Title: Recent results on Kitaev interactions in Co based magnets

Speakers: Peter Armitage

Series: Quantum Matter

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Abstract: Kitaev quantum spin liquids (QSLs) are exotic states of matter that are predicted to host Majorana fermions and gauge flux excitations. However, so far all known Kitaev QSL candidates are known to have appreciable non-Kitaev interactions that pushes these systems far from the QSL regime. Co based magnets have been proposed to be perhaps a more ideal platform for realizing Kitaev QSLs. In this talk I will show evidence for a Kitaev interactions in both the quasi-one-dimensional ferromagnet CoNb2O6 as well as the hexagonal magnet BaCo2(AsO4). Although it is usually believed to be the best material realization of a 1D Ising chain, by combining terahertz spectroscopy and calculations we have shown that CoNb2O6 is well described by a model with bond-dependent interactions. We call this model the 'twisted Kitaev chain', as these interactions are similar to those of the honeycomb Kitaev spin liquid. The ferromagnetic ground state of CoNb2O6 arises from the compromise between two axes. Owing to this frustration, even at zero field domain walls have quantum motion, which is described by the celebrated Su-Schrieffer-Heeger model of polyacetylene and shows rich behavior as a function of field. Most recently, we have shown also that the honeycomb cobalt-based Kitaev QSL candidate, BaCo2(AsO4)2, has dominant Kitaev interactions. Due to only small non-Kitaev terms a magnetic continuum consistent with Majorana fermions and the existence of a Kitaev QSL can be induced by a small out-of-plane-magnetic field. Our results demonstrate BaCo2(AsO4)2 as a far more ideal version of Kitaev QSL compared with other candidates.

C. M Morris et al. "Hierarchy of bound states in the one-dimensional ferromagnetic Ising chain CoNb2O6 investigated by high-resolution time-domain terahertz spectroscopy." Phys. Rev. Lett. 112.13 137403 (2014).

C.M. Morris et al. "Duality and domain wall dynamics in a twisted Kitaev chain", Nature Physics

volume 17, pages 832-836 (2021).

X. Zhang, et al., "In- and out-of-plane field induced quantum spin-liquid states in a more ideal Kitaev material: BaCo2(AsO4)", https://arxiv.org/abs/2106.13418

Zoom Link: https://pitp.zoom.us/meeting/register/tJcqc-ihqzMvHdW-YBm7mYd_XP9Amhypv5vO

Recent results on Kitaev interactions in Co based magnets: chains and honeycomb

N. Peter Armitage

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Dept. of Physics and Astronomy
The Johns Hopkins University

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Recent results on Kitaev interactions in Co based magne

$CoNb_2O_6$, best material realization of "Ising's model"

-THz experiments on $CoNb_2O_6$ in zero field; 9 "meson" bound states at low temperature.

-Ising chain in transverse magnetic field; simplest examp of a quantum phase transition; Kramers-Wannier duality; twisted Kitaev chain

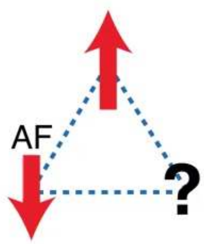
Quantum spin-liquid states in a more ideal Kitaev material: $BaCo_2(AsO_4)_2$

-small J and Γ terms.

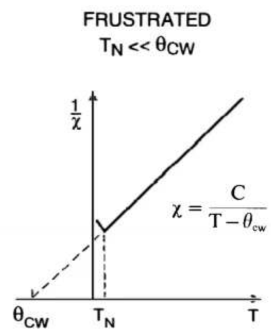
- out-of-plane field of a few T can induce a QSL.

Morris et al. PRL 2014
Steinberg, NPA, et al. PRB 2019
Morris et al. Nature Physics 2021
Zhang et al. arXiv 2106.13418.

Frustrated magnets



$$H = -\frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i \bullet \mathbf{S}_j$$



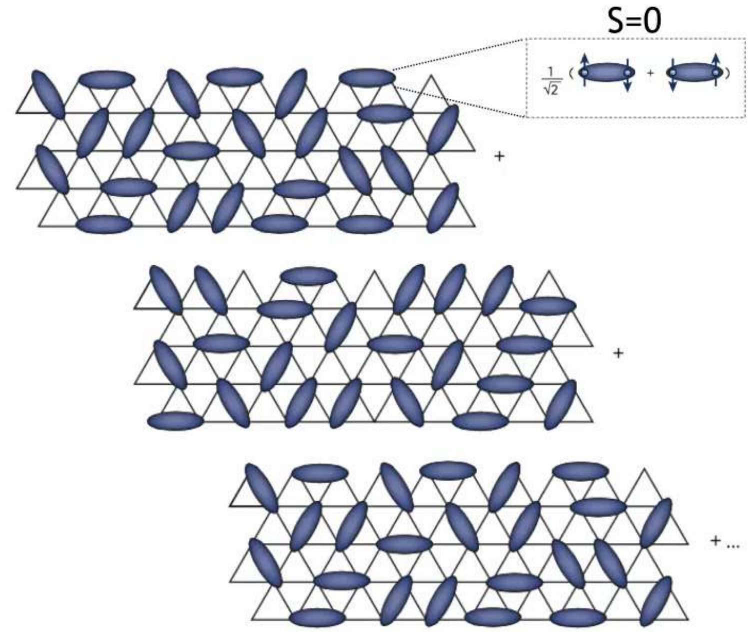
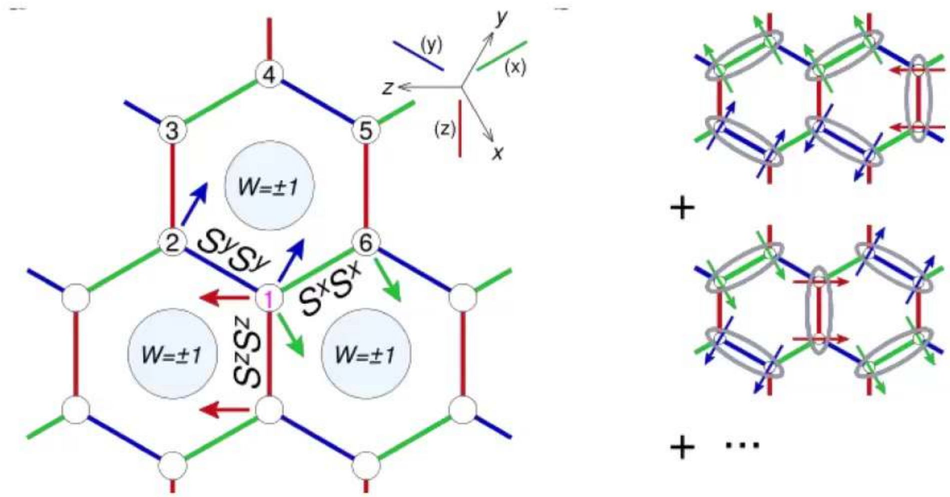


Image courtesy of L. Balents

Kitaev interaction in honeycomb lattice



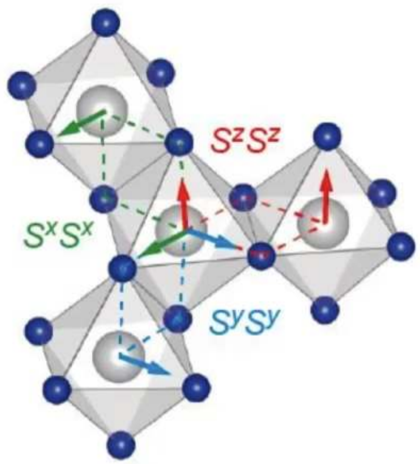
Takagi et al.

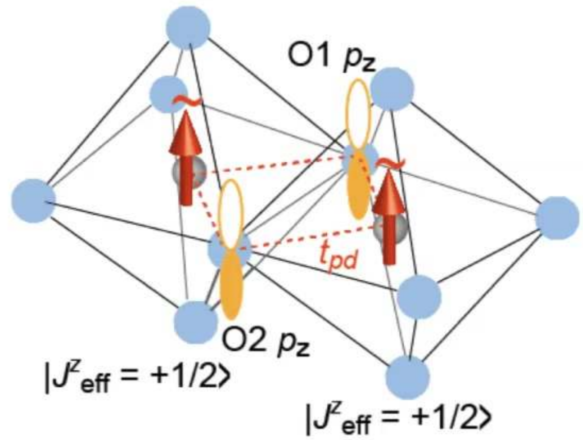
Kitaev demonstrated exactly solvable model of a spin liquid with each bond with Ising interaction in different direction.

$$H_K = \sum_{i,j} K^{\gamma} S_i^{\gamma} S_j^{\gamma}$$

5

Kitaev interaction in honeycomb lattice



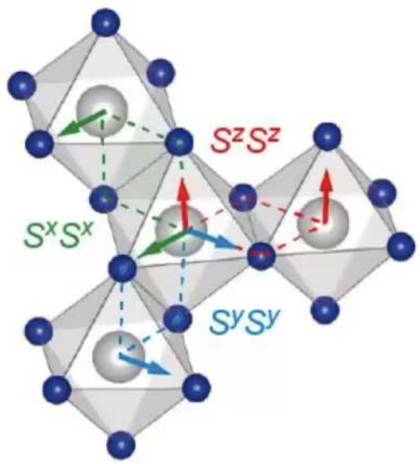


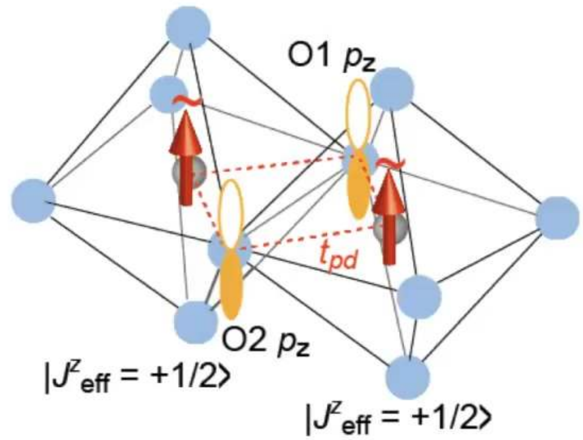
Jackeli and Khaliullin showed possible in edge sharing octahedra with strong SOC. But other interactions exist (Heisenberg etc.)

