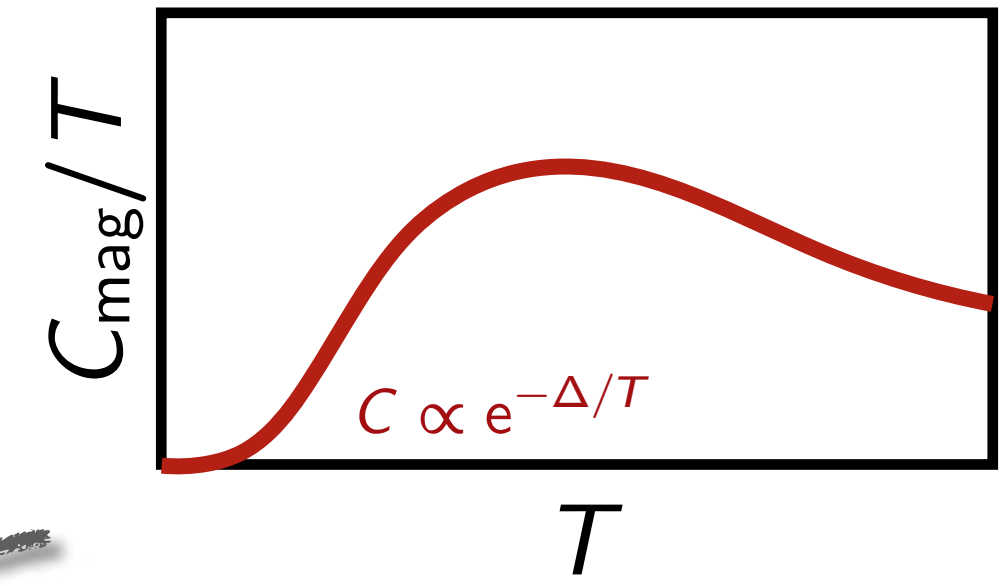
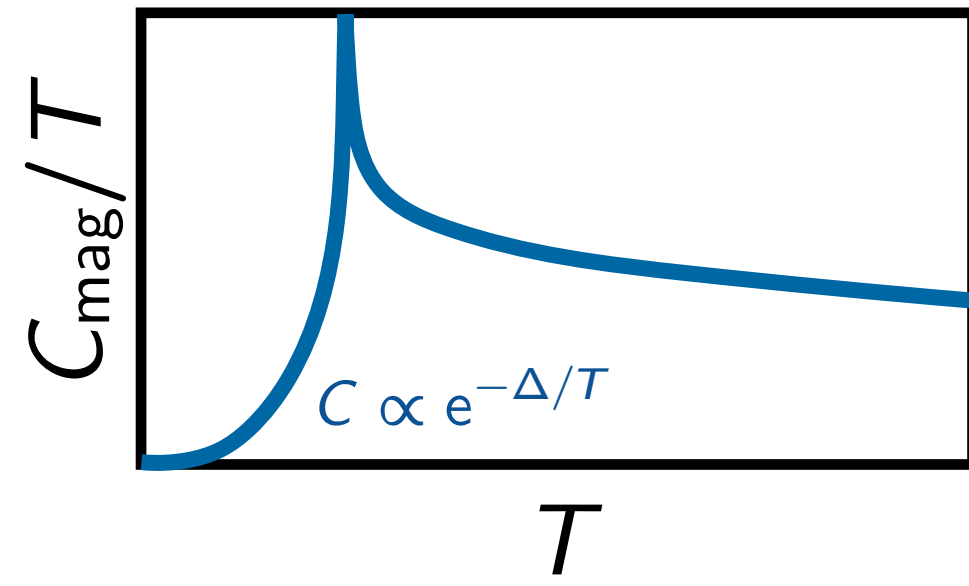
illustrationsource.com



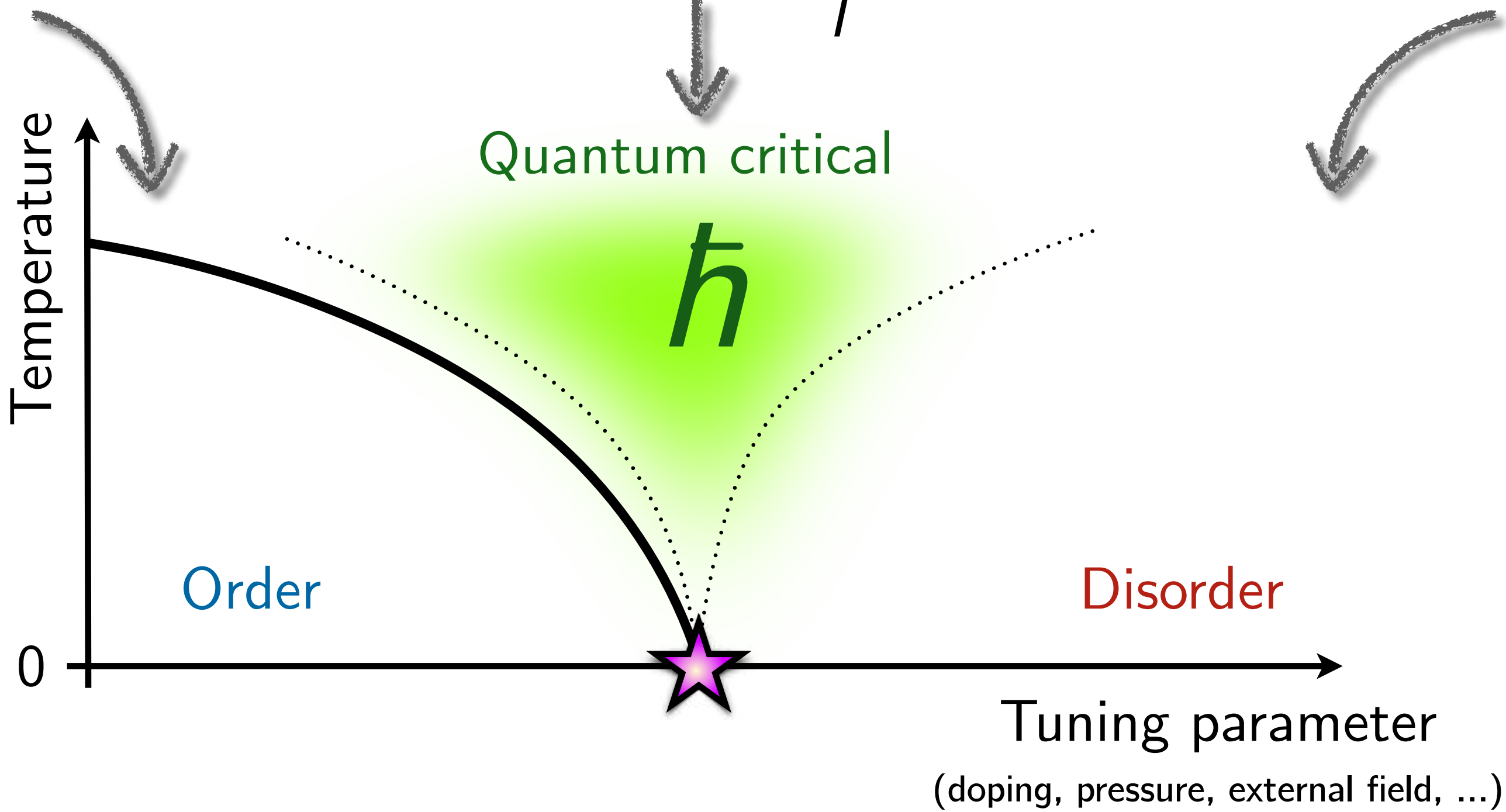
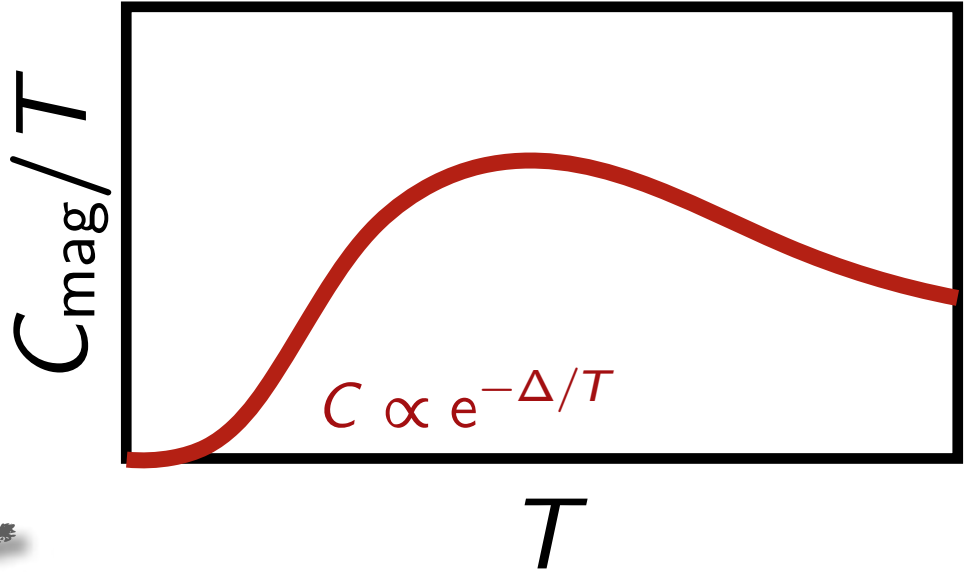
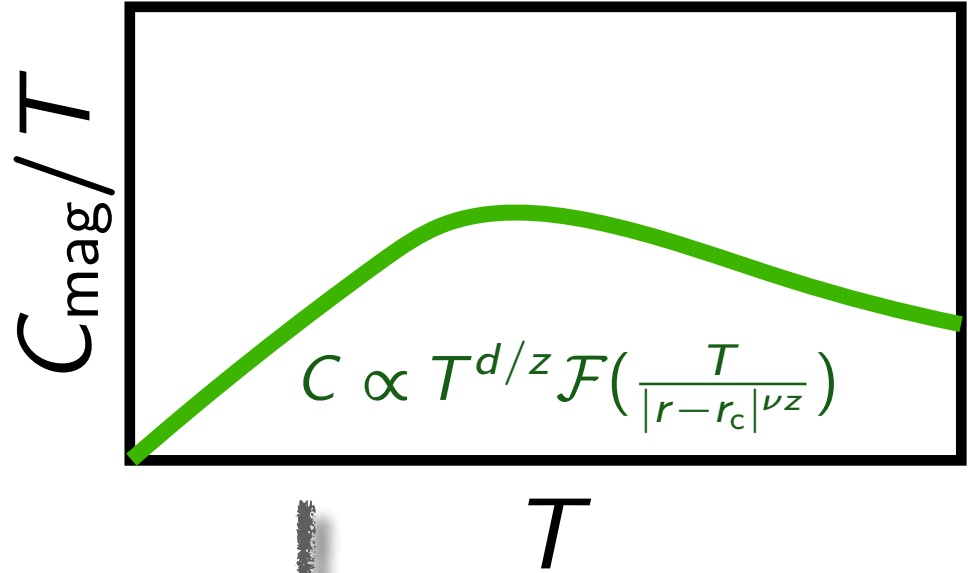
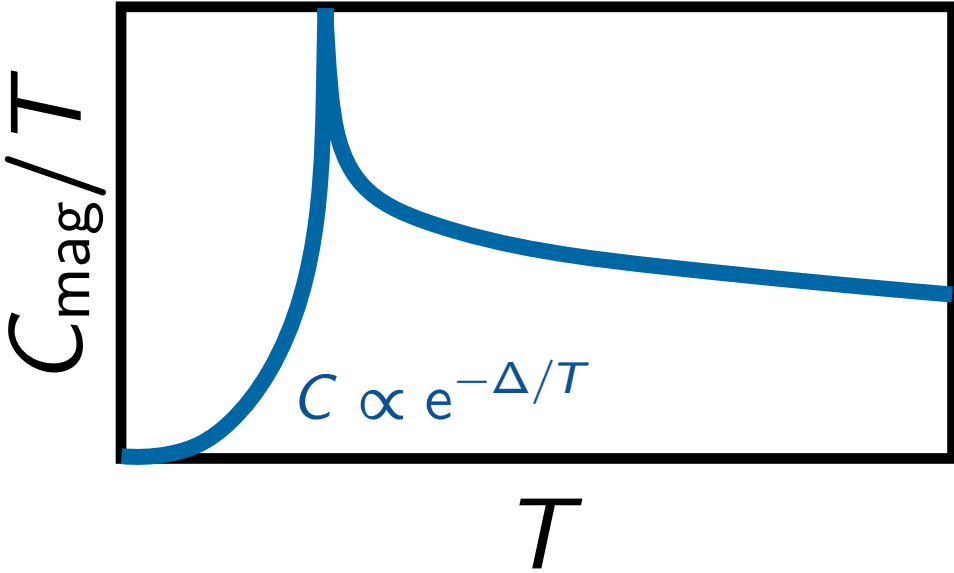
Ingredient #3: Quantum Criticality



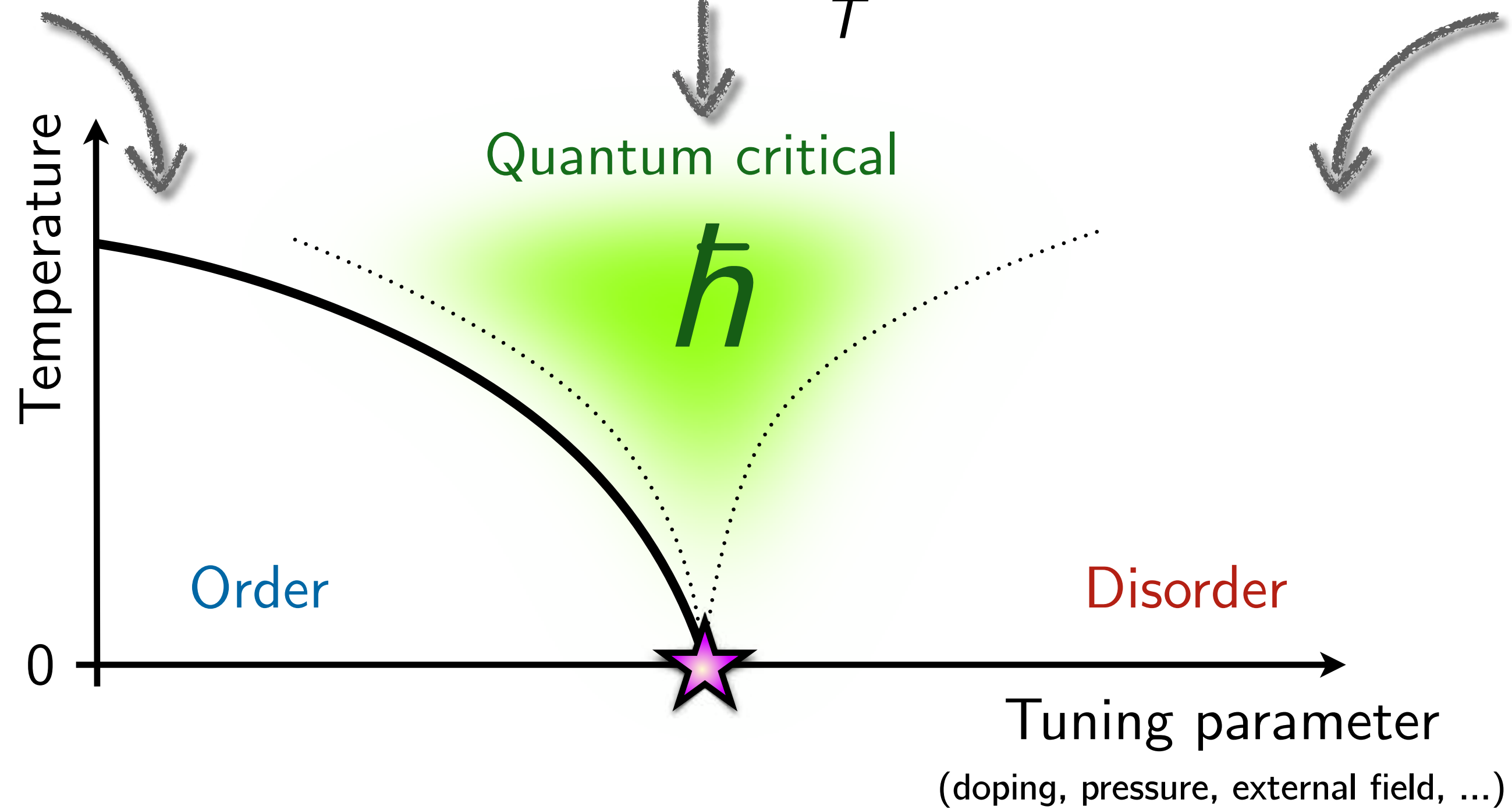
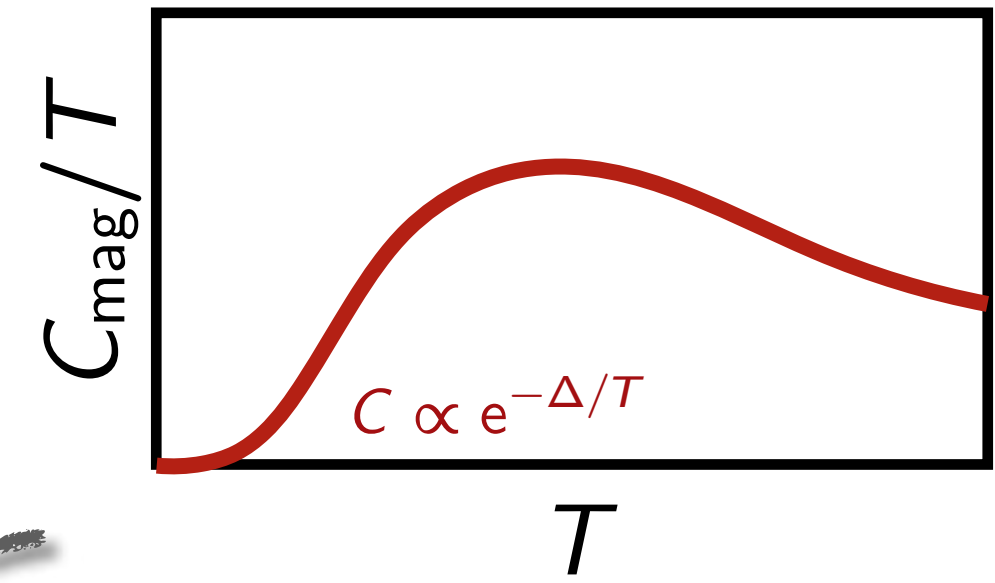
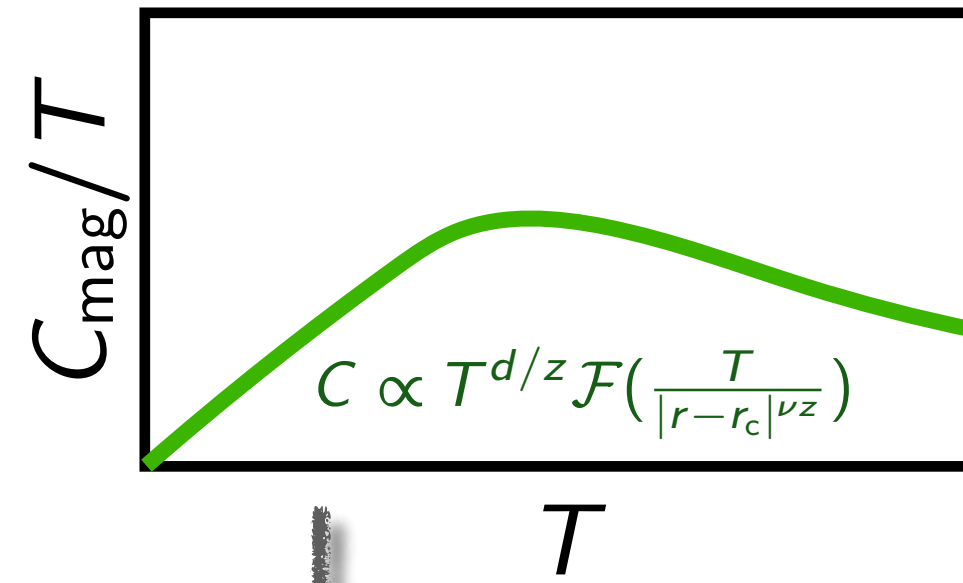
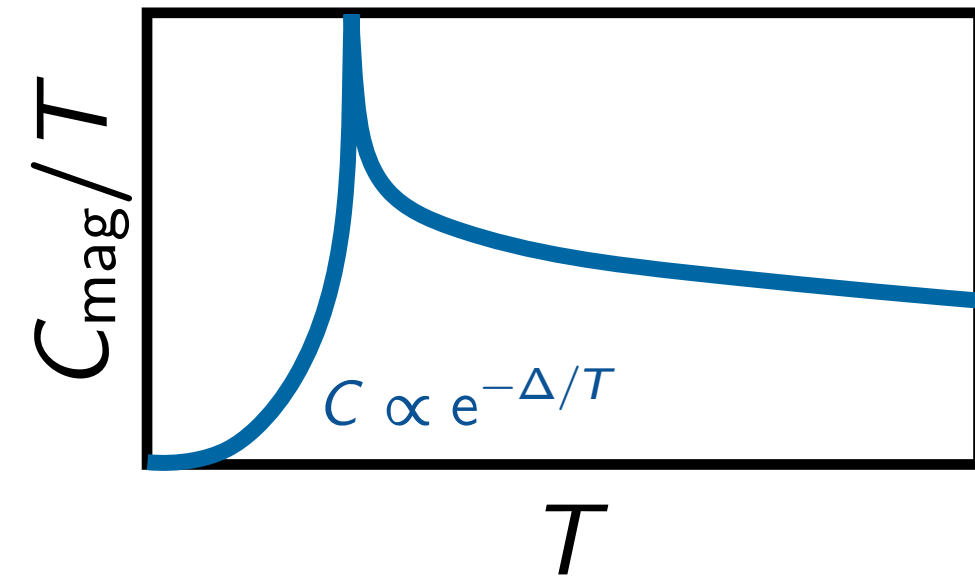
Ingredient #3: Quantum Criticality



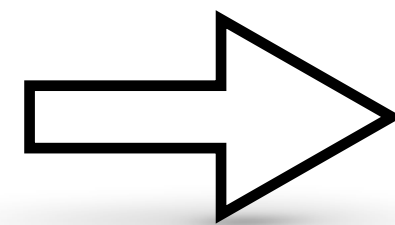
Ingredient #3: Quantum Criticality



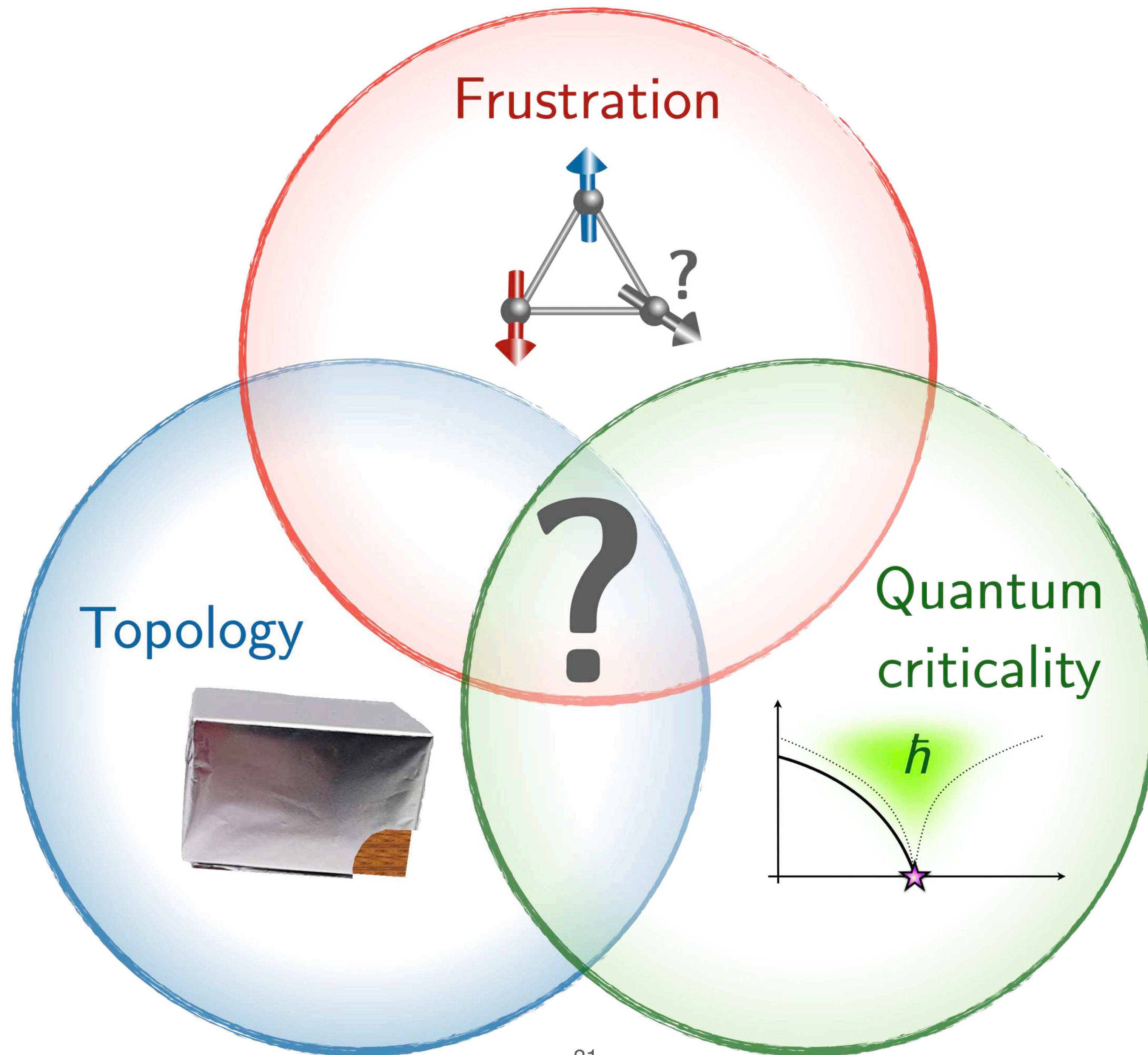
Ingredient #3: Quantum Criticality



Strong correlations



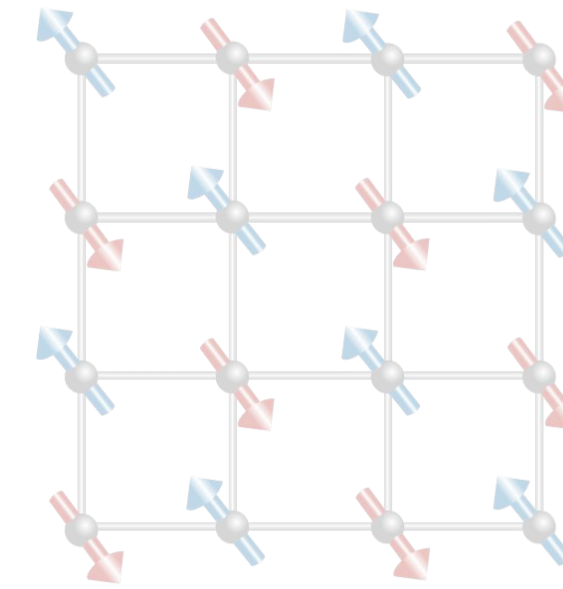
Novel states without conventional quasiparticles?



Outline

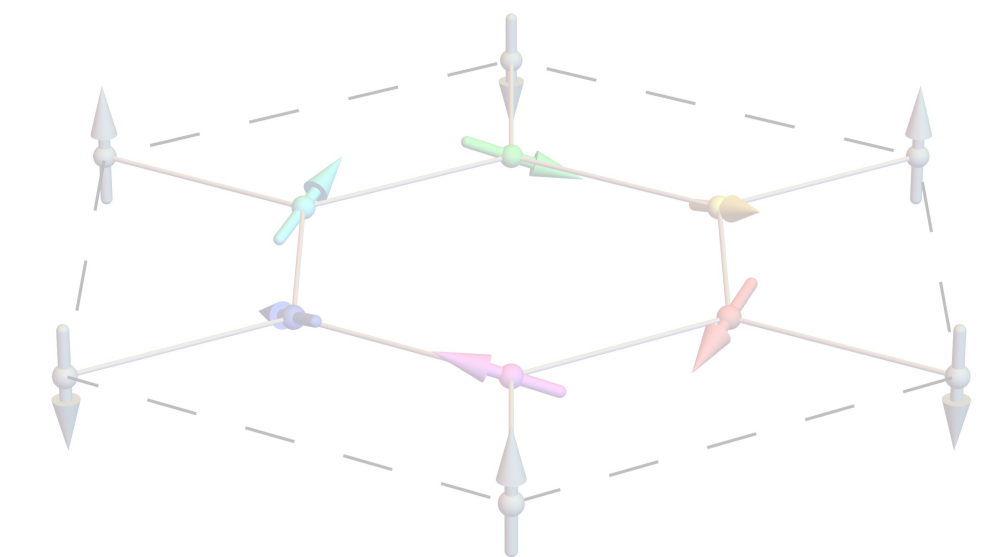
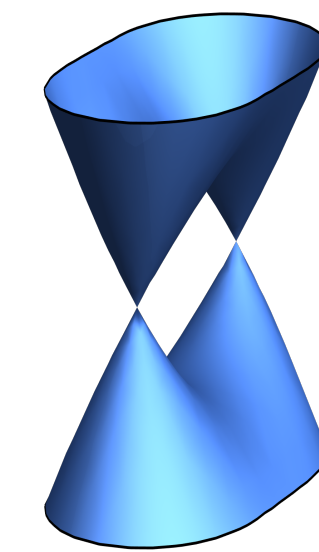
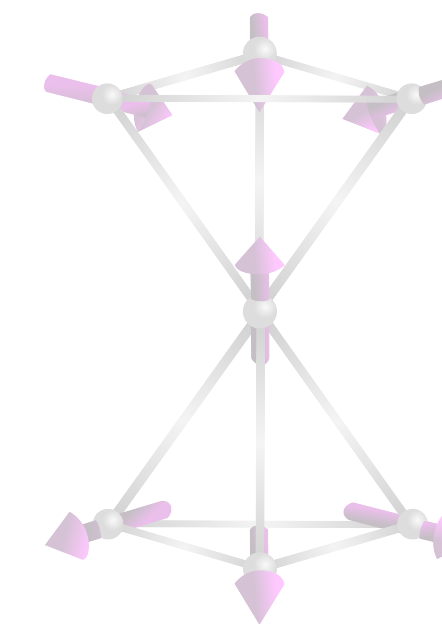
(1) Introduction

- ▶ Research Motivation
- ▶ Research Goals

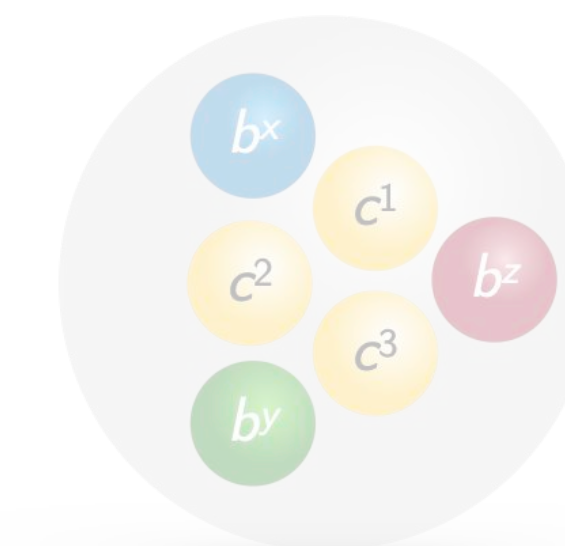


(2) Emergent Phenomena in Quantum Materials

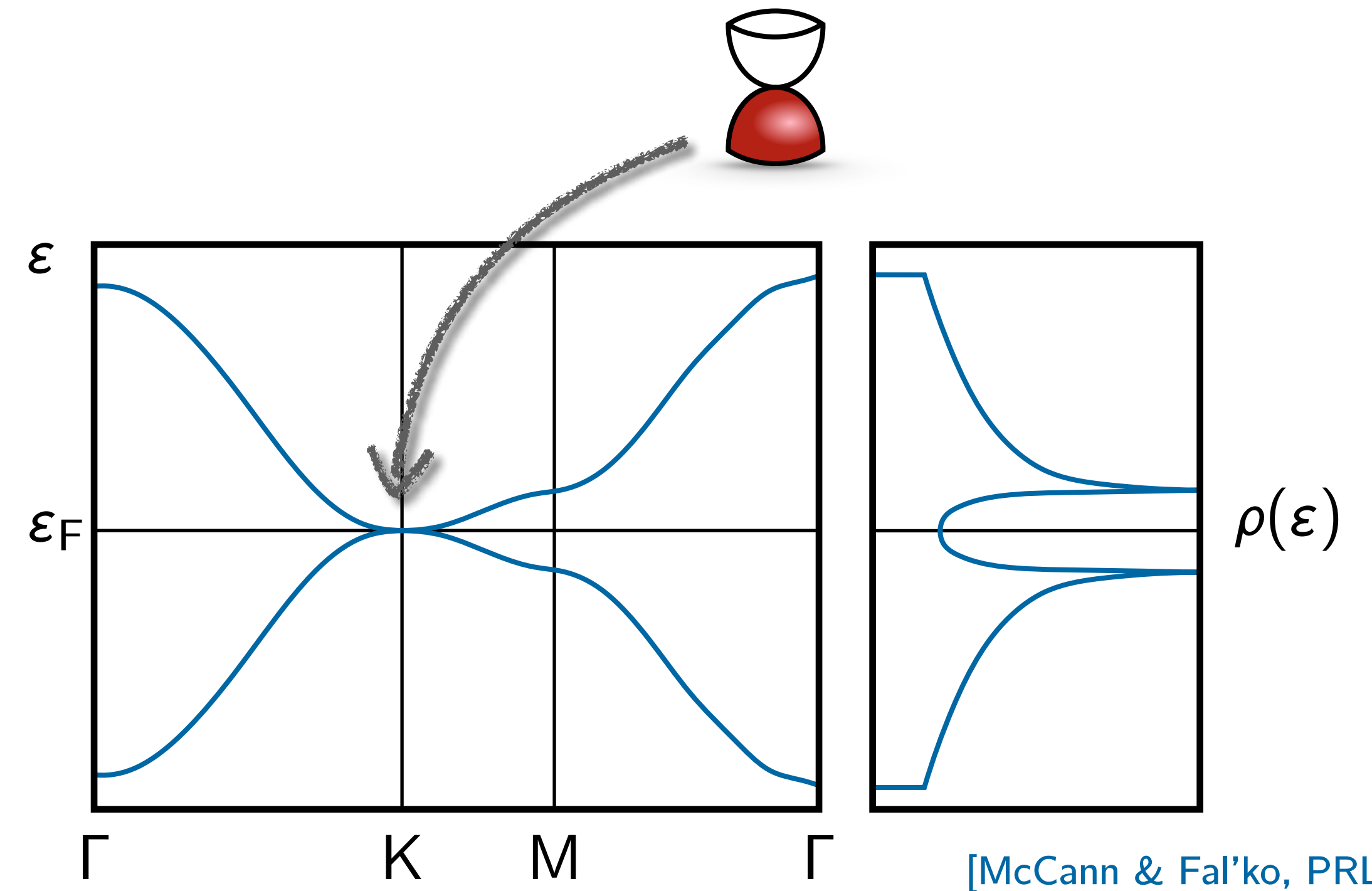
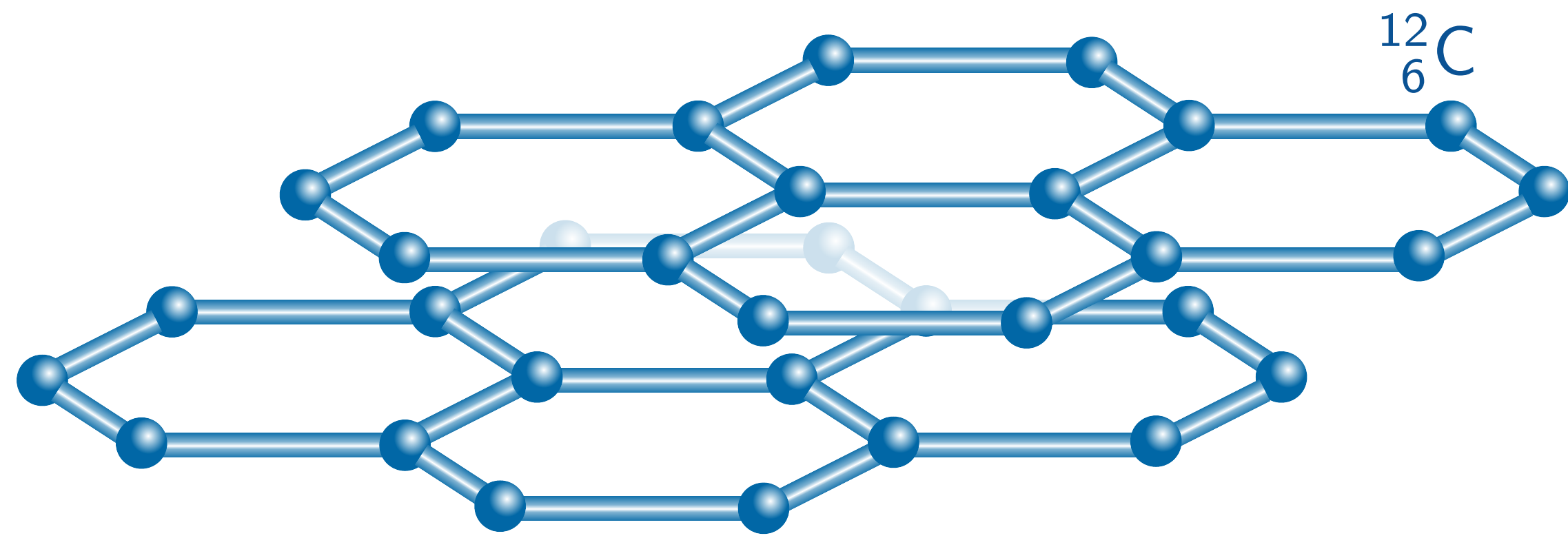
- ▶ Emergent Symmetries
- ▶ Emergent Topology
- ▶ Emergent Orders
- ▶ Emergent Particles



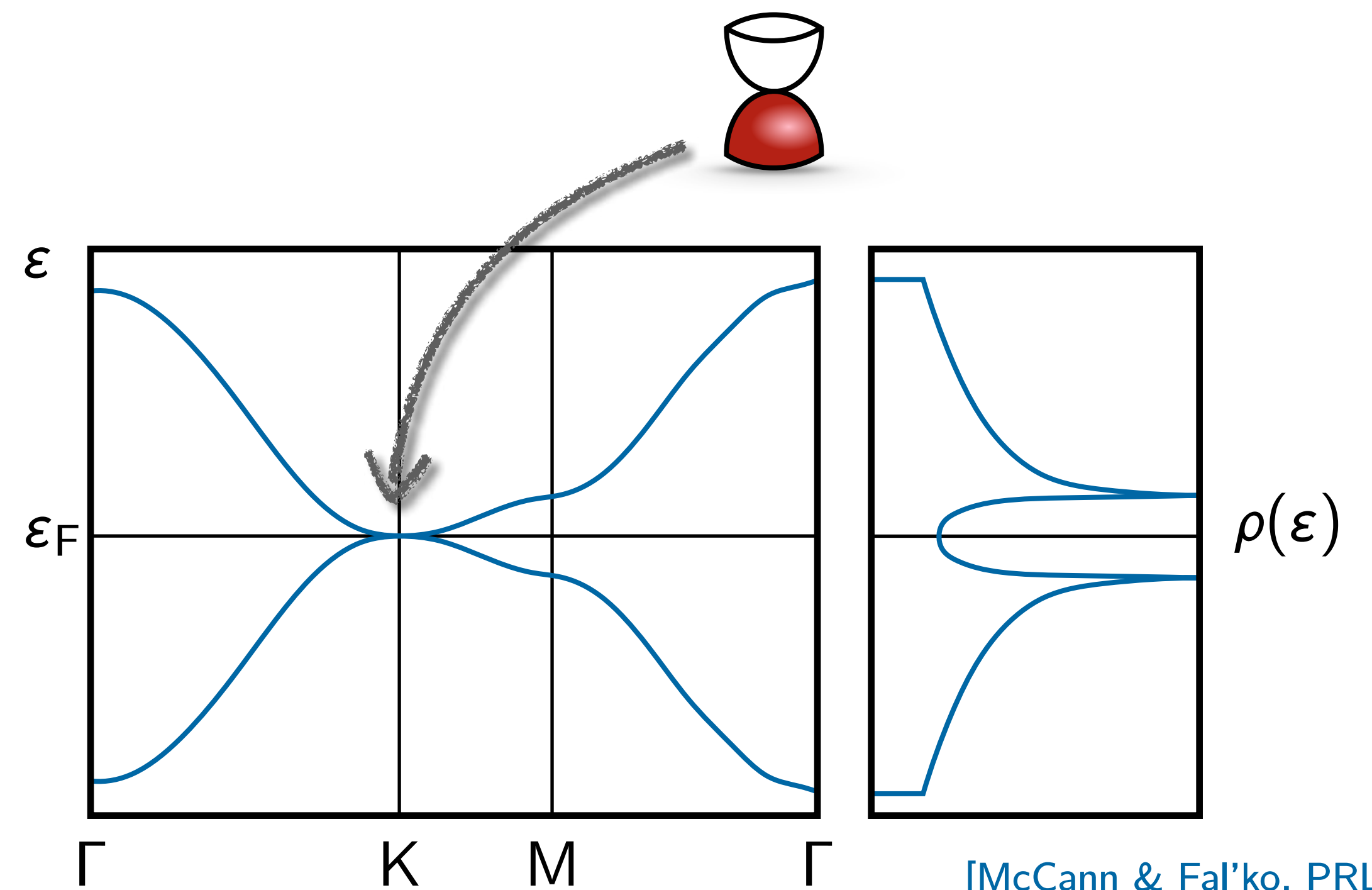
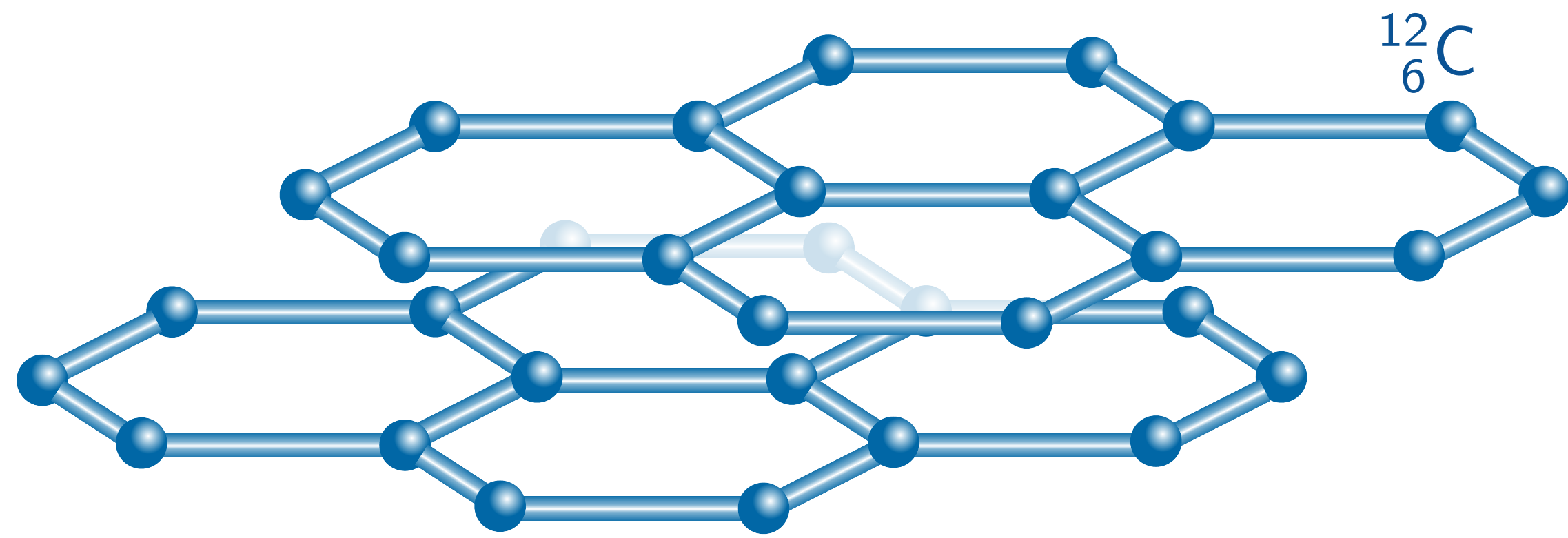
(3) Summary



Example #1: Bilayer Graphene

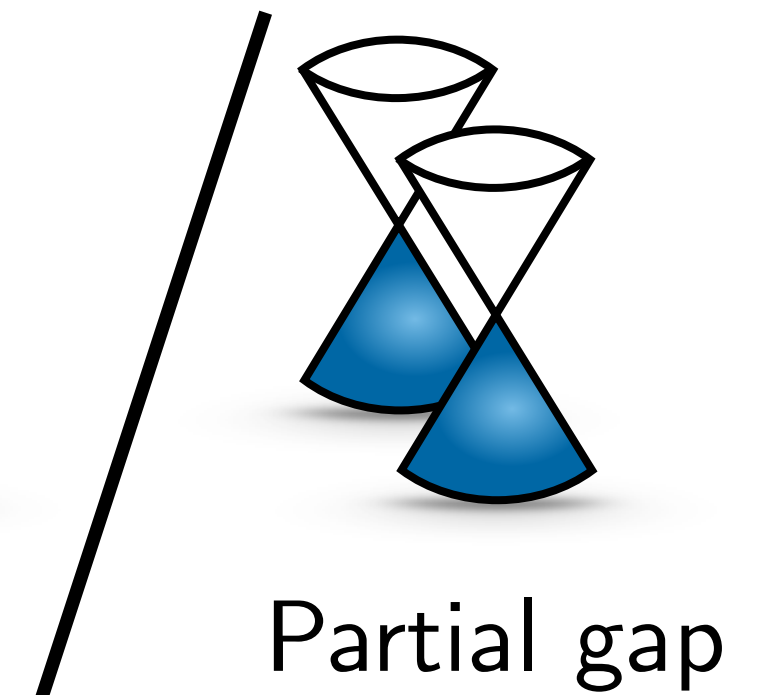
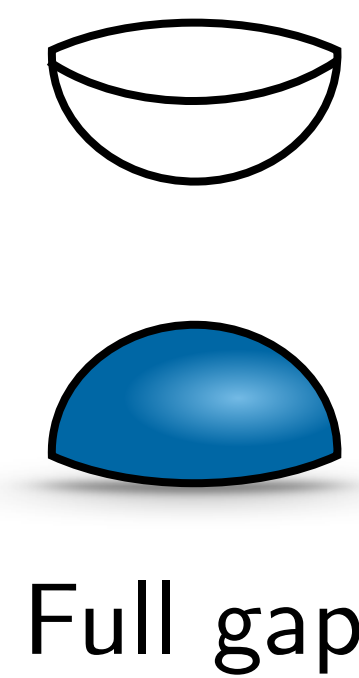
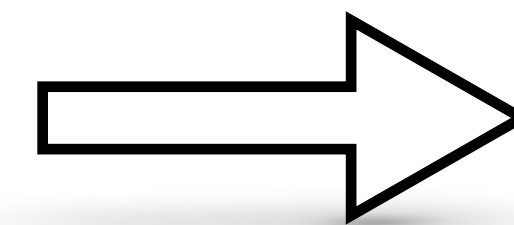
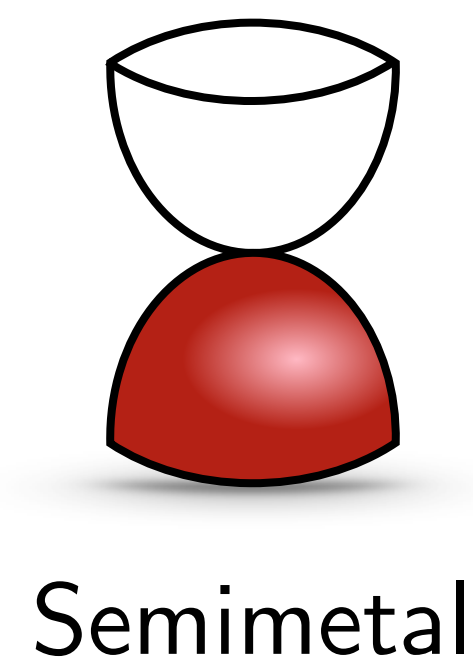
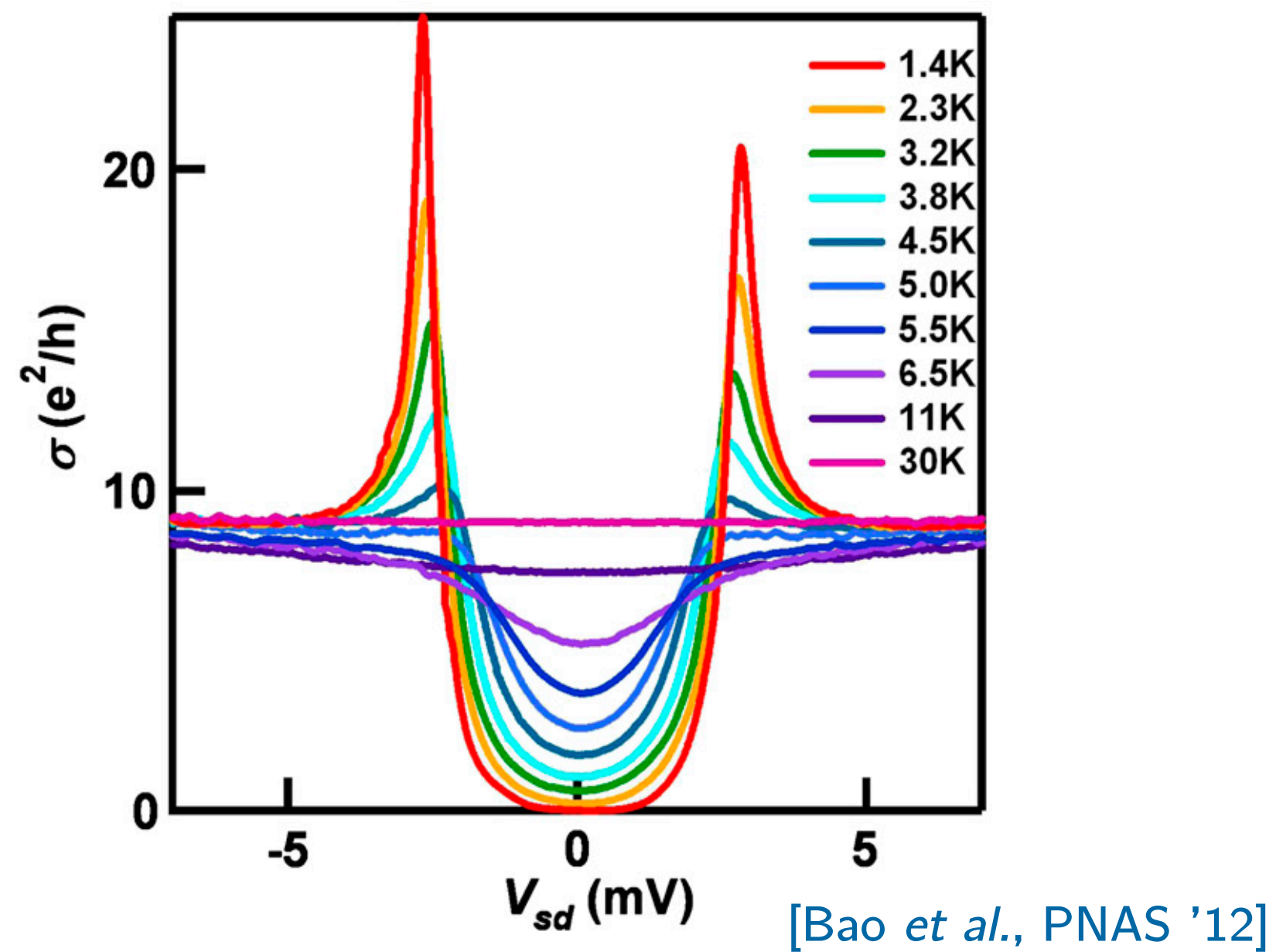


Example #1: Bilayer Graphene



[McCann & Fal'ko, PRL '06]

Instability:



[Velasco *et al.*, Nat. Nano. '12]

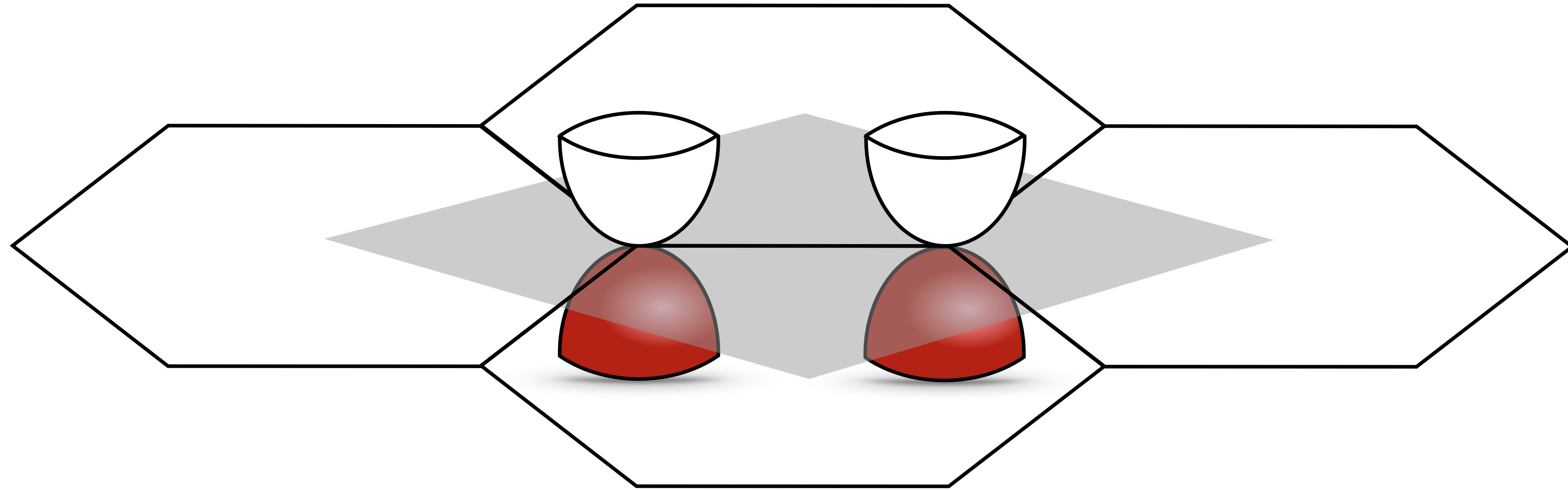
[Freitag *et al.*, PRL '12]

