

*Tutorial:*

# Magnon-magnon interactions in spin-wave theory:

*Spontaneous decay, renormalization &  
implications for topological excitations*

**Jeffrey G. Rau**

*University of Windsor*

*SPICE-Workshop on Quantum Geometry and Transport of Collective Excitations  
in (Non-)Magnetic Insulators – May 8<sup>th</sup>, 2025*



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# Outline

1. History
2. Linear spin-waves
3. Non-linear spin waves
4. Applications

# Outline

~~1. History~~

2. Linear spin-waves

3. Non-linear spin waves

4. Applications

# Some Useful References

*Colloquium: Spontaneous magnon decays*, M. E. Zhitomirsky and A. L. Chernyshev, Rev. Mod. Phys. **85**, 219 (2013)

*Spin waves in a triangular lattice antiferromagnet: Decays, spectrum renormalization, and singularities*, A. L. Chernyshev and M. E. Zhitomirsky, Phys. Rev. B **79**, 144416 (2009)

*Dynamical structure factor of the triangular-lattice antiferromagnet*, M. Mourigal, W. T. Fuhrman, A. L. Chernyshev, and M. E. Zhitomirsky, Phys. Rev. B **88**, 094407 (2013)

*Quantum Many-Particle Physics*, Negele and Orland (1998)

*Spin Waves*, Akhiezer, A. I., V. G. Bar'yakhtar, and S. V. Peletminskii (1968)

*Spin Waves*, J. Van Kranendonk and J. H. Van Vleck, Rev. Mod. Phys. **30**, 1 (1958)

...

# Linear Spin Waves

# Review: *Spin-wave Theory*

- ◆ Consider a general (bilinear) spin model in *classical* limit ( $1/S = 0$ )

$$H = \frac{1}{2} \sum_{rr'} \mathbf{S}_r \mathbf{J}_{rr'} \mathbf{S}_{r'}$$

- ◆ *Find a classical ground state*: unit vectors  $\mathbf{z}_r$  such that  $\mathbf{S}_r = S \mathbf{z}_r$  minimizes the energy

**Goal:** Describe the physics *near* the  $1/S = 0$  where quantum and/or thermal fluctuations allow the spins to weakly deviate from the classical ordering direction

# Local Basis

- Can define *local frame* using this ordering: a right-handed (mutually orthogonal) coordinate system at each site

$$\hat{\mathbf{x}}_r \quad \hat{\mathbf{y}}_r \quad \hat{\mathbf{z}}_r$$

- Work in frame aligned with local frame at each site

$$\mathbf{S}_r = S_r^+ \hat{\mathbf{e}}_{r,-} + S_r^- \hat{\mathbf{e}}_{r,+} + S_r^z \hat{\mathbf{e}}_{r,0} \quad \begin{aligned} \hat{\mathbf{e}}_{r,\pm} &= (\hat{\mathbf{x}}_r \pm i\hat{\mathbf{y}}_r) / \sqrt{2} \\ \hat{\mathbf{e}}_{r,0} &= \hat{\mathbf{z}}_r \end{aligned}$$

- Spin Hamiltonian is re-expressed as

$$= \frac{1}{2} \sum_{rr'} \left[ \mathcal{J}_{rr'}^{00} S_r^0 S_{r'}^0 + \left( \mathcal{J}_{rr'}^{++} S_r^- S_{r'}^- + \mathcal{J}_{rr'}^{+0} S_r^- S_{r'}^0 + \mathcal{J}_{rr'}^{0+} S_r^0 S_{r'}^- + \mathcal{J}_{rr'}^{+-} S_r^- S_{r'}^+ + \text{h.c.} \right) \right]$$

*Longitudinal terms*
*Transverse terms*
*Transverse-Longitudinal terms*

# Holstein-Primakoff Expansion

- ◆ Bosonic representation of spin operators with respect to classical ground state

$$S_r = \sqrt{S} \left[ \left(1 - \frac{n_r}{2S}\right)^{1/2} a_r \hat{\mathbf{e}}_{r,-} + a_r^\dagger \left(1 - \frac{n_r}{2S}\right)^{1/2} \hat{\mathbf{e}}_{r,+} \right] + (S - n_r) \hat{\mathbf{e}}_{r,0}$$

*Transverse part*

- ◆ where we have that  $[a_r, a_{r'}^\dagger] = \delta_{rr'}$  and  $n_r \equiv a_r^\dagger a_r$  *Longitudinal part*
- ◆ **Non-linear** in boson number
- ◆ Natural expansion parameter - *boson occupancy*

$$\frac{n_r}{2S} \ll 1$$

# Linear Spin-Wave Theory

- ◆ Leading order expansion – drop the roots

$$\left(1 - \frac{n_r}{2S}\right)^{1/2} \approx 1$$

- ◆ Representation

$$\mathbf{S}_r \approx \sqrt{S} \left( a_r \hat{\mathbf{e}}_{r,-} + a_r^\dagger \hat{\mathbf{e}}_{r,+} \right) + (S - n_r) \hat{\mathbf{e}}_{r,0}$$

- ◆ Bosons represent spin raising/lowering operators in direction *transverse to the ordering*

# Linear Spin-Wave Theory

- ◆ Plug this back into Hamiltonian and keep only leading terms in  $1/S$

$$H = S^2 E_0 + S H_2 + \dots$$

- ◆ Constant part at  $O(S^2)$  is classical energy  $E_0 = \frac{1}{2} \sum_{rr'} \hat{\mathbf{z}}_r^\top \mathbf{J}_{rr'} \hat{\mathbf{z}}_{r'}$
- ◆ Quadratic boson Hamiltonian at  $O(S)$

$$S H_2 = \sum_{rr'} \left[ \underbrace{A_{rr'} a_r^\dagger a_{r'}}_{\substack{\text{“Hopping”} \\ \text{like terms}}} + \frac{1}{2!} \left( \underbrace{B_{rr'} a_r^\dagger a_{r'}^\dagger}_{\substack{\text{“Pairing”} \\ \text{like terms}}} + \text{h.c.} \right) \right]$$

# Linear Spin-Wave Theory

- ◆ In Fourier space this becomes

$$S H_2 = \sum_{\mathbf{k}} \sum_{\alpha\alpha'} \left[ A_{\mathbf{k}}^{\alpha\alpha'} a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha'} + \frac{1}{2!} \left( B_{\mathbf{k}}^{\alpha\alpha'} a_{\mathbf{k}\alpha}^\dagger a_{-\mathbf{k}\alpha'}^\dagger + \text{h.c.} \right) \right]$$

- ◆ The matrices given by

$$A_{\mathbf{k}}^{\alpha\alpha'} = S \left( \mathcal{J}_{\mathbf{k},\alpha\alpha'}^{+-} - \delta_{\alpha\alpha'} \sum_{\mu} \mathcal{J}_{\mathbf{0},\alpha\mu}^{00} \right)$$

$$B_{\mathbf{k}}^{\alpha\alpha'} = S \mathcal{J}_{\mathbf{k}}^{++}$$

Group into enlarged matrix

$$\mathbf{M}_{\mathbf{k}} = \begin{pmatrix} \mathbf{A}_{\mathbf{k}} & \mathbf{B}_{\mathbf{k}} \\ \mathbf{B}_{-\mathbf{k}}^* & \mathbf{A}_{-\mathbf{k}}^* \end{pmatrix}$$

# Linear Spin-Wave Theory

- ◆ Stability of classical ground state restricts spin-wave Hamiltonian

*Condition #1:* Linear terms in bosons must vanish

- Since the ground state is an extremum of the energy

*Condition #2:* Matrix  $\mathbf{M}_k$  must be positive definite

- Since the ground state is a *minimum* of the energy

- ◆ Linear terms can be removed by shift of bosons
- ◆ Interaction effects can sometimes allow expansion about *unstable* ground state

# Linear Spin-Wave Theory

- ◆ Can diagonalize by Bogoliubov transformation

$$\sigma_3 \mathbf{M}_k = \begin{pmatrix} \mathbf{A}_k & \mathbf{B}_k \\ -\mathbf{B}_{-k}^* & -\mathbf{A}_{-k}^* \end{pmatrix} \xrightarrow{\text{Diagonalize}} \sigma_z \mathbf{M}_k \mathbf{V}_{k\alpha} = \underset{\text{Eigenvector}}{\epsilon_{k\alpha}} \underset{\text{Eigenvalue}}{\mathbf{V}_{k\alpha}}$$

- ◆ Yields independent new bosonic degrees of freedom

$$\sum_{k\alpha} \epsilon_{k\alpha} \left( \gamma_{k\alpha}^\dagger \gamma_{k\alpha} + \frac{1}{2} \right)$$

- ◆ Ground state energy at  $O(S)$  acquires zero-point correct; zero  $\gamma$  bosons in the ground state

# Beyond Linear Spin-Wave Theory

- ♦ Many reasons why we often need to go beyond LSWT

**Quantitative comparisons:** Need more accurate spin-wave dispersion for comparison to other model calculations or experimental data

**Intrinsic interactions effects:** Physics of interest only appears at next to leading order (*pseudo-Goldstone gaps, spontaneous decay*)

**Transport properties:** Many require interactions to avoid unphysical results due to non-interacting particles (*thermal conductivity*)

# Non-linear Spin Waves

# Magnon-Magnon Interactions

- ◆ Continue to next order in  $O(1/S)$

$$\left(1 - \frac{n_r}{2S}\right)^{1/2} \approx 1 - \frac{n_r}{4S} + \dots$$

- ◆ Will introduce cubic and quartic interactions between the magnons
- ◆ **General expressions are quite complicated**

Will show you the formalism for simpler case:

- One sublattice with inversion symmetry at zero temperature

$$a_{k\alpha} \rightarrow a_k \qquad k \leftrightarrow -k \qquad T = 0$$

- ◆ Leading order parts are  $O(S)^{1/2}$  and  $O(S)$

$$H_2 = \sum_{r_1 r_2} \left[ A_{r_1 r_2} a_{r_1}^\dagger a_{r_2} + \frac{1}{2!} \left( B_{r_1 r_2} a_{r_1}^\dagger a_{r_2}^\dagger + \bar{B}_{r_1 r_2} a_{r_1} a_{r_2} \right) \right],$$

$$H_3 = \frac{1}{2!} \sum_{r_1 r_2 r_3} \left[ T_{r_1 r_2 r_3} a_{r_1}^\dagger a_{r_2}^\dagger a_{r_3} + \bar{T}_{r_1 r_2 r_3} a_{r_3}^\dagger a_{r_2} a_{r_1} \right],$$

$$H_4 = \sum_{r_1 r_2 r_3 r_4} \left[ \frac{1}{(2!)^2} V_{r_1 r_2 r_3 r_4} a_{r_1}^\dagger a_{r_2}^\dagger a_{r_3} a_{r_4} + \frac{1}{3!} \left( D_{r_1 r_2 r_3 r_4} a_{r_1}^\dagger a_{r_2}^\dagger a_{r_3}^\dagger a_{r_4} + \bar{D}_{r_1 r_2 r_3 r_4} a_{r_4}^\dagger a_{r_3} a_{r_2} a_{r_1} \right) \right]$$

*Symmetrization factors  
simplify perturbative  
expansion*

- ◆ Interactions **do not conserve boson number** (from  $D$  and  $T$ )
- ◆ Interactions **do not conserve boson number mod 2** (from  $T$ )

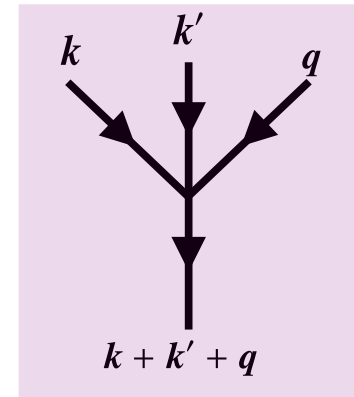
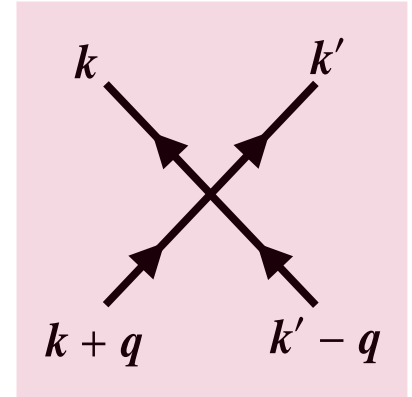
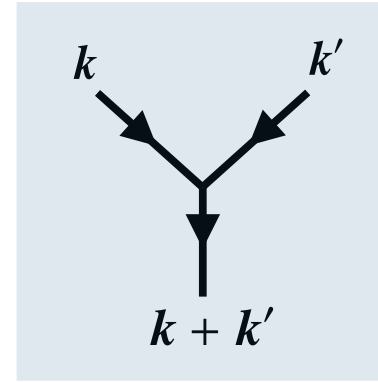
- ◆ More natural in Fourier space; momentum conserved in each interaction

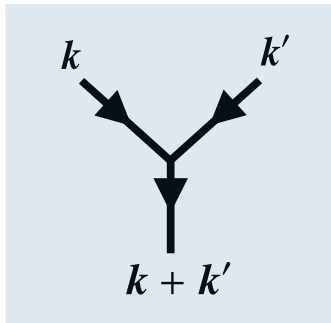
$$H_2 = \sum_k \left[ A_k a_k^\dagger a_k + \frac{1}{2!} \left( B_k a_k^\dagger a_{-k}^\dagger + \text{h.c.} \right) \right]$$

$$H_3 = \frac{1}{\sqrt{N}} \sum_{kk'} \left( T_{kk'} a_k^\dagger a_{k'}^\dagger a_{k+k'} + \text{h.c.} \right)$$

$$H_4 = \frac{1}{N} \sum_{kk'q} \frac{1}{(2!)^2} V_{kk'q} a_{k+q}^\dagger a_{k'-q}^\dagger a_k a_{k'}$$

$$H'_4 = \frac{1}{N} \sum_{kk'q} \frac{1}{3!} \left( D_{kk'q} a_k^\dagger a_{k'}^\dagger a_q^\dagger a_{k+k'+q} + \text{h.c.} \right)$$

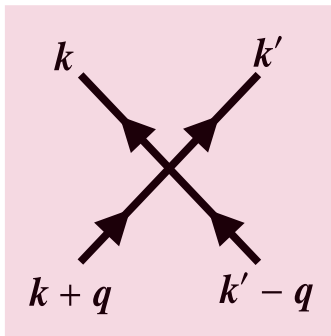




$$A_k = S \left( \mathcal{J}_k^{+-} - \mathcal{J}_0^{00} \right)$$

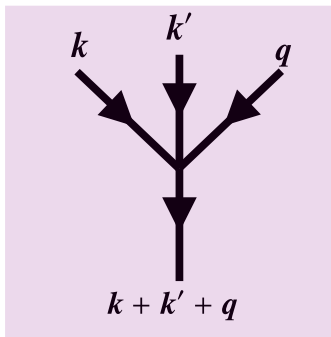
$$B_k = S \mathcal{J}_k^{++}$$

- ◆ Vertices are (somewhat) simple functions of local exchange matrices



$$T_{kk'} = -S^{1/2} \left( \mathcal{J}_k^{+0} + \mathcal{J}_{k'}^{+0} \right)$$

$$V_{kk'}[q] = \frac{1}{2} \left( \mathcal{J}_{k-k'+q}^{00} + \mathcal{J}_{k'-k-q}^{00} + \mathcal{J}_q^{00} + \mathcal{J}_{-q}^{00} \right) \\ - \frac{1}{2} \left( \mathcal{J}_k^{+-} + \mathcal{J}_{k'}^{+-} + \mathcal{J}_{k'-q}^{+-} + \mathcal{J}_{k+q}^{+-} \right)$$



$$D_{kk'q} = -\frac{1}{2} \left( \mathcal{J}_k^{++} + \mathcal{J}_{k'}^{++} + \mathcal{J}_q^{++} \right)$$

# Free theory

- ◆ Use (diagrammatic) many-body perturbation theory about free limit

$$H_0 = \sum_k \left[ A_k a_k^\dagger a_k + \frac{1}{2!} (B_k a_k^\dagger a_{-k}^\dagger + \text{h.c.}) \right]$$

- ◆ Need **Green's function** for this free theory
- ◆ Work in *imaginary time*

$$a_k(\tau) \equiv e^{\tau H_0} a_k e^{-\tau H_0}$$

- ◆ Consider **normal** and **anomalous** propagators

# Free Theory

*(Imaginary) time ordered*

$$g^{-+}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}(\tau) a_{\mathbf{k}}^\dagger(0) \rangle_0$$

$$g^{+-}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}^\dagger(\tau) a_{\mathbf{k}}(0) \rangle_0$$

*Normal parts*

$$g^{++}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}^\dagger(\tau) a_{\mathbf{k}}^\dagger(0) \rangle_0$$

$$g^{--}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}(\tau) a_{\mathbf{k}}(0) \rangle_0$$