Possible in Na_2IrO_3, ∝-$RuCl_3$ and $H_3LiIr_2O_6$ and also proposed for Co^{+2} systems

$$\mathcal{H}_1 = \sum_{\langle ij \rangle_\gamma} K S_i^\gamma S_j^\gamma$$

Kitaev interaction in honeycomb lattice





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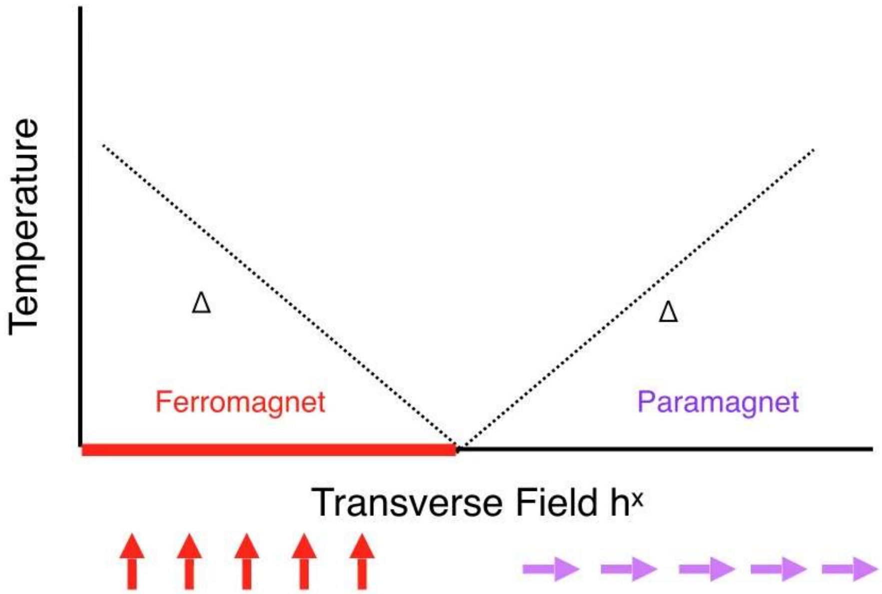
$$\mathcal{H}_1 = \sum_{\langle ij\rangle_\gamma} \left[K S_i^\gamma S_j^\gamma + J \mathbf{S}_i \cdot \mathbf{S}_j + \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) + \Gamma' \left(S_i^\gamma S_j^\alpha + S_i^\gamma S_j^\beta + S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma \right) \right]$$
$$+ J_3 \sum_{\langle ij\rangle_3} \mathbf{S}_i \cdot \mathbf{S}_j + \mu_B \sum_{\langle i\rangle} \mathbf{B} \cdot \mathbf{g} \cdot \mathbf{S}_i,$$

The Ising chain in transverse field

Energy scales collapse near a quantum phase transiti



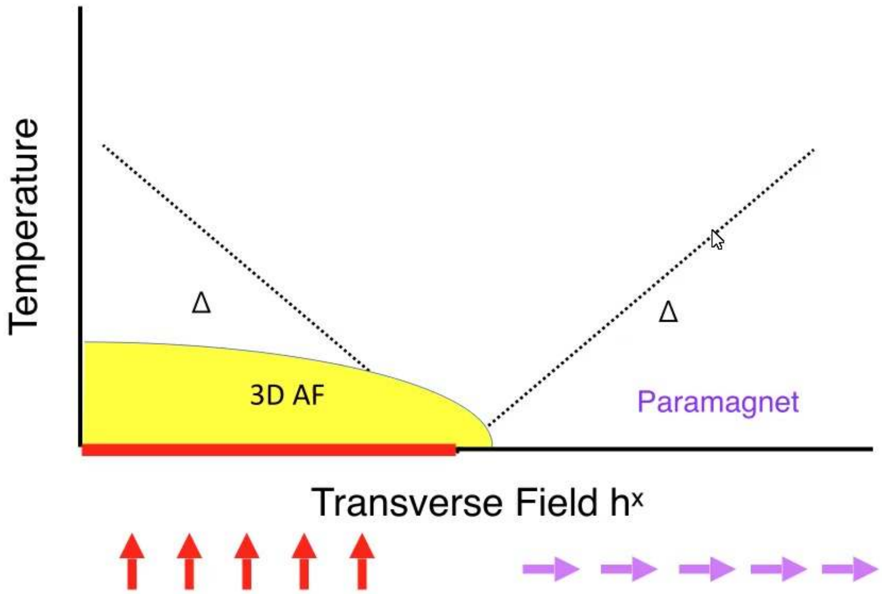
$$H = -J' \sum_n S_n^z S_{n+1}^z - h^x \sum_n S_n^x$$

Limits of high field and low field are well defined.

There must be a QPT as ground state changes degeneracy

General phenomena → changing of ground state as function of non-thermal parameter; phase transition

Energy scales collapse near a quantum phase transiti



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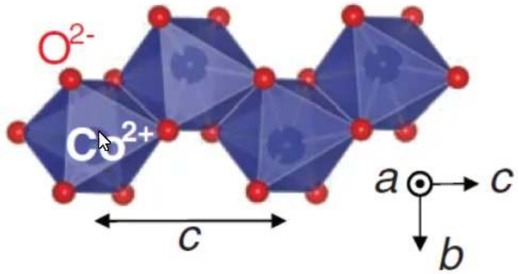
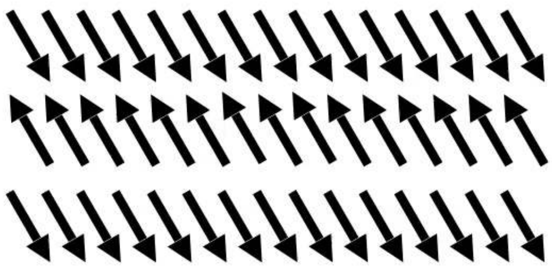
$CoNb_2O_6$ – Columbite - Ising chain material

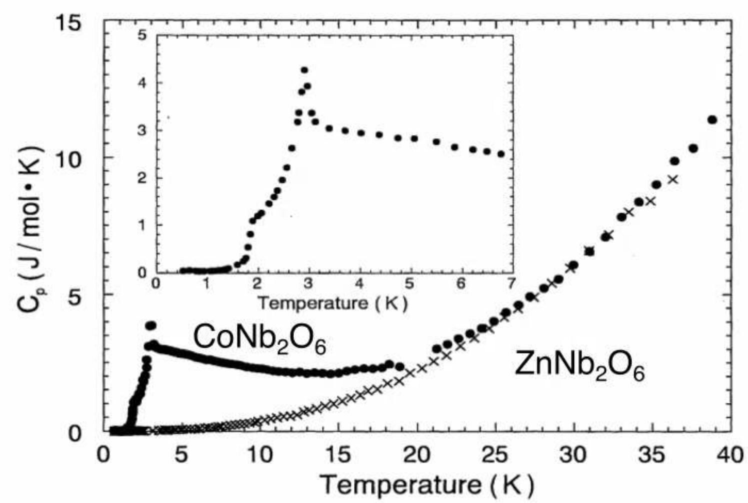


R. Coldea et. al., Science **327**, 177 (2010)

Spins point in a-c plane

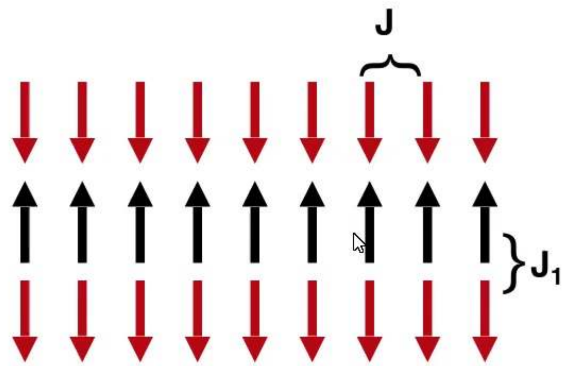
- T_{N1} = 2.95 K, incommensurate AF ordering of FM chains
- T_{N2} = 1.97 K, commensurate AF ordering of FM chains
- Interesting QCP @ H_b = 5.5 Tesla





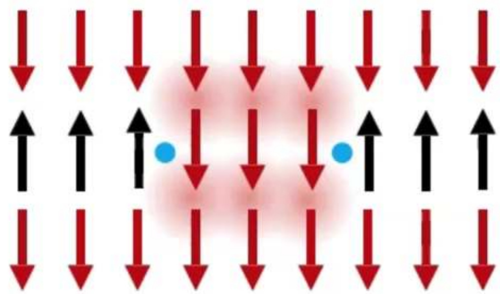
T. Hanawa et. al., J. Phys. Soc. Jap. **63**, 2706 (1994)

$CoNb_2O_6$ – Ising chain material - Excitations



Below T_{N2}, interchain mean field gives effective confining potential linear in separation of domain walls. Strong S_zS_{z+1} interaction.

$E_n = 2(J/2) + n\,J_1$
n is # of flipped spins



But real materials are not pure Ising! → S_x, S_y and inter-chain couplings give "kink" motion.

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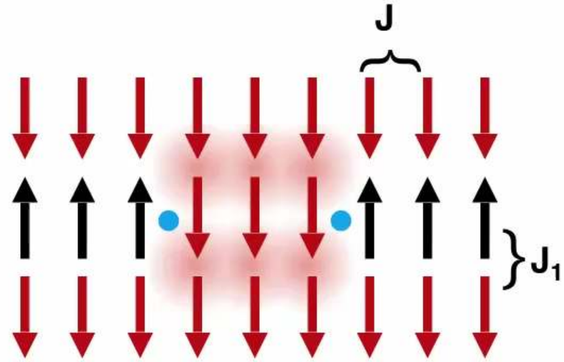

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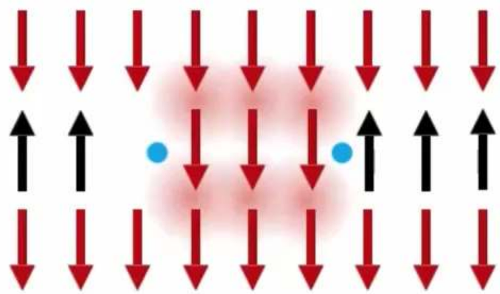

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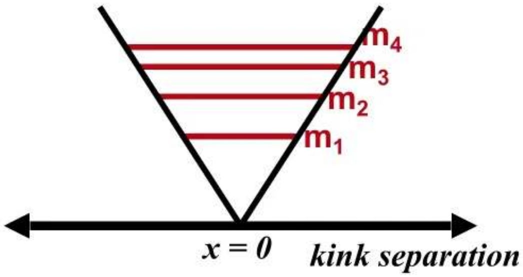
$CoNb_2O_6$ – Ising chain material - Excitations

Rewrite equations of motion with kink as fundamental particle



$$V(x) = \lambda x$$

$$-\frac{\hbar^2}{\mu}\frac{d^2\varphi}{dx^2} + \lambda|x|\varphi = (m - 2m_0)\varphi \qquad (2)$$

$$m_j = 2m_0 + z_j\lambda^{2/3}\left(\frac{\hbar^2}{\mu}\right)^{1/3} \qquad j = 1, 2, 3, \ldots$$

Mapping to continuum 1D Schrodinger equation with linearly confining potential

Solutions are Airy functions, z_j are the negative roots to Airy functions (z_j = 2.34, 4.09, 5.52, 6.79, 7.94, 9.02,…)

PHYSICAL REVIEW D VOLUME 18, NUMBER 4 15 AUGUST 1978

Two-dimensional Ising field theory in a magnetic field: Breakup of the cut in the two-point function

Barry M. McCoy
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794

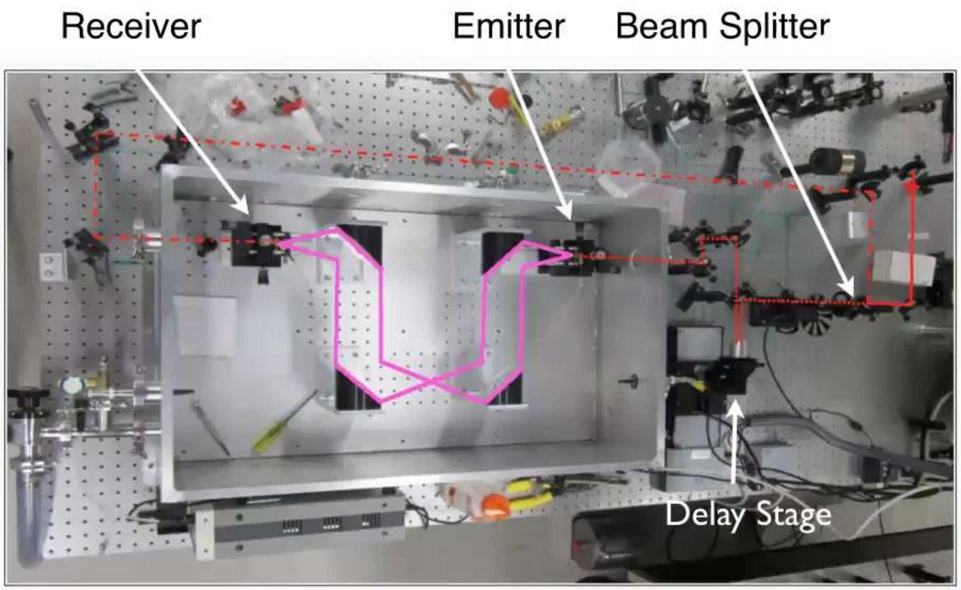
Tai Tsun Wu*
Institute for Theoretical Physics, Utrecht, The Netherlands

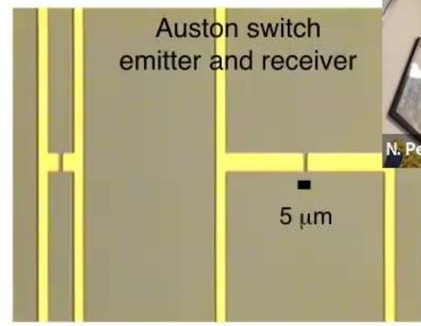
(Received 12 April 1978)

We demonstrate that the cut which is present as the leading singularity in the two-point function of the Ising field theory for $T < T_c$ and $H = 0$ breaks up into a sequence of poles for $H \neq 0$. Both the positions and the residues of the low-lying poles are calculated.