[Mayorov *et al.*, Science '11]

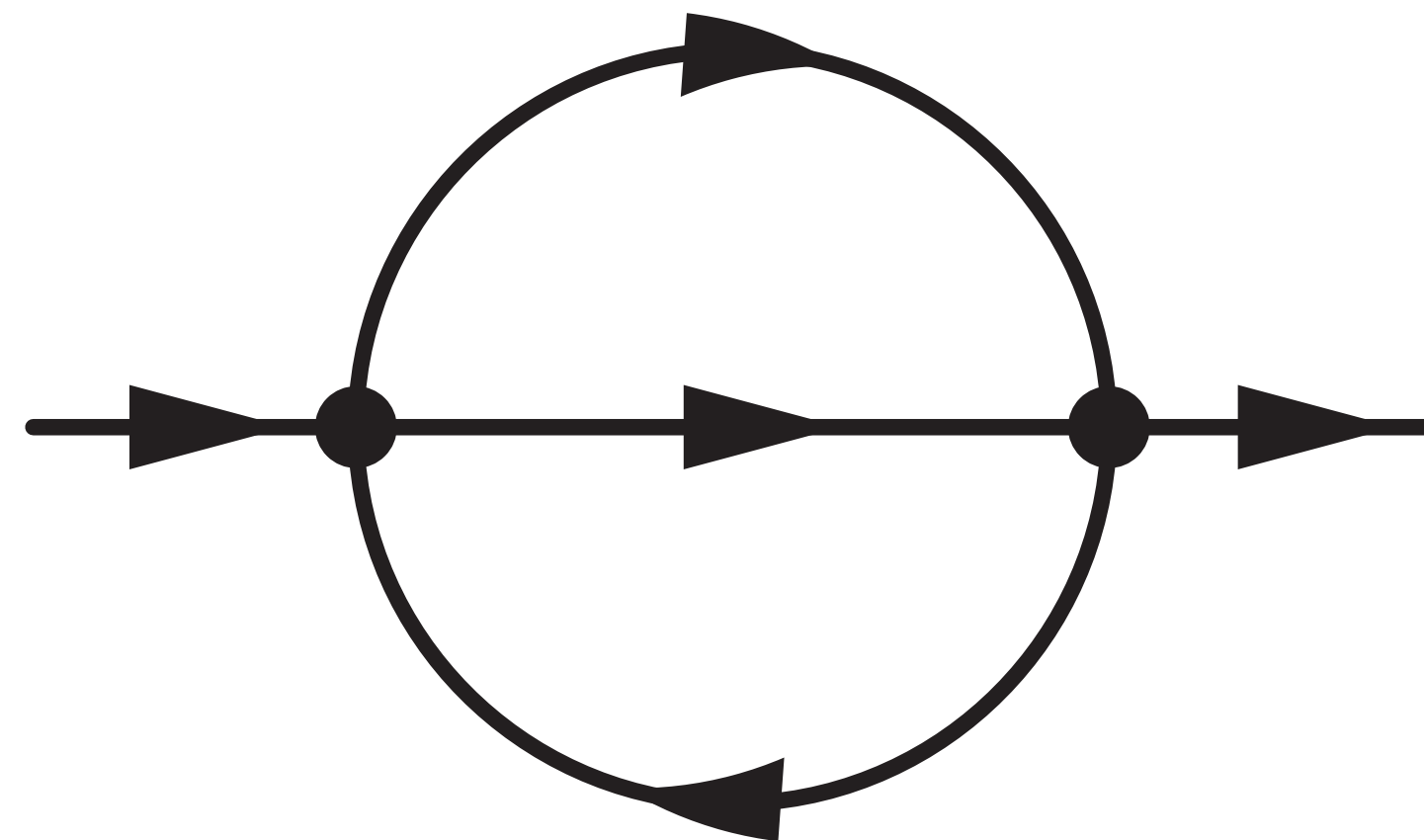
Emergent Lorentz Symmetry I



Shouryya Ray

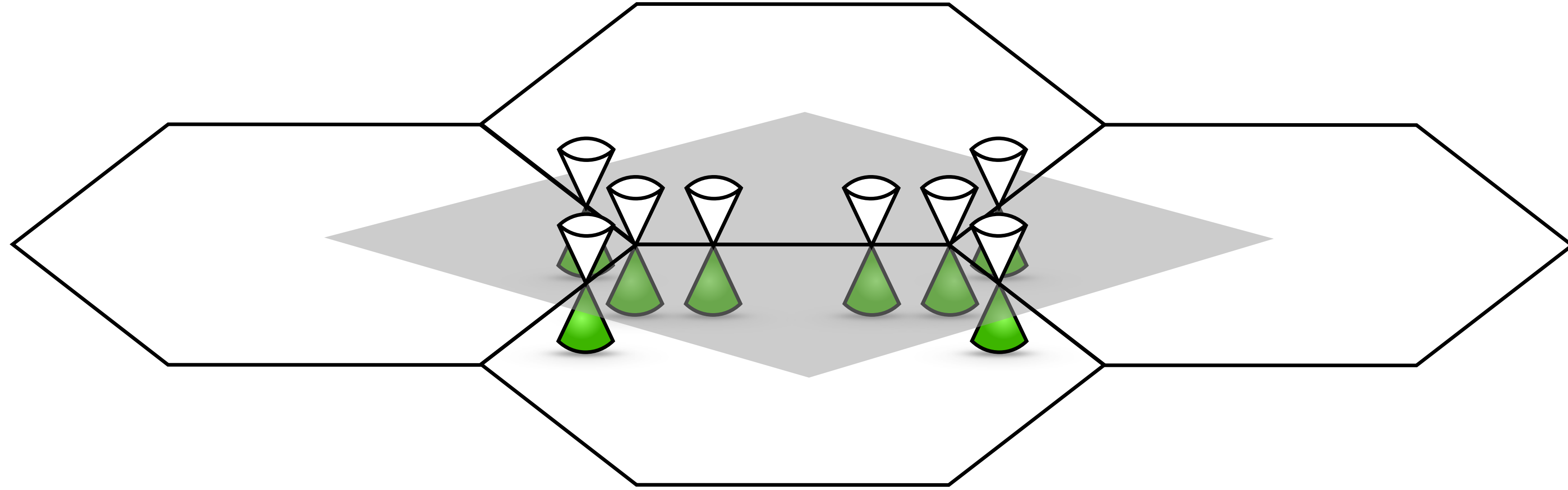


+



[Ray, Vojta, LJ, PRB '18 (Editors' Suggestion)]

Emergent Lorentz Symmetry I

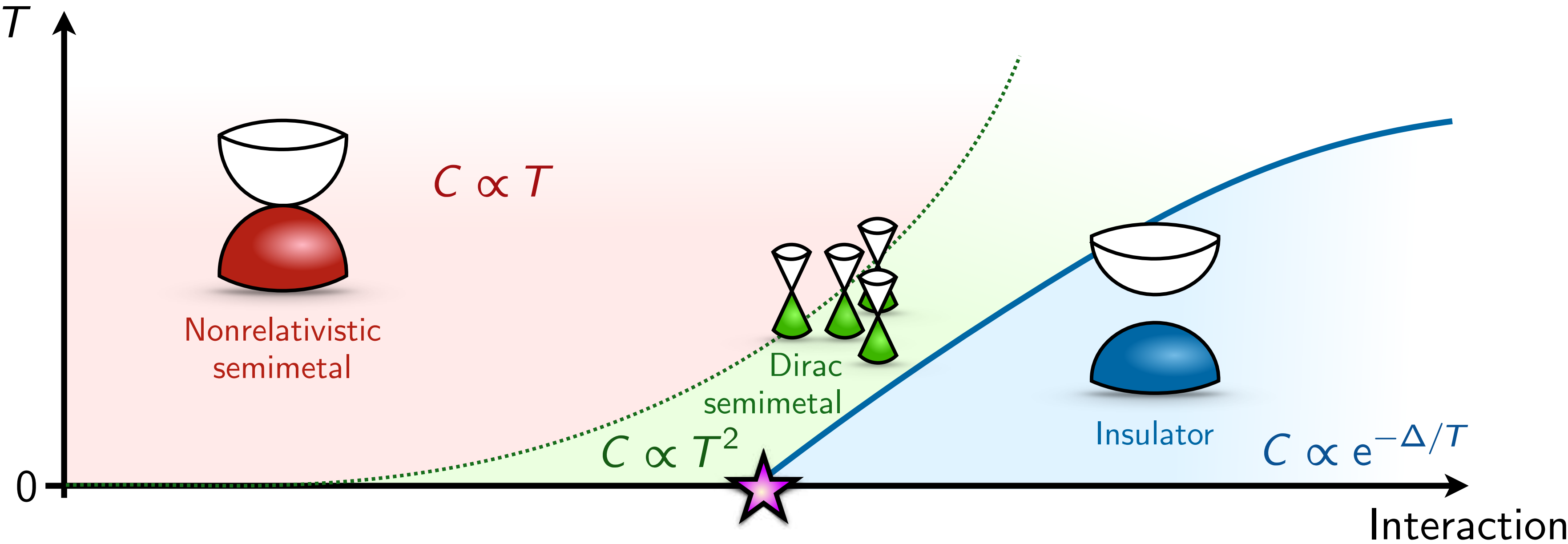
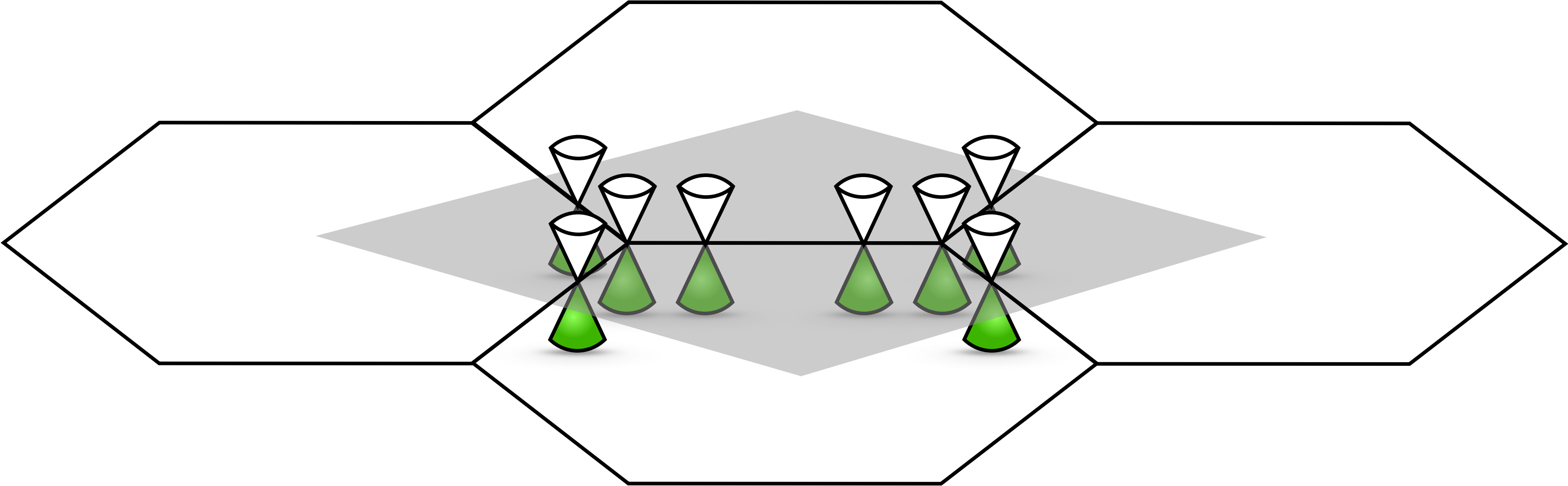


Shouryya Ray

Emergent Lorentz Symmetry I



Shouryya Ray



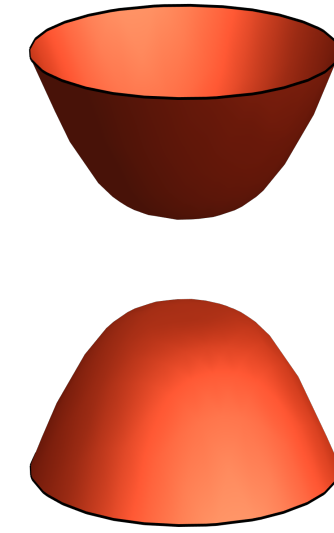
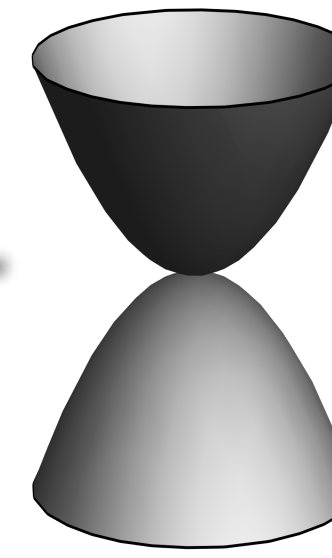
[Ray, Vojta, LJ, PRB '18 (Editors' Suggestion)]

see also: [Pujari, Lang, Murthy, Kaul, PRL '16]

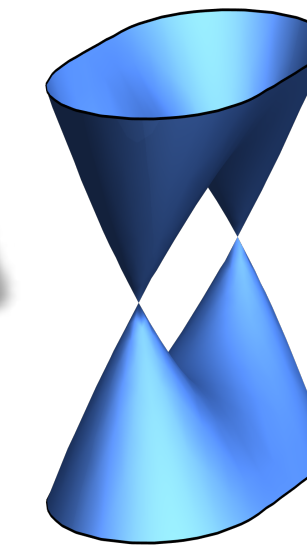
Emergent Lorentz Symmetry II

Lagrangian:

$$\mathcal{L} = \psi^\dagger [\partial_\tau + d_a (-i\nabla)(\Gamma_a \otimes \mathbb{1}_2)] \psi - g [\psi^\dagger (\Gamma_z \otimes \vec{\sigma}) \psi]^2 - g' [\psi^\dagger (\Gamma_a \otimes \mathbb{1}_2) \psi]^2$$



Antiferromagnetic insulator



Nematic semimetal



Shouryya Ray

Emergent Lorentz Symmetry II

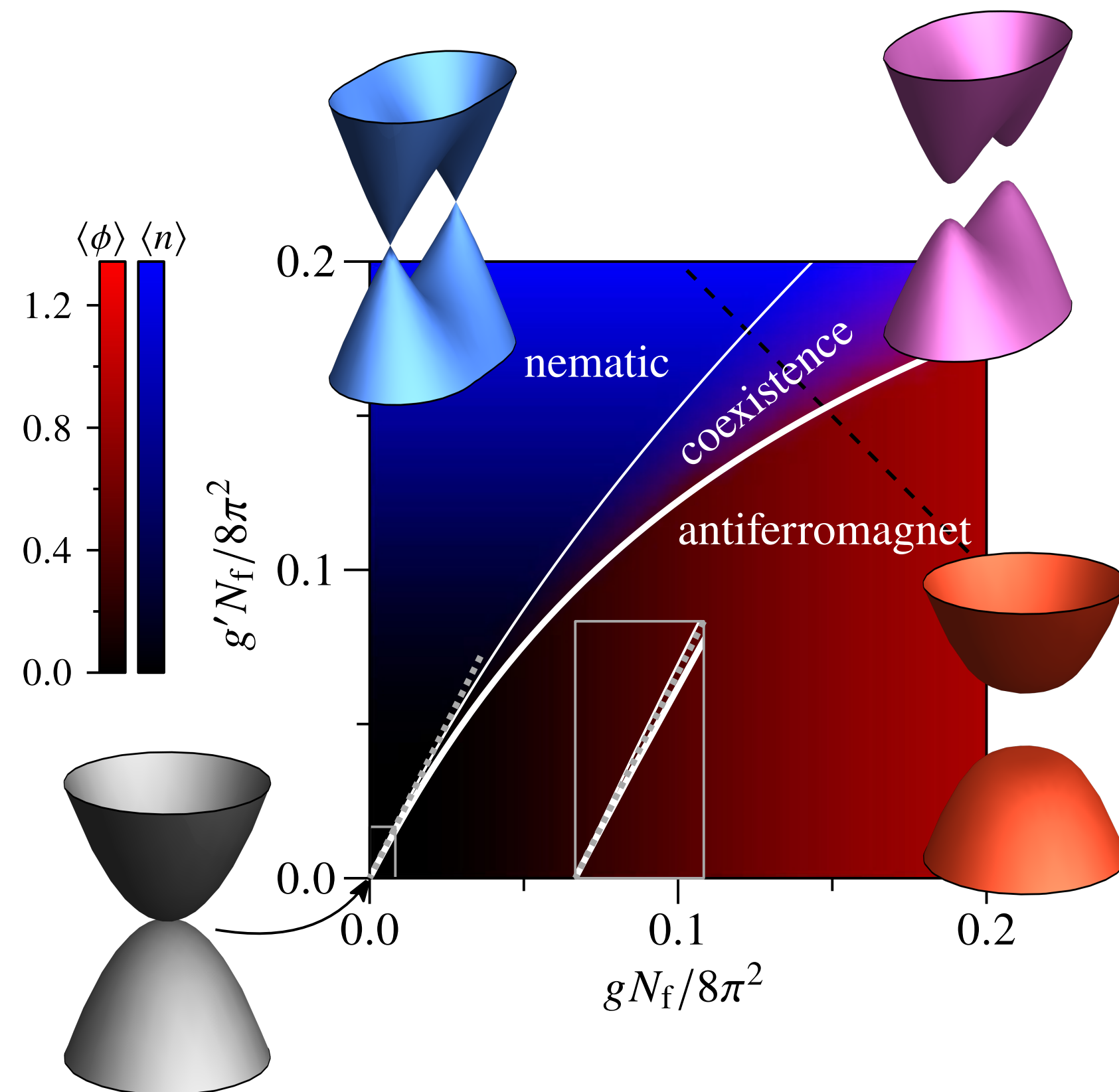
Lagrangian:

$$\mathcal{L} = \psi^\dagger [\partial_\tau + d_a (-i\nabla)(\Gamma_a \otimes \mathbb{1}_2)] \psi - g [\psi^\dagger (\Gamma_z \otimes \vec{\sigma}) \psi]^2 - g' [\psi^\dagger (\Gamma_a \otimes \mathbb{1}_2) \psi]^2$$



Shouryya Ray

Phase diagram:



Emergent Lorentz Symmetry II

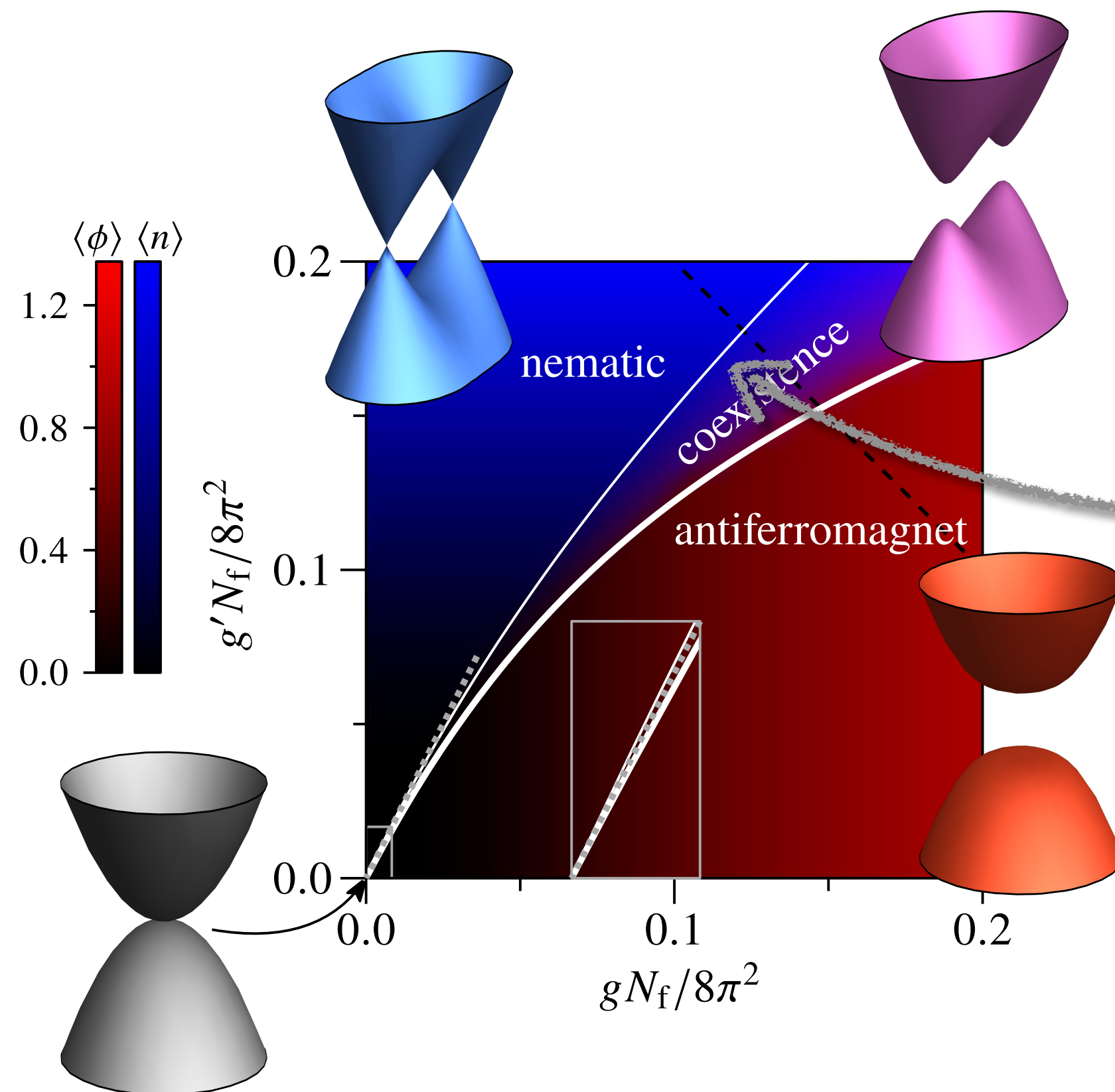


Shouryya Ray

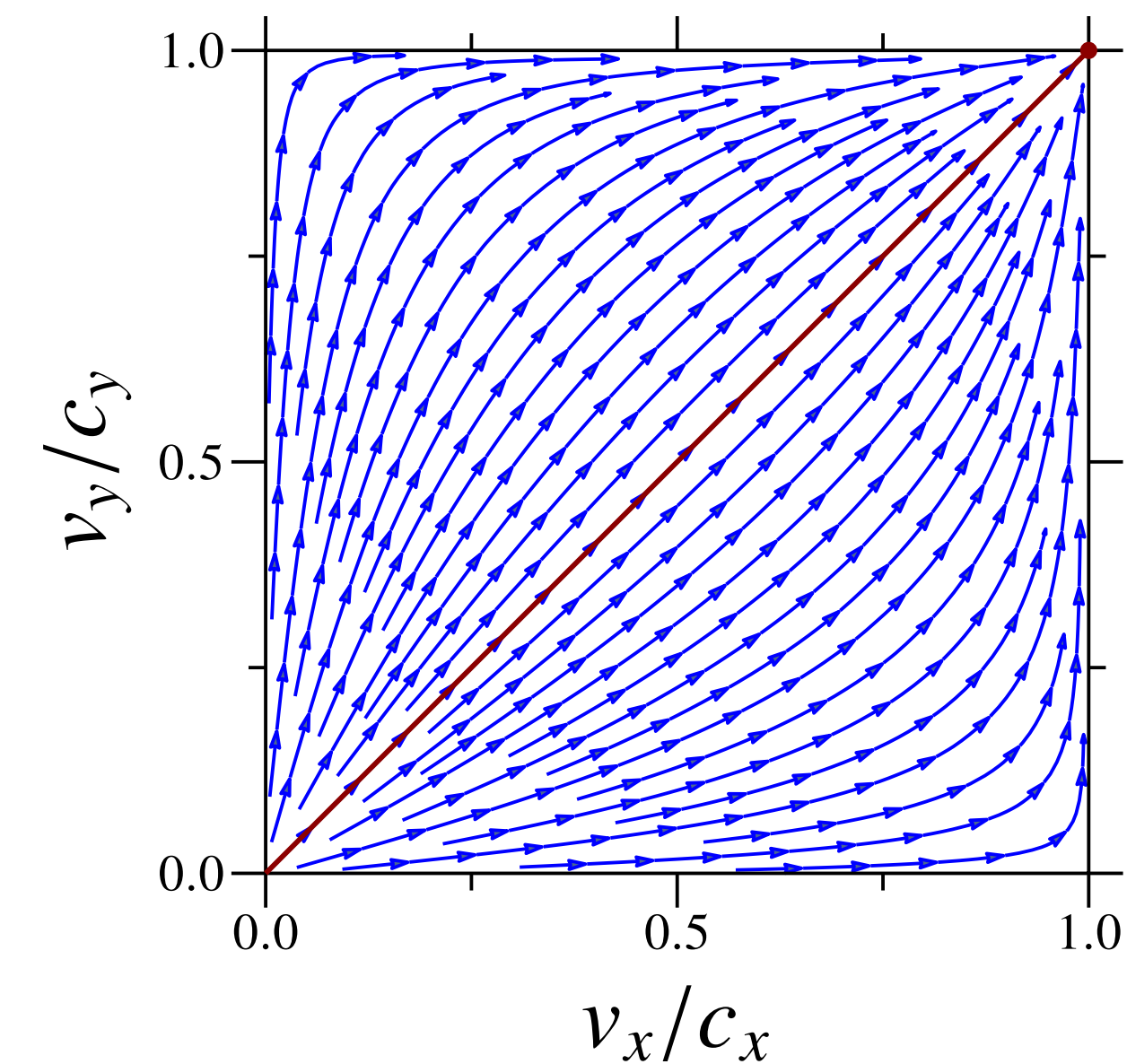
Lagrangian:

$$\mathcal{L} = \psi^\dagger [\partial_\tau + d_a(-i\nabla)(\Gamma_a \otimes \mathbb{1}_2)]\psi - g[\psi^\dagger(\Gamma_z \otimes \vec{\sigma})\psi]^2 - g'[\psi^\dagger(\Gamma_a \otimes \mathbb{1}_2)\psi]^2$$

Phase diagram:



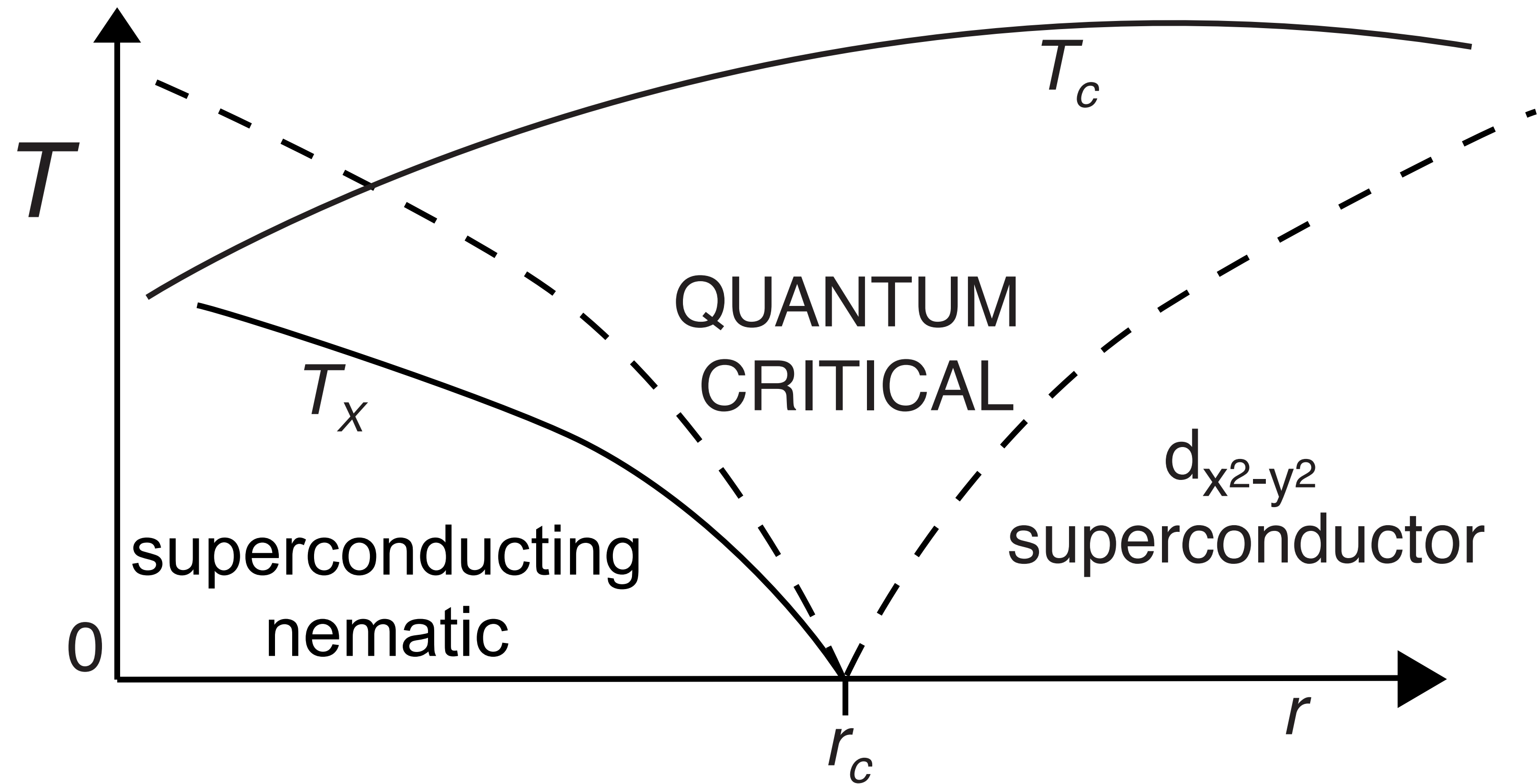
Velocity flow:



➡ emergent Lorentz symmetry!

Counterexample: Emergent Anisotropy

Phase diagram of a d -wave superconductor:

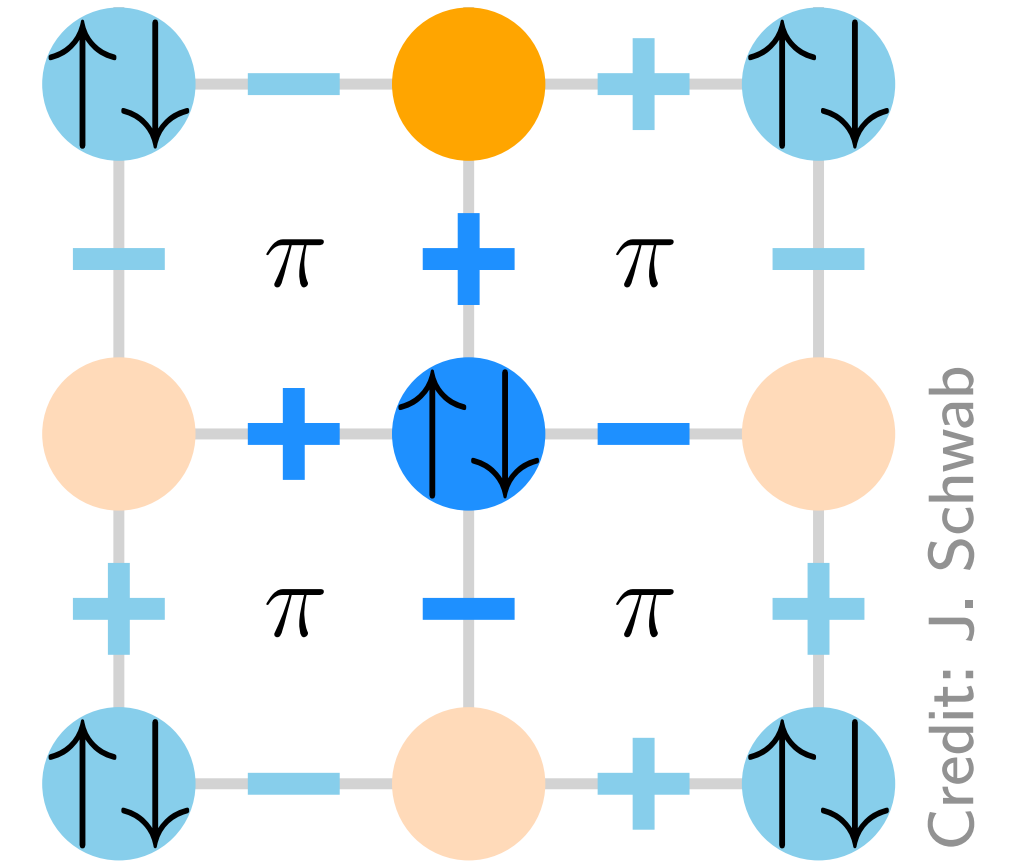


[Vojta, Zhang, Sachdev, PRL '00]

Counterexample: Emergent Anisotropy

Hamiltonian:

$$\mathcal{H} = - \sum_{\langle ij \rangle} (t_{ij} + \xi_{ij} S_i^z) c_i^\dagger c_j + \text{h.c.} \\ - J \sum_{\langle\langle i, i' \rangle\rangle} S_i^z S_{i'}^z - h \sum_{i \in A} S_i^x$$

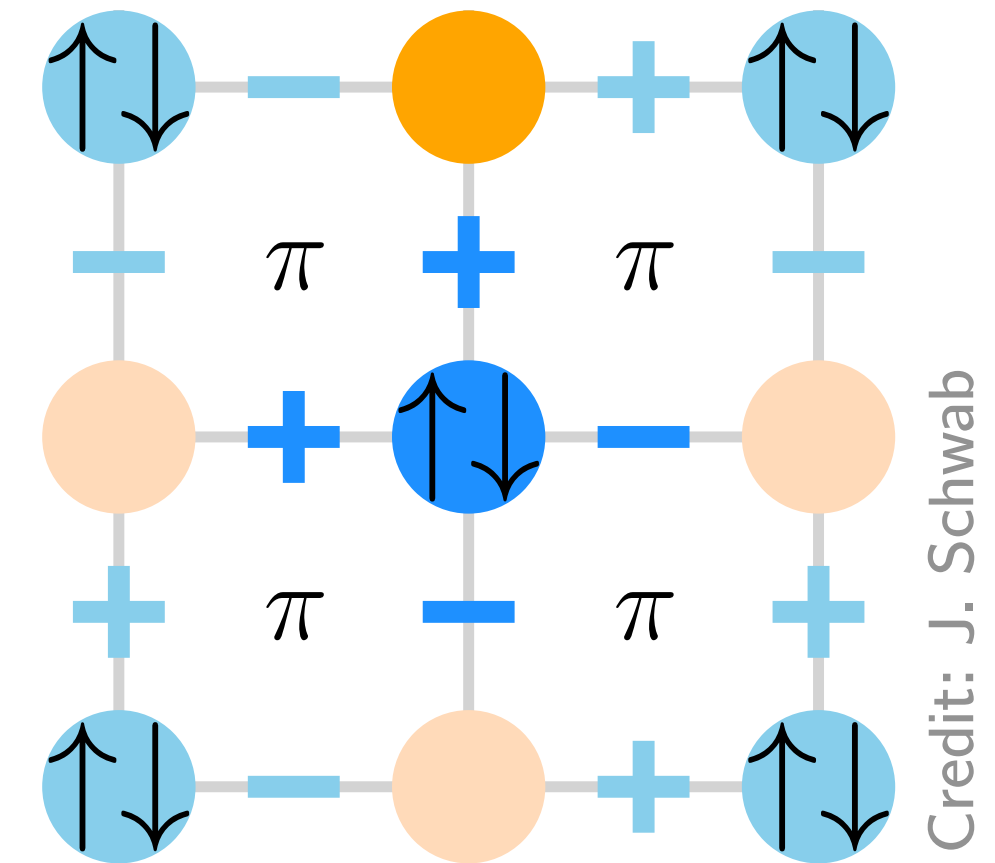


Credit: J. Schwab

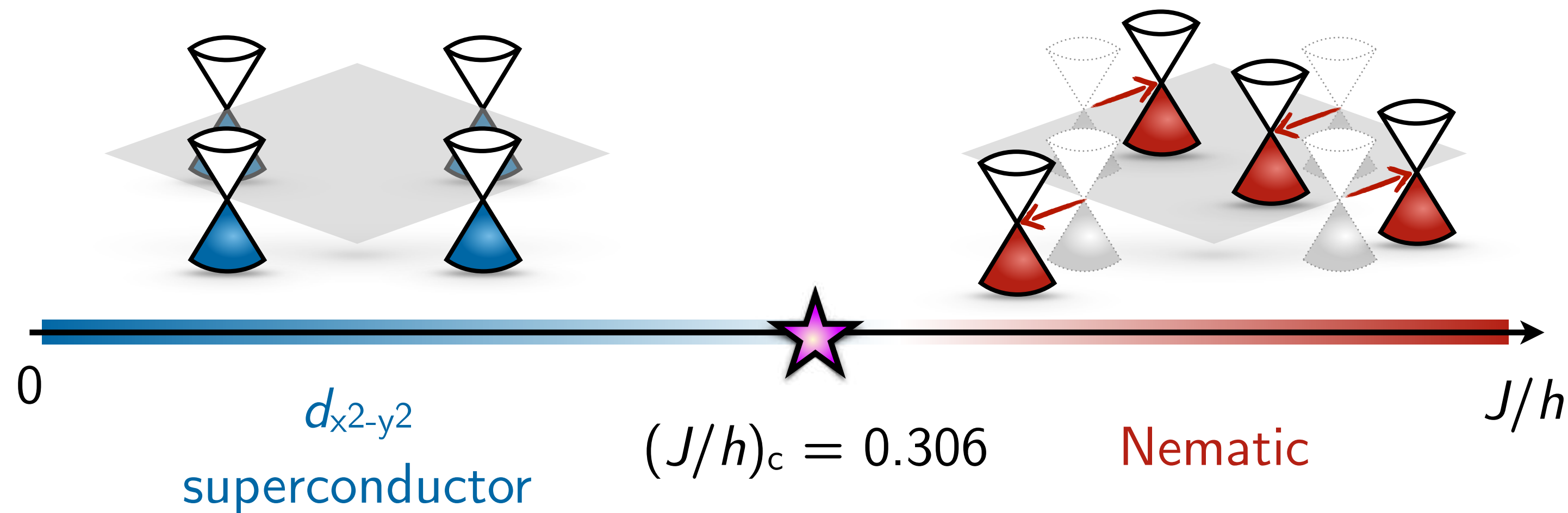
Counterexample: Emergent Anisotropy

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$$\mathcal{H} = - \sum_{\langle ij \rangle} (t_{ij} + \xi_{ij} S_i^z) c_i^\dagger c_j + \text{h.c.} \\ - J \sum_{\langle\langle i, i' \rangle\rangle} S_i^z S_{i'}^z - h \sum_{i \in A} S_i^x$$



Phase diagram:

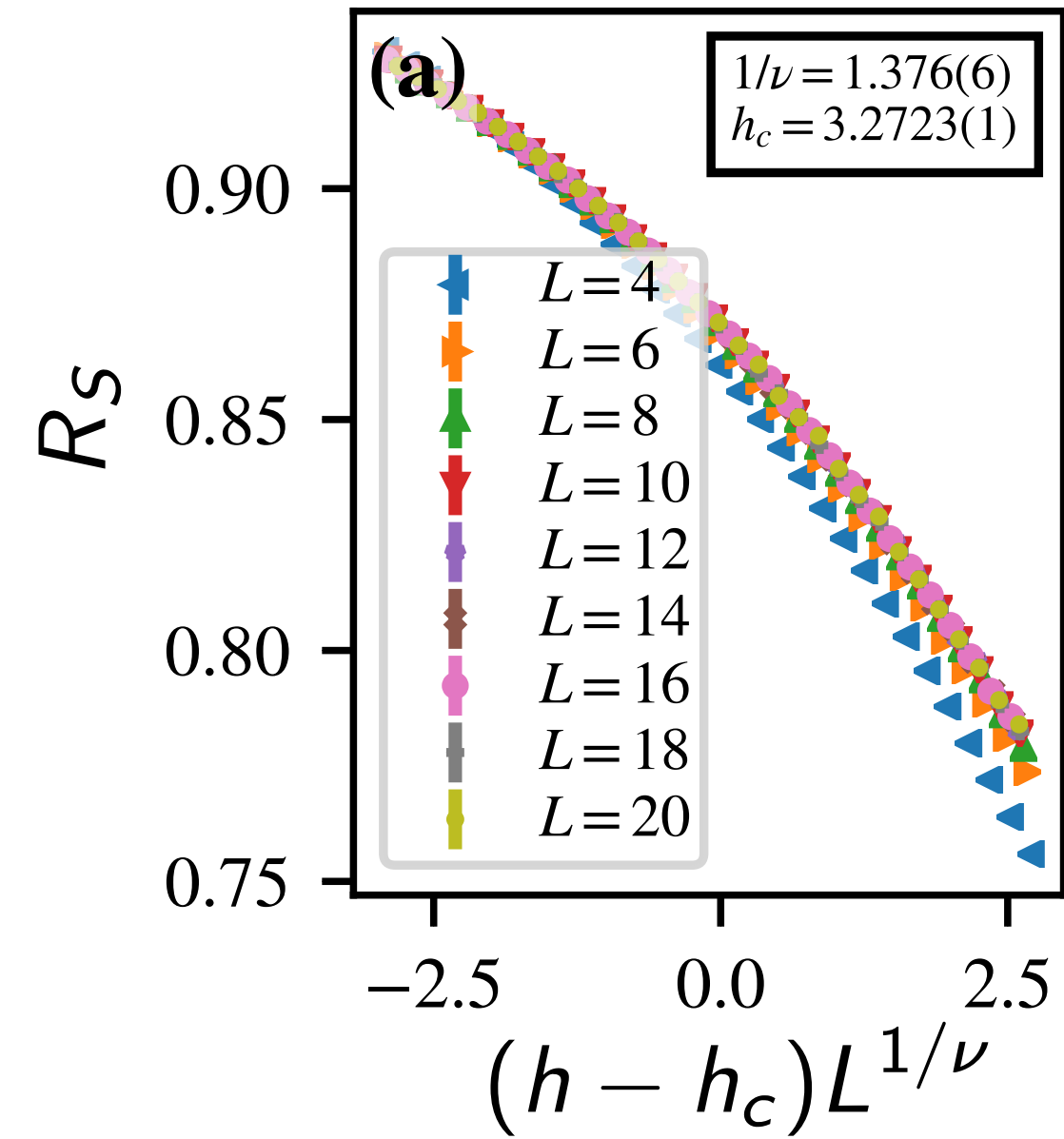


[Schwab, LJ, Sun, Meng, *et int.*, Assaad, PRL '22]

Counterexample: Emergent Anisotropy

Correlation ratio:

$$R_S = 1 - \frac{S(\Gamma + d\vec{k})}{S(\Gamma)}$$



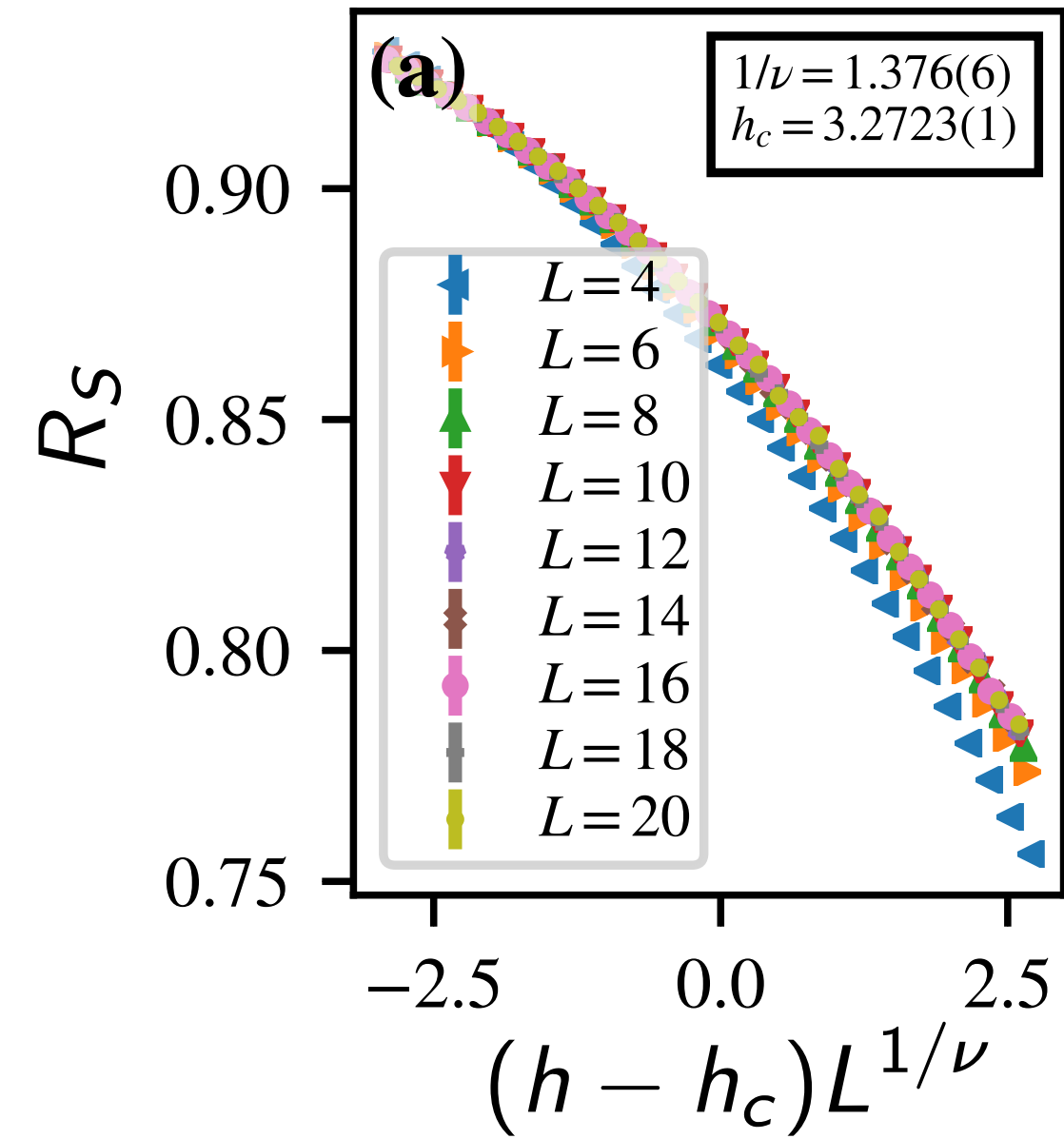
Algorithms
Lattice
Fermions

Continuous transition ...

Counterexample: Emergent Anisotropy

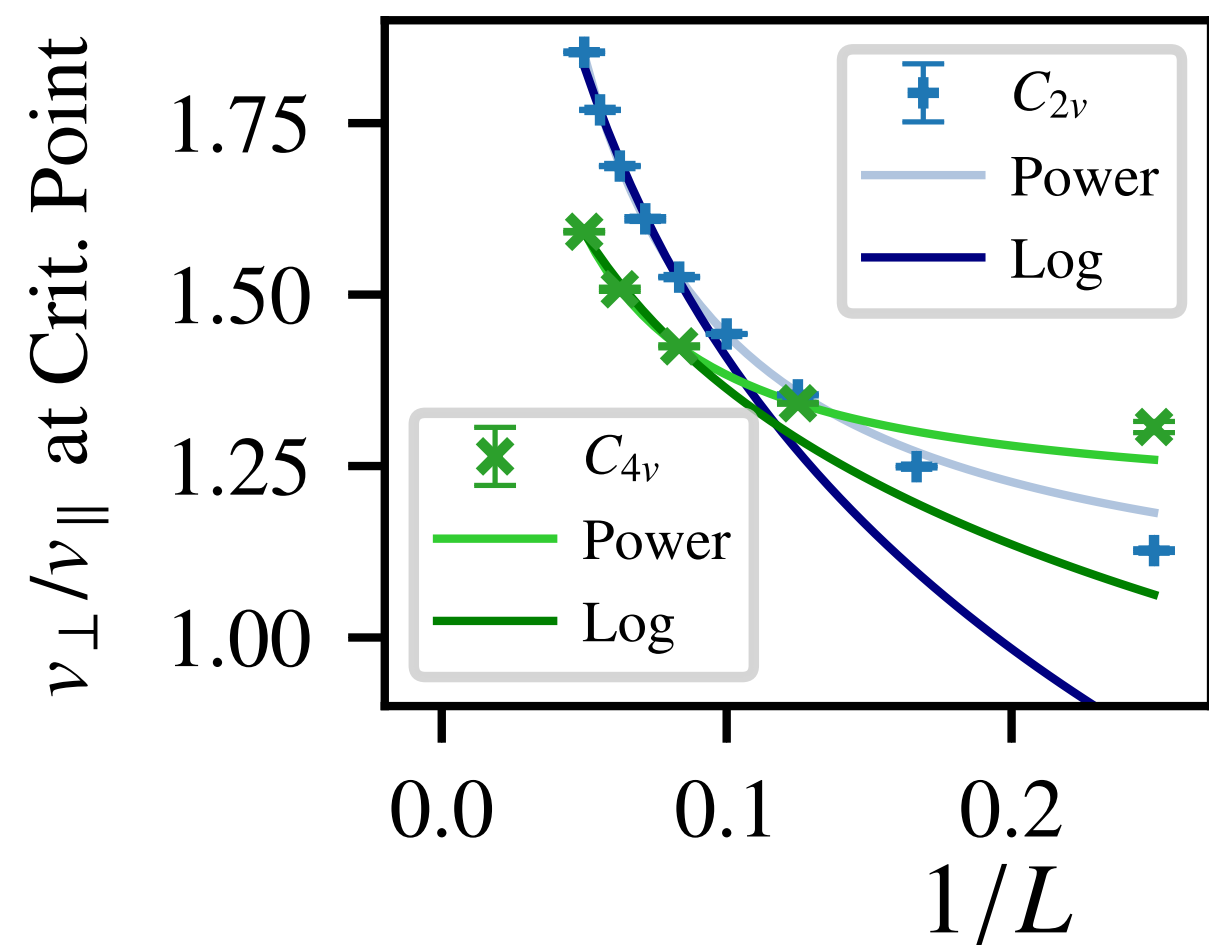
Correlation ratio:

$$R_S = 1 - \frac{S(\Gamma + d\vec{k})}{S(\Gamma)}$$

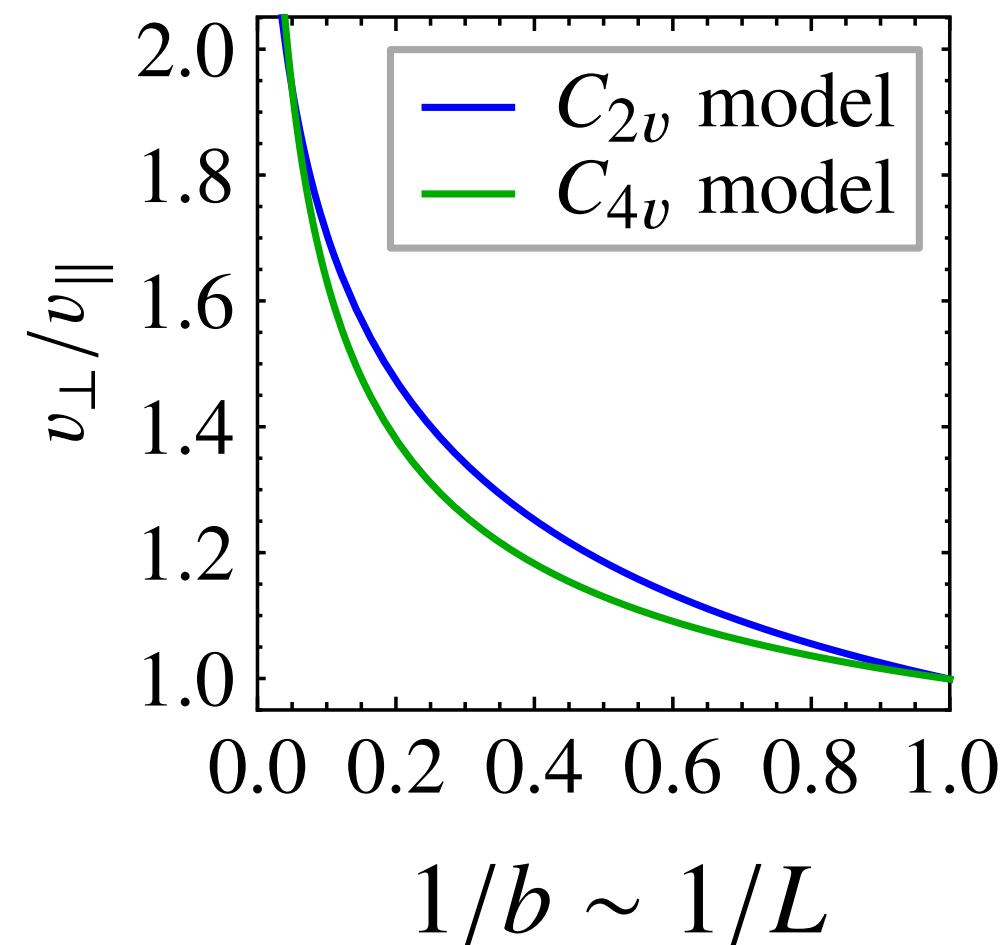


Continuous transition ...
... with emergent **anisotropy**!