*Anomalous parts*

Organize into 2 by 2 matrix mirroring the  $\mathbf{M}_{\mathbf{k}}$

$$\mathbf{g}(\mathbf{k}, \omega) \equiv \begin{pmatrix} g^{-+}(\mathbf{k}, \omega) & g^{--}(\mathbf{k}, \omega) \\ g^{++}(\mathbf{k}, \omega) & g^{+-}(\mathbf{k}, \omega) \end{pmatrix}$$

# Free Theory

$$\begin{pmatrix} a_k(\tau) \\ a_{-k}^\dagger(\tau) \end{pmatrix} = e^{-\tau \sigma_z M_k} \begin{pmatrix} a_k \\ a_{-k}^\dagger \end{pmatrix}$$

- ♦ Can calculate explicitly (assume inversion so that  $A_k = A_{-k}$ )

$$g(\mathbf{k}, \omega) = [-i\omega \sigma_z + \mathbf{M}_k]^{-1}$$

- ♦ Alternatively:

$$g^{-+}(\mathbf{k}, \omega) = g^{+-}(-\mathbf{k}, -\omega) = \frac{|u_k|^2}{-i\omega + \epsilon_k} + \frac{|v_k|^2}{-i\omega + \epsilon_k}$$

$$g^{--}(\mathbf{k}, \omega) = g^{++}(\mathbf{k}, \omega)^* = \frac{2\epsilon_k u_k v_k^*}{\omega^2 + \epsilon_k^2}$$

$$\epsilon_k = \sqrt{A_k^2 - |B_k|^2}$$

# Green's Function

$$G^{-+}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}(\tau) a_{\mathbf{k}}^\dagger(0) \rangle$$

$$G^{+-}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}^\dagger(\tau) a_{\mathbf{k}}(0) \rangle$$

$$G^{++}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}^\dagger(\tau) a_{\mathbf{k}}^\dagger(0) \rangle$$

$$G^{--}(\mathbf{k}, \omega) \equiv \int_0^\beta d\tau e^{i\omega\tau} \langle \mathcal{T} a_{\mathbf{k}}(\tau) a_{\mathbf{k}}(0) \rangle$$

- ◆ Compute these Green's functions perturbatively in the interactions
- ◆ Only *two* of these are independent
  - $G^{+-}(\mathbf{k}, \omega)$  and  $G^{-+}(\mathbf{k}, \omega)$  are related by symmetry
  - $G^{++}(\mathbf{k}, \omega)$  and  $G^{--}(\mathbf{k}, \omega)$  are related by symmetry

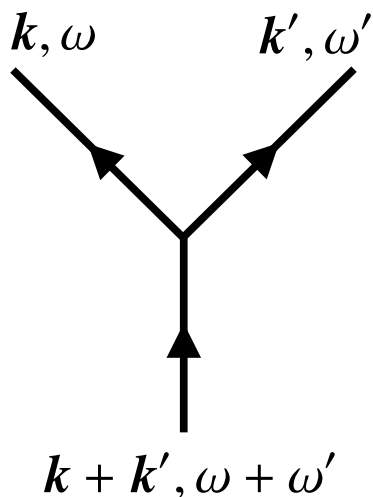
# Diagrammatic Rules

- ◆ Compute perturbative contributions diagrammatically
  - Green's function can be computed as sum of diagrams
- ◆ Since have normal and anomalous Green's function have *four kinds of free propagators*

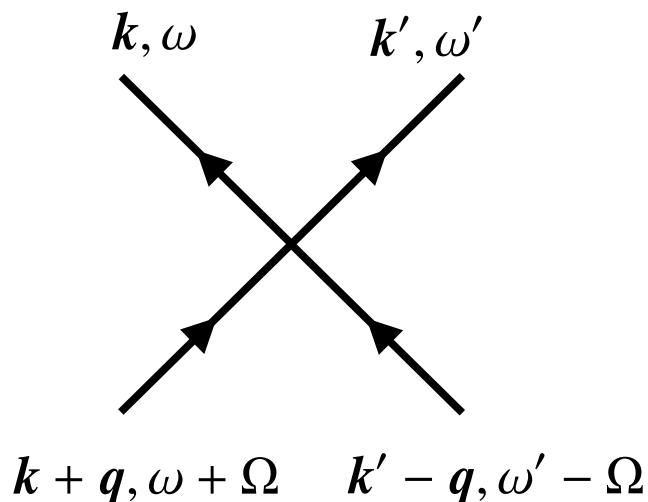
$$\overrightarrow{k, \omega} \equiv g^{-+}(k, \omega) \qquad \overleftarrow{-k, -\omega} \overrightarrow{k, \omega} \equiv g^{++}(k, \omega)$$

$$\overleftarrow{k, \omega} \equiv g^{+-}(k, \omega) \qquad \overrightarrow{k, \omega} \overleftarrow{-k, -\omega} \equiv g^{--}(k, \omega)$$

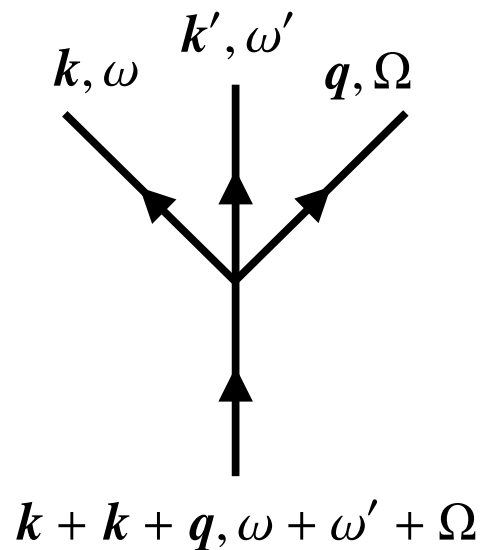
- ◆ Three kinds of interaction vertices: two particle scattering, two magnon decay and three magnon decay



$$-\frac{1}{\sqrt{\beta N}} T_{kk'}^*$$



$$-\frac{1}{\beta N} V_{kk'[q]}$$



$$-\frac{1}{\beta N} D_{kk'q}^*$$

1. Draw all distinct connected diagrams consisting of  $n_4$  four point vertices (of type  $V, D$ ),  $n_3$  three point vertices (of type  $T$ ), connected by normal or anomalous propagators. Order is  $n_4 + n_3/2$
2. For each line assign a momentum and Matsubara frequency, consistent with conservation of wave-vector and frequency at each vertex and sums over them
3. For each line include the correct free Green's function from  $g(\mathbf{k}, \omega)$
4. For each vertex include the appropriate factor of  $V, D, T$ . Vertices with more outgoing lines than incoming lines always have a conjugation.
5. Compute the symmetry factor  $\sigma$  and multiply by  $1/\sigma$  *Overcounting of permutations*
6. For each bundle of  $m$  lines starting at the same vertex with a  $m_1$ -fold redundancy and ending at the same vertex with a  $m_2$ -fold redundancy multiply by  $1/[m!(m_1 - m)!(m_2 - m)!]$ .

*Often easier just to manually count contractions*

Finally, let  $a_\alpha|\phi\rangle = 0$  for all annihilation operators. Show that  $\hat{A}_i\hat{A}_j$  is the propagator  $\langle\phi|T\hat{A}_i\hat{A}_j|\phi\rangle$  and that

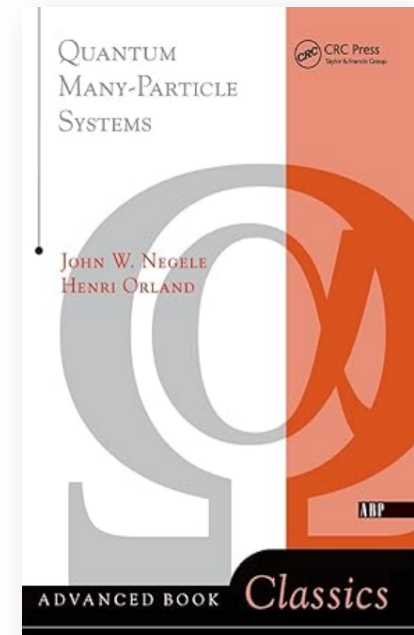
$$\langle\phi|T\hat{A}_1\hat{A}_2\cdots\hat{A}_n|\phi\rangle = \sum_{\text{all complete contractions}} \overbrace{\hat{A}_1\hat{A}_2} \cdots \overbrace{\hat{A}_{n-1}\hat{A}_n}$$

where

$$\overbrace{\hat{A}_1\hat{A}_2} = \langle\phi|T\hat{A}_1\hat{A}_2|\phi\rangle \quad .$$

**PROBLEM 2.9** Generalize the Hugenholtz diagram rules to the case in which  $V$  contains one-body, two-body, ... up to  $n$ -body interactions. The principal issue is what to do about  $m$ -tuples of equivalent lines. Note that in general an  $m$ -tuple of equivalent lines could start at an  $n_1$ -body vertex and terminate at an  $n_2$ -body vertex and that multiple  $m$ -tuples could originate or terminate at the same vertex.

**PROBLEM 2.10 The Linked-Cluster Theorem.** Show that the exponential of the sum of all linked graphs yields the sum of all diagrams with the appropriate factors using unlabeled Feynman diagrams. First, let  $a_c$  denote the contribution of some linked cluster and consider a graph composed of  $n$  of these clusters. Explain why the symmetry factor is  $n!s_c^n$  where  $s_c$  is the symmetry factor in  $a_c$ . Hence, show that the contribution of any number (including 0) of clusters  $a_c$  is  $\sum_{n=0}^{\infty} \frac{a_c^n}{n!} e^{a_c}$ . Generalize to show that  $e^{\sum_c a_c}$  yields the sum of all diagrams with the correct symmetry factors.



Negele & Orland,  
*Quantum Many-Particle Systems*

# Self-Energy

- ◆ Resummation of diagrams ala Dyson/Gorkov gives **self-energy**

$$\begin{array}{c}
 \rightarrow \text{---} \bigcirc G^{--+} \text{---} \rightarrow = \text{---} \rightarrow + \text{---} \bigcirc \Sigma^{--+} \text{---} \bigcirc G^{--+} \text{---} \rightarrow \\
 \\
 \text{New piece due to anomalous parts} + \text{---} \bigcirc \Sigma^{--} \text{---} \bigcirc G^{++} \text{---} \rightarrow
 \end{array}$$

- ◆ Self-energy and Dyson series *also* has normal and anomalous parts

# Self-Energy

- ◆ Doing this for all Green's functions gives the form

$$\mathbf{G}(\mathbf{k}, \omega) \equiv [-i\omega\boldsymbol{\sigma}_z + \mathbf{M}_k + \boldsymbol{\Sigma}(\mathbf{k}, \omega)]^{-1}$$

- ◆ Self-energy is now a 2 by 2 matrix like Green's function

$$\boldsymbol{\Sigma}(\mathbf{k}, \omega) \equiv \begin{pmatrix} \Sigma^{-+}(\mathbf{k}, \omega) & \Sigma^{--}(\mathbf{k}, \omega) \\ \Sigma^{++}(\mathbf{k}, \omega) & \Sigma^{+-}(\mathbf{k}, \omega) \end{pmatrix}$$

- ◆ **The self-energy will be the focus of our calculations**

# Continuing to Real Time

- ◆ To extract information about the magnons, we need to analytically continue to **real-time**
- ◆ Effectively substitution of frequency  $i\omega \rightarrow \omega + i0^+$
- ◆ Retarded Green's function given by

$$\mathbf{G}_R(\mathbf{k}, \omega) \equiv -\mathbf{G}(\mathbf{k}, -i\omega + 0^+) = [\omega\boldsymbol{\sigma}_z - \mathbf{M}_\mathbf{k} - \boldsymbol{\Sigma}_R(\mathbf{k}, \omega)]^{-1}$$

- ◆ Similar definition for the retarded self-energy

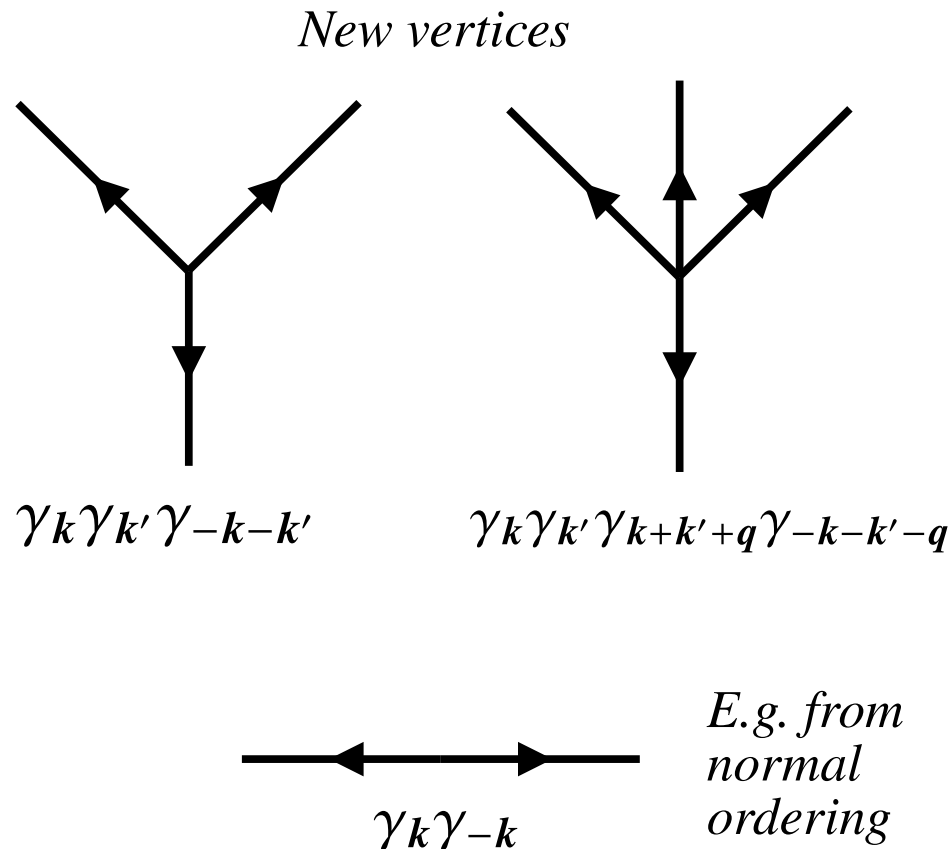
$$\boldsymbol{\Sigma}_R(\mathbf{k}, \omega) \equiv -\boldsymbol{\Sigma}(\mathbf{k}, -i\omega + 0^+)$$

# Aside: Choice of Basis

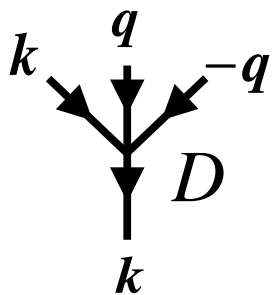
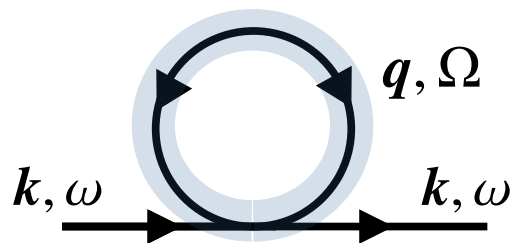
- ◆ I showed you this in *original* basis of magnons
- ◆ This perturbation theory (usually) is carried out in the *diagonalized basis*

## Practically:

- Write in terms of  $\gamma_k$
- Normal order the operators
- Perturbation theory but with larger set of vertices



# Example: Normal Self-Energy



$$g^{++}(k, \omega) = \frac{2u_k^* v_k \epsilon_k}{\omega^2 + \epsilon_k^2}$$

$$\equiv -\frac{1}{2} \cdot \frac{1}{\beta N} \sum_{q\Omega} g^{++}(q, \Omega) D_{k,q,-q}$$

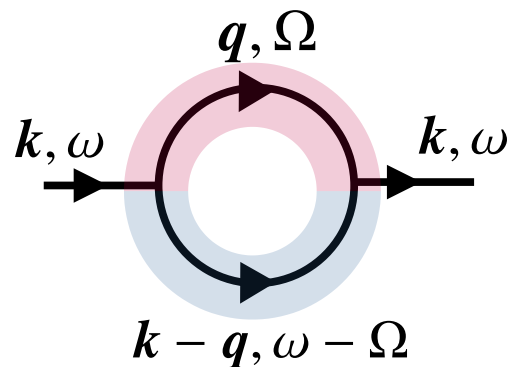
*Perform  
sum at  $T=0$*

$$= -\frac{1}{2} \sum_q \langle a_q^\dagger a_{-q}^\dagger \rangle_0 D_{k,q,-q}$$

*Analytic  
continue to  
real time*

$$\rightarrow +\frac{1}{2} \sum_q \langle a_q^\dagger a_{-q}^\dagger \rangle_0 D_{k,q,-q}$$

