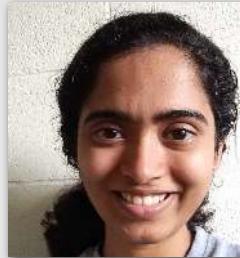


# Duality & Domain Wall Dynamics in $\text{CoNb}_2\text{O}_6$

**Ribhu Kaul**  
Penn State University

# Collaborators



**Nisheeta Desai**  
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C. M. Morris, N. Desai, J. Viirok, D. Huvonen, U. Nagel, T. Room,  
J. W. Krizan, R. J. Cava, T. M. McQueen, S. M. Koohpayeh,  
R. K. Kaul\*, N. P. Armitage\*

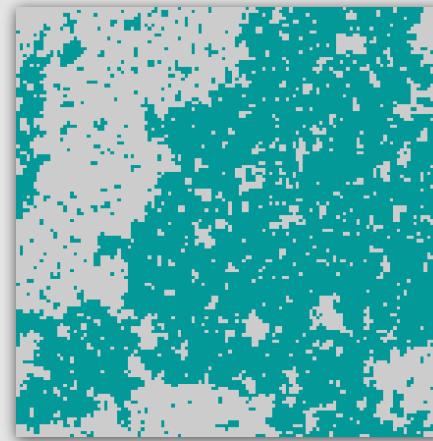
Nature Physics **17**, 832–836 (2021)



# Ising Model D=2

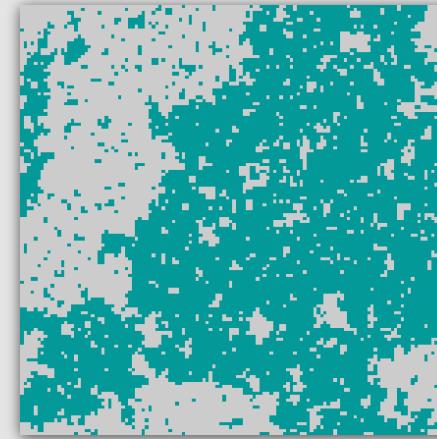
$$E = -J \sum_{\langle ij \rangle} s_i s_j$$

$$Z = \sum_c e^{-E_c/k_B T}$$



# Ising Model D=2

$$E = -J \sum_{\langle ij \rangle} s_i s_j$$



$$Z = \sum_c e^{-E_c/k_B T}$$

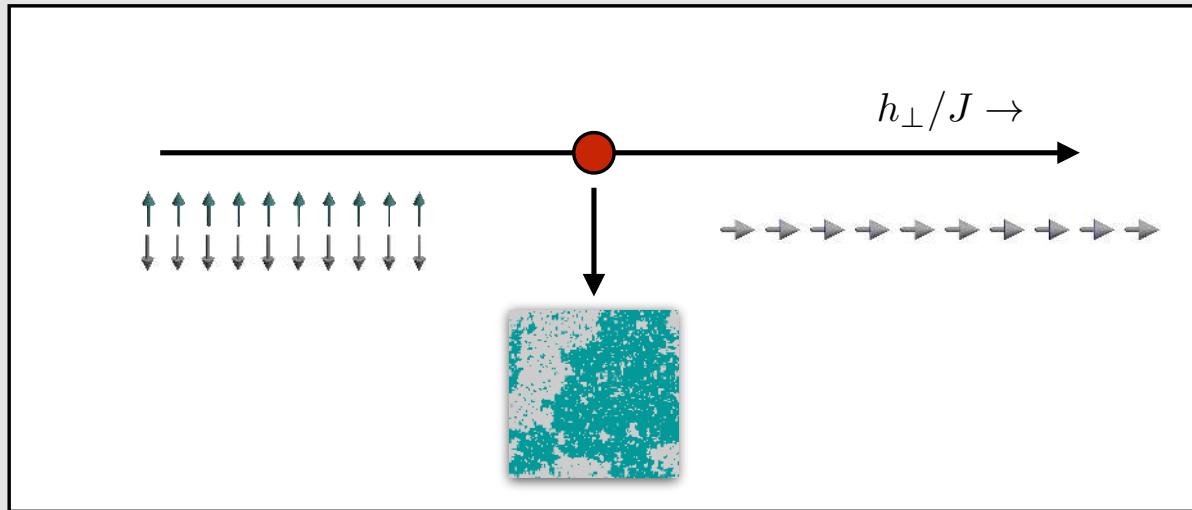
Stat. Mech (D=2) & Quantum MB (D=1+1)



$$H = - \sum_i \left( J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + h_{\perp} \hat{\sigma}_i^x + h_{\parallel} \hat{\sigma}_i^z \right)$$

# Ising Model D=2

$$H = - \sum_i (J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + h_{\perp} \hat{\sigma}_i^x + h_{\parallel} \hat{\sigma}_i^z)$$

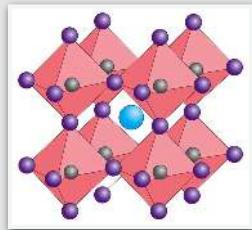


spontaneous symmetry breaking (1920s)  
duality (1940s)  
critical phenomena/RG (1960-70s)  
conformal field theory (1970-80s)

# Quantum Magnetism

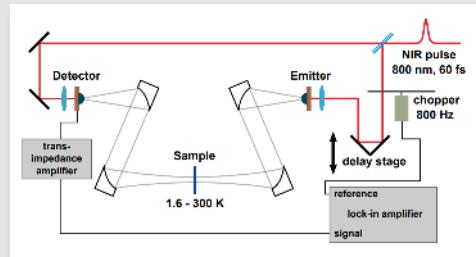
## Quantum Materials

pyrochlores, spinels, perovskites ...  
rare earths, transition metals...  
oxides, chalcogenides ...  
vdW...



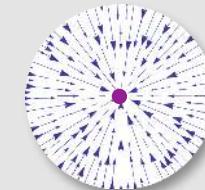
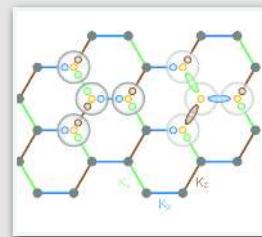
## Advanced Probes

neutrons  
THz  
transport  
resonant inelastic X-ray



## Theoretical

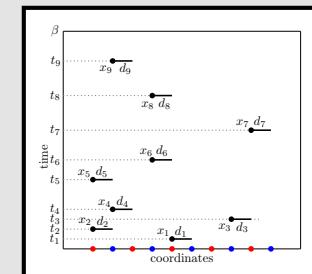
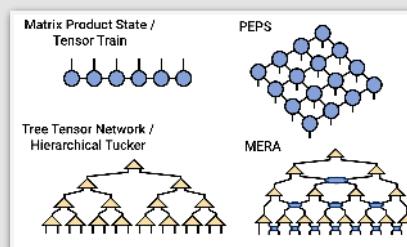
topological quantum spin liquid  
quantum spin ice  
quantum criticality (1+1, 2+1)  
critical points and critical phases



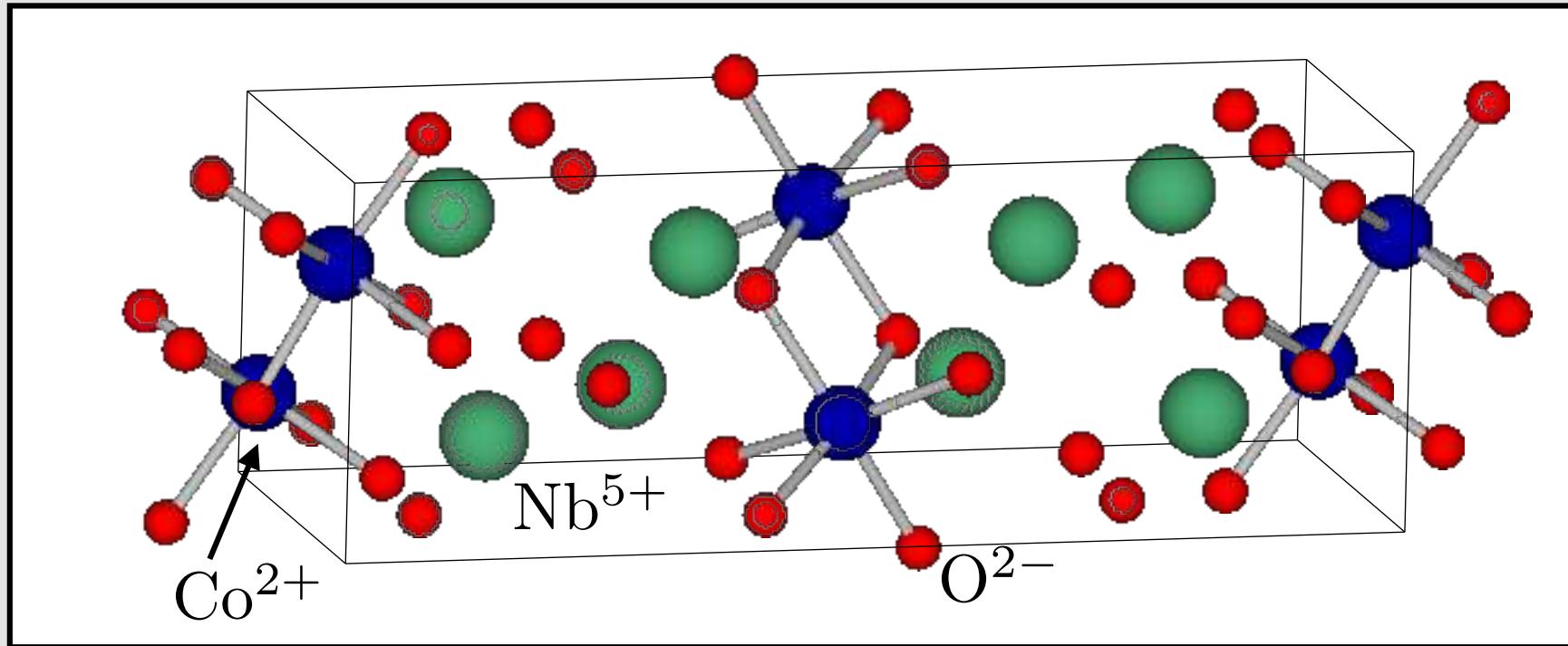
$$\mathcal{L} = \bar{\Psi}_j \gamma^\mu (\partial_\mu + i a_\mu) \Psi_j + \frac{1}{8\pi e^2} f_{\mu\nu} f^{\mu\nu}$$

## Numerical

Matrix-product/tensors/density matrix RG  
quantum Monte Carlo  
series expansions  
exact diagonalization

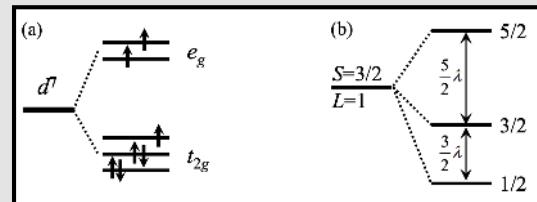
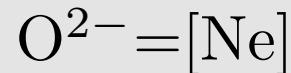
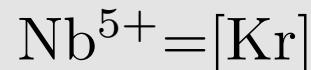
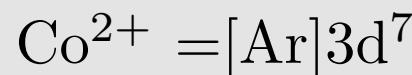
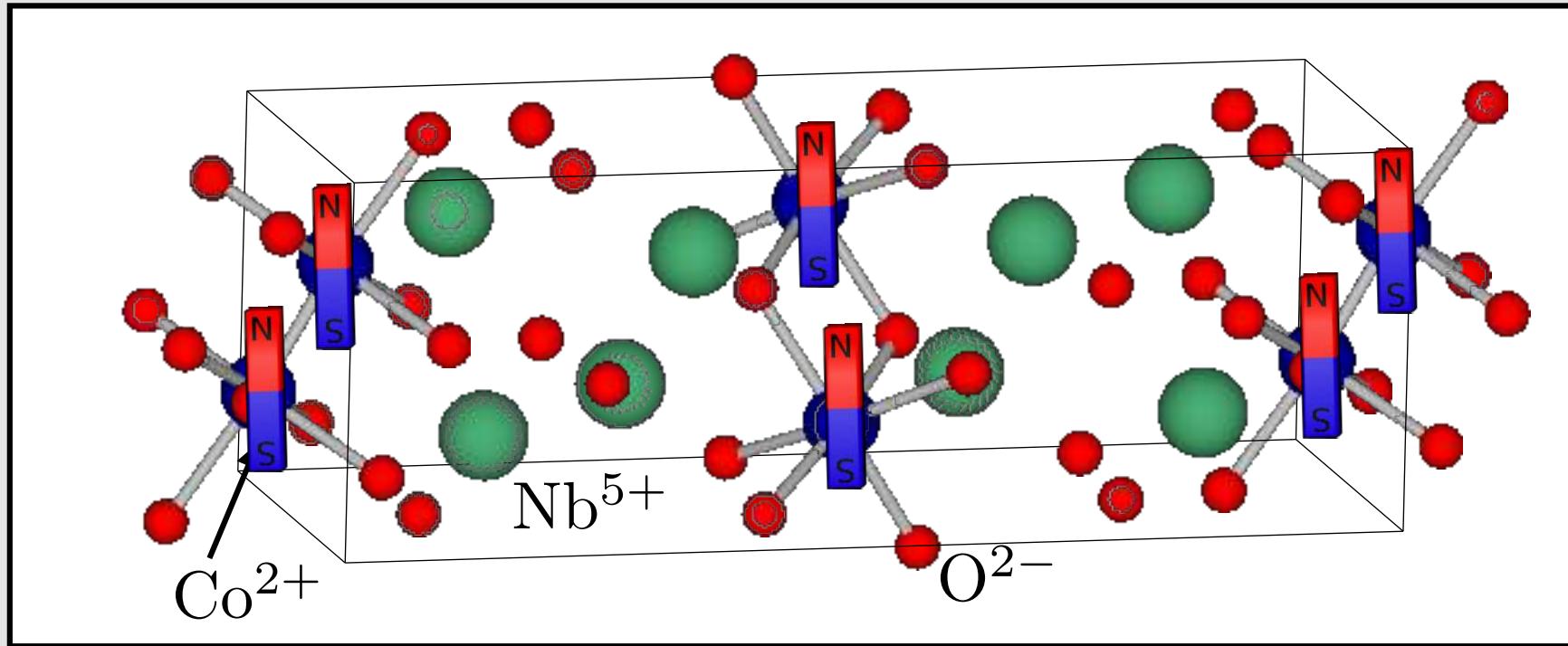