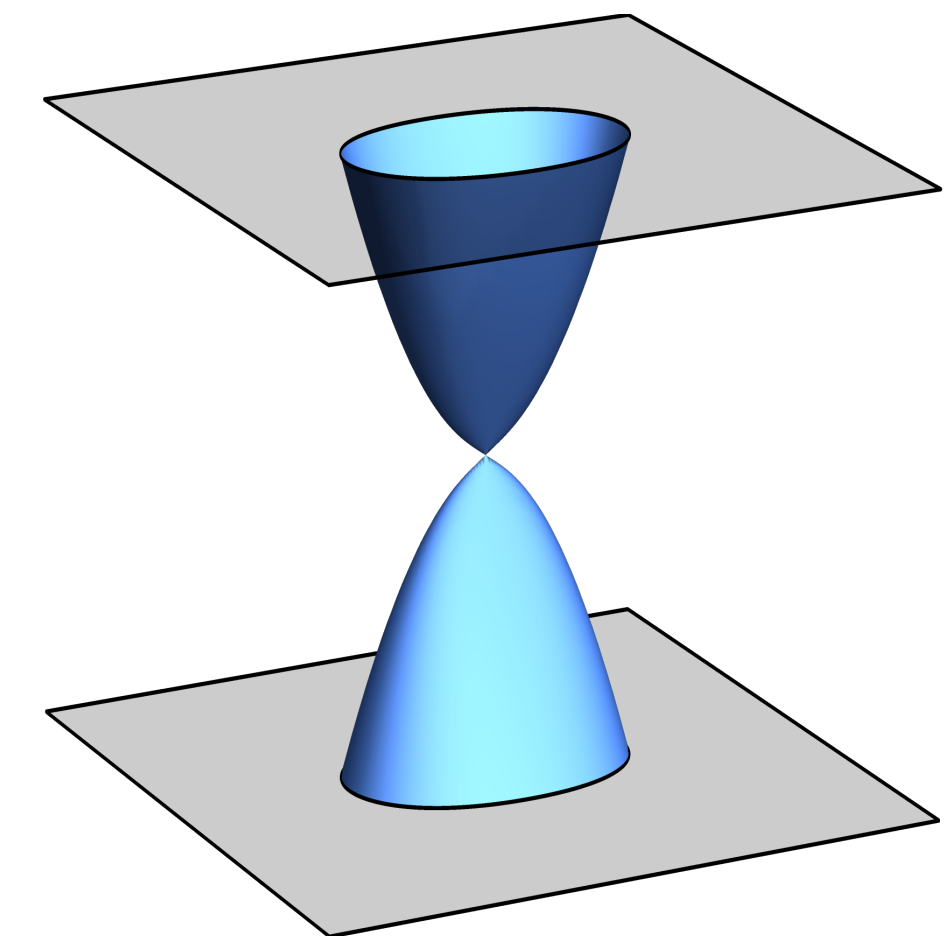
Velocity flow:



Quantum Monte Carlo



ϵ expansion

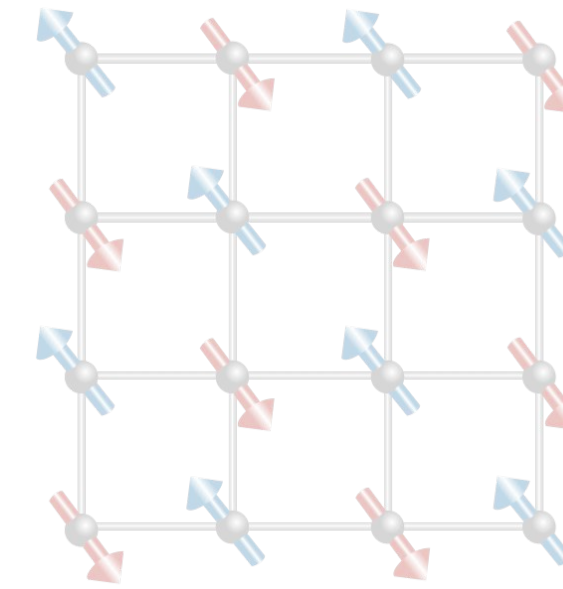


[Schwab, LJ, Sun, Meng, *et int.*, Assaad, PRL '22]

Outline

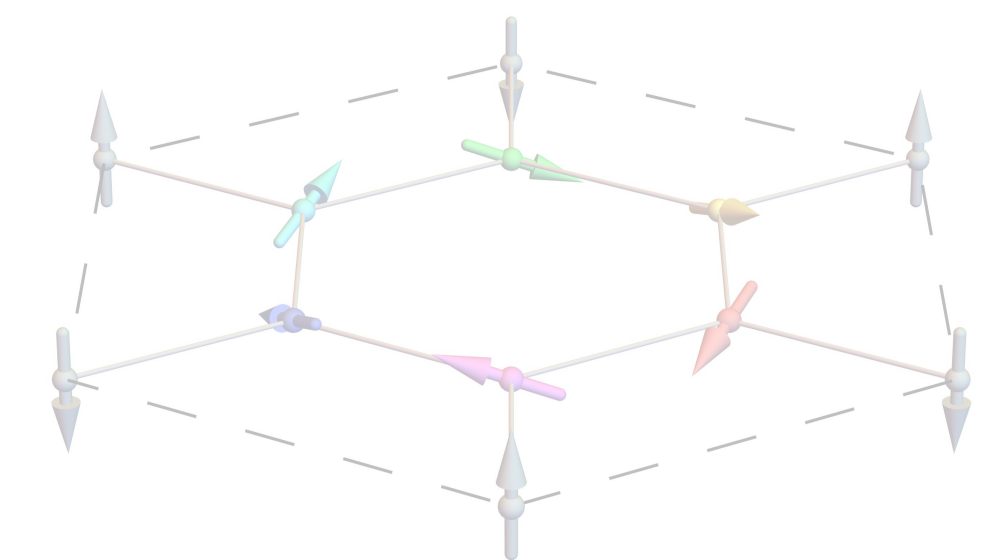
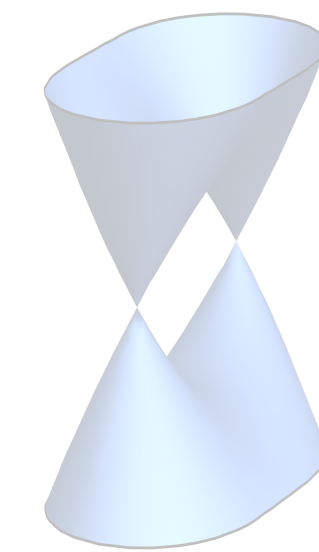
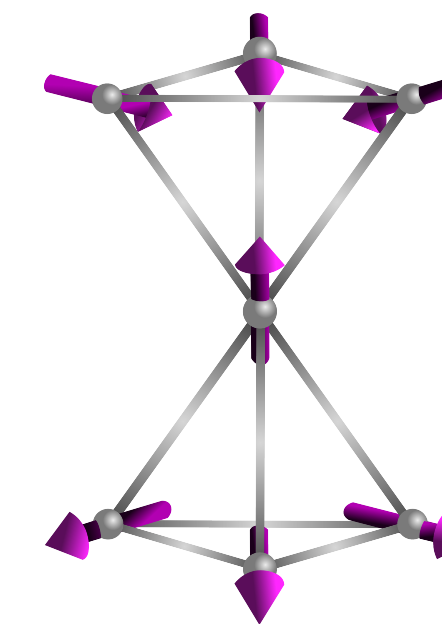
(1) Introduction

- ▶ Research Motivation
- ▶ Research Goals

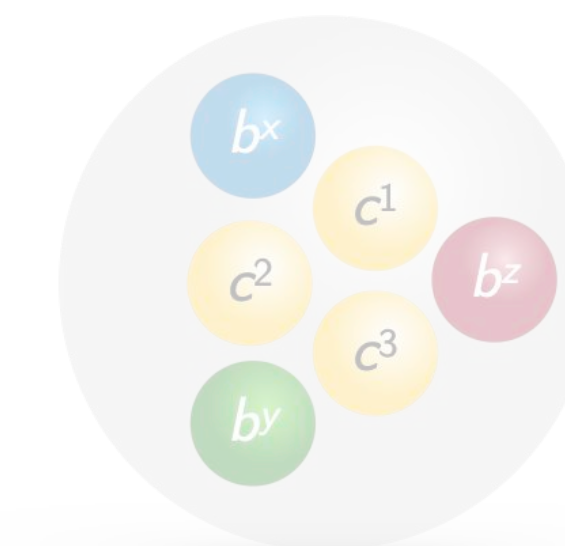


(2) Emergent Phenomena in Quantum Materials

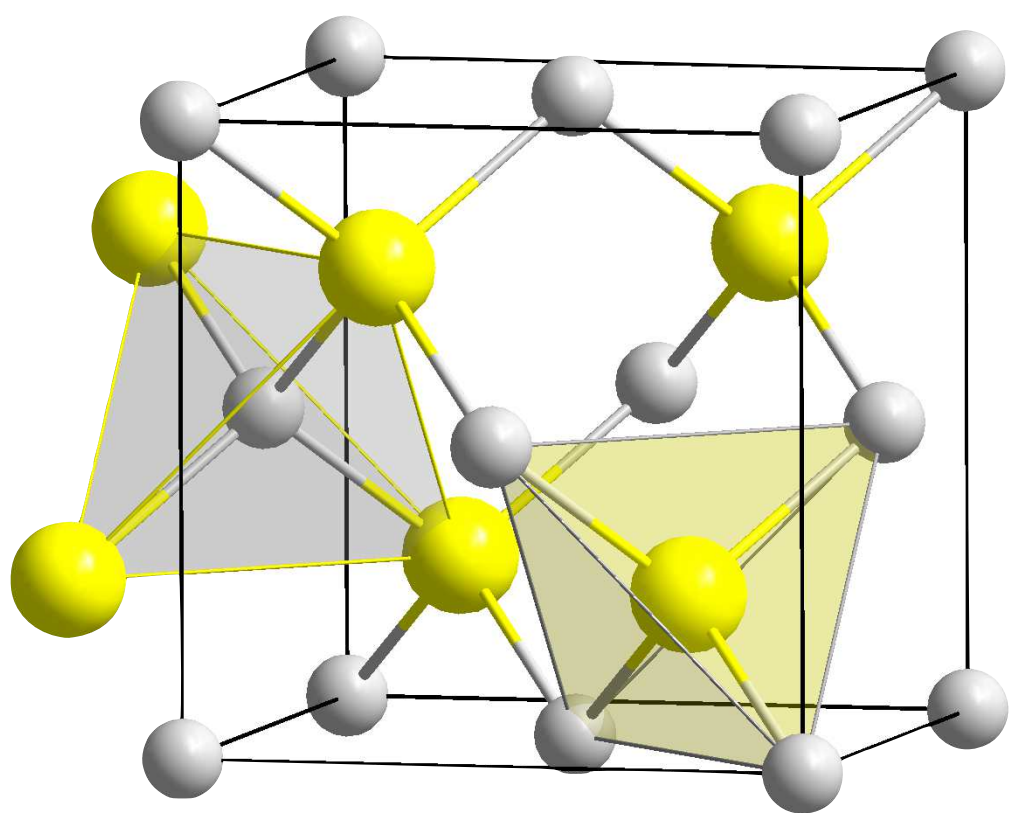
- ▶ Emergent Symmetries
- ▶ **Emergent Topology**
- ▶ Emergent Orders
- ▶ Emergent Particles



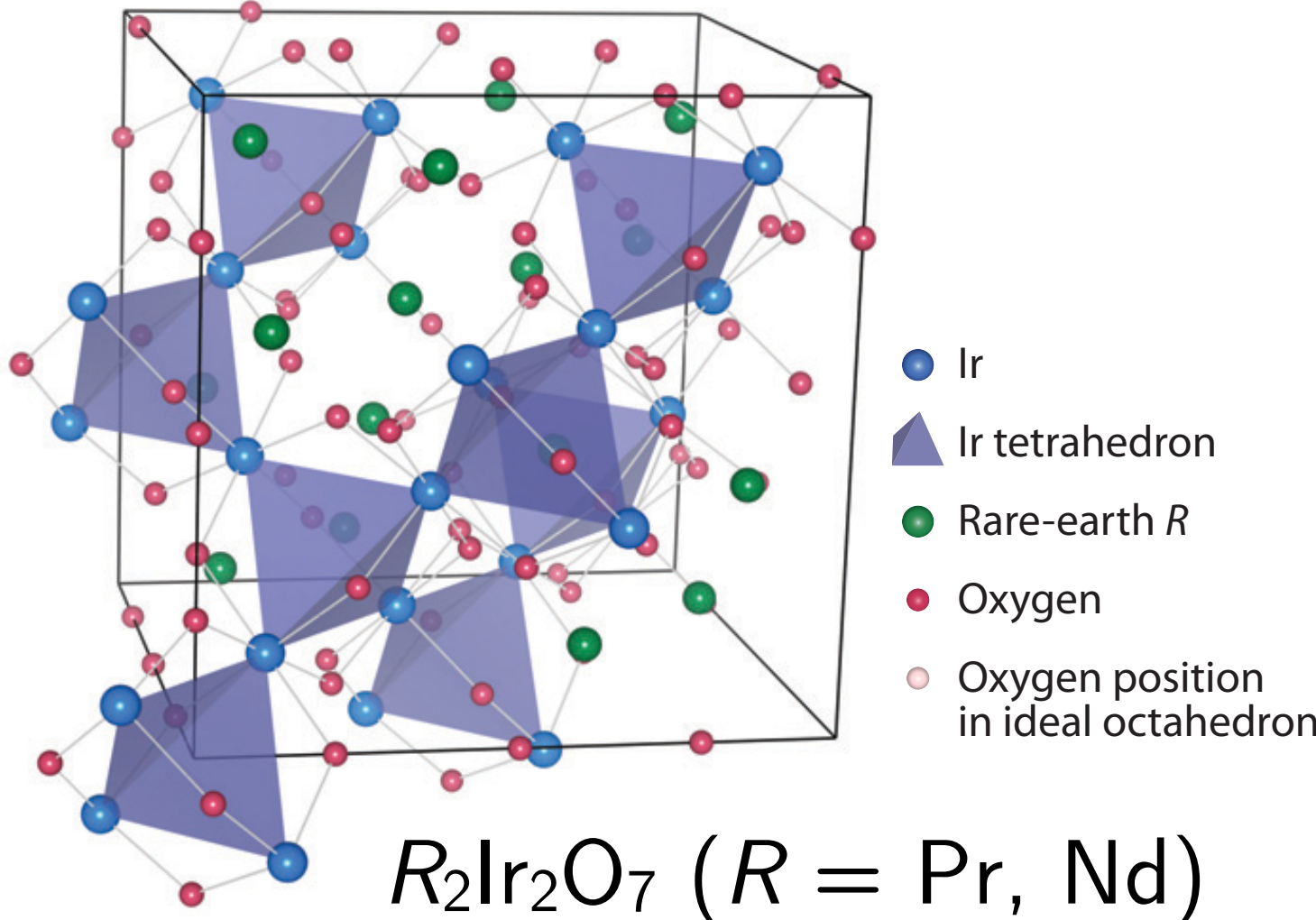
(3) Summary



Example #2: Luttinger Semimetals

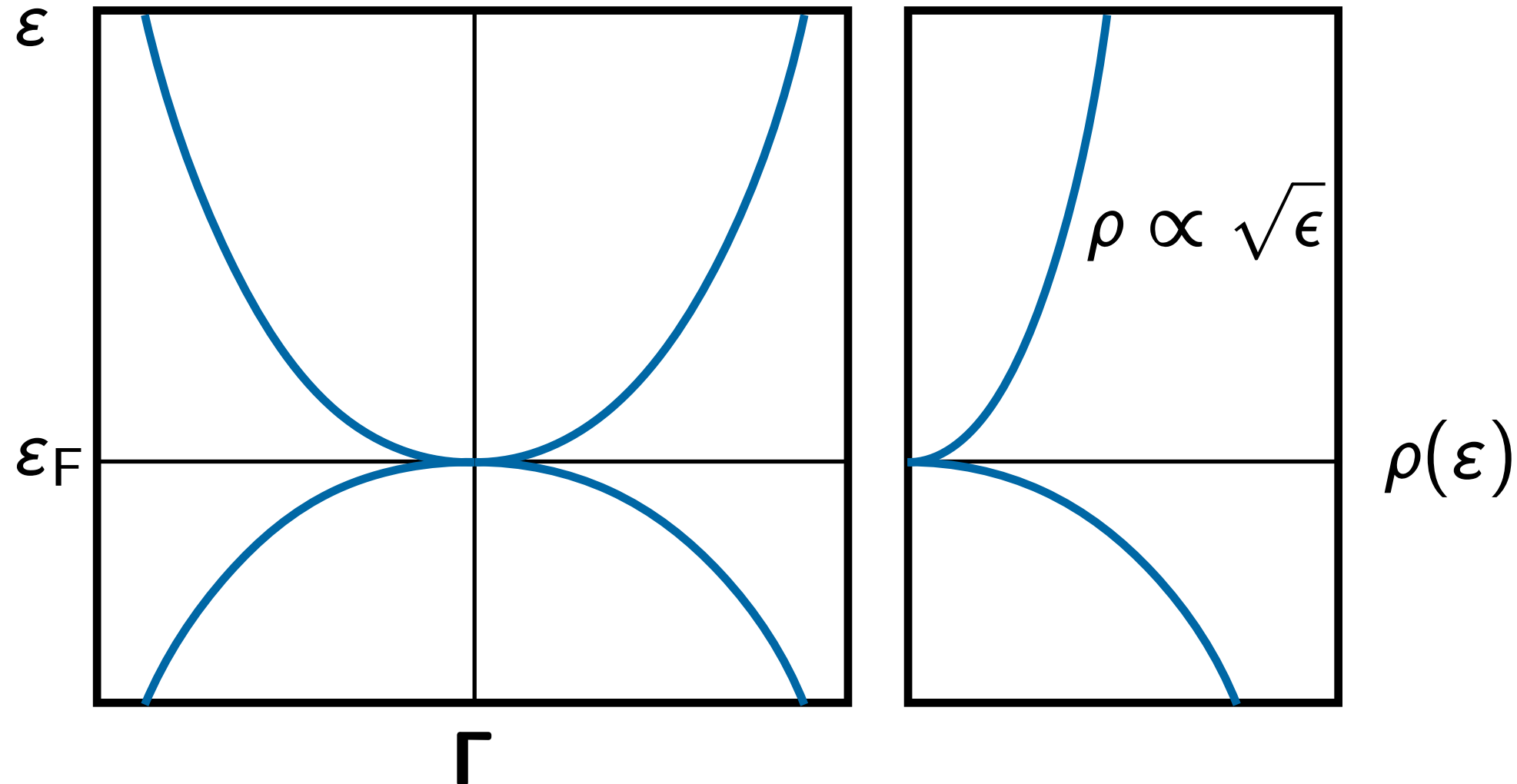


α -Sn, HgTe



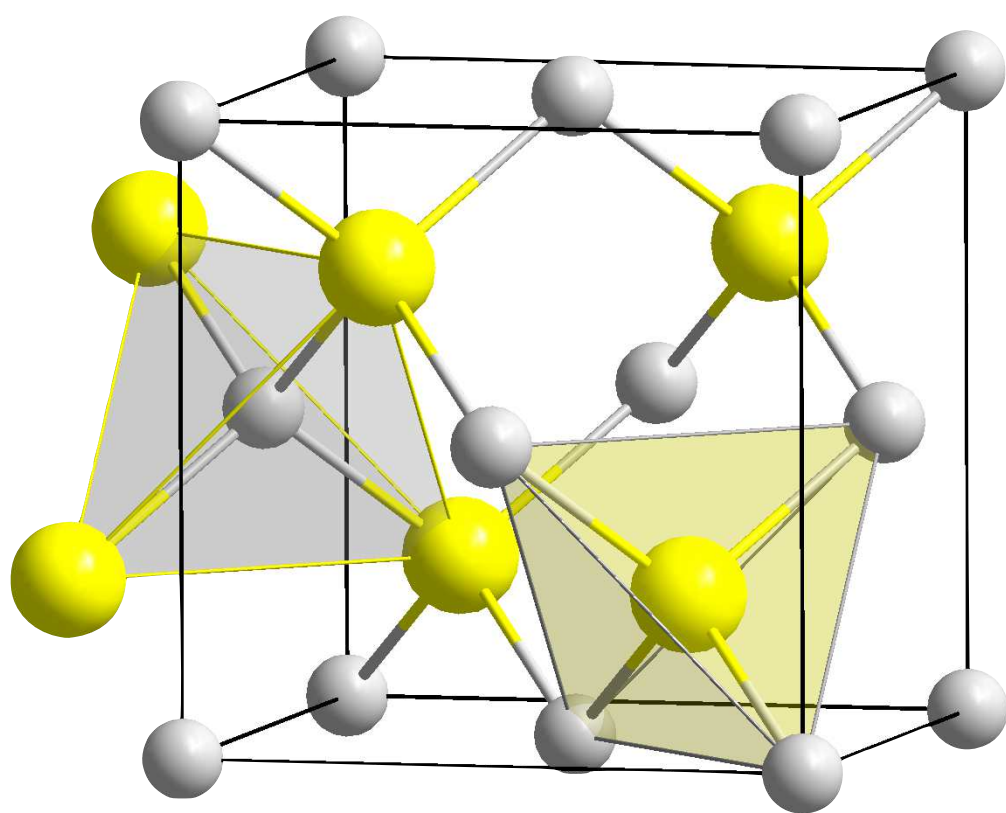
$R_2\text{Ir}_2\text{O}_7$ ($R = \text{Pr}, \text{Nd}$)

[Kondo *et al.*, Nat. Comm. '15]
 [Wang *et al.*, Nat. Phys. '20]

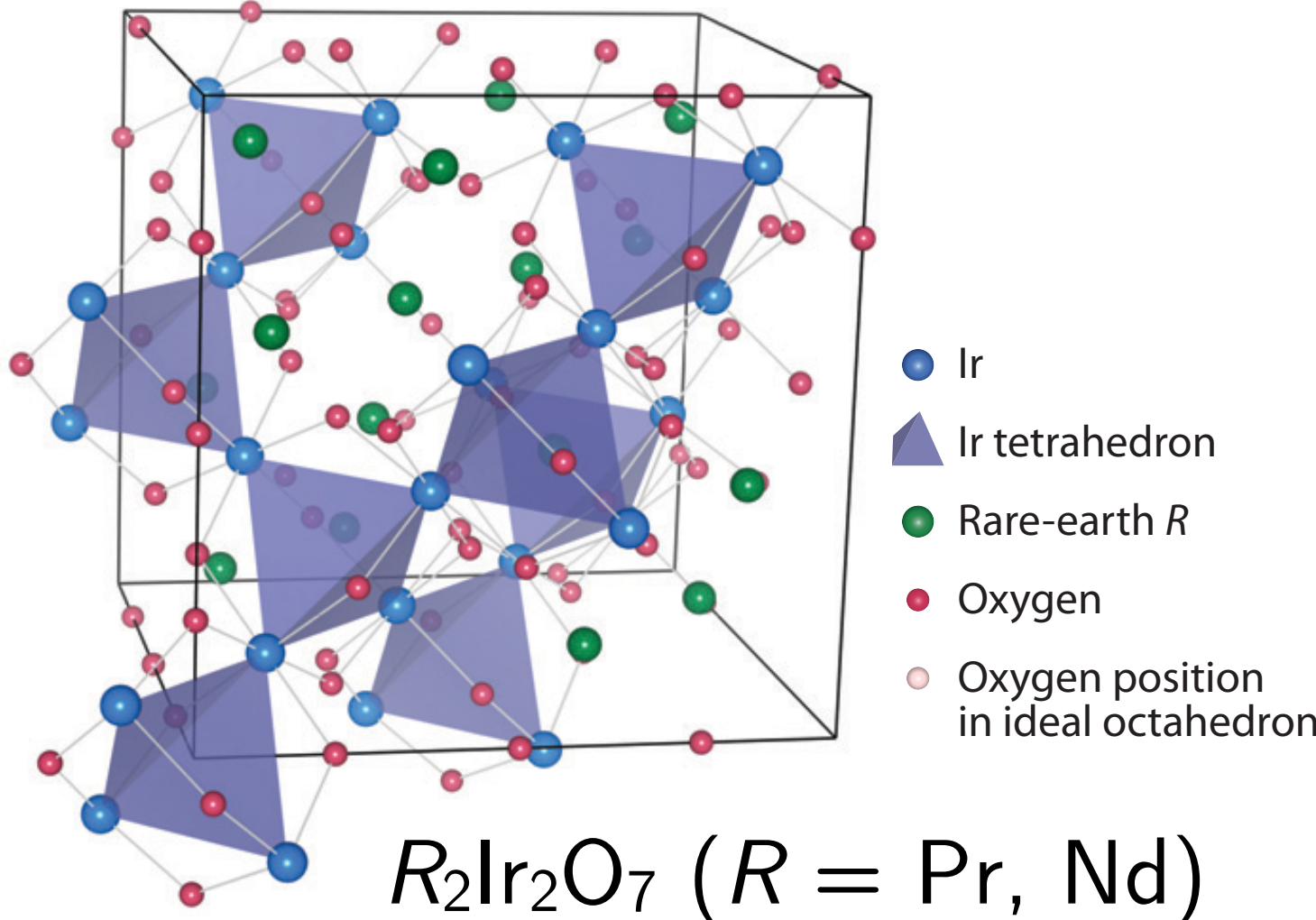


[Witczak-Krempa *et al.*, ARCMP '14]
 [Armitage, Mele, Vishwanath, RMP '18]

Example #2: Luttinger Semimetals

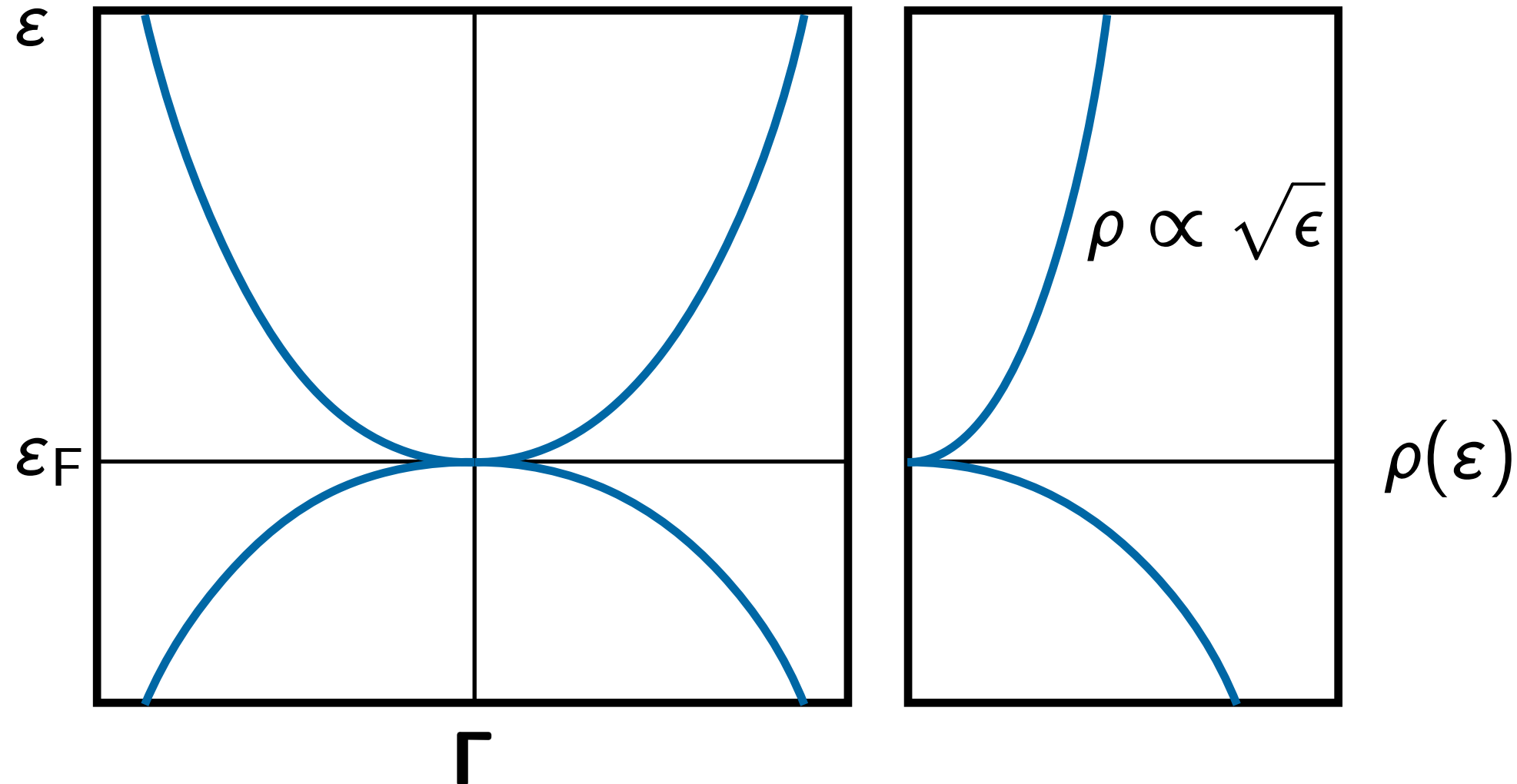


α -Sn, HgTe



$R_2Ir_2O_7$ ($R = Pr, Nd$)

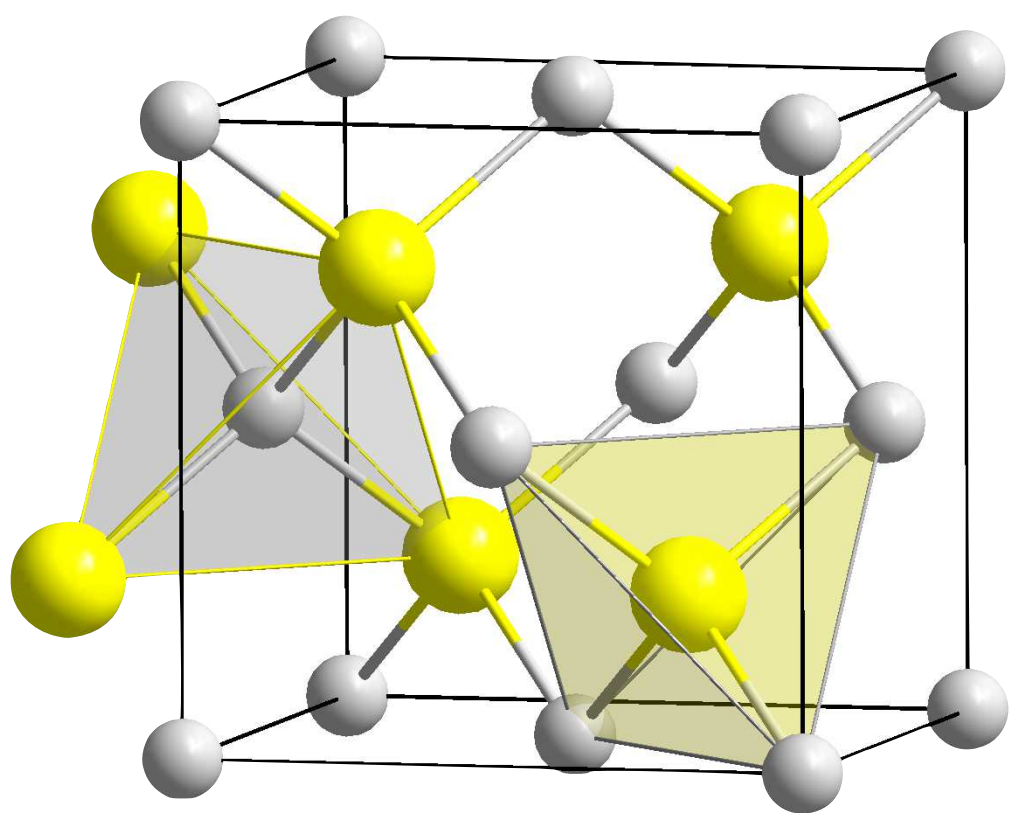
[Kondo *et al.*, Nat. Comm. '15]
 [Wang *et al.*, Nat. Phys. '20]



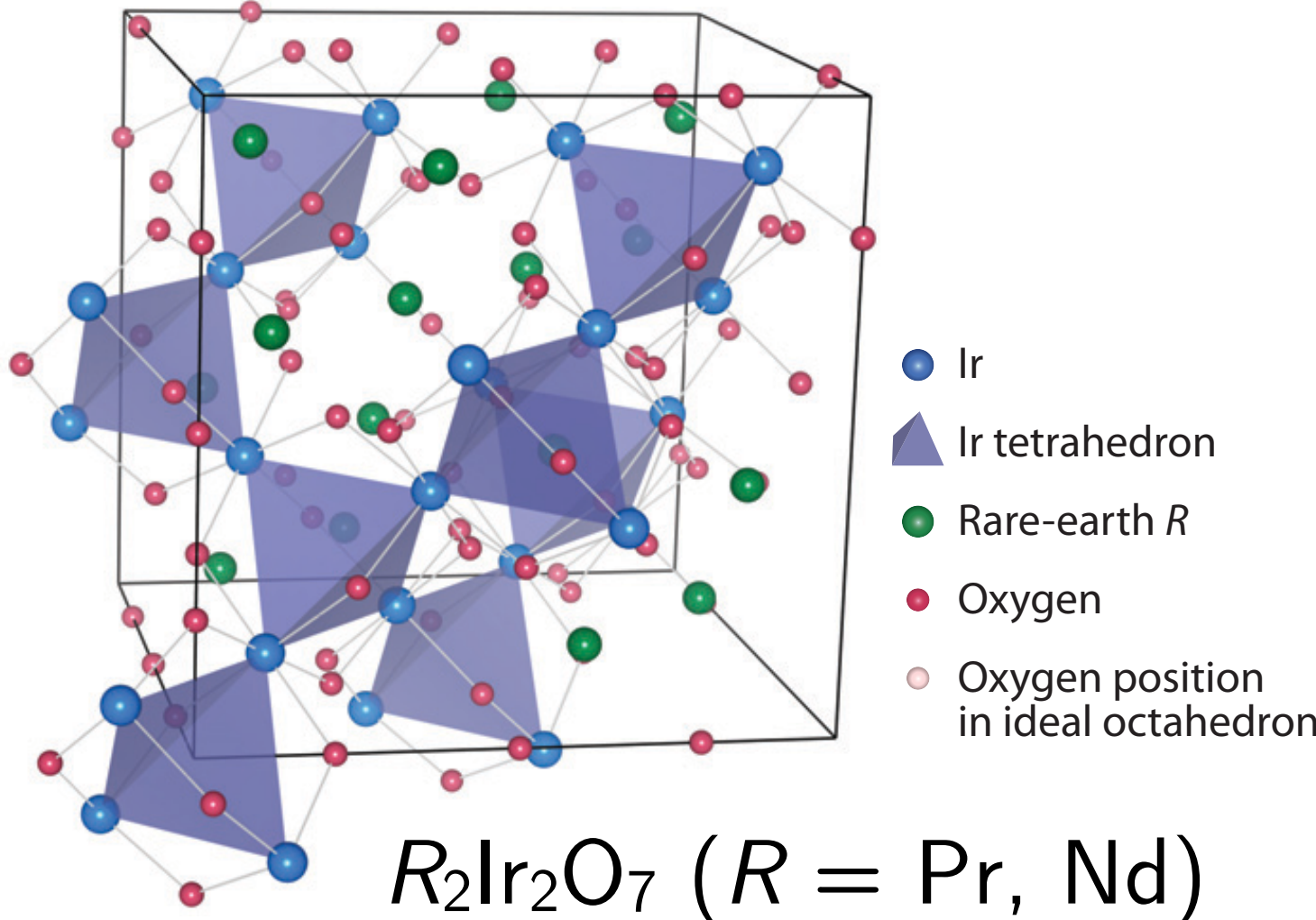
[Witczak-Krempa *et al.*, ARCMP '14]
 [Armitage, Mele, Vishwanath, RMP '18]

Short-range interactions: Irrelevant

Example #2: Luttinger Semimetals

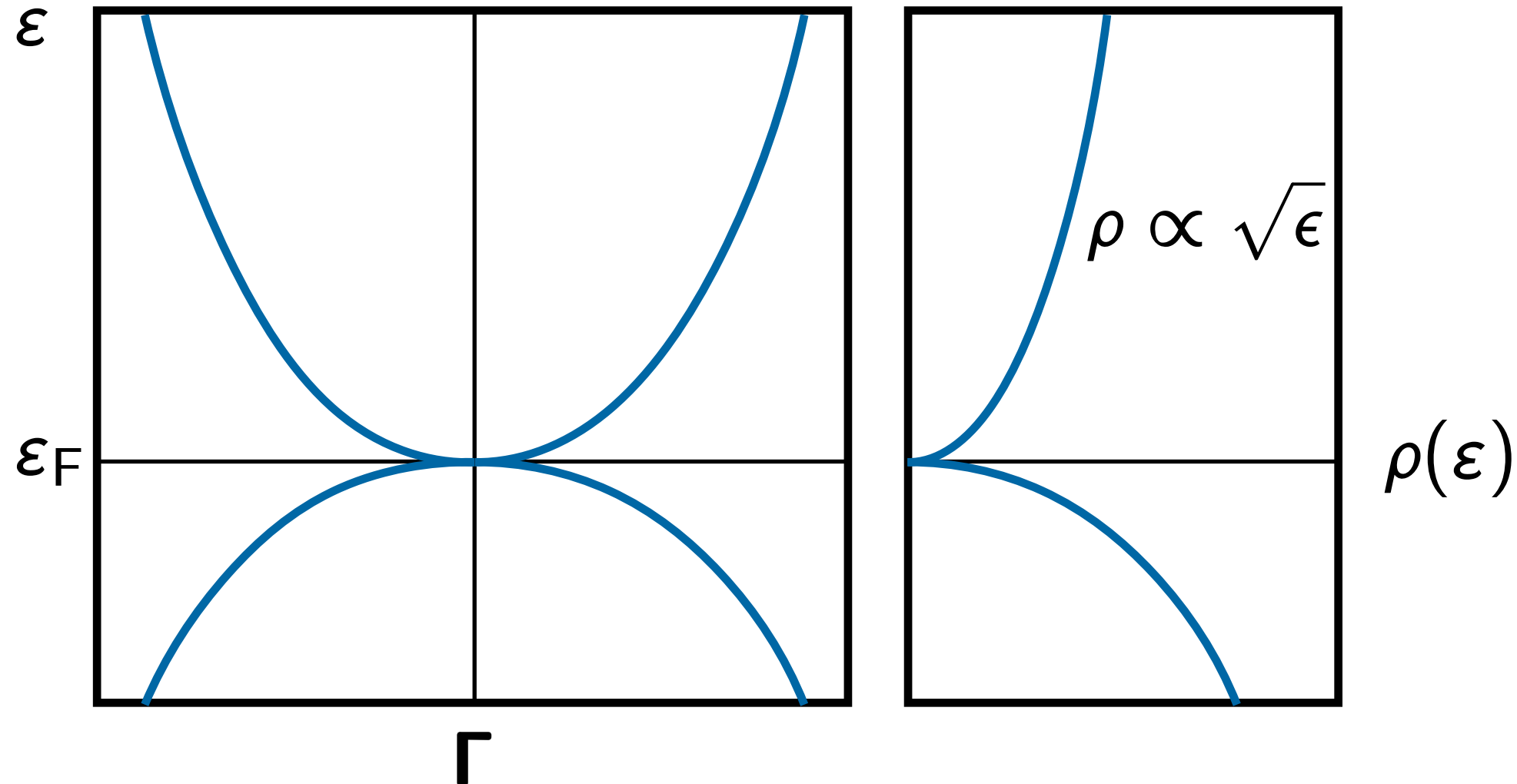


α -Sn, HgTe



$R_2Ir_2O_7$ ($R = Pr, Nd$)

[Kondo *et al.*, Nat. Comm. '15]
[Wang *et al.*, Nat. Phys. '20]



[Witczak-Krempa *et al.*, ARCMP '14]
[Armitage, Mele, Vishwanath, RMP '18]

Short-range interactions: Irrelevant

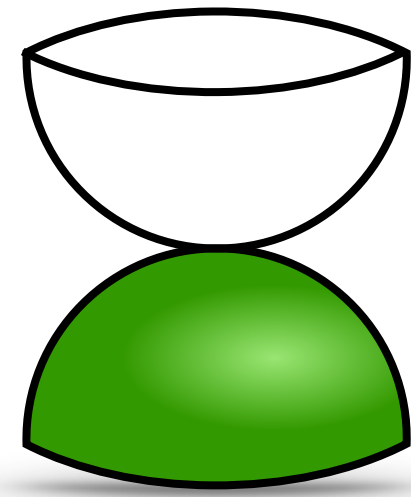
Coulomb interaction: $V_0(r) \propto \frac{1}{r} \rightarrow V_{\text{eff}} \propto \frac{1}{r^z}, \quad z \approx 1.8$

[Moon, Xu, Kim, Balents, PRL '13]

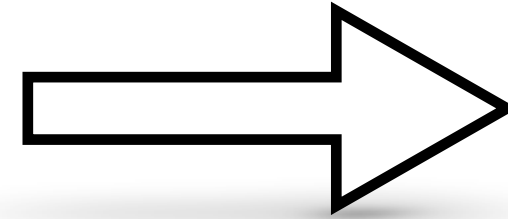
Emergent Topological Phases

Coulomb-driven
instability:

Semimetal

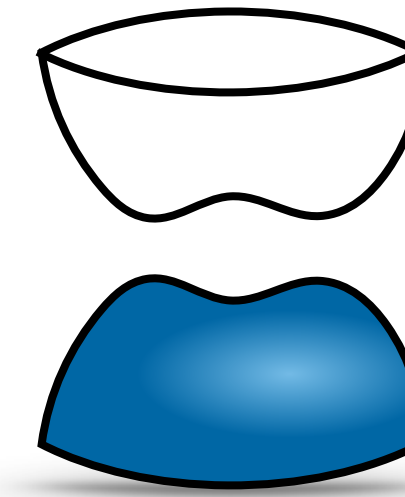


$R_2Ir_2O_7$



Cooling

Topological insulator



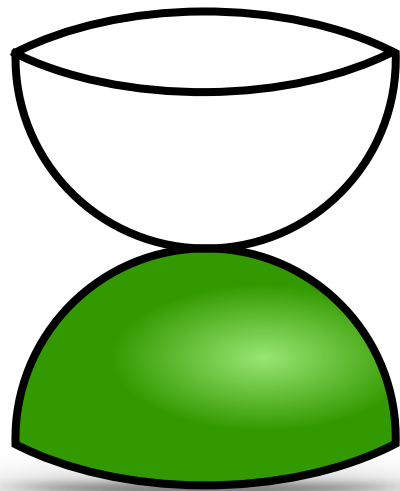
Cooled $R_2Ir_2O_7$

[Herbut & LJ, PRL '14]
[LJ & Herbut, PRB '17]

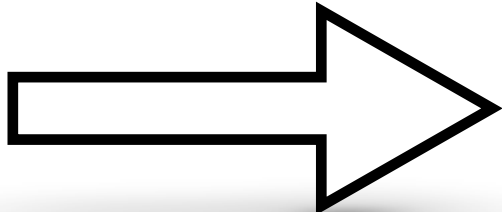
Emergent Topological Phases

Coulomb-driven instability:

Semimetal

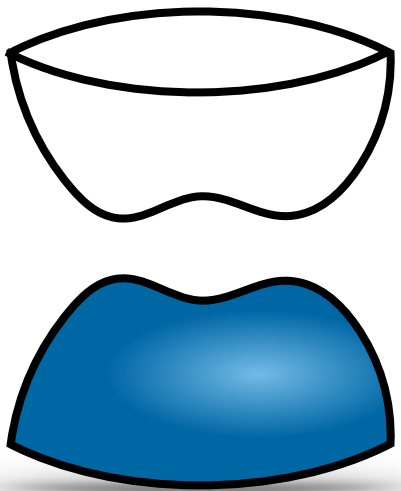


$R_2Ir_2O_7$



Cooling

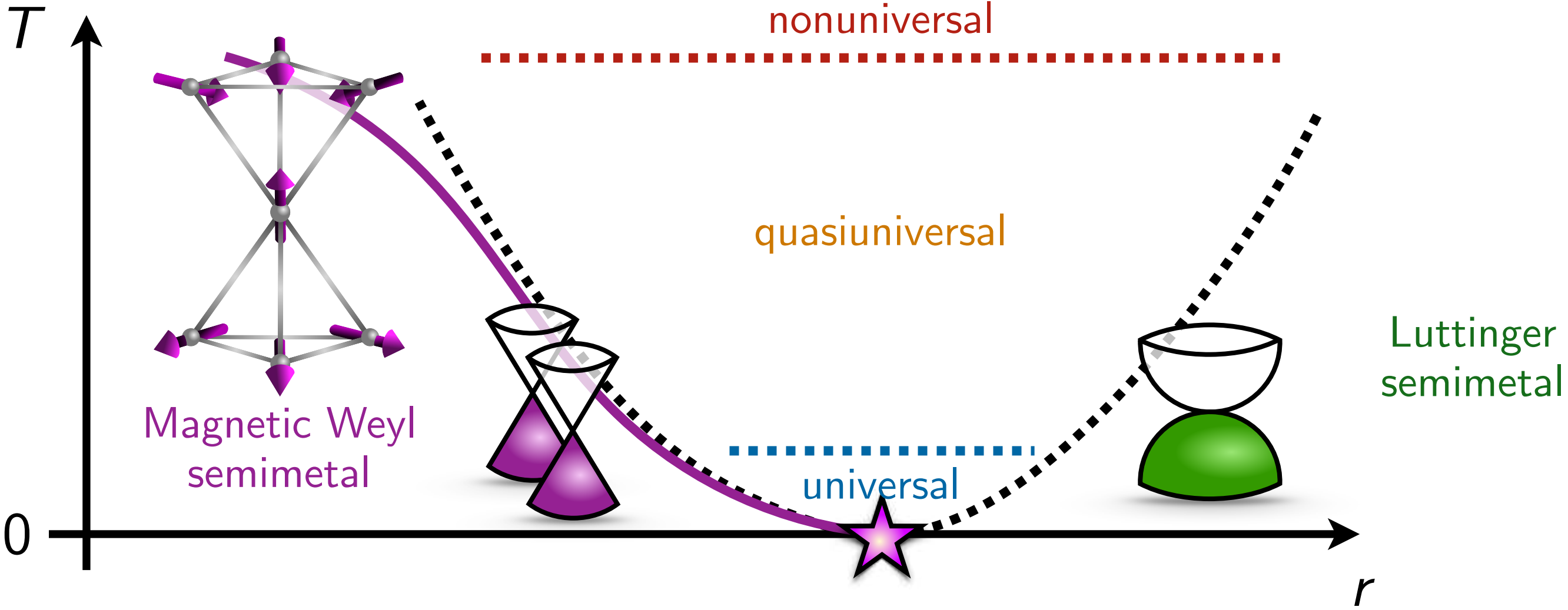
Topological insulator



Cooled $R_2Ir_2O_7$

[Herbut & LJ, PRL '14]
[LJ & Herbut, PRB '17]

Strong short-range interactions:



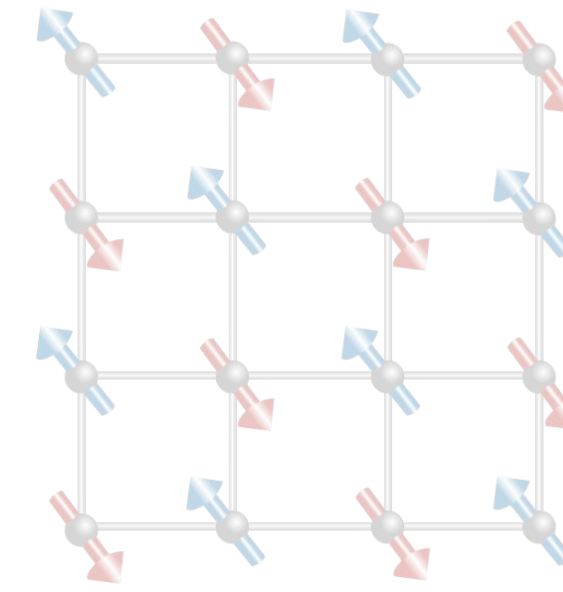
David Moser

[Moser & LJ, in preparation]
see also: [Boettcher & Herbut, PRB '17]

Outline

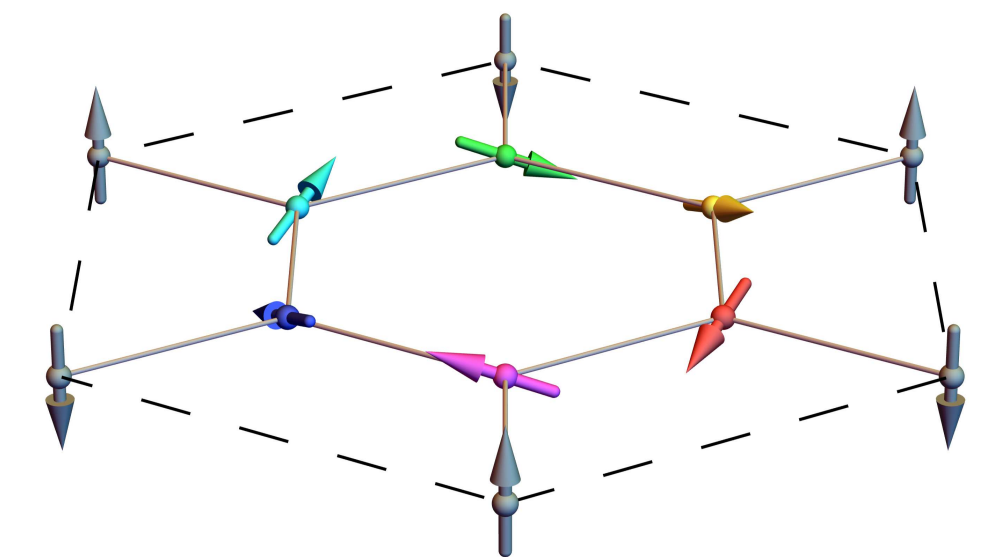
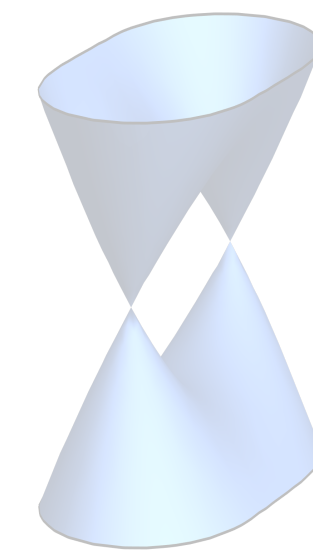
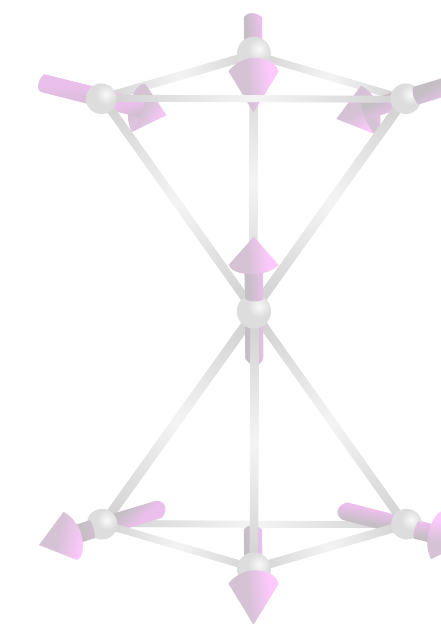
(1) Introduction

- ▶ Research Motivation
- ▶ Research Goals

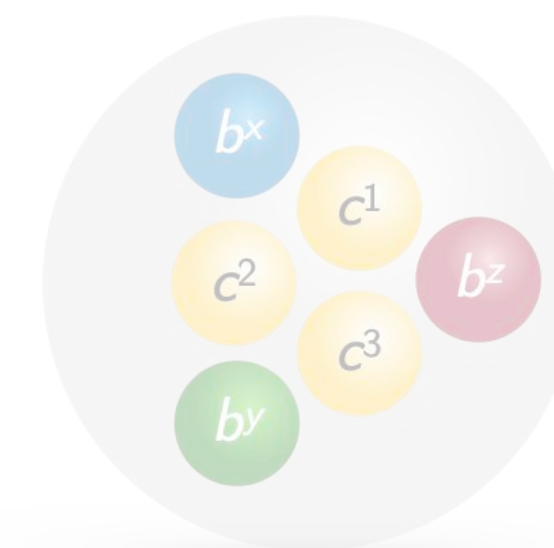


(2) Emergent Phenomena in Quantum Materials

- ▶ Emergent Symmetries
- ▶ Emergent Topology
- ▶ **Emergent Orders**
- ▶ Emergent Particles



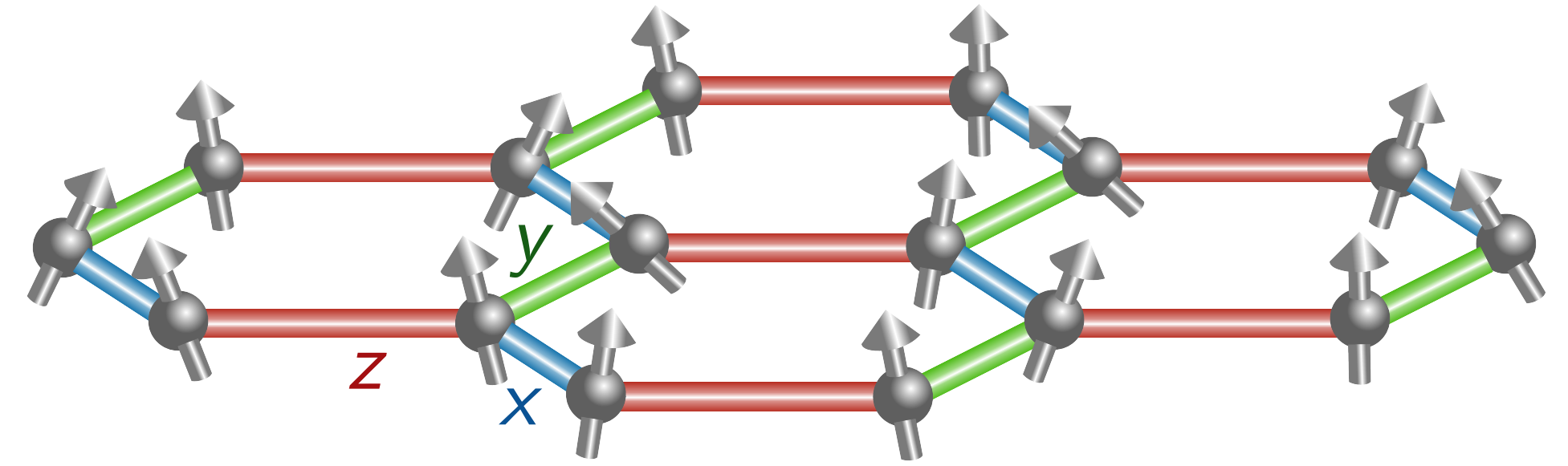
(3) Summary



Example #2: Kitaev magnets

Hamiltonian:

$$\mathcal{H} = K \left(\sum_{\langle ij \rangle_x} S_i^x S_j^x + \sum_{\langle ij \rangle_y} S_i^y S_j^y + \sum_{\langle ij \rangle_z} S_i^z S_j^z \right)$$