# Example: Normal Self-Energy



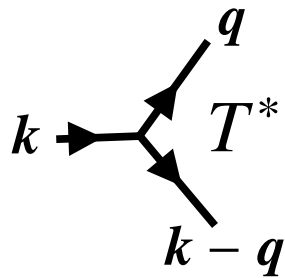
$$g^{-+}(k, \omega) = \frac{|u_k|^2}{-i\omega + \epsilon_k} + \frac{|v_k|^2}{i\omega + \epsilon_k}$$

$$\equiv \frac{1}{2} \cdot \frac{1}{\beta N} \sum_{q\Omega} g^{-+}(q, \Omega) g^{-+}(k-q, \omega-\Omega) T_{q,k-q}^* T_{q,k-q}$$

*Evaluate sum at T=0*

$$= \frac{1}{2N} \sum_q |T_{q,k-q}|^2 \left[ \frac{|u_q|^2 |u_{k-q}|^2}{-i\omega + \epsilon_q + \epsilon_{k-q}} + \frac{|v_q|^2 |v_{k-q}|^2}{i\omega + \epsilon_q + \epsilon_{k-q}} \right] \quad \text{To real time}$$

$$= \frac{1}{2N} \sum_q |T_{q,k-q}|^2 \left[ \frac{|u_q|^2 |u_{k-q}|^2}{\omega - \epsilon_q - \epsilon_{k-q} + i0^+} - \frac{|v_q|^2 |v_{k-q}|^2}{\omega + \epsilon_q + \epsilon_{k-q} + i0^+} \right]$$



# Quasi-particle poles

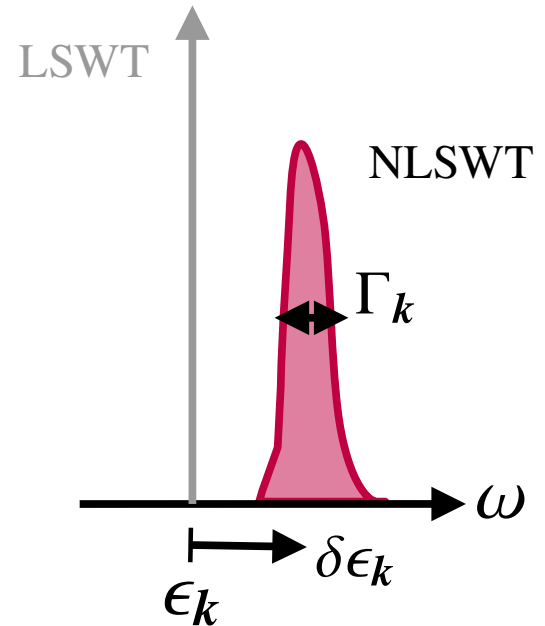
- Excitations appear as **poles**

$$\det [\omega \sigma_z - M_k - \Sigma_R(k, \omega)] = 0$$

- If interactions are well-behaved can solve via perturbation theory

$$\omega = \epsilon_k + V_k^\dagger \Sigma_R(k, \epsilon_k) V_k$$

- Solution for poles can be **complex**; real and imaginary part



$$\delta\epsilon_k = \text{Re}[V_k^\dagger \Sigma_R(k, \epsilon_k) V_k]$$

$$\Gamma_k = -\text{Im}[V_k^\dagger \Sigma_R(k, \epsilon_k) V_k]$$

# Spontaneous Decay

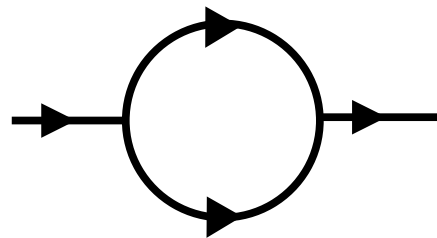
- ◆ *When* do we get an imaginary contribution?
- ◆ Non-zero if frequency in two-magnon continuum

$$\text{Re}\Sigma^{-+}(\mathbf{k}, \omega) = \frac{1}{2N} \mathcal{P} \sum_q \frac{|T_{q, \mathbf{k}-q}|^2}{\omega - \epsilon_q - \epsilon_{\mathbf{k}-q}}$$

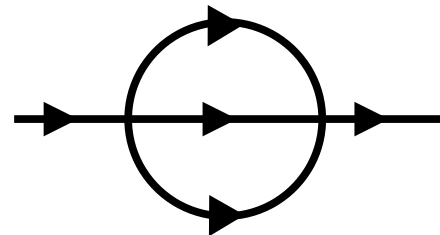
Non-zero when  
 $\omega = \epsilon_q + \epsilon_{q-k}$

$$-\text{Im}\Sigma^{-+}(\mathbf{k}, \omega) = \frac{1}{2N} \sum_q |T_{q, \mathbf{k}-q}|^2 \delta(\omega - \epsilon_q - \epsilon_{\mathbf{k}-q})$$

- ◆ If  $T$  vertex vanishes, leading process can be  $O(D^2)$



*Set  $u_k = 1$ ,  $v_k = 0$   
for simplicity*



# Dynamical Structure Factor

- Computing the dynamical structure factor not *entirely* from the magnon Green's function

*Just  $G^{-+}$*

*Renormalize/mix the usual Green's functions*

$$\langle S_r^+(\tau) S_{r'}^-(0) \rangle_c \approx S \langle a_r(\tau) a_{r'}^\dagger(0) \rangle - \frac{1}{4} \left( \langle a_r(\tau) a_{r'}^\dagger(0) n_{r'}(0) \rangle + \langle n_r(\tau) a_r(\tau) a_{r'}^\dagger(0) \rangle \right)$$

$$\langle S_r^z(\tau) S_{r'}^z(0) \rangle_c \approx \langle n_r(\tau) n_{r'}(0) \rangle$$

*Density-density: Probes two-magnon properties*

$$\langle S_r^z(\tau) S_{r'}^+(0) \rangle_c \approx -S^{1/2} \langle n_r(\tau) a_{r'}^\dagger(0) \rangle$$

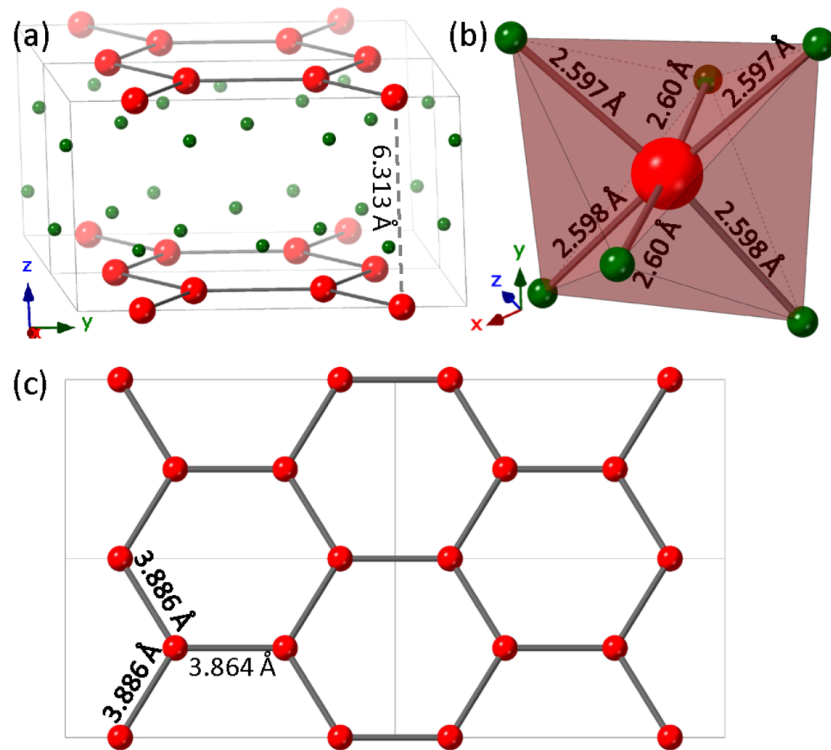
*Renormalize/mix the usual Green's functions & involve "bubbles"*

# Effects of Interactions

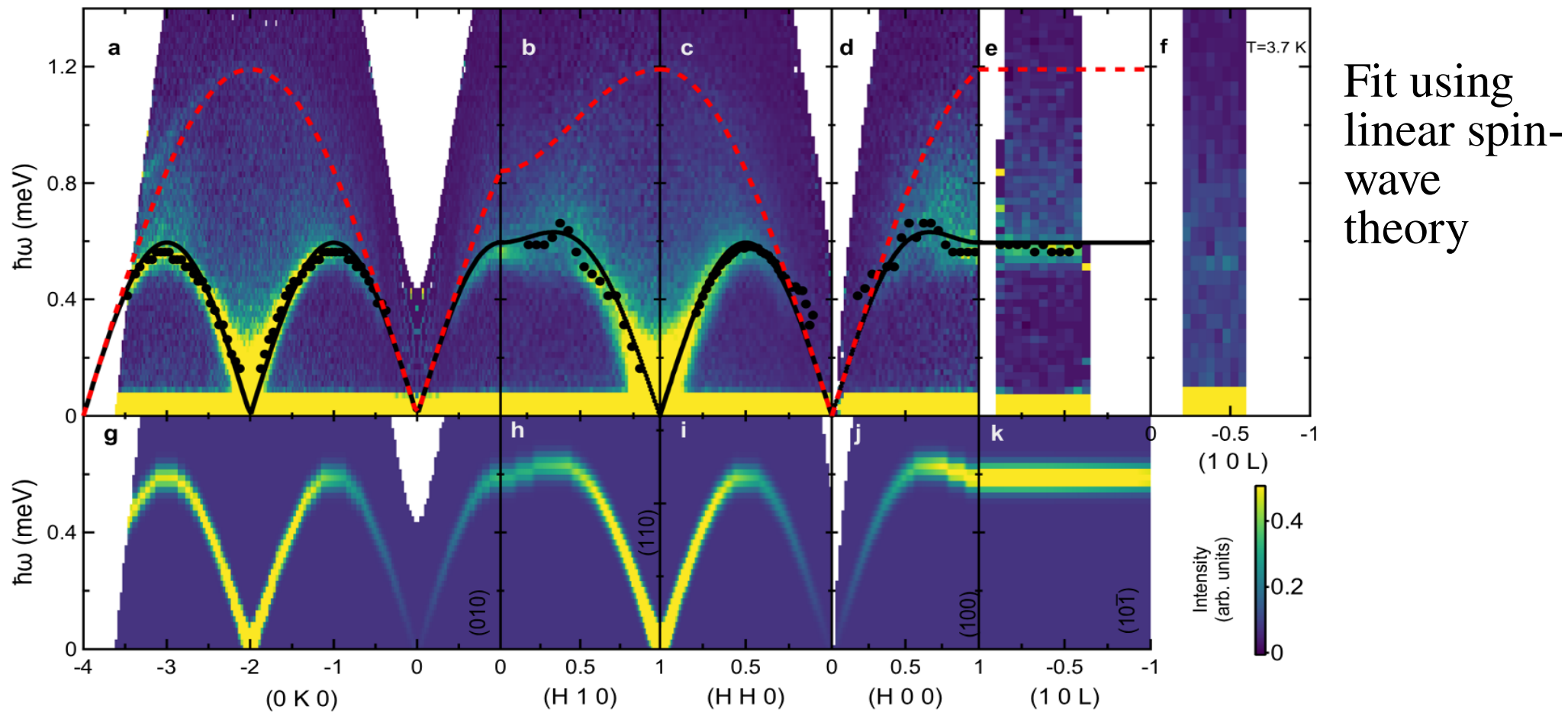
# Example: Renormalization

- ◆ Rare-earth magnet:  $\text{YbCl}_3$
- ◆ Honeycomb lattice antiferromagnet ( $S_{\text{eff}} = 1/2$ )
- ◆ Neel order below  $\sim 0.6$  K
- ◆ **Surprisingly isotropic exchange interactions**
- ◆ Model with Heisenberg exchange

$$H = \frac{1}{2} \sum_{rr'} J_{rr'} \mathbf{S}_r \cdot \mathbf{S}_{r'}$$



Xing et al, Phys. Rev. B **102**, 014427 (2020)  
Sala *et al*, Phys. Rev. B **100**, 180406 (2019);  
Rau & Gingras, Phys. Rev. B **98**, 054408 (2018)



$$J = 0.421 \text{ meV}$$

- ◆ Non-linear effects renormalize spectrum

- ◆ At leading order rescales

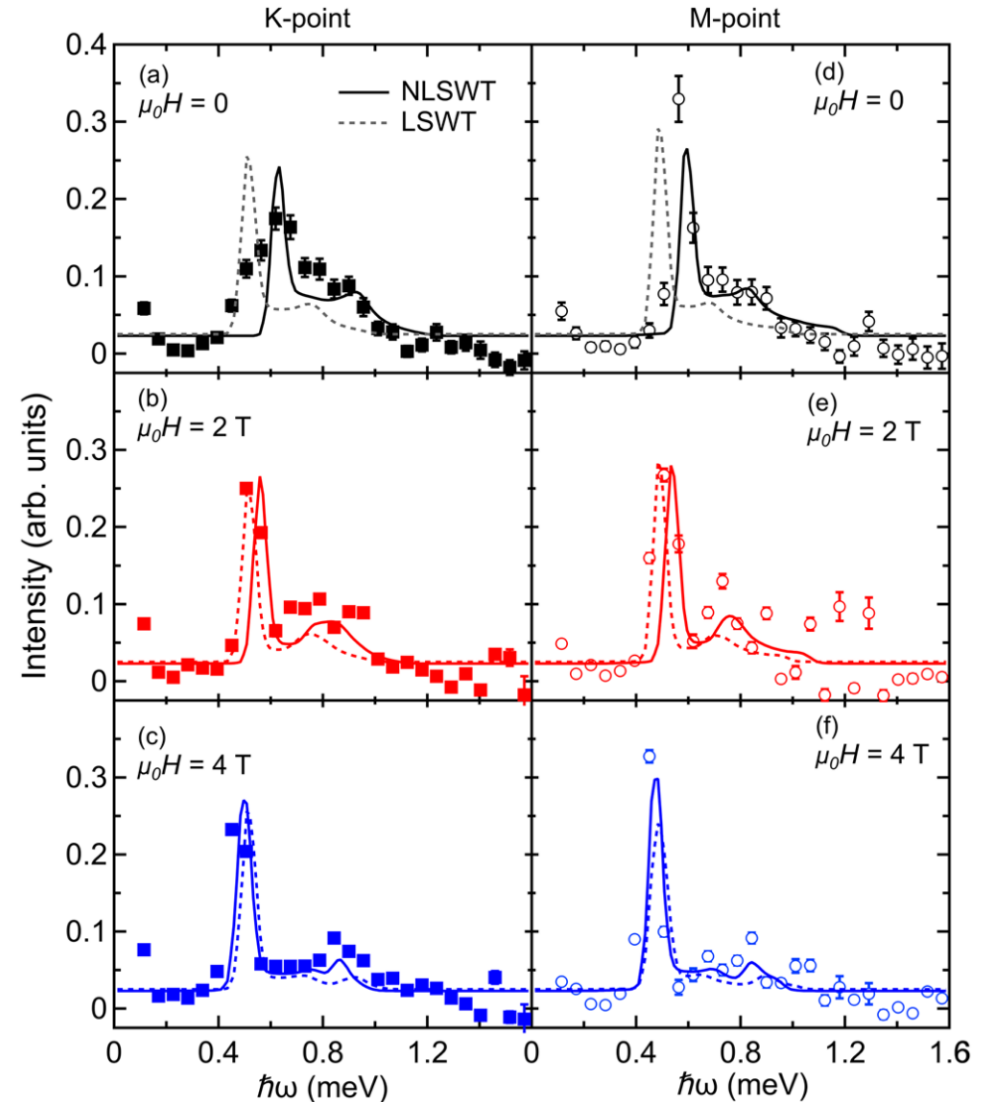
$$\epsilon_k + \delta\epsilon_k \approx Z\epsilon_k$$

