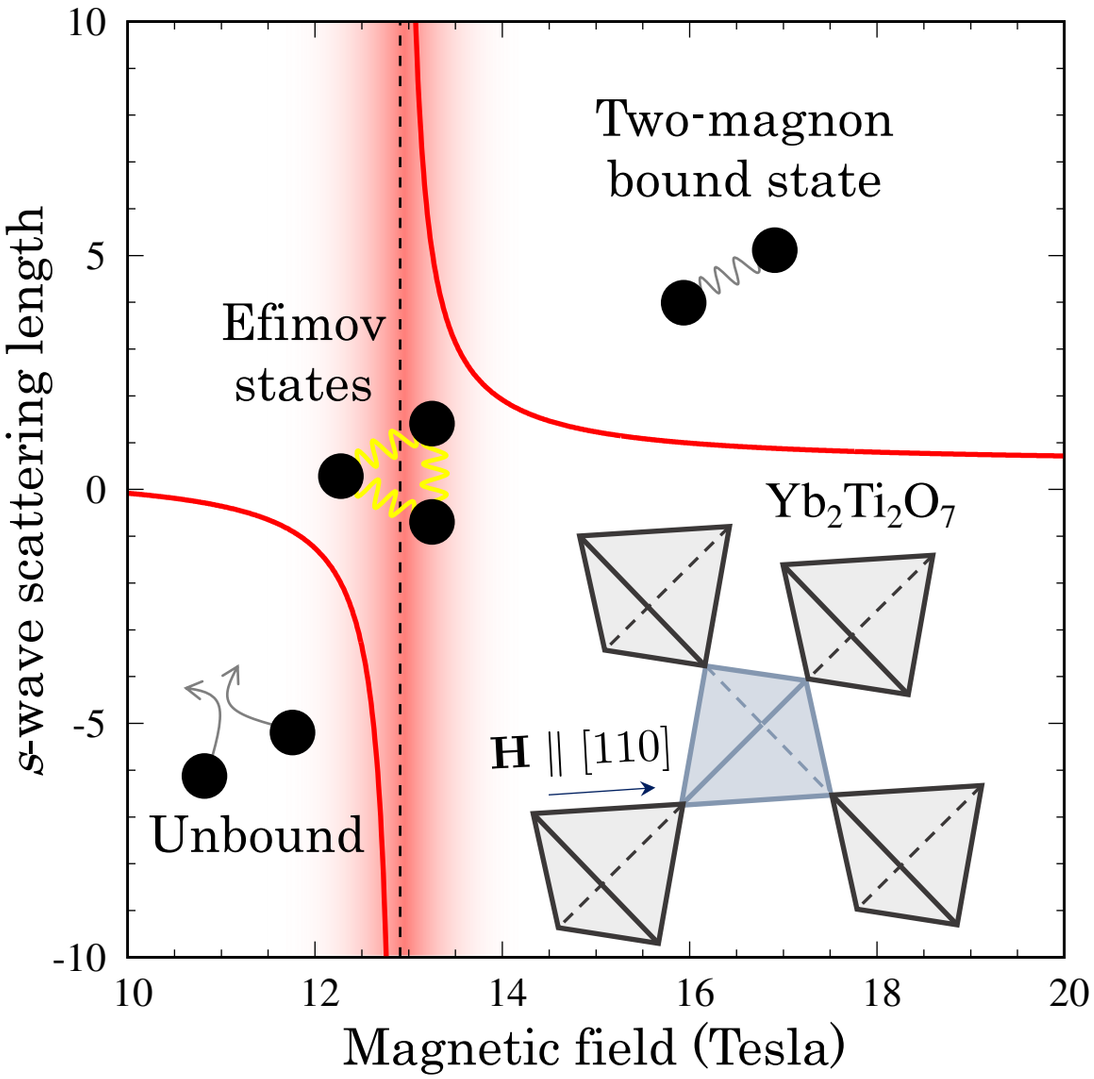
Magnetic-field-induced tunability of magnon bound states: Scattering resonances and Efimov states in $Yb_2Ti_2O_7$

Key takeaways:

- The scattering length between magnons is tunable by a uniform magnetic field. (Counterpart of Feshbach resonance in ultracold atomic gases)
- Efimov bound states are expected in the vicinity of the unitarity limit.



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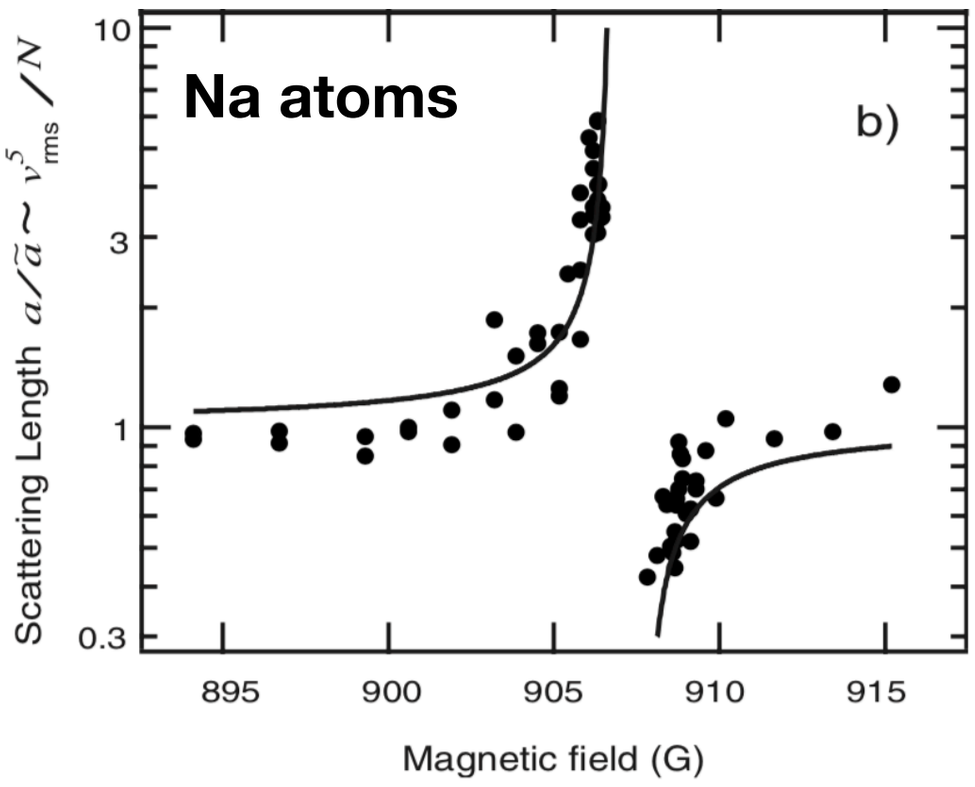
Publication: Phys. Rev. Research **2**, 033024 (2020).