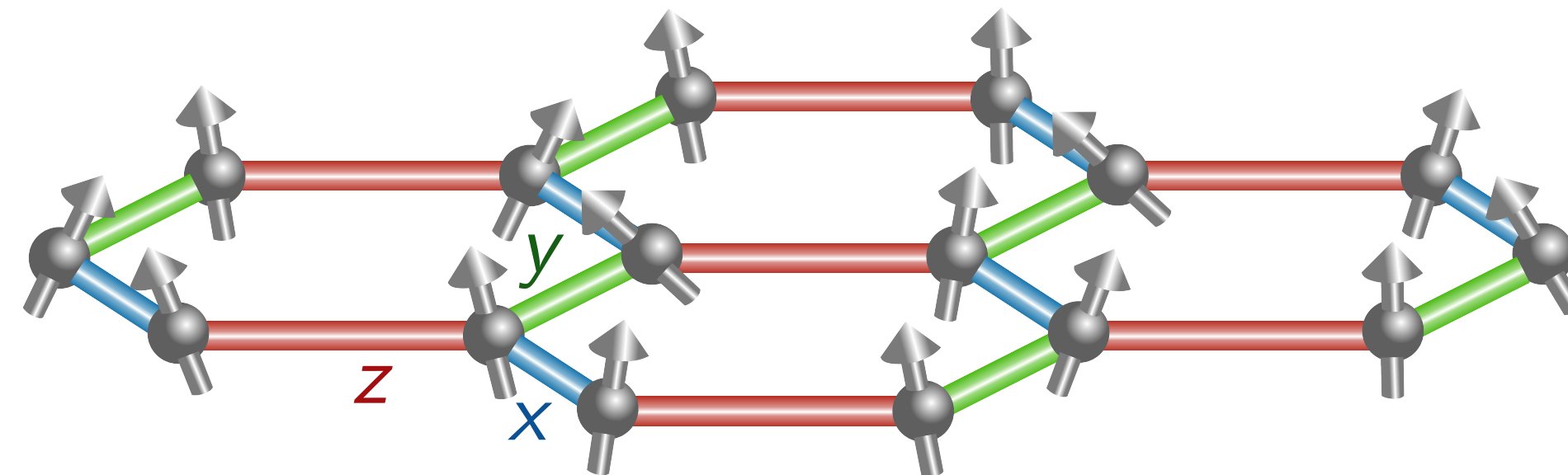
[Kitaev, Ann. Phys. '06]

Review: [LJ & Vojta, JPCM '19]

Example #2: Kitaev magnets

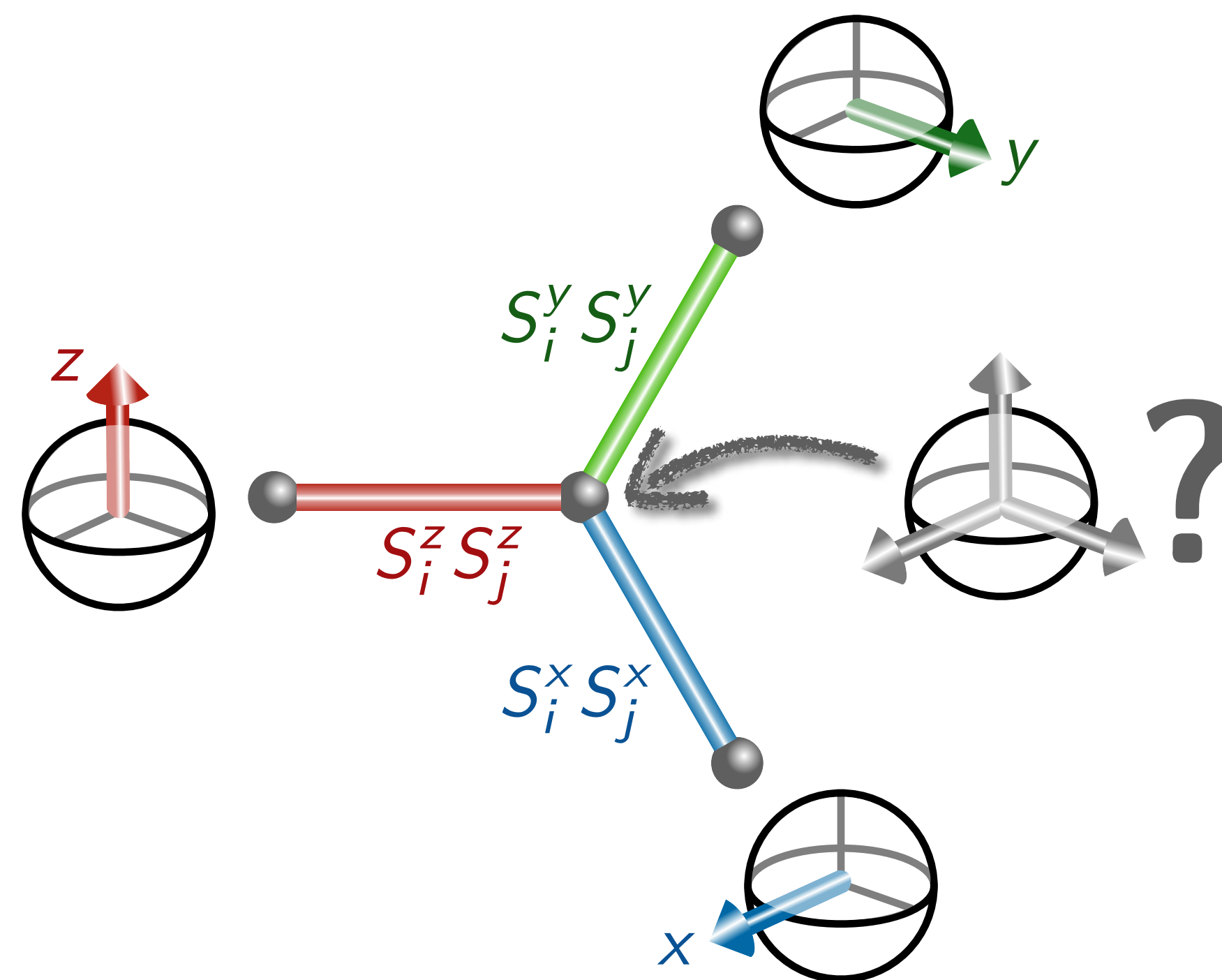
Hamiltonian:

$$\mathcal{H} = K \left(\sum_{\langle ij \rangle_x} S_i^x S_j^x + \sum_{\langle ij \rangle_y} S_i^y S_j^y + \sum_{\langle ij \rangle_z} S_i^z S_j^z \right)$$



[Kitaev, Ann. Phys. '06]

Frustration:



Review: [LJ & Vojta, JPCM '19]

Kitaev-Heisenberg Physics in Magnetic Fields

Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\alpha} S_i^\alpha S_j^\alpha + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i$$

$$J = A \cos \varphi$$
$$K = 2A \sin \varphi$$

Kitaev-Heisenberg Physics in Magnetic Fields

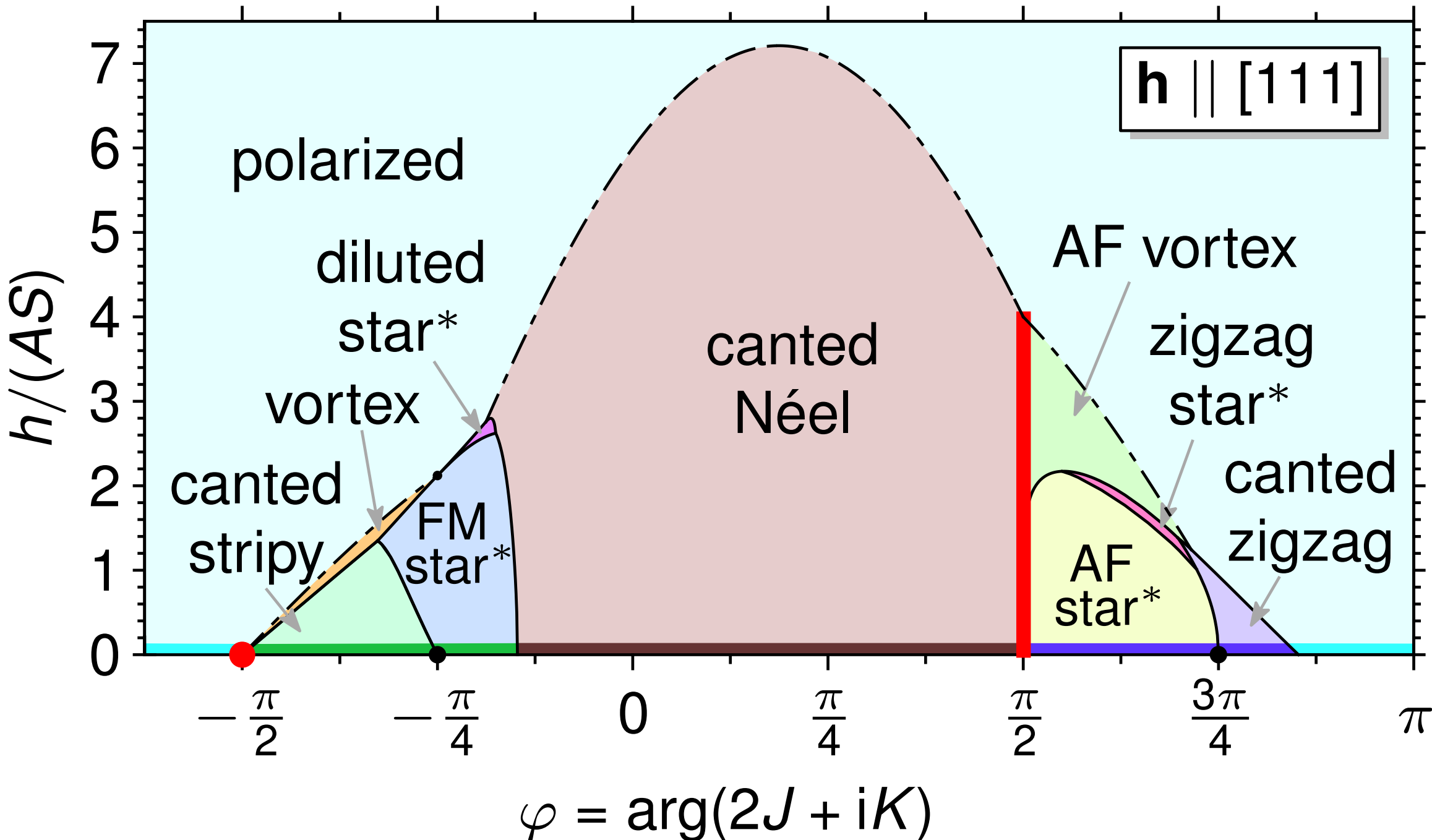
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$$\mathcal{H} = K \sum_{\langle ij \rangle_\alpha} S_i^\alpha S_j^\alpha + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i$$

$$J = A \cos \varphi$$

$$K = 2A \sin \varphi$$

Phase diagram:



[LJ, Andrade, Vojta, PRL '16]

[Cônsoi, LJ, Vojta, Andrade, PRB '20]

Kitaev-Heisenberg Physics in Magnetic Fields

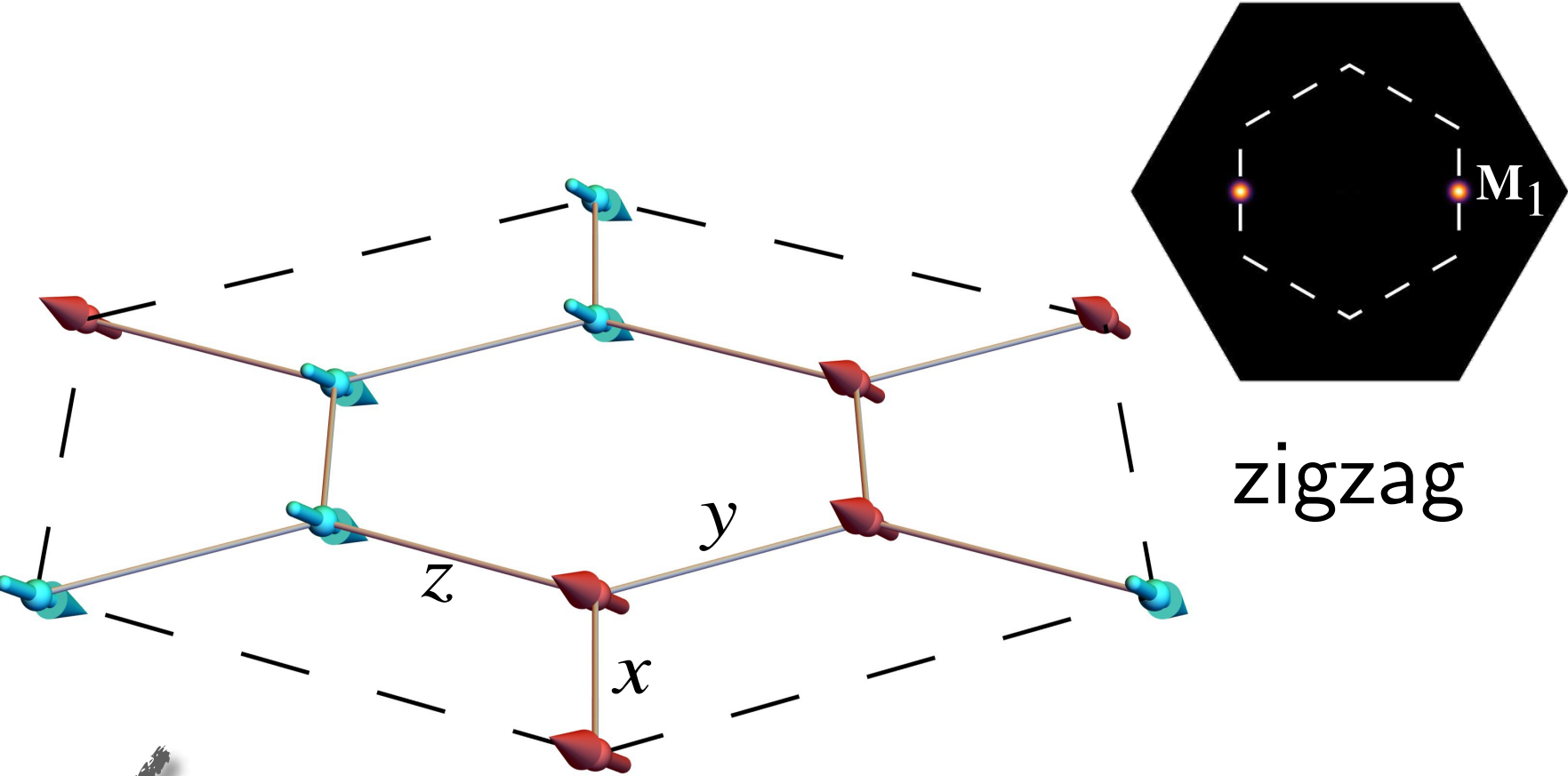
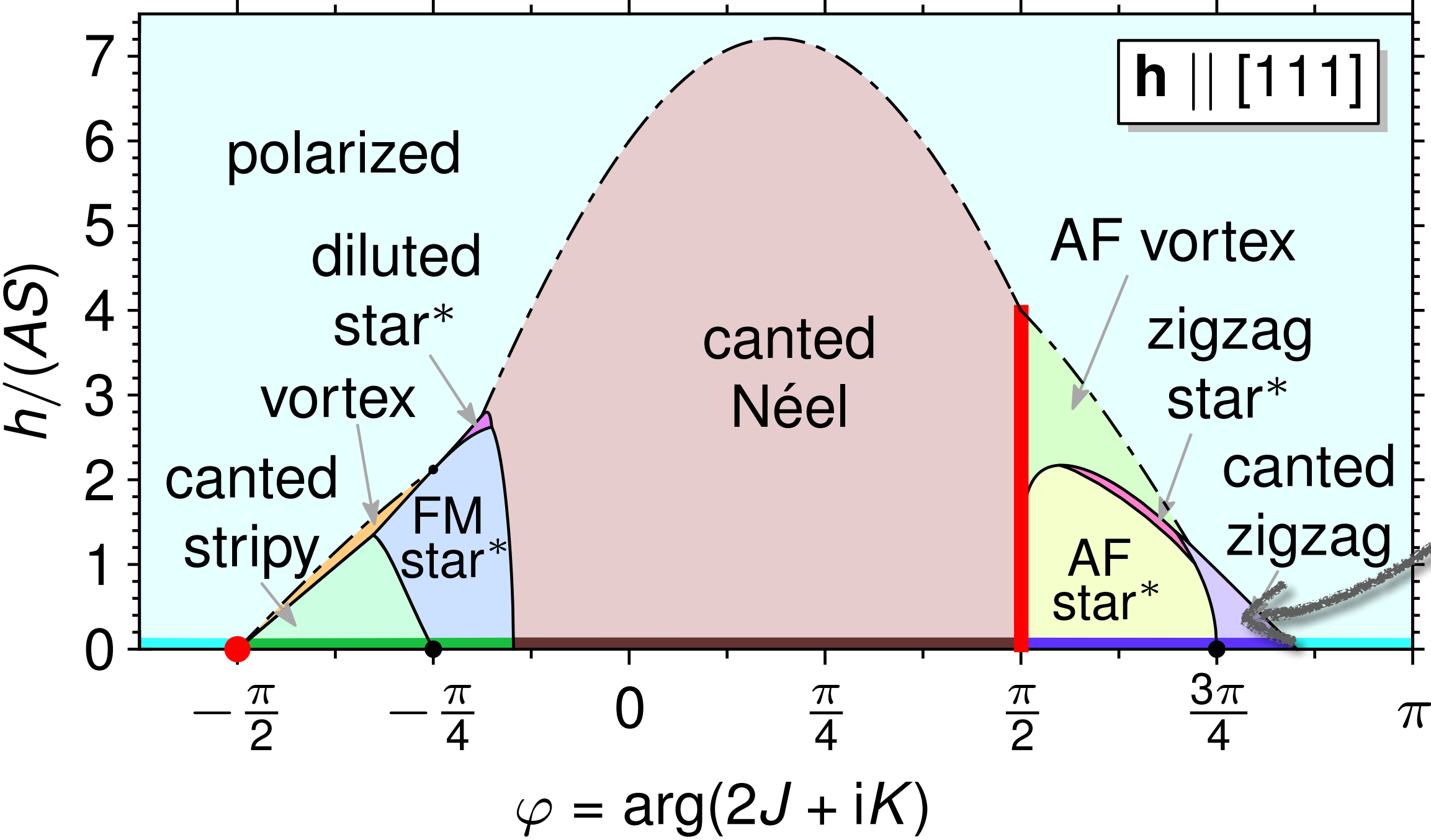
Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\alpha} S_i^\alpha S_j^\alpha + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i$$

$$J = A \cos \varphi$$

$$K = 2A \sin \varphi$$

Phase diagram:



[LJ, Andrade, Vojta, PRL '16]
 [Cônsoi, LJ, Vojta, Andrade, PRB '20]

Kitaev-Heisenberg Physics in Magnetic Fields

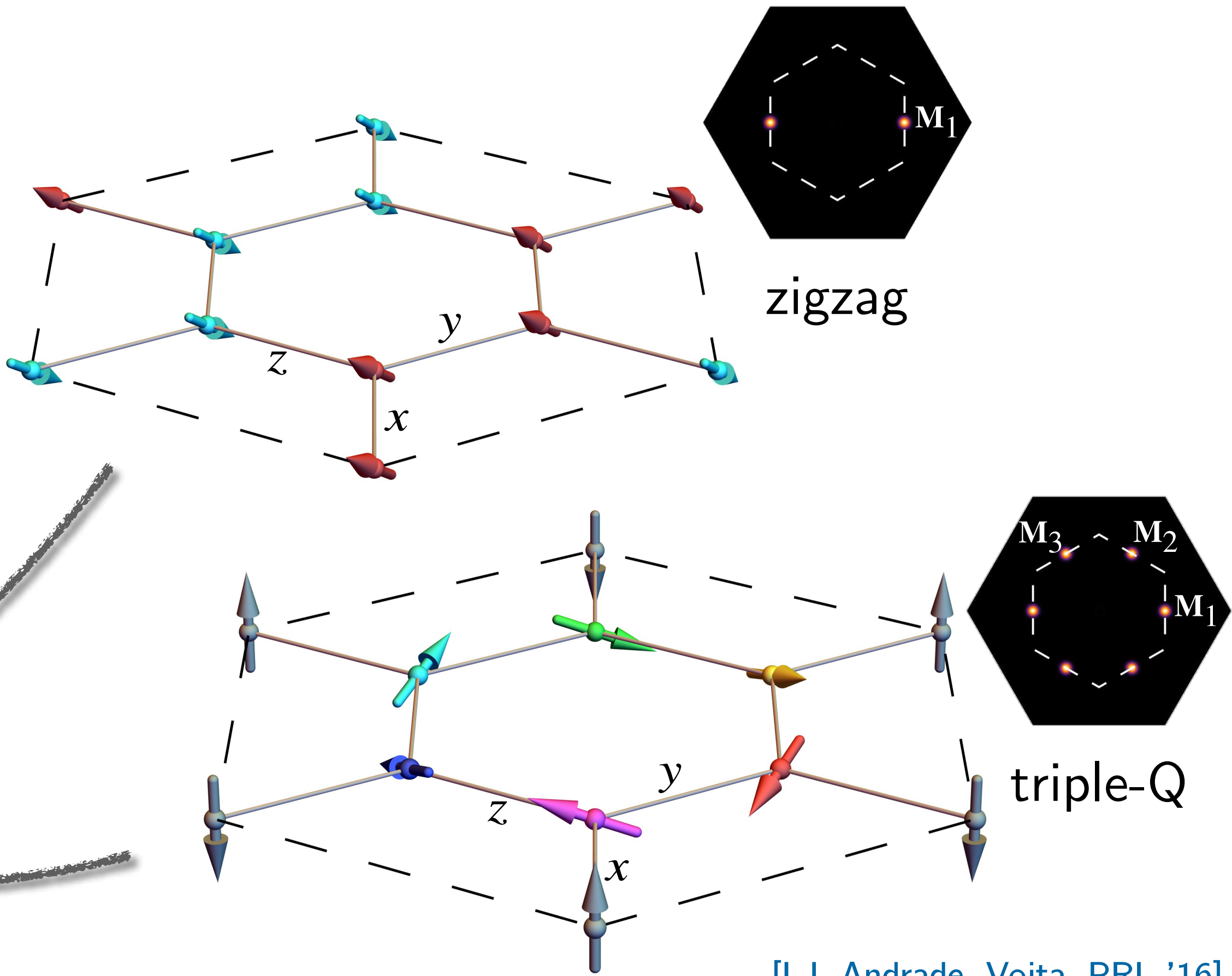
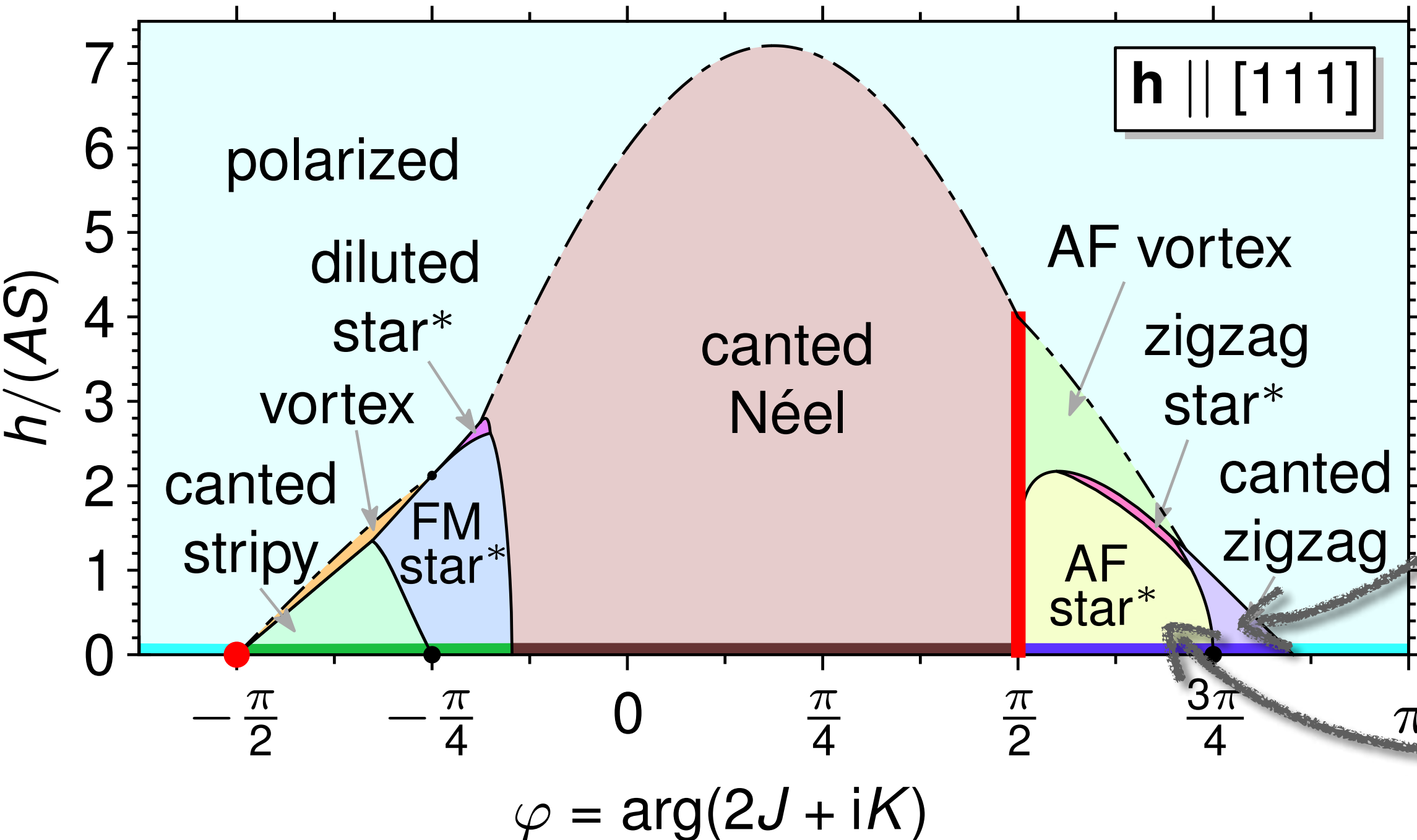
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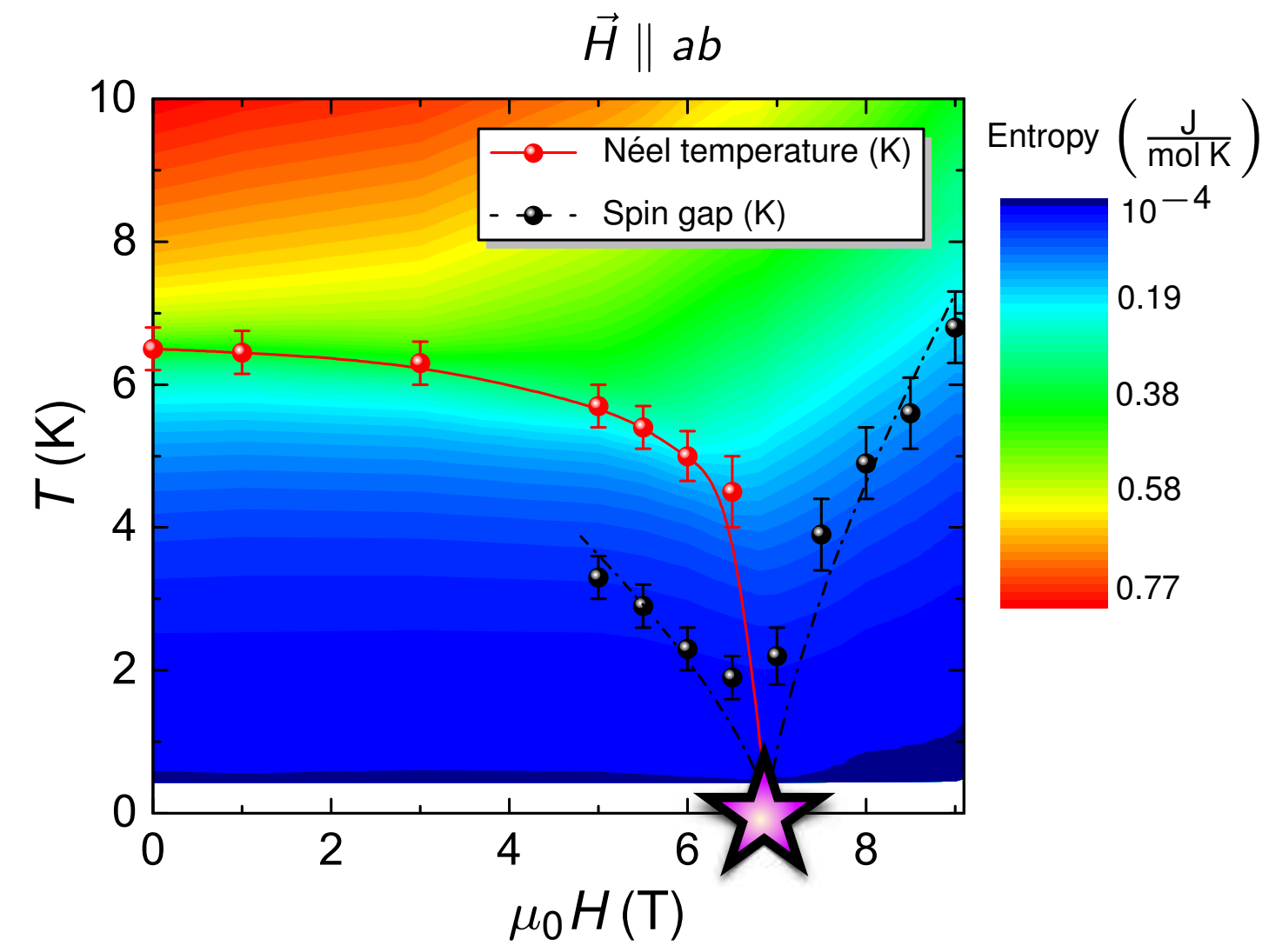
Phase diagram:



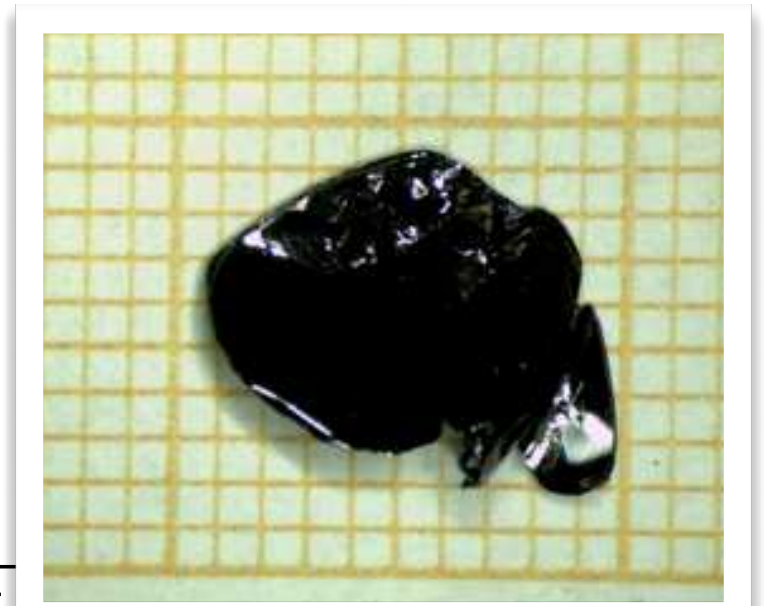
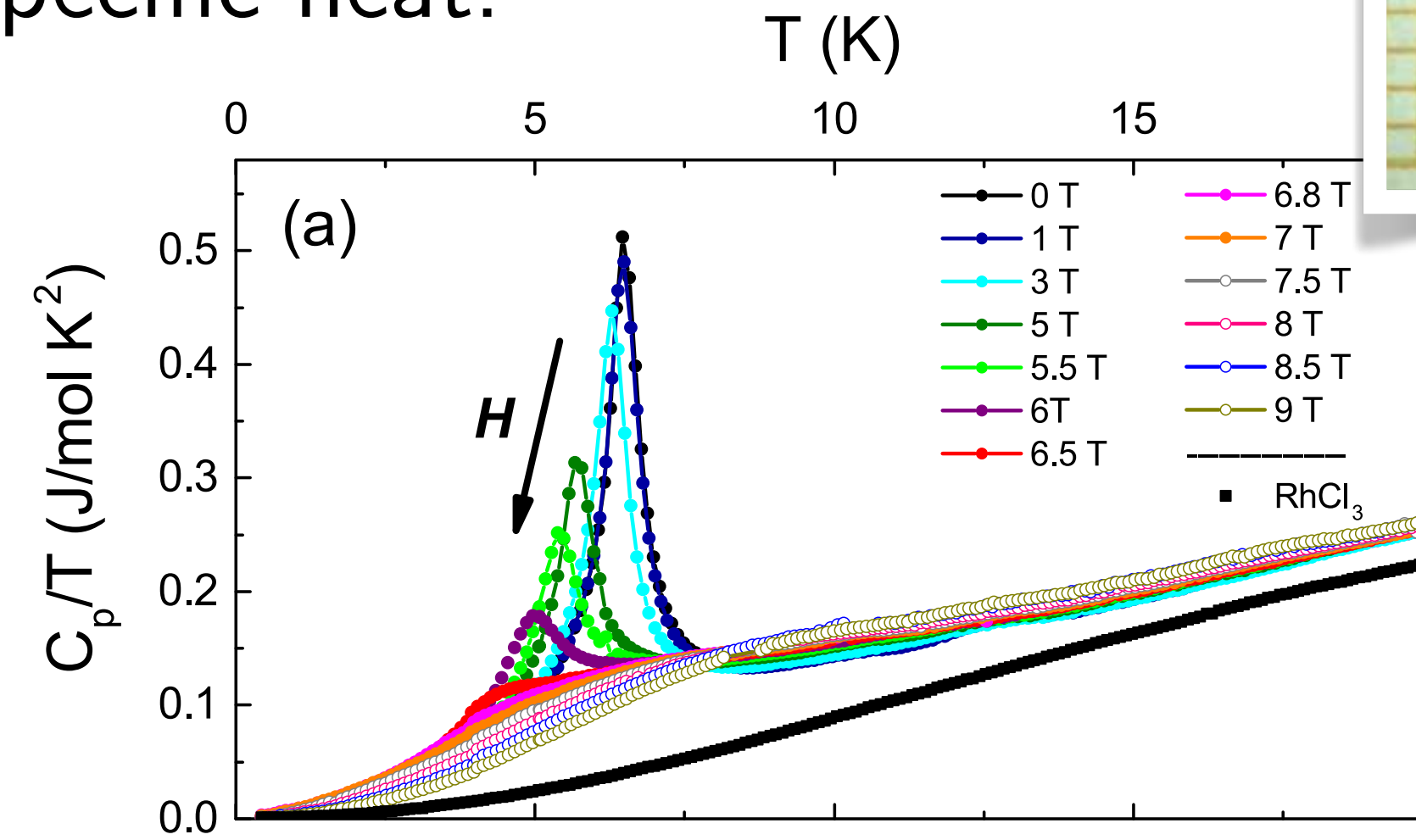
[LJ, Andrade, Vojta, PRL '16]
[Cônsoi, LJ, Vojta, Andrade, PRB '20]

α -RuCl₃ in Magnetic Field

Phase diagram:



Specific heat:

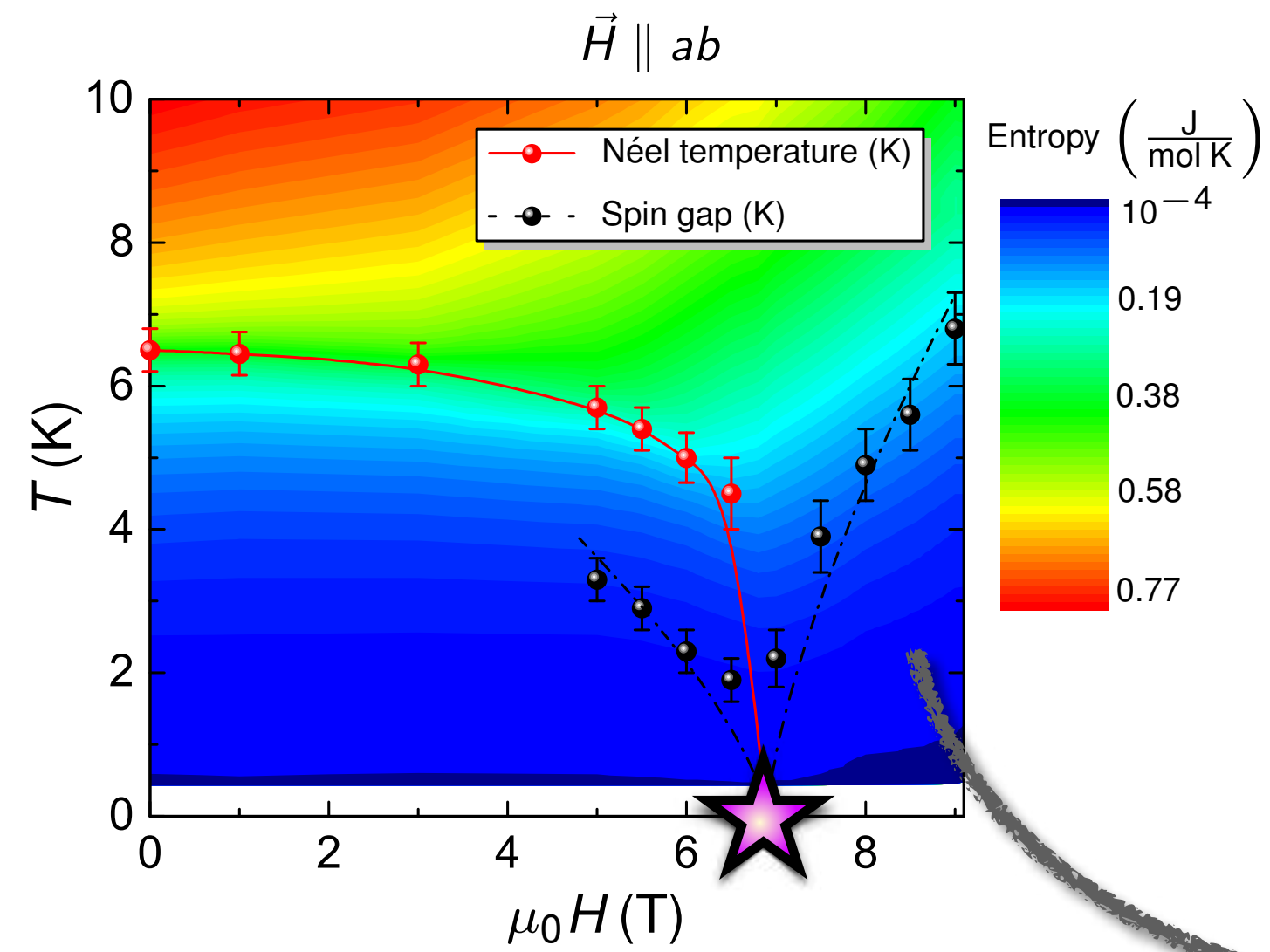


Credit: S. Wurmehl

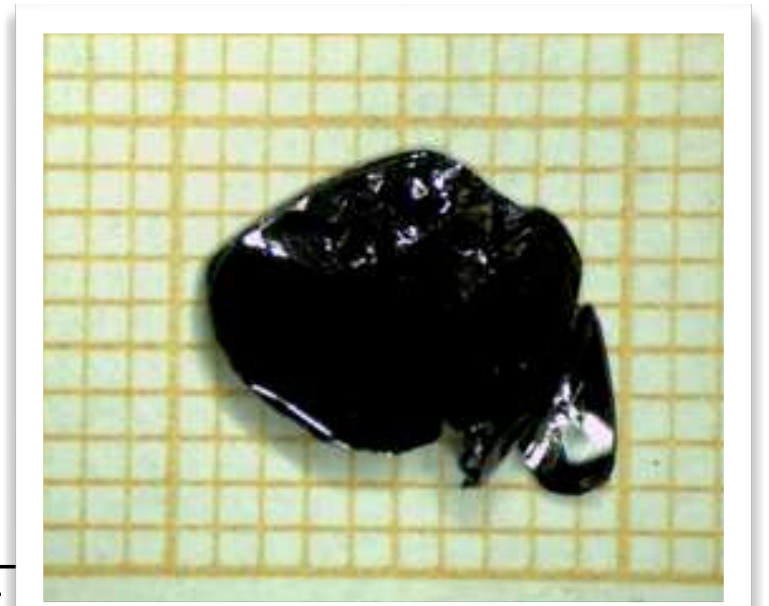
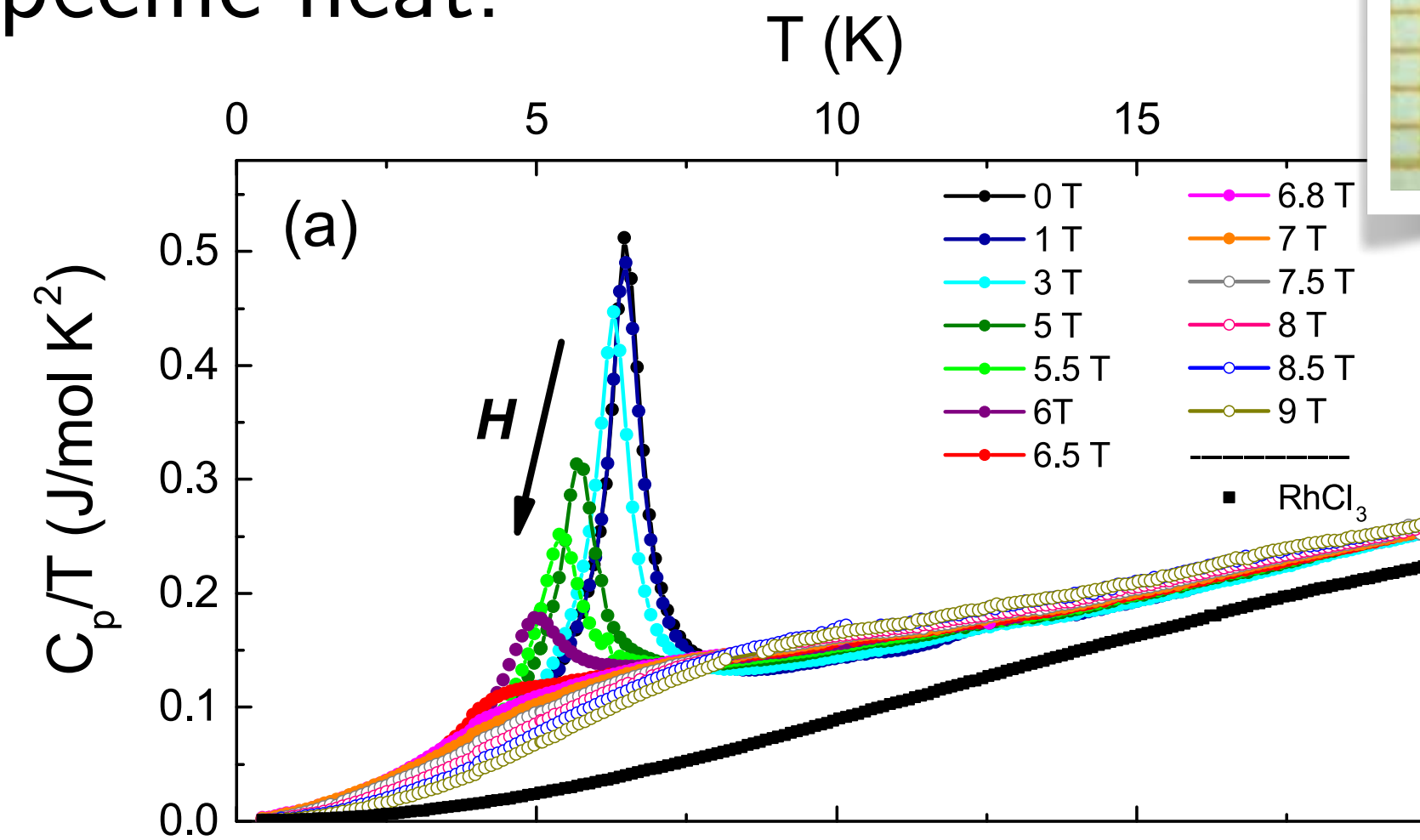
[Wolter, Corredor, LJ, et al., PRB '17]

α -RuCl₃ in Magnetic Field

Phase diagram:



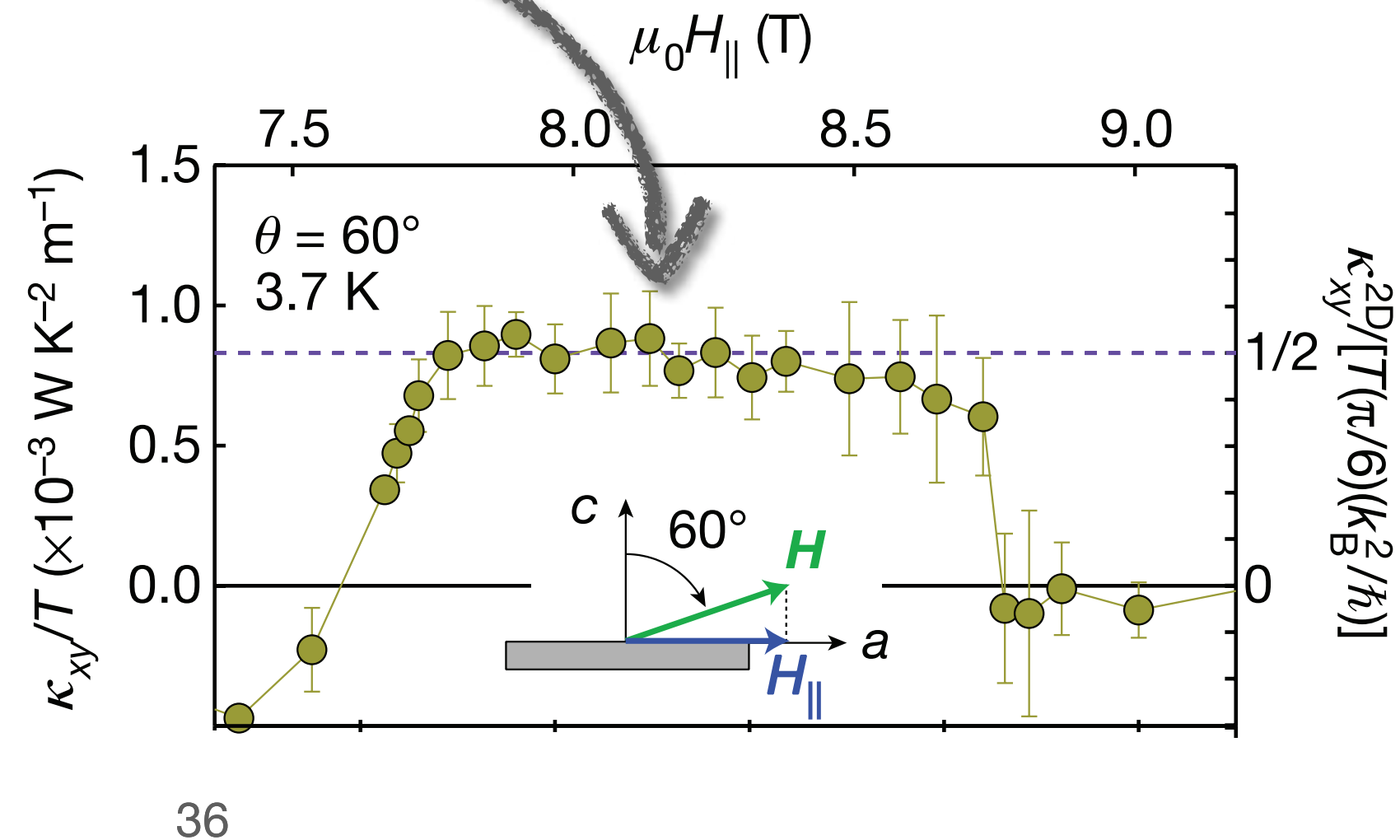
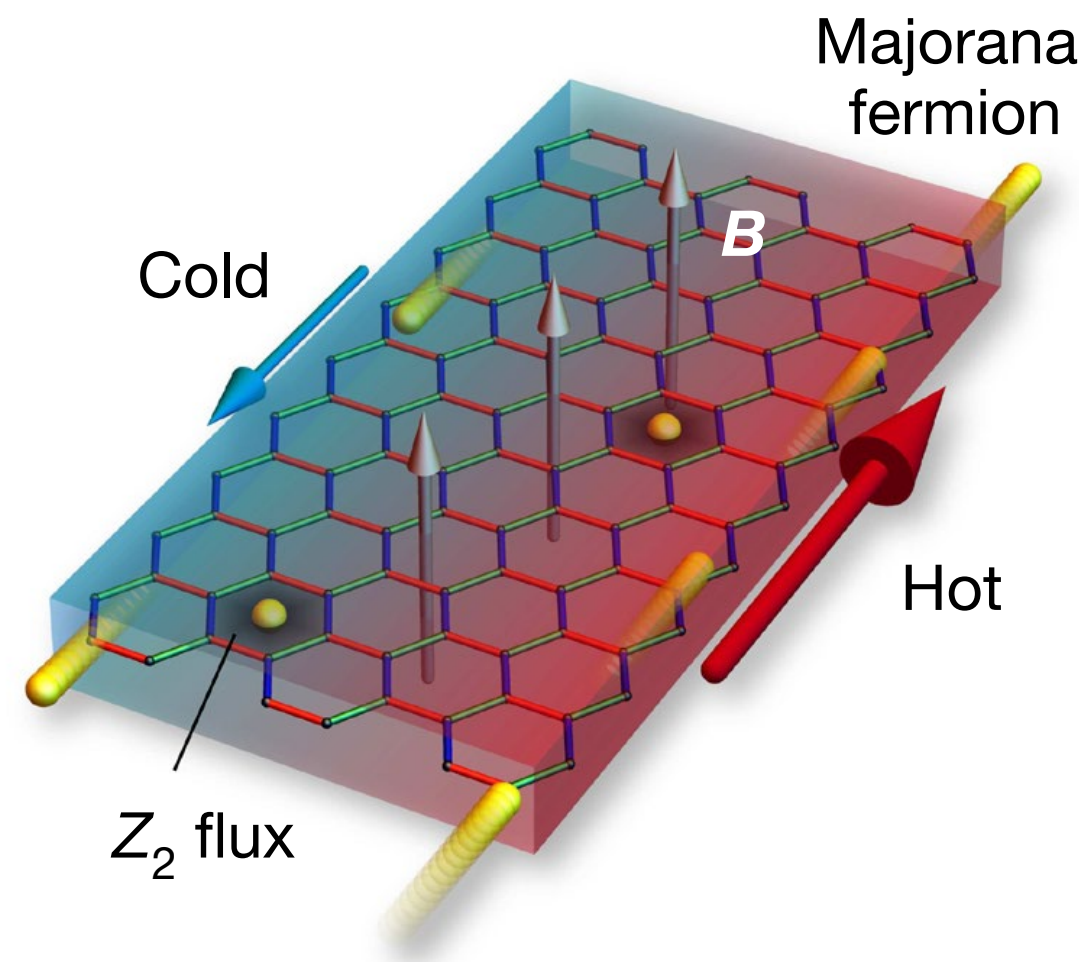
Specific heat:



Credit: S. Wurmehl

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

Half-integer quantum Hall effect:



[Kasahara et al., Nature '18]

[Yokoi et al., Science '21]

α -RuCl₃: Zigzag

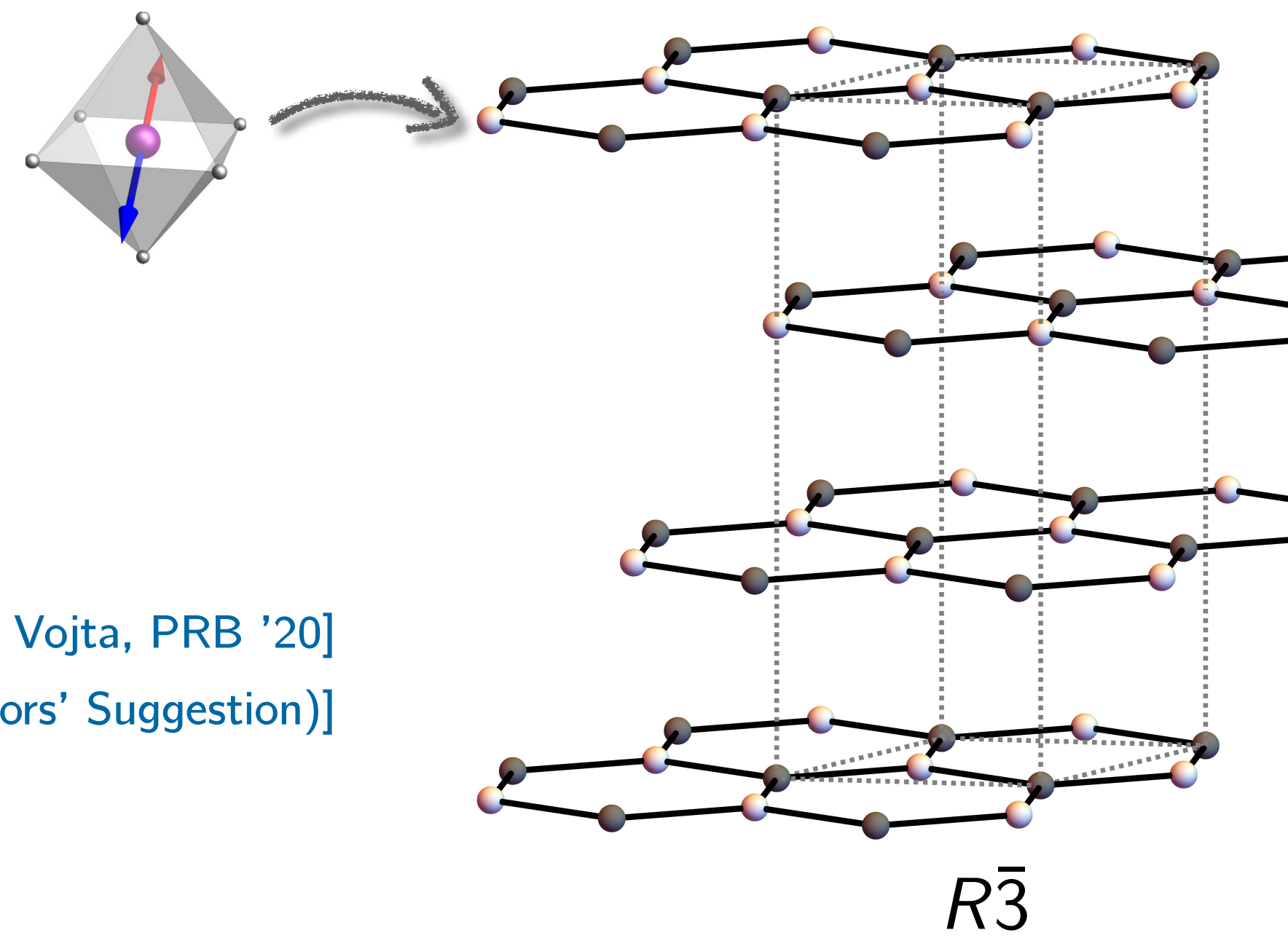
Hamiltonian:

$$\mathcal{H}_{3D} = \mathcal{H}_{2D} + J_{\perp} \sum_{\langle ni, mi \rangle} \vec{S}_{n,i} \cdot \vec{S}_{m,i} + \dots$$