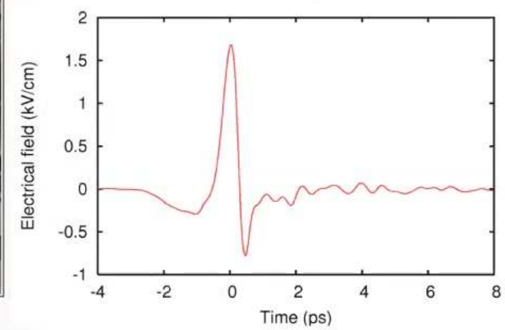
Analogy to quark confinement in QCD
kinks are quarks, bound state is a meson

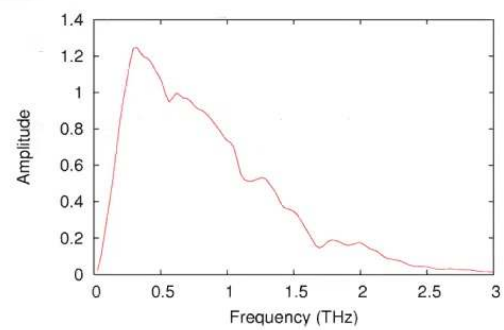
Time Domain THz Spectroscopy





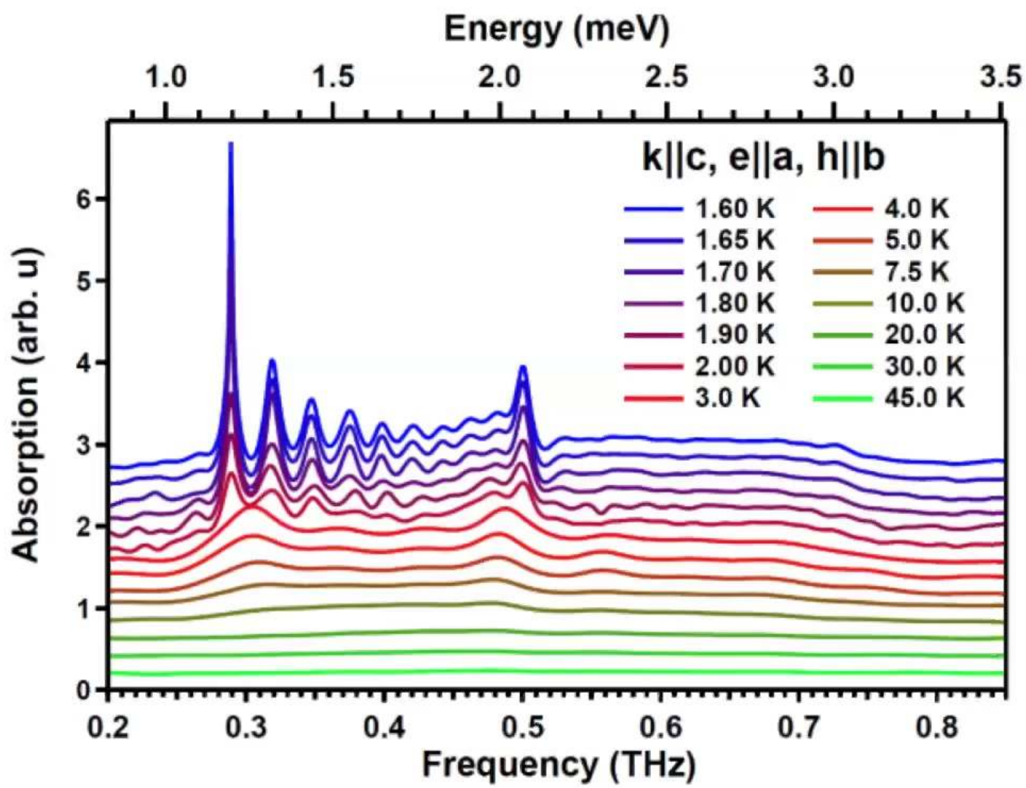
Laser
800nm
60fs



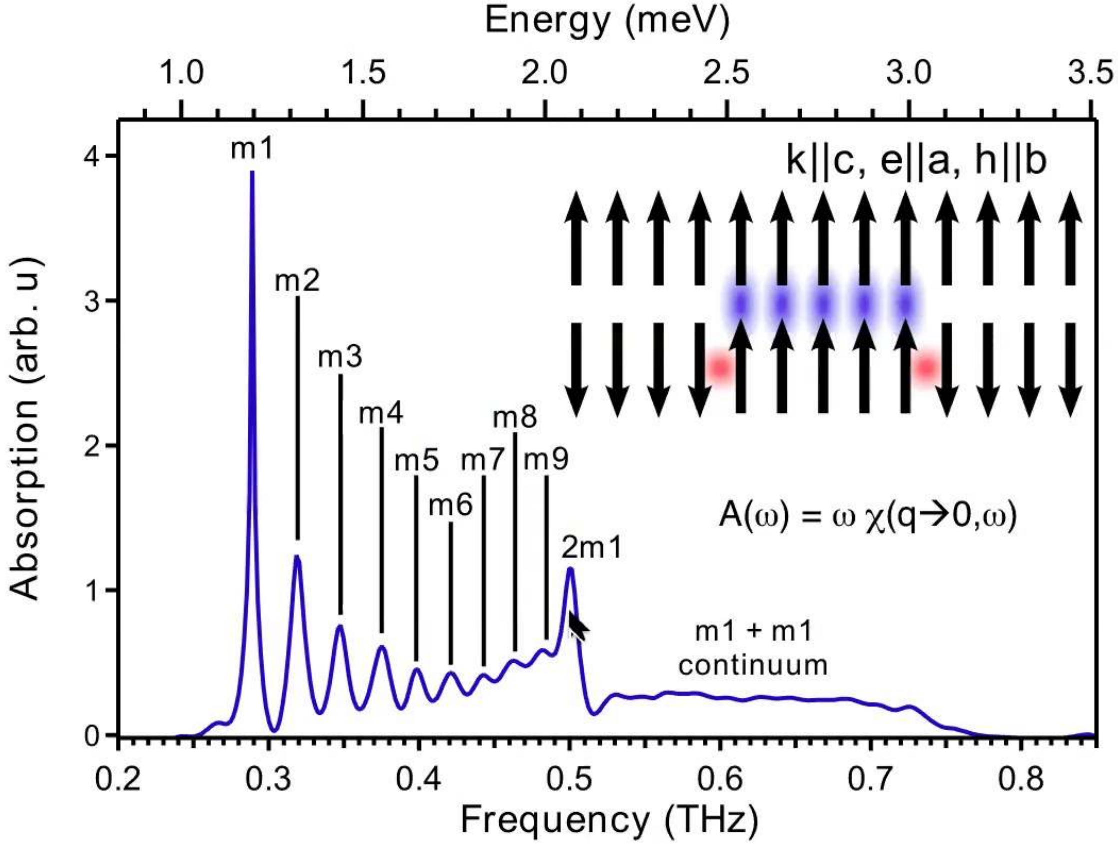


- fs laser excites photoconductive emitter and receiver. Coherent detection of field allows **complex** optical response functions to be measured: 100 GHz - 3 THz (0.8 meV - 12 meV), @ 1.4K - 300K.
- Usually light couples to charge, but can excite **magnetic** dipoles with THz B field
- Broad band THz electron spin resonance (ESR)
- Transmission —> ln(T(ω)) ~ -ωχ(q~0,ω)

Temperature Dependence



Nine “meson” bound states



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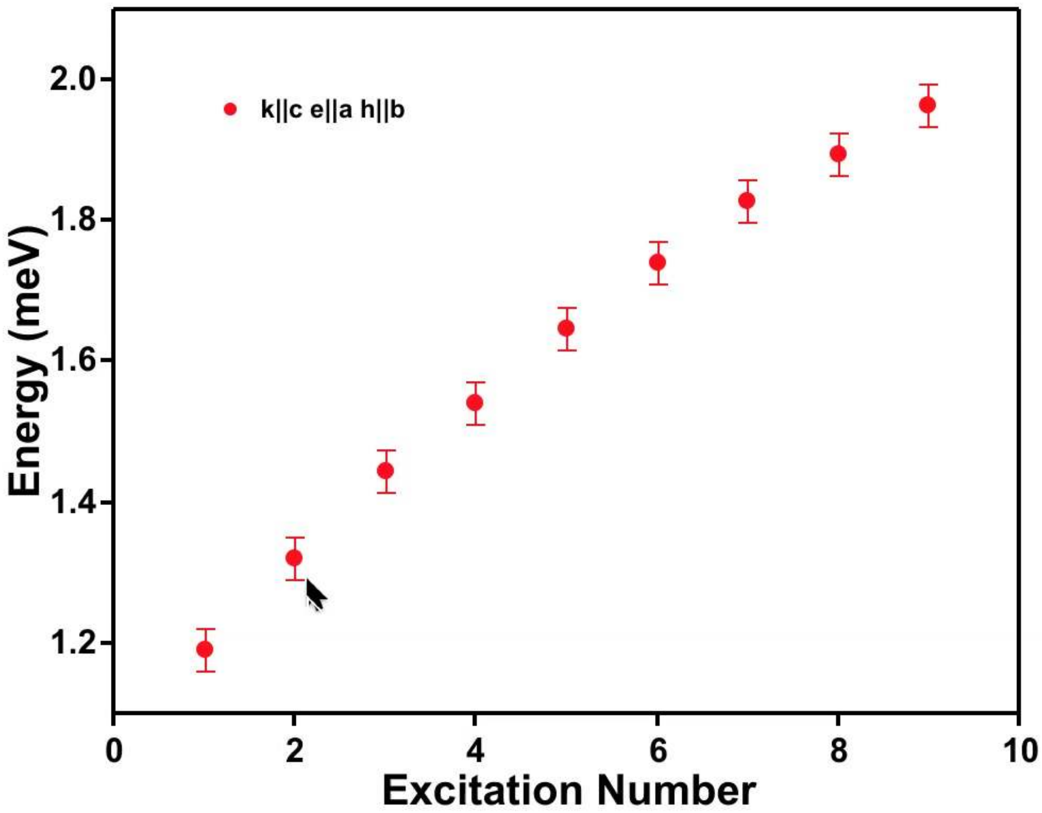