2021/03/25

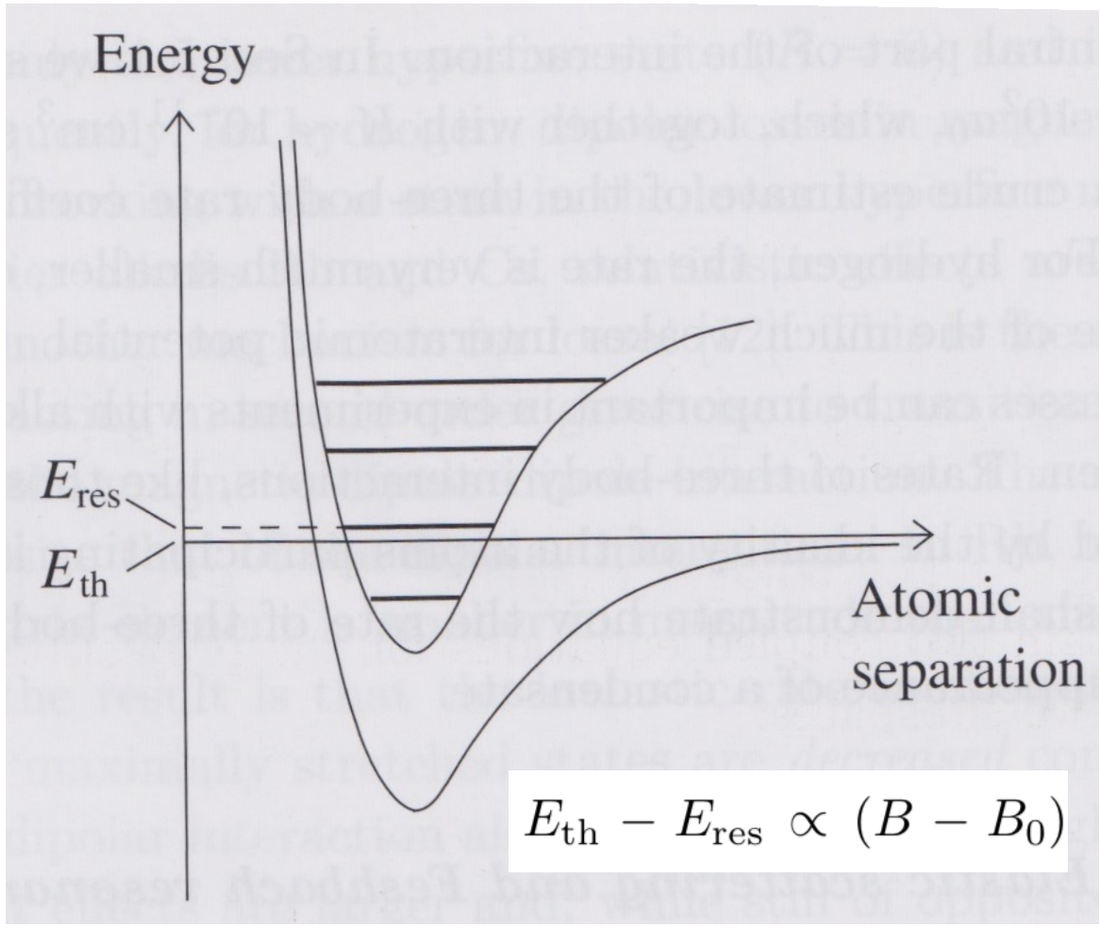
Feshbach resonance in ultracold atomic gases

Bound ↔ Unbound



S. Inouye *et al*., PRL (2004)

Review article: C. Chin *et al*., RMP 2010.



C. J. Pethick & H. Smith, ”Bose-Einstein Condensation in Dilute Gases (2nd Ed)”, Cambridge Univ. Press (2008).

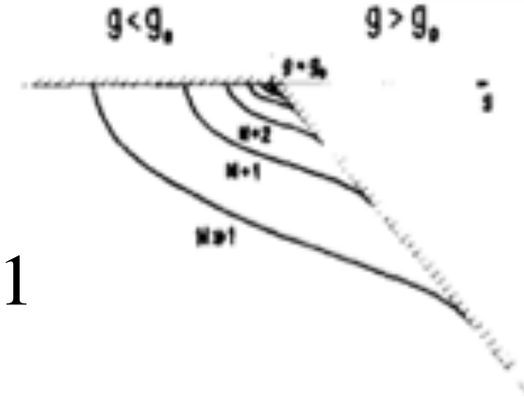
The *s*-wave scattering length a can be varied by applying a uniform magnetic field.
→ Efimov bound states are found in ultracold atomic gases [T. Kraemer et al., Nature (2006)]**.**

Efimov effect

Volume 33B, number 8 PHYSICS LETTERS 21 December 1970

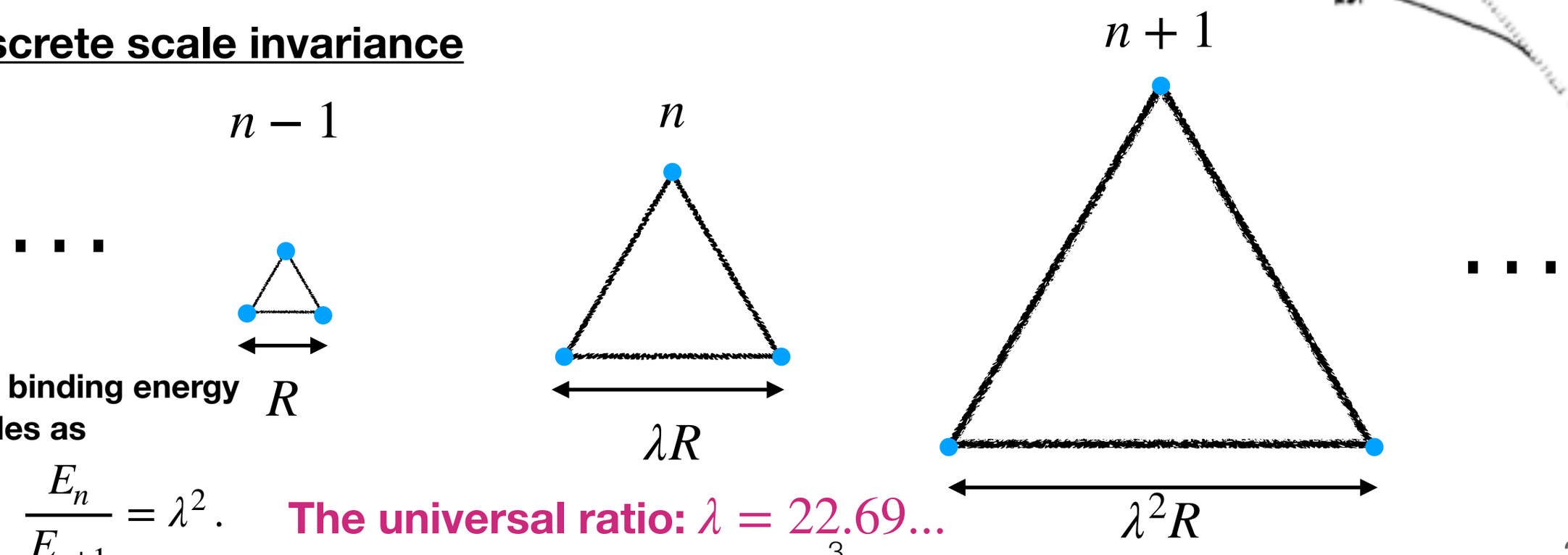
ENERGY LEVELS ARISING FROM RESONANT TWO-BODY FORCES IN A THREE-BODY SYSTEM

V. EFIMOV



When two bosons interact with $a = \pm\infty$, three bosons form an infinite tower of three-body bound states in 3D.