[LJ, Koch, Vojta, PRB '20]

[Balz, LJ, *et int.*, Nagler, PRB '21 (Editors' Suggestion)]

● Cl⁻
● Ru³⁺

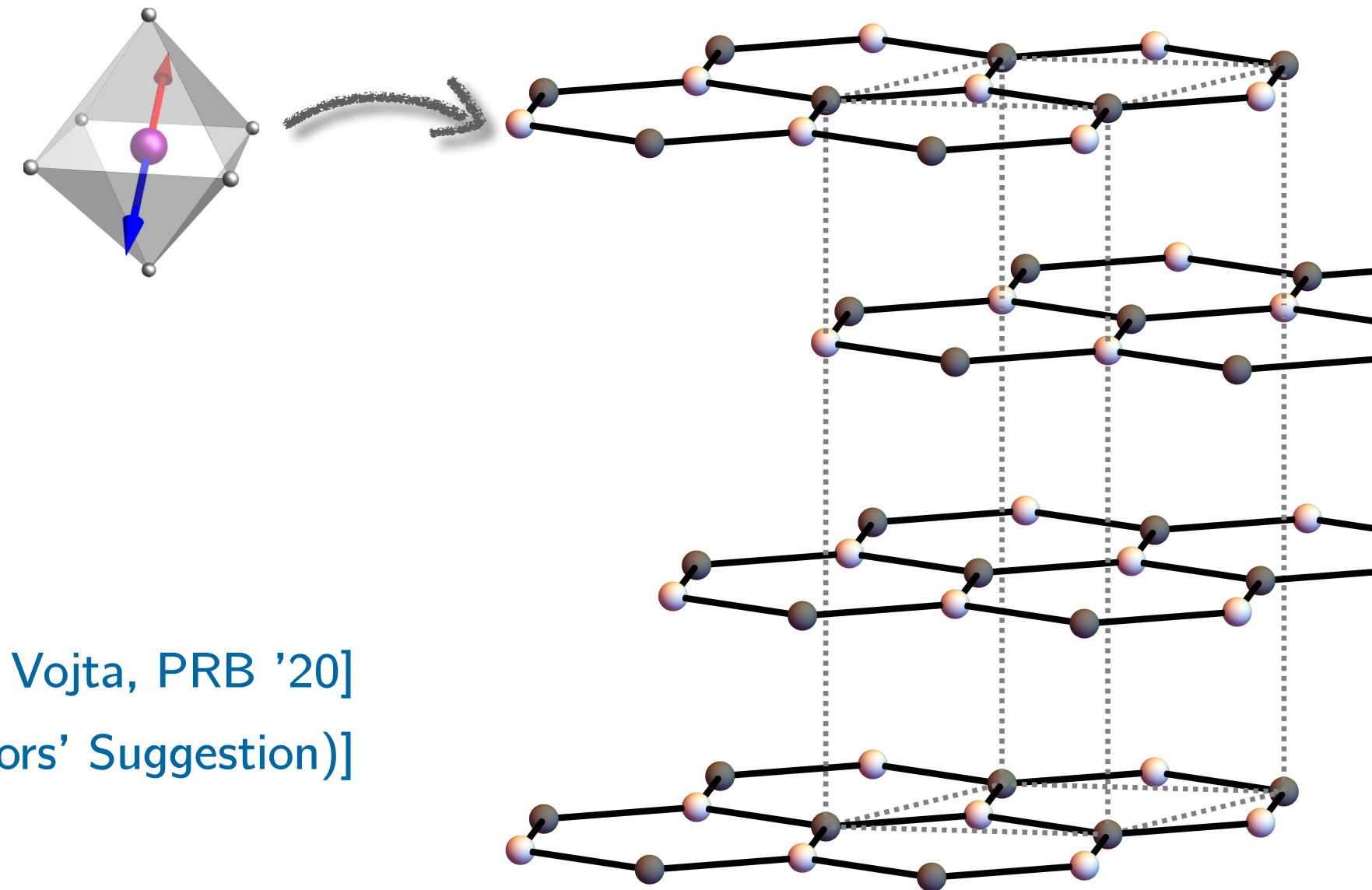


α -RuCl₃: Zigzag

Hamiltonian:

$$\mathcal{H}_{3D} = \mathcal{H}_{2D} + J_{\perp} \sum_{\langle ni, mi \rangle} \vec{S}_{n,i} \cdot \vec{S}_{m,i} + \dots$$

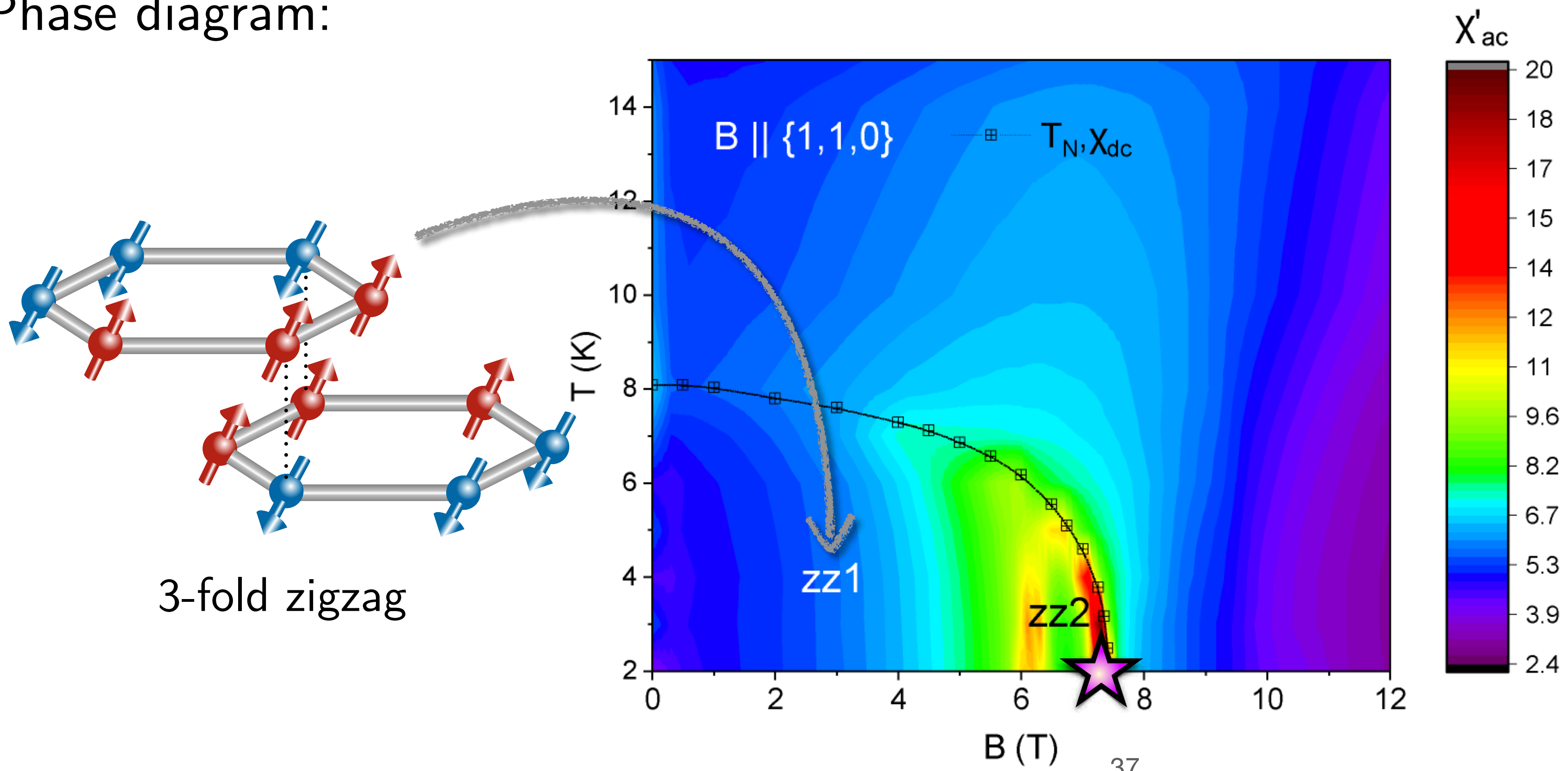
● Cl⁻
● Ru³⁺



[LJ, Koch, Vojta, PRB '20]

[Balz, LJ, *et int.*, Nagler, PRB '21 (Editors' Suggestion)]

Phase diagram:



$R\bar{3}$

α -RuCl₃: Zigzag

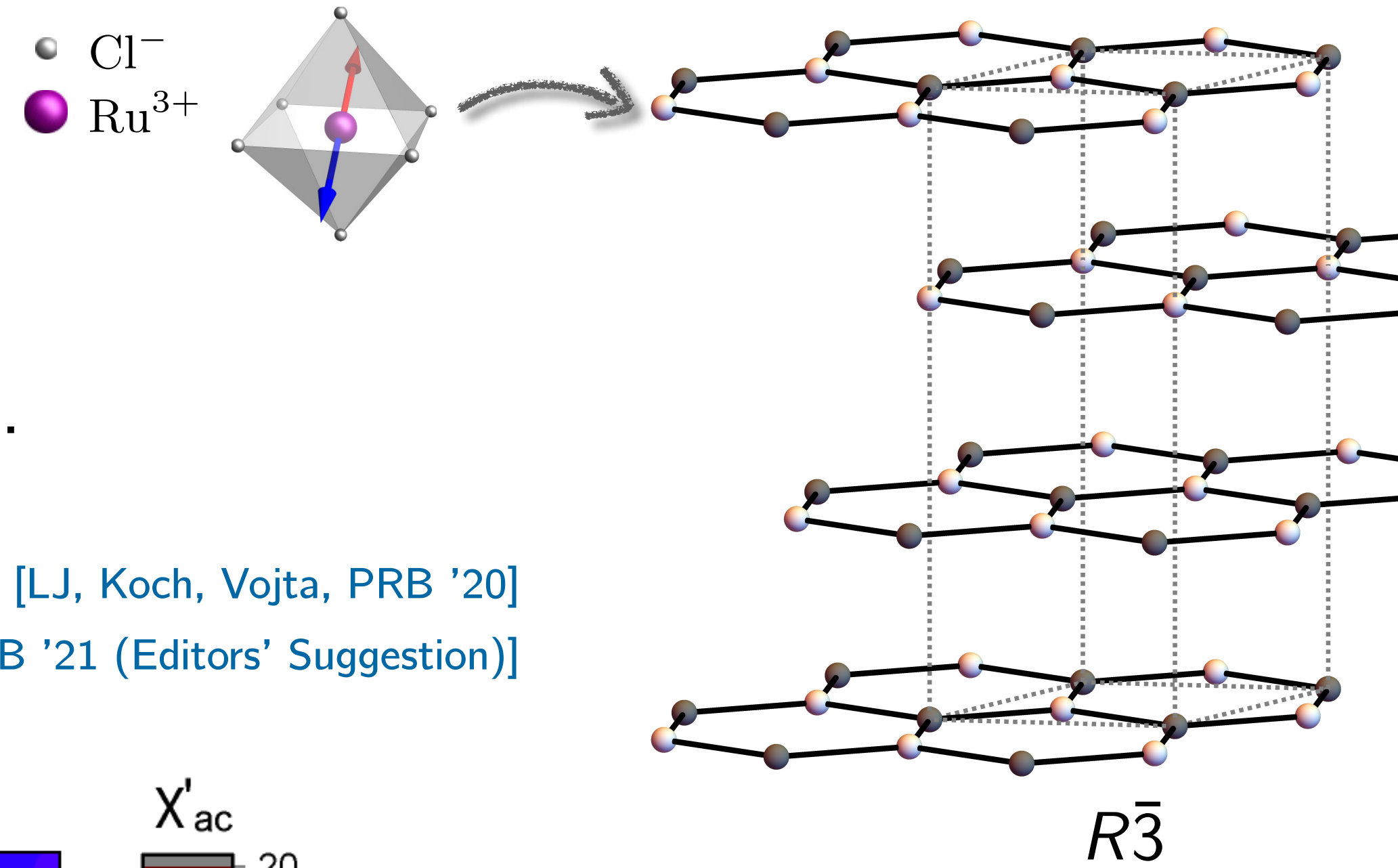
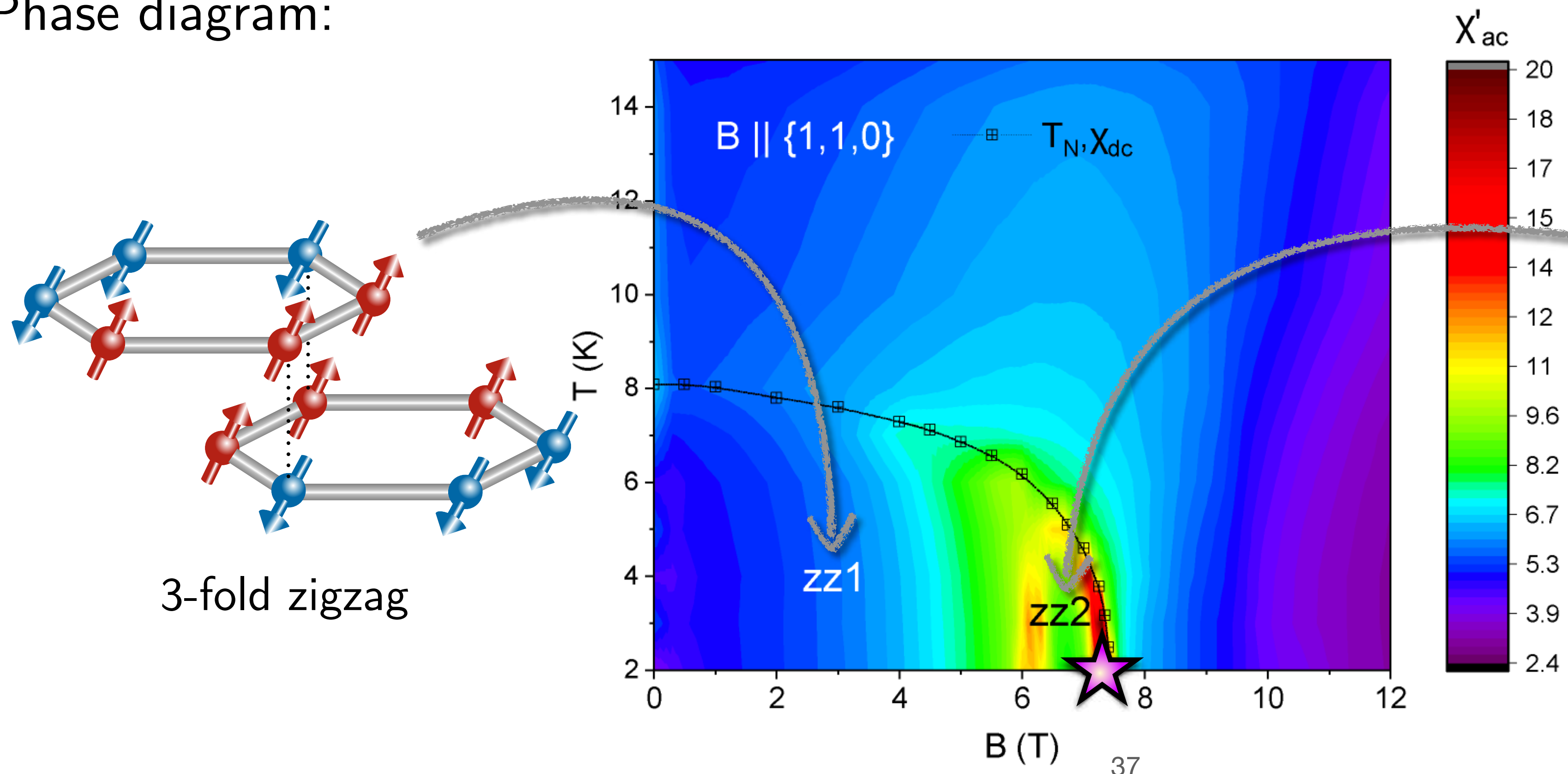
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[LJ, Koch, Vojta, PRB '20]

[Balz, LJ, *et int.*, Nagler, PRB '21 (Editors' Suggestion)]

Phase diagram:



α -RuCl₃: Zigzag

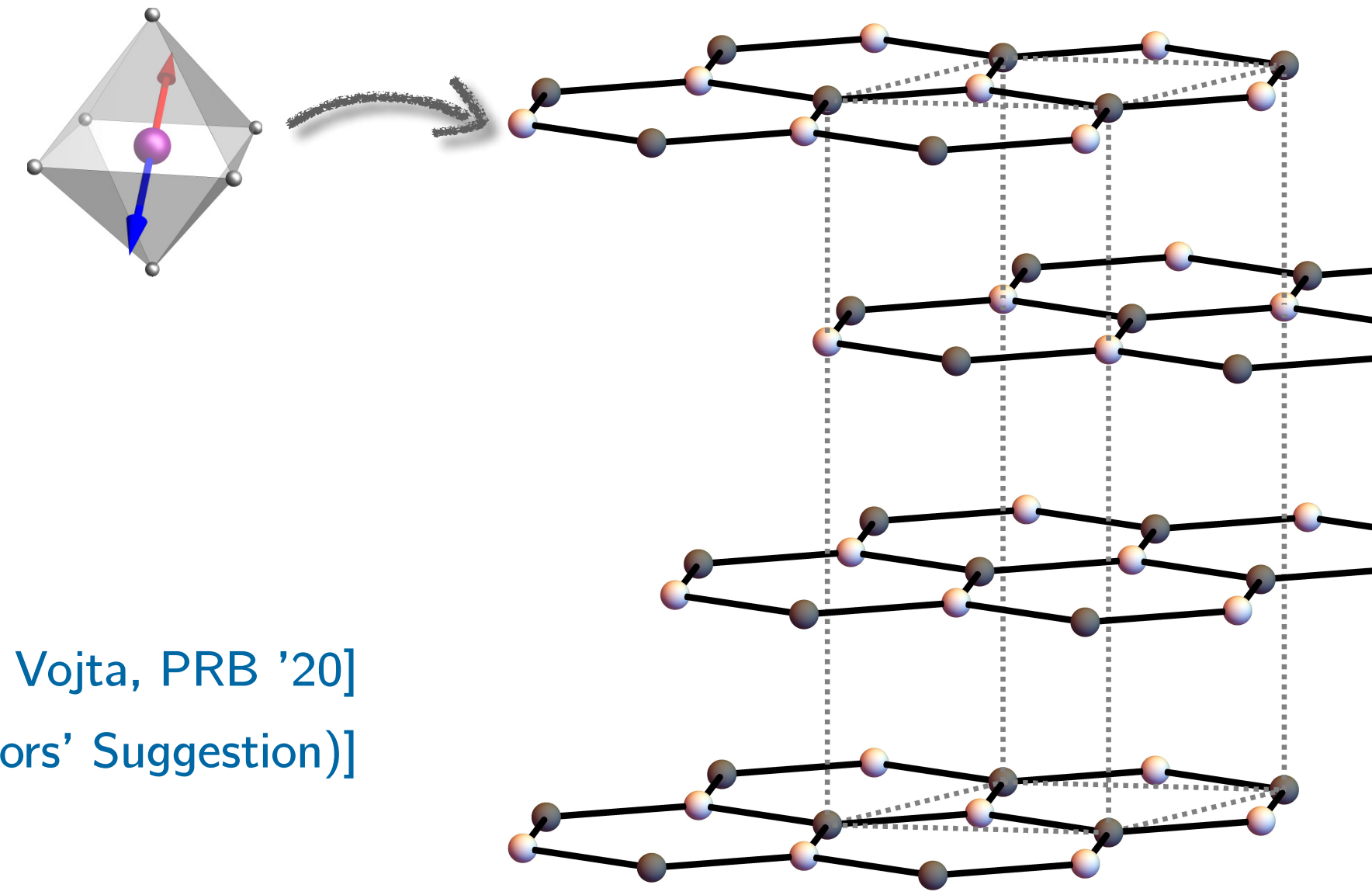
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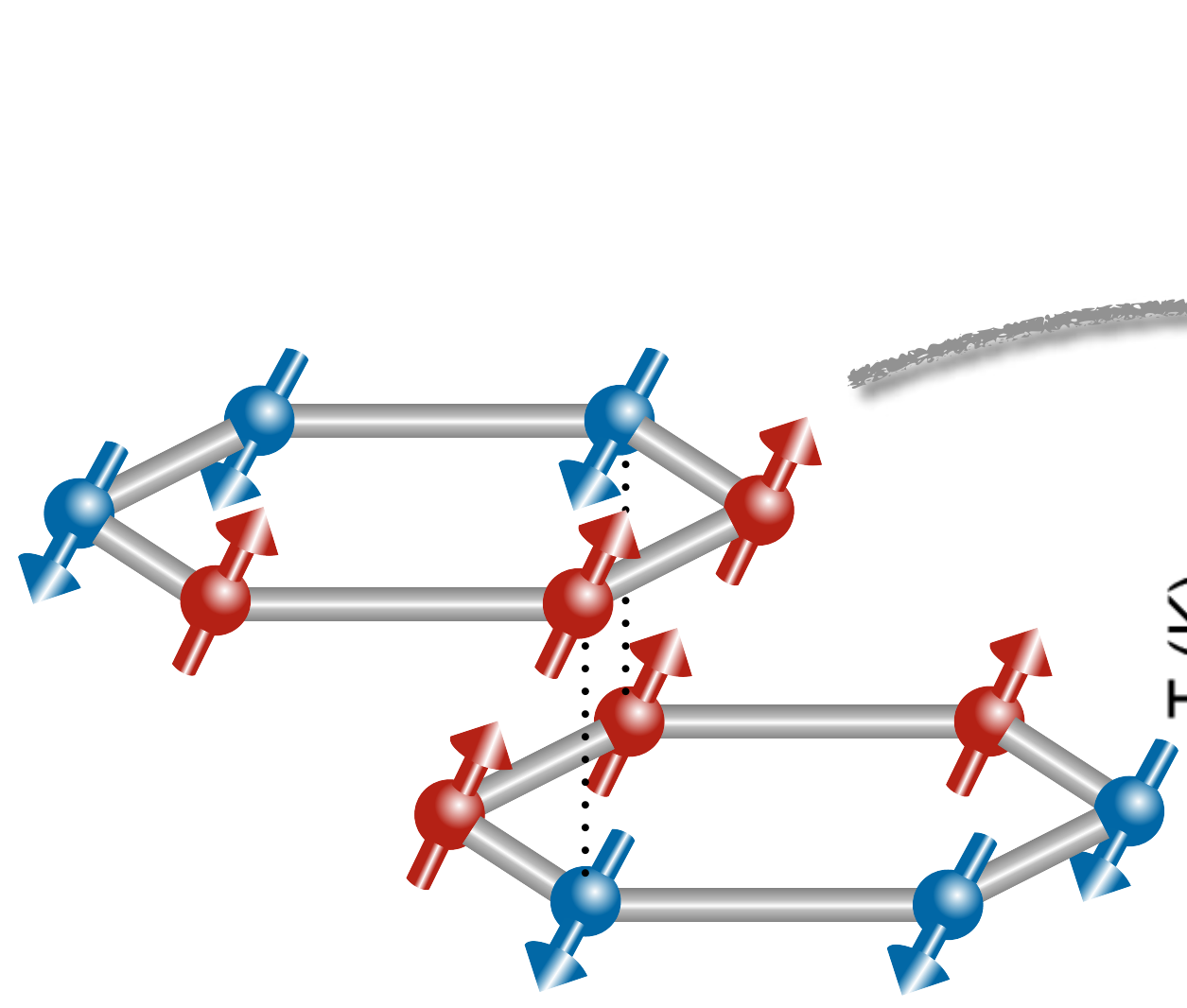
[LJ, Koch, Vojta, PRB '20]

[Balz, LJ, *et int.*, Nagler, PRB '21 (Editors' Suggestion)]

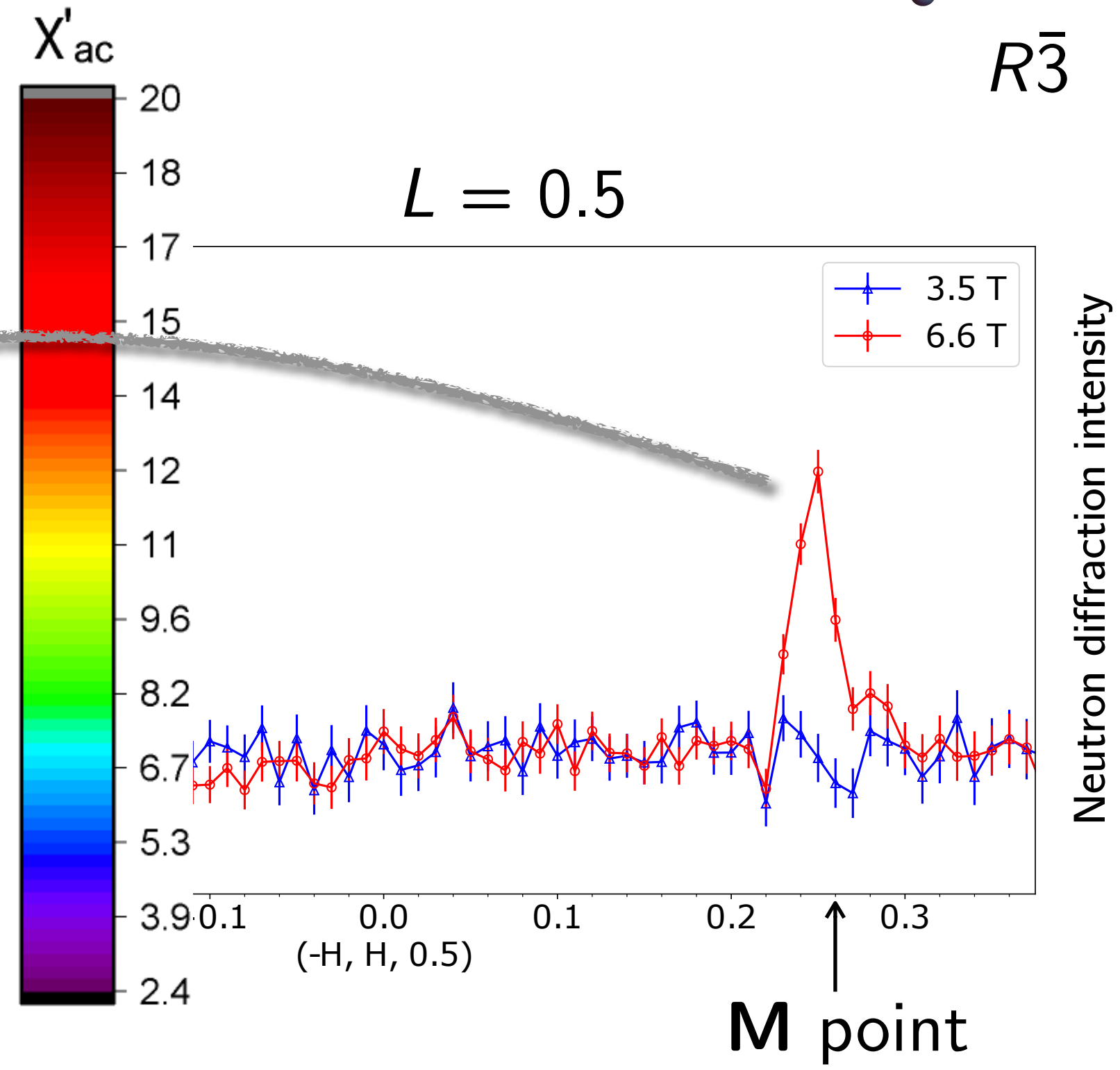
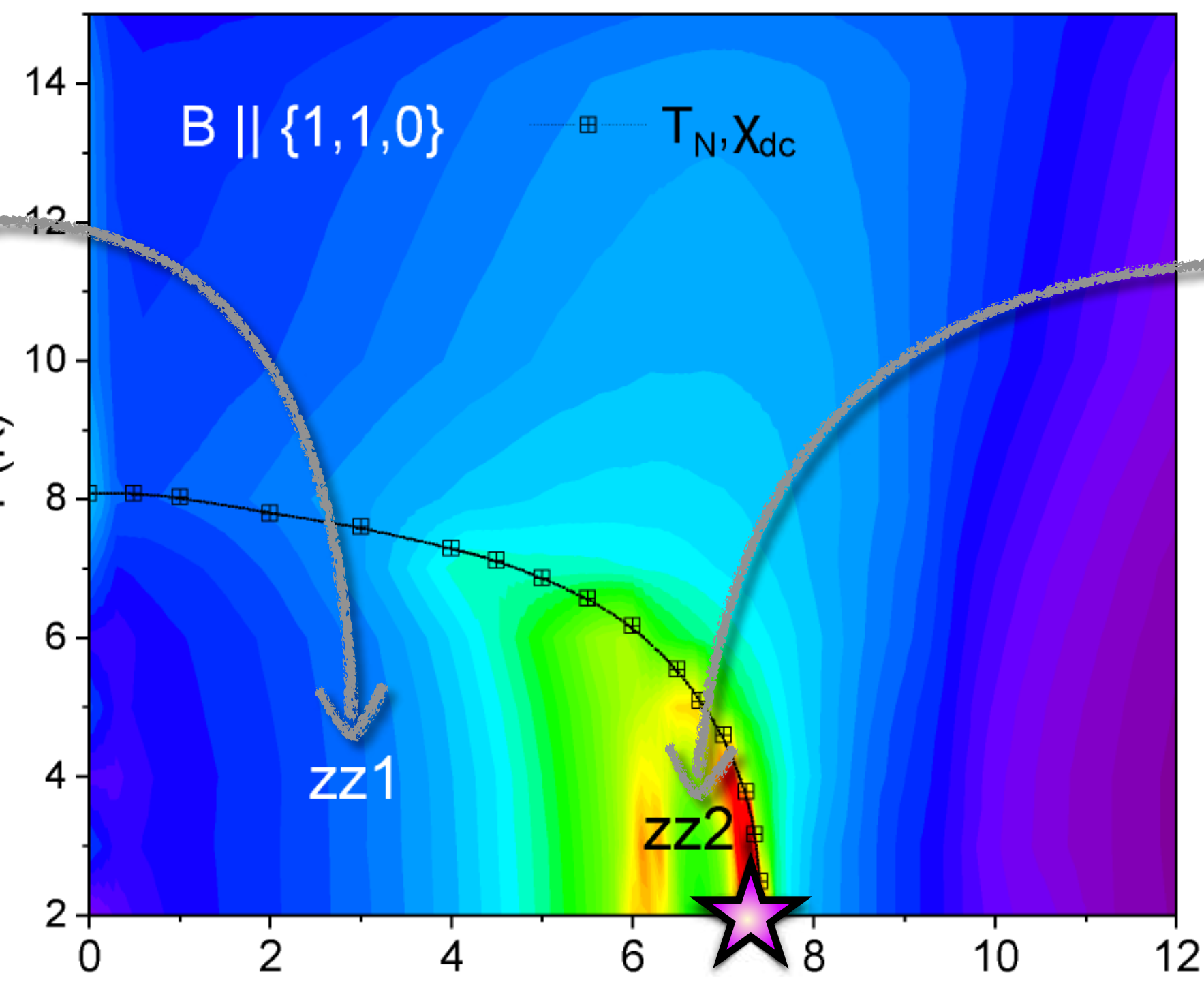
● Cl⁻
● Ru³⁺



Phase diagram:



3-fold zigzag



α -RuCl₃: Zigzag

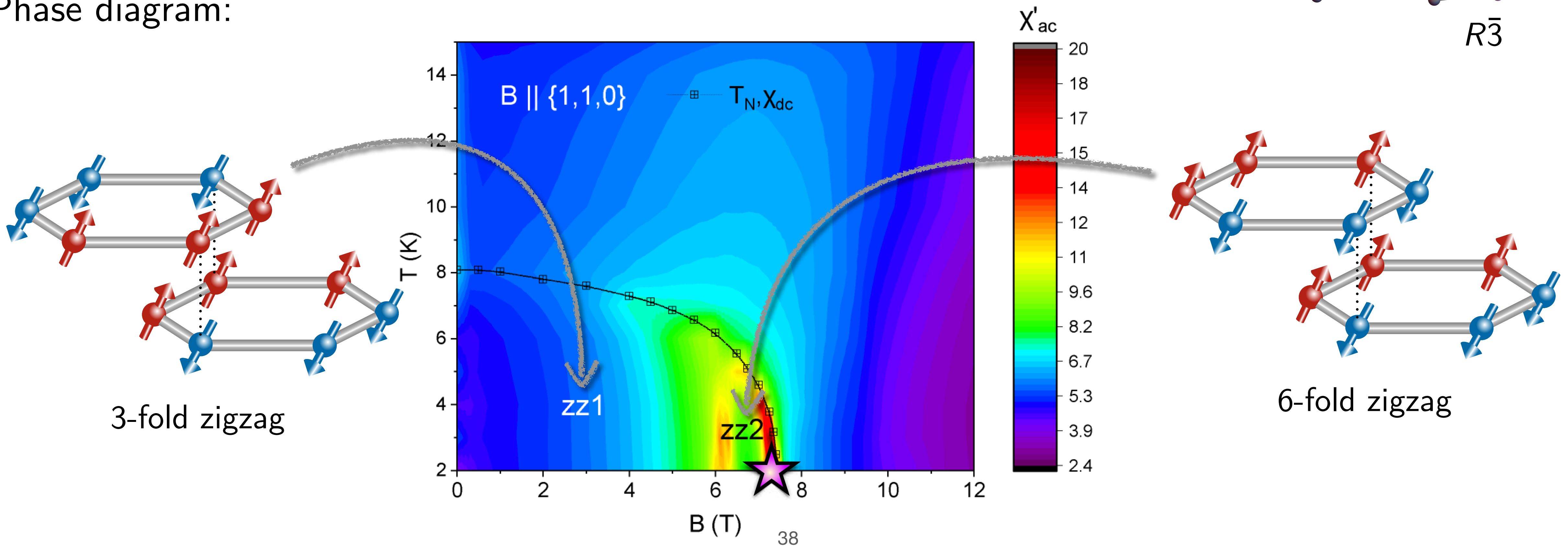
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[LJ, Koch, Vojta, PRB '20]

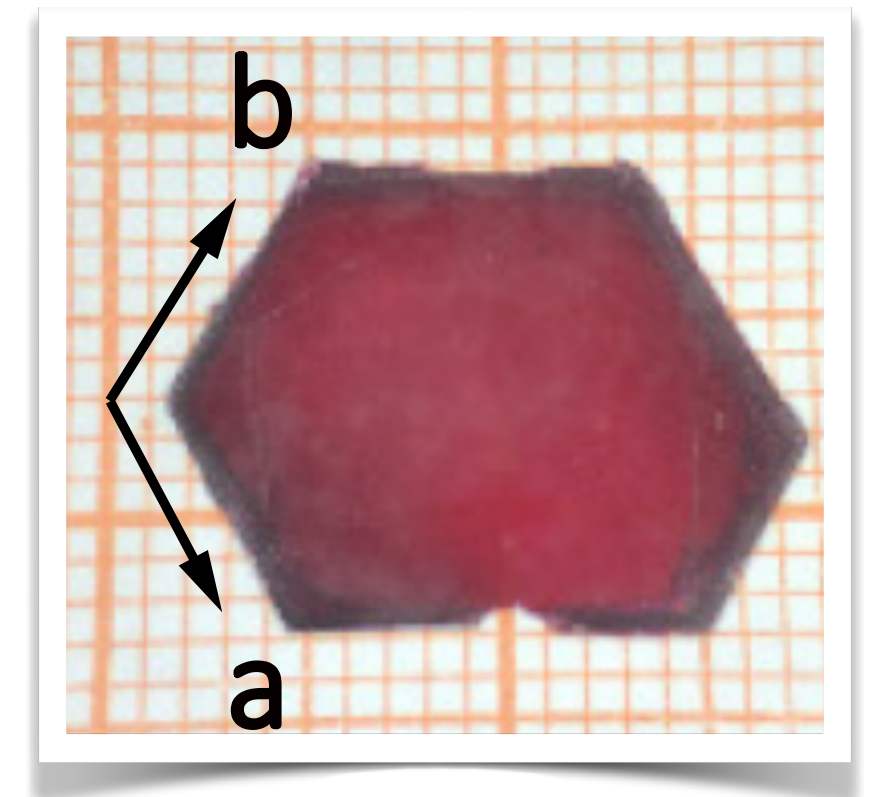
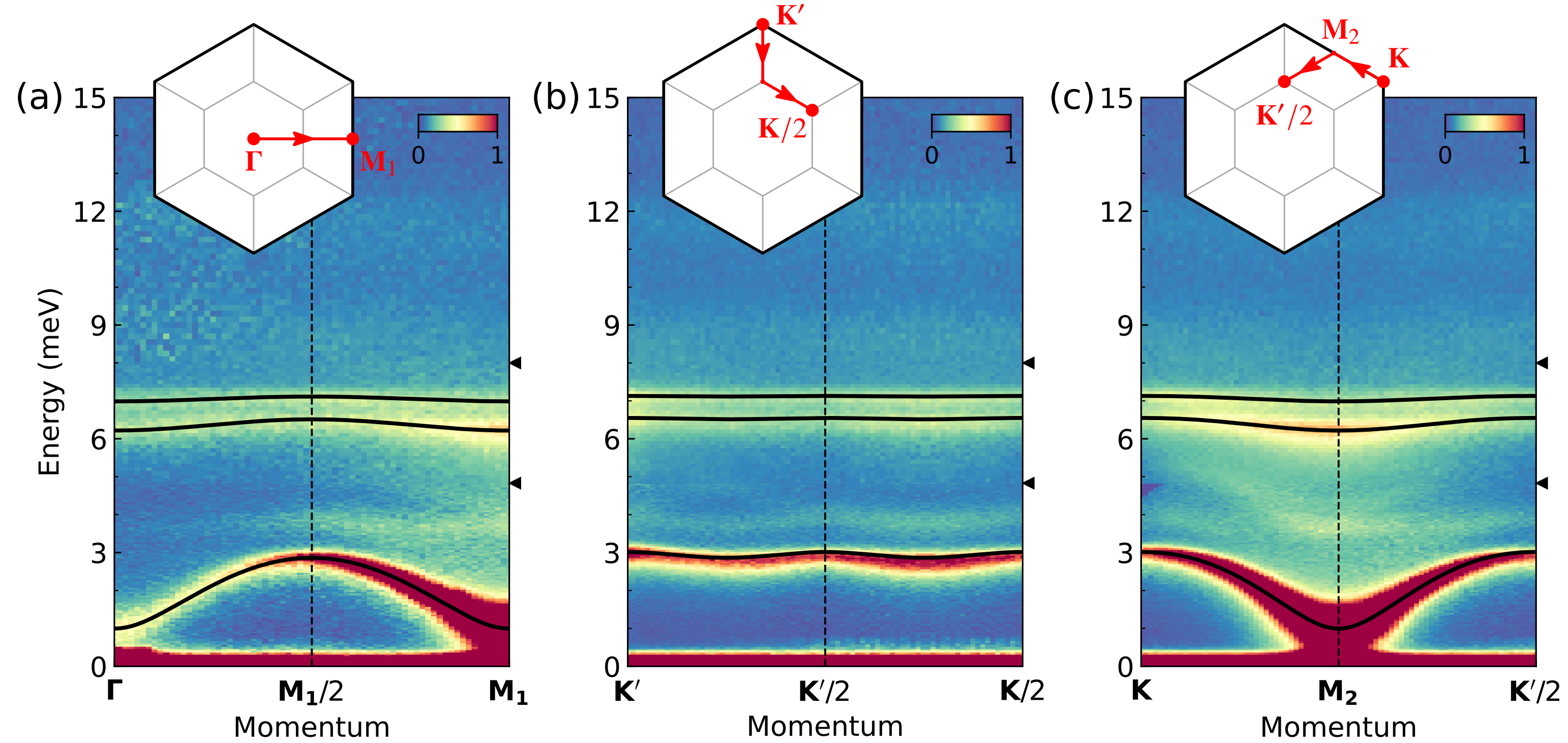
[Balz, LJ, *et int.*, Nagler, PRB '21 (Editors' Suggestion)]

Phase diagram:



Na₂Co₂TeO₆: Triple-Q

Inelastic neutron spectrum:



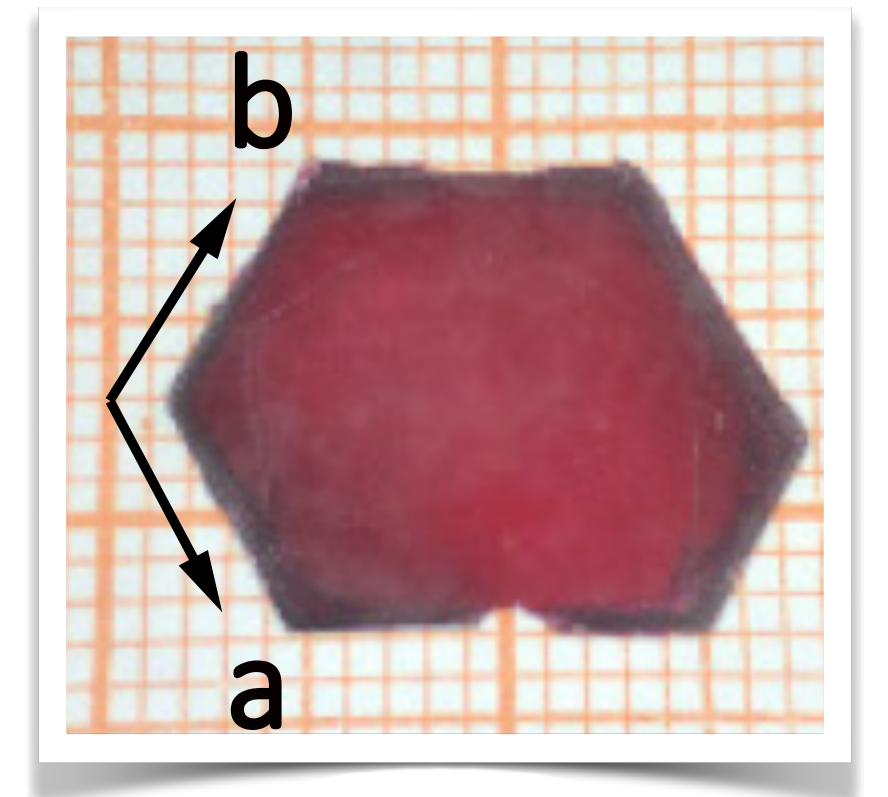
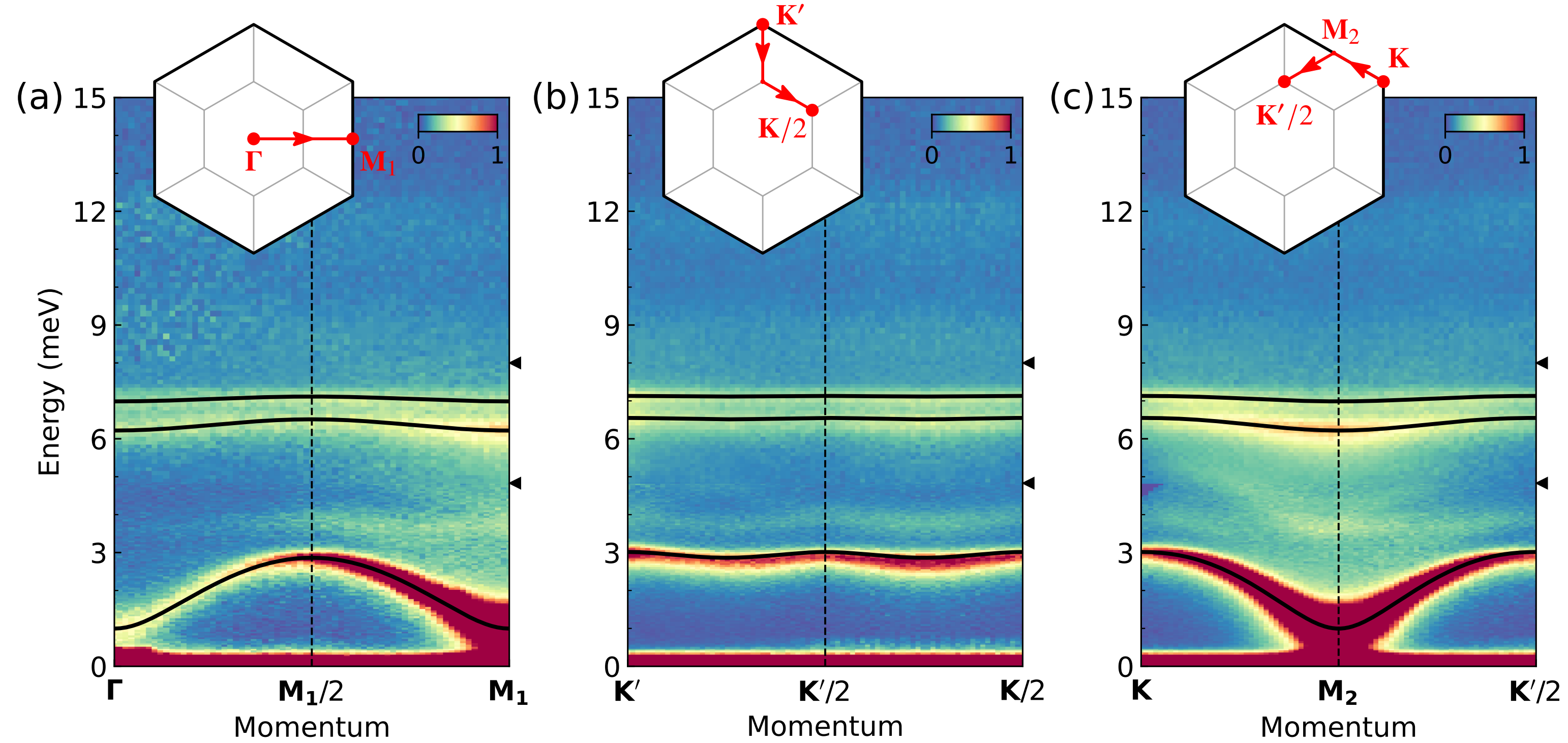
Credit: Yuan Li



Wilhelm Krüger

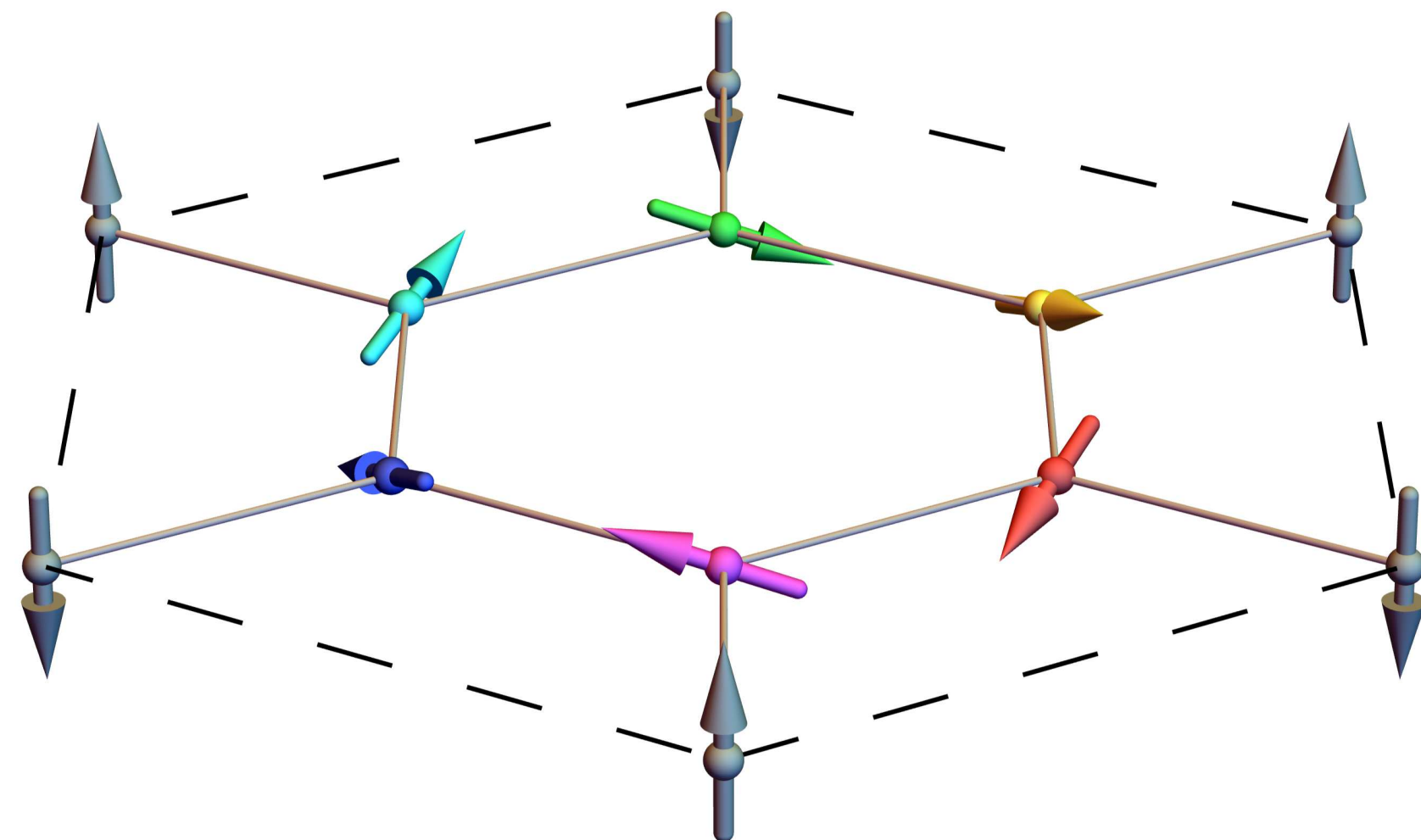
Na₂Co₂TeO₆: Triple-Q

Inelastic neutron spectrum:



Credit: Yuan Li

Ground state:



⇒ triple-Q order



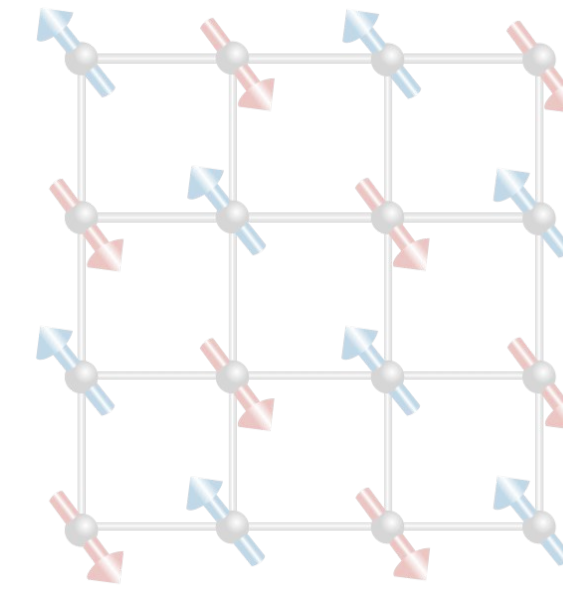
Wilhelm Krüger

[Krüger, Chen, Jin, Li, LJ, arXiv:2211.16957]

Outline

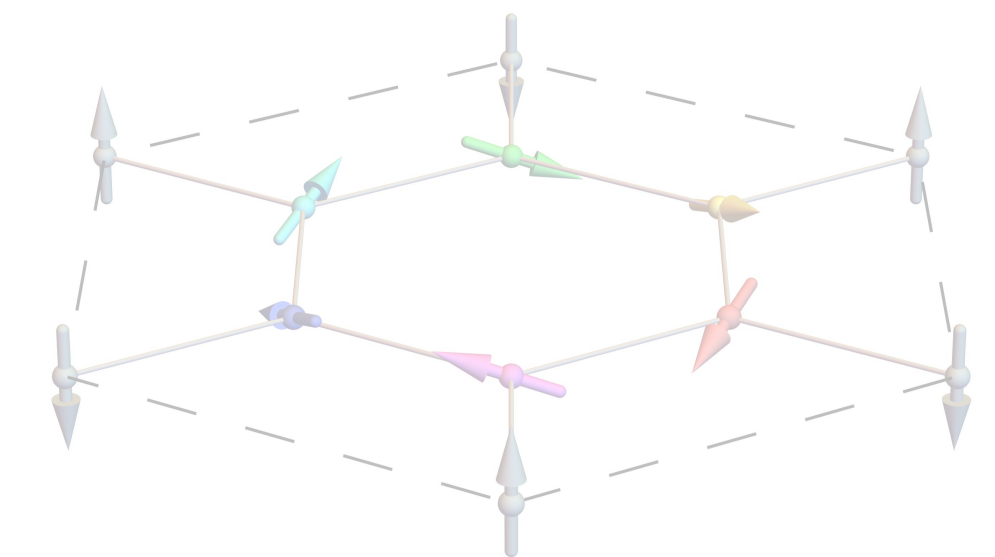
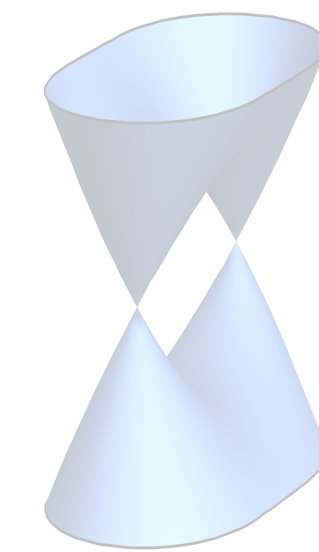
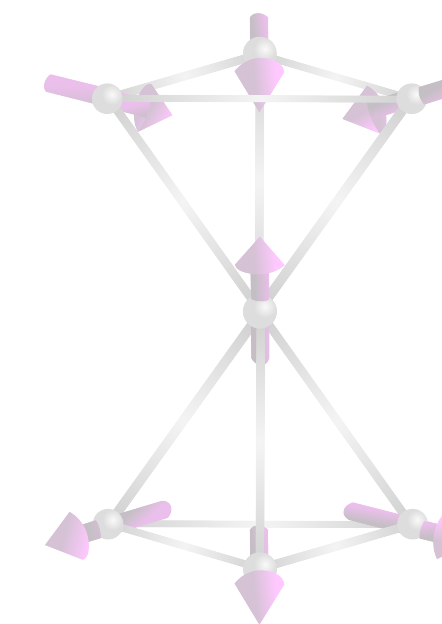
(1) Introduction