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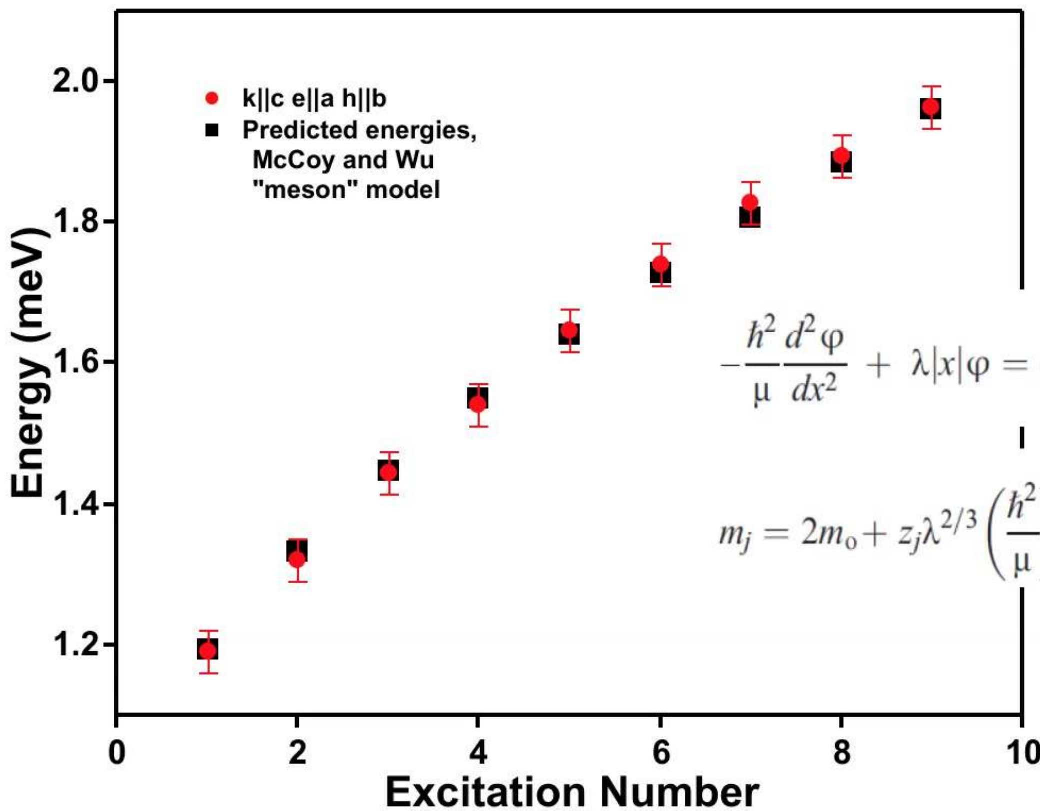

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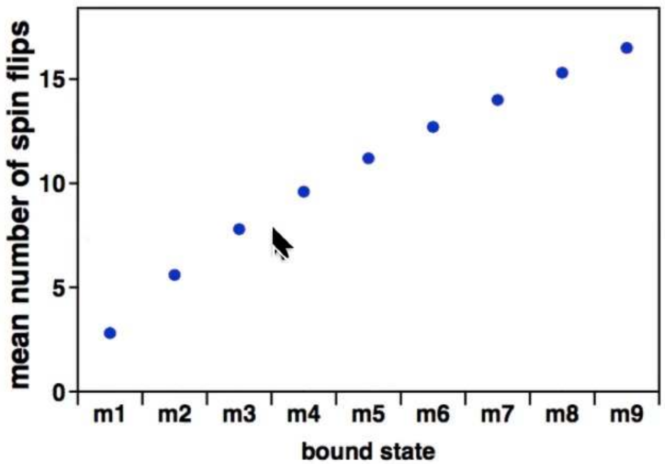
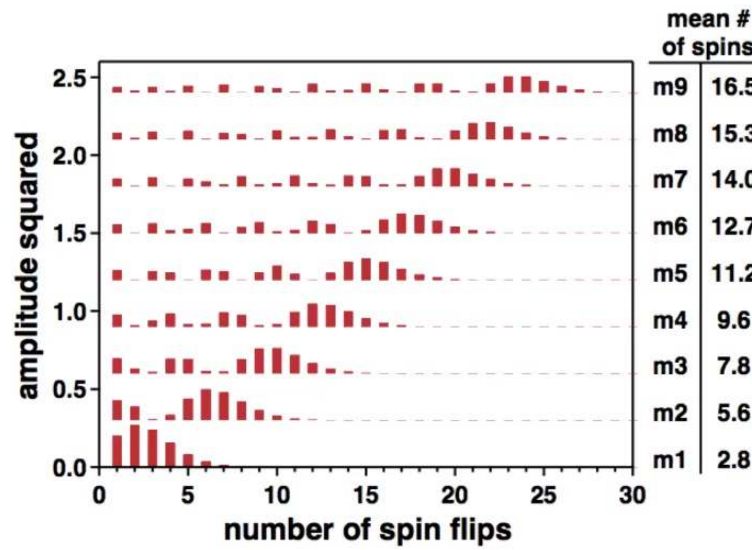
Numerics of the 1D Ising Chain





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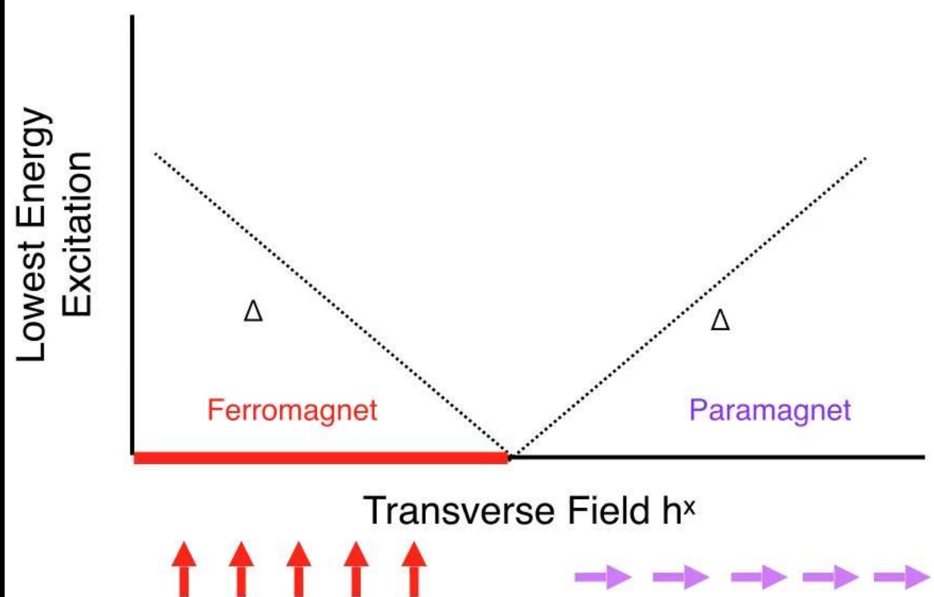
Energy scales collapse near a quantum phase transiti



Limits of high field and low field are well defined.

There must be a QPT as ground state changes degeneracy

General phenomena → changing of ground state as function of non-thermal parameter; phase transition

$$H = -J' \sum_n S_n^z S_{n+1}^z$$

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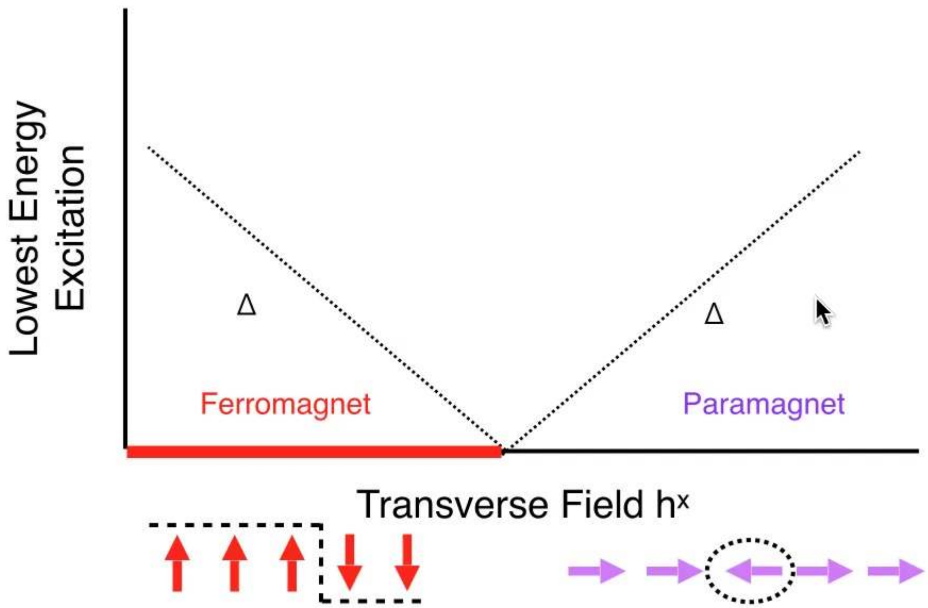

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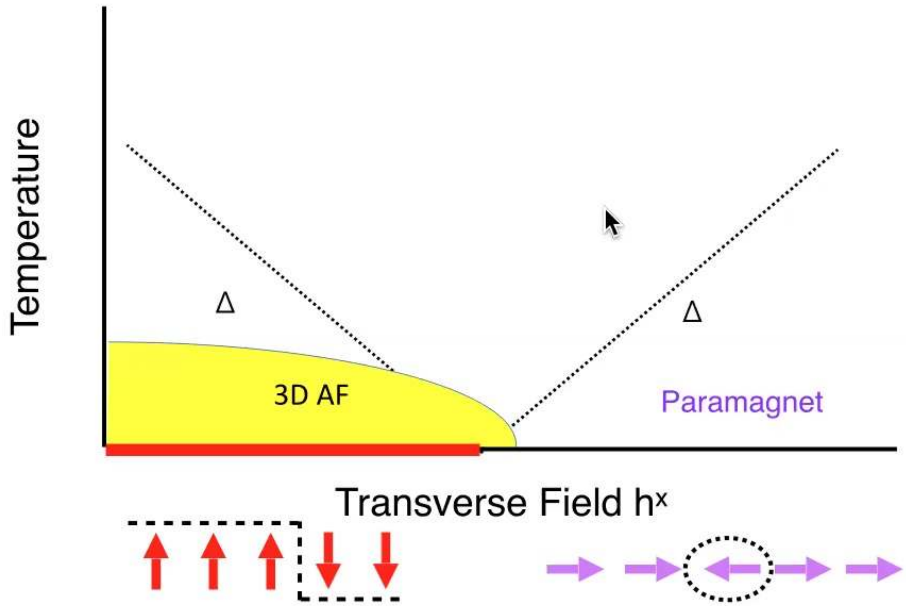