Discrete scale invariance



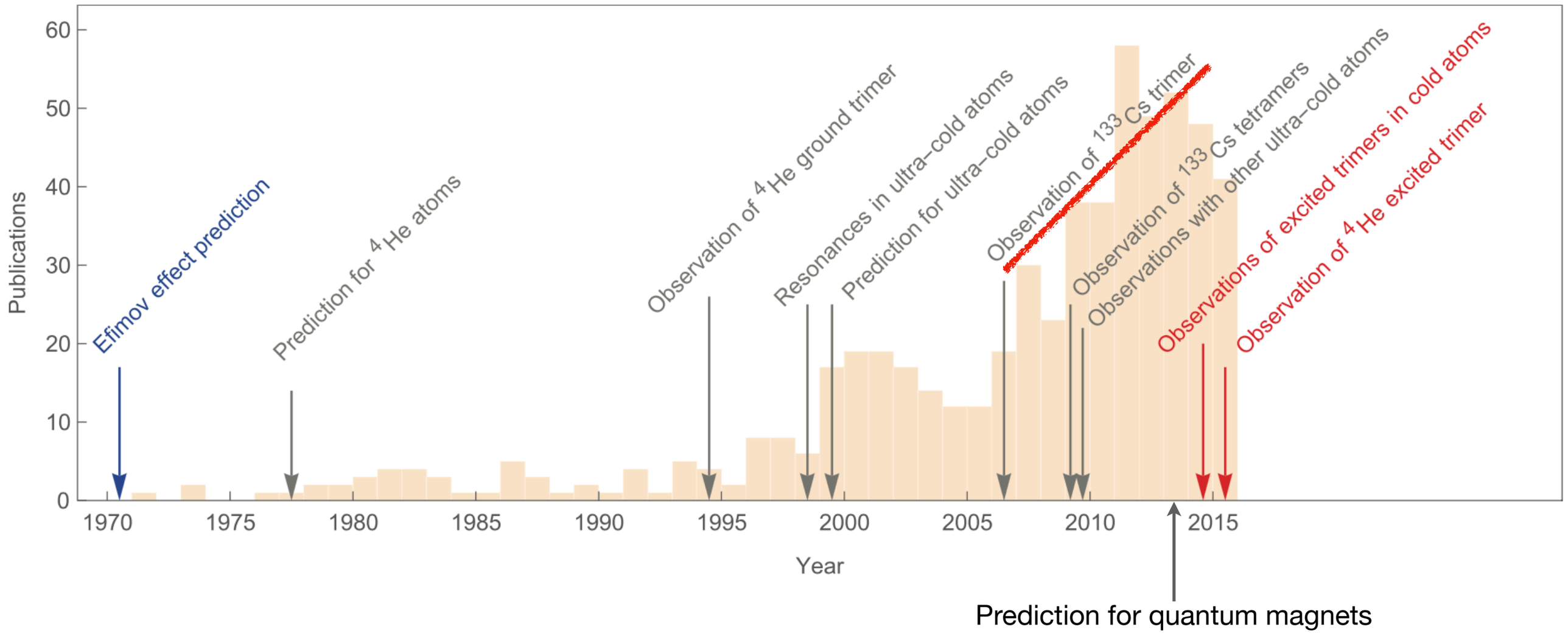
The binding energy scales as

$$\frac{E_n}{E_{n+1}} = \lambda^2 .$$

The universal ratio: $\lambda = 22.69...$

Efimov effect

P. Naidon & S. Endo, *Rep. Prog. Phys.* **80** 056001 (2017)



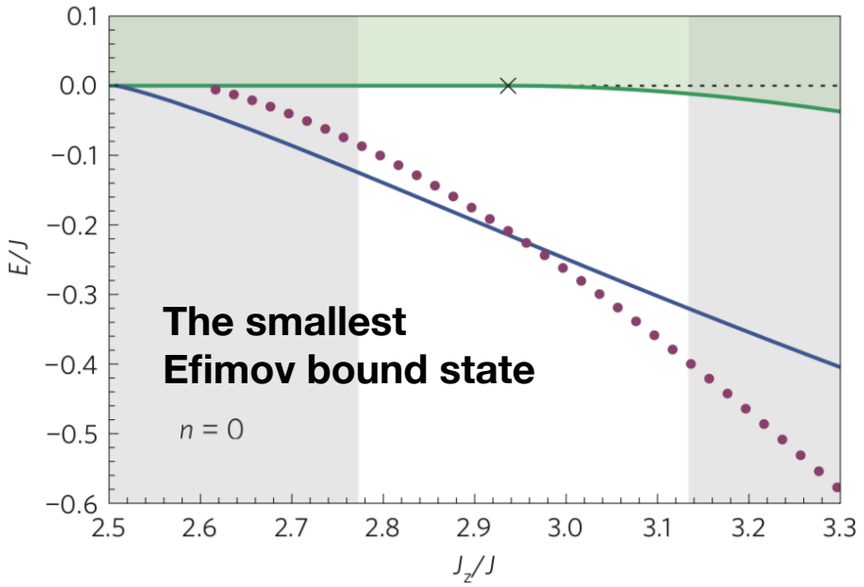
Efimov states have been observed in very limited systems due to the requirement of proximity to a scattering resonance.

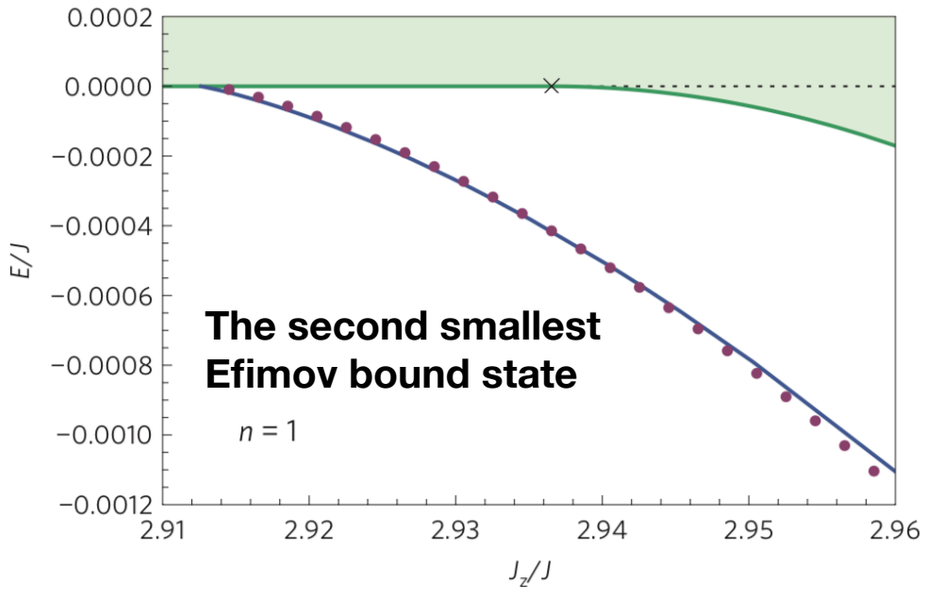
Efimov effect in magnets were predicted but has not been observed yet.

Efimov effect in quantum magnets

Y. Nishida, Y.K. & C.D. Batista, Nat. Phys. 9, 93 (2013).

$S = 1/2$ and $S = 1$ XXZ model and $S = 1$ Heisenberg model with uniaxial anisotropy on a simple cubic lattice





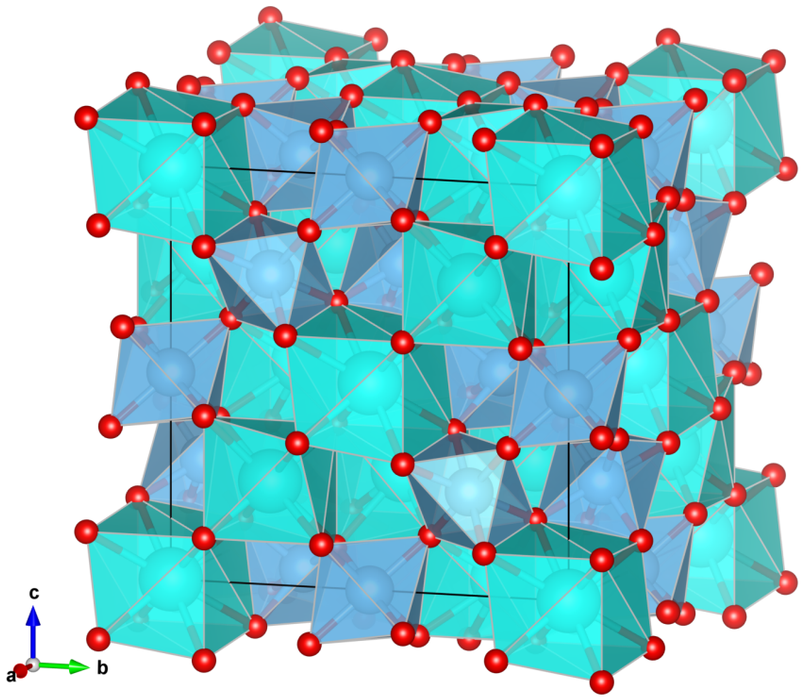
Two lowest binding energies of three magnons for $S = 1/2$ near the two-magnon resonance.