# The Quantum Material



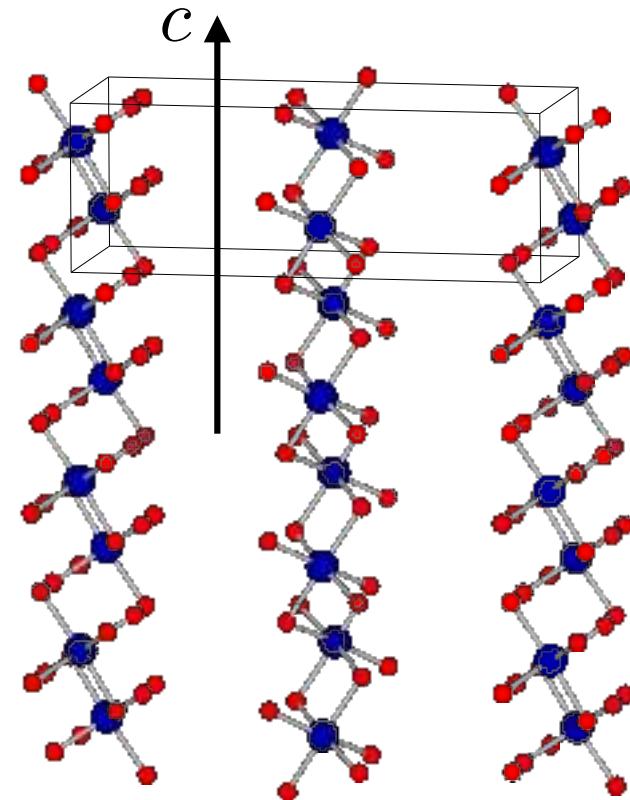
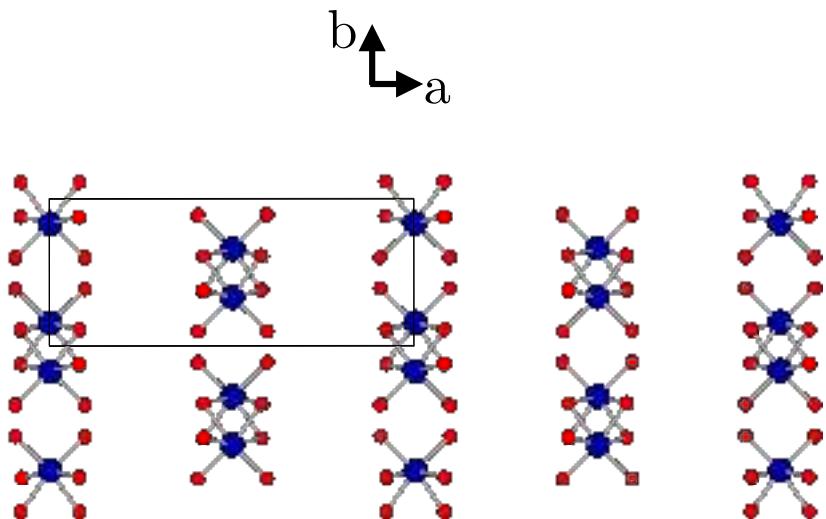
Space Group: Pbcn (Orthorhombic)  
“Mott Insulator”

# The Quantum Material



Liu, Khalliulin (2018)

# The Quantum Material



# Experimental Observations

C. Heid et al., J. Magn. Magn. Mater. 151, 123 (1995). S. Kobayashi et al., Phys. Rev. B 60, 3331 (1999).

I. Maartense, I. Yaeger, B. M. Wanklyn, Solid State Commun. 21, 93 (1977).

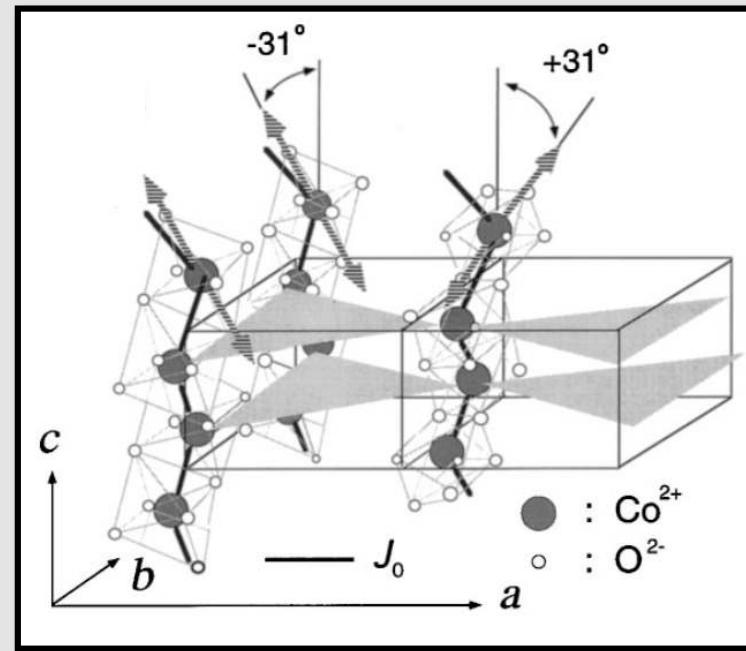
**R. Coldea et al Science (2010)**

Easy-axis magnet ( $T_N = 2.95$  K)

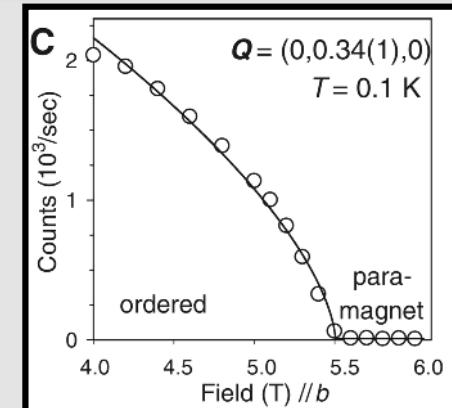
Ferromagnet along chains

Moments lie in a-c plane

$B_b = 5.5$  T “transverse field”

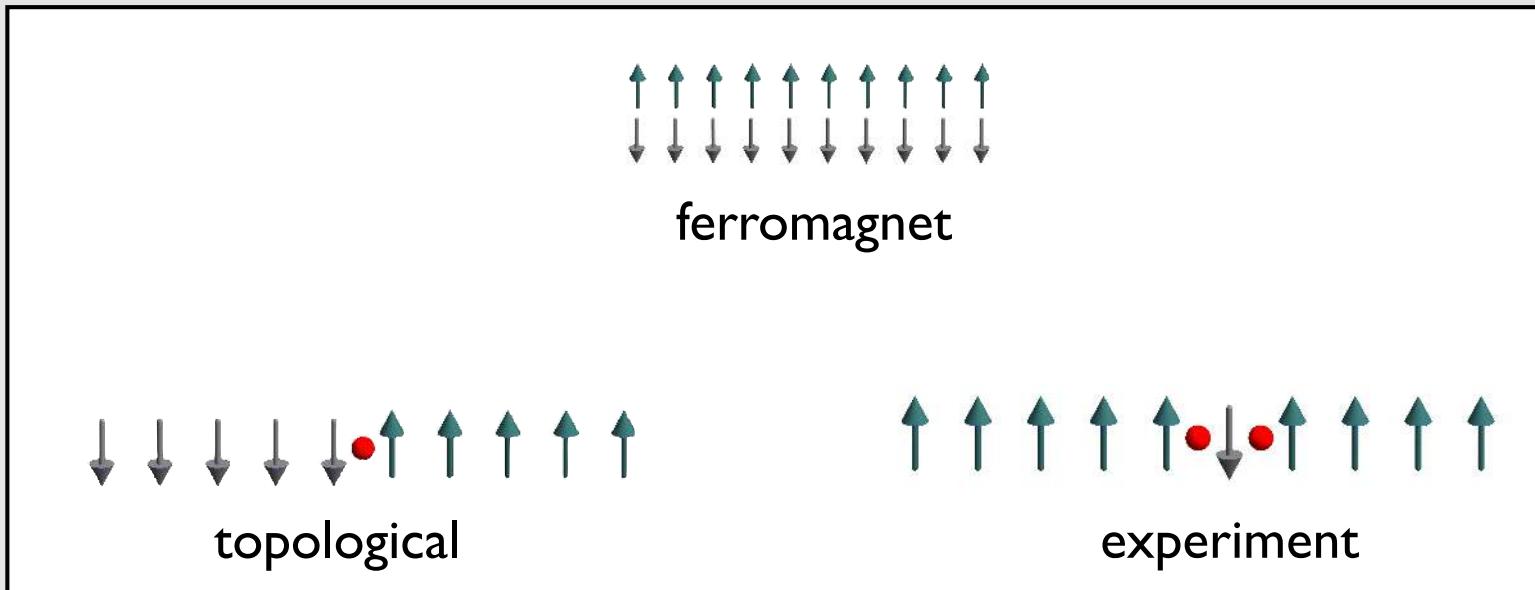


Transverse Field Ising Chain?



# Domain-Wall Excitations

$$H = - \sum_i (J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + h_{\perp} \hat{\sigma}_i^x + h_{\parallel} \hat{\sigma}_i^z)$$



$$h_{\parallel} = 0$$

domain walls move freely

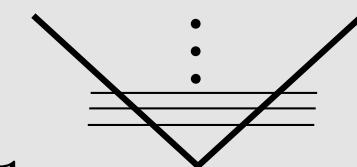
$$h_{\parallel} \neq 0$$

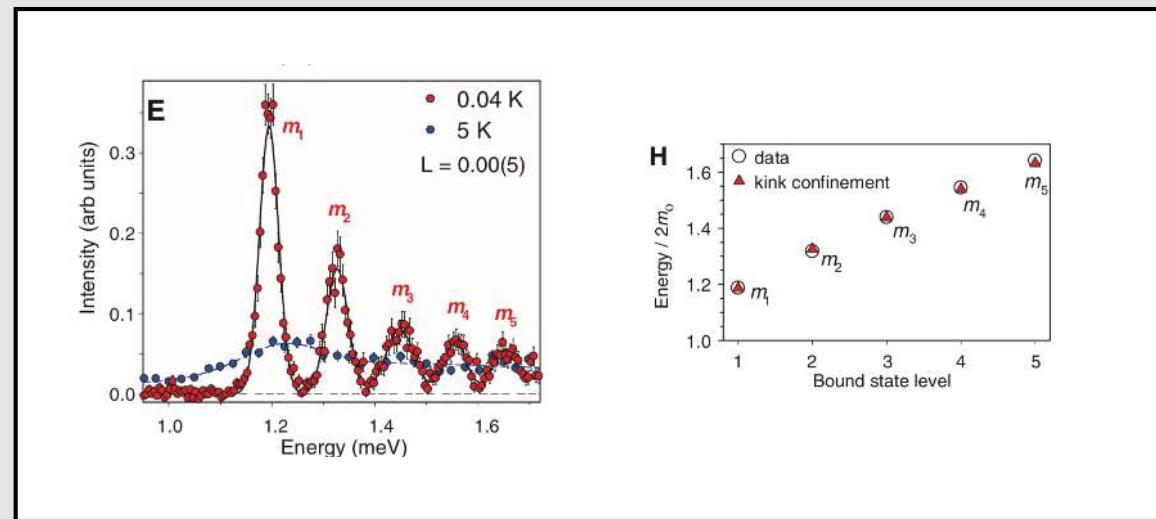
domain wall feel linear potential

# Neutron spectra

R. Coldea *et al* Science (2010)

## 2-p bound states

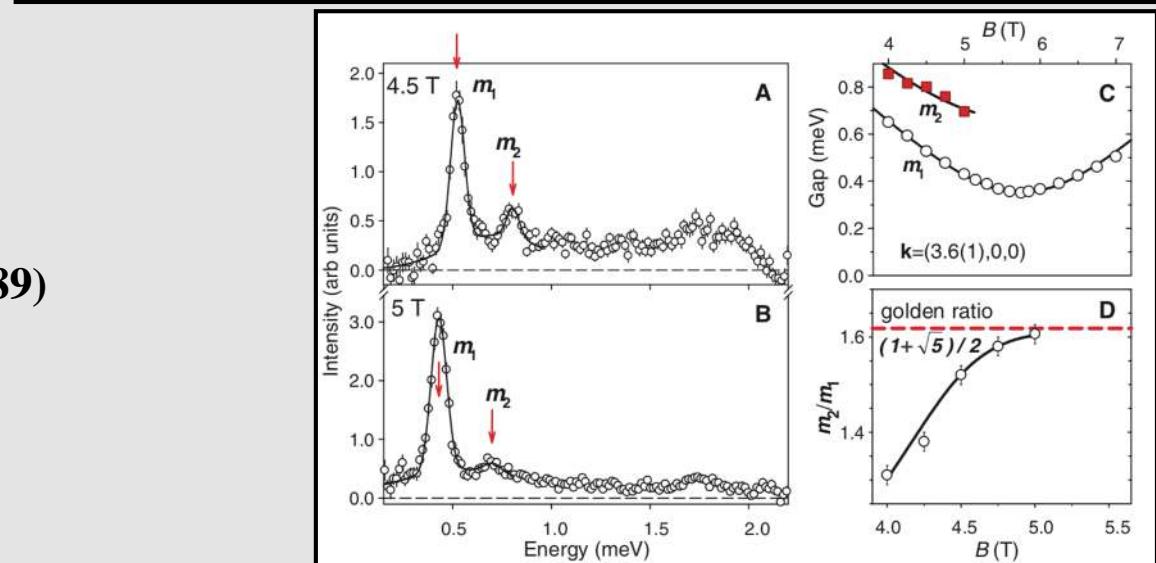
$$H = -\frac{1}{m} \partial_x^2 + \alpha|x|$$




## critical point

A. B. Zamolodchikov, (1989)

$$\frac{m_2}{m_1} = \frac{1 + \sqrt{5}}{2}$$

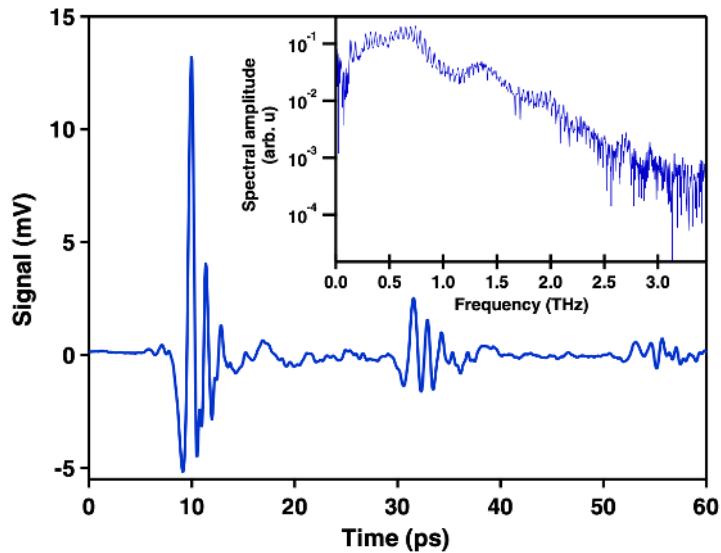
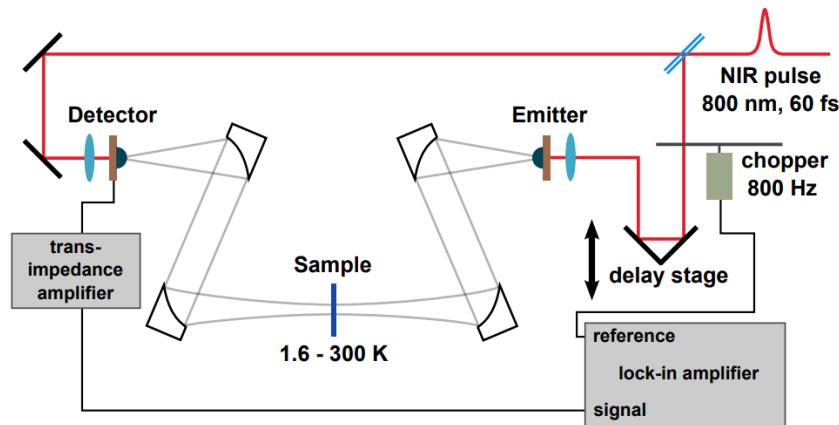


How are these pictures connected?