- ◆ Factor is approximately  $Z \sim 1.3$

- ◆ If fit with NLSWT would find

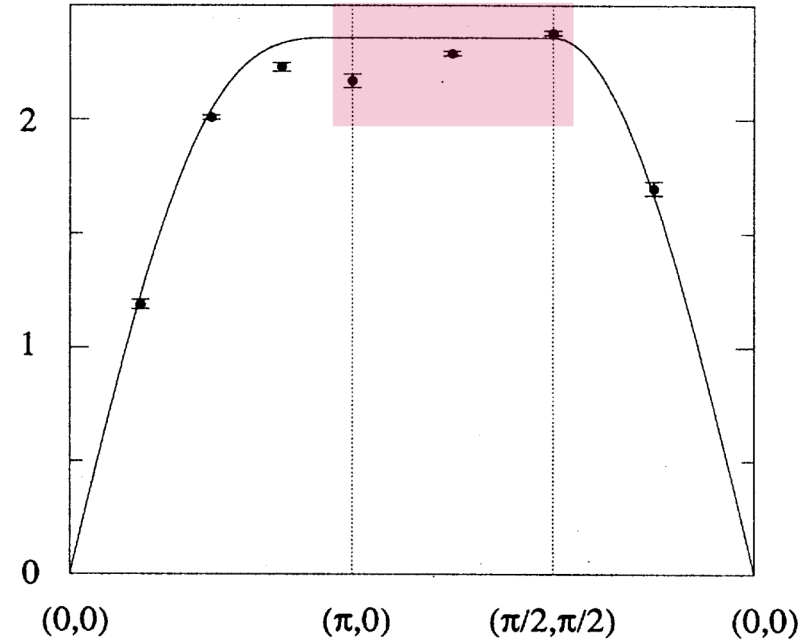
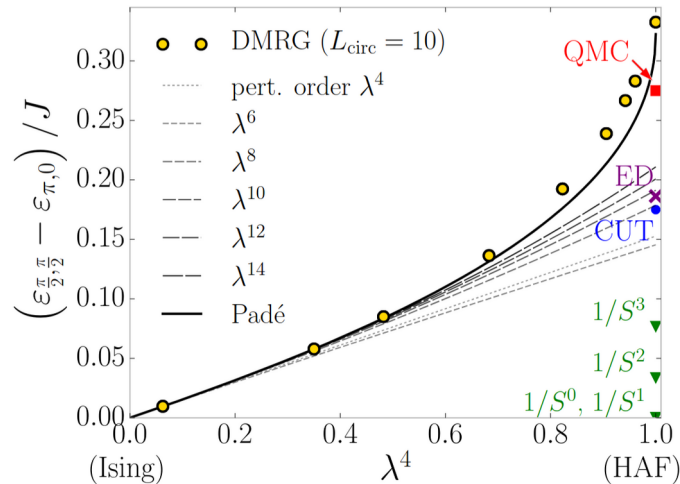
$$J = 0.344 \text{ meV}$$

- ◆ Validated by high-field experiment; LSWT becomes exact when  $|\mathbf{B}|/J$  large



# Example: Renormalization

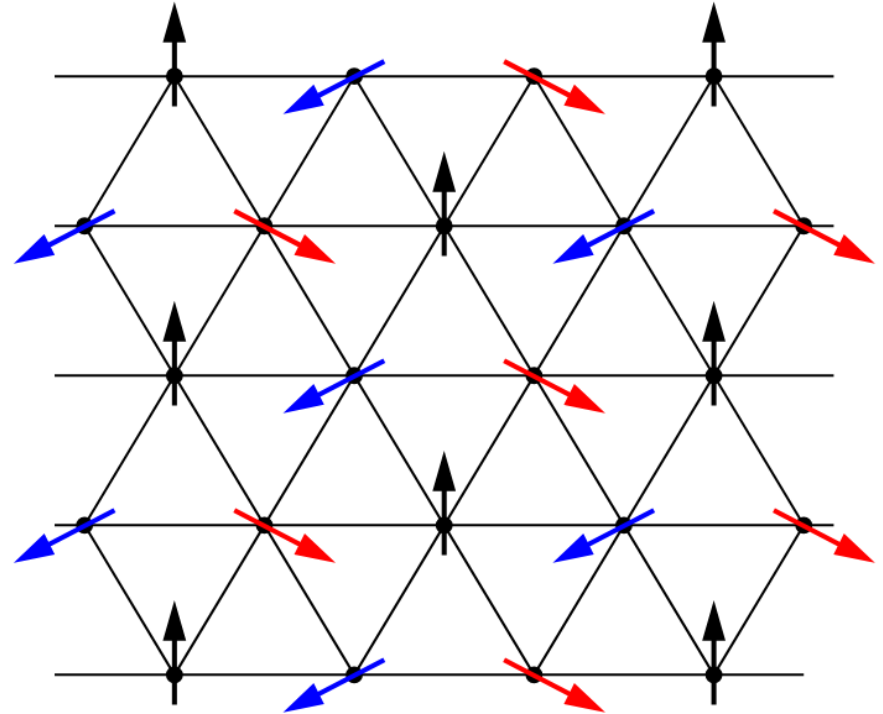
- ◆ ... some well known cases where interactions aren't enough
- ◆ Square lattice Heisenberg antiferromagnet



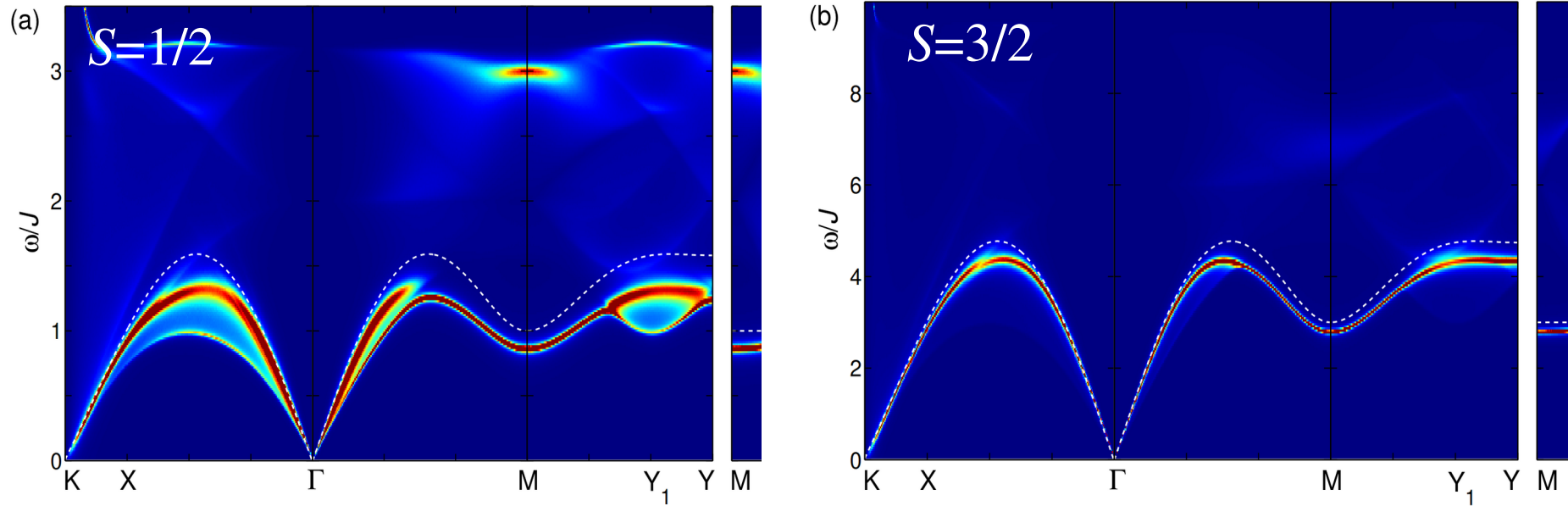
- ◆ Spin-waves are **flat** along line at leading order in interactions

# Example: *Spontaneous Decay*

- ◆ Triangular Heisenberg anti-ferromagnet
- ◆ Isotropic interactions, but non-collinear order
- ◆ **Spontaneous magnon decay is allowed**
- ◆ Presence of gapless Goldstone mode means kinematic condition not too hard to satisfy

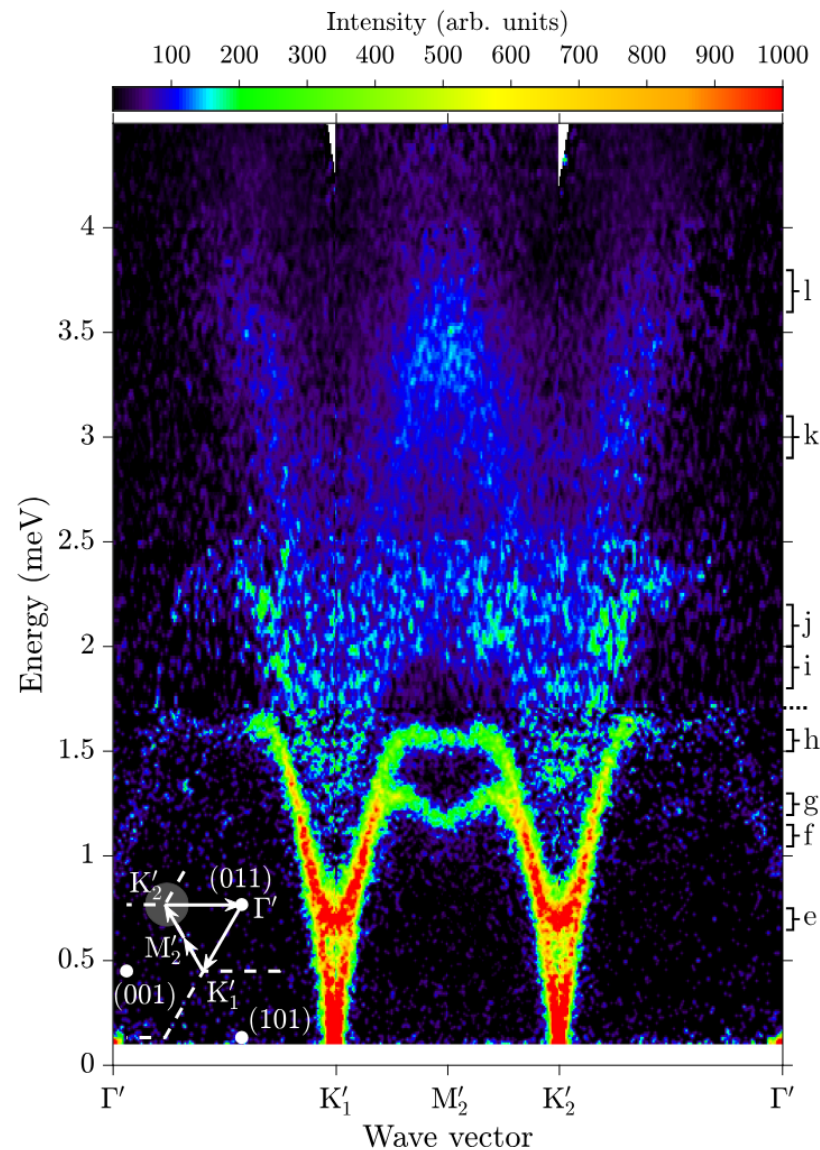
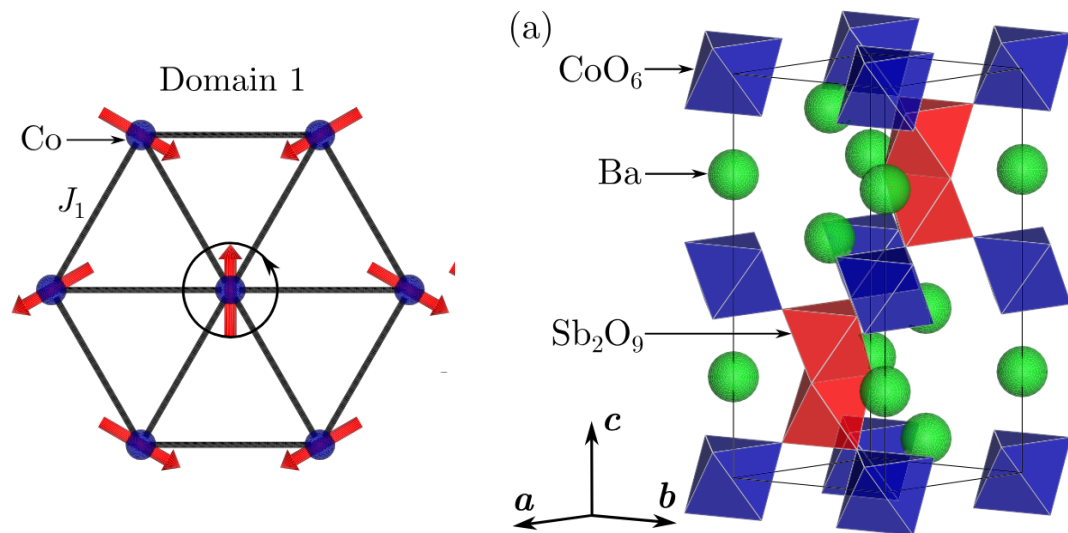


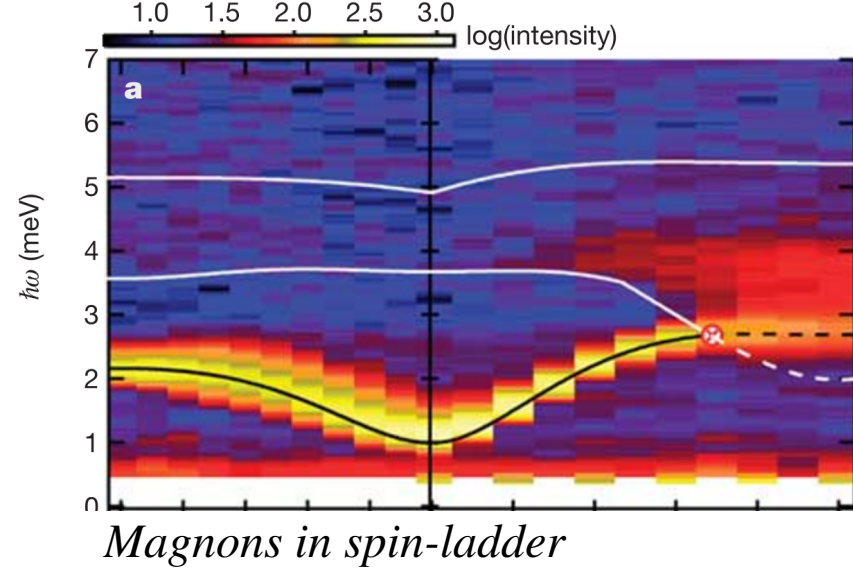
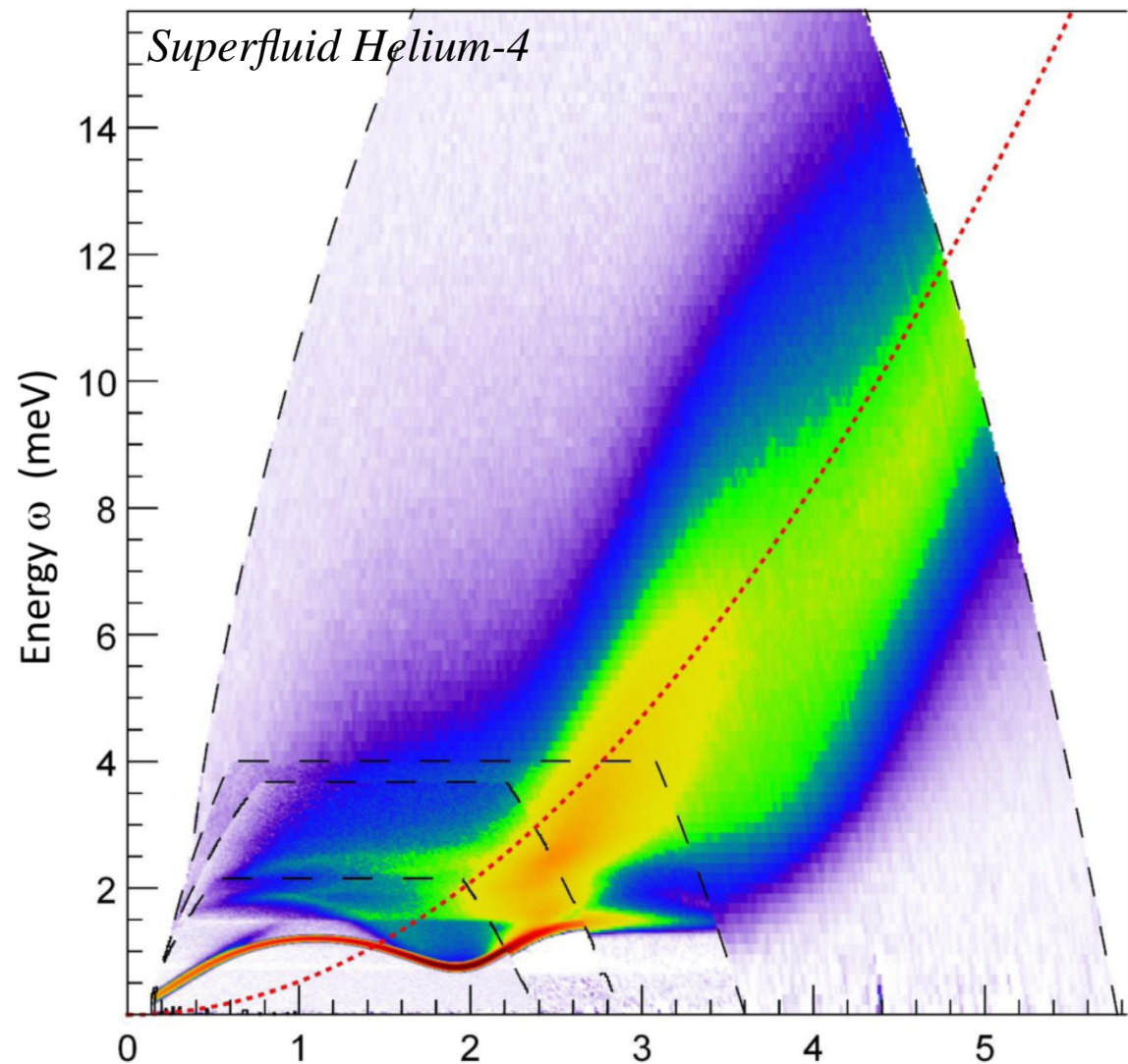
# Example: *Spontaneous Decay*