Table 1 | Few lowest binding energies of three magnons right at the two-magnon resonances.

S	J_z/J	D/J	n	E_n/J	$\sqrt{E_{n-1}/E_n}$
1/2	2.93654	—	0	-2.09×10^{-1}	—
			1	-4.15×10^{-4}	22.4
			2	-8.08×10^{-7}	22.7
1	4.87307	0	0	-5.16×10^{-1}	—
			1	-1.02×10^{-3}	22.4
			2	-2.00×10^{-6}	22.7
1	+1	4.76874	0	-5.50×10^{-2}	—
			1	-1.16×10^{-4}	21.8
1	−1	5.12703	0	-4.36×10^{-3}	—
			1	-8.88×10^{-6}	22.2
—	—	—	∞	—	22.6944

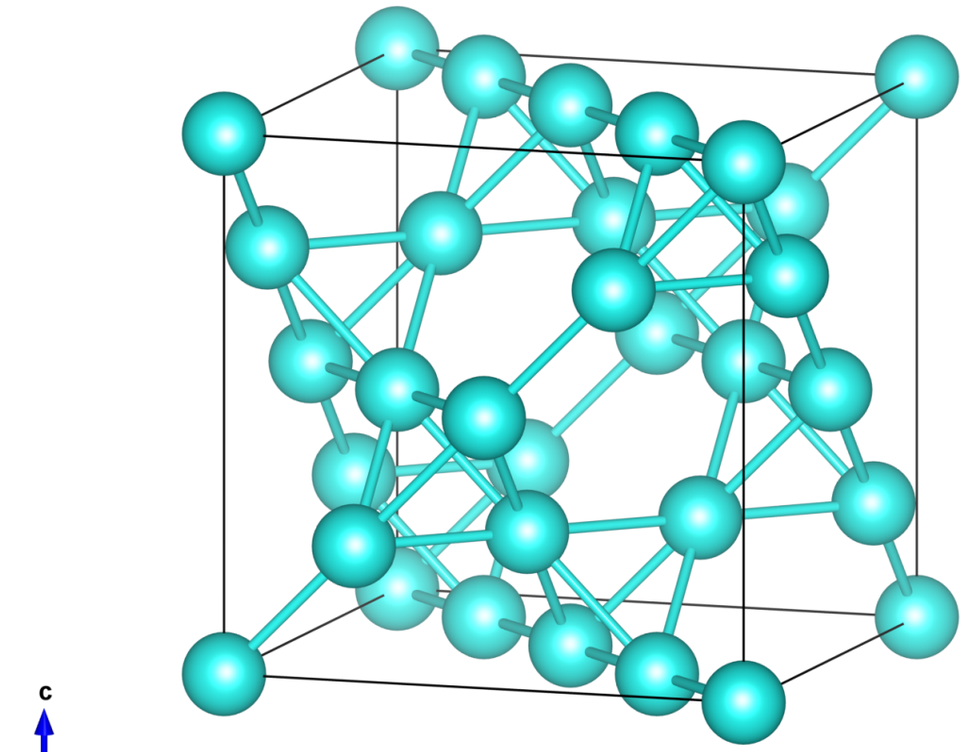
Universal ratio $\lambda \sim 22.7$ is confirmed.
Efimov effect in quantum magnets is predicted.

Candidate material: $Yb_2Ti_2O_7$



H. Blöte et al., Physica **43**, 549 (1969)
A.V. Shlyakhtina *et al*., Solid State Ionics **179**, 1004 (2008)

Yb^{3+} ions form a pyrochlore lattice.



Yb^{3+}: $4f^{13}$ (J = 7/2)
Spin orbit coupling & crystalline electric field
→ GS Kramers doublet:= spin-1/2

Detailed analysis: J. Gaudet *et al*., PRB **92**, 134420 (2015)

Focused material $Yb_2Ti_2O_7$

- **ferromagnetically ordered at 270 mK**
- **competition between ferromagnetism and antiferromagnetism**
- **magnetic ground state remains a matter of debate at zero field**

Model and methods

Model

◉ Spin Hamiltonian (four-sublattice)

↓ exact mapping

◉ Hard-core boson model

↓ perturbation theory

◉ Effective boson model (two-sublattice)
(★ number conserved)

spin-1/2 degree of freedom on Yb^{3+}

$$\mathcal{H}_{\rm spin} = \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \left[J_{zz} \mathsf{S}^z_{\mathbf{r}} \mathsf{S}^z_{\mathbf{r}'} - J_{\pm} \left(\mathsf{S}^+_{\mathbf{r}} \mathsf{S}^-_{\mathbf{r}'} + \text{h.c.} \right) \right.$$
$$+ J_{\pm\pm} \left(\gamma_{\alpha_{\mathbf{r}} \alpha_{\mathbf{r}'}} \mathsf{S}^+_{\mathbf{r}} \mathsf{S}^+_{\mathbf{r}'} + \text{h.c.} \right)$$
$$\left. + J_{z\pm} \left\{ \mathsf{S}^z_{\mathbf{r}} \left(\zeta_{\alpha_{\mathbf{r}} \alpha_{\mathbf{r}'}} \mathsf{S}^+_{\mathbf{r}'} + \text{h.c.} \right) + (\mathbf{r} \leftrightarrow \mathbf{r}') \right\} \right]$$
$$- \mu_{\rm B} \mu_0 H^\mu \sum_{\mathbf{r}} g^{\mu\nu}_{\alpha_{\mathbf{r}}} \mathsf{S}^\nu_{\mathbf{r}} . \qquad \mathbf{H} \parallel [110]$$

Methods

◉ Exact diagonalization

◉ Lippmann-Schwinger equation

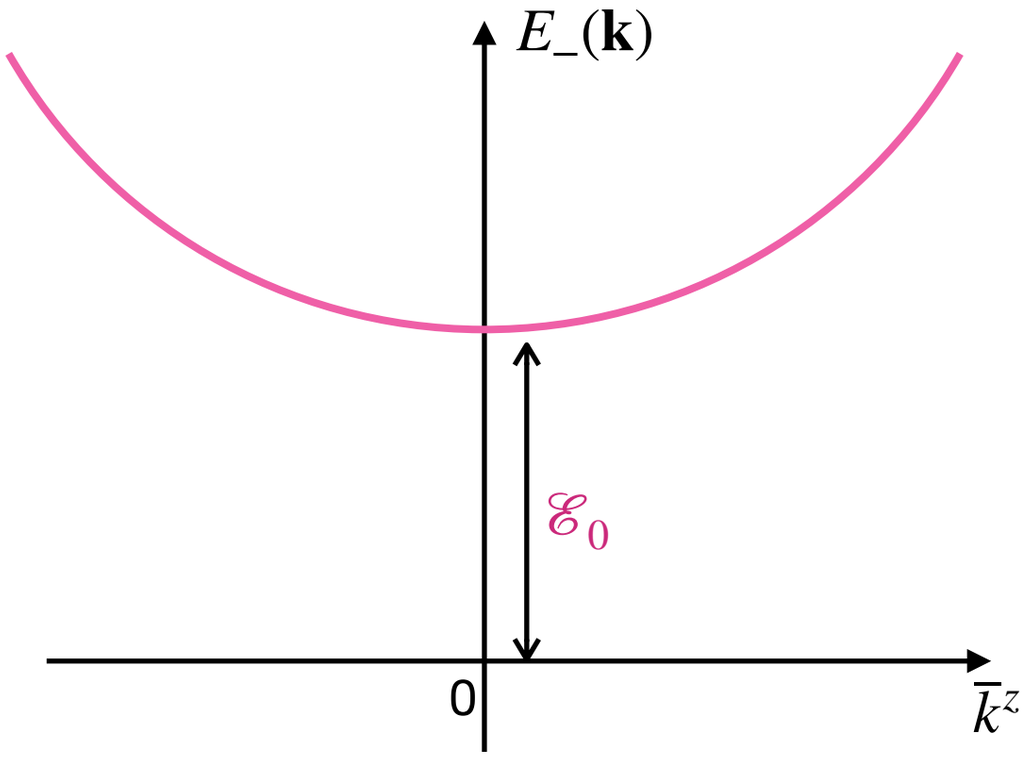
Parameter sets determined by the inelastic neutron scattering experiment [e.g., J.D. Thompson *et al*., PRL 2017].