# THz absorption: linear response

Nature Physics (2021)

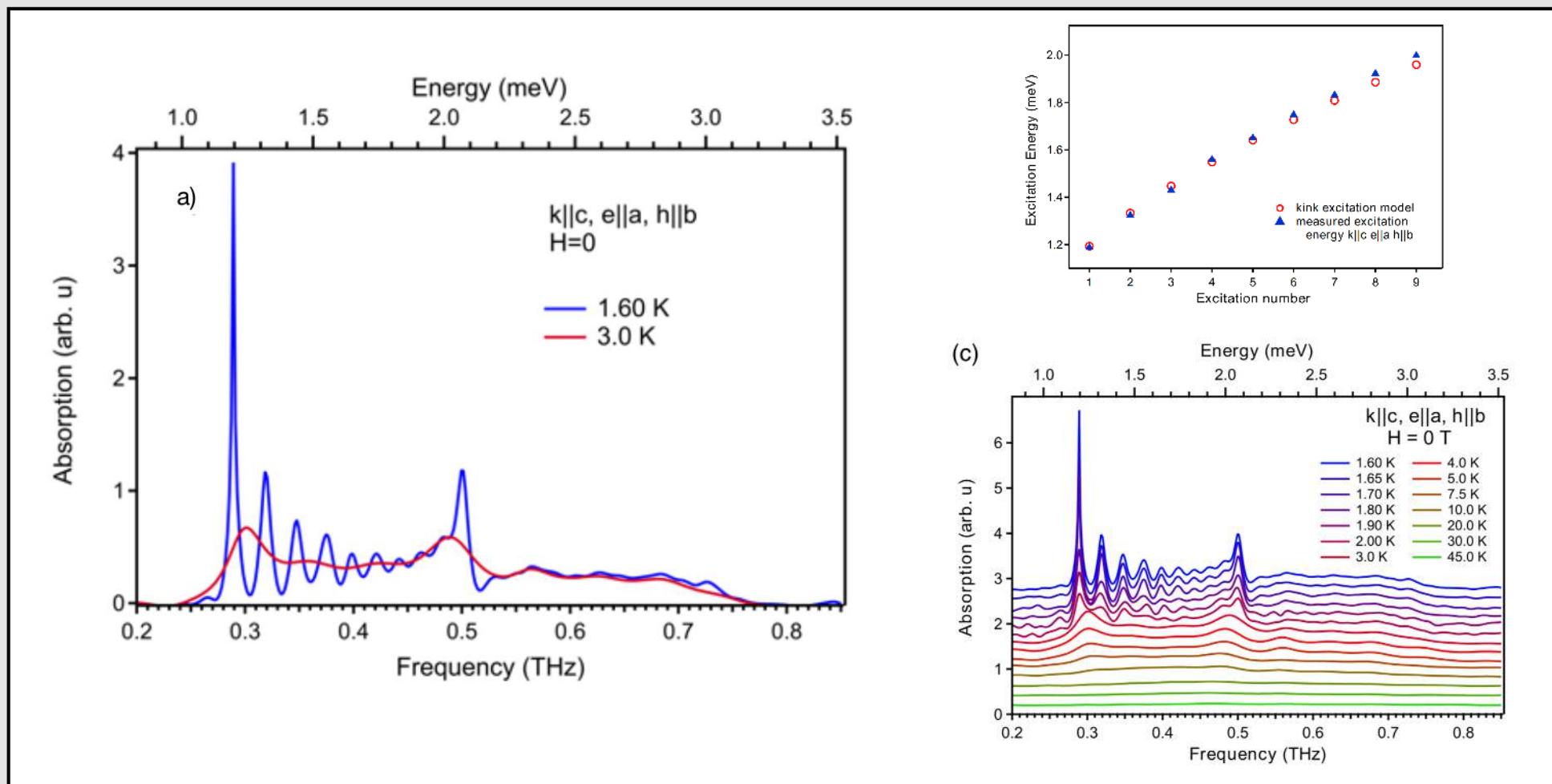
C. M. Morris et al PRL (2014)



# THz absorption

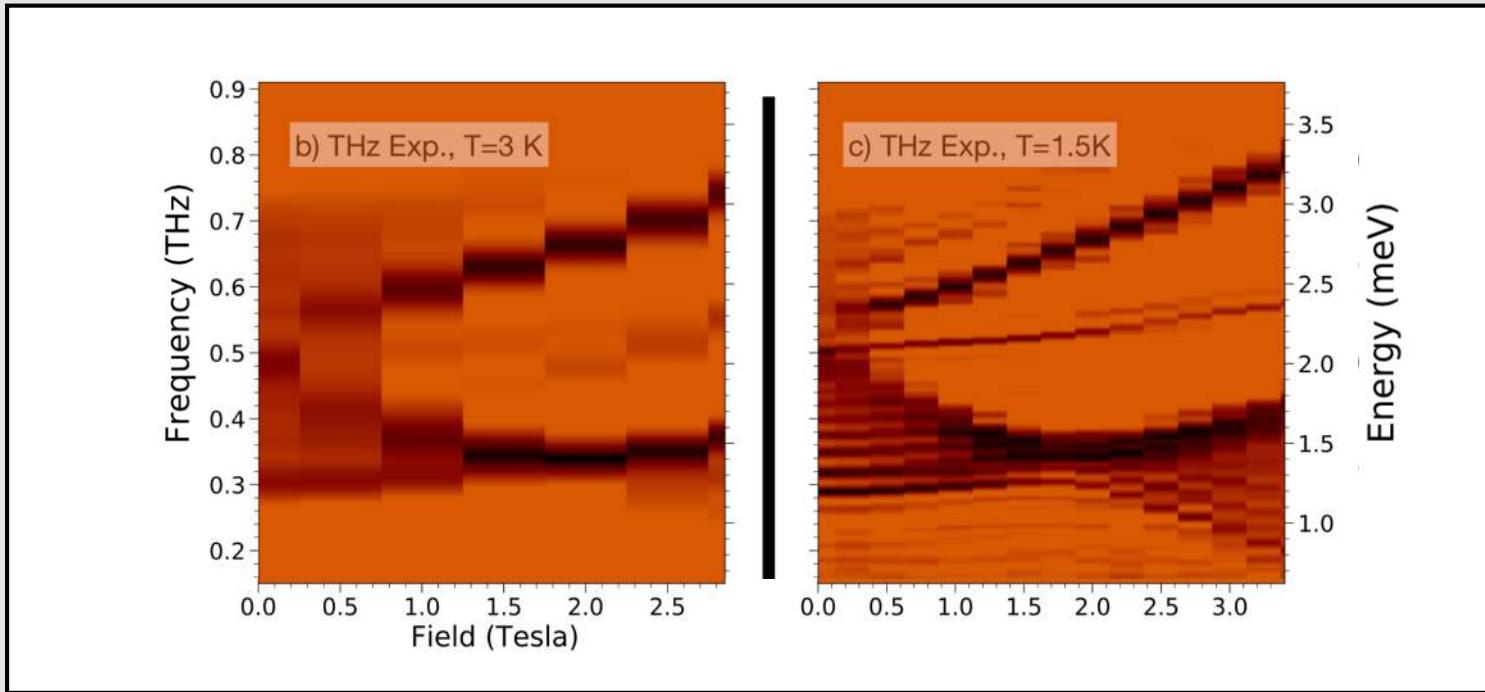
Nature Physics (2021)

C. M. Morris et al PRL (2014)



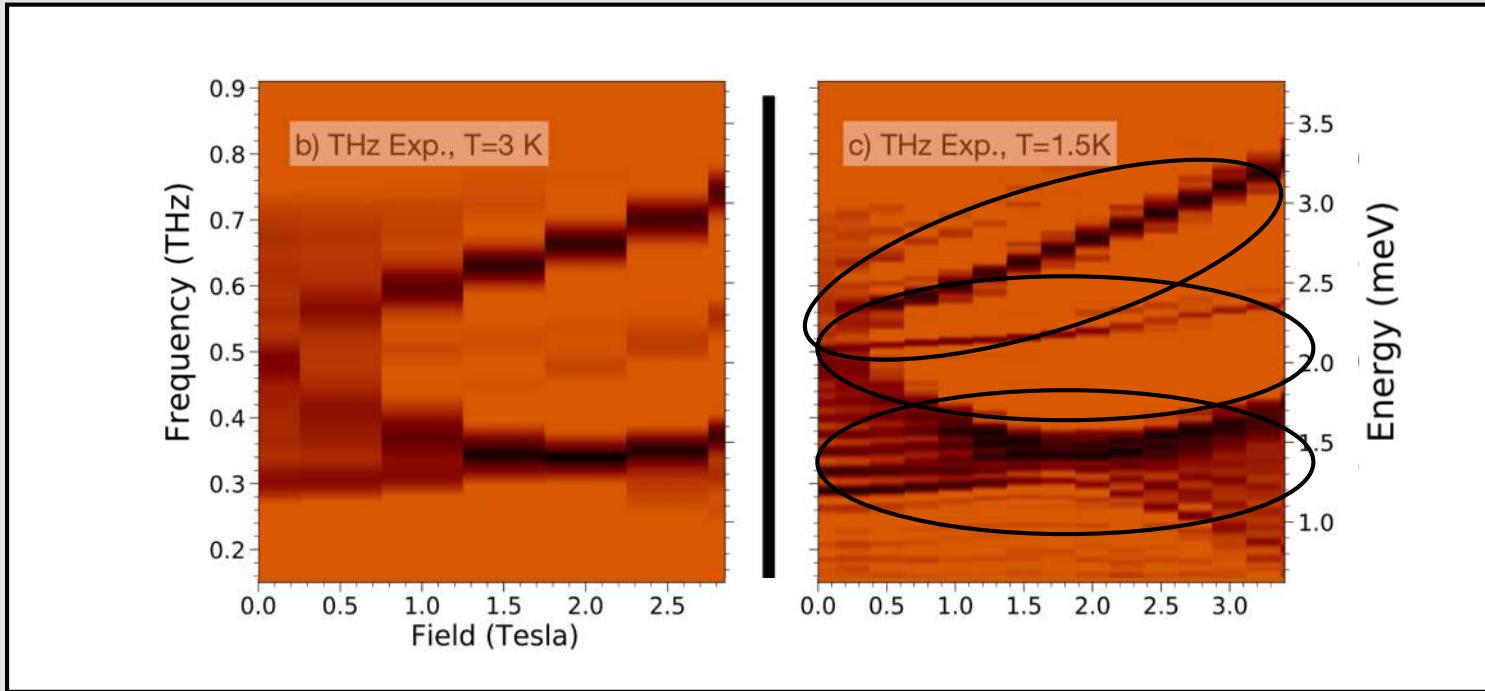
# Evolution in transverse field

Nature Physics (2021)

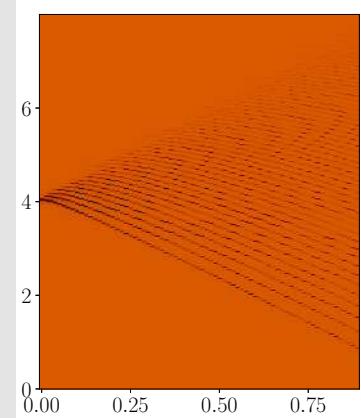


# Evolution in transverse field

Nature Physics (2021)

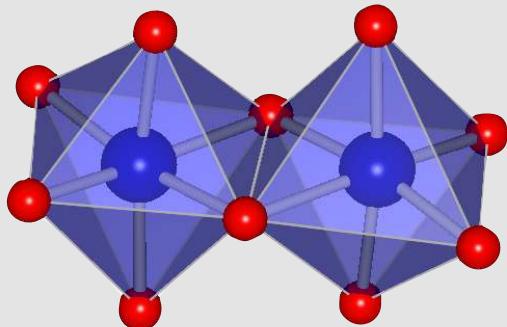


Does not look at all like TFIM!  
-Domain wall dispersion at zero field  
-Non-monotonic gap  
-Three features

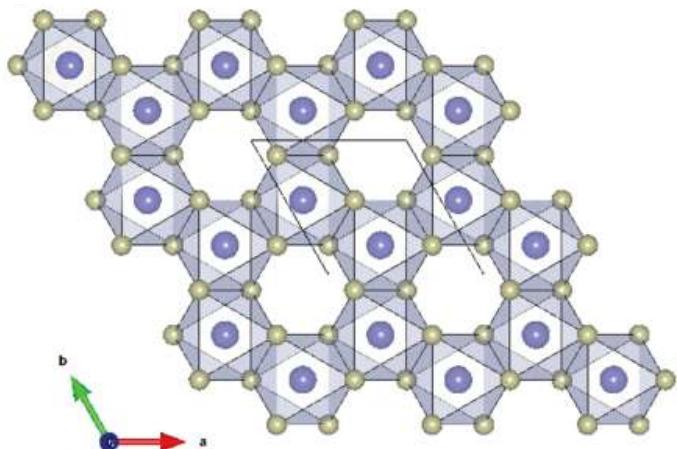


# Bond Dependent Interactions?

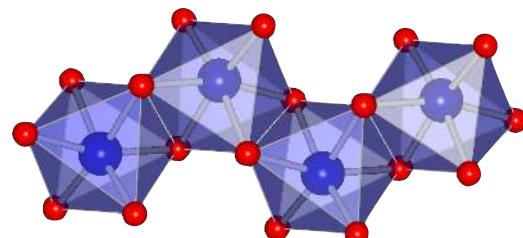
Jackeli & Khaliulin PRL (2009)  
Liu & Khaliulin; Sano, Kato, Motome (2018)