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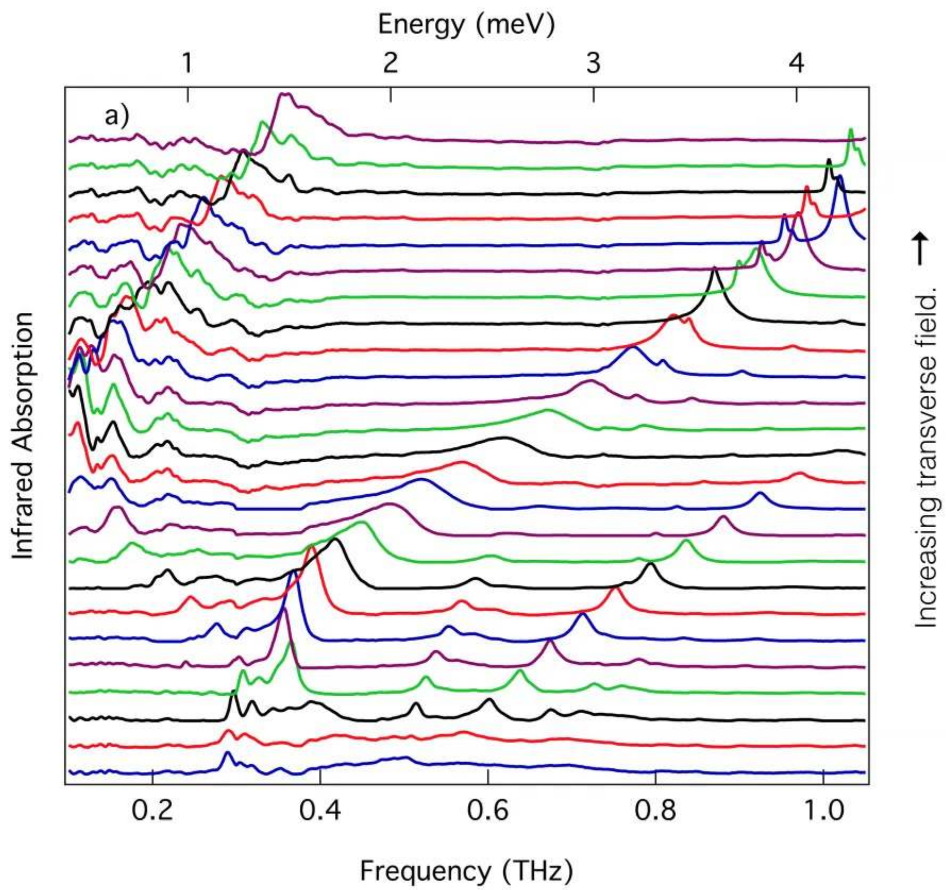
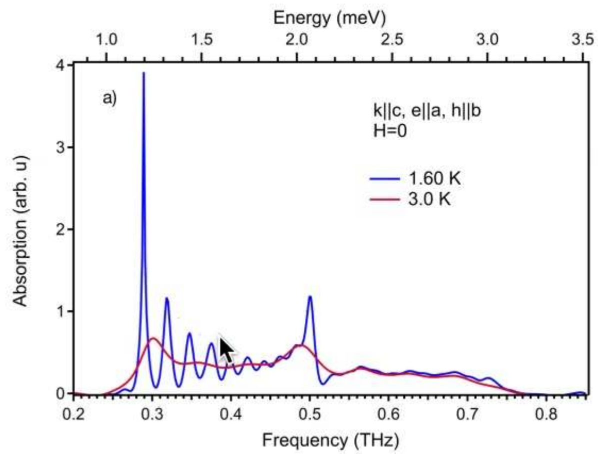
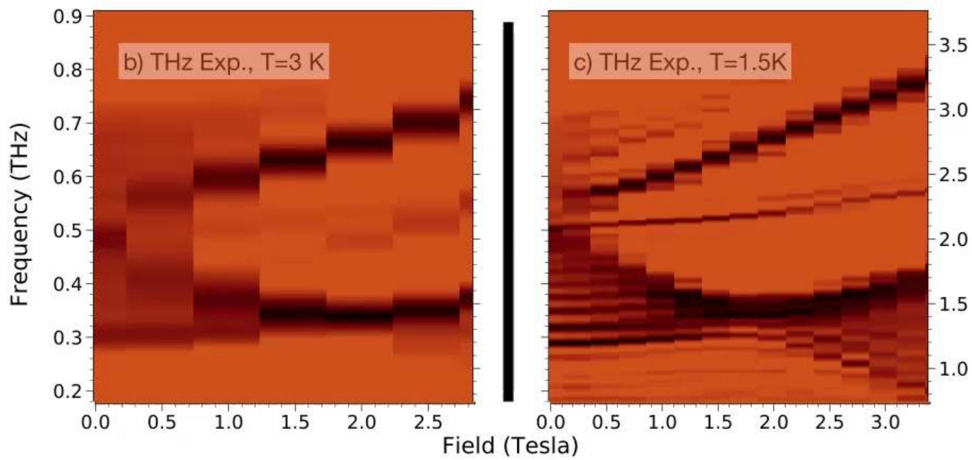
Quantum phase transition of Ising chain in transverse fie



$CoNb_2O_6$ in transverse magnetic field





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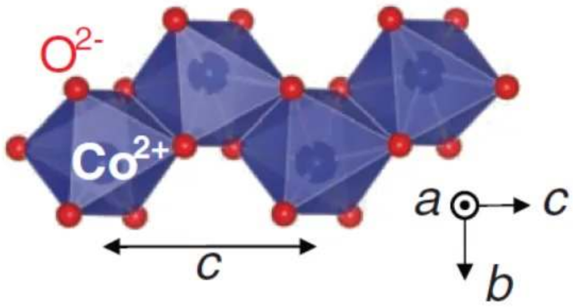
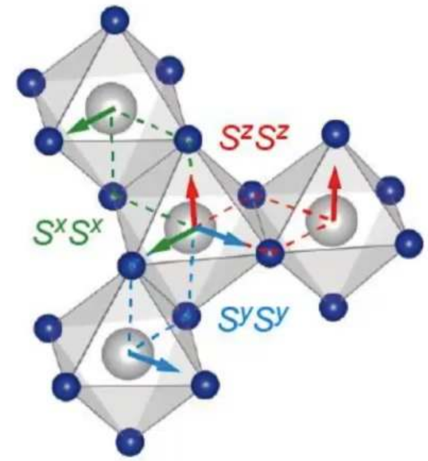
The twisted Kitaev chain





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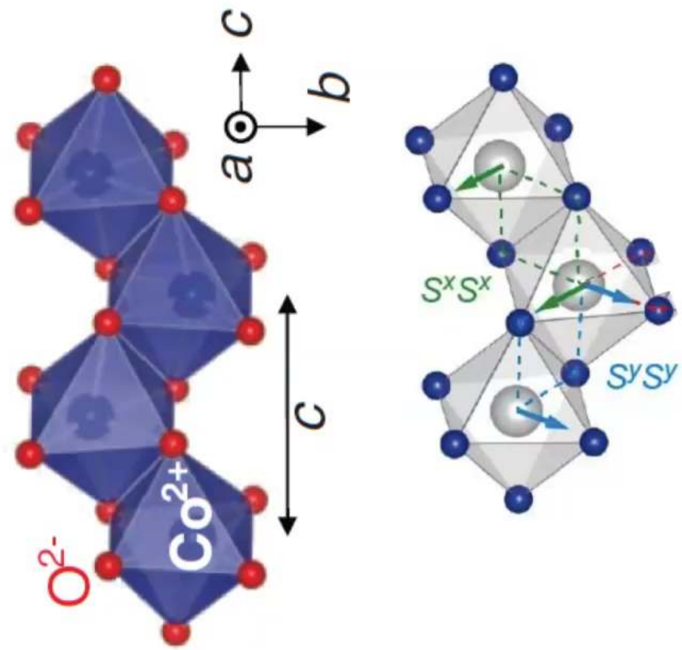
The twisted Kitaev chain



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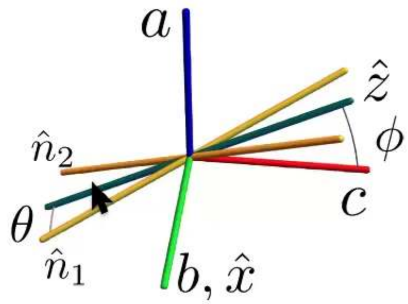
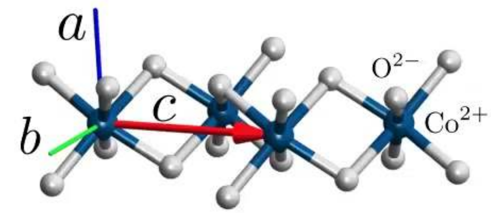


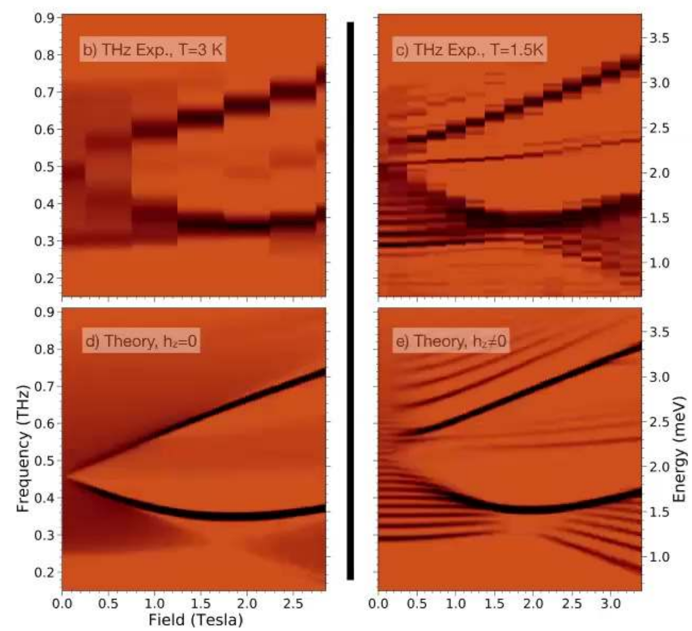
$$\mathcal{H}_K = -K \sum_{i \in e} \left(\tau_i^{\hat{n}_1} \tau_{i+1}^{\hat{n}_1} + \tau_{i+1}^{\hat{n}_2} \tau_{i+2}^{\hat{n}_2} \right)$$

Local axes alternates sign of ň θ
between octahedra

For $\theta, h_x/K, h_z/K \ll 1$

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





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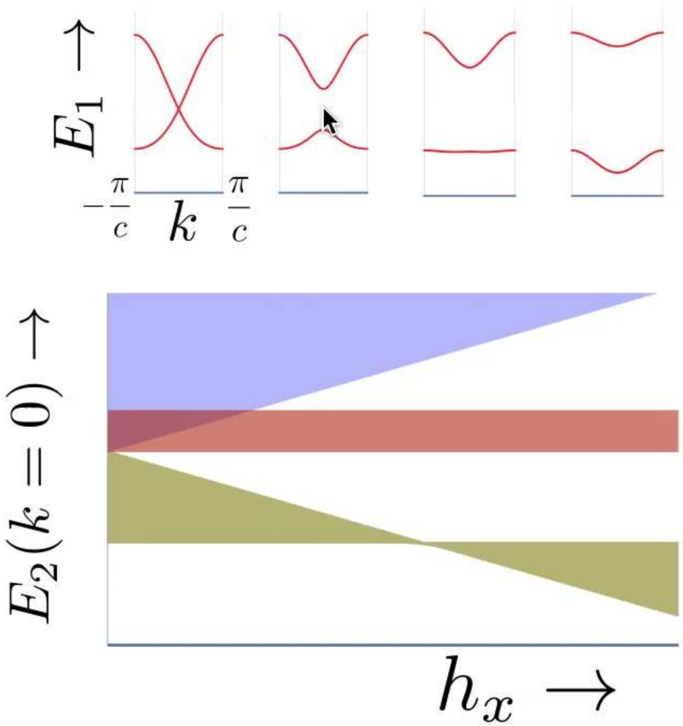
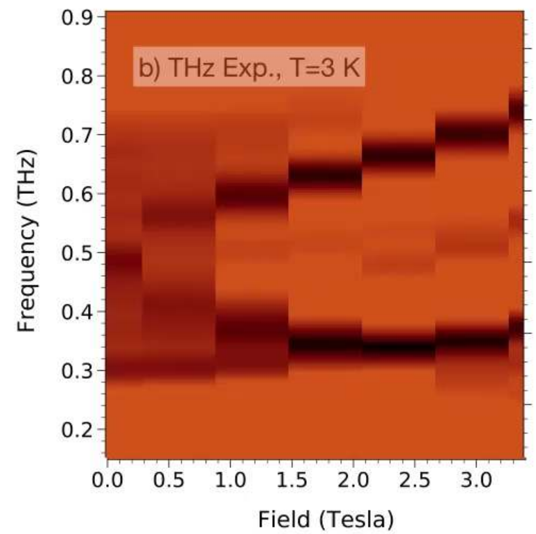
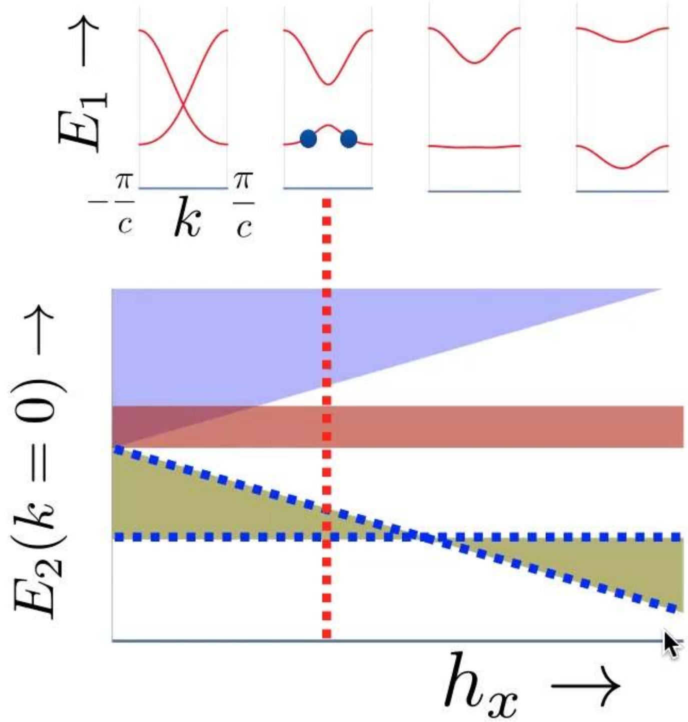
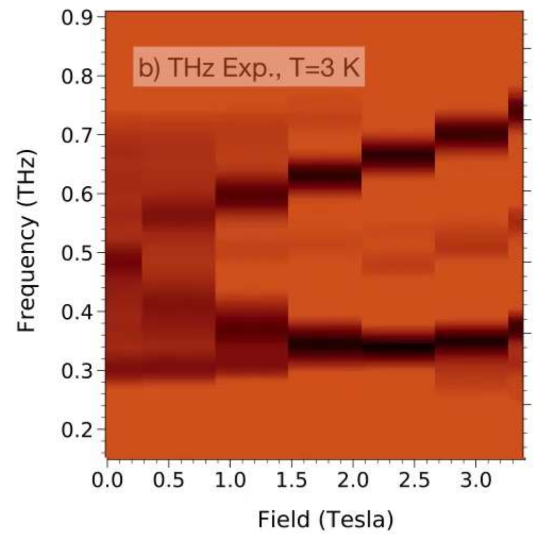




$$\mathcal{H}_d = -\sum_n \Big[(h_x + (-1)^n K \sin(2\theta)) \, (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) + K \sin^2(\theta) (d_n^\dagger d_{n+2} + d_{n+2}^\dagger d_n) \Big] \, ,$$