$$J_{zz} = 0.026(3)\ \text{meV}, \quad J_{\pm\pm} = 0.048(2)\ \text{meV},$$
$$J_{\pm} = 0.074(2)\ \text{meV}, \quad J_{z\pm} = -0.159(2)\ \text{meV},$$
$$g_{\parallel} = 2.14(3), \qquad g_{\perp} = 4.17(2)\,.$$

Results

- Single-magnon spectrum
- Two-magnon resonance
- Three-magnon Efimov states

Single-magnon spectrum



Lower branch of the dispersion:

$$E_-(\mathbf{k}) \simeq \mathscr{E}_0 + \frac{\overline{\mathbf{k}}^2}{2m_z} \quad \left(|\overline{\mathbf{k}}| \ll 1\right)$$

$\overline{\mathbf{k}}$: Normalized wave vector

$$\begin{cases} m_z^{-1} = 0.0399 \text{ meV} \\ m_x^{-1} = 0.0425 \text{ meV} \end{cases} \text{ at } \mu_0 H = 12.91 \text{ T}$$

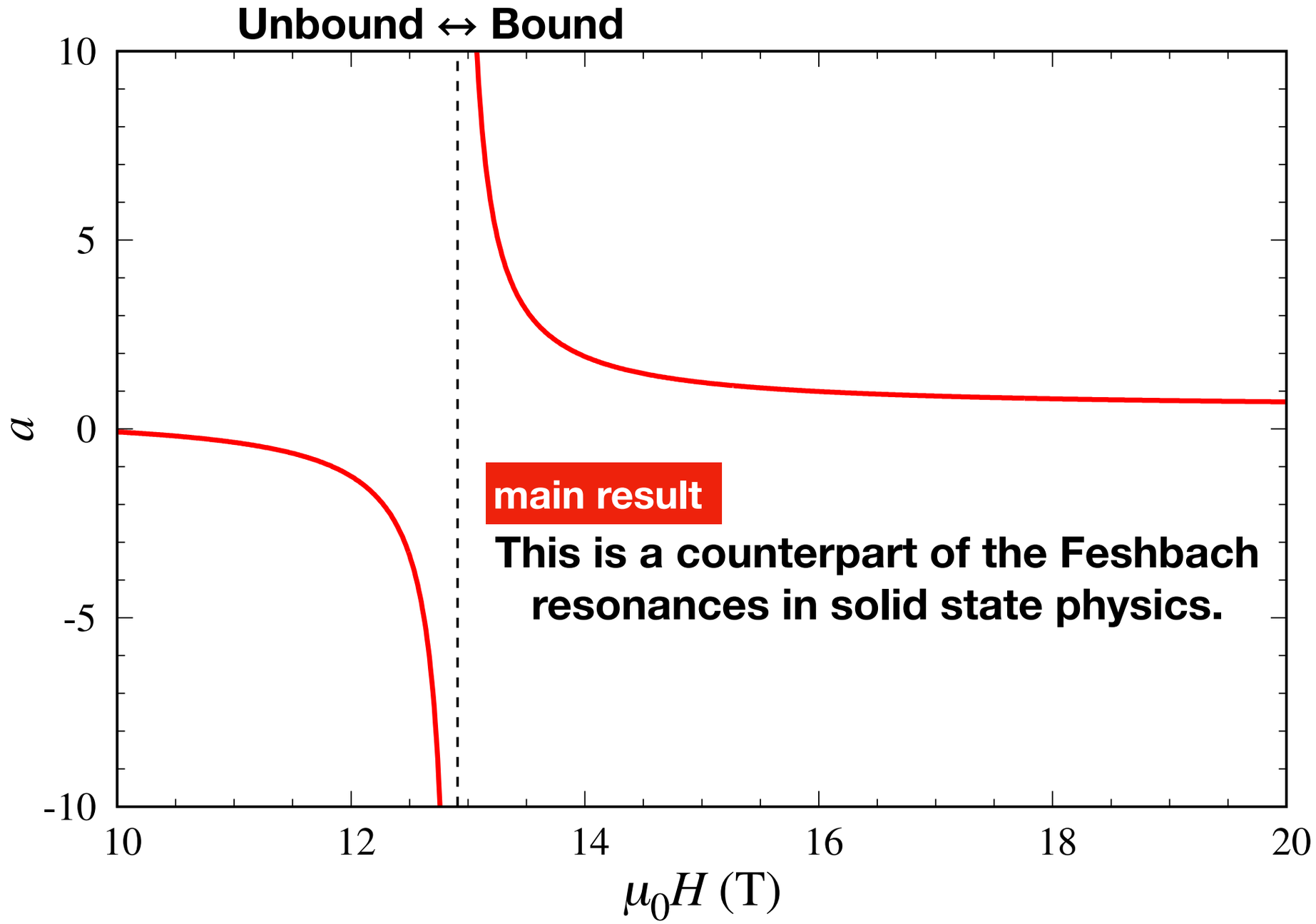
(almost isotropic)

m_z: mass for $\mathbf{k} \parallel [110]$

m_x: mass for $\mathbf{k} \perp [110]$

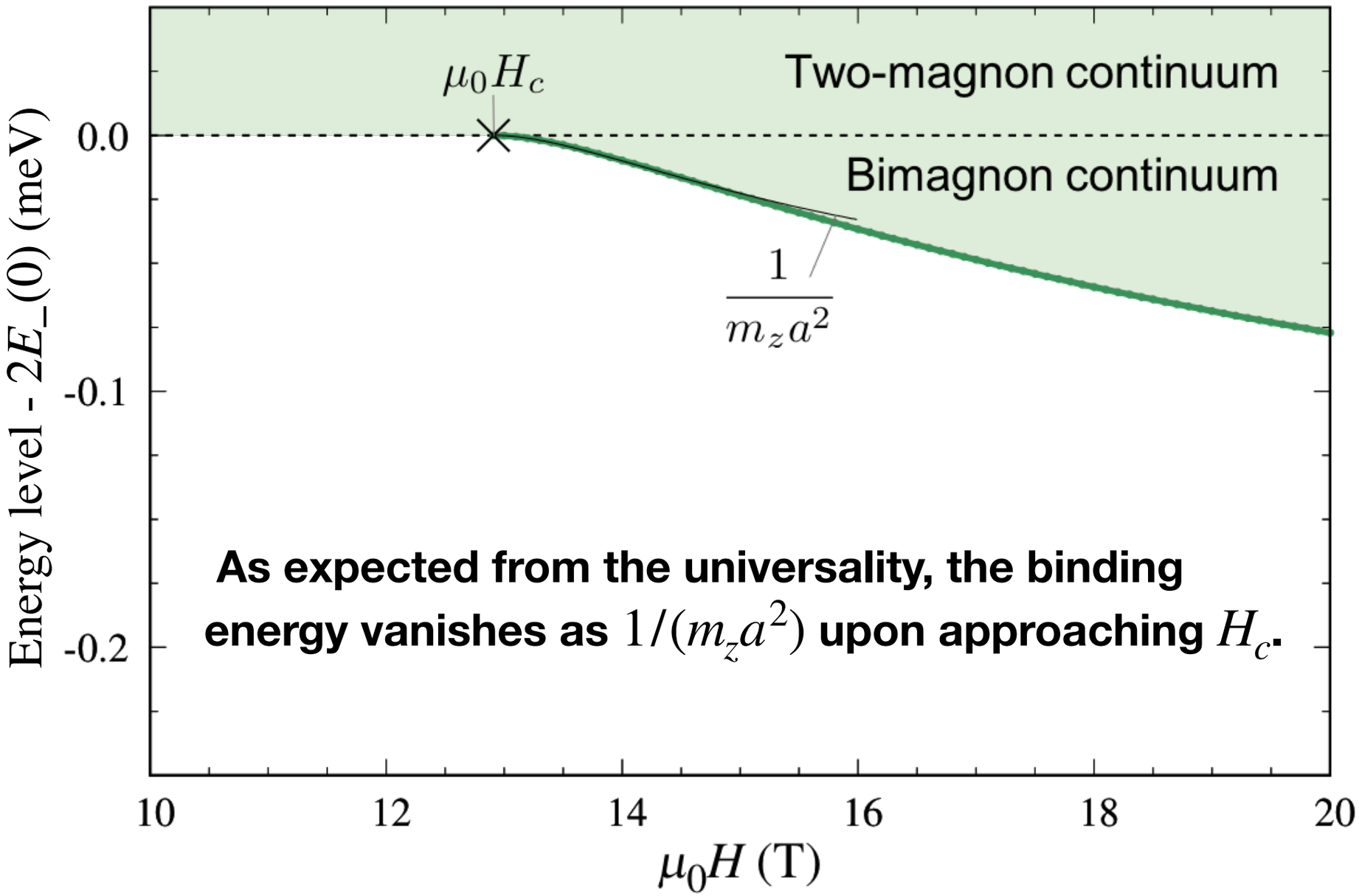
The low-energy physics of $Yb_2Ti_2O_7$ is described by bosons in continuous space with the anisotropic mass tensor.