$\text{Na}_2\text{IrO}_3$     $\text{RuCl}_3$

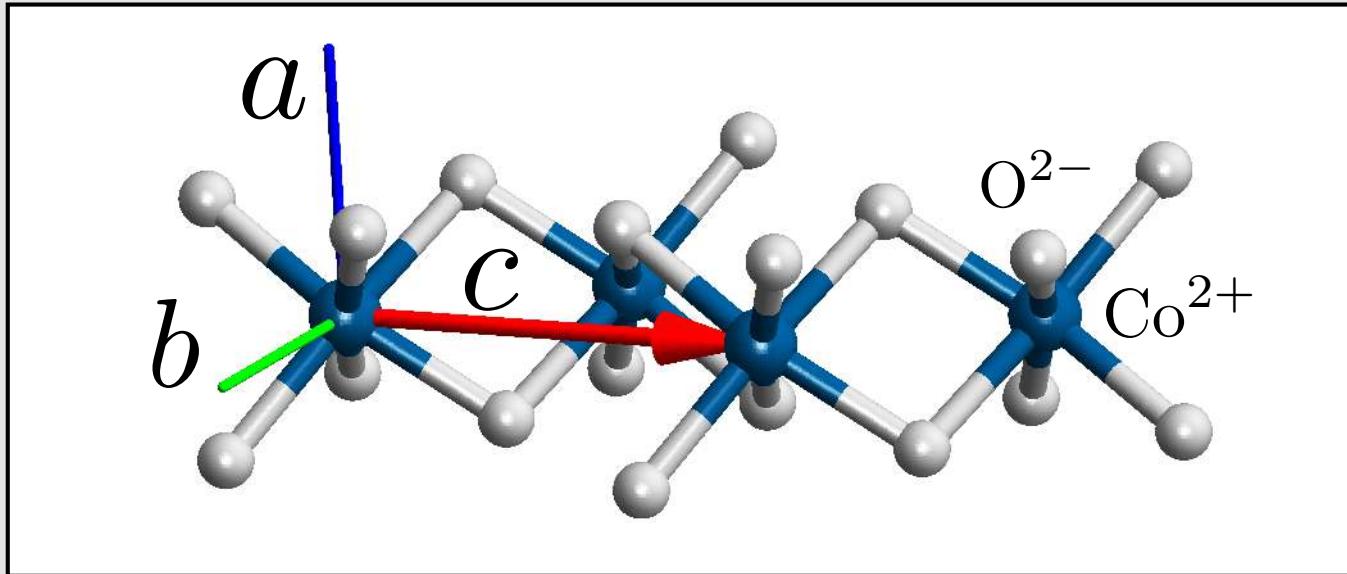


$\text{CoNb}_2\text{O}_6$



# Crystal Structure of Chain

Nature Physics (2021)

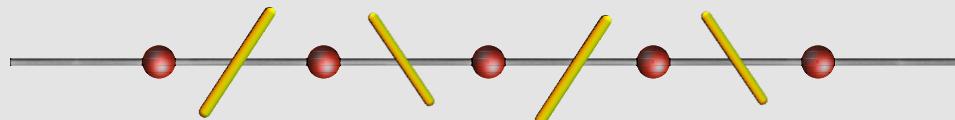


zig-zag chain  
cannot have a uniform Ising axes

$$H_{\text{Ising}} = \tau_i^{\hat{n}} \tau_j^{\hat{n}}$$

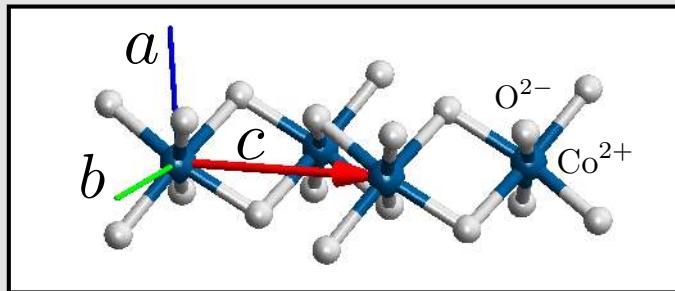
$$\tau^{\hat{n}} \equiv \vec{\tau} \cdot \hat{n}$$

Ising axes must alternate along chain!



# Twisted Kitaev model

Nature Physics (2021)

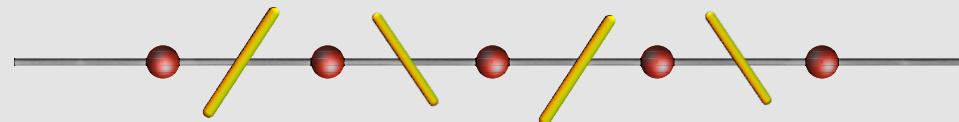
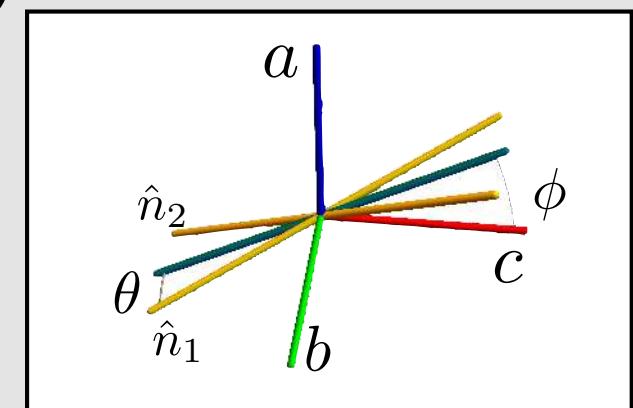


Space group “Pbcn” fixes all Ising axes once one is known!

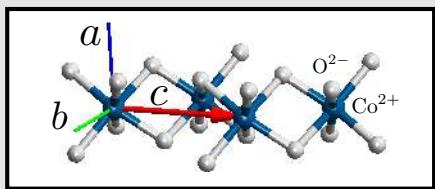
e.g.  $C_2^b$  (passing through Co site)

$$\mathcal{H}_K = -K \sum_{i \in e} \left( \tau_i^{\hat{n}_1} \tau_{i+1}^{\hat{n}_1} + \tau_{i+1}^{\hat{n}_2} \tau_{i+2}^{\hat{n}_2} \right)$$

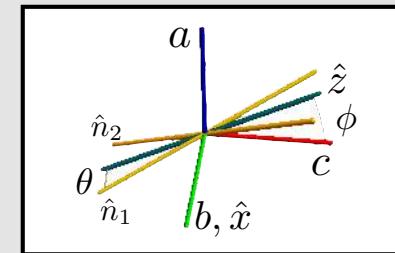
“twisted Kitaev model”



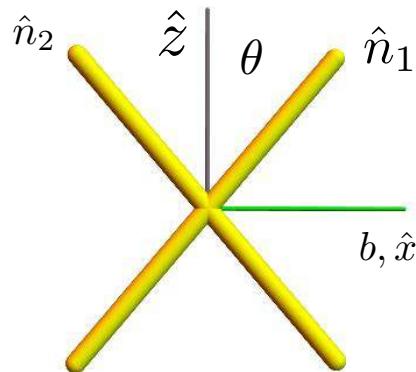
# Twisted Kitaev: Ground State



Nature Physics (2021)



$$\mathcal{H}_K = -K \sum_{i \in e} \left( \tau_i^{\hat{n}_1} \tau_{i+1}^{\hat{n}_1} + \tau_{i+1}^{\hat{n}_2} \tau_{i+2}^{\hat{n}_2} \right)$$



$\mathcal{C}_2^b$  (Ising symmetry)

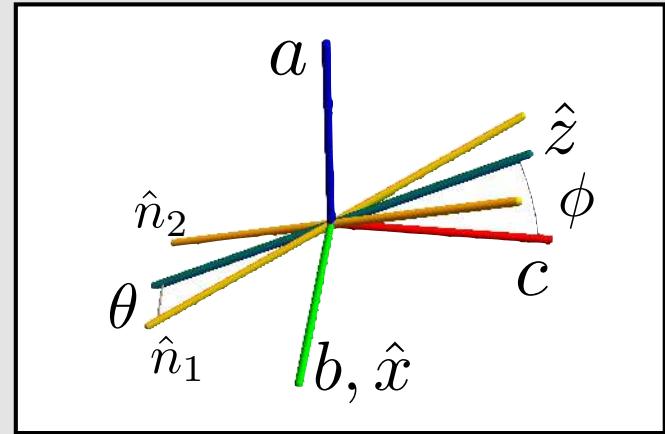
uniform polarization in a-c plane.

z-polarization breaks  $\mathcal{C}_2^b$ .

# Twisted Kitaev: Excitations

Nature Physics (2021)

$$\mathcal{H}_K = -K \sum_{i \in e} \left( \tau_i^{\hat{n}_1} \tau_{i+1}^{\hat{n}_1} + \tau_{i+1}^{\hat{n}_2} \tau_{i+2}^{\hat{n}_2} \right)$$



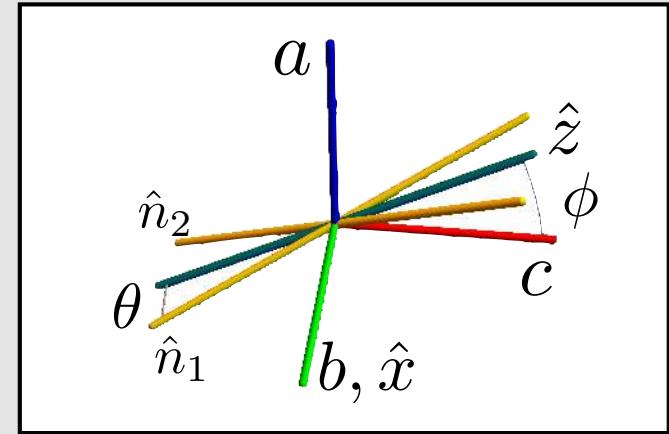
$$\begin{aligned}\mathcal{H} &= -K \sum_i \left[ \cos^2(\theta) \tau_i^z \tau_{i+1}^z + \sin^2(\theta) \tau_i^x \tau_{i+1}^x \right. \\ &\quad \left. + \frac{\sin(2\theta)}{2} (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) \right] \\ &\quad - h_x \sum_i \tau_i^x - h_z \sum_i \tau_i^z\end{aligned}$$

cf. Fava, Coldea, Parameswaran (2020)

# Twisted Kitaev: Excitations

Nature Physics (2021)

$$\mathcal{H}_K = -K \sum_{i \in e} \left( \tau_i^{\hat{n}_1} \tau_{i+1}^{\hat{n}_1} + \tau_{i+1}^{\hat{n}_2} \tau_{i+2}^{\hat{n}_2} \right)$$



$$\begin{aligned} \mathcal{H} &= -K \sum_i \left[ \cos^2(\theta) \tau_i^z \tau_{i+1}^z + \sin^2(\theta) \tau_i^x \tau_{i+1}^x \right. \\ &\quad \left. + \frac{\sin(2\theta)}{2} (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) \right] \\ &\quad - h_x \sum_i \tau_i^x - h_z \sum_i \tau_i^z \end{aligned}$$

cf. Fava, Coldea, Parameswaran (2020)

# Twisted Kitaev: Excitations

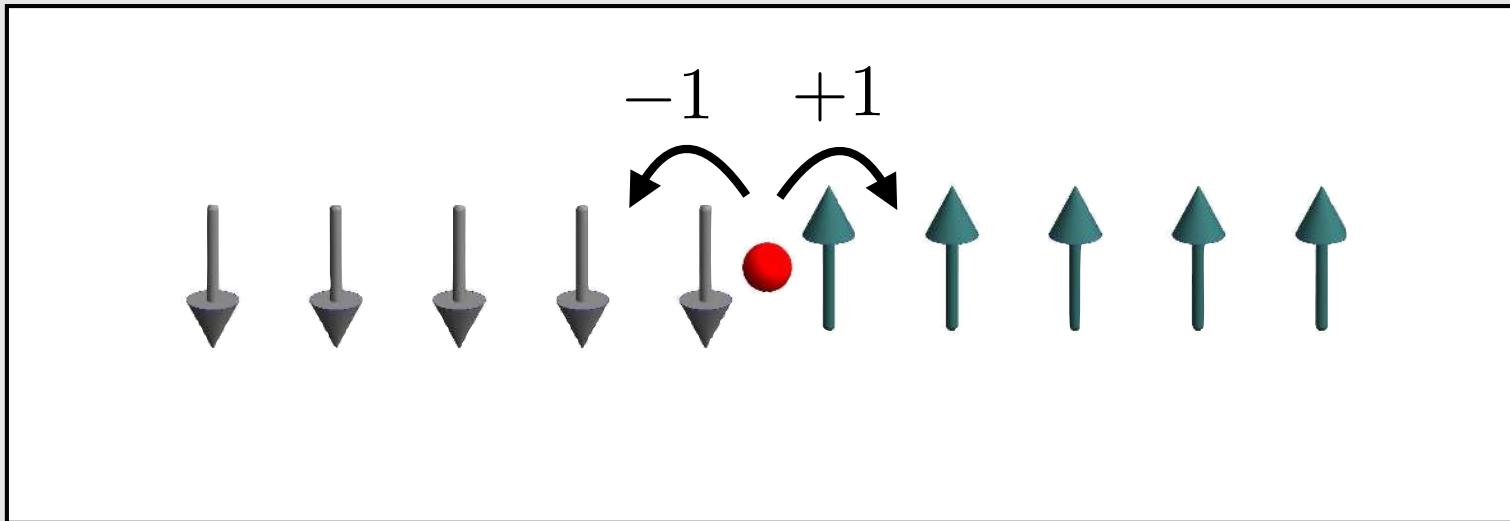
Nature Physics (2021)

$$\sum_i (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) = \sum_i (-1)^i (\tau_{i+1}^z - \tau_{i-1}^z) \tau_i^x$$

# Twisted Kitaev: Deg Pert theory

Nature Physics (2021)