- ▶ Research Motivation
- ▶ Research Goals

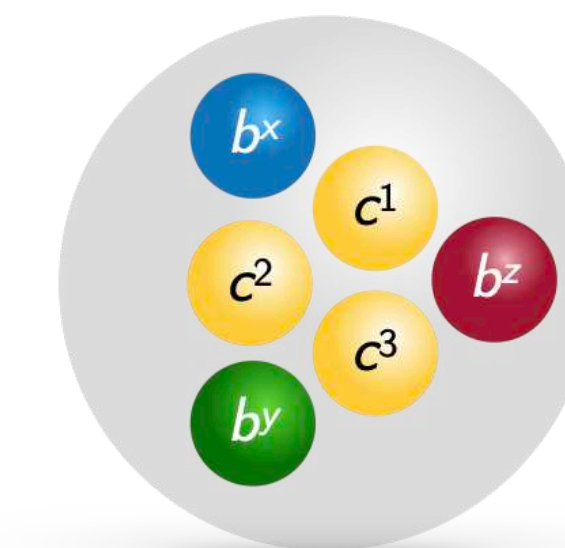


(2) Emergent Phenomena in Quantum Materials

- ▶ Emergent Symmetries
- ▶ Emergent Topology
- ▶ Emergent Orders
- ▶ Emergent Particles



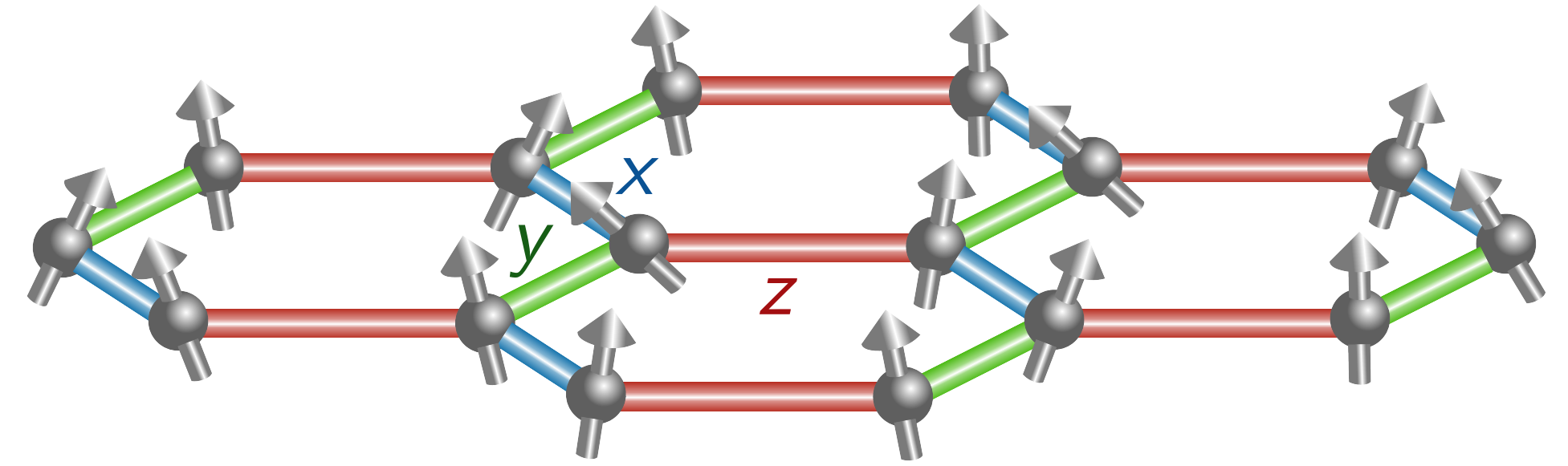
(3) Summary



Example #3: Fractionalized Systems

Kitaev spin-1/2 model:

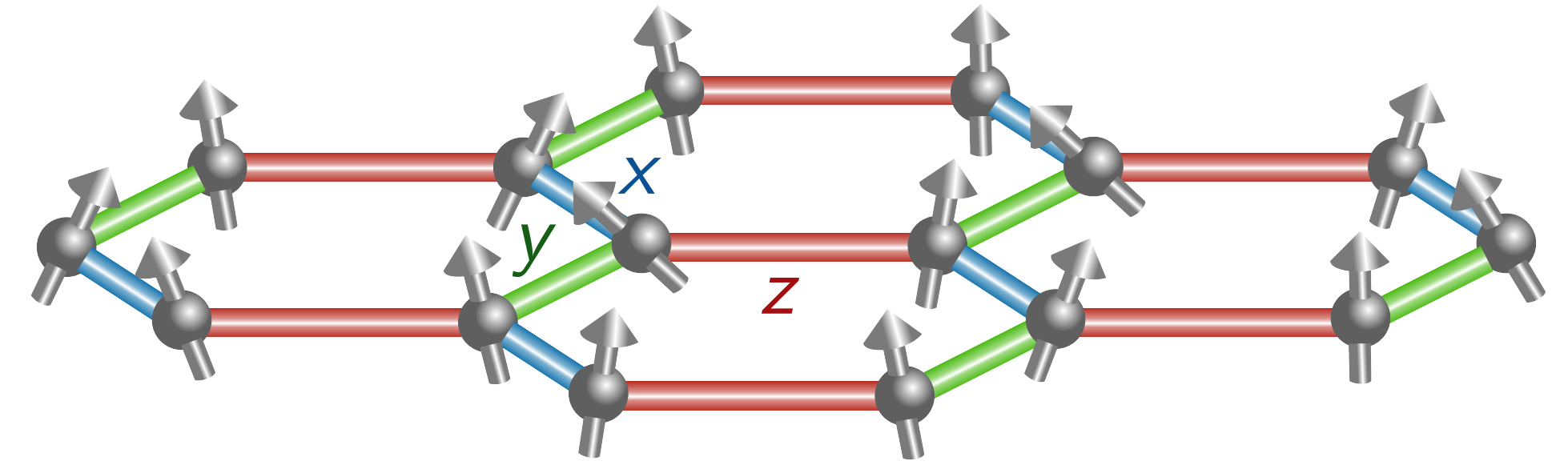
$$\mathcal{H} = K \left(\sum_{\langle ij \rangle_x} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle_y} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle_z} \sigma_i^z \sigma_j^z \right)$$



Example #3: Fractionalized Systems

Kitaev spin-1/2 model:

$$\mathcal{H} = K \left(\sum_{\langle ij \rangle_x} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle_y} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle_z} \sigma_i^z \sigma_j^z \right)$$

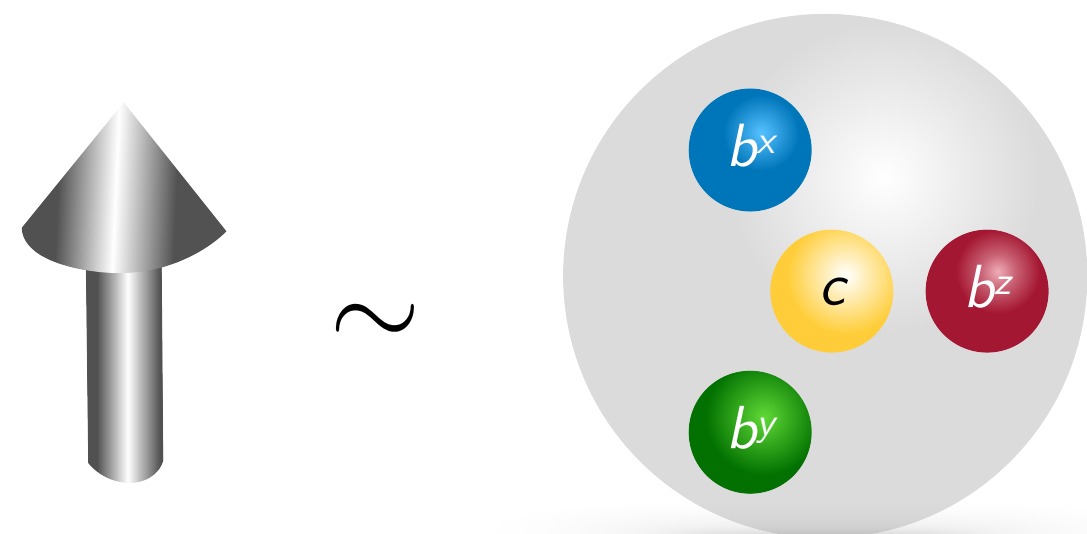


Majorana representation:

$$\sigma^x \sim i b^x c$$

$$\sigma^y \sim i b^y c$$

$$\sigma^z \sim i b^z c$$



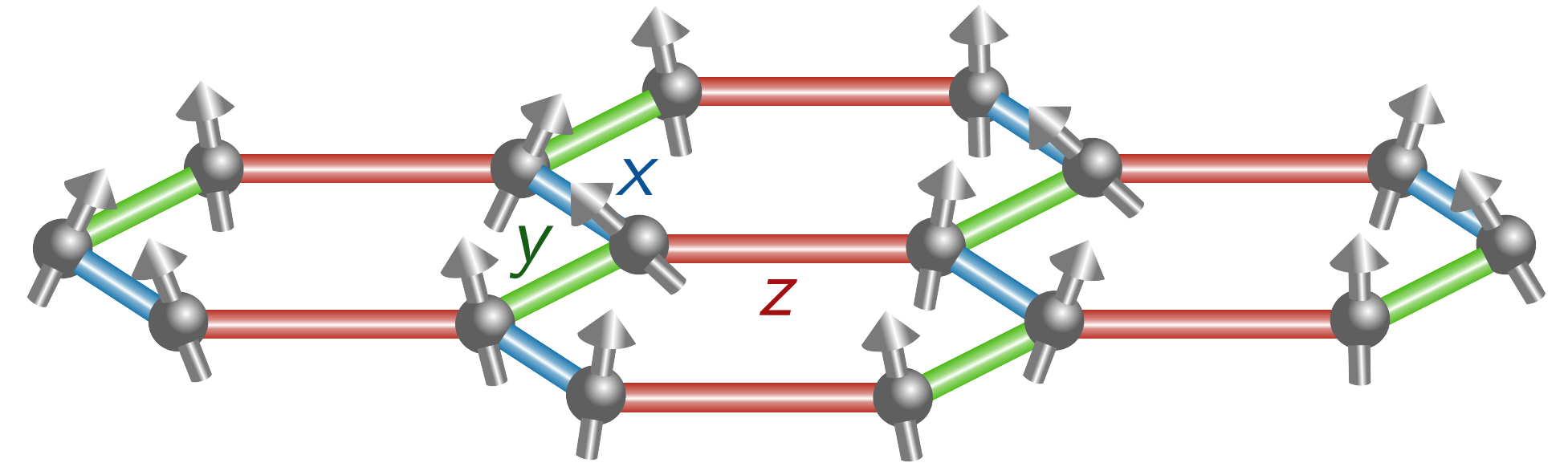
spin

4 Majoranas
with gauge constraint

Example #3: Fractionalized Systems

Kitaev spin-1/2 model:

$$\mathcal{H} = K \left(\sum_{\langle ij \rangle_x} \sigma_i^x \sigma_j^x + \sum_{\langle ij \rangle_y} \sigma_i^y \sigma_j^y + \sum_{\langle ij \rangle_z} \sigma_i^z \sigma_j^z \right)$$

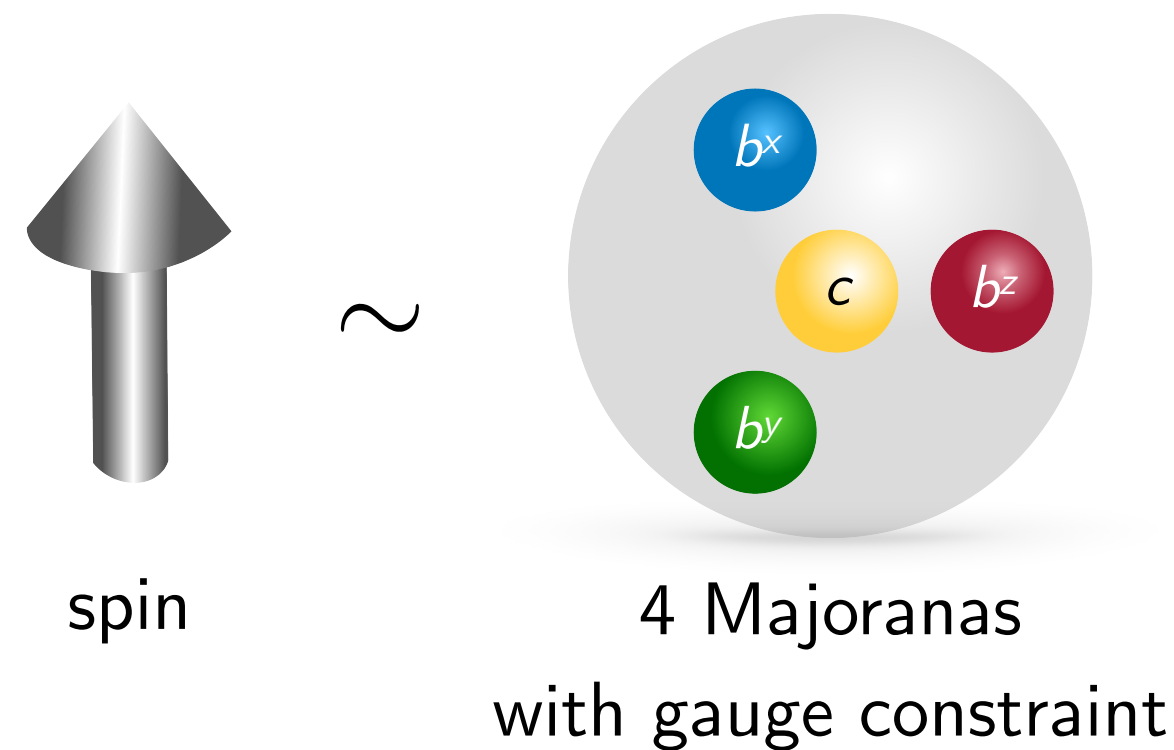


Majorana representation:

$$\sigma^x \sim i b^x c$$

$$\sigma^y \sim i b^y c$$

$$\sigma^z \sim i b^z c$$



Fractionalization:

$$\mathcal{H} \sim iK \sum_{\langle ij \rangle_\alpha} \underbrace{(i b_i^\alpha b_j^\alpha)}_{\equiv \hat{u}_{ij} = \hat{u}_{ij}^\dagger} c_i c_j$$

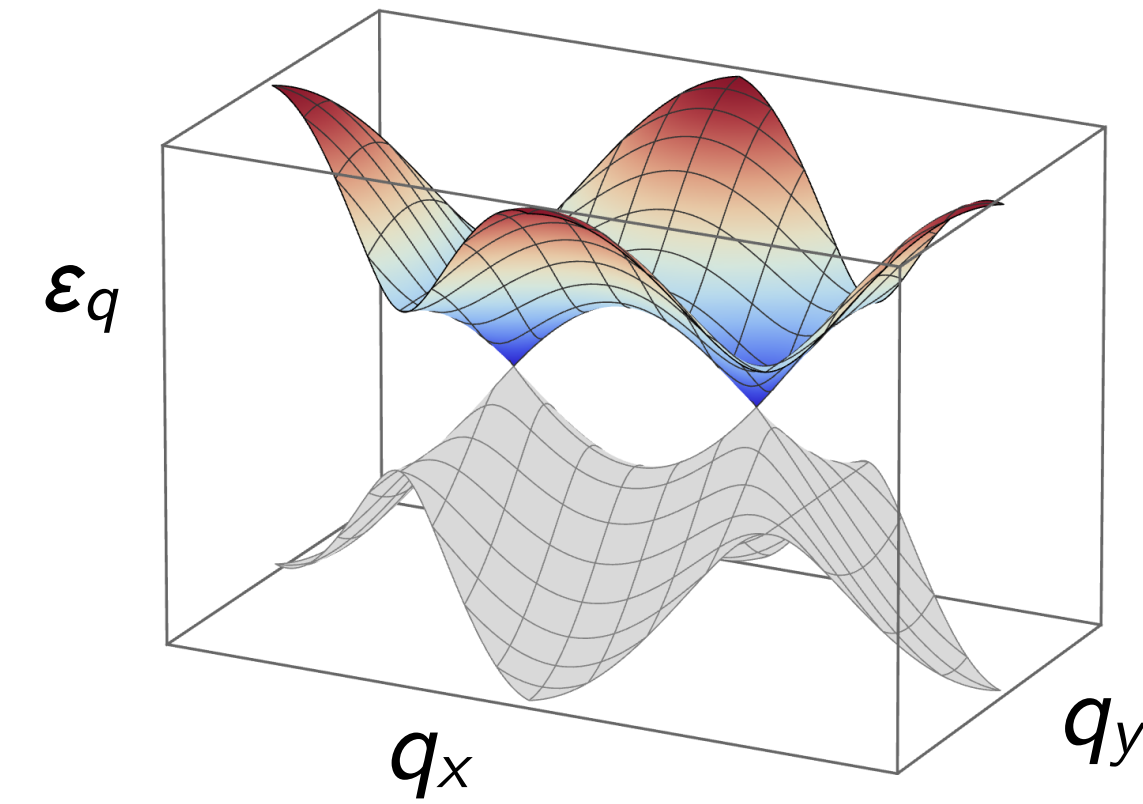
with $[\hat{u}_{ij}, \tilde{\mathcal{H}}] = 0 \Rightarrow$ static \mathbb{Z}_2 gauge field!

Kitaev quantum spin liquid

Ground state:

$$\hat{u}_{ij} \mapsto u_{ij} \equiv 1 \quad \Rightarrow \quad \mathcal{H} \sim iK \sum_{\langle ij \rangle} c_i c_j$$

Majorana spectrum:



Kitaev quantum spin liquid

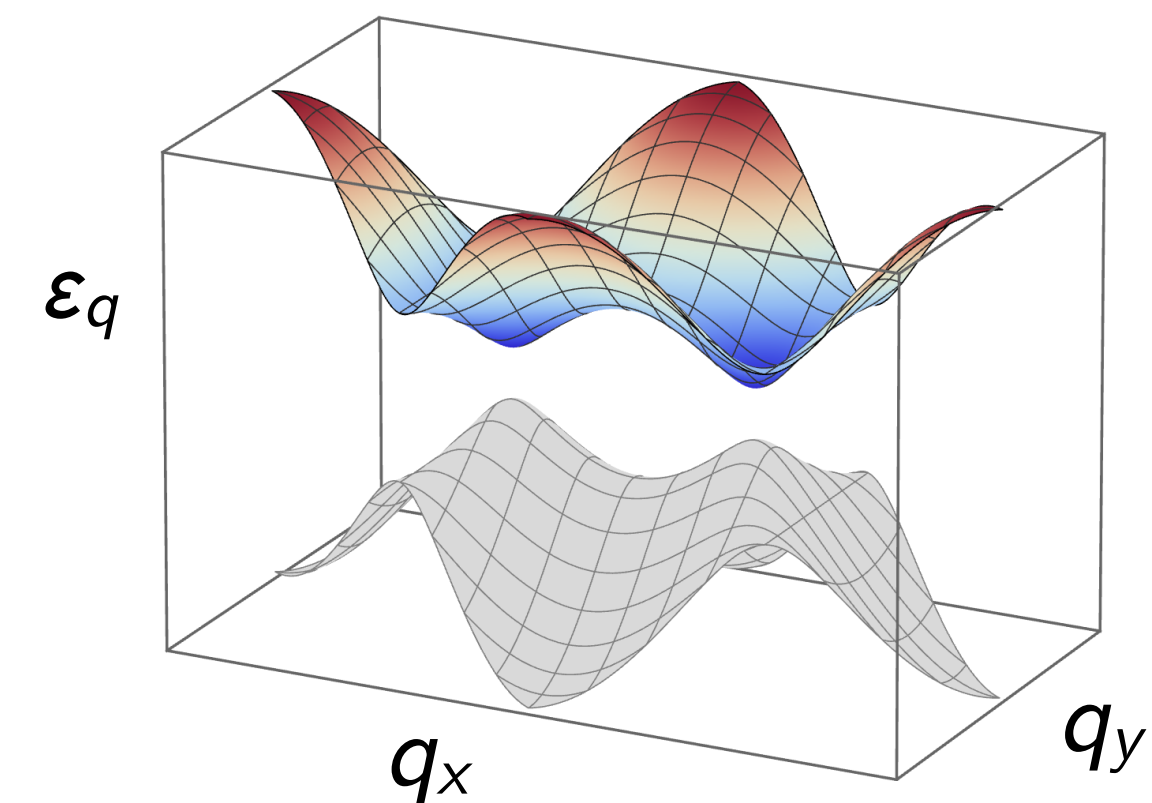
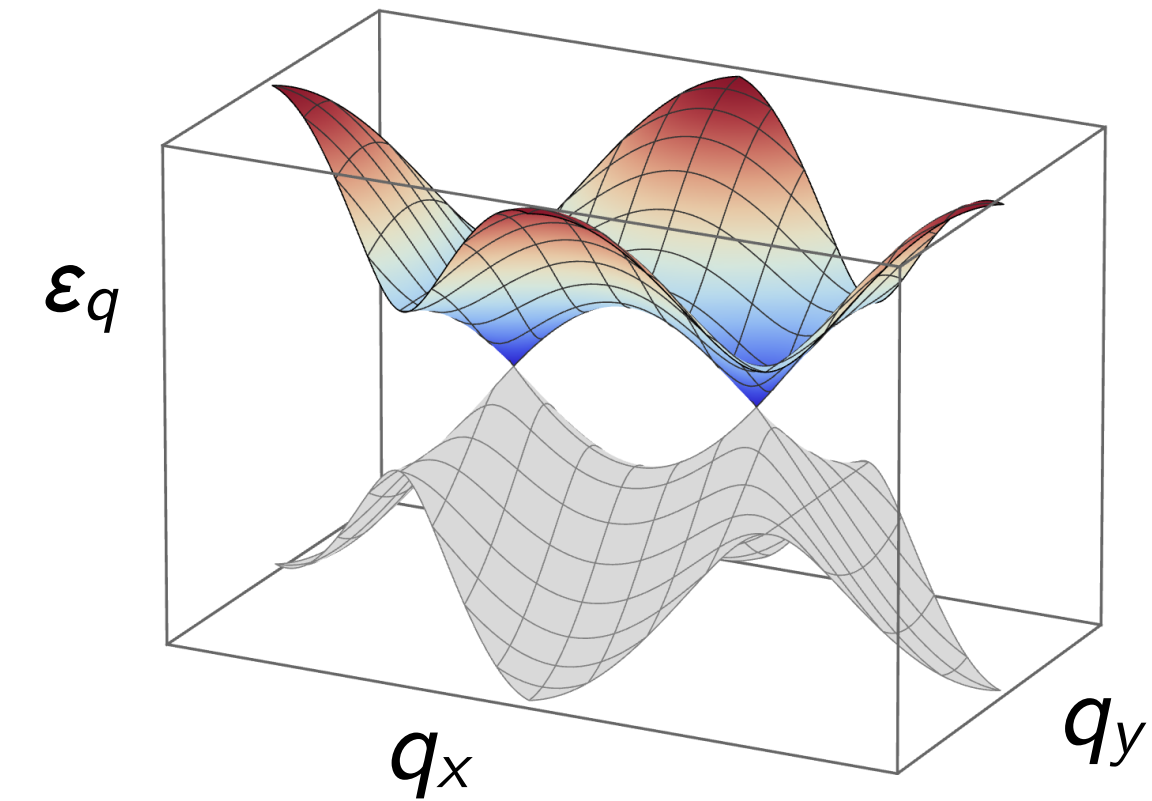
Ground state:

$$\hat{u}_{ij} \mapsto u_{ij} \equiv 1 \quad \longrightarrow \quad \mathcal{H} \sim iK \sum_{\langle ij \rangle} c_i c_j$$

External field $\vec{h} \parallel [111]$:

$$\mathcal{H} \mapsto \mathcal{H} - \vec{h} \cdot \sum_i \vec{\sigma}_i$$

Majorana spectrum:



with $\nu = 1$!

Kitaev quantum spin liquid

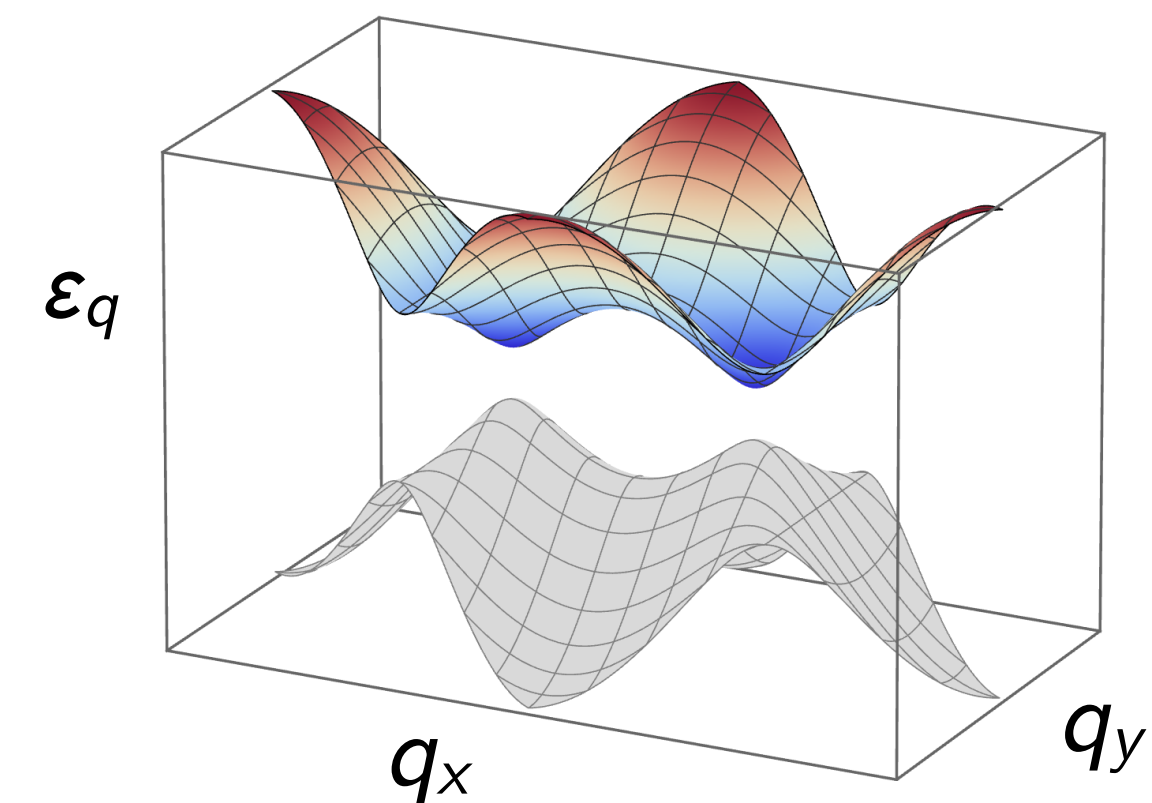
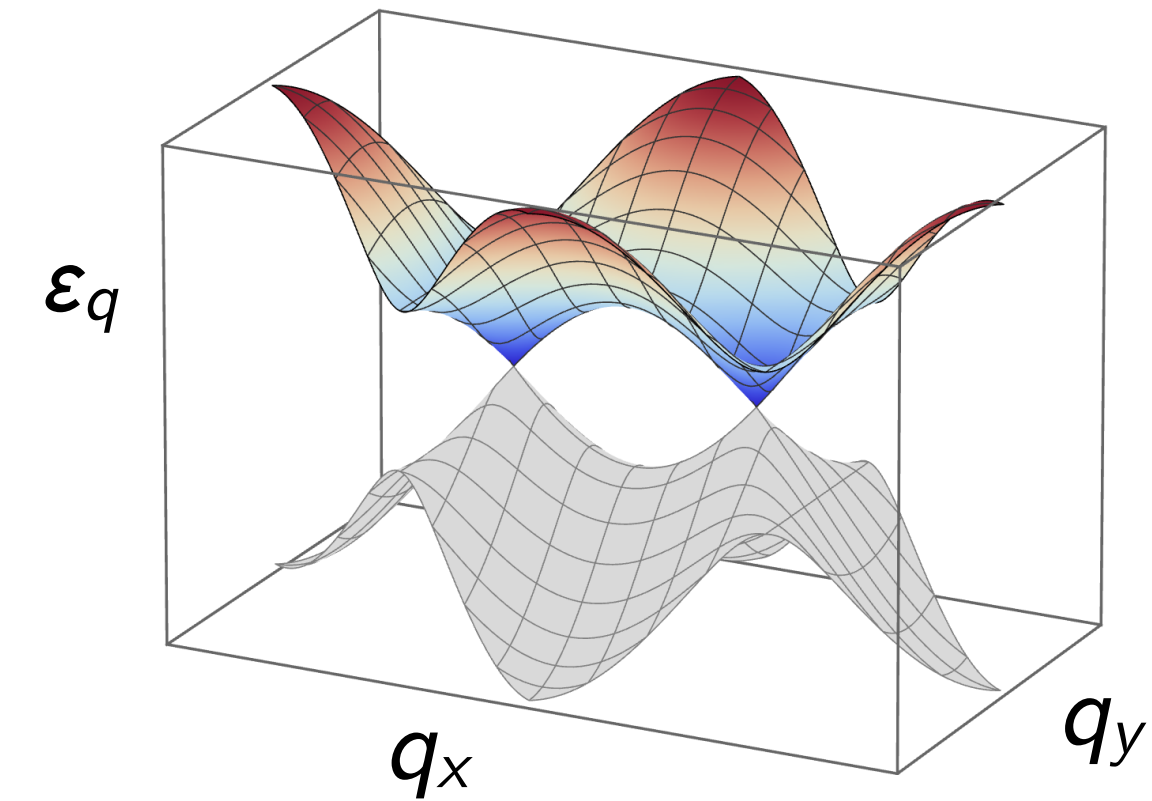
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External field $\vec{h} \parallel [111]$:

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Majorana spectrum:

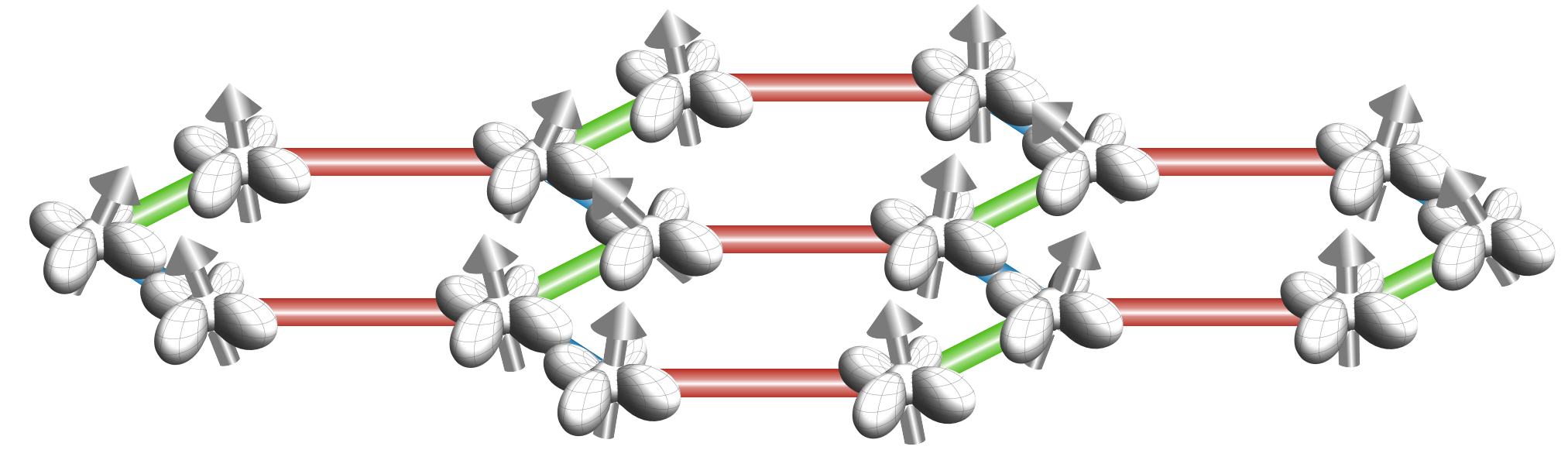


with $\nu = 1$!

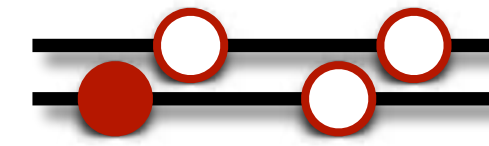
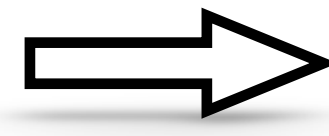
\Rightarrow Fractionalized version of topological insulator!

Beyond Kitaev spin-1/2

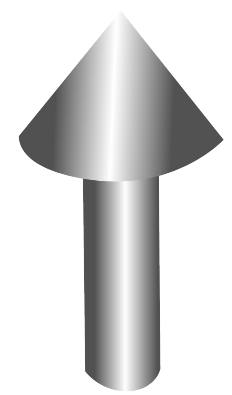
Spin-orbital generalization:



$$\sigma^\alpha \quad 2 \times 2$$

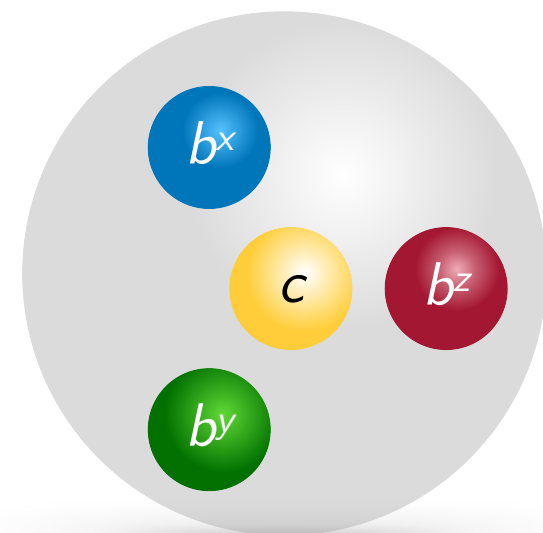


$$\gamma^i = \sigma^\alpha \otimes \tau^\beta \quad 4 \times 4$$

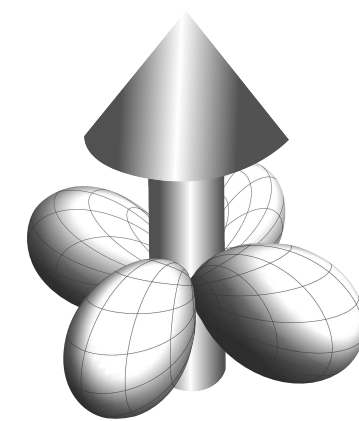


spin

~

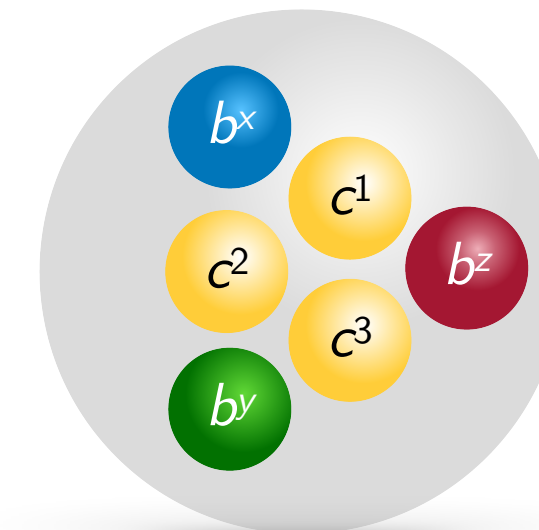


4 Majoranas
with gauge constraint



spin + orbital

~

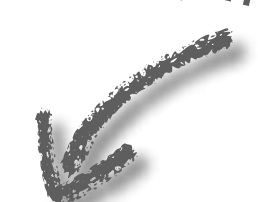


6 Majoranas
with gauge constraint

Kitaev-Heisenberg spin-orbital models

Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\alpha} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\alpha \tau_j^\alpha}_{\mapsto \hat{u}_{ij} c_i^\top c_j} + J \sum_{\langle ij \rangle} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j}_{\mapsto \frac{1}{4} (c_i^\top \vec{L} c_i) \cdot (c_j^\top \vec{L} c_j)}$$

spin-1 matrices 

with $[\hat{u}_{ij}, \mathcal{H}] = 0$ still static!

Kitaev-Heisenberg spin-orbital models

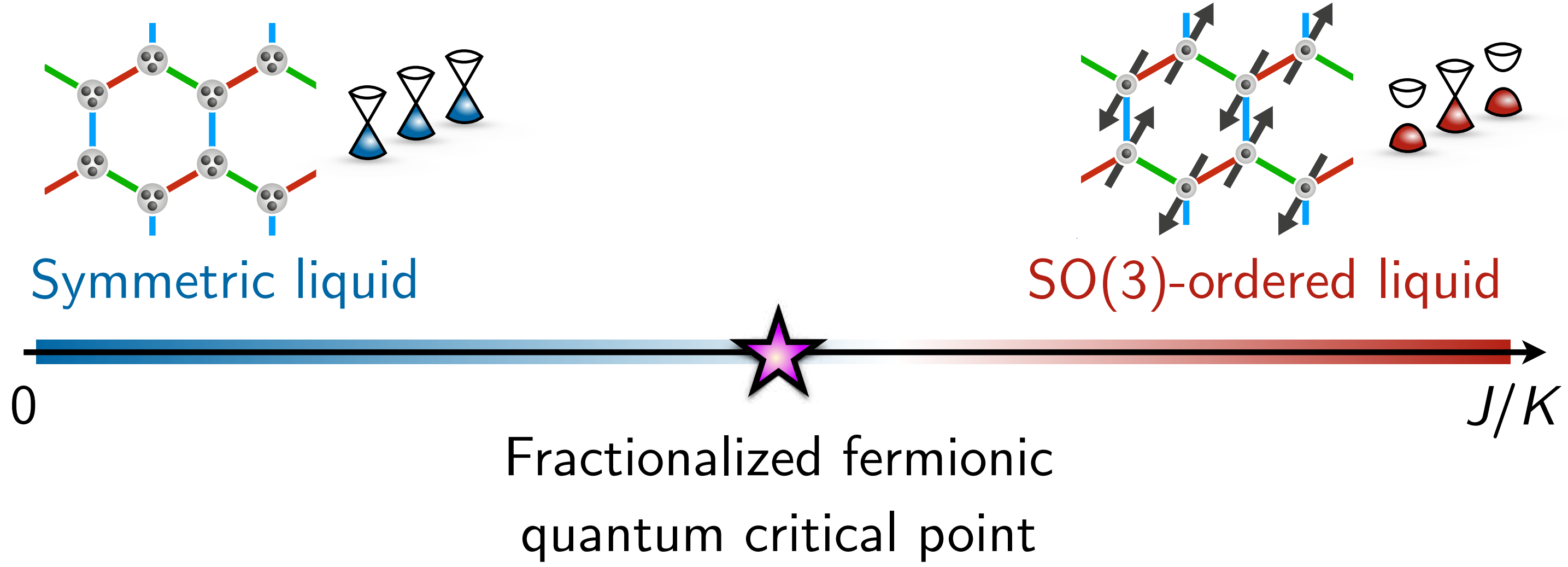
Hamiltonian:

$$\mathcal{H} = K \sum_{\langle ij \rangle_\alpha} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \tau_i^\alpha \tau_j^\alpha}_{\mapsto \hat{u}_{ij} c_i^\top c_j} + J \sum_{\langle ij \rangle} \underbrace{\vec{\sigma}_i \cdot \vec{\sigma}_j \otimes \mathbb{1}_i \mathbb{1}_j}_{\mapsto \frac{1}{4} (c_i^\top \vec{L} c_i) \cdot (c_j^\top \vec{L} c_j)}$$

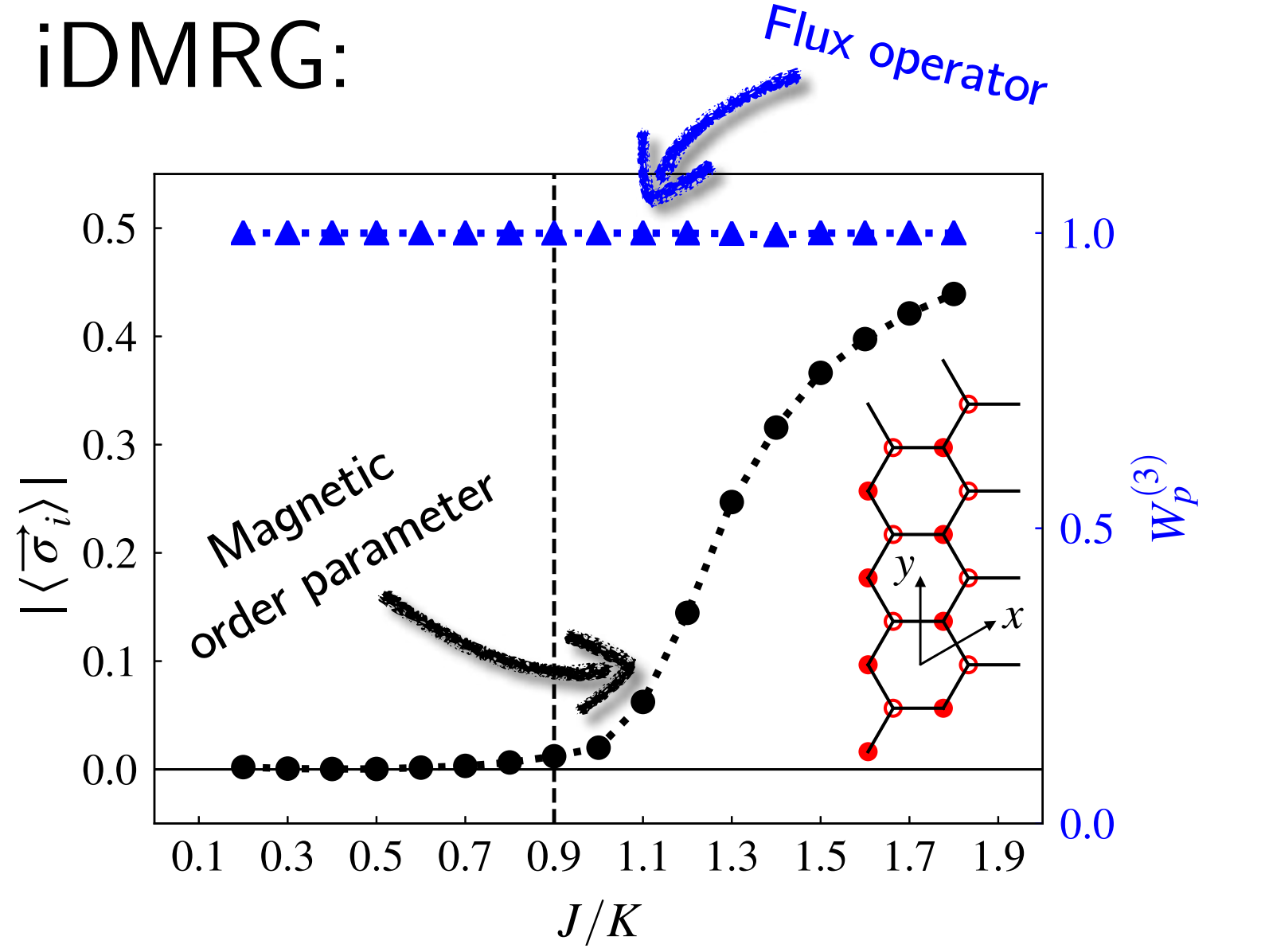
spin-1 matrices

with $[\hat{u}_{ij}, \mathcal{H}] = 0$ still static!

Phase diagram:



iDMRG:

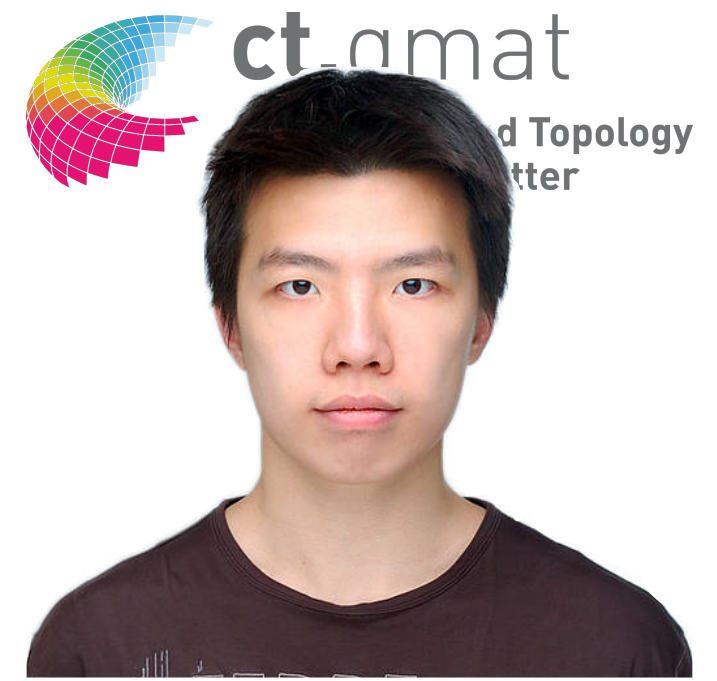
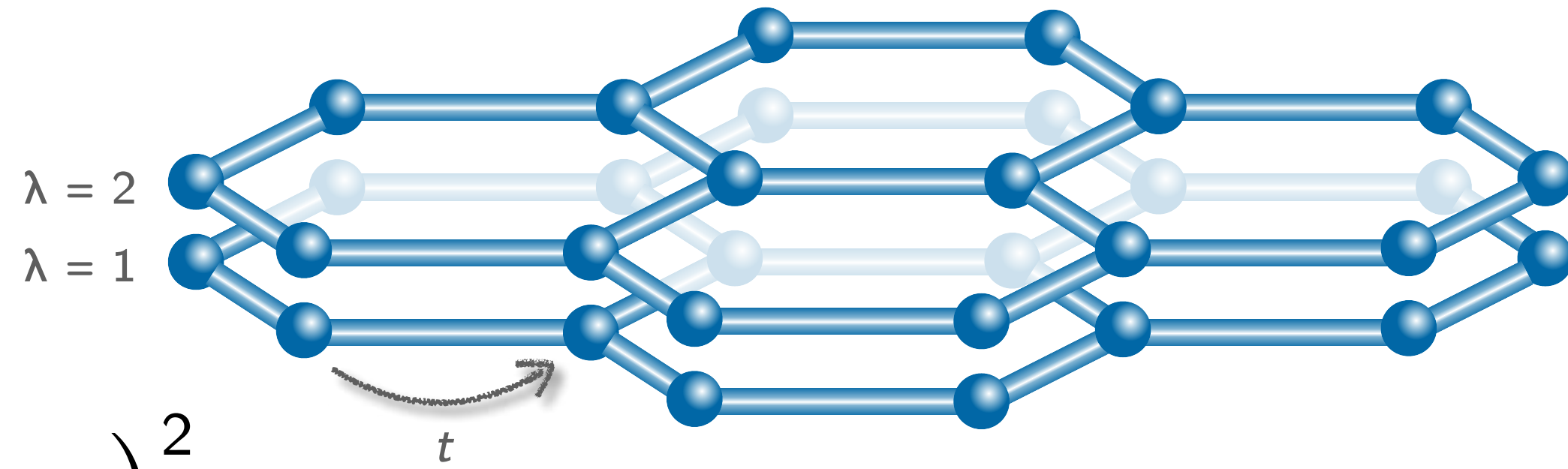


[Seifert, Dong, et int., LJ, PRL '20]

Effective low-energy model

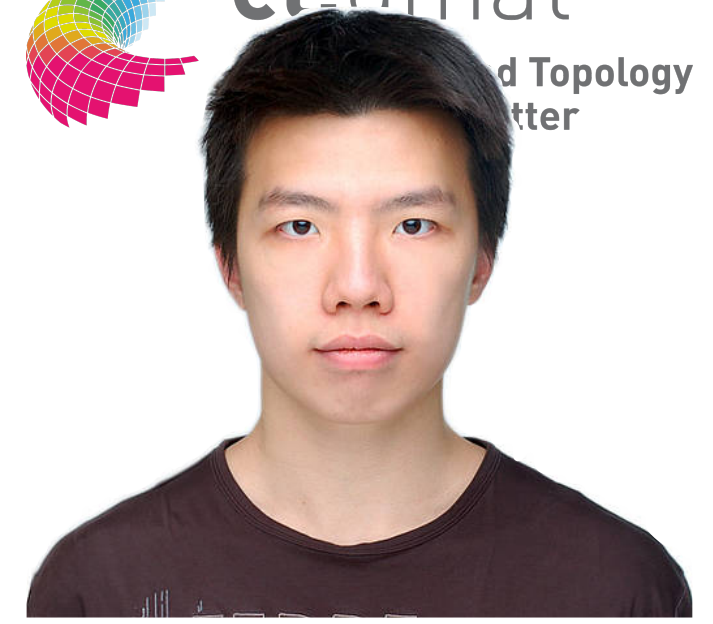
Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_{i\lambda}^\dagger c_{j\lambda} - J \sum_i \left(c_{i\lambda}^\dagger \vec{L} \tau_{\lambda\lambda'}^z c_{i\lambda'} \right)^2$$



Zihong Liu

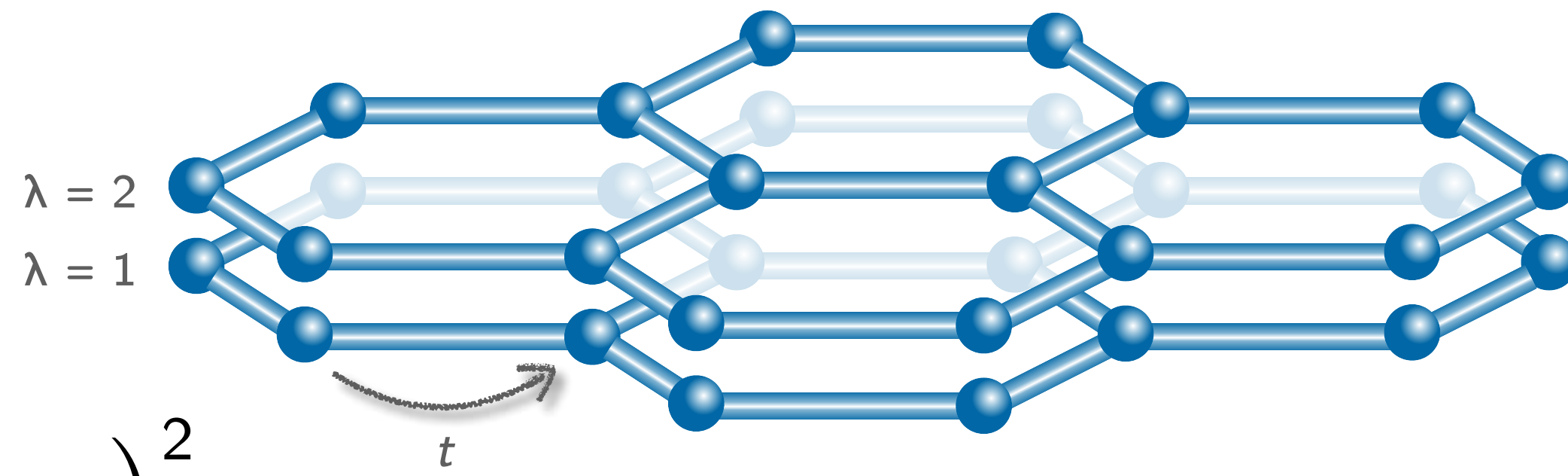
Effective low-energy model



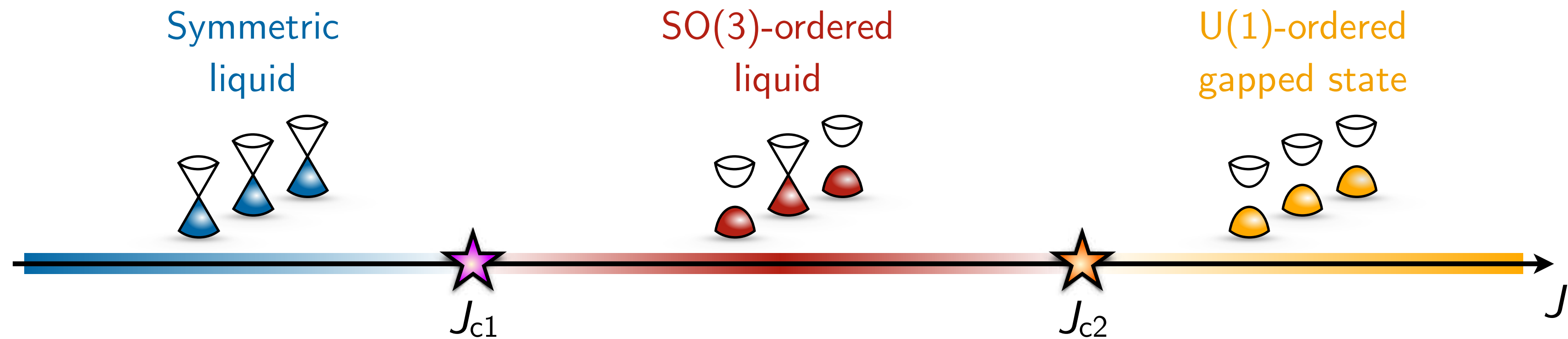
Zihong Liu

Hamiltonian:

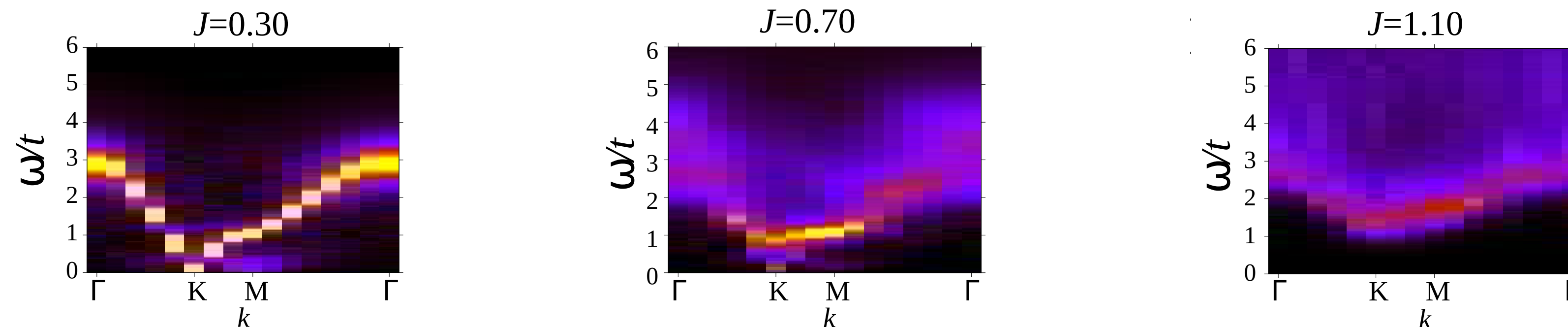
$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_{i\lambda}^\dagger c_{j\lambda} - J \sum_i \left(c_{i\lambda}^\dagger \vec{L} \tau_{\lambda\lambda'}^z c_{i\lambda'} \right)^2$$



Phase diagram:



Fermion spectral function:

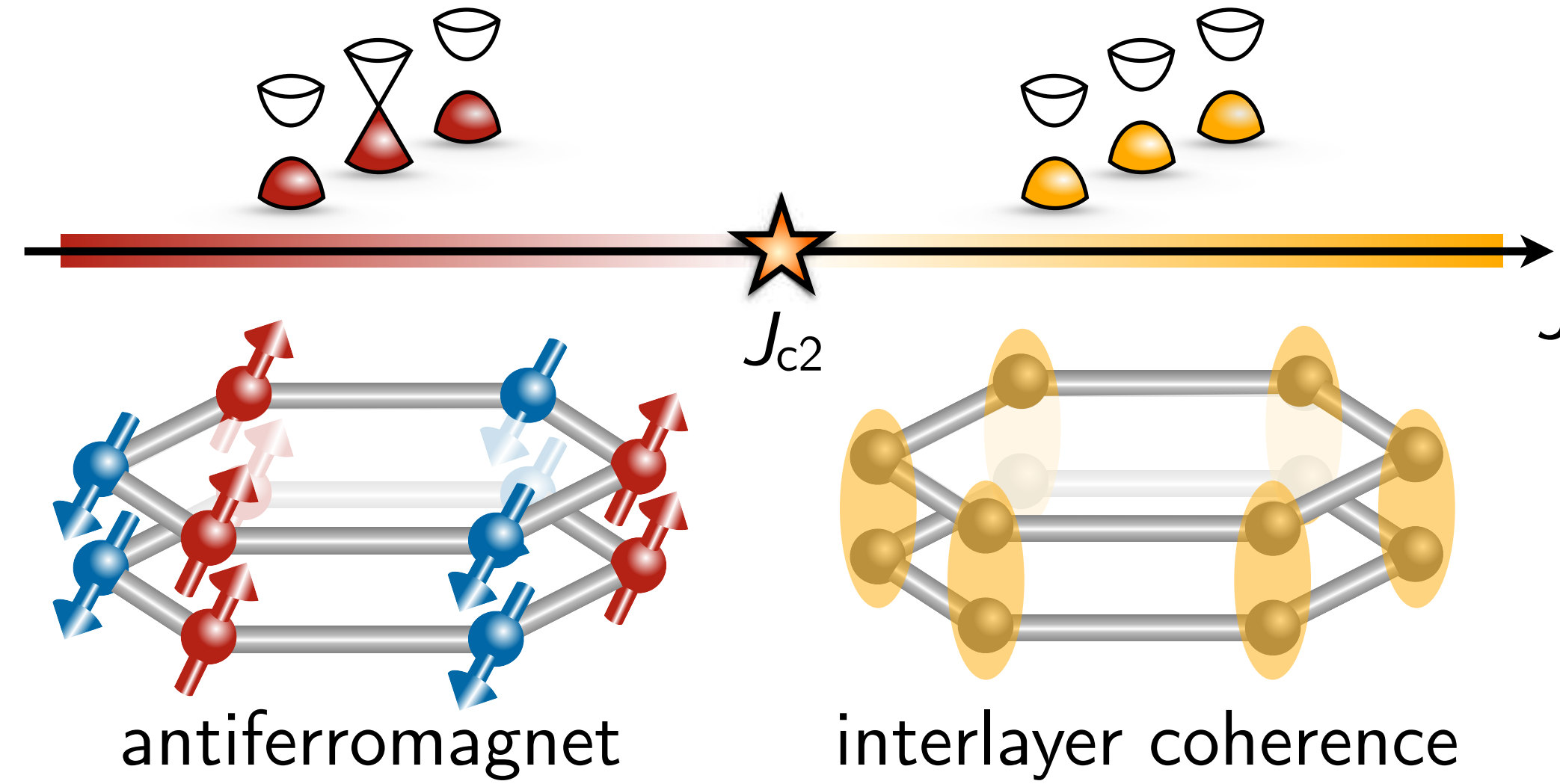


Deconfined Metal-Insulator Transition



Zihong Liu

Competing orders:

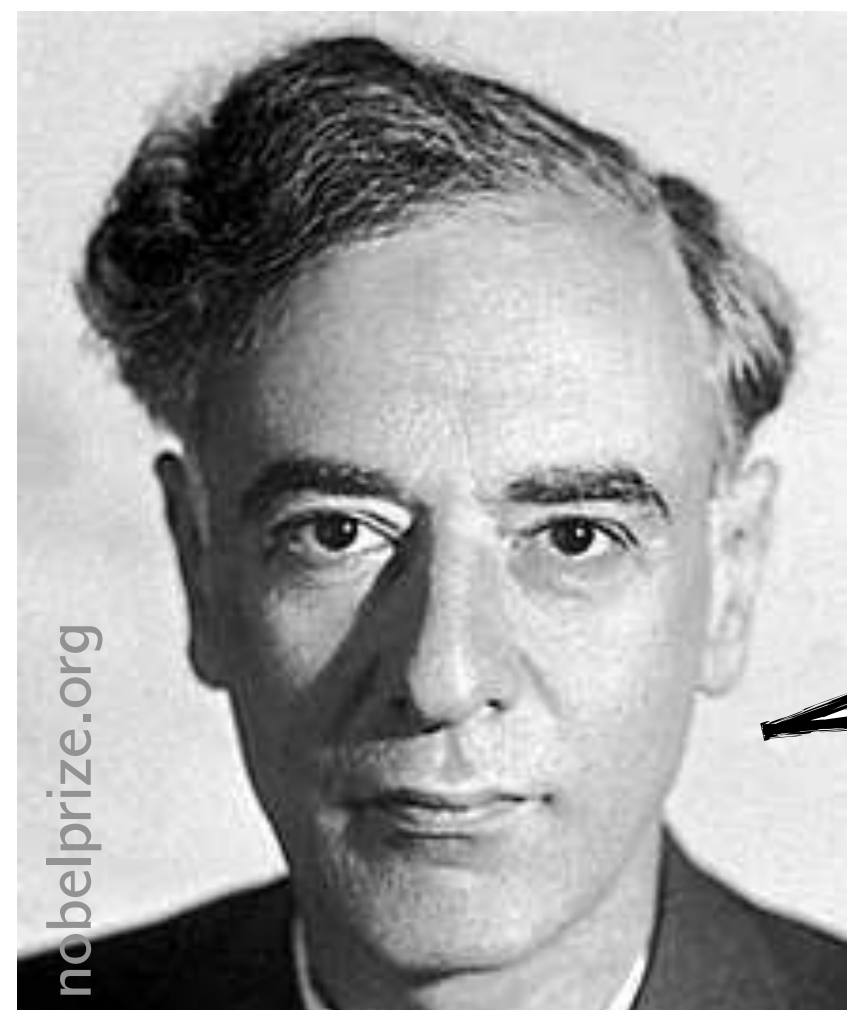
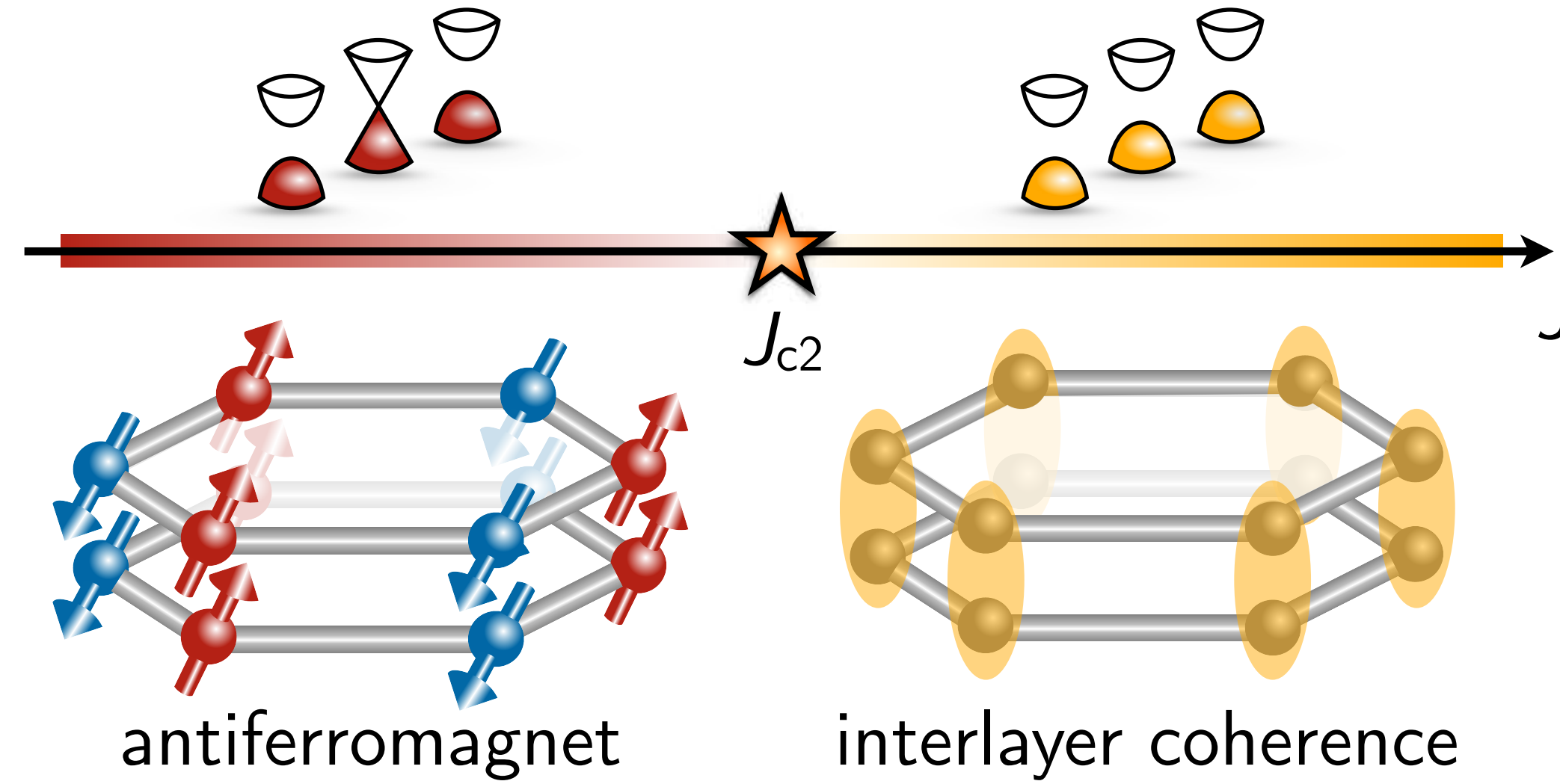


Deconfined Metal-Insulator Transition

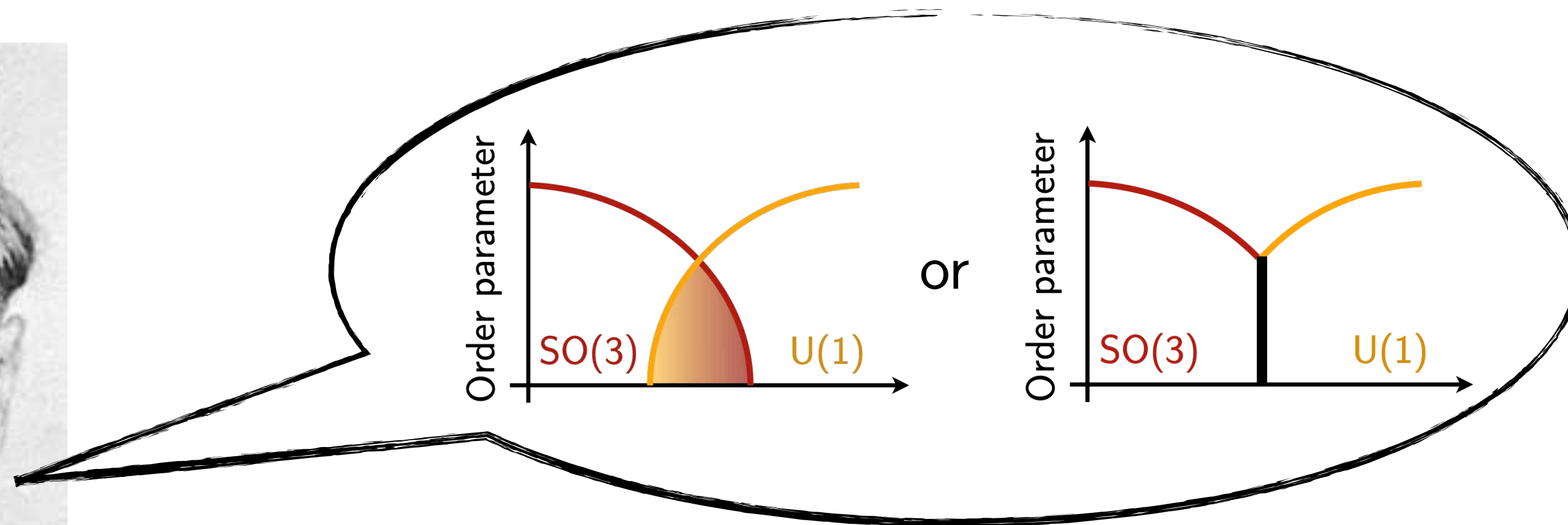


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Competing orders:



Landau

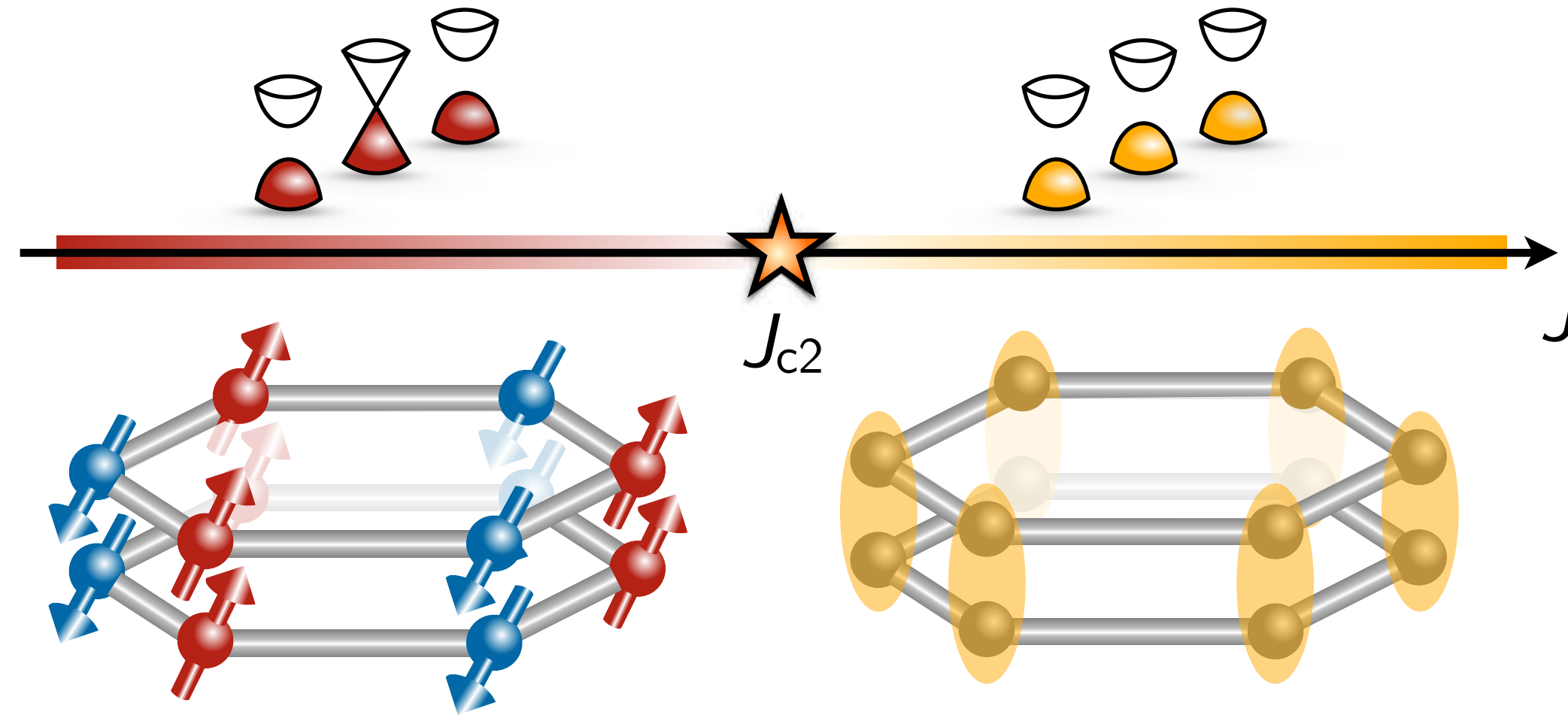


Deconfined Metal-Insulator Transition

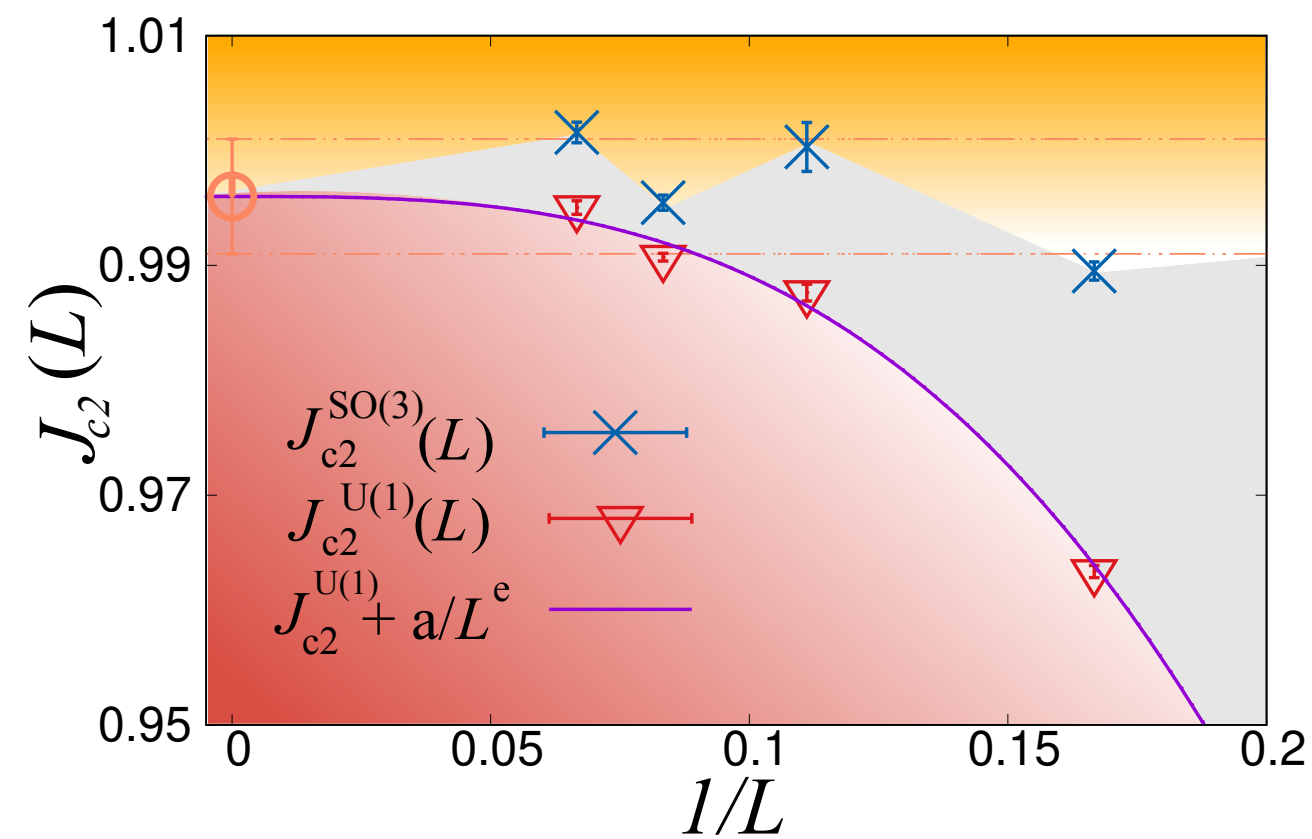


Zihong Liu

Competing orders:

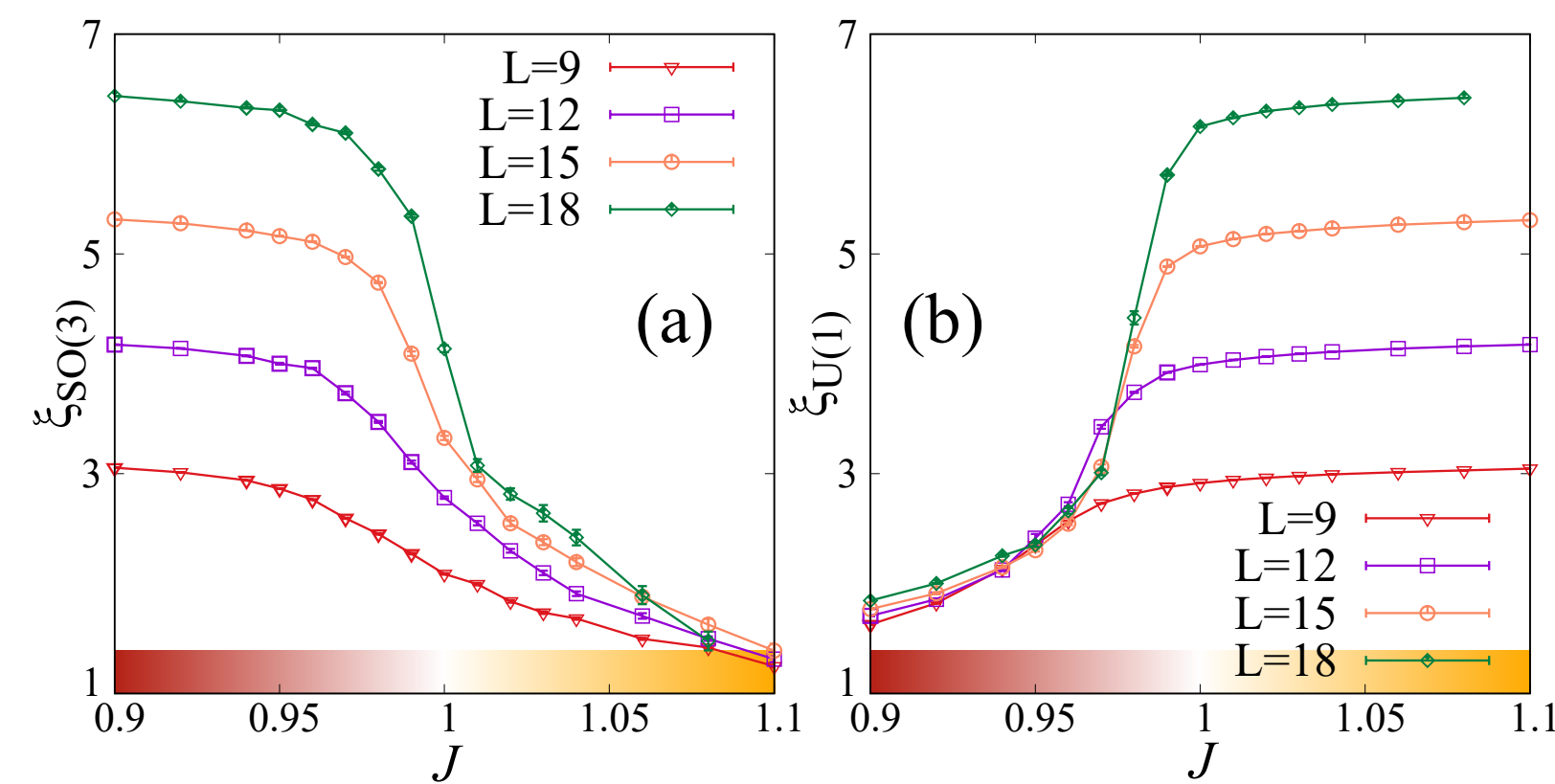


Quantum Monte Carlo:



direct ...

&



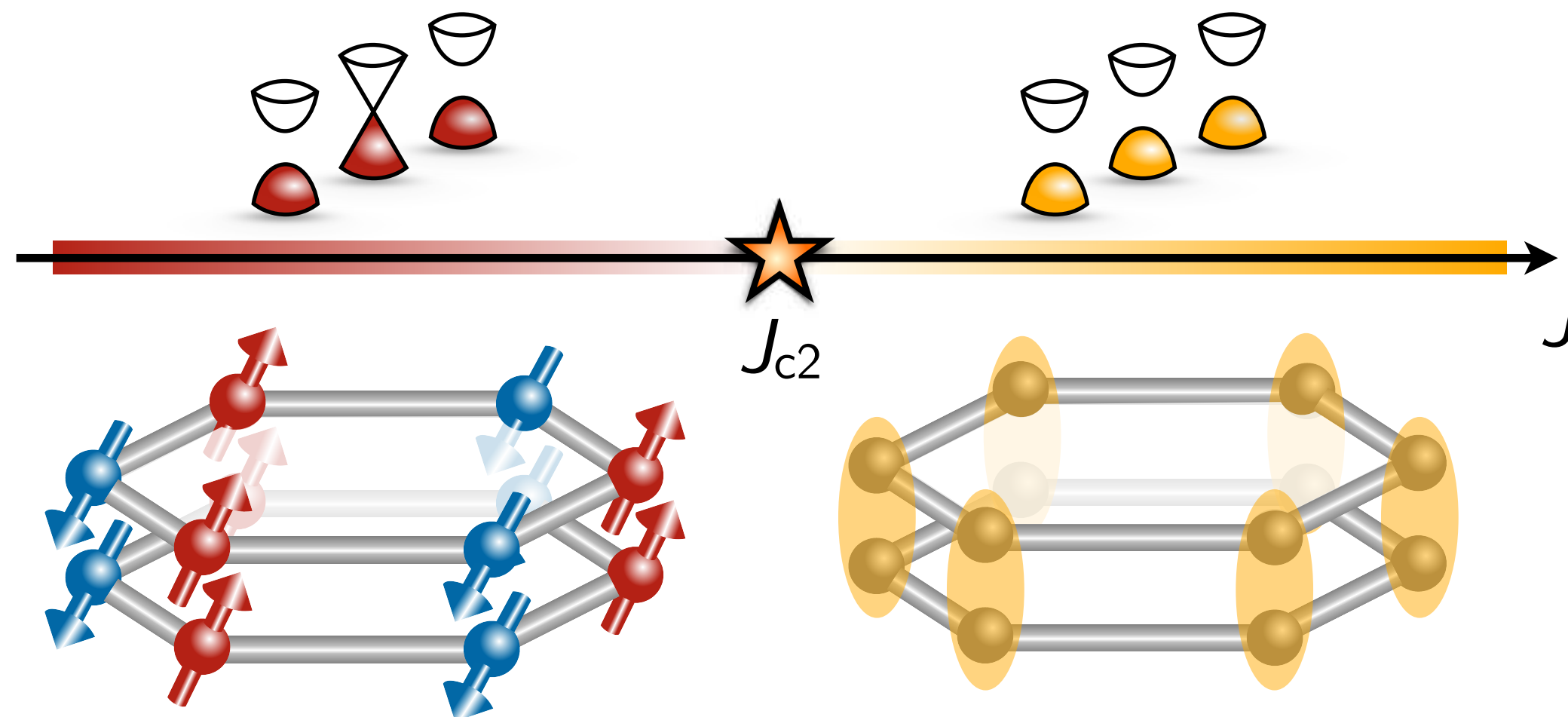
... continuous

Deconfined Metal-Insulator Transition

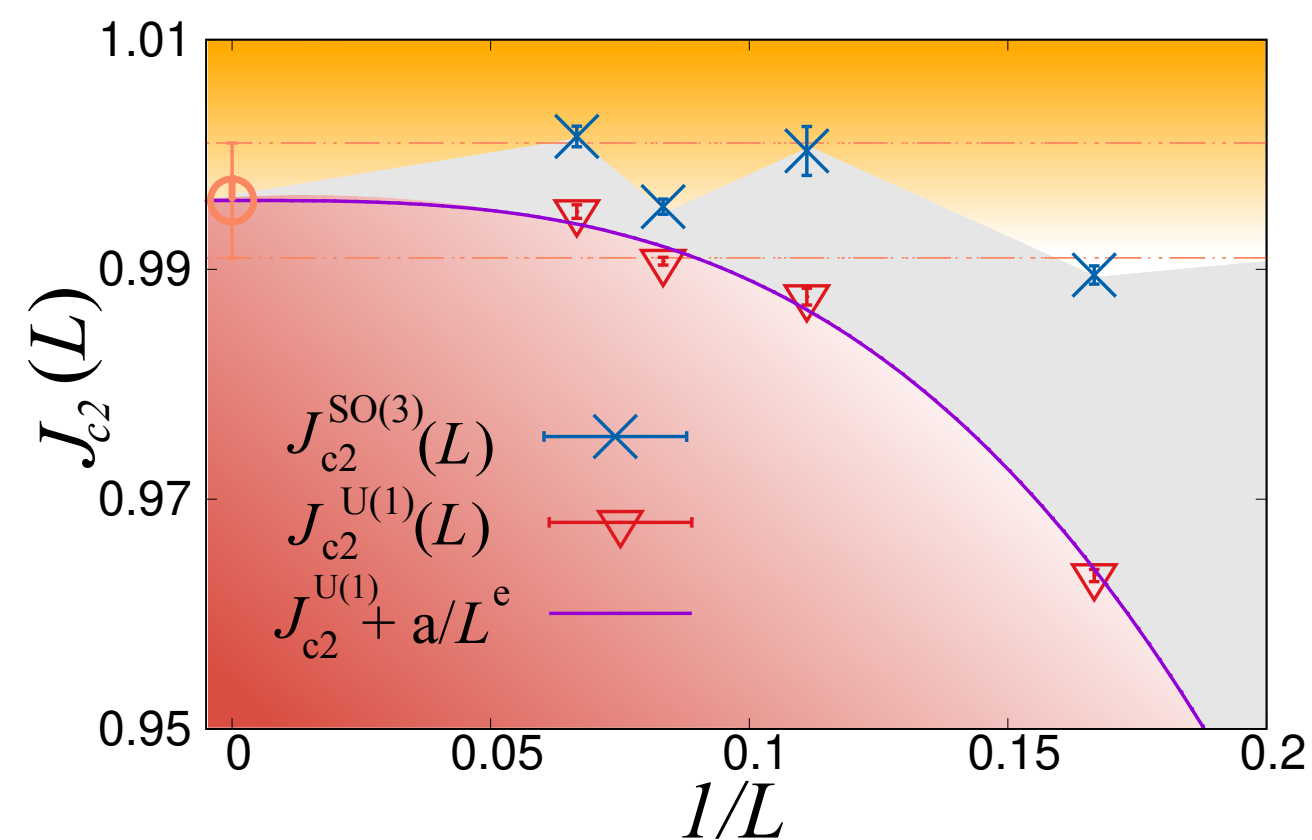


Zihong Liu

Competing orders:



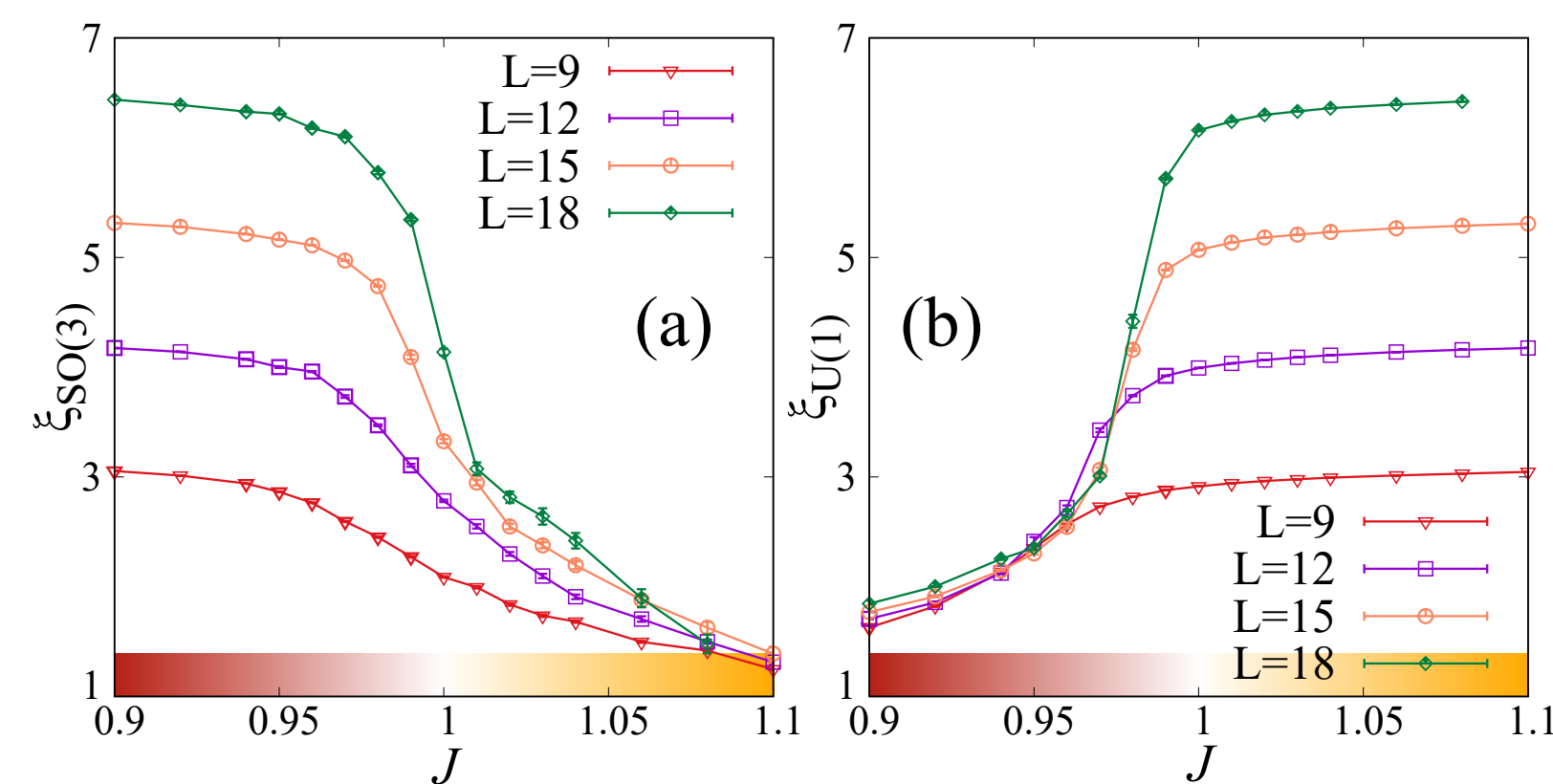
Quantum Monte Carlo:



direct ...

&

... continuous

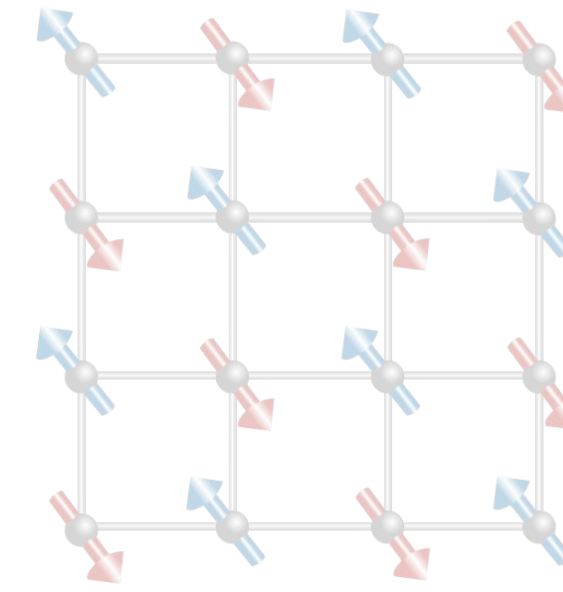


➔ Metallic deconfined quantum critical point!

Outline

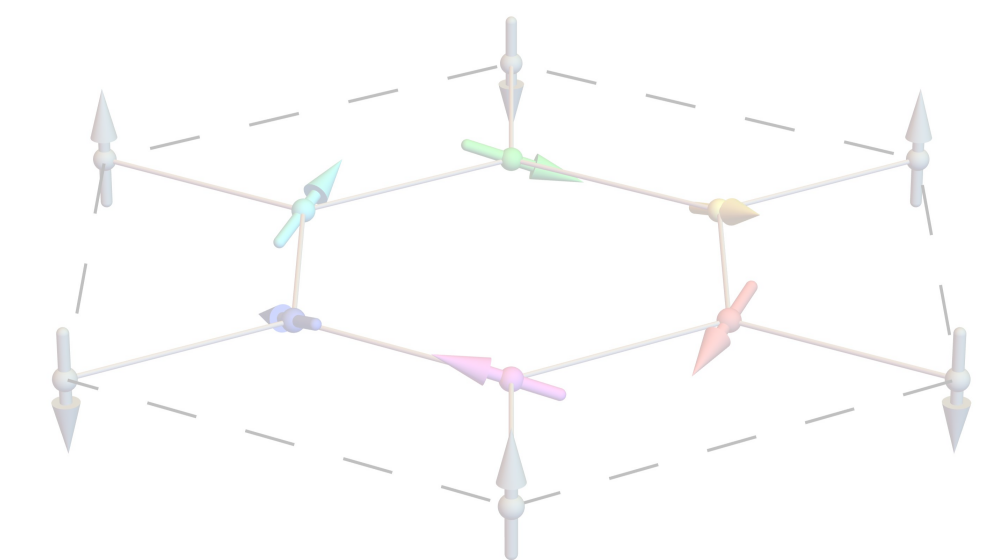
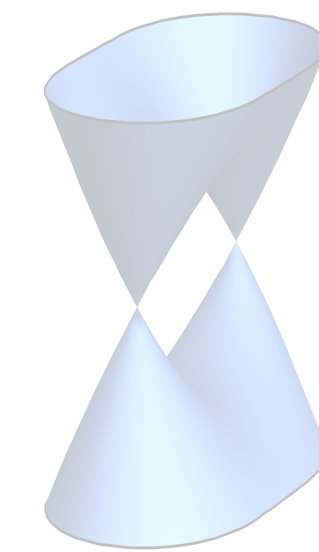
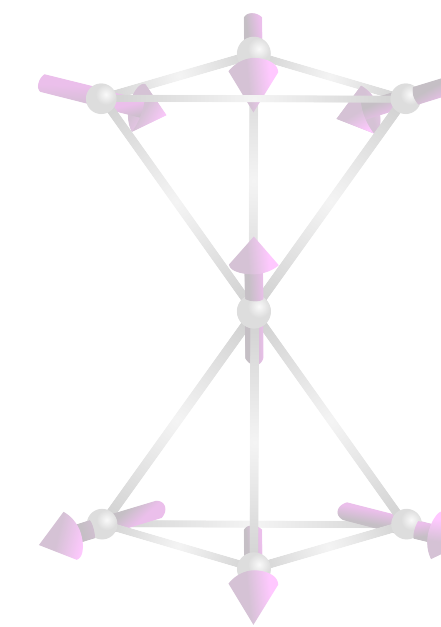
(1) Introduction

- ▶ Research Motivation
- ▶ Research Goals

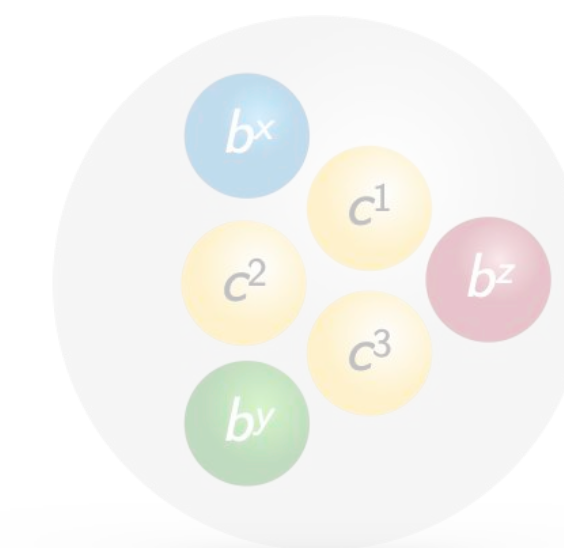


(2) Emergent Phenomena in Quantum Materials

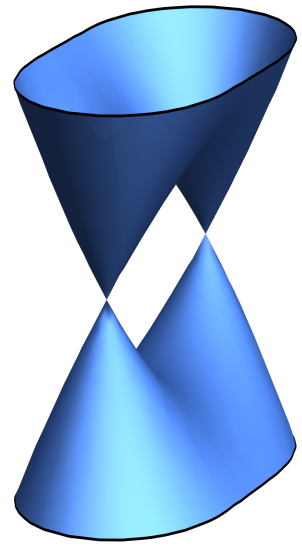
- ▶ Emergent Symmetries
- ▶ Emergent Topology
- ▶ Emergent Orders
- ▶ Emergent Particles



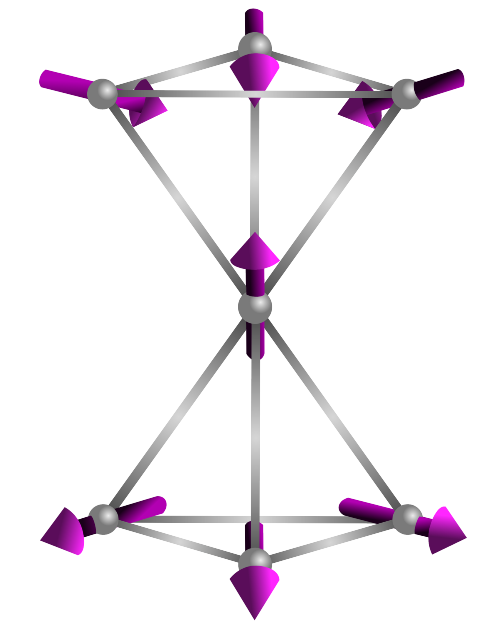
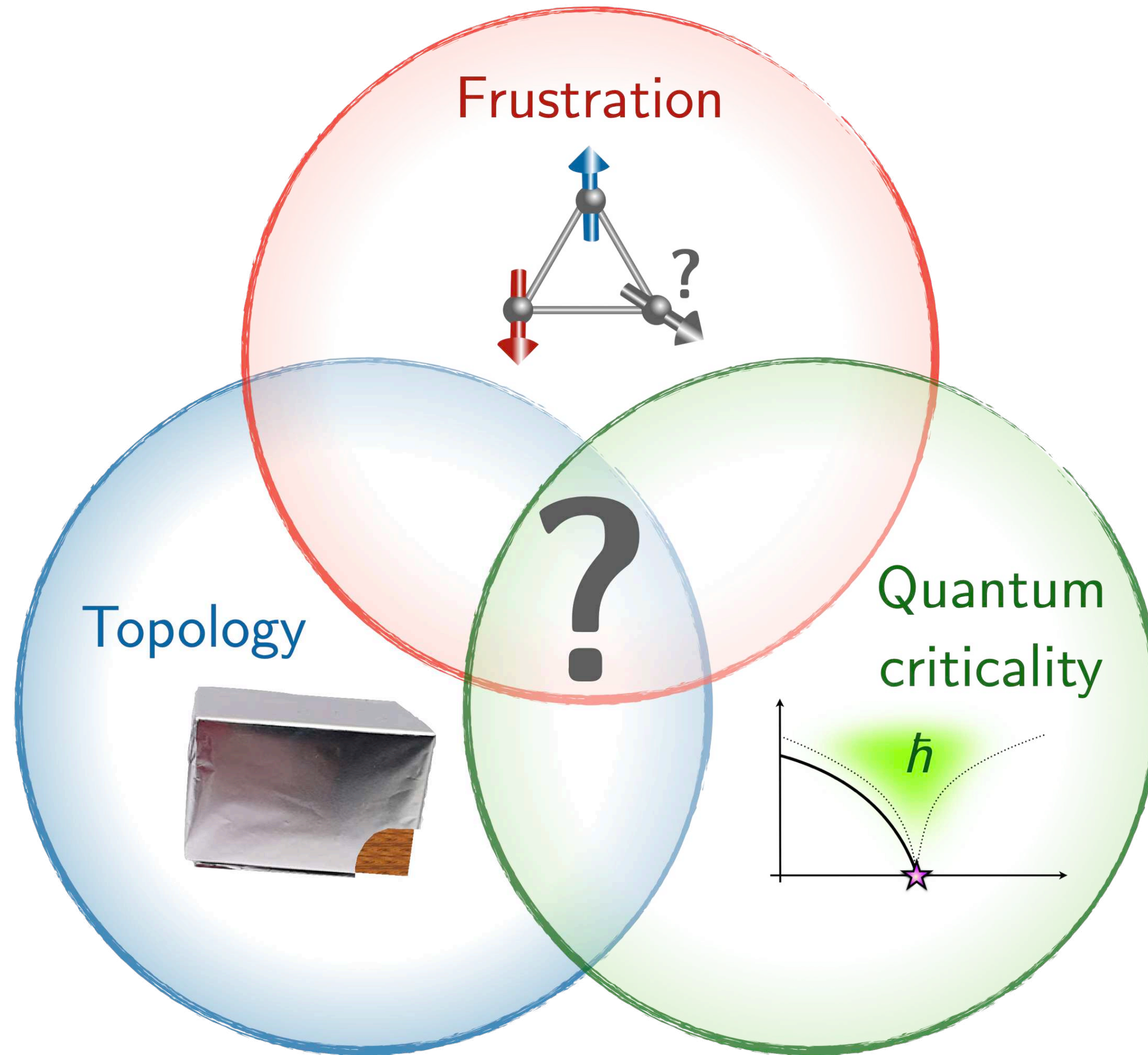
(3) Summary



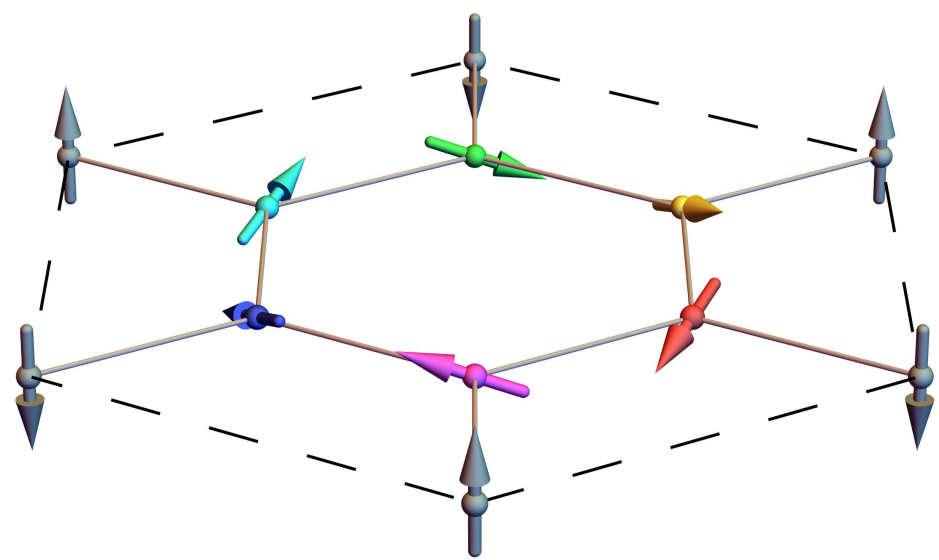
Emergent Phenomena in Quantum Materials



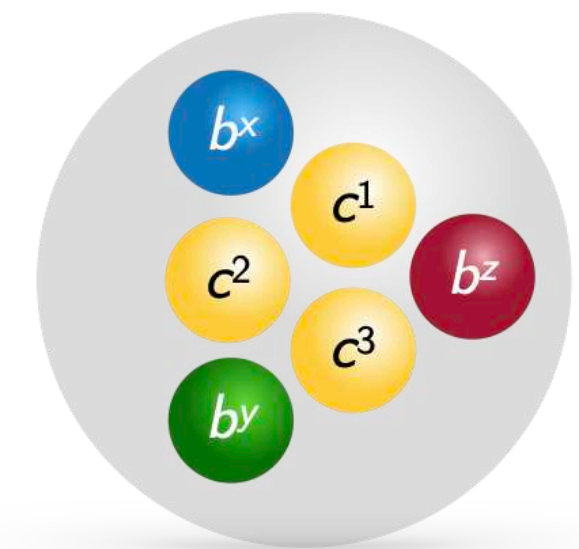
Emergent symmetries



Emergent topology



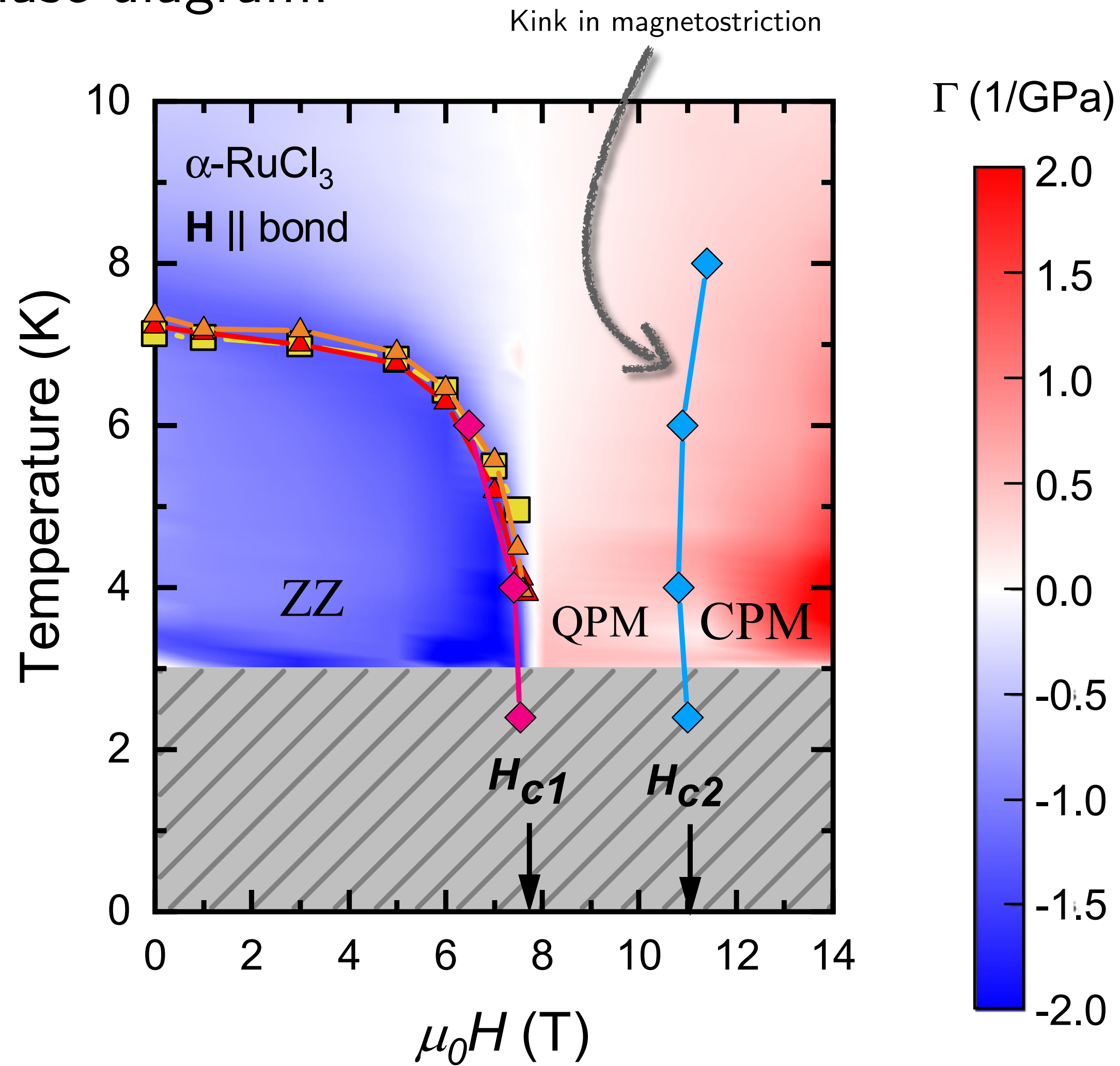
Emergent orders



Emergent particles

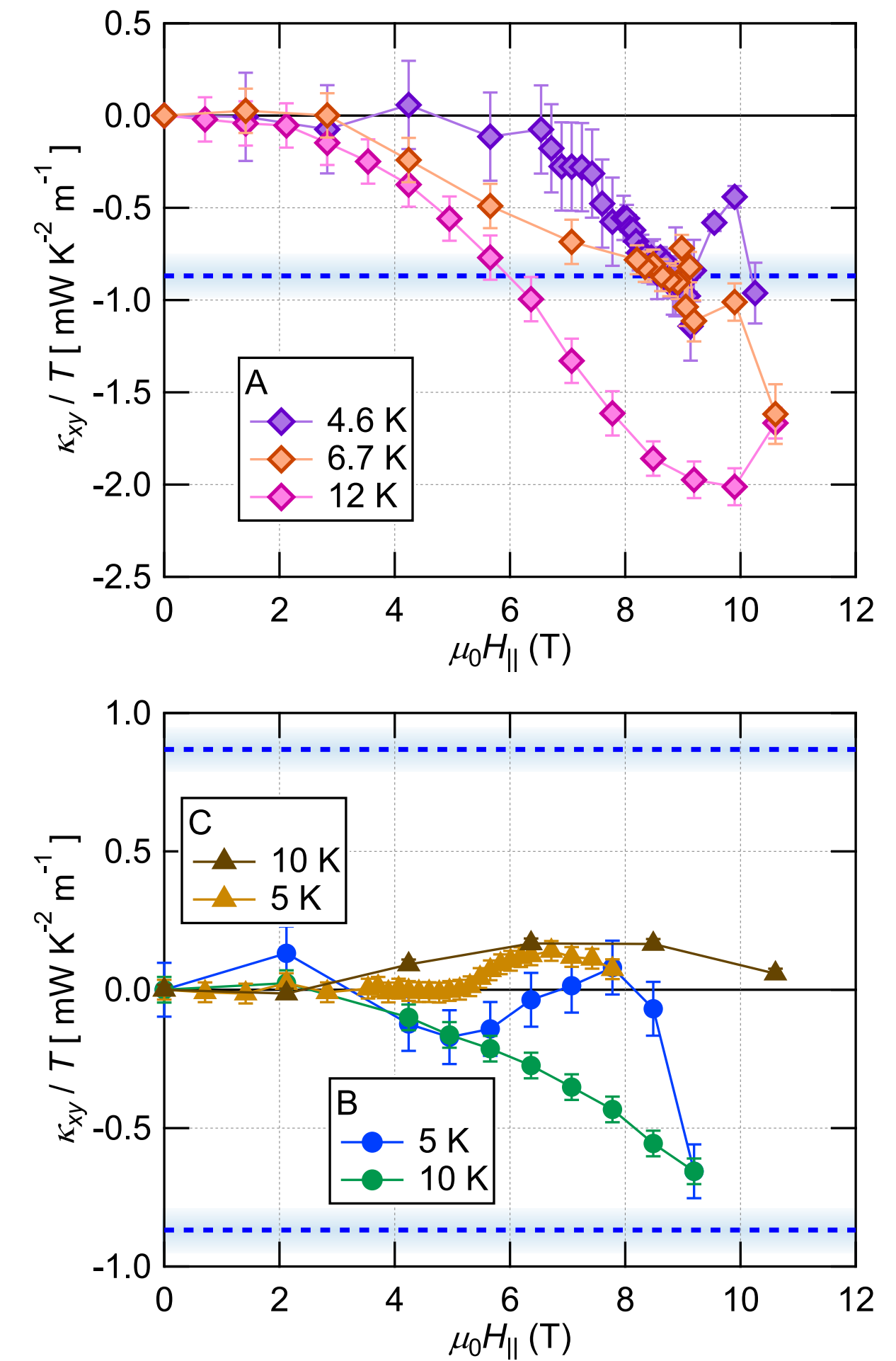
Field-Induced Quantum Paramagnet in α -RuCl₃