Two-magnon resonance



The s-wave scattering length is expected to be diverge at $\mu_0 H_c = 12.91$ T.

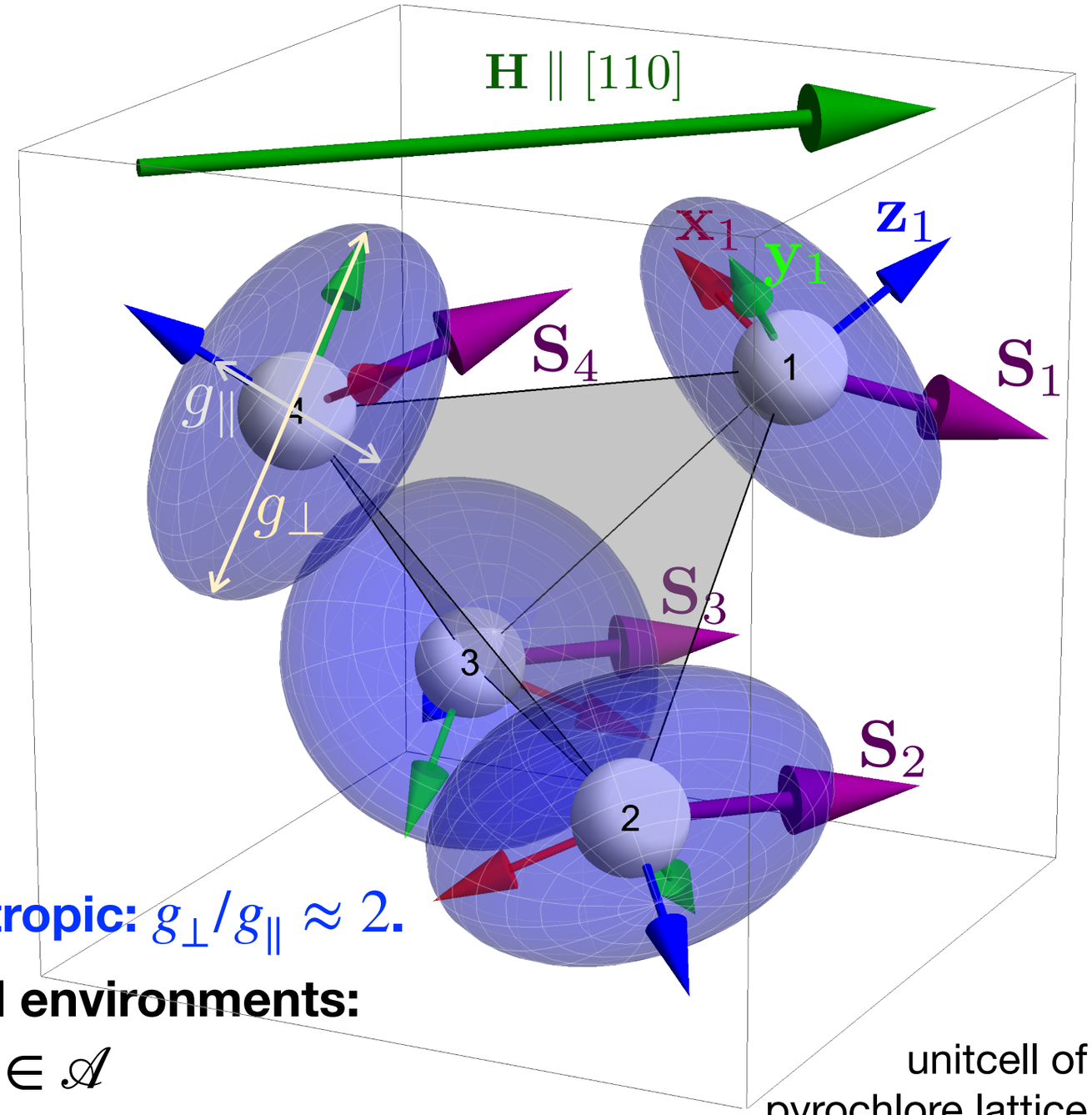
Two-magnon resonance

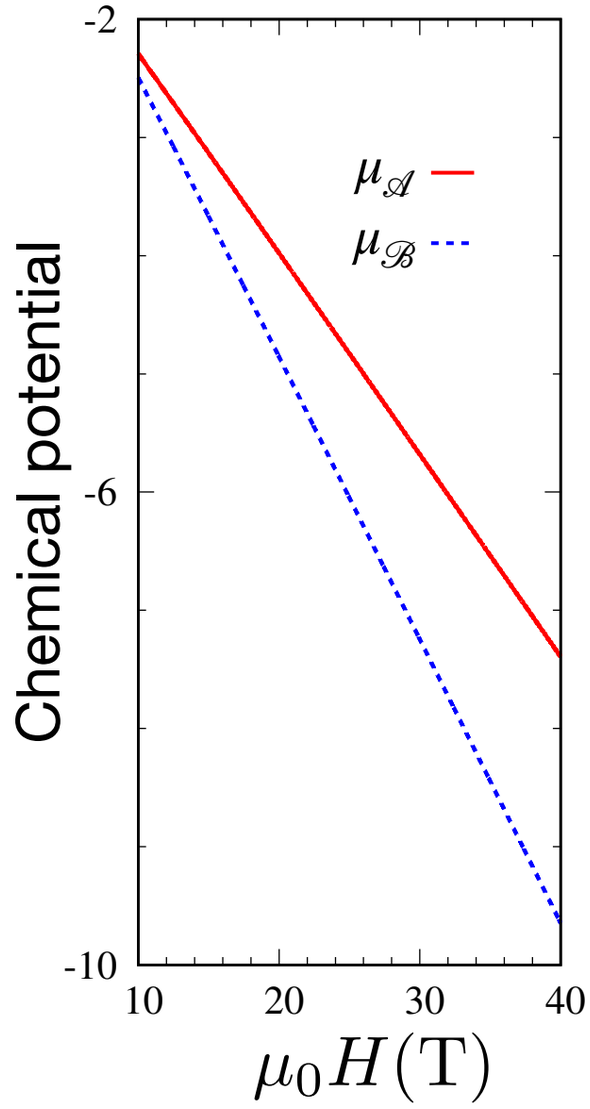


As expected from the universality, the binding energy vanishes as $1/(m_z a^2)$ upon approaching H_c.