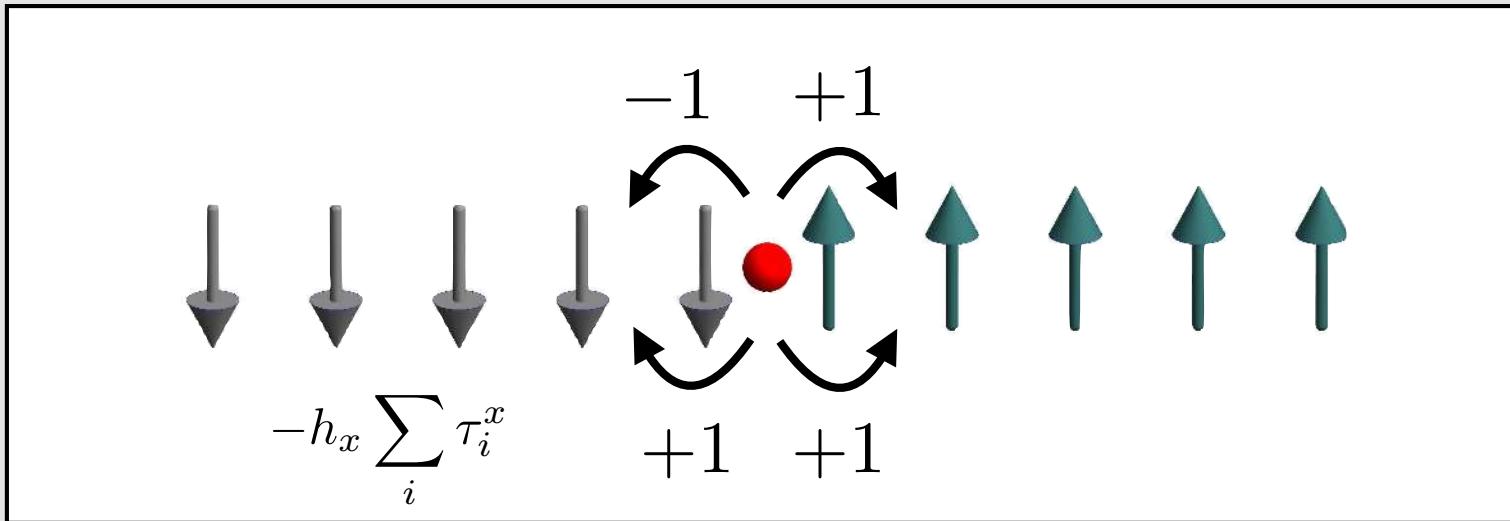
$$\sum_i (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) = \sum_i (-1)^i (\tau_{i+1}^z - \tau_{i-1}^z) \tau_i^x$$



# Twisted Kitaev: Deg Pert theory

Nature Physics (2021)

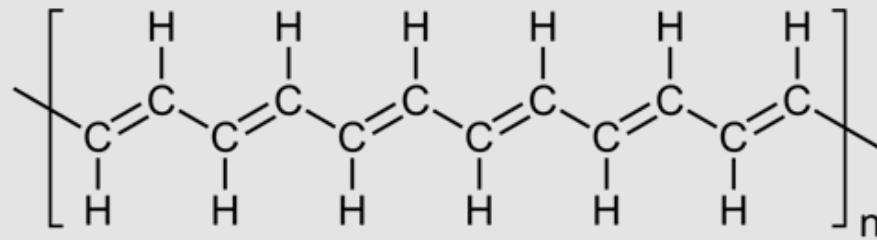
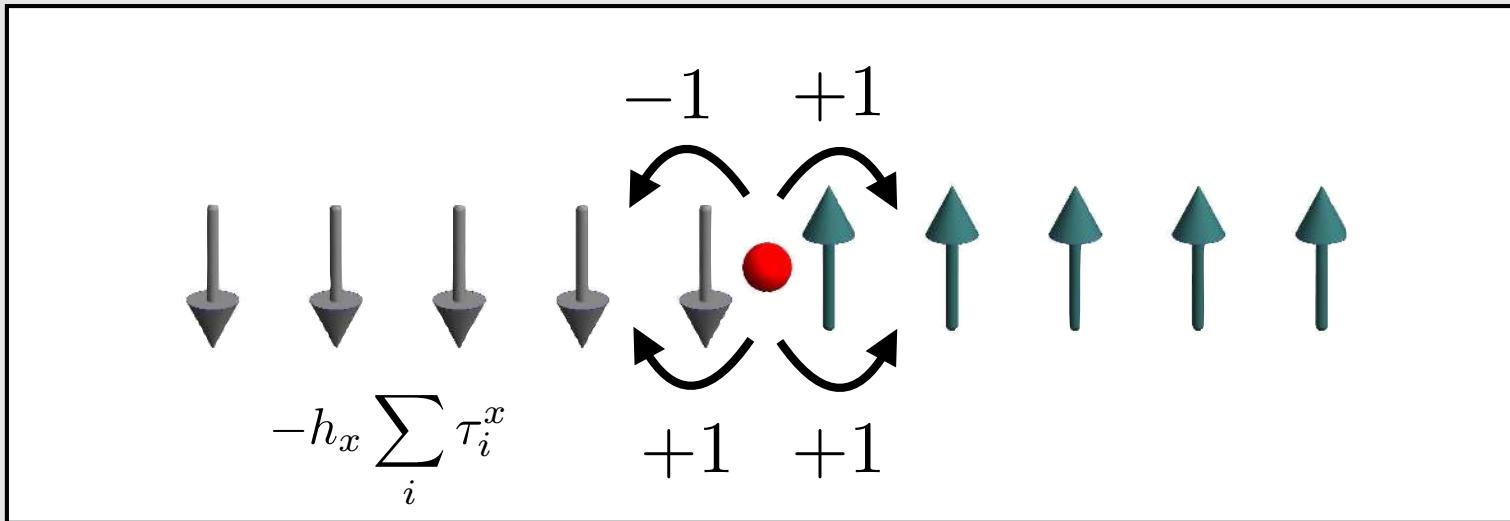
$$\sum_i (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) = \sum_i (-1)^i (\tau_{i+1}^z - \tau_{i-1}^z) \tau_i^x$$



# Twisted Kitaev: Deg Pert theory

Nature Physics (2021)

$$\sum_i (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) = \sum_i (-1)^i (\tau_{i+1}^z - \tau_{i-1}^z) \tau_i^x$$



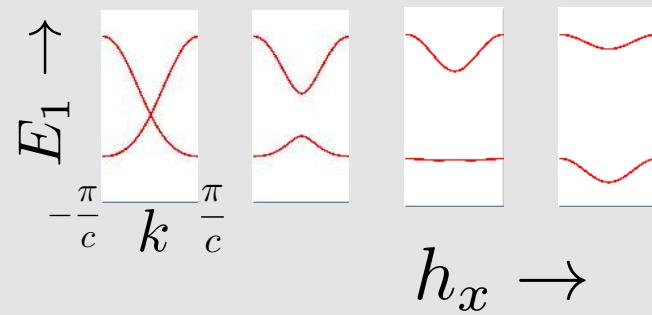
Su-Schrieffer-Heeger

# Twisted Kitaev: Deg Pert theory

Nature Physics (2021)

$$\mathcal{H}_d = - \sum_n \left[ (h_x + (-1)^n K \sin(2\theta)) (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) \right]$$

Two-bands. Su-Schrieffer-Heeger model!

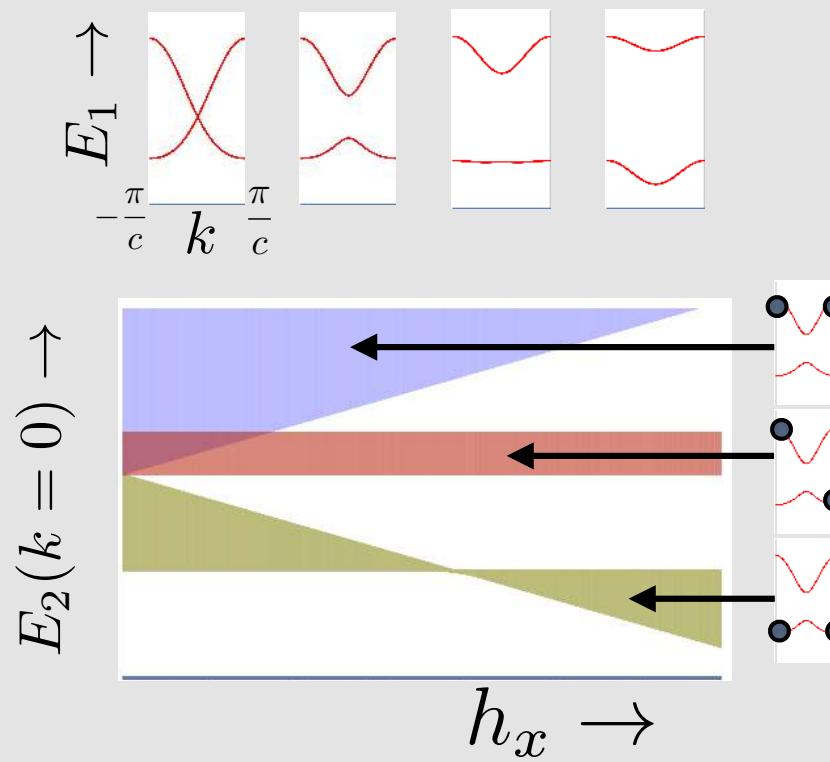
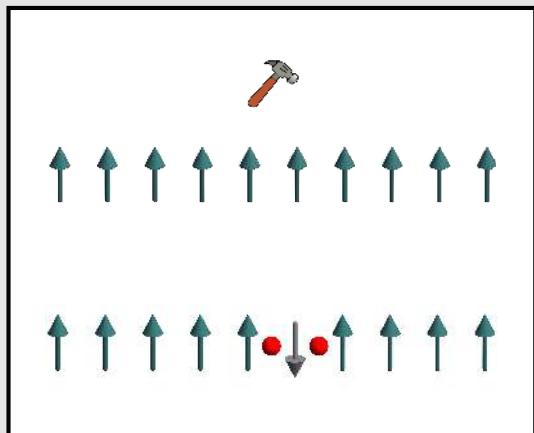


# Twisted Kitaev: Deg Pert theory

Nature Physics (2021)

$$\mathcal{H}_d = - \sum_n \left[ (h_x + (-1)^n K \sin(2\theta)) (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) \right]$$

Two-bands. Su-Schrieffer-Heeger model!

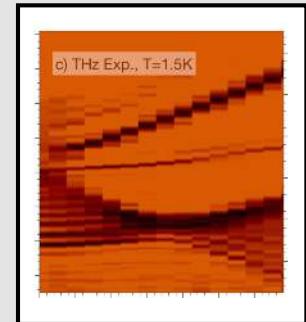
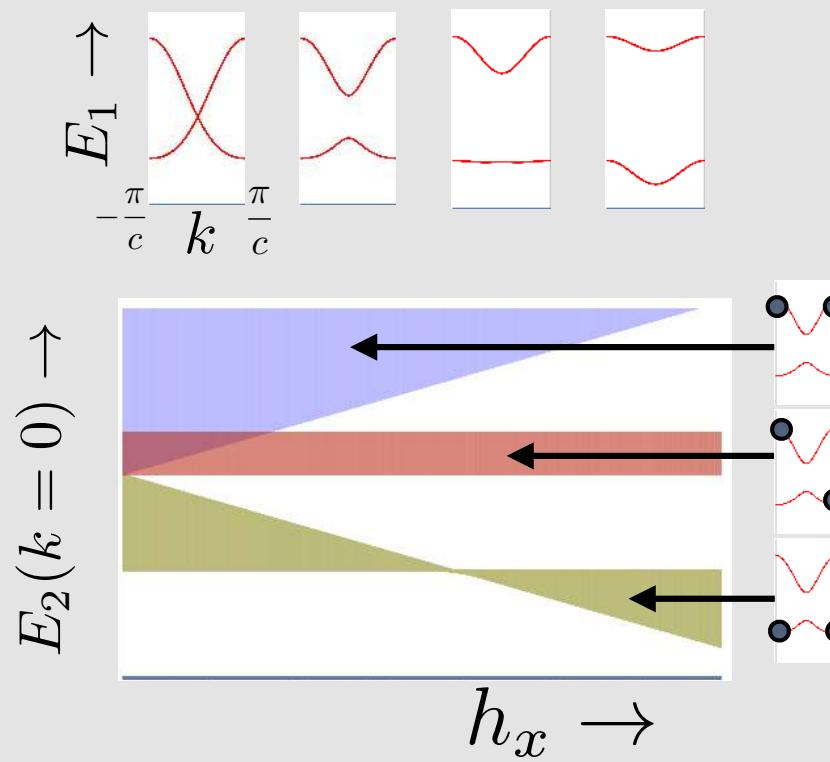
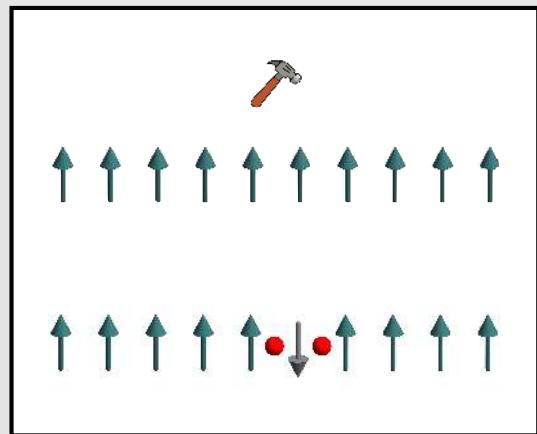


# Twisted Kitaev: Deg Pert theory

Nature Physics (2021)

$$\mathcal{H}_d = - \sum_n \left[ (h_x + (-1)^n K \sin(2\theta)) (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) \right]$$

Two-bands. Su-Schrieffer-Heeger model!



# Twisted Kitaev: DMRG

White (1992); Vidal (2003); White & Feiguin (2004);

Need to go beyond perturbation theory

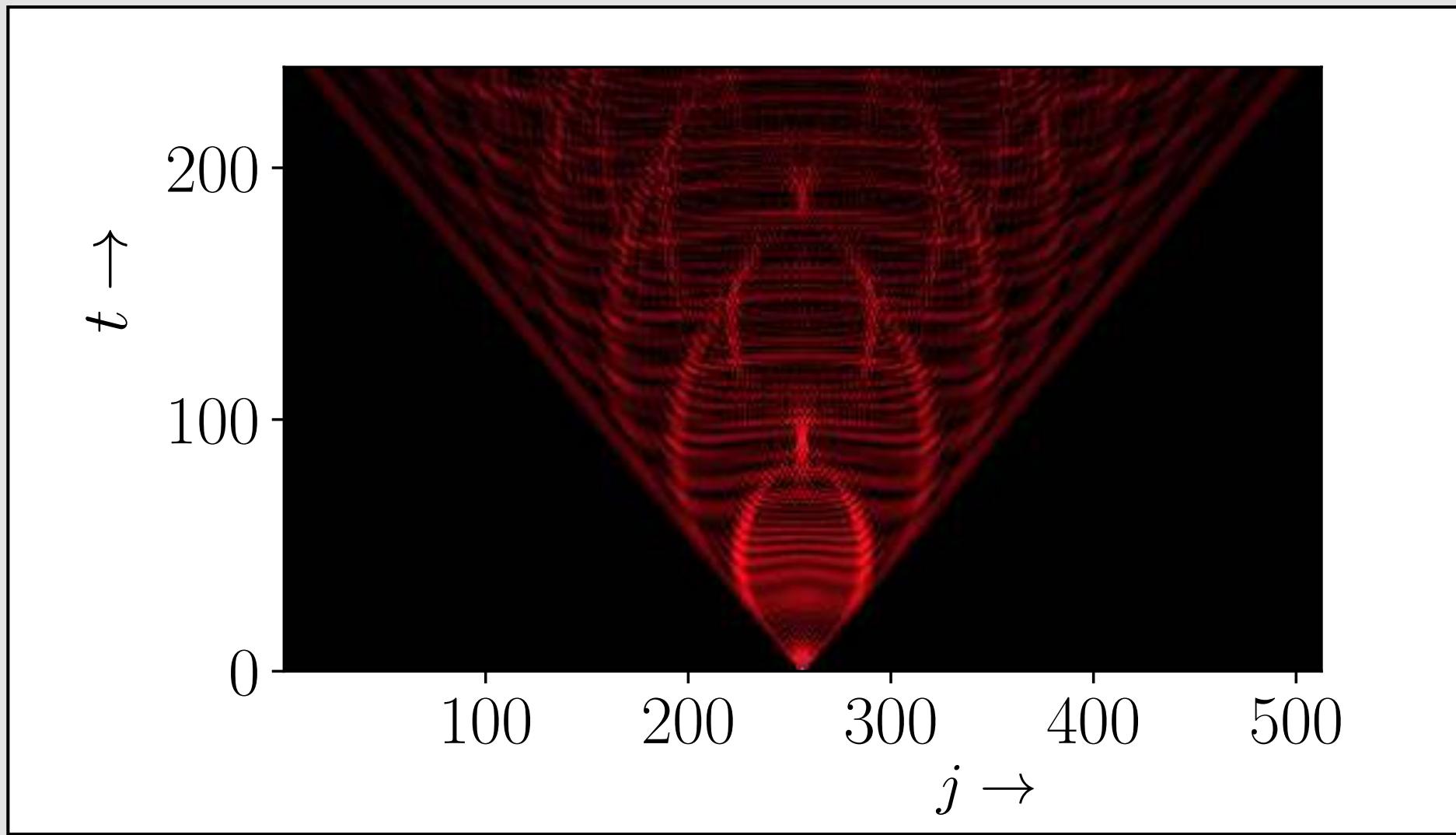
$$\begin{aligned}\mathcal{H} = & -K \sum_i \left[ \cos^2(\theta) \tau_i^z \tau_{i+1}^z + \sin^2(\theta) \tau_i^x \tau_{i+1}^x \right. \\ & + \frac{\sin(2\theta)}{2} (-1)^i (\tau_i^x \tau_{i+1}^z + \tau_i^z \tau_{i+1}^x) \Big] \\ & - h_x \sum_i \tau_i^x - h_z \sum_i \tau_i^z\end{aligned}$$