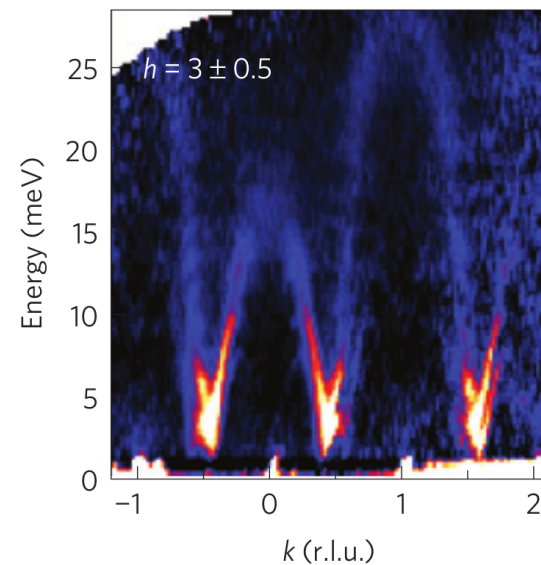
- ◆ Significant decay at small  $S$ ; approaches LSWT as  $S$  increases

- ◆ Not always apparent in real materials
- ◆  $\text{Ba}_3\text{CoSb}_2\text{O}_9$  is (near) ideal triangular  $S=1/2$  HAFM
- ◆ **Quasi-particle decay (mostly) avoided**

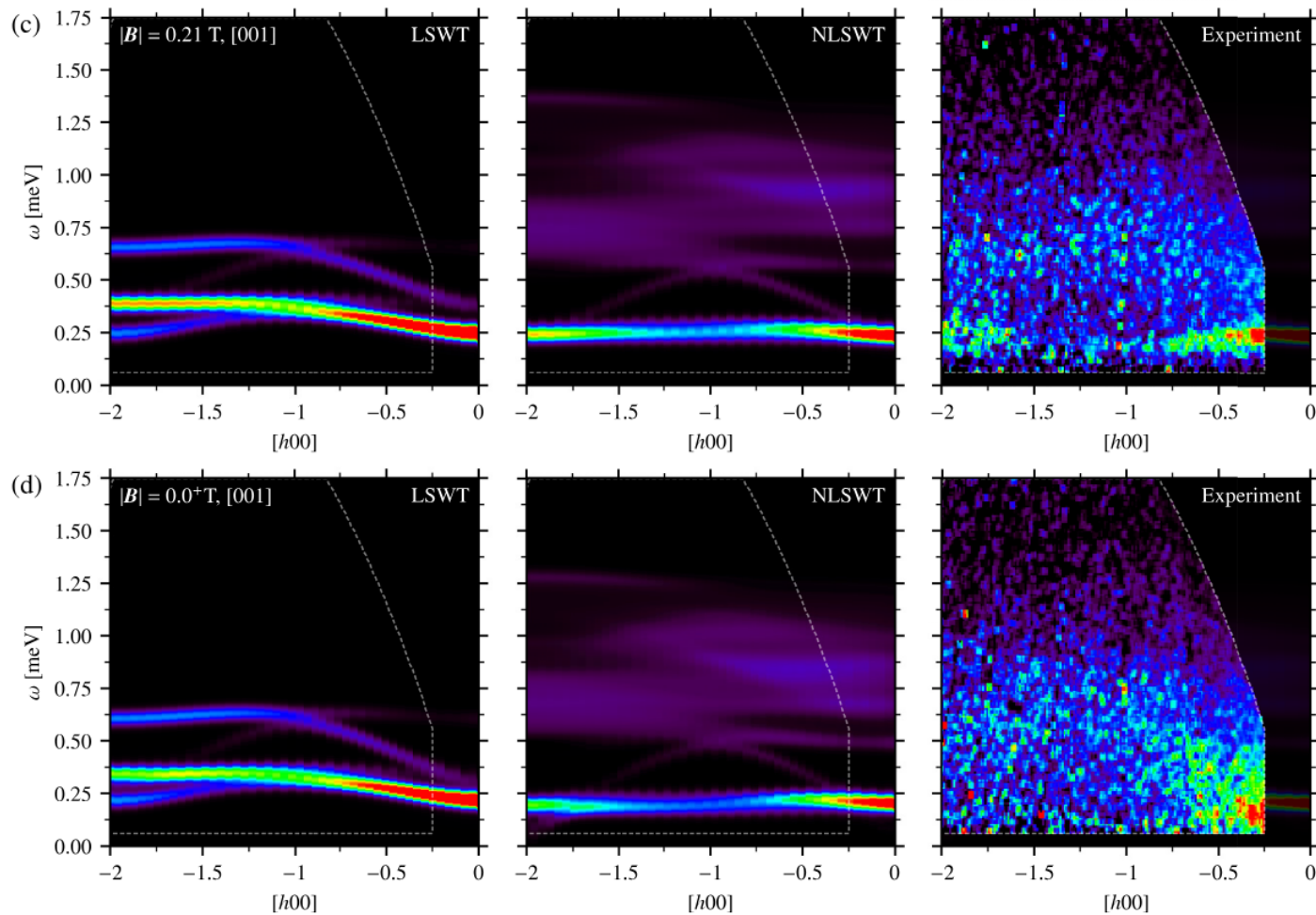




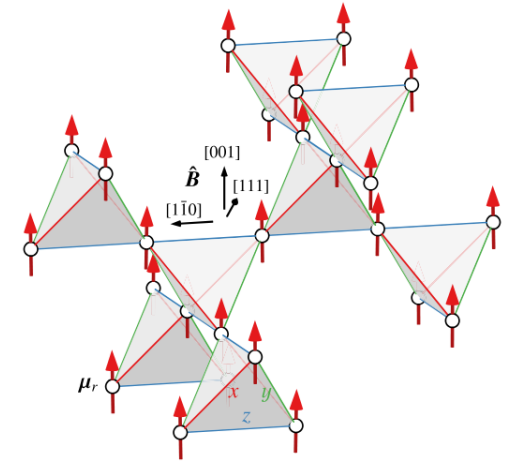
*Triplons in  
Dimerized  
magnet*



*Beauvois et al, PRB (2018); Stone et al, Nature (2005), Plumb et al, Nat Phys (2016)*



## $\text{Yb}_2\text{Ti}_2\text{O}_7$ (anisotropic FM)



- ◆ ... often amount of (apparent) decay isn't *enough* as compared to experiment

# Pseudo-Goldstone Modes

# Pseudo-Goldstone Modes

- ♦ Rotation of spins in “soft” direction is *shift of bosons*

$$a_r \rightarrow a_r + \lambda_r$$

*Determined by ordering  
pattern & direction of  
deformation*

- ♦ Accidental degeneracy implies **zero mode**

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^\dagger & \mathbf{A}^\top \end{pmatrix} \begin{pmatrix} \lambda \\ \lambda^\dagger \end{pmatrix} = 0$$

*Two kinds of zero modes*

- **Type I:** Conjugate momentum is “hard”
- **Type II:** Conjugate momentum also soft

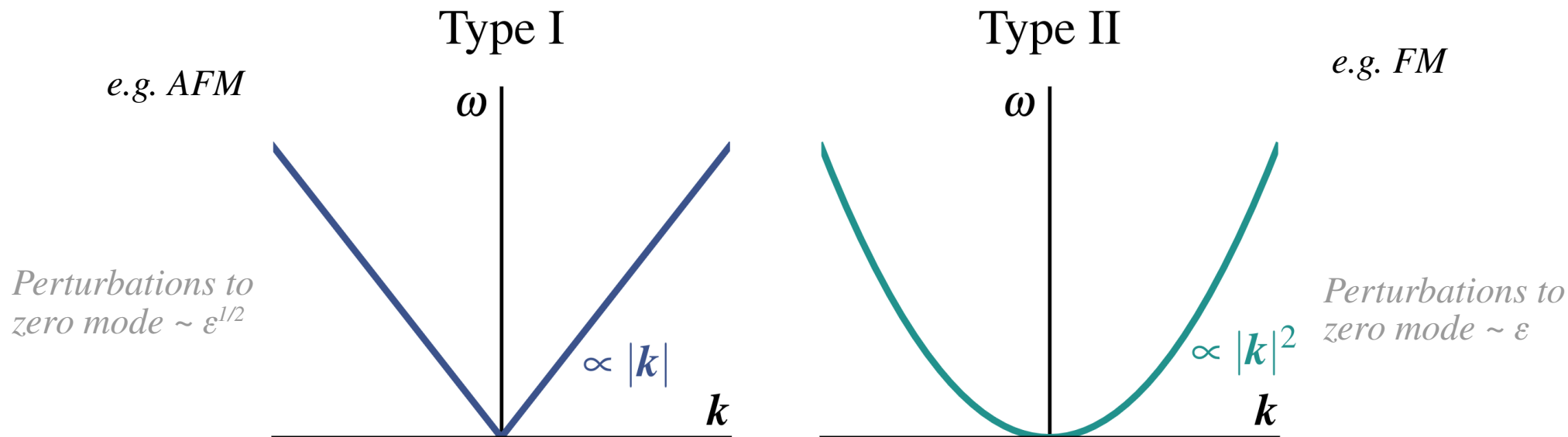
*i.e.  $H \sim P^2$*

*i.e.  $H = 0$*

- More mathematically for a mode at  $k = 0$ :

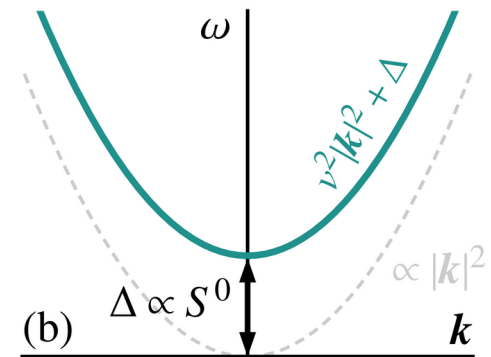
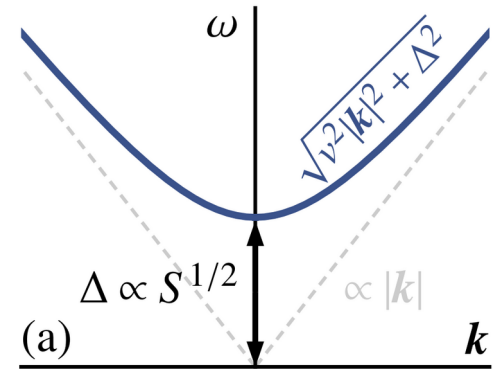
$$\begin{pmatrix} A_k & B_k \\ -B_k^* & -A_k \end{pmatrix} \xrightarrow{\text{at } k=0} \begin{pmatrix} A_0 & A_0 \\ -A_0 & -A_0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

*Non-diagonalizable (Jordan block)*

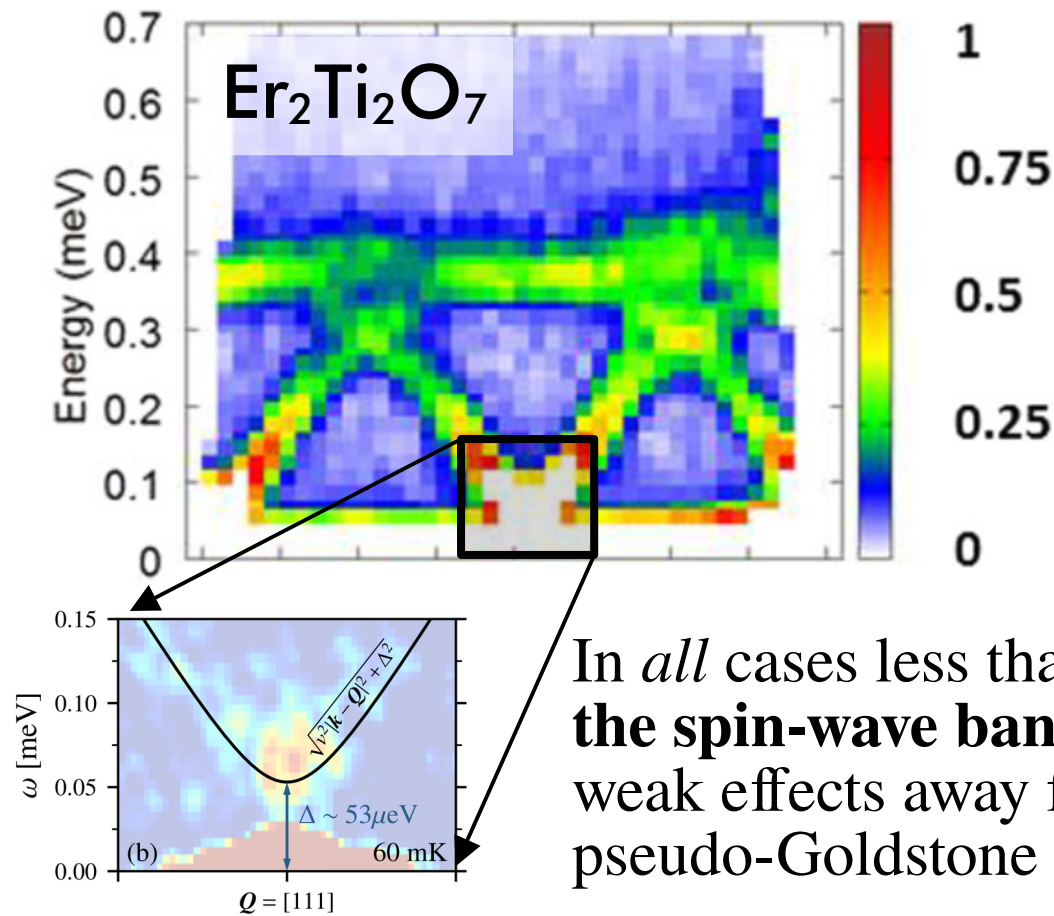


# Pseudo-Goldstone gaps

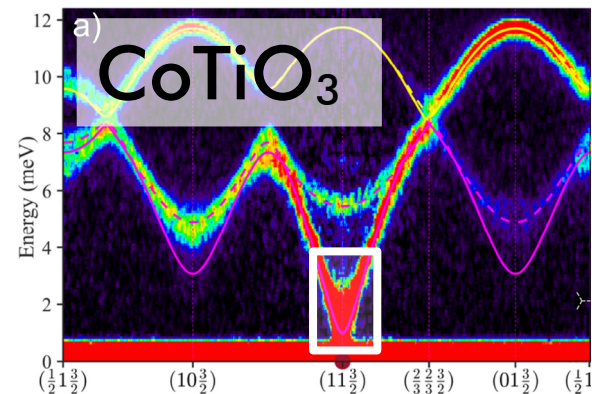
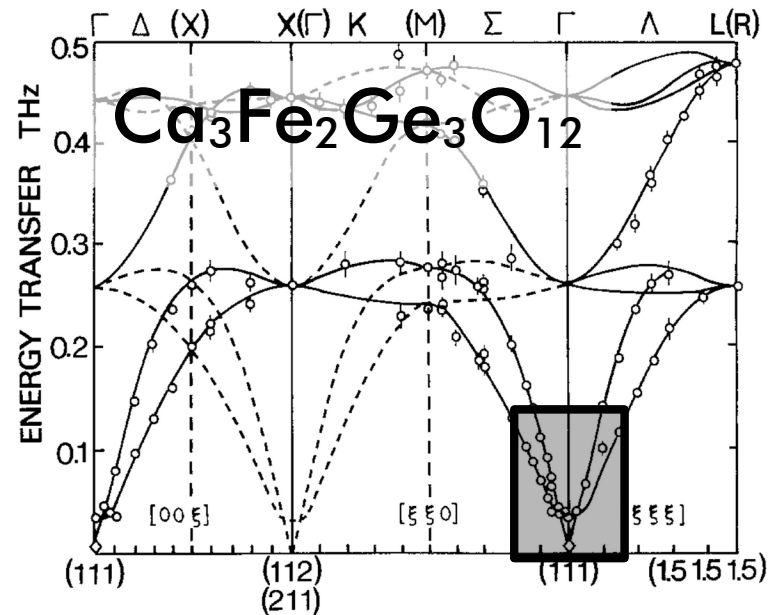
- ◆ Generated by *quantum fluctuations*
- ◆ Can be calculated at  $O(1/S^2)$  in spin-wave theory
  - Directly via perturbation theory in magnon-magnon interactions
  - Indirectly via **curvature formula\*** involving fluctuation corrected energy density
- ◆ **Intrinsic interaction effect**
- ◆ Expect (*hope*) they are small, perturbative in  $1/S$