Phase diagram:



[Gass, *et int.*, LJ, *et al.*, PRB '20]

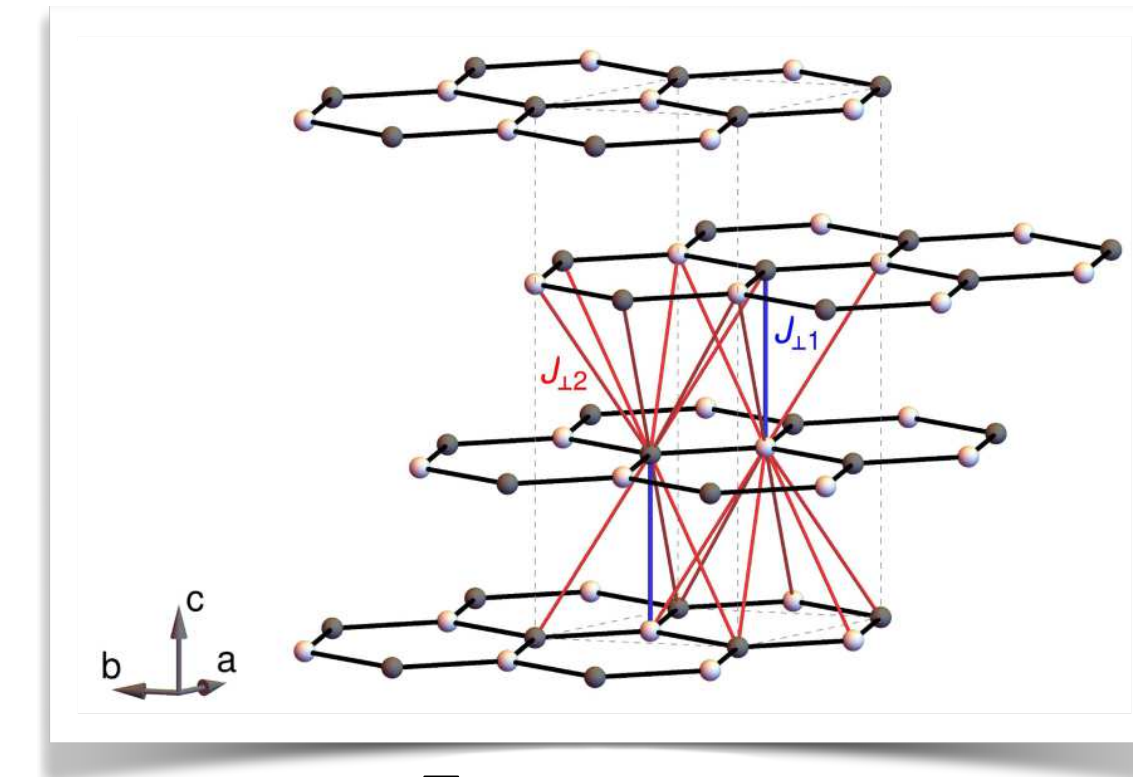
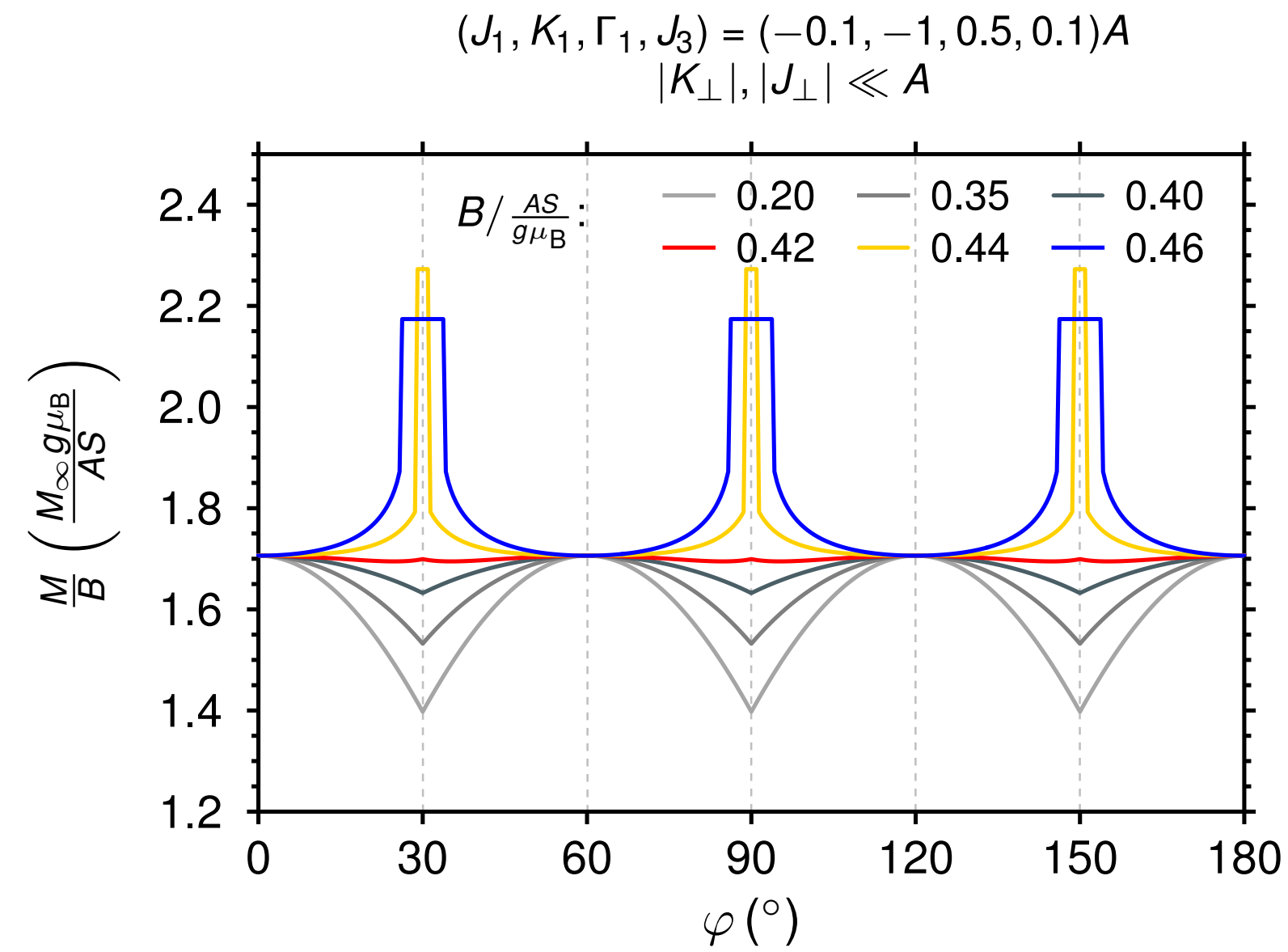
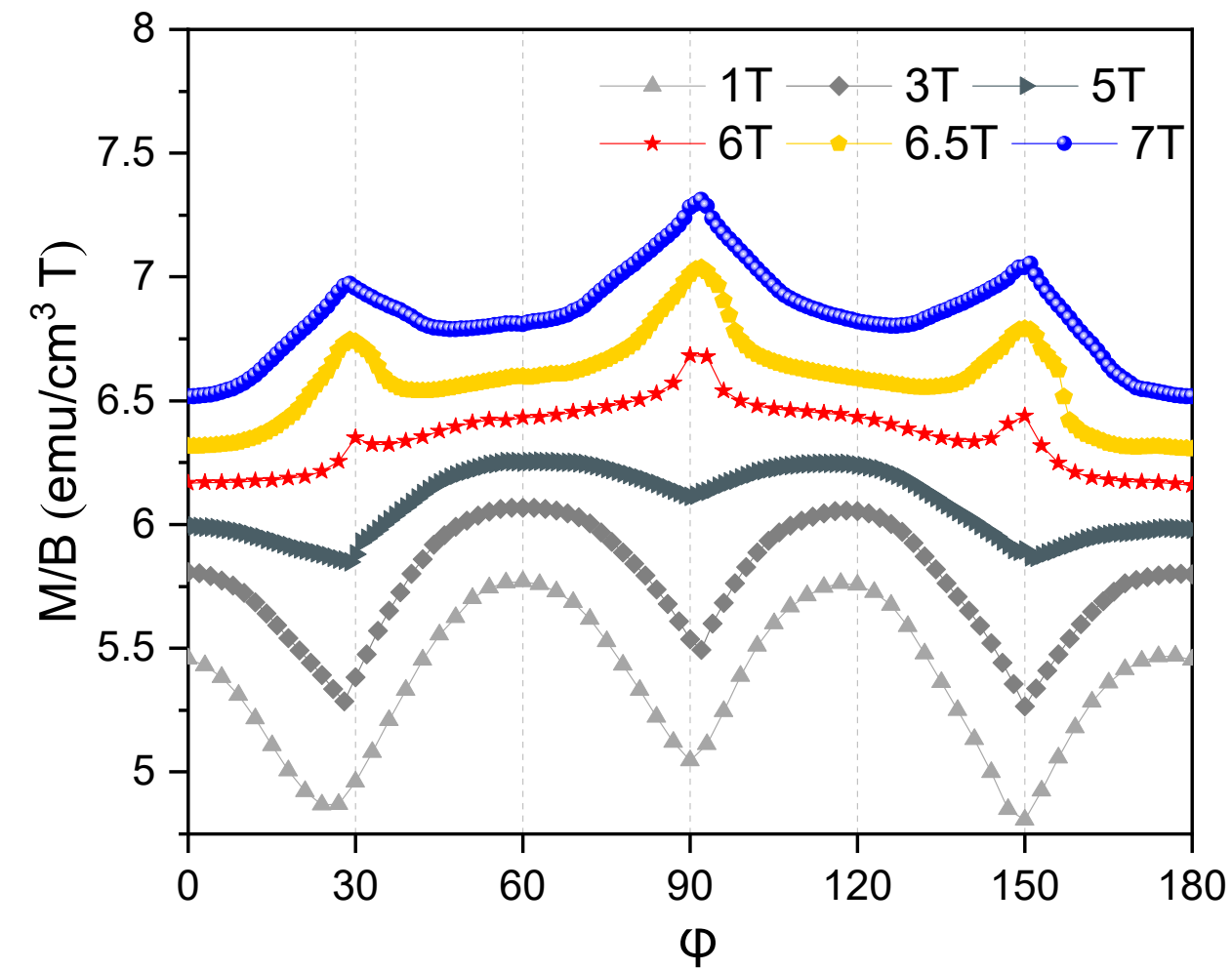
Sample dependence:



[Yamashita *et al.*, PRB '20]

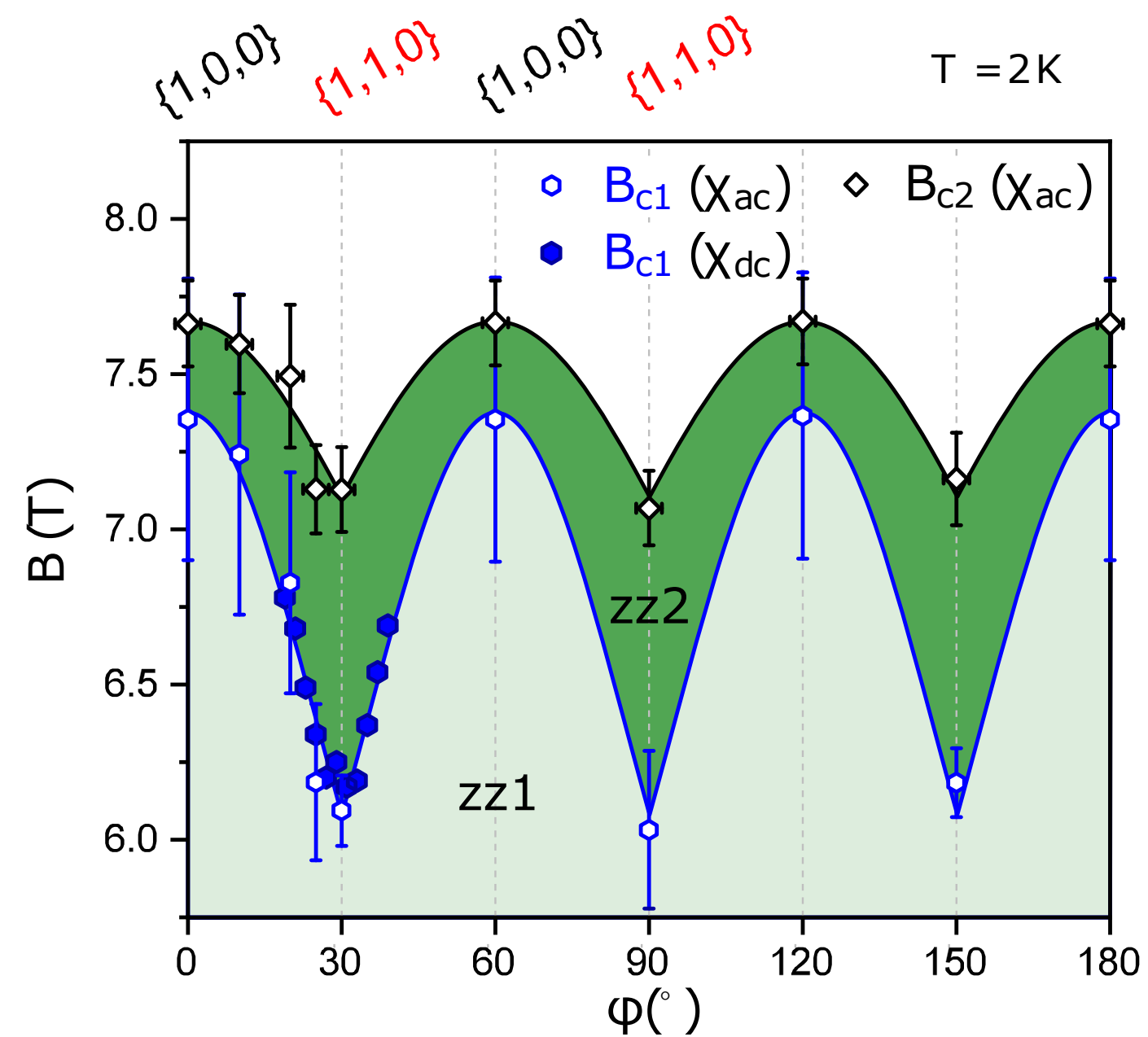
Magnetic Anisotropy in α -RuCl₃

Susceptibility:

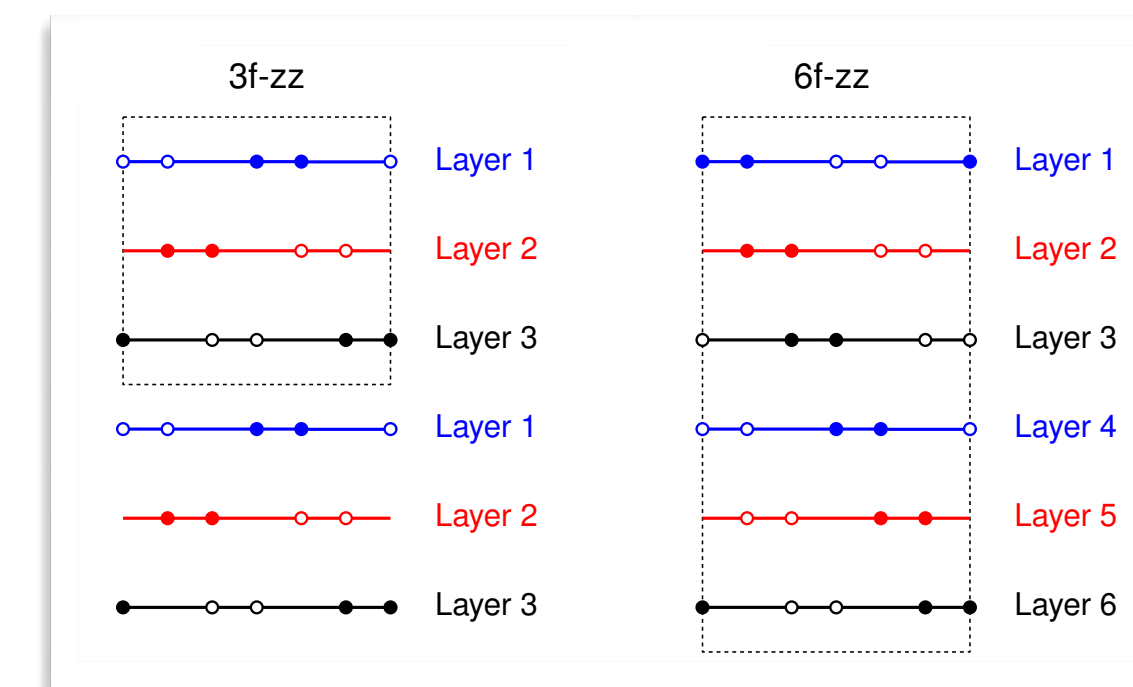
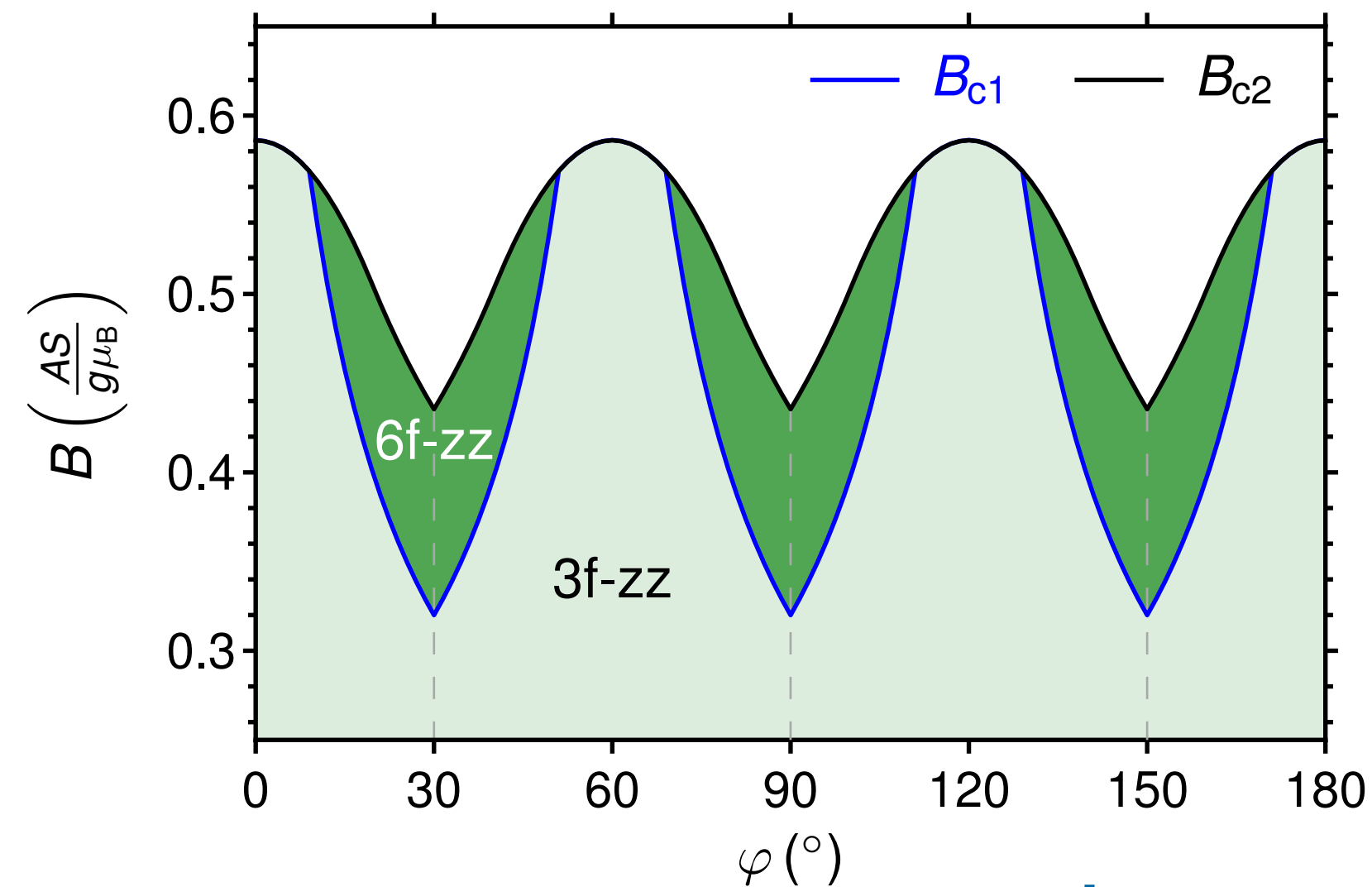


$R\bar{3}$ crystal structure

Phase diagram:



$(J_1, K_1, \Gamma_1, J_3) = (-0.1, -1, 0.5, 0.1)A$
 $K_{\perp}/J_{\perp} = -1.14, J_{\perp} > 0$

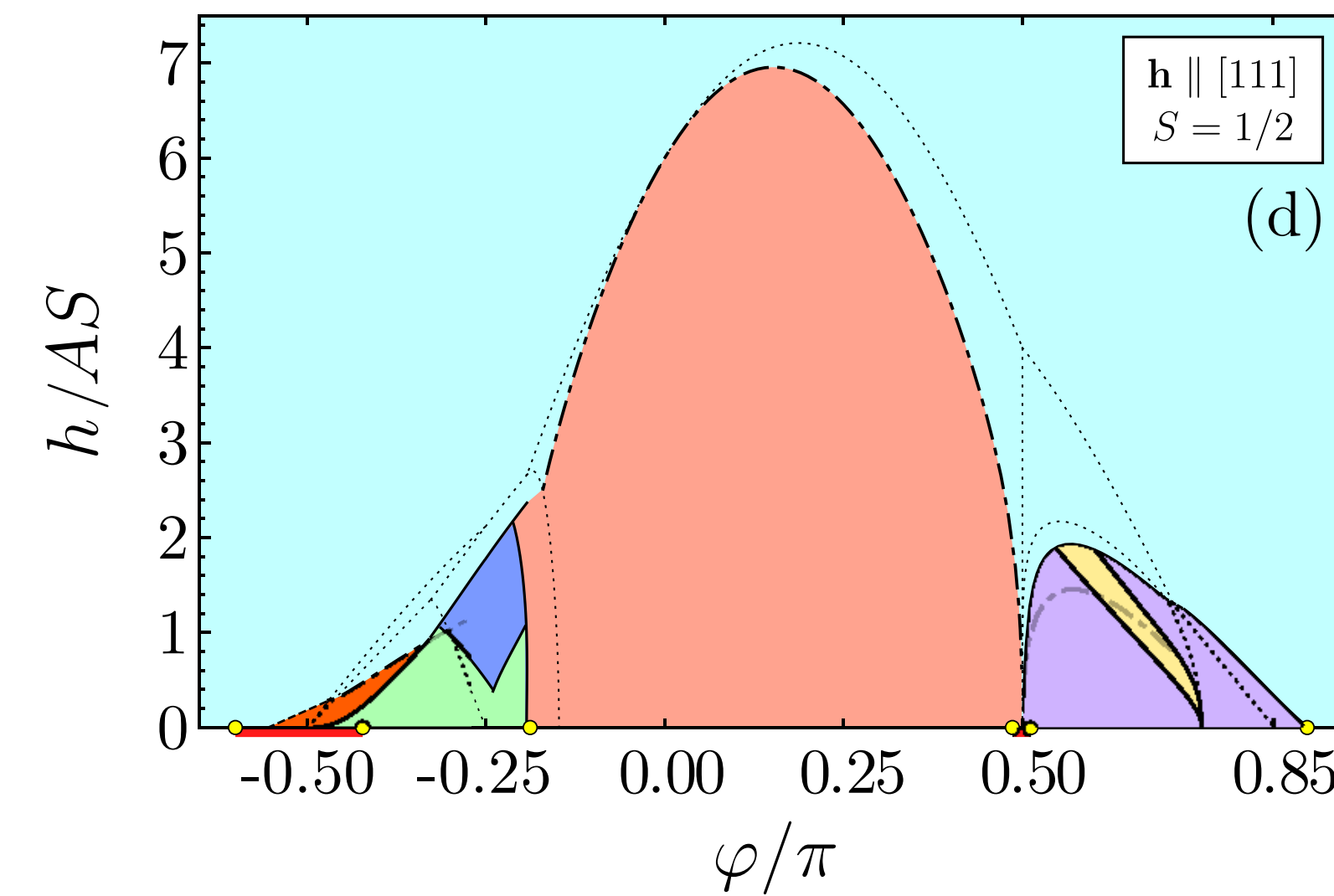
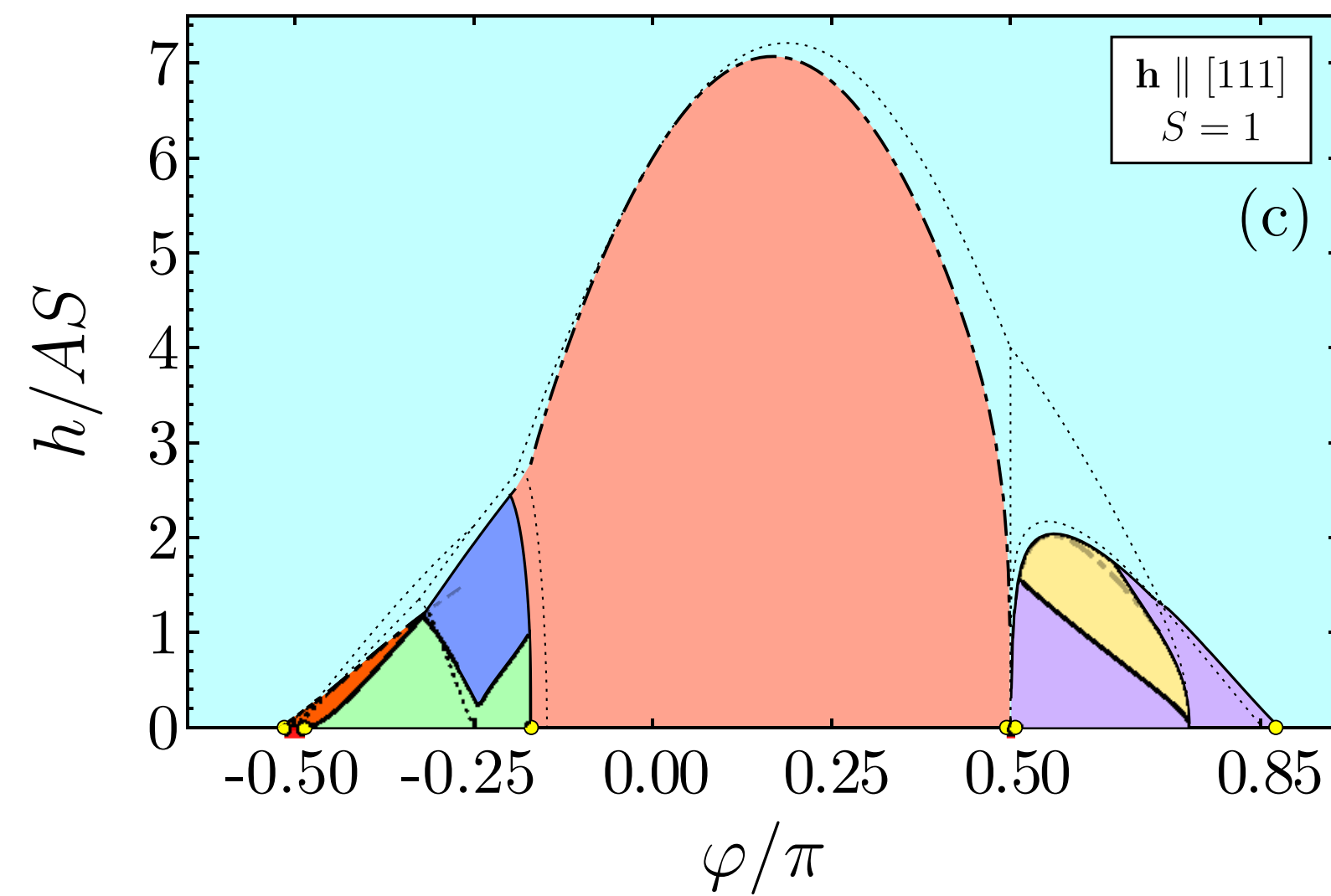
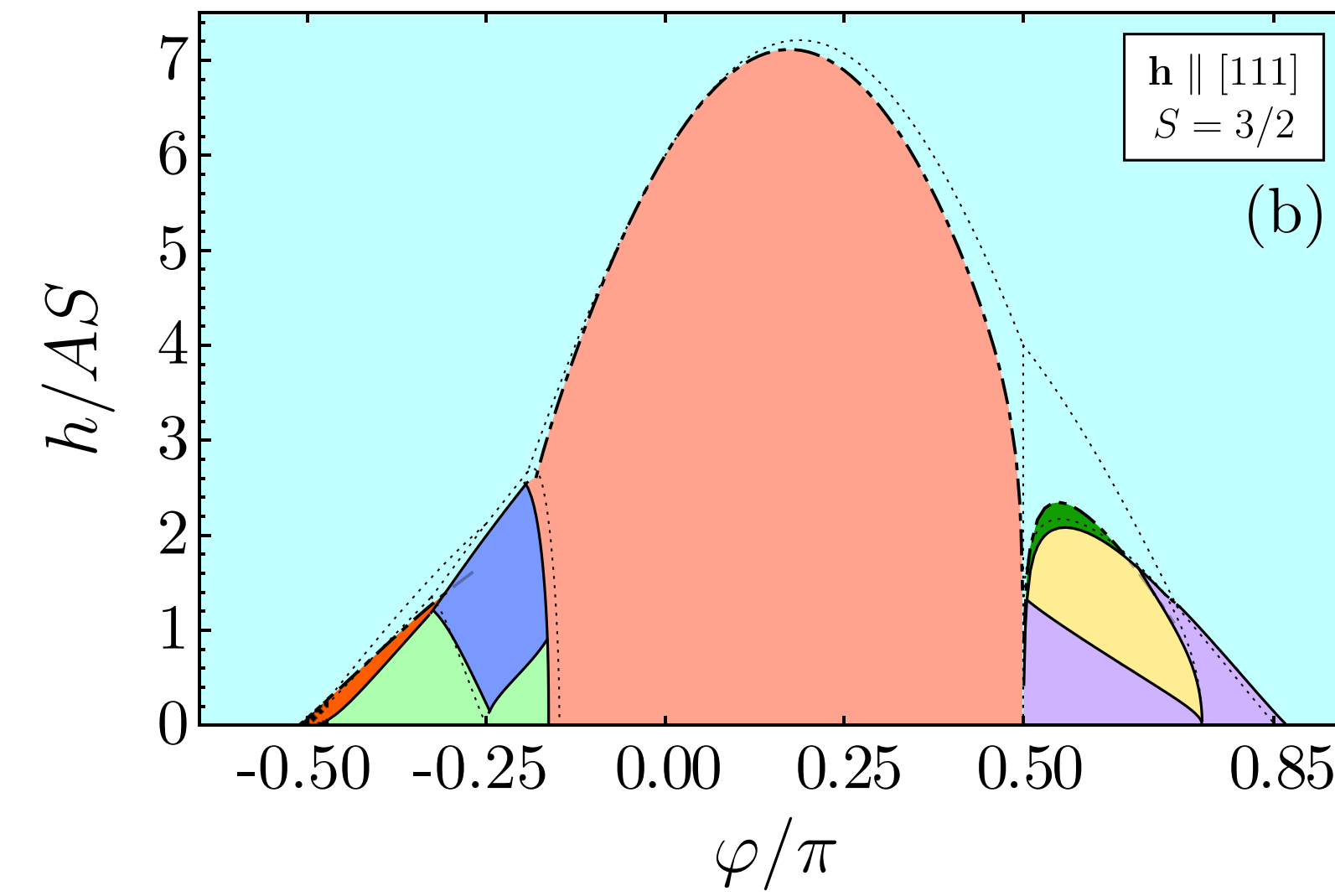
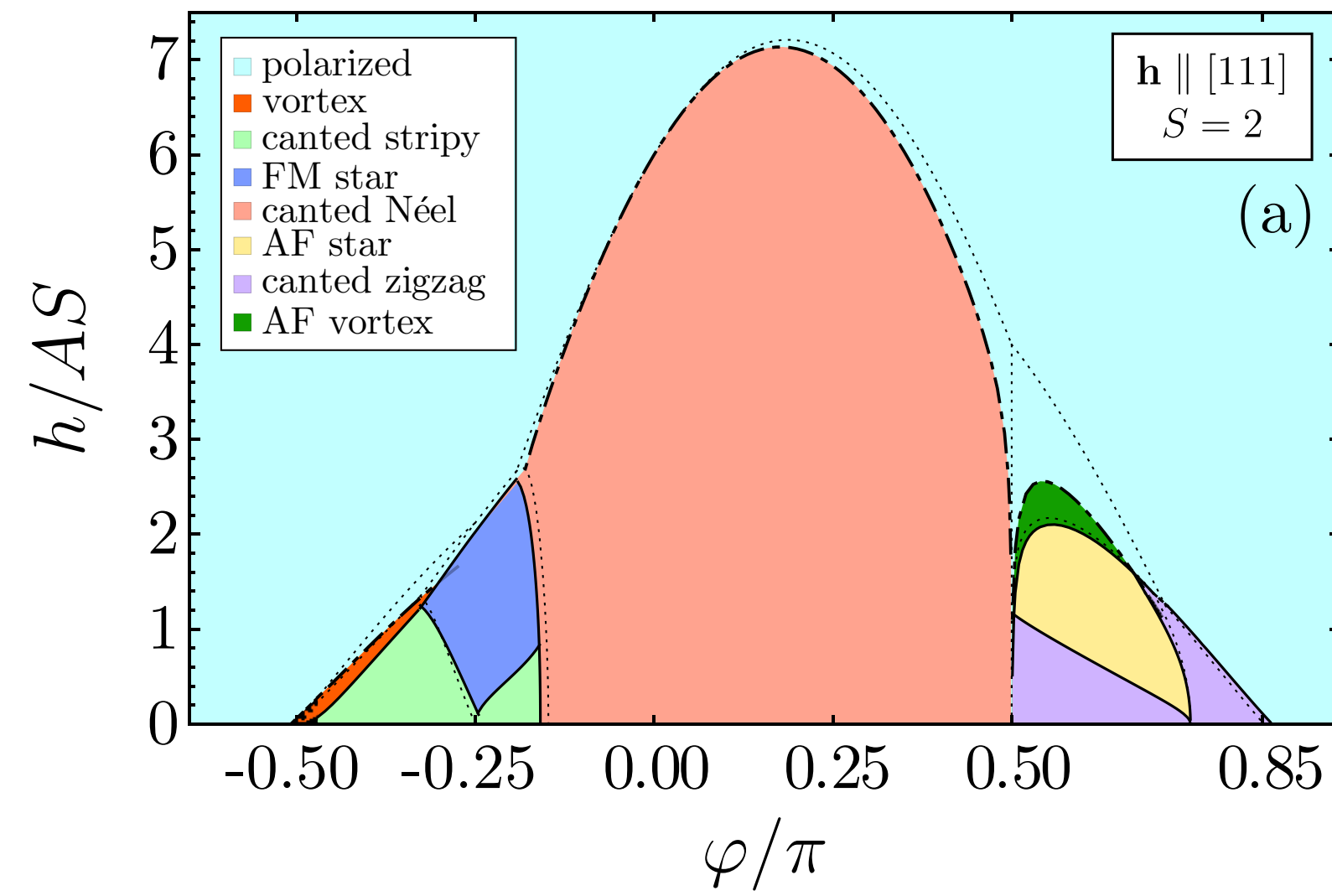


Magnetic structures: Side view

[LJ, Koch, Vojta, PRB '20]

[Balz, LJ, *et int.*, Nagler, PRB '21 (Editors' Suggestion)]

Kitaev-Heisenberg model in external field: $1/S$ expansion



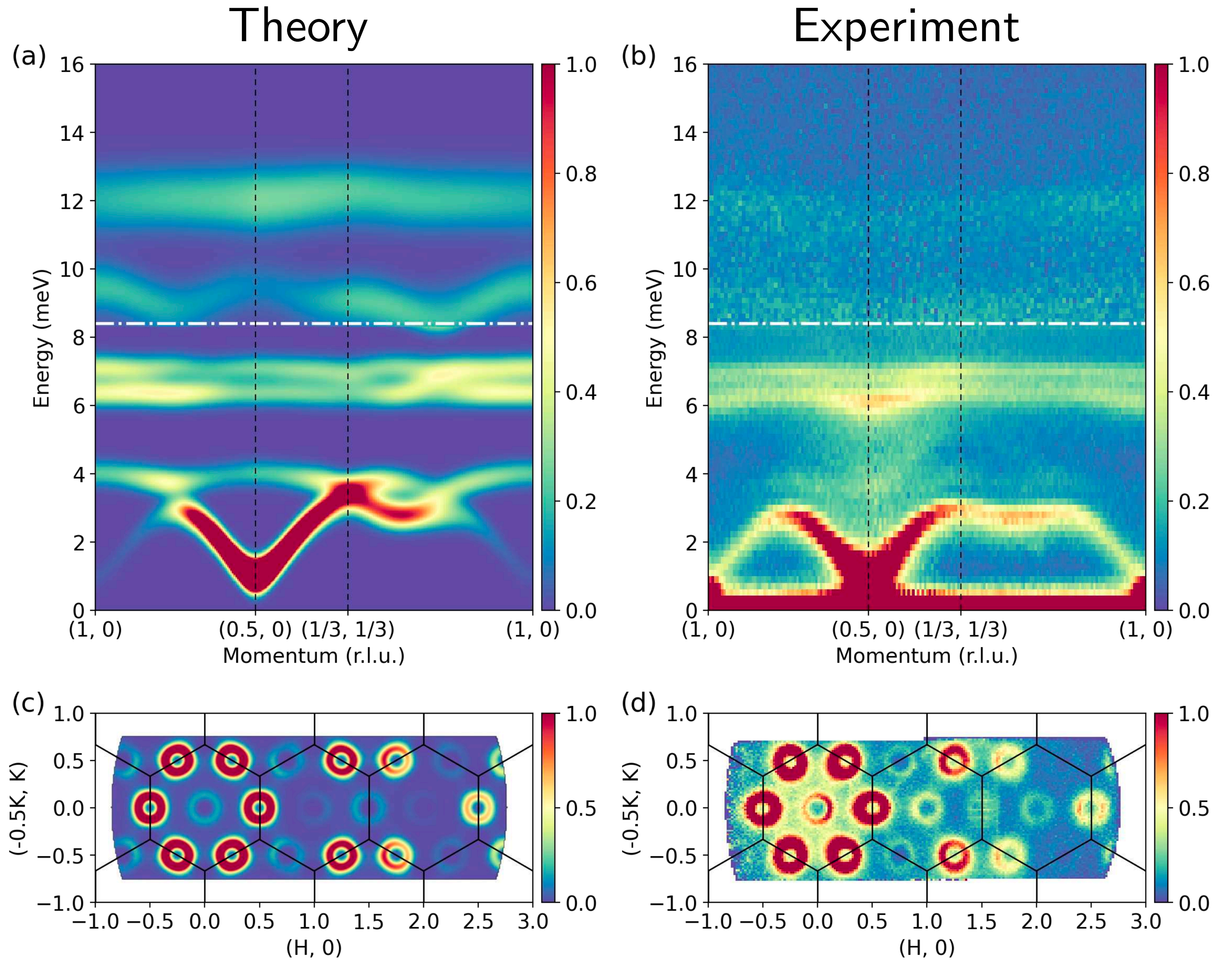
$$J = A \cos \varphi$$

$$K = 2A \sin \varphi$$

Na₂Co₂TeO₆: Inelastic Neutron Spectrum

$$(J, K, \Gamma, \Gamma') = (1.2, -8.3, 1.9, -2.3, 0.5) \text{ meV}$$
$$(J_3, J_2^A, J_2^B) = (1.5, 0.32, -0.24) \text{ eV}$$

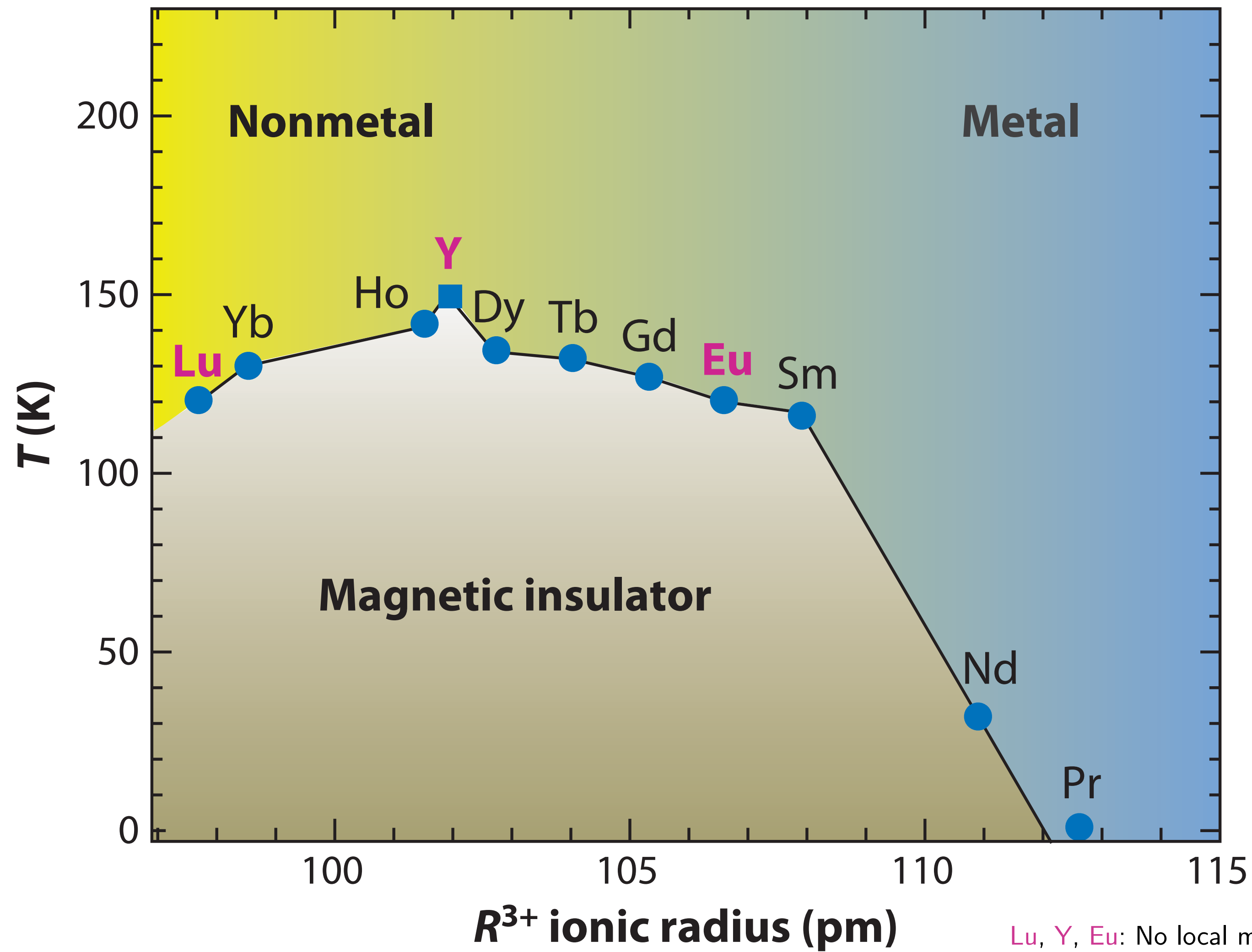
+ ring exchange



[Krüger, Chen, Jin, Li, LJ, arXiv:2211.16957]

[Yao *et al.*, arXiv:2203.00282]

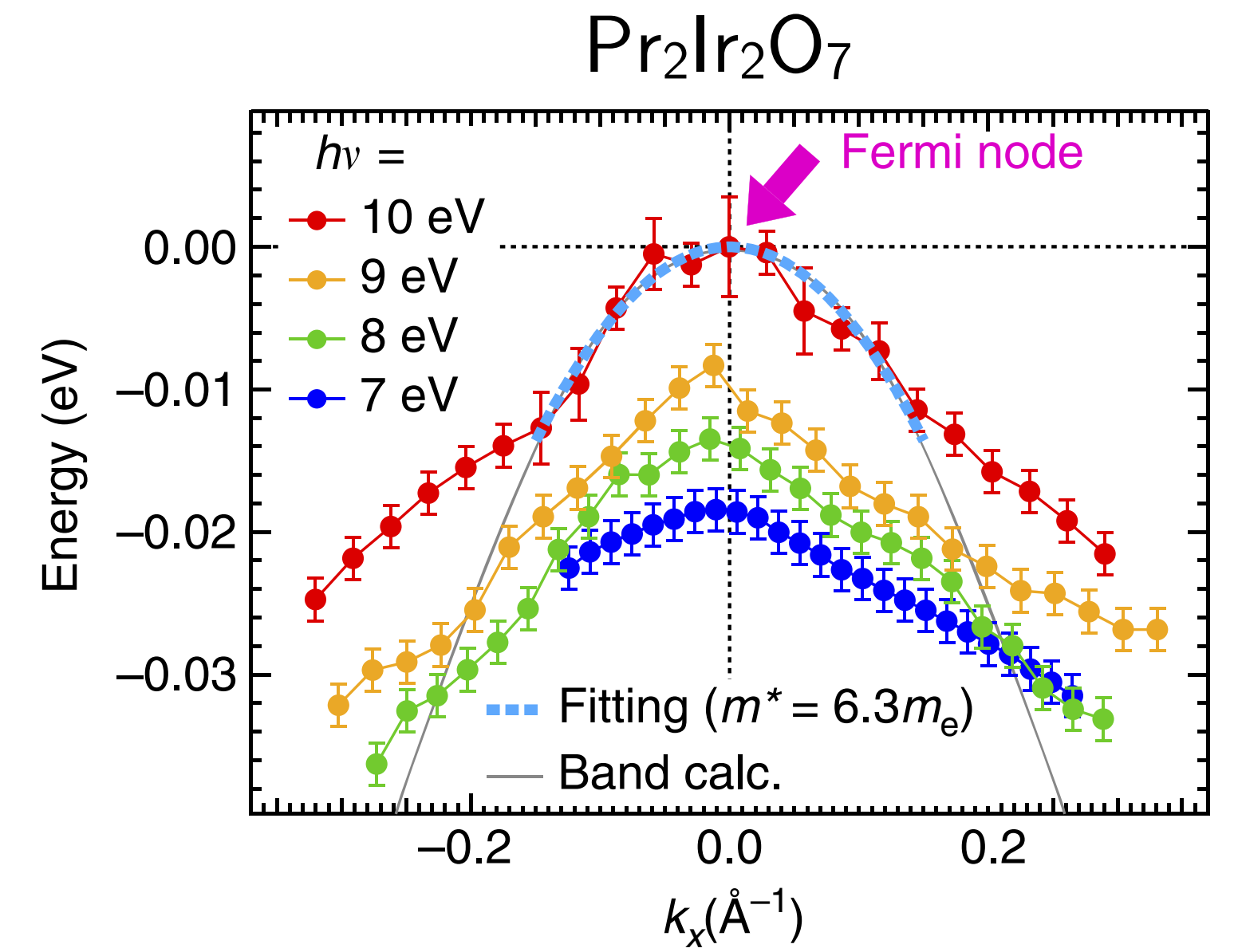
Phase diagram of $R_2\text{Ir}_2\text{O}_7$



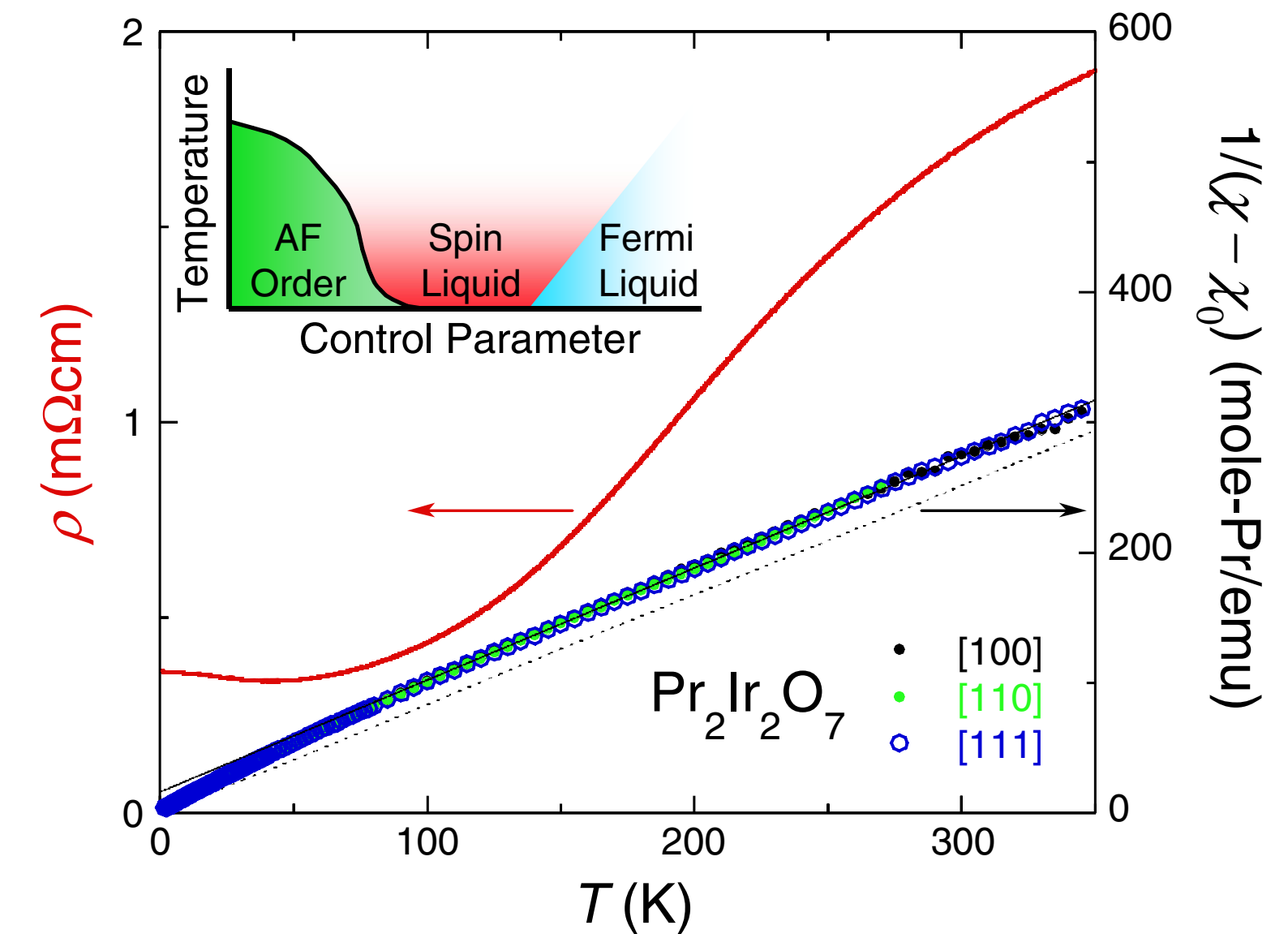
Lu, Y, Eu: No local moment

Y: Non-lanthanoid rare earth

[Witczak-Krempa *et al.*, ARCMP '14]



[Kondo *et al.*, Nat. Comm. '15]



[Nakatsuji *et al.*, PRL '06]