DMRG: Store  $|\Psi\rangle$  as a “matrix product state”

$$\mathcal{S}^{\alpha\beta}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt \sum_j e^{i\mathbf{k} \cdot \mathbf{x}_j - i\omega t} \langle S_j^\alpha(t) S_0^\beta(0) \rangle$$

# DMRG: Time Evolution

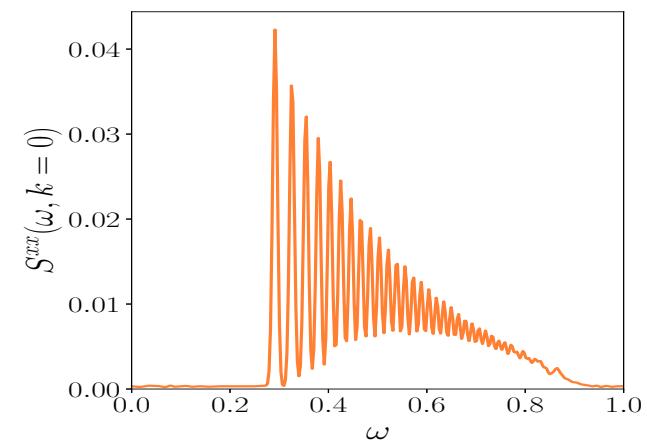
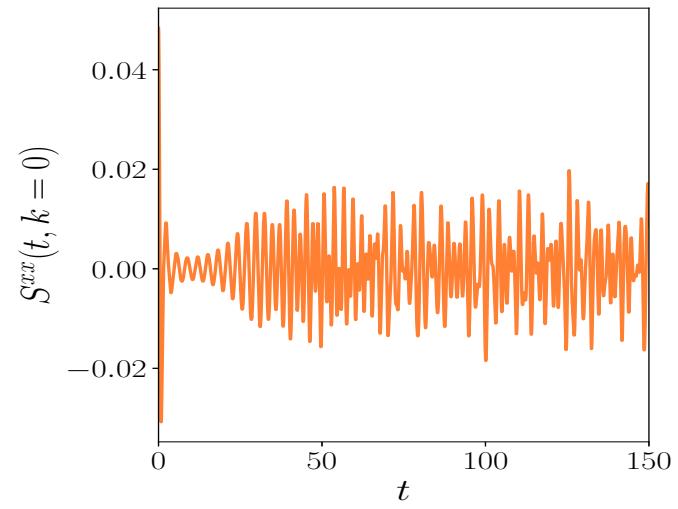
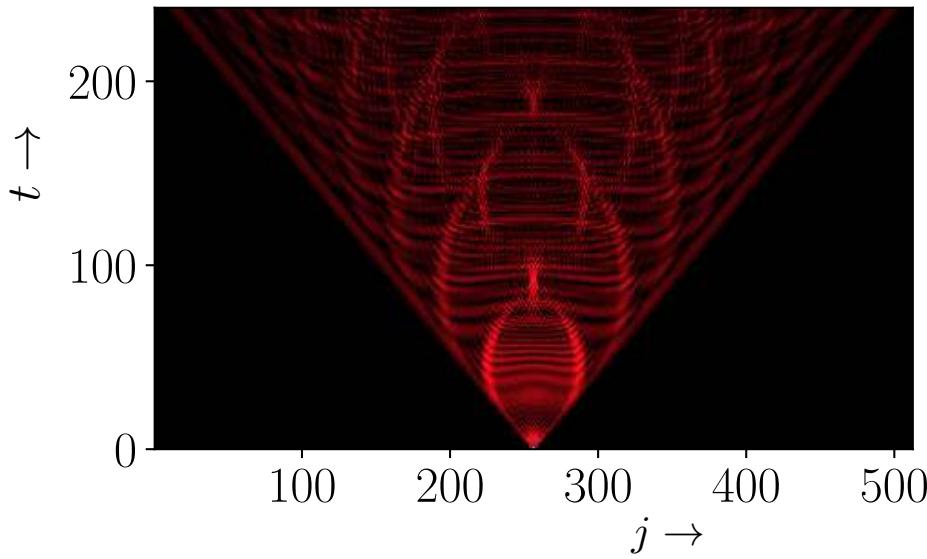
$$\langle S_j^x(t) S_0^x \rangle = \langle \Psi_{\text{gs}} | S_j^x e^{-i(H-E_0)t} S_0^x | \Psi_{\text{gs}} \rangle$$



# DMRG: Time Evolution

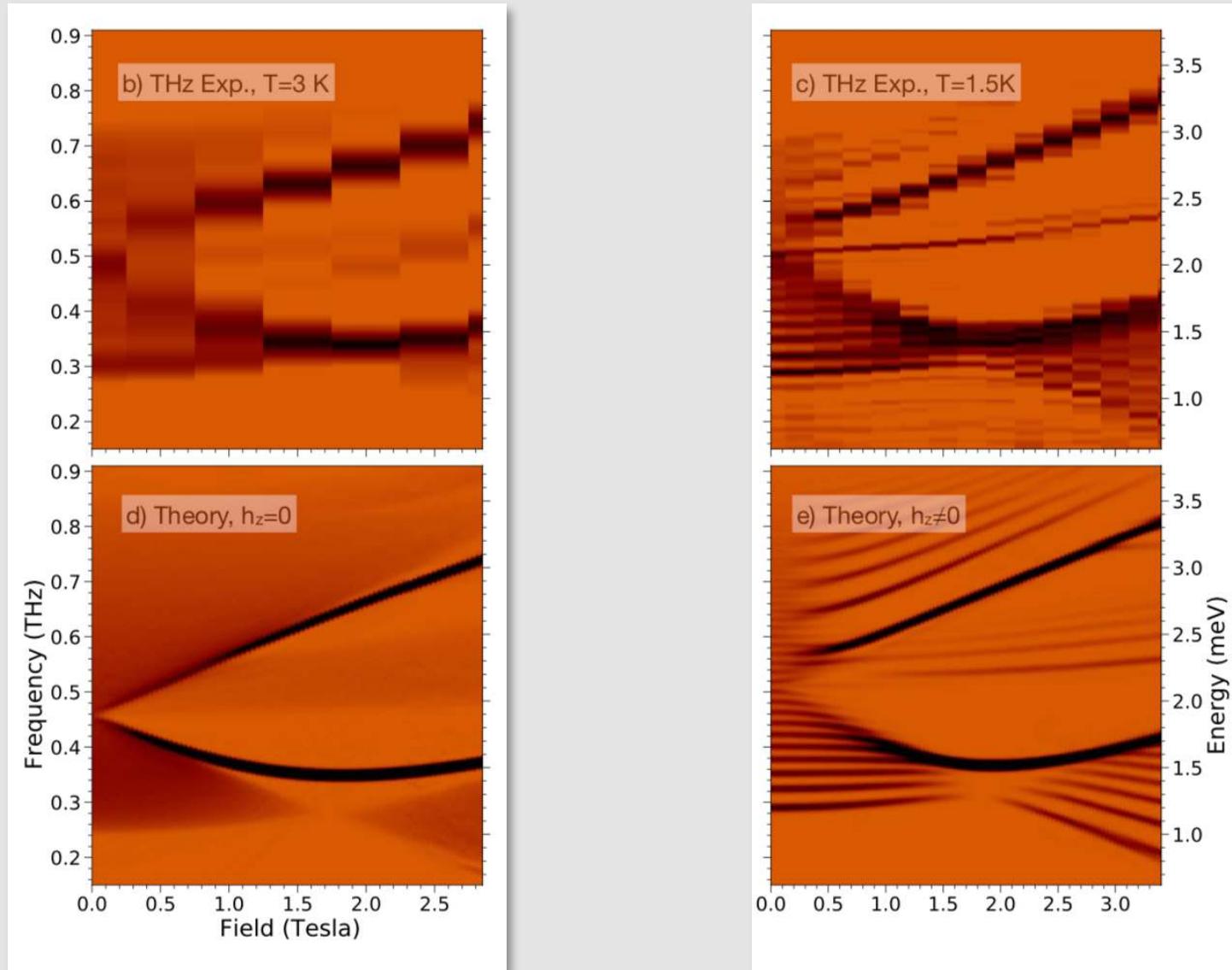
$$\langle S_j^x(t) S_0^x \rangle = \langle \Psi_{\text{gs}} | S_j^x e^{-i(H-E_0)t} S_0^x | \Psi_{\text{gs}} \rangle$$

$$\mathcal{S}^{\alpha\beta}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt \sum_j e^{i\mathbf{k}\cdot\mathbf{x}_j - i\omega t} \langle S_j^\alpha(t) S_0^\beta(0) \rangle$$



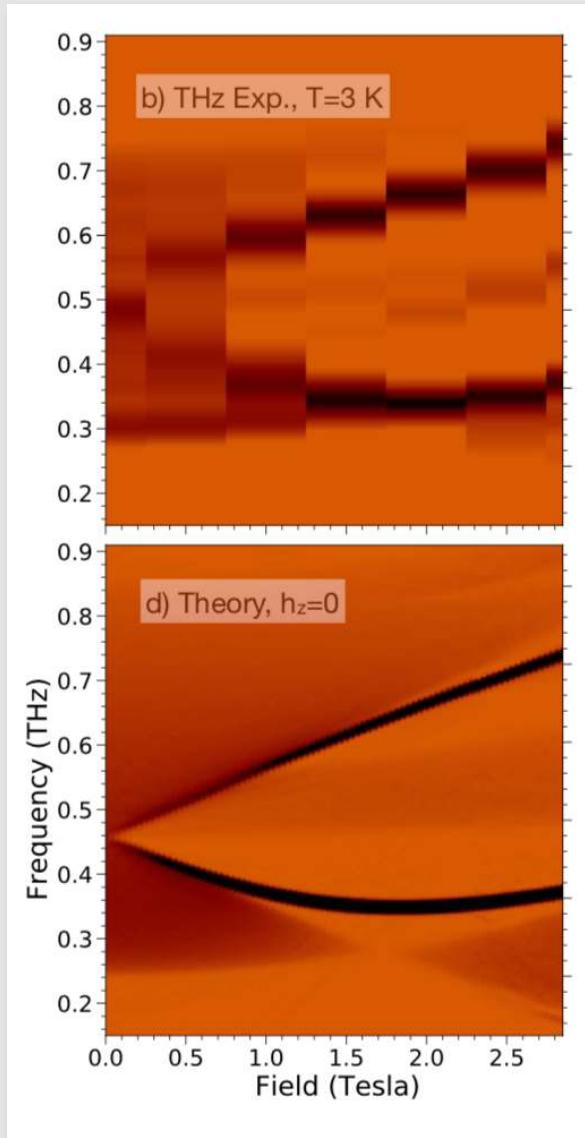
# DMRG

Nature Physics (2021)



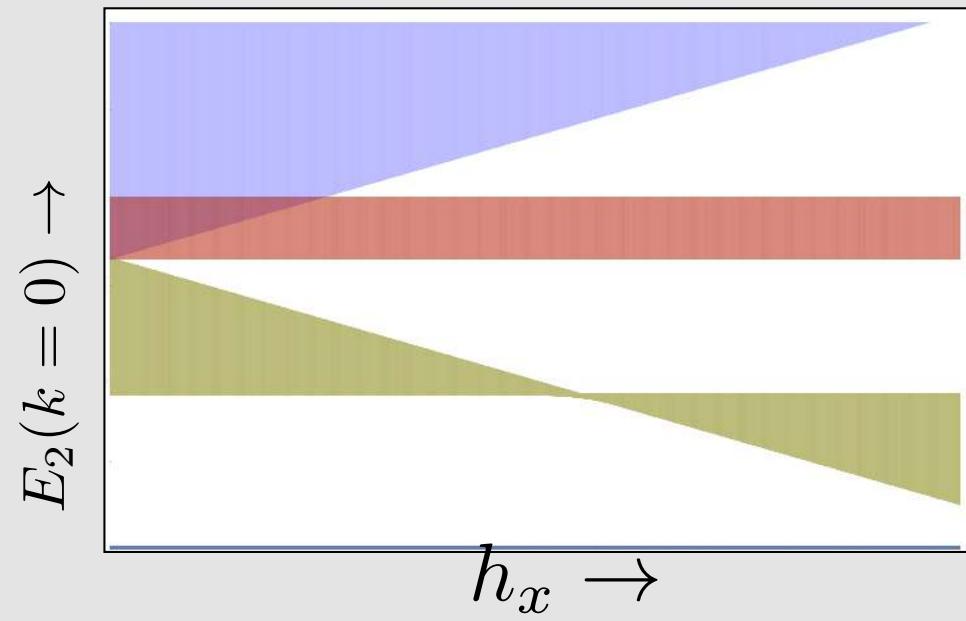
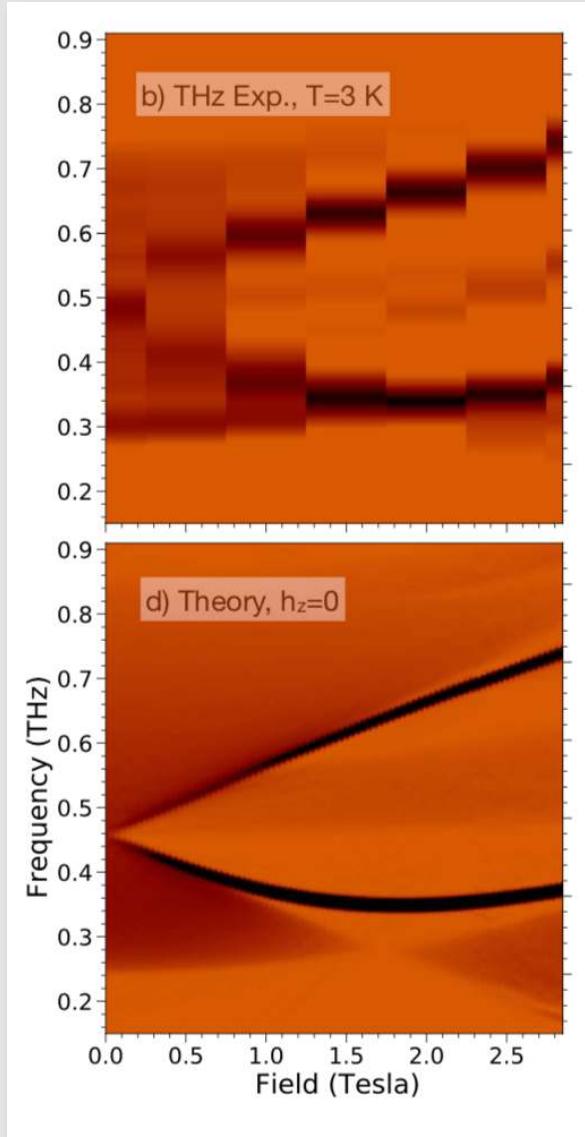
# DMRG