\*Rau et al, Phys. Rev. Lett **121**, 237201 (2018)



In *all* cases less than **~10%** of the spin-wave bandwidth, weak effects away from pseudo-Goldstone mode

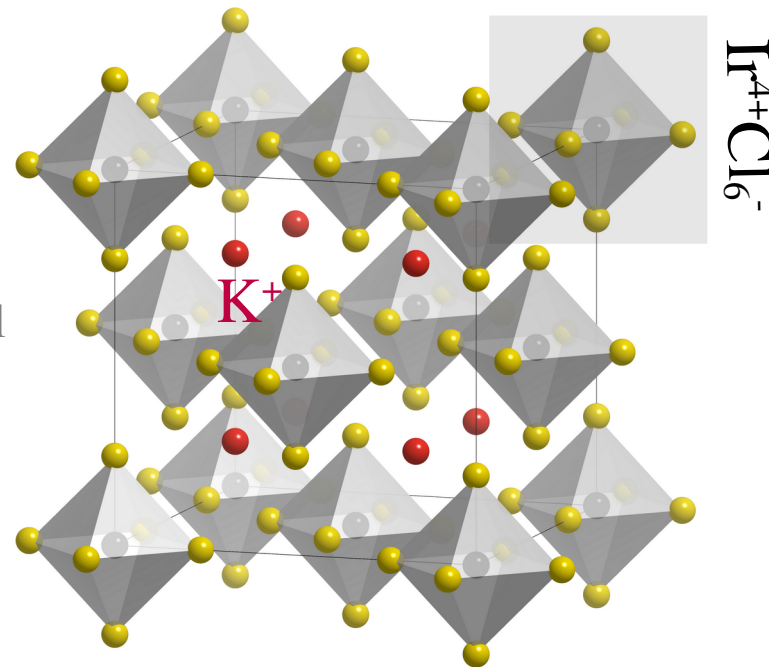


Ross *et al*, Phys. Rev. Lett. **112**, 057201 (2014), Petit *et al*, Phys. Rev. B **90**, 060410(R) (2014); T. Bruekel *et al*, Z. Phys. B **72**, 477 (1988), Elliot *et al*, Nat. Comm. **12** 3936 (2021), ....

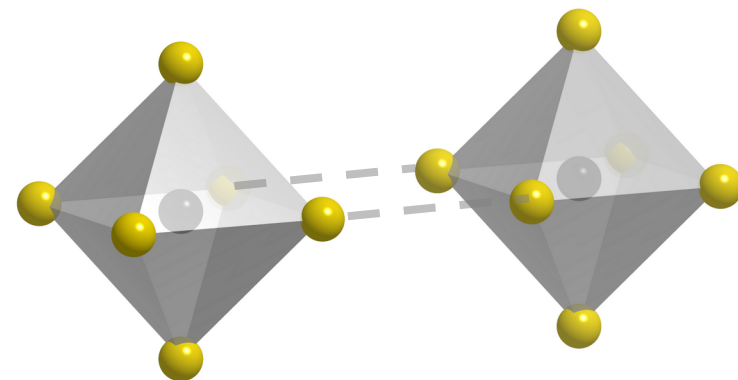
# $\text{K}_2\text{IrCl}_6$

- ◆ Cubic crystal (SG #225)
- ◆ Magnetic  $\text{Ir}^{4+}$  ions ( $5d^5$ )
  - Octahedral  $\text{Cl}^-$  cages
  - *Strong spin-orbit coupling*
  - $J_{\text{eff}} = 1/2$  doublets
- ◆ **Face-centered cubic lattice**  
(no detectable distortion)
- ◆ Same bond *symmetry* as in  
(idealized) Kitaev materials

No trigonal  
or tetragonal  
distortions



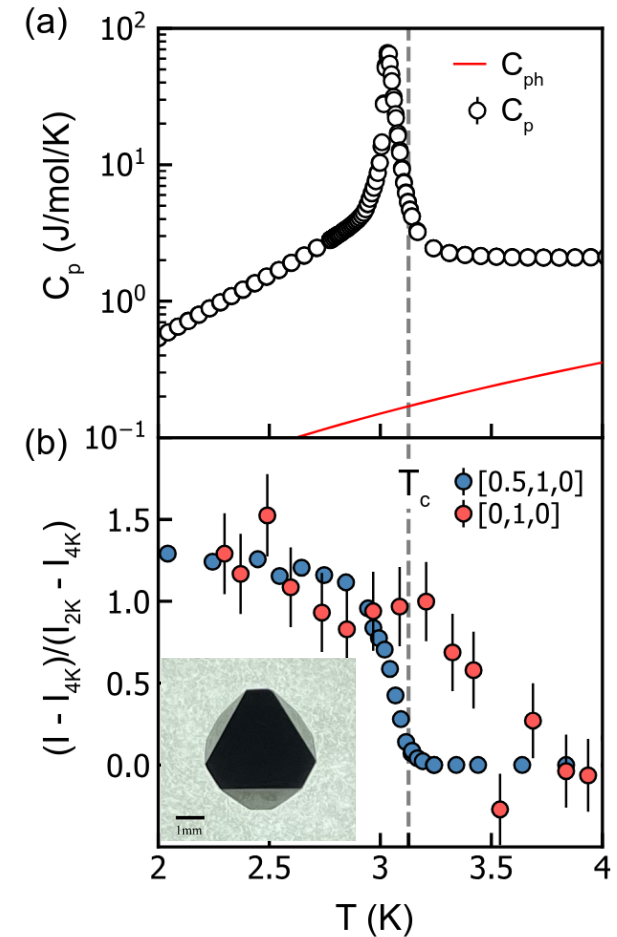
*Separated;*  
not edge-  
shared



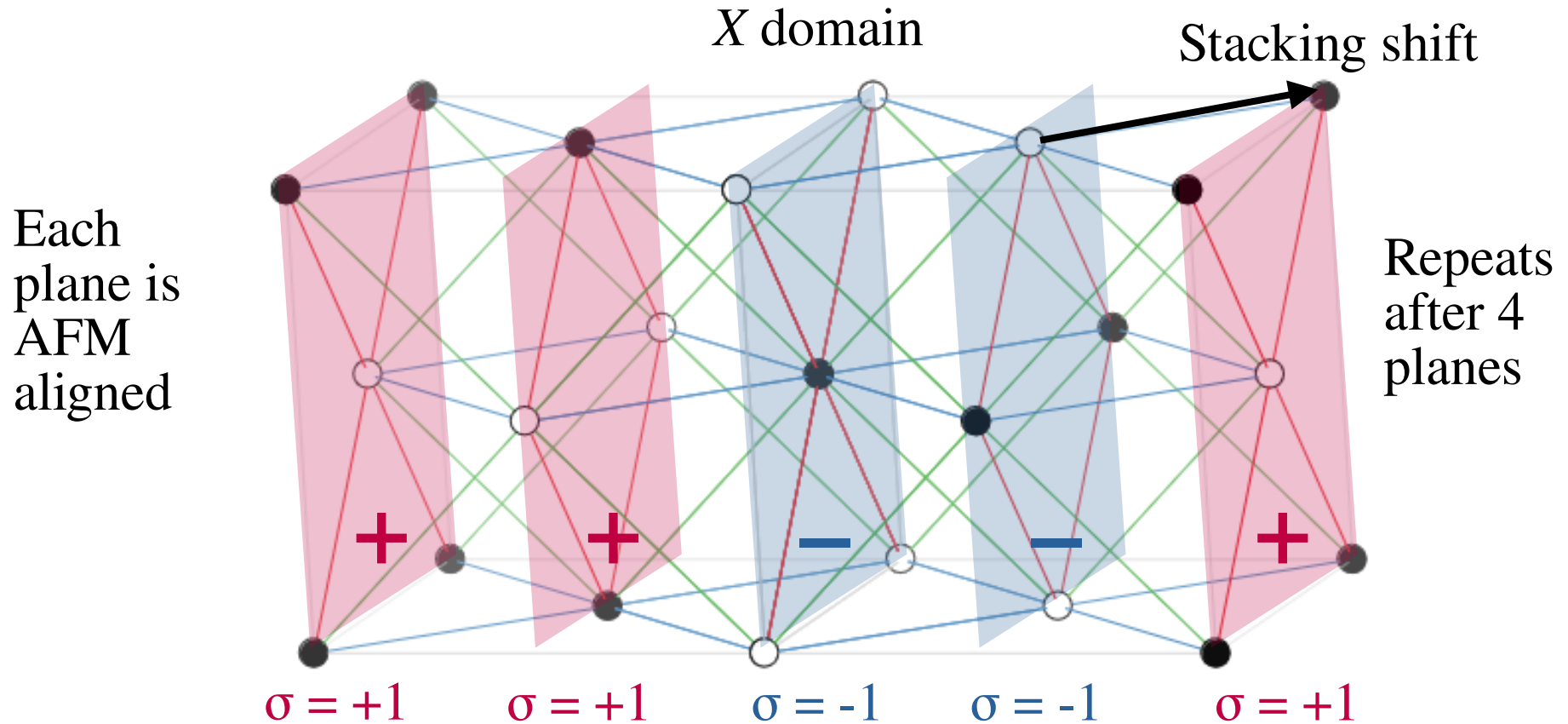
# Magnetic Order

- ◆ Order appears at low temperature  $T_N \sim 3$  K via sharp phase transition
  - Curie-Weiss temperature estimated to be  $\Theta_{CW} \sim 30$  K
  - **Highly frustrated**
- ◆ Bragg peaks appear at  $[\frac{1}{2}, 1, 0]$  and equivalents below  $T_N$ 
  - Antiferromagnetic “Type III” order
- ◆ Polarization analysis yields moment *parallel* to  $\frac{1}{2}$  direction

Looks continuous



# Type-III: AFM planes stacked $++--\dots$



# Model

- ◆ Anisotropic spin-1/2 exchange model on FCC lattice

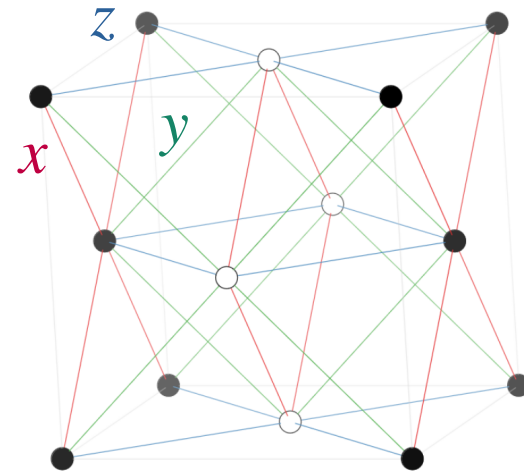
$$H = \sum_{\langle ij \rangle_{\alpha\beta(\gamma)}} \left[ JS_i \cdot S_j + KS_i^\gamma S_j^\gamma + (-1)^{\sigma_{ij}^{\alpha\beta}} \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right] + J_2 \sum_{\langle ij \rangle_2} S_i \cdot S_j$$

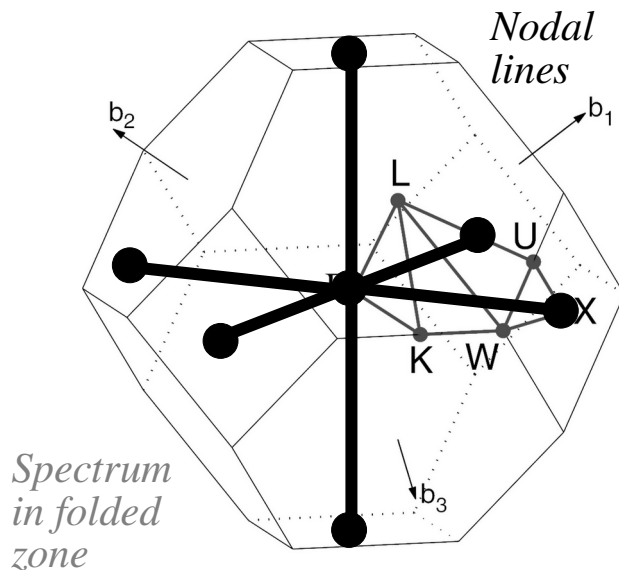
- ◆ Three bond types:  $x$ ,  $y$ ,  $z$ .  $\alpha\beta(\gamma)$  is cyclic permutation
- ◆  $\Gamma$  has sign structure determined by

$$\sigma_{ij}^{\alpha\beta} \equiv \text{sgn}(d_{ij}^\alpha d_{ij}^\beta)$$

where  $\mathbf{d}_{ij} = \mathbf{r}_i - \mathbf{r}_j$  is the bond direction

- ◆ Isotropic  $J_2$  for simplicity



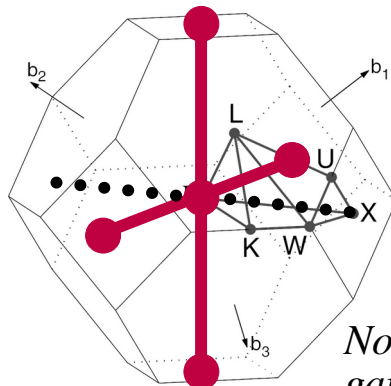


# Ordered Phase Excitations

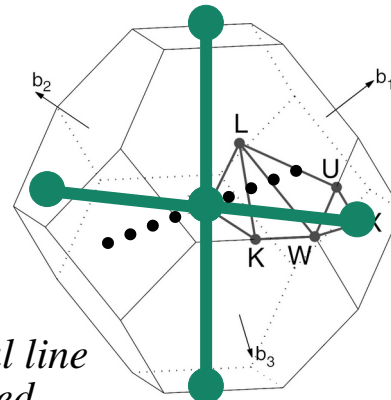
- ◆ **Three nodal lines** in *all* ground states in Heisenberg limit
- ◆ Correspond to continuous mixing with other stacked states – “**pseudo-Goldstone modes**”

- ◆ Nodal line **along stacking direction** is **lifted** by Kitaev interaction
- ◆ **Two nodal lines left**