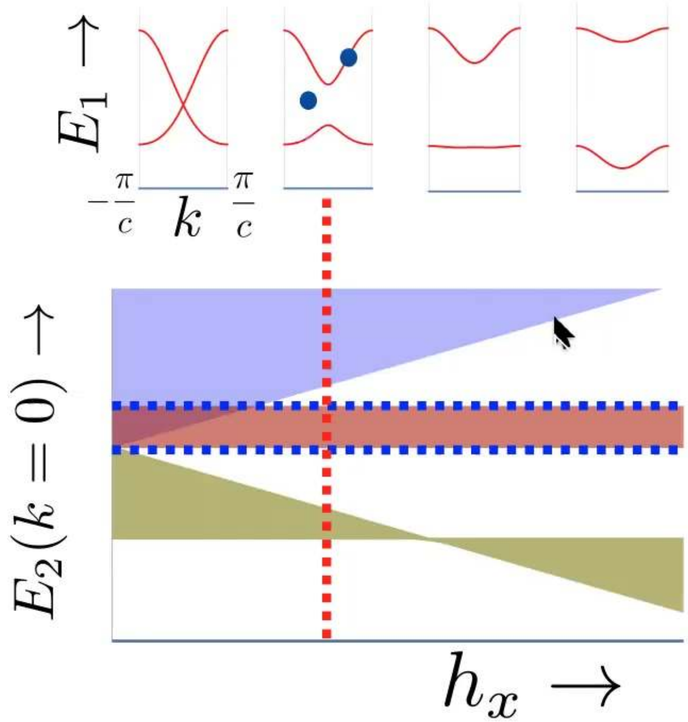
The twisted Kitaev chain

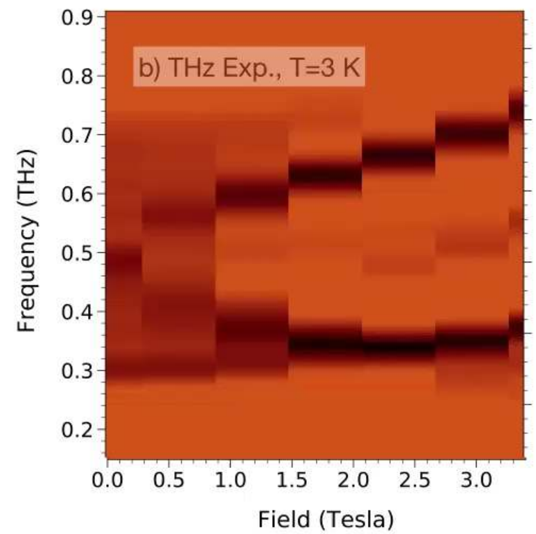




$$\mathcal{H}_d = -\sum_n \Big[(h_x + (-1)^n K \sin(2\theta)) (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) + K \sin^2(\theta)(d_n^\dagger d_{n+2} + d_{n+2}^\dagger d_n) \Big],$$

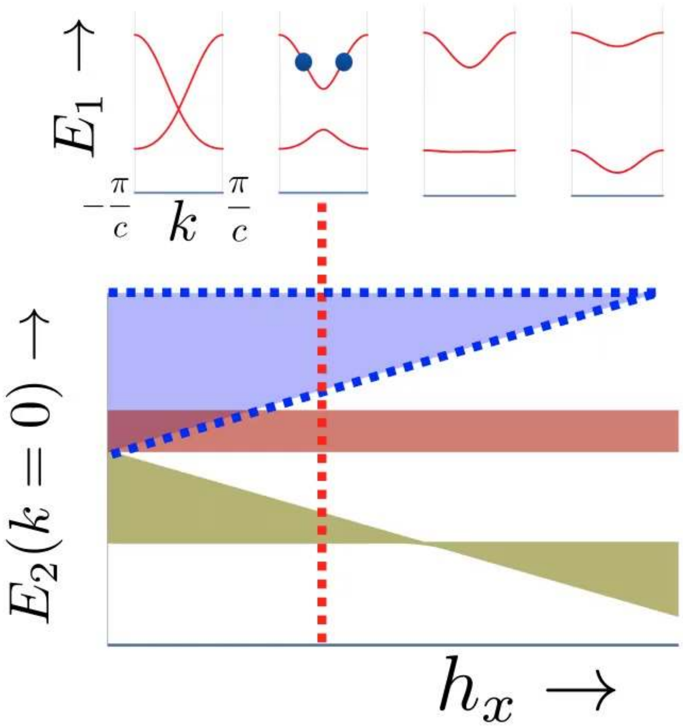
The twisted Kitaev chain

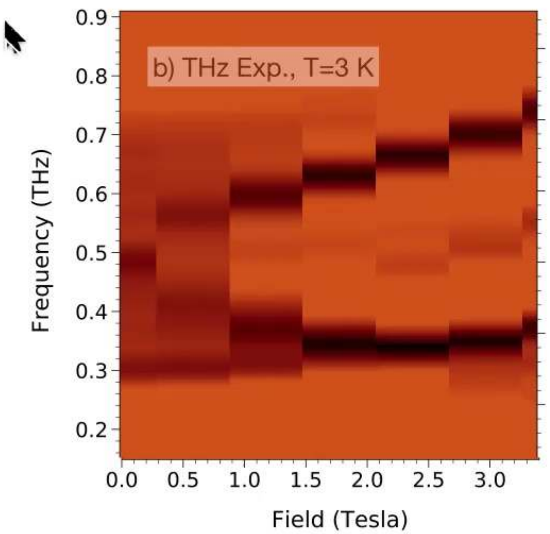




$$\mathcal{H}_d = -\sum_n \Big[(h_x + (-1)^n K \sin(2\theta)) \, (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) + K \sin^2(\theta) (d_n^\dagger d_{n+2} + d_{n+2}^\dagger d_n) \Big] ,$$

The twisted Kitaev chain





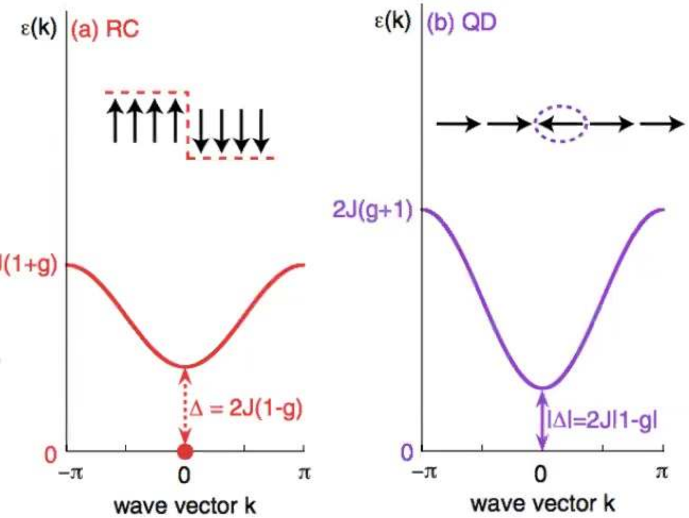
$$\mathcal{H}_d = -\sum_n \Big[(h_x + (-1)^n K \sin(2\theta)) (d_n^\dagger d_{n+1} + d_{n+1}^\dagger d_n) + K \sin^2(\theta)(d_n^\dagger d_{n+2} + d_{n+2}^\dagger d_n) \Big] ,$$

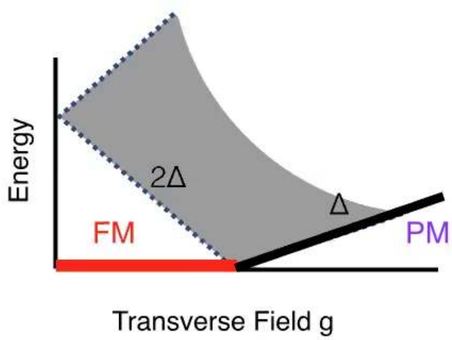
Quantum phase transition in transverse magnetic fie

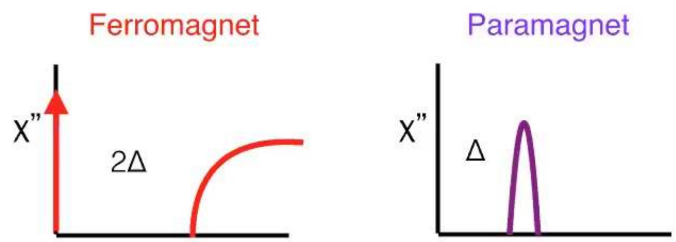
$$H = -J\sum_{n}\left(S_n^z S_{n+1}^z + g S_n^x\right)$$

In FM kinks are elementary excitations, but only pairs of kinks can be excited.

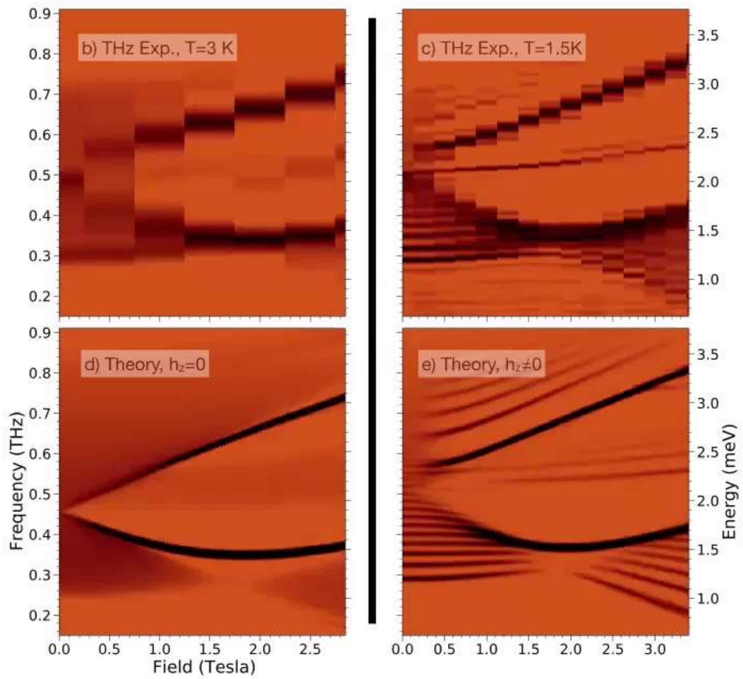
On paramagnetic side, spin flips are elementary excitations