Nature Physics (2021)



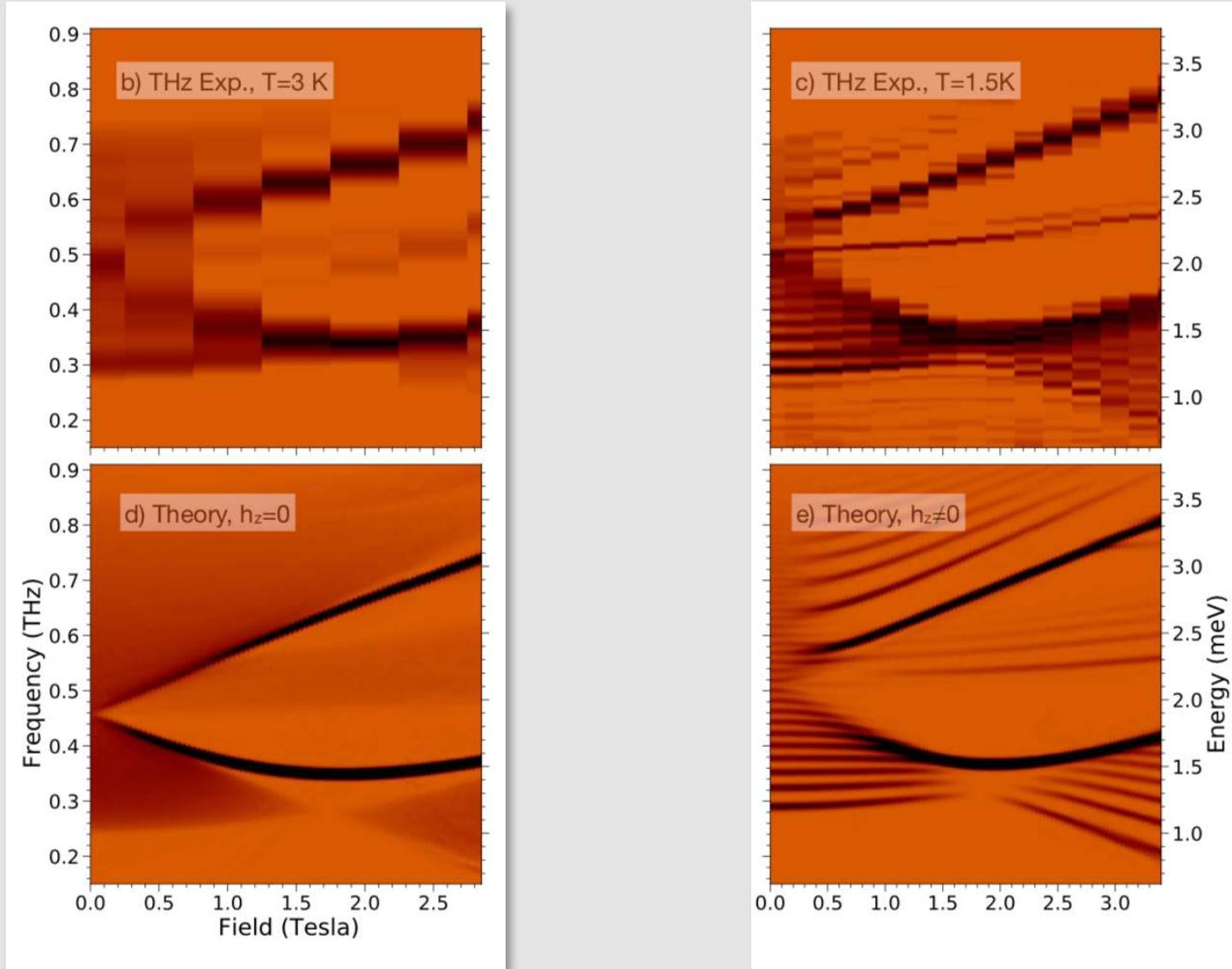
# DMRG

Nature Physics (2021)



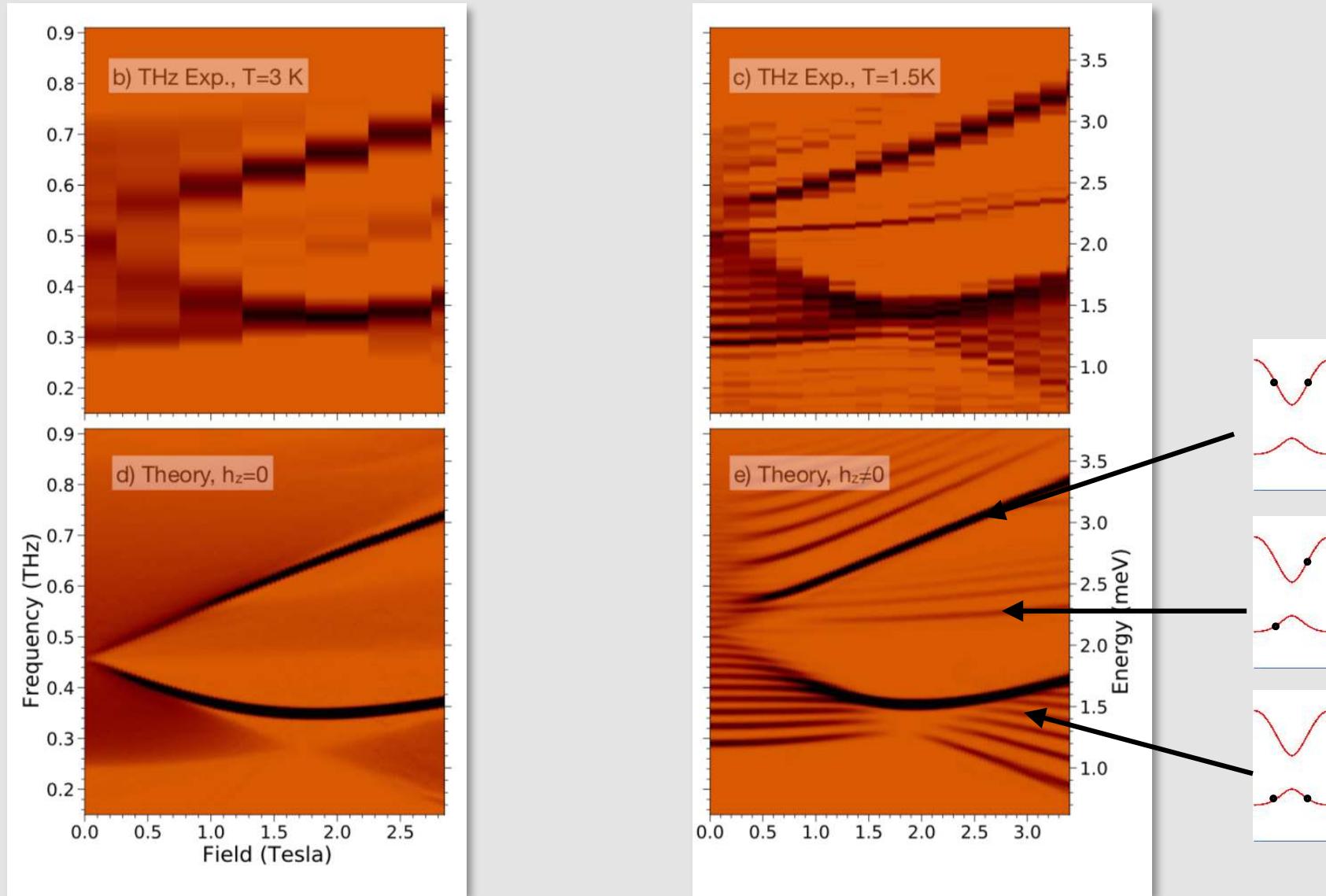
# DMRG

Nature Physics (2021)

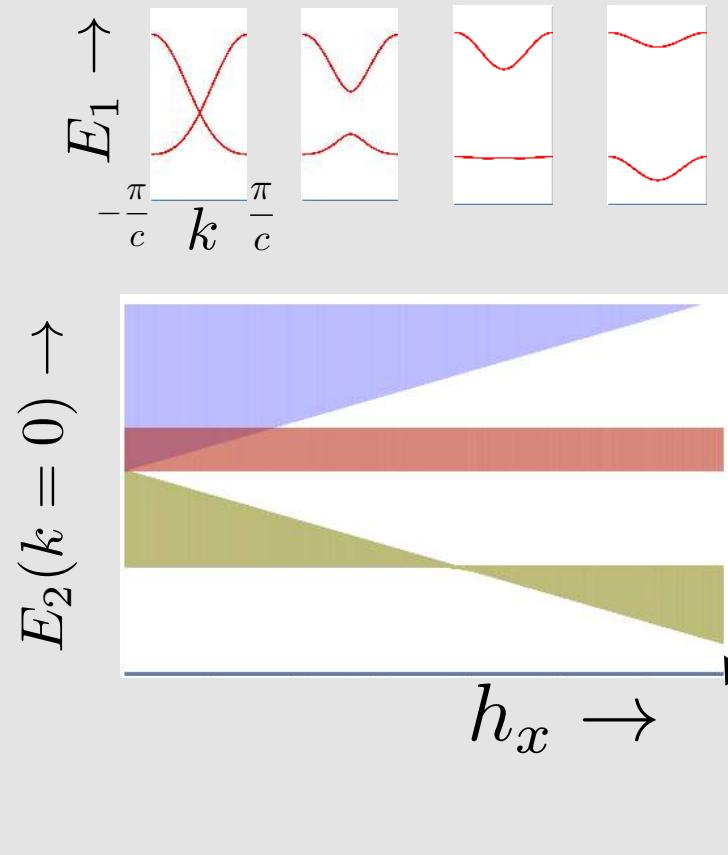


# DMRG

Nature Physics (2021)

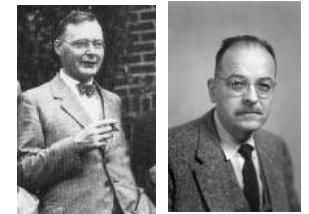


# K-W duality

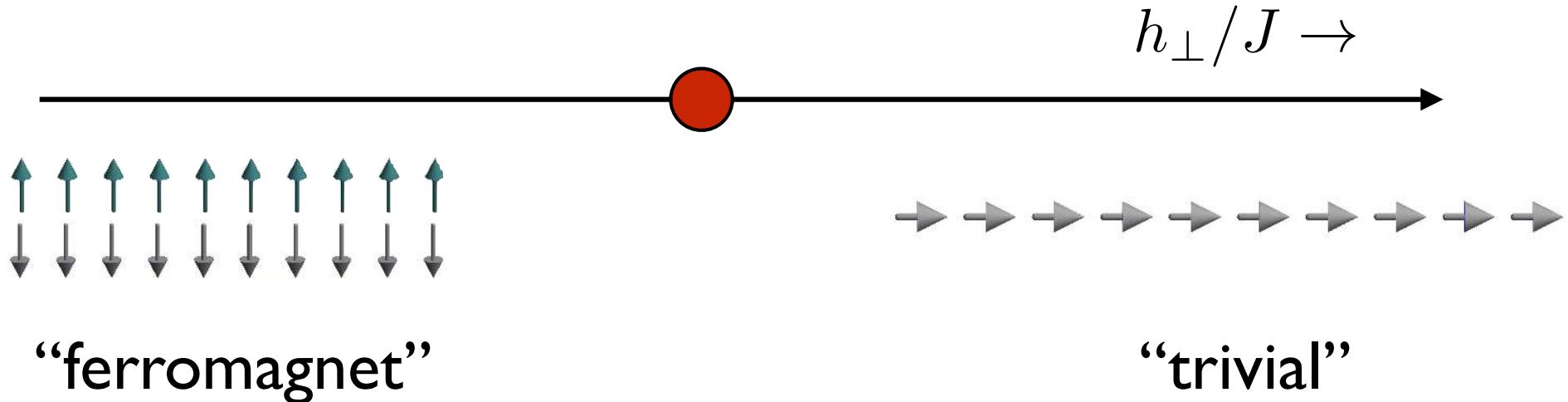


Transition happens through domain-wall condensation

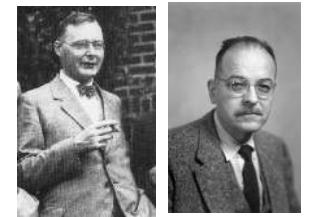
# Kramers-Wannier Duality (1941)



$$H = - \sum_i (J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + h_{\perp} \hat{\sigma}_i^x)$$