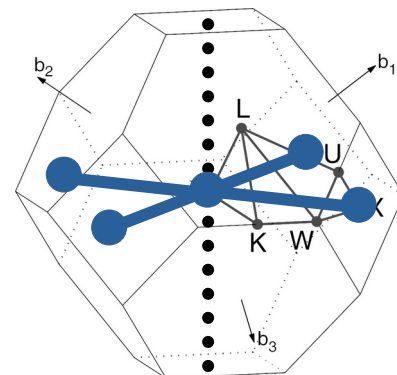
**X** stacked



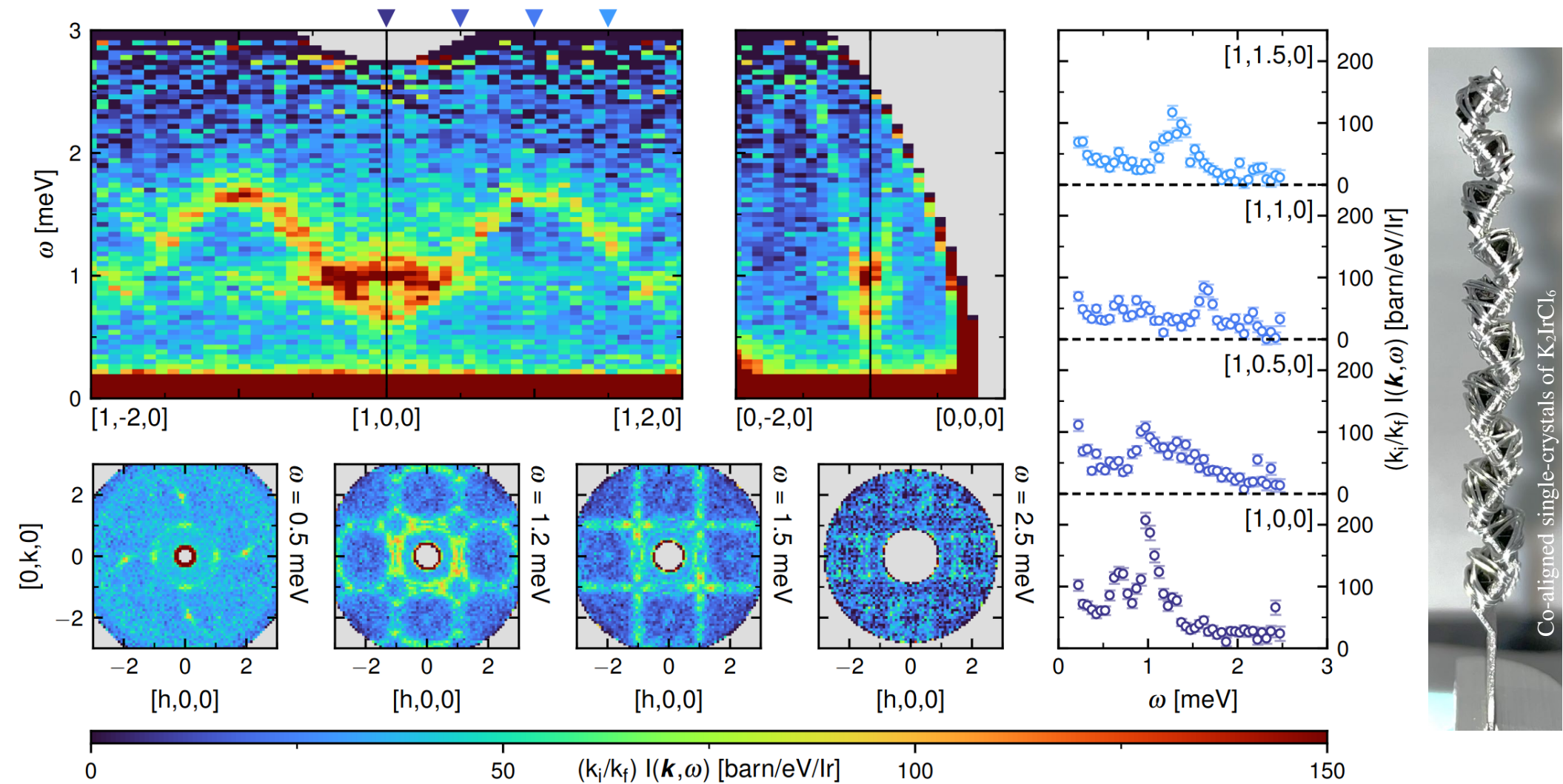
**Y** stacked



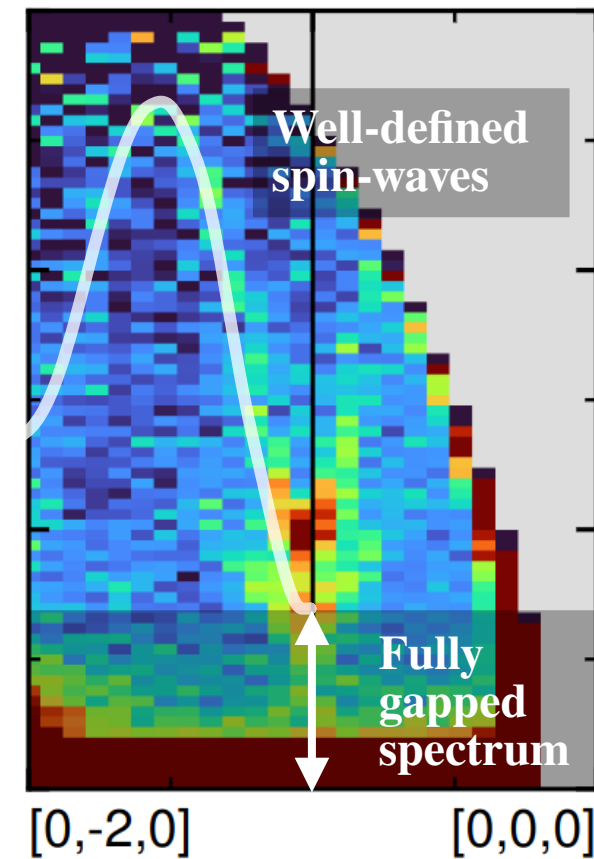
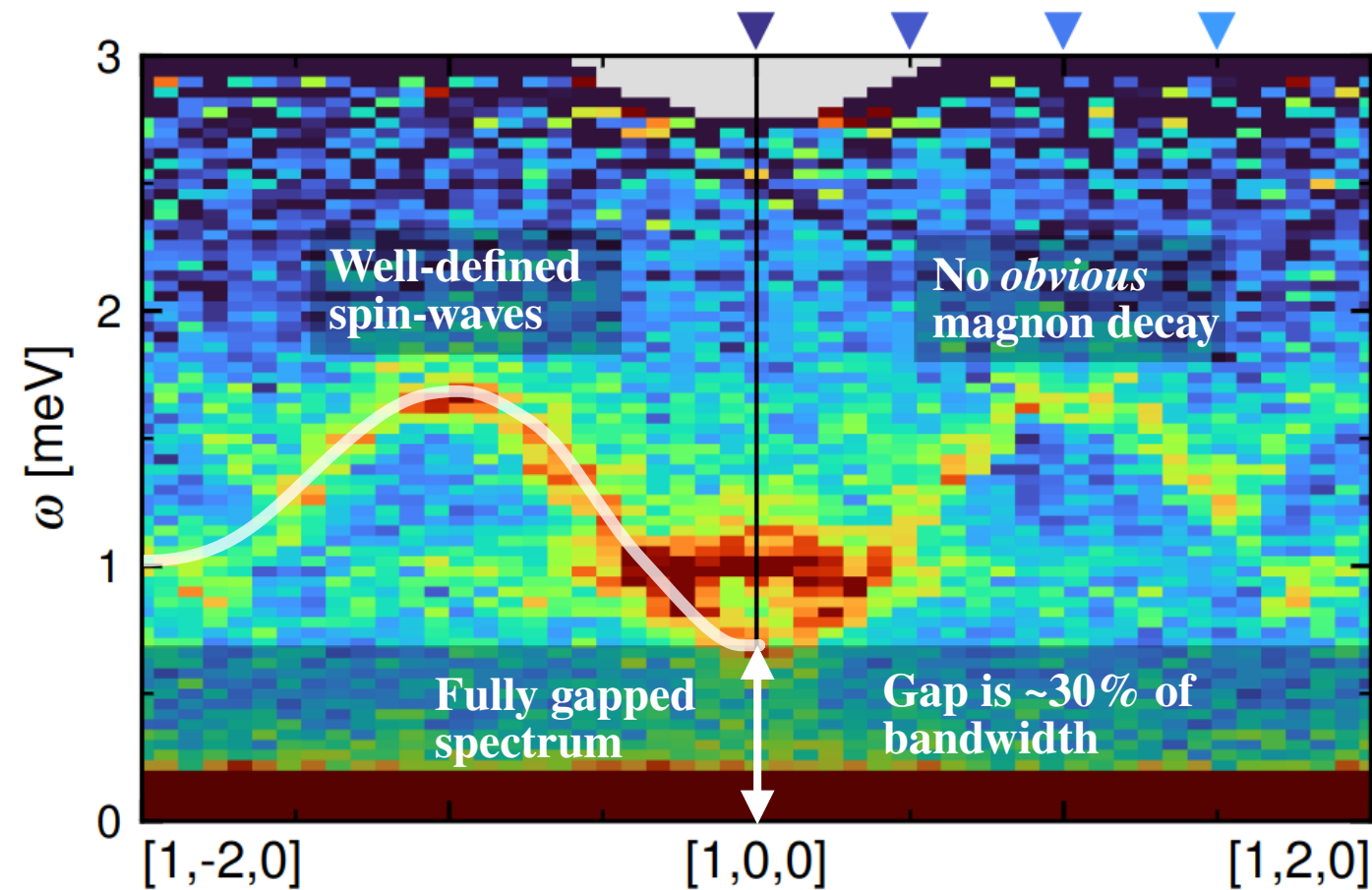
**Z** stacked