The twisted Kitaev chain



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

K = 0.57 meV, g = 3.5 and θ = 17○

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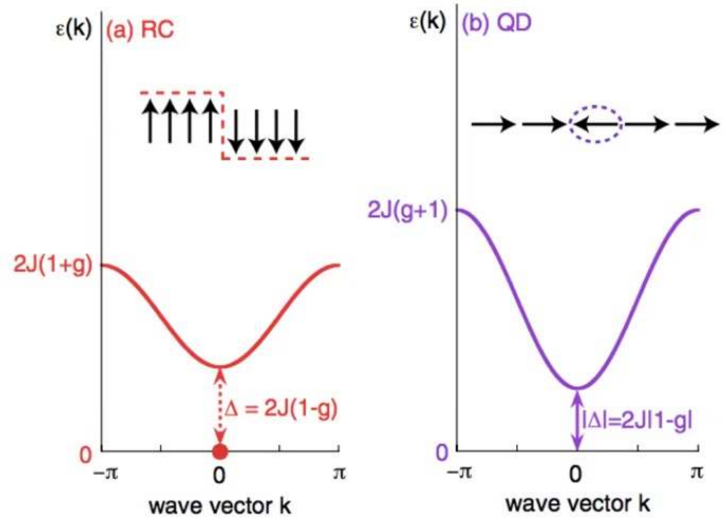
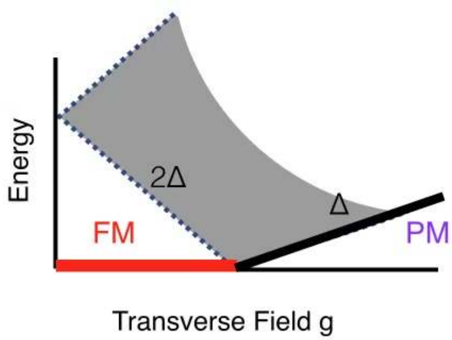
Quantum phase transition in transverse magnetic fie

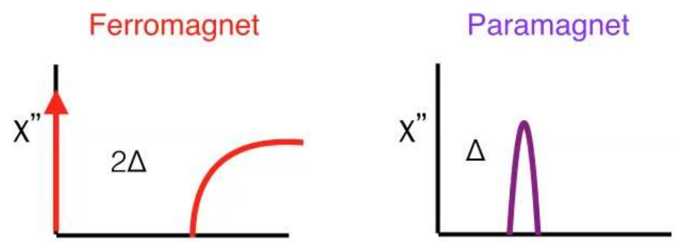
$$H = -J\sum_{n}\left(S_n^z S_{n+1}^z + gS_n^x\right)$$

In FM kinks are elementary excitations, but only pairs of kinks can be excited.

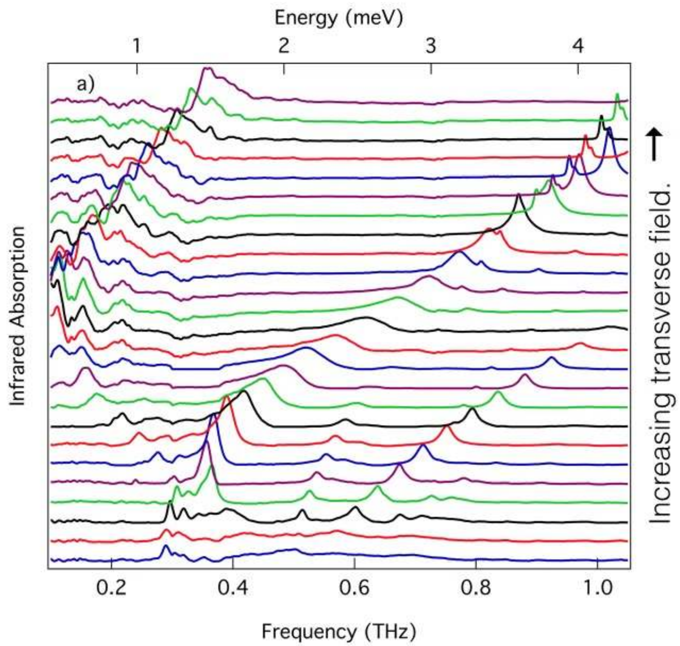
On paramagnetic side, spin flips are elementary excitations

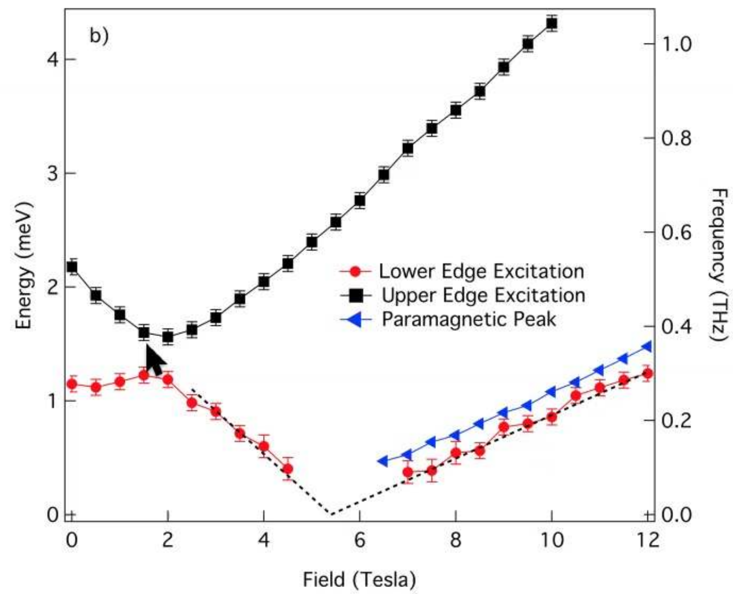






Quantum phase transition of Ising chain in transverse fie





Gap is suppressed twice as fast on FM side

Evidence for free fermion description of Ising chain

In FM kinks are elementary excitations, but only pairs of kinks can be excited.

On paramagnetic side, spin flips are elementary excitations

PHYSICAL REVIEW X **4**, 031008 (2014)

Evolution of Quantum Fluctuations Near the Quantum Critical Point of the Transverse Field Ising Chain System $CoNb_2O_6$

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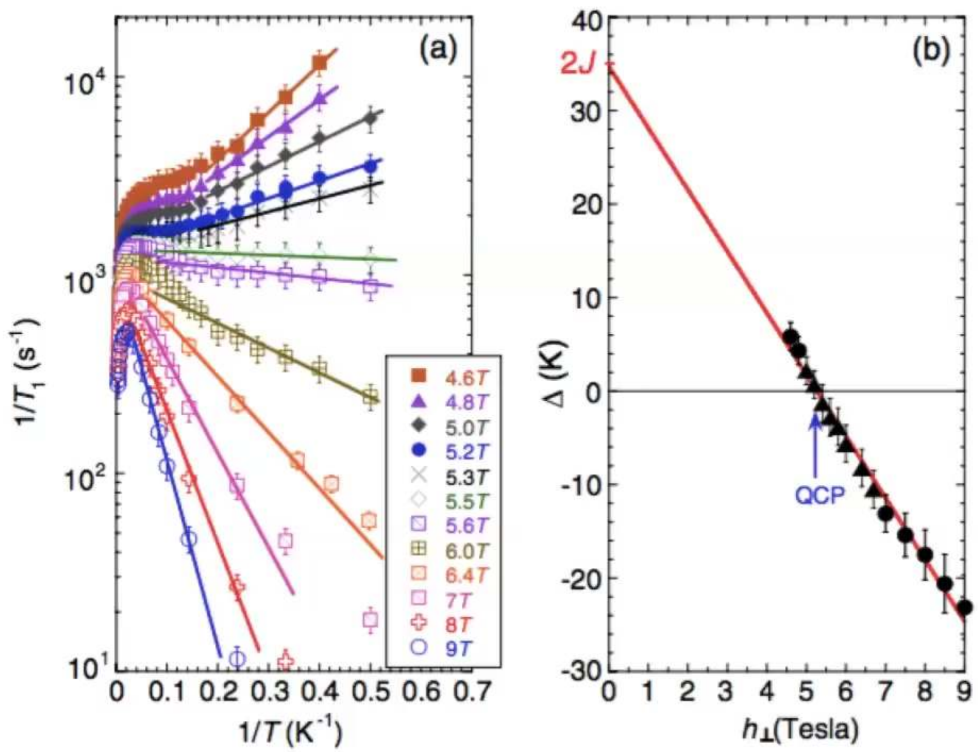
(Received 21 March 2014; published 14 July 2014)



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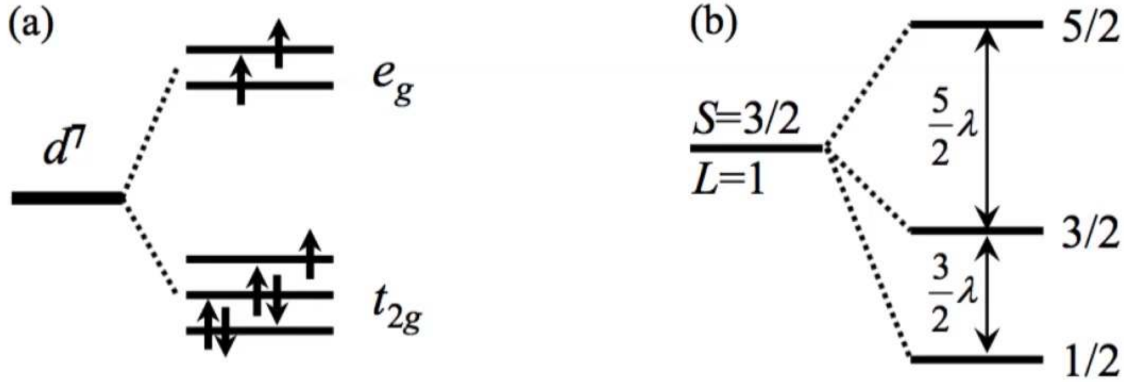
A more ideal Kitaev material?: $BaCo_2(AsO_4)_2$

Pseudospin interactions in d7 cobalt compounds



L = 1 and S=3/2 with negative spin orbit coupling parameter makes lowest Kramers doublet with J=1/2

$$\left|+\frac{\tilde{1}}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|\frac{3}{2},-1\right\rangle - \frac{1}{\sqrt{3}}\left|\frac{1}{2},0\right\rangle + \frac{1}{\sqrt{6}}\left|-\frac{1}{2},1\right\rangle,$$
$$\left|-\frac{\tilde{1}}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|-\frac{3}{2},1\right\rangle - \frac{1}{\sqrt{3}}\left|-\frac{1}{2},0\right\rangle + \frac{1}{\sqrt{6}}\left|\frac{1}{2},-1\right\rangle. \quad (1)$$