# Kramers-Wannier Duality (1941)

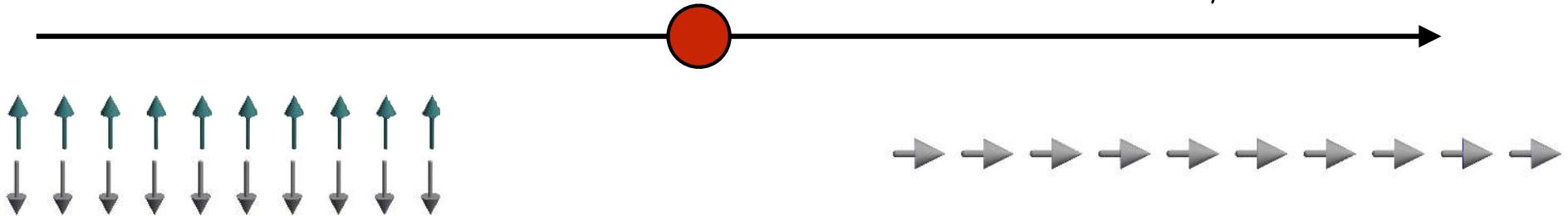


$$H = - \sum_i (J \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z + h_{\perp} \hat{\sigma}_i^x)$$



$$H = - \sum_i (h_{\perp} \hat{\tau}_i^z \hat{\tau}_{i+1}^z + J \hat{\tau}_i^x)$$

$h_{\perp}/J \rightarrow$

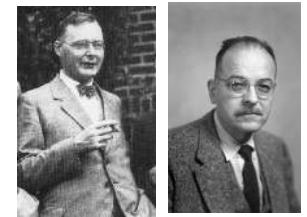


“ferromagnet”

“trivial”

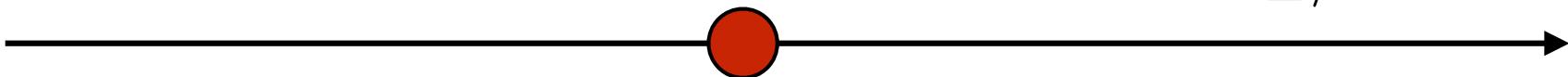
# Kramers-Wannier Duality (1941)

$$H(J, h_{\perp}) \leftrightarrow H(h_{\perp}, J)$$



$$(J/h_{\perp})_c = 1$$

$$h_{\perp}/J \rightarrow$$



domain wall qp



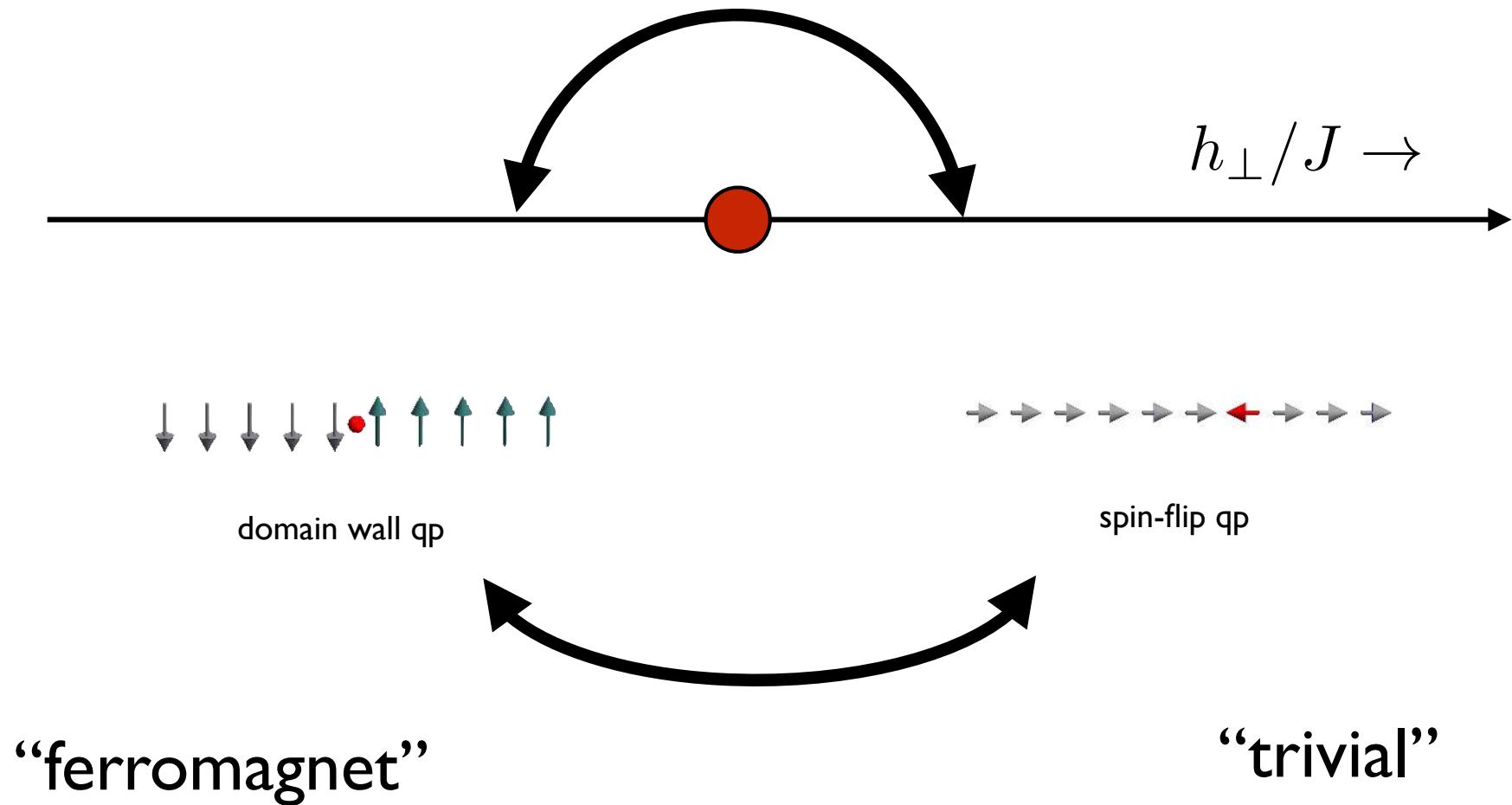
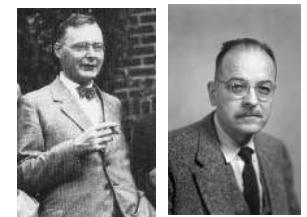
spin-flip qp

“ferromagnet”

“trivial”

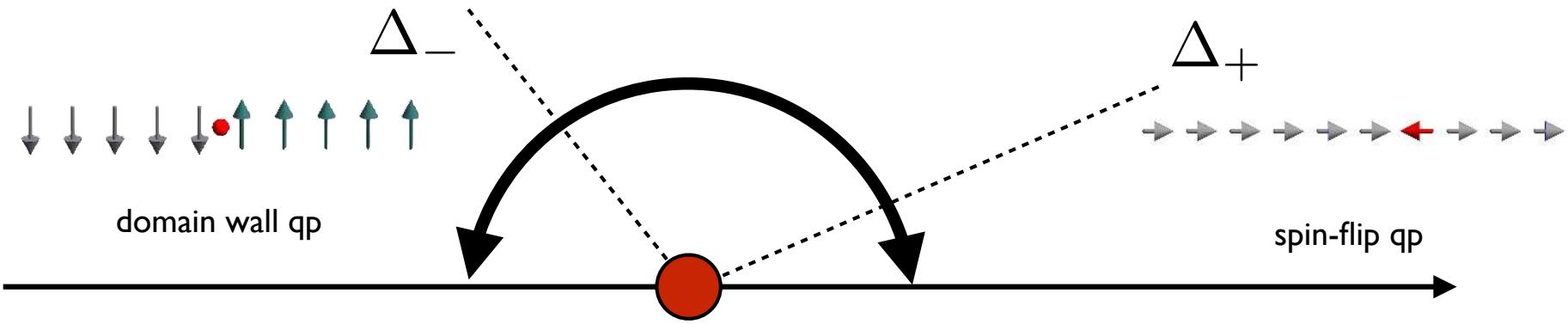
# Kramers-Wannier Duality (1941)

$$H(J, h_{\perp}) \leftrightarrow H(h_{\perp}, J)$$



# K-W duality

$$H(J, h_{\perp}) \leftrightarrow H(h_{\perp}, J)$$



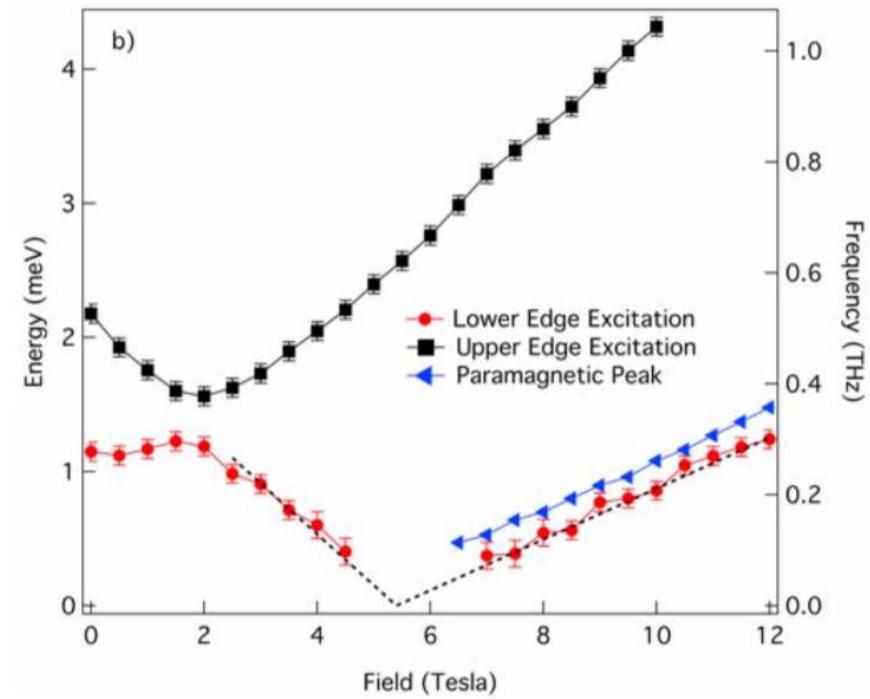
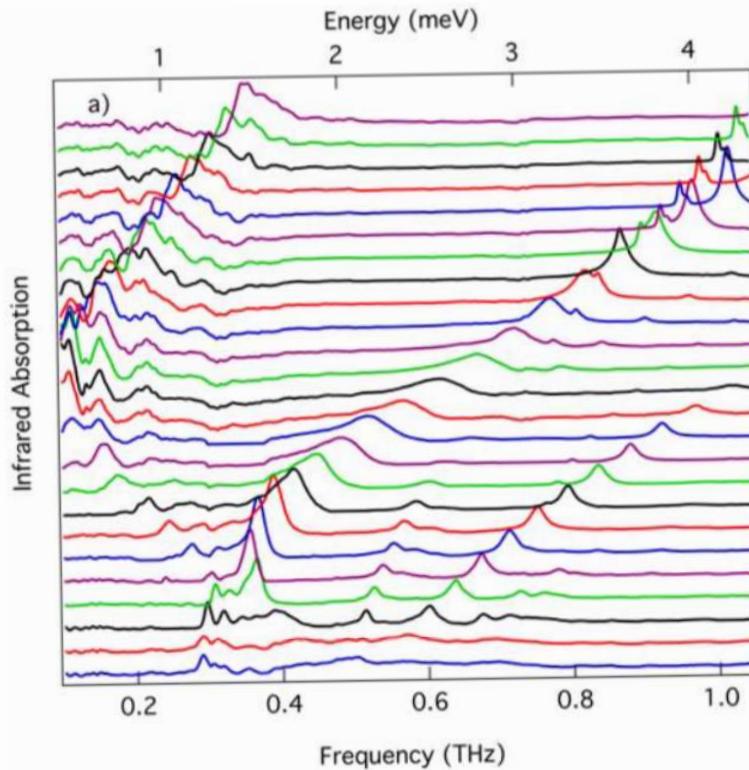
$$h_{\perp}/J \rightarrow$$
$$\Delta_{\pm} \sim \mathcal{A}_{\pm} |t|^{z\nu}$$

Amplitude ratio universal!

$$\frac{\mathcal{A}_-}{\mathcal{A}_+} = 2$$

# K-W duality

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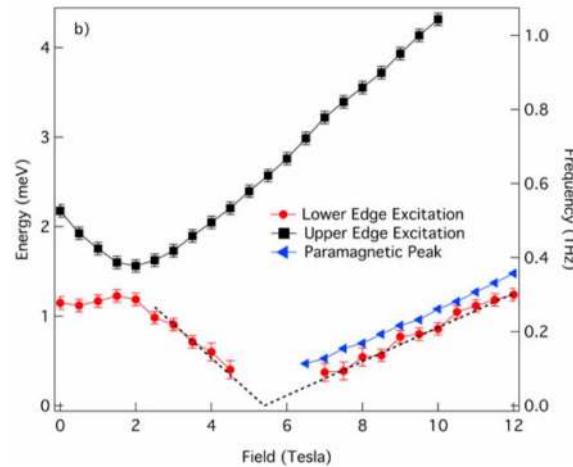


$$\Delta_{\pm} \sim \mathcal{A}_{\pm} |t|^{z\nu}$$

$$t \equiv (B_b - B_b^c)/B_b^c$$

# K-W duality

Nature Physics (2021)



$$\Delta_{\pm} \sim \mathcal{A}_{\pm} |t|^{z\nu}$$

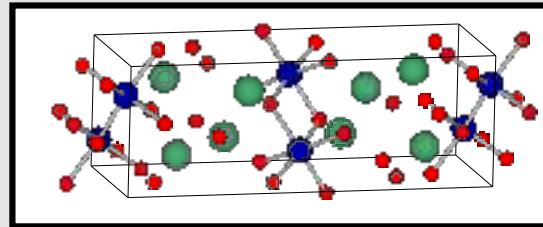
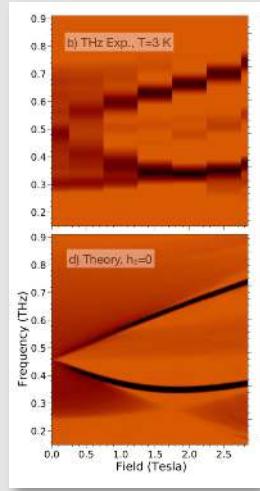


Experiment: I.9(I)

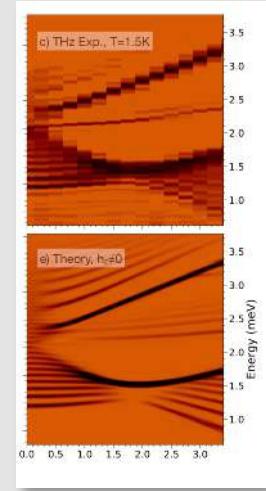
Direct evidence for the Kramers-Wannier duality!

# Quantum Magnetism

Nature Physics (2021)



CoNb<sub>2</sub>O<sub>6</sub>



Theory & Exp for fundamental many body models

**Low Field:** Domain Walls, SSH model

**High Field:** KW duality

bond-dependent interactions in Co  
non-linear response