*Nodal line gapped*

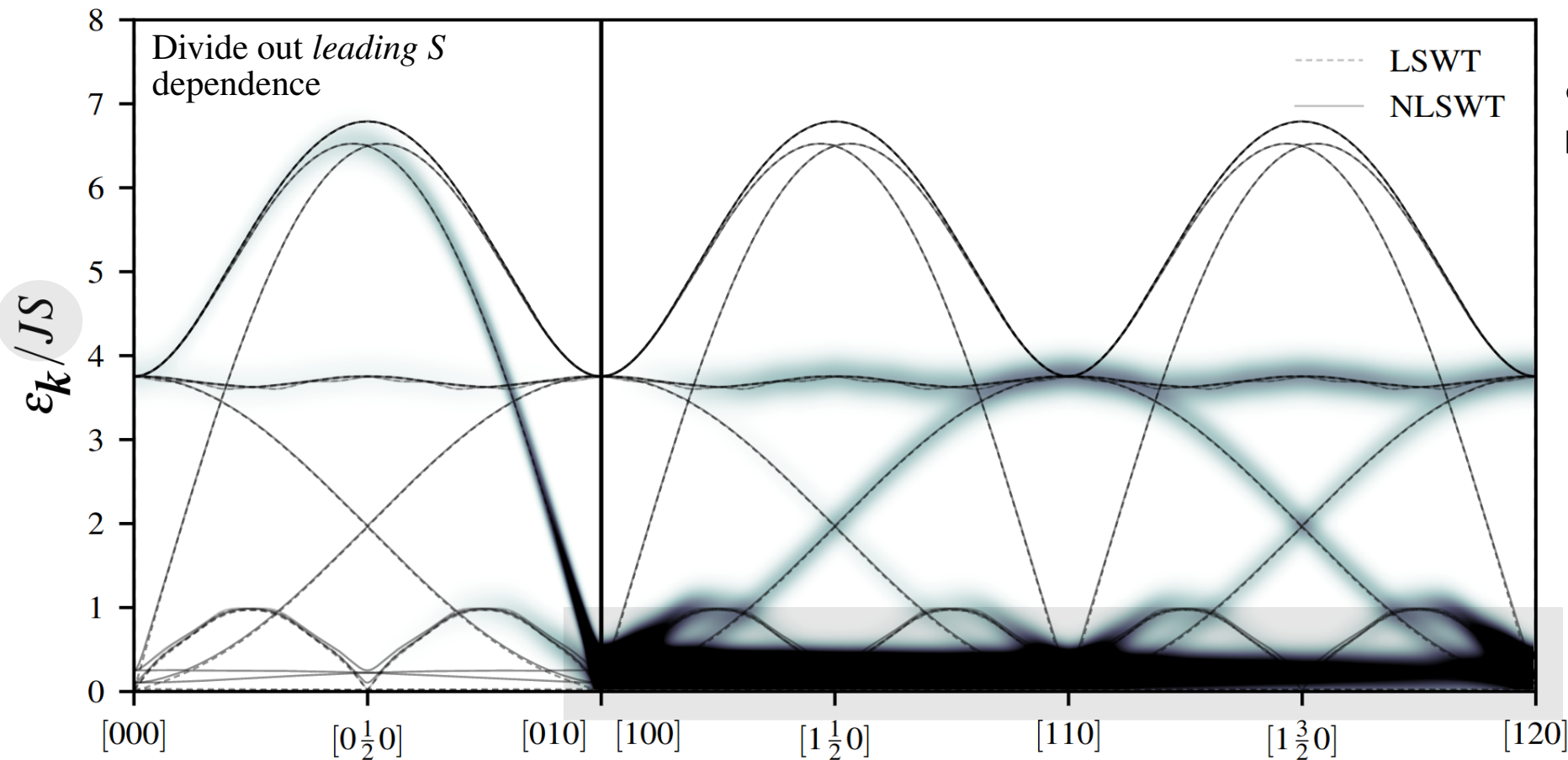


\*Iridium is strong neutron absorber



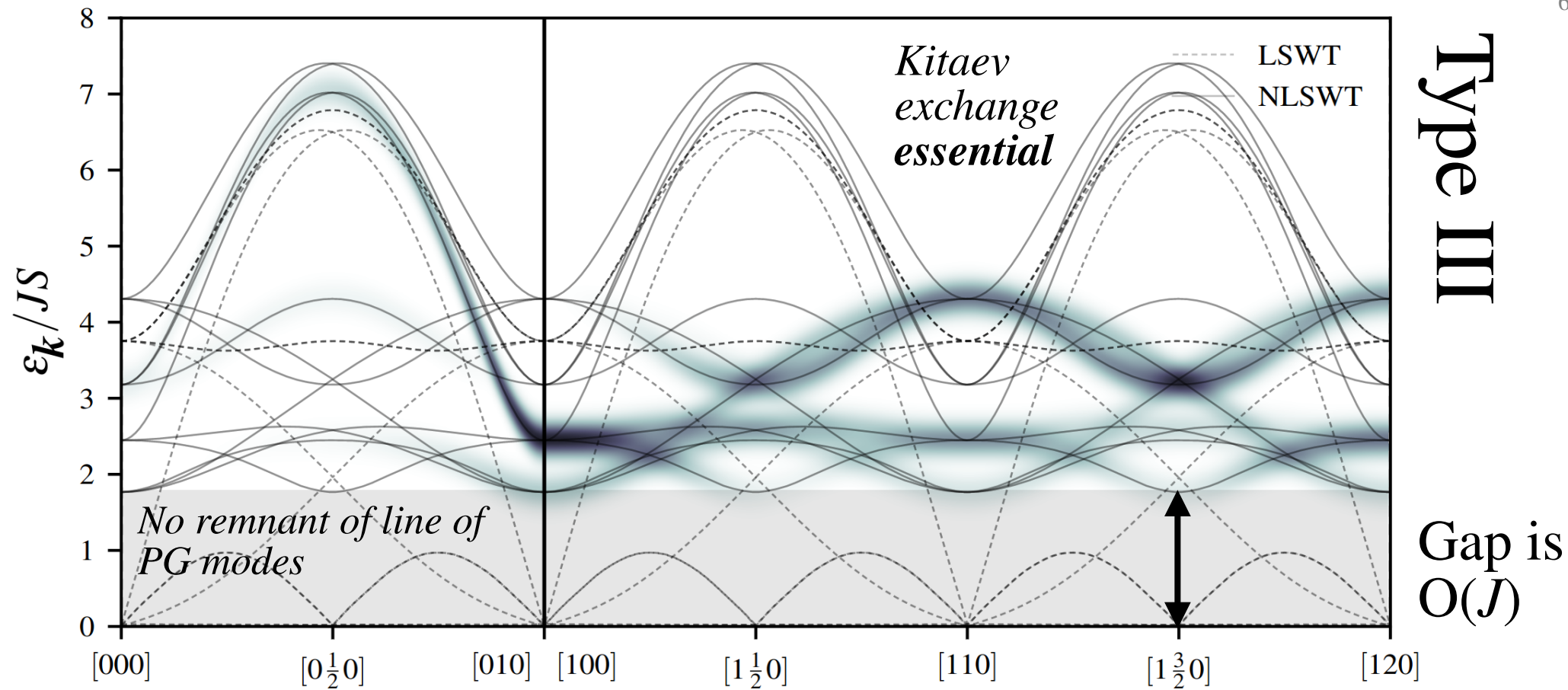
*Very different than expectations!*

## Type III



$$K/J = 0.20, 1/S \rightarrow 0$$

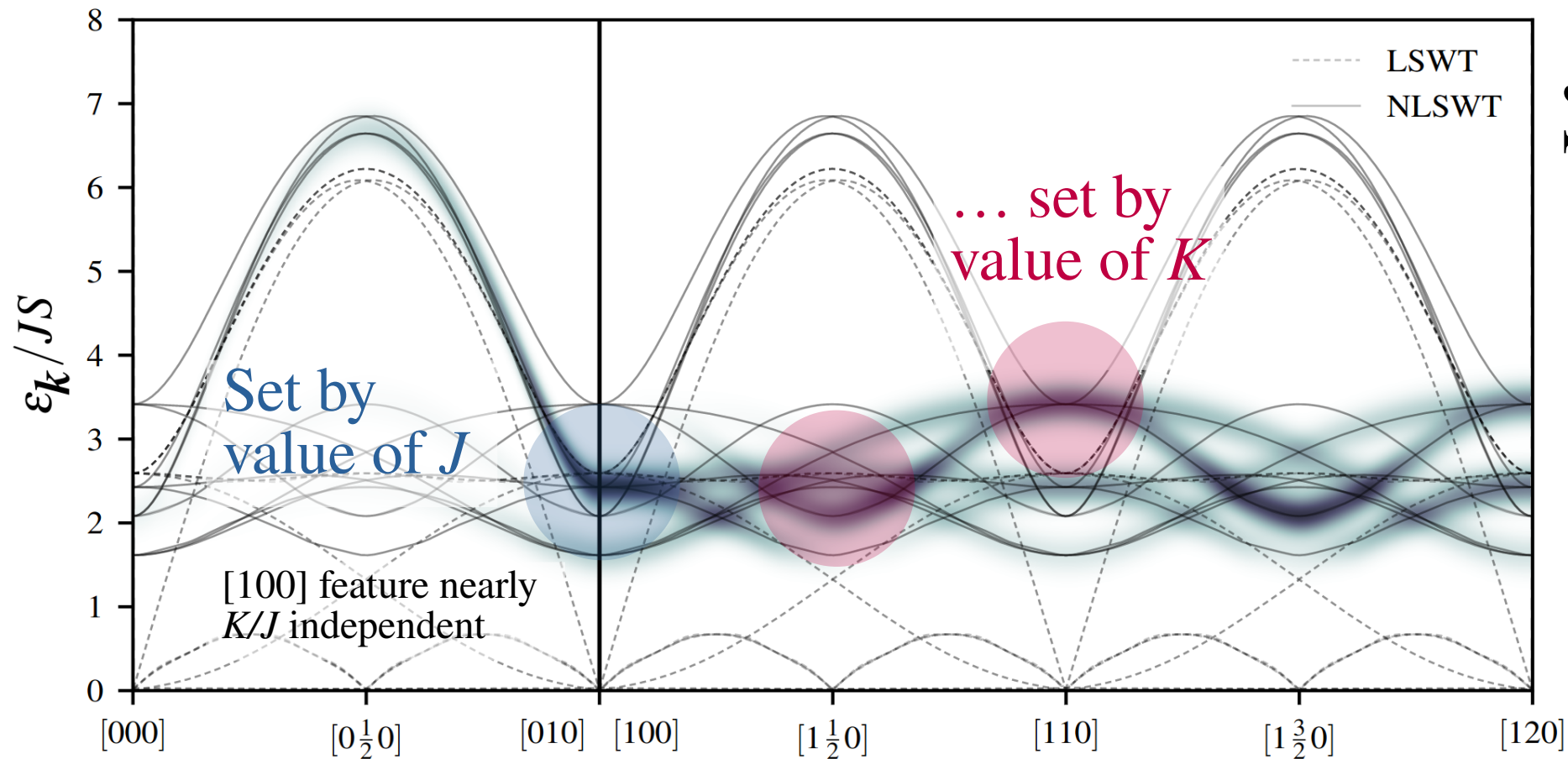
LSWT



$$K/J = 0.20, S = 1/2$$

NLSWT

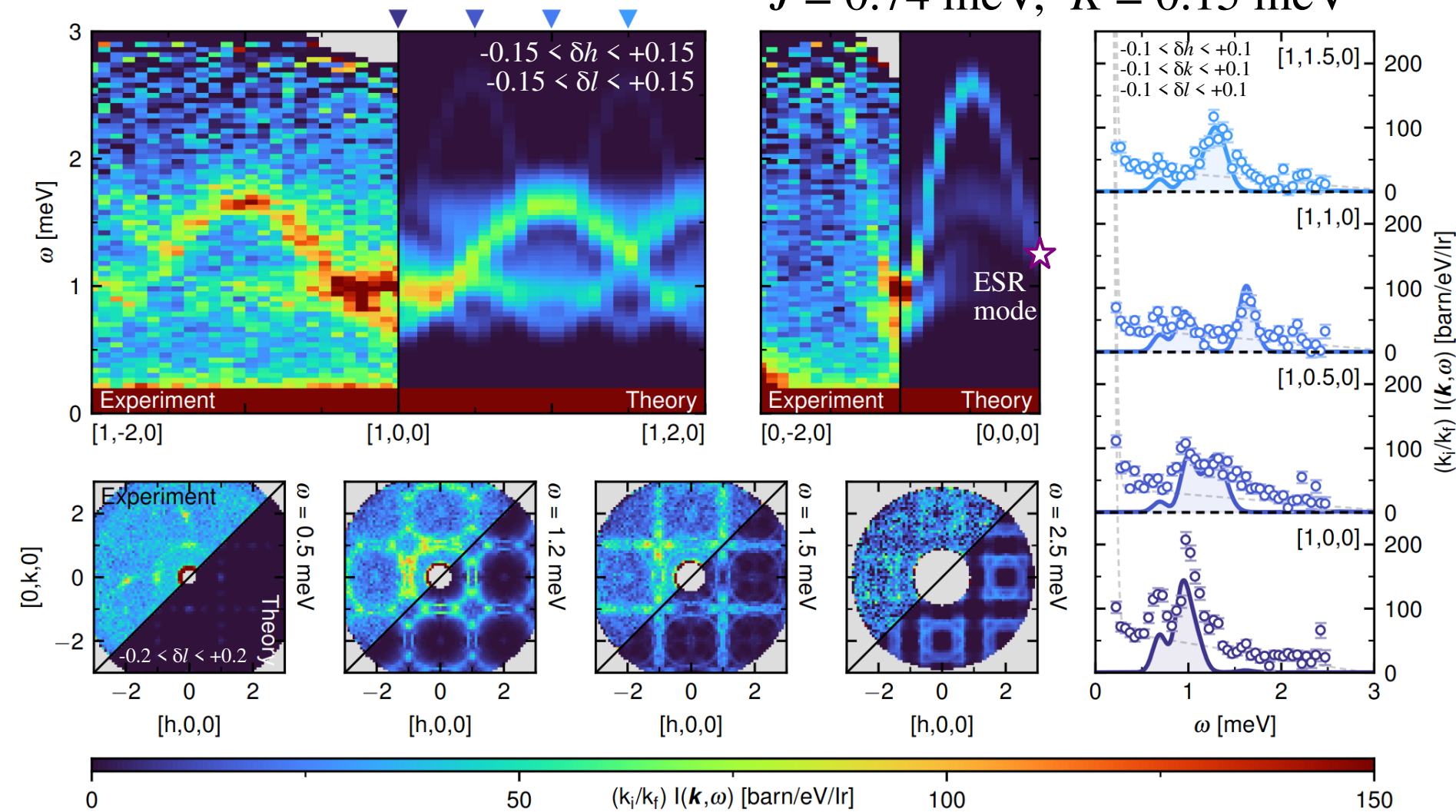
## Type III



Set  $\Gamma = 0$  (no decay) and  $J_2 = 0$  (simplicity)

Including: Experimental averaging,  $\text{Ir}^{4+}$  form factor

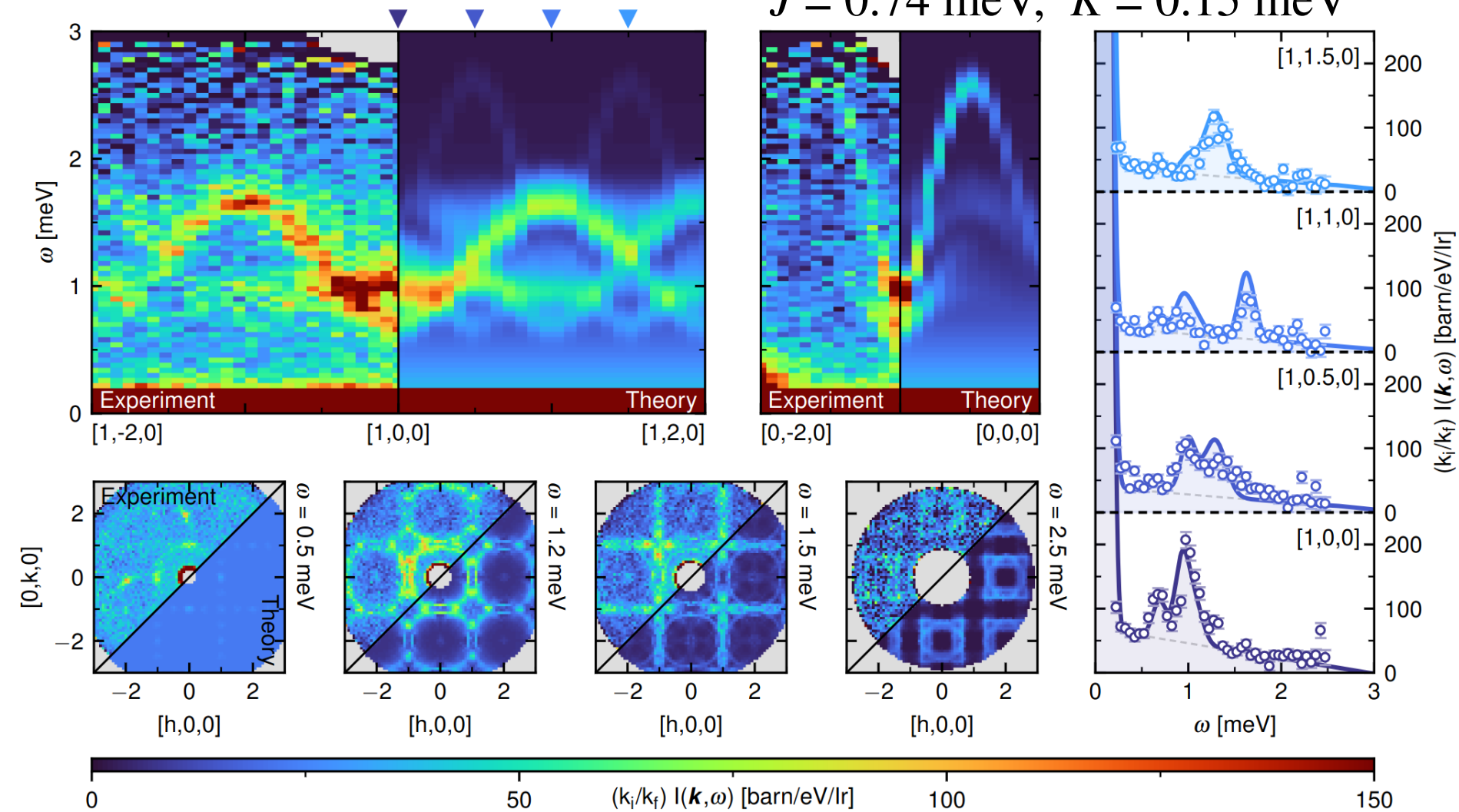
$$J = 0.74 \text{ meV}, K = 0.15 \text{ meV}$$



\*Also gives  $\Theta_{\text{CW}} \sim 27.5 \text{ K}$  and mode at  $1.22 \text{ meV}$  ( $\mathbf{q} = 0$ ) mode from ESR [Bhaskaran *et al.*, Phys. Rev. B **104**, 184404 (2021)]

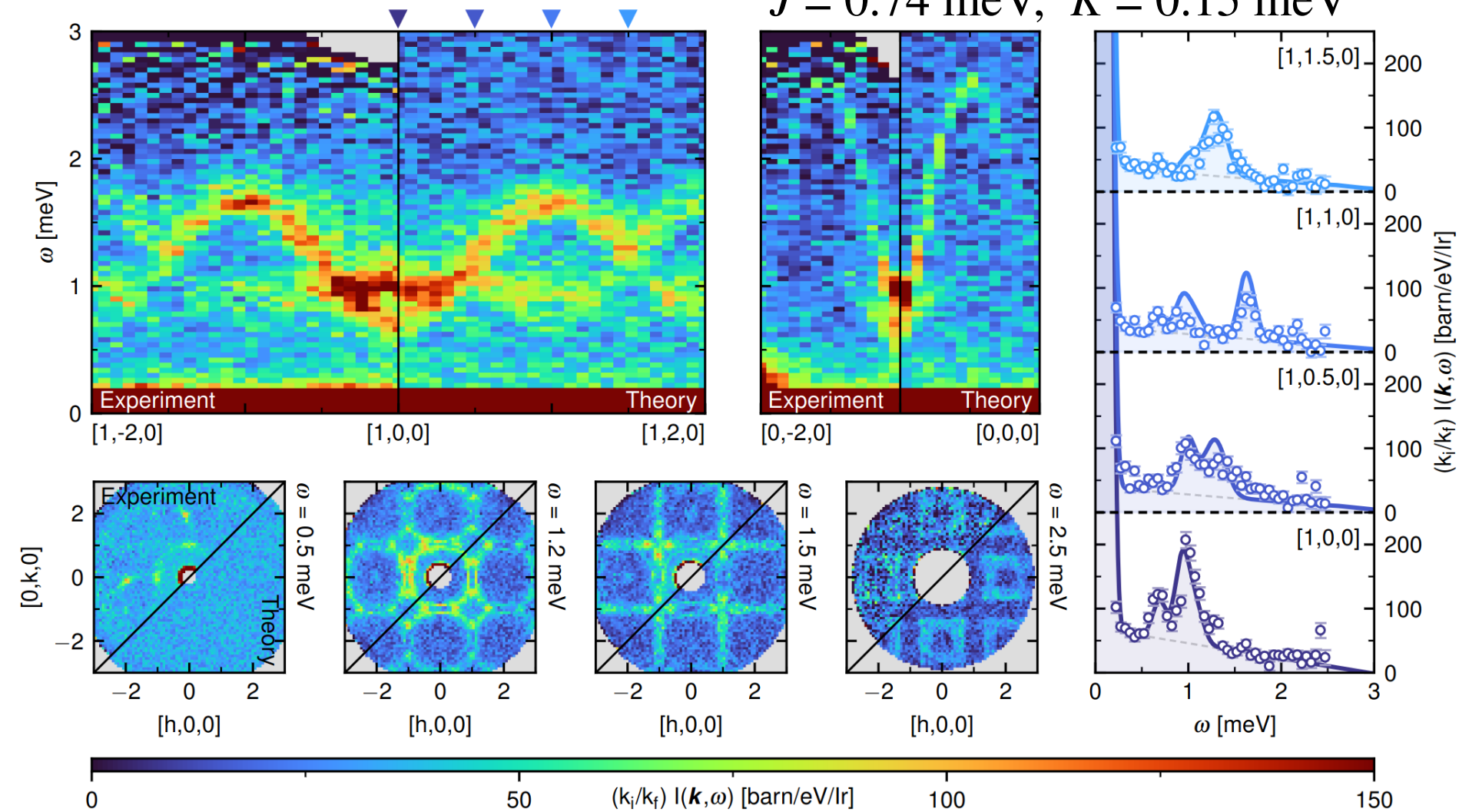
$$J = 0.74 \text{ meV}, \quad K = 0.15 \text{ meV}$$

**Including: Experimental averaging,  $\text{Ir}^{4+}$  form factor + background**



$$J = 0.74 \text{ meV}, \quad K = 0.15 \text{ meV}$$

**Including: Experimental averaging,  $\text{Ir}^{4+}$  form factor + background + noise**



# Conclusion

- ◆ Spin-wave theory can describe the excitations of ordered states of quantum magnets
- ◆ Often linear spin-waves work surprising well even at  $S = 1/2$

## **... but magnon-magnon interactions can often be important**

- (More) quantitative comparison to small  $S$  limit (& experiment)
- Magnons are not always sharp; spontaneous decay can imbue them a finite lifetime
- Other features also *require* interactions to describe at any level: pseudo-Goldstone modes, transport, ...

# Self-consistent mean-field theory

- ◆ Corrections are *static* (no frequency dependence)
- ◆ Can be thought of as modifications of linear spin wave dispersion

$$\delta A_k = \frac{1}{N} \sum_q \left[ V_{k,q,0} \langle a_q^\dagger a_q \rangle + \frac{1}{2} \left( D_{q,-q,k} \langle a_q^\dagger a_{-q}^\dagger \rangle + \text{c.c.} \right) \right]$$

$$\delta B_k = \frac{1}{N} \sum_q \left[ D_{k,-k,q} \langle a_q^\dagger a_q \rangle + \frac{1}{2} V_{q,-q,k-q} \langle a_q a_{-q} \rangle \right]$$

- ◆ *Alternatively*: from a Hartree-Fock like “decoupling” of the four-boson interactions into all hopping and pairing channels

# Self-consistent mean-field theory

- ◆ Add and subtract corrections to quadratic part

$$\delta H_2 = \sum_k \left[ \delta A_k a_k^\dagger a_k + \frac{1}{2!} \left( \delta B_k a_k^\dagger a_{-k}^\dagger + \text{h.c.} \right) \right]$$

- ◆ Treat added part with LSWT and subtracted part perturbatively

$$H_2 + H_4 = (H_2 + \delta H_2) + (H_4 - \delta H_2)$$

*Modifies LSWT energies,  
eigenvectors*

*Perturbative contribution  
depends on  $\delta A_k, \delta B_k$*

# Self-consistent mean-field theory

- ◆ Choose the correction terms so that they cancel the interaction corrections

$$\begin{array}{l}
 \text{Static} \\
 \text{correction} \\
 \text{from } H_4
 \end{array}
 \begin{array}{l}
 \Sigma_s^{-+}(k) - \delta A_k = 0, \\
 \Sigma_s^{--}(k) - \delta B_k = 0.
 \end{array}
 \begin{array}{l}
 \text{Depends on} \\
 \text{value of } \delta A_k, \delta B_k
 \end{array}$$

- ◆ Practically: Self-consistent iteration for the correction terms

$$\begin{aligned}
 \delta A_k^{(n+1)} &= \Sigma_s^{-+}(k) \big|_{\delta A^{(n)}, \delta B^{(n)}} \\
 \delta B_k^{(n+1)} &= \Sigma_s^{--}(k) \big|_{\delta A^{(n)}, \delta B^{(n)}}
 \end{aligned}$$

*Iterate until maximum error falls below threshold  $\varepsilon$*