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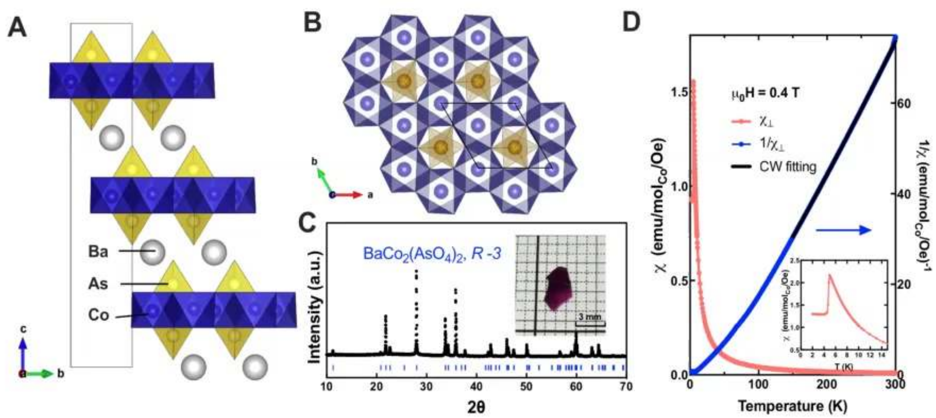
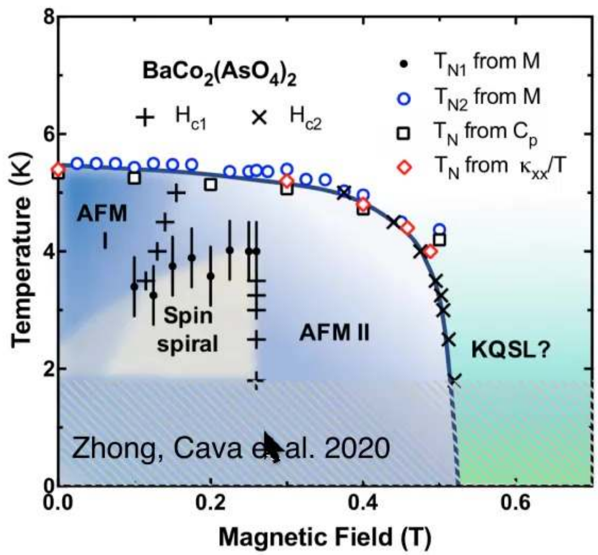
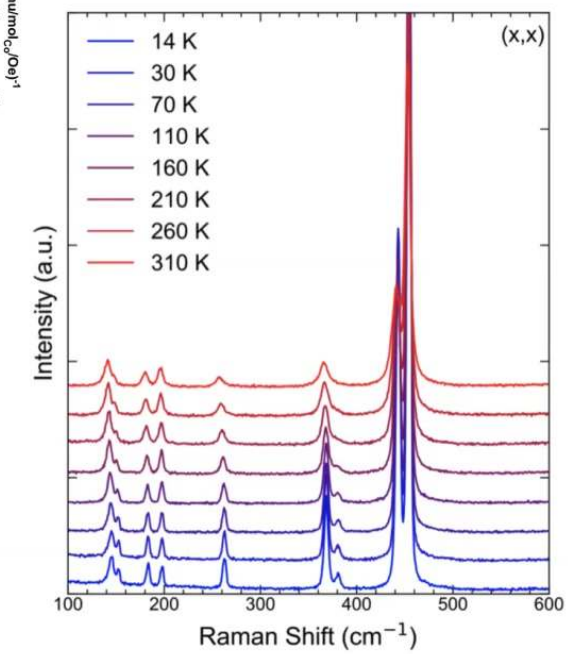
Sano, Kato, Motome (2018) and Liu, Khalullin (2018)

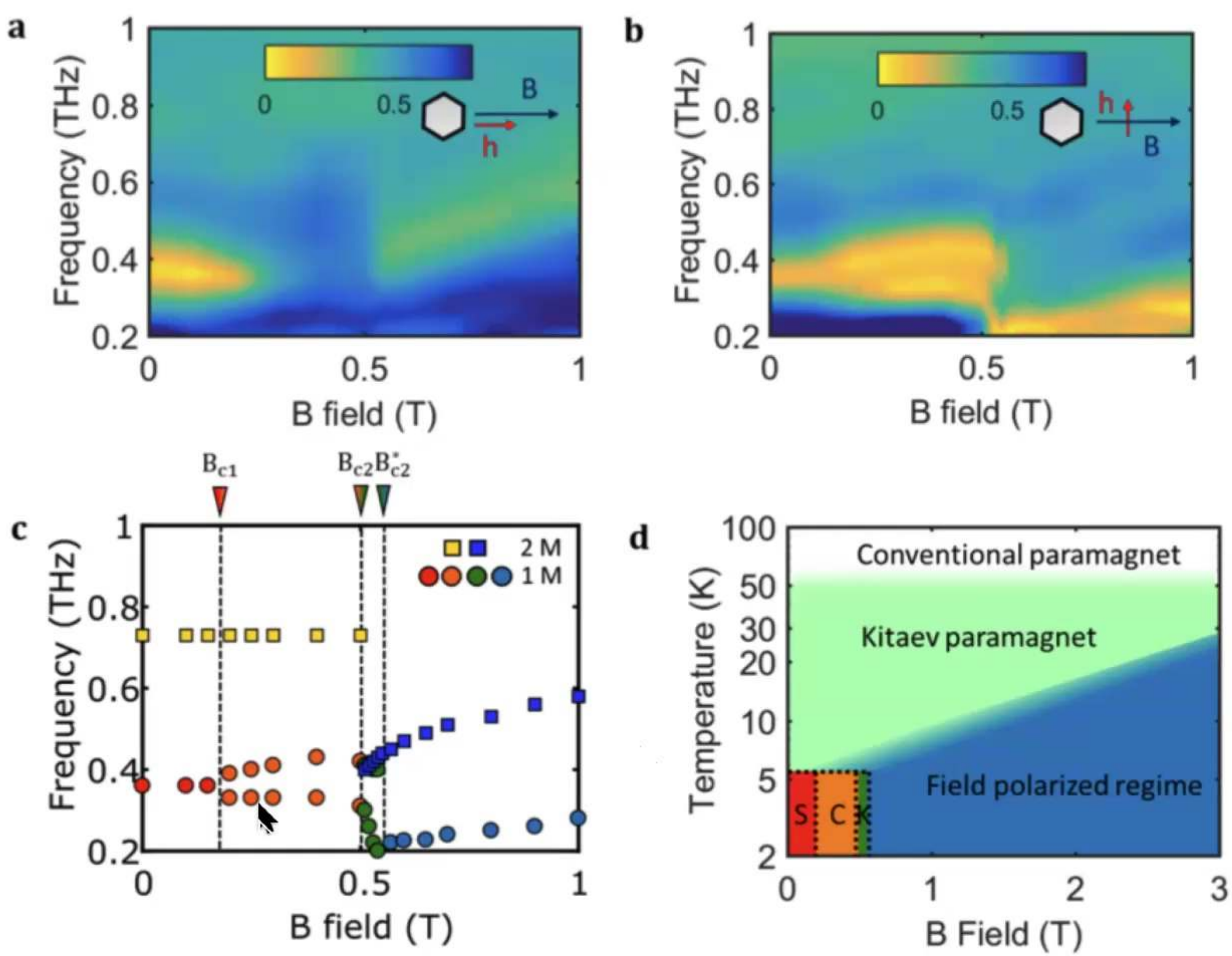
A more ideal Kitaev material?: $BaCo_2(AsO_4)_2$

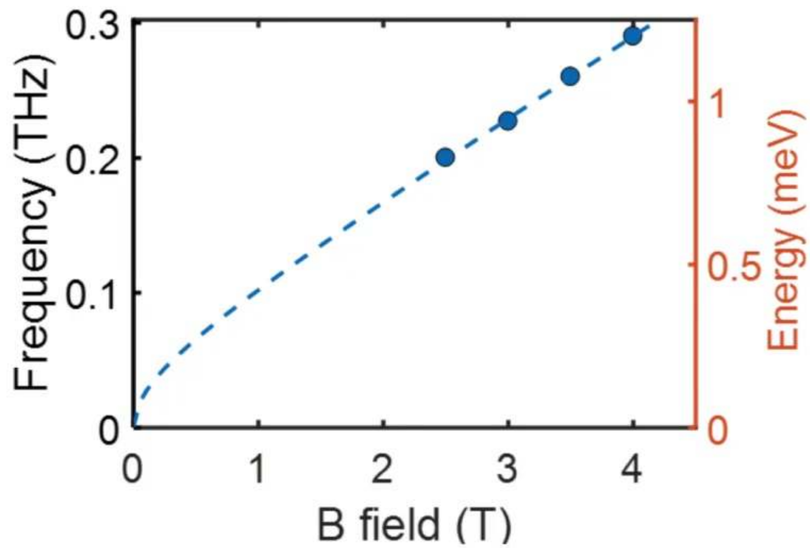






THz spectra of BaCo2(AsO4)2 with in-plane field



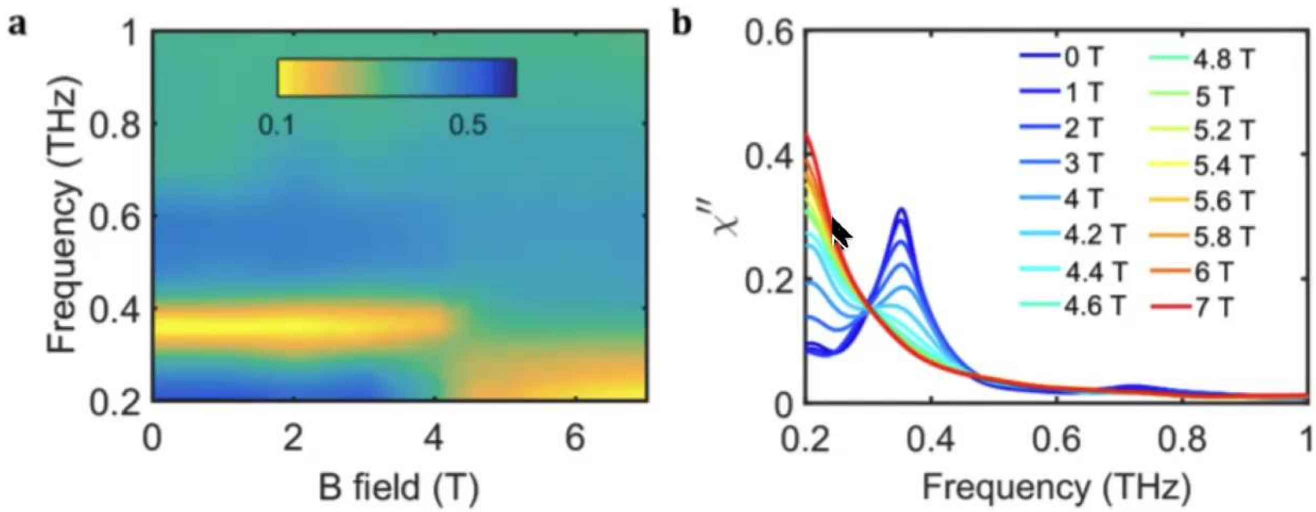


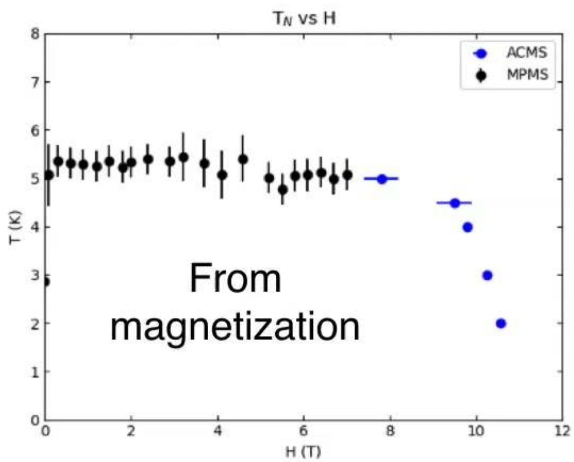
$$\mathcal{H}_1 = \sum_{\langle ij \rangle_\gamma} \left[K S_i^\gamma S_j^\gamma + J \mathbf{S}_i \cdot \mathbf{S}_j + \Gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) + \Gamma' \left(S_i^\gamma S_j^\alpha + S_i^\gamma S_j^\beta + S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma \right) \right]$$

$$\varepsilon_0^{(0)} = \sqrt{g\mu_B B \big(g\mu_B B + 3S(\Gamma + 2\Gamma')\big)}.$$

$\mathbf{\Gamma}_{\text{total}} = \mathbf{\Gamma} + 2\mathbf{\Gamma} = 0.32$ meV

THz spectra of $BaCo_2(AsO_4)_2$ with out-of-plane fie





In-plane easy axis. Likely mixed field character to our THz data.

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Recent results on Kitaev interactions in Co based magne

$CoNb_2O_6$, best material realization of “Ising’s model”

-THz experiments on $CoNb_2O_6$ in zero field; 9 “meson” bound states at low temperature.

-Ising chain in transverse magnetic field; simplest examp of a quantum phase transition; Kramers-Wannier duality; twisted Kitaev chain

Quantum spin-liquid states in a more ideal Kitaev material: $BaCo_2(AsO_4)_2$

-small J and Γ terms.

- out-of-plane field of a few T can induce a QSL.

Morris et al. PRL 2014
Steinberg, NPA, et al. PRB 2019
Morris et al. Nature Physics 2021
Zhang et al. arXiv 2106.13418.