Mechanism (1/3)

Spin orientation in large $\mathbf{H} \parallel [110]$ limit





unitcell of
pyrochlore lattice

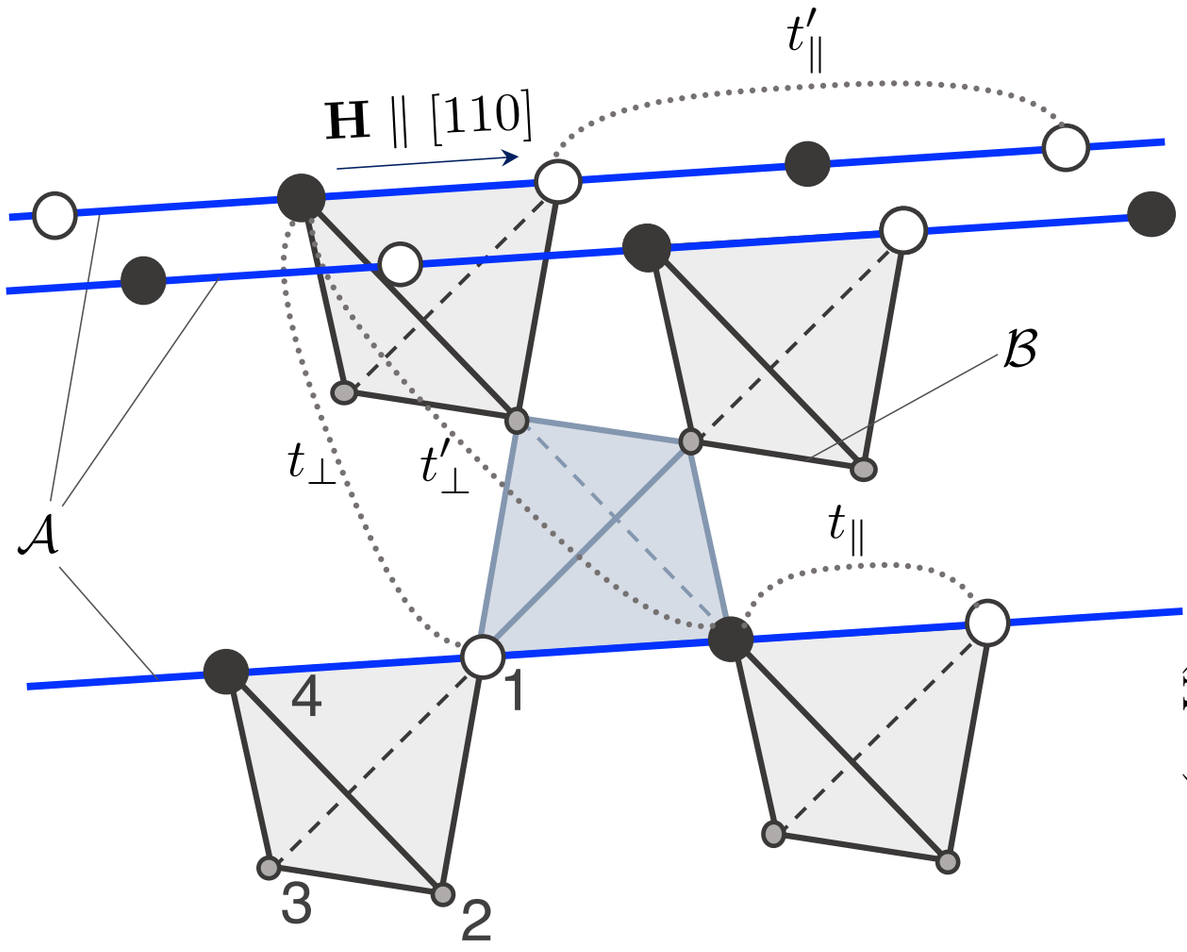
g-tenser is anisotropic: $g_\perp / g_\parallel \approx 2$.

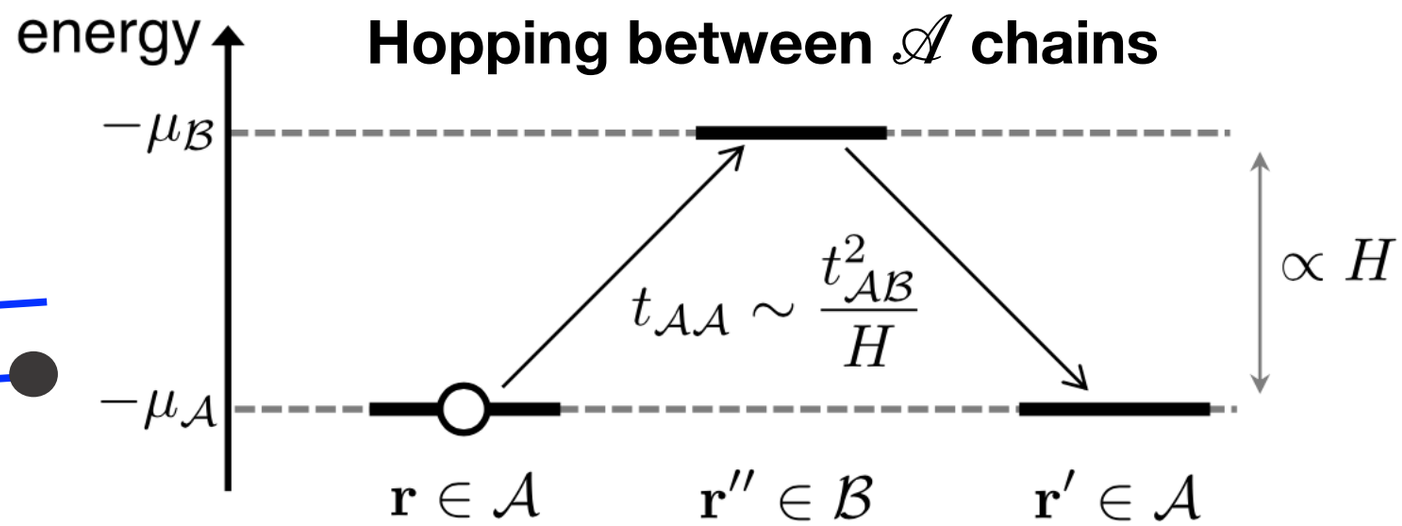
Two different local environments:

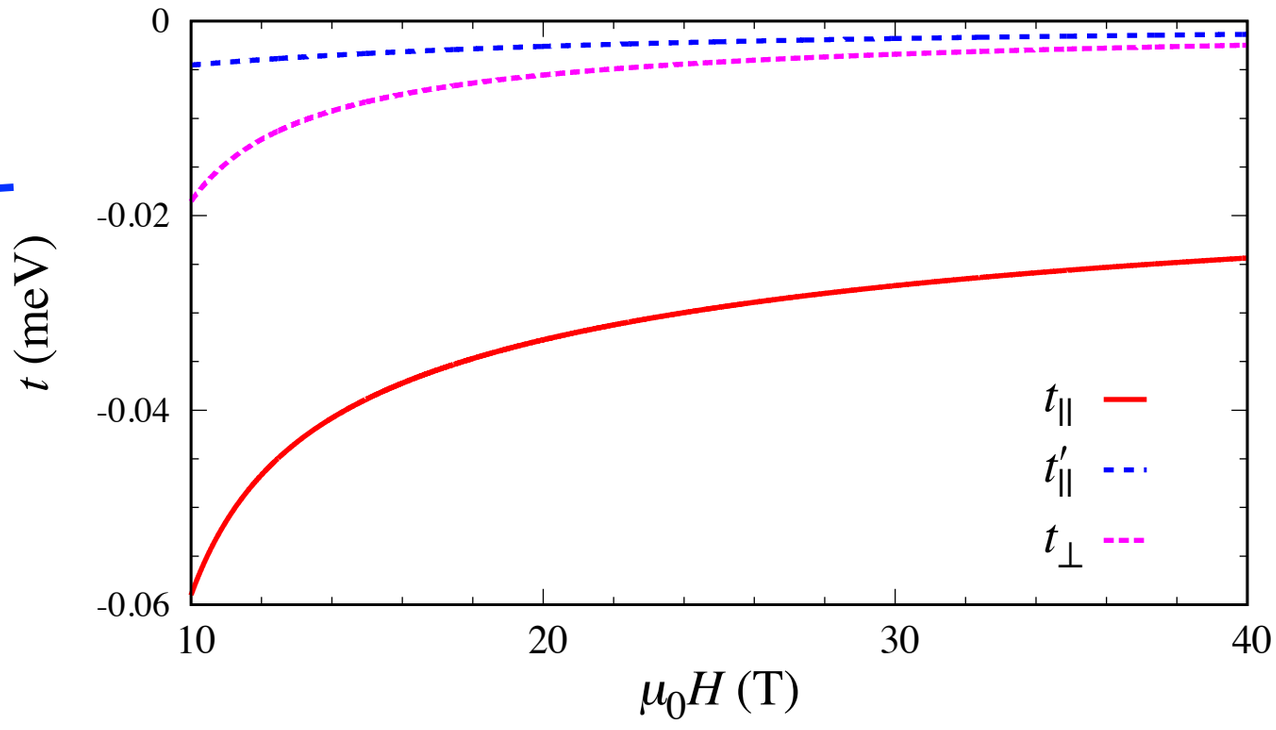
sublattice 1 and 4 $\in \mathscr{A}$

sublattice 2 and 3 $\in \mathscr{B}$

Mechanism (2/3)



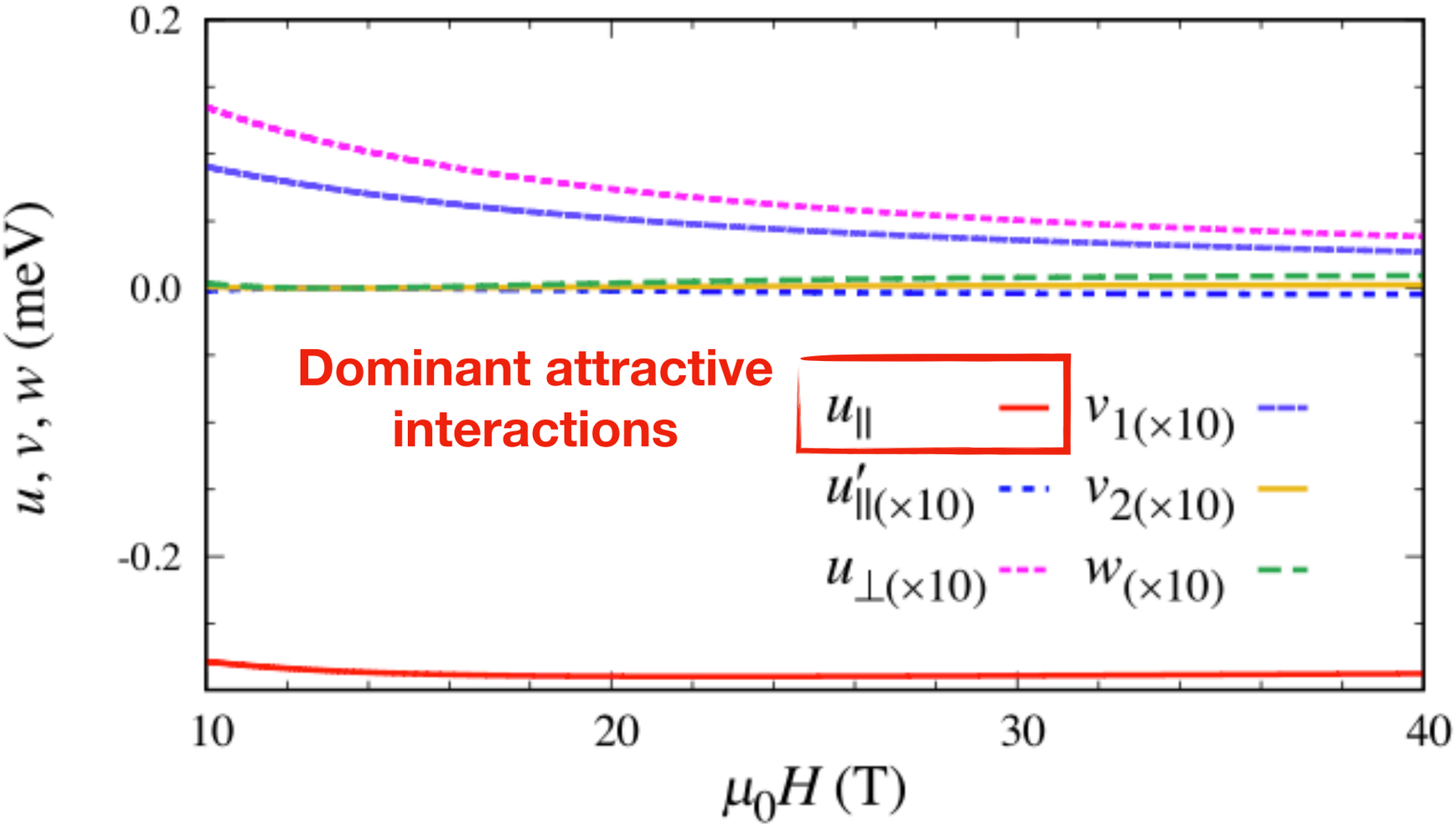


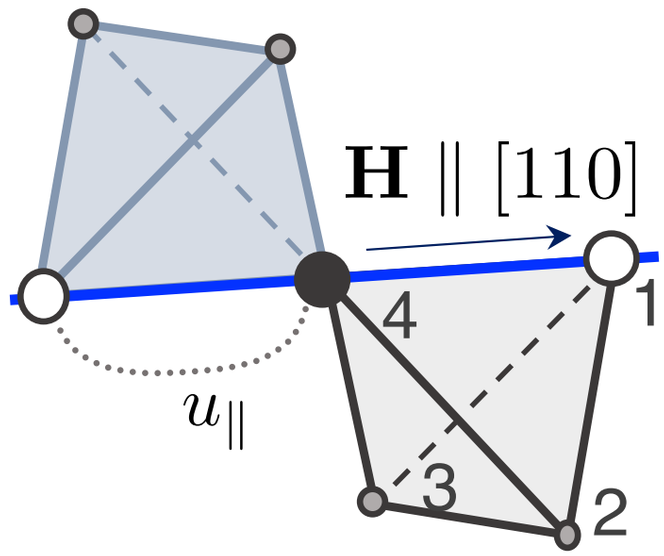


A part of kinetic energy is suppressed by an external magnetic field.

Mechanism (3/3)

Attractive interaction is insensitive to the external magnetic field.





Dominant attractive interaction in large $\mathbf{H} \parallel [110]$ limit:

$$u_{\parallel} \approx \frac{2}{2g_{\parallel}^2 + g_{\perp}^2}\left[2\sqrt{2}g_{\parallel}g_{\perp}J_{z\pm} + g_{\perp}^2(J_{\pm} - J_{\pm\pm}) - g_{\parallel}^2 J_{zz}\right]$$

The main factor of the large $u_{\parallel}$ is due to the large $-J_{z\pm}$.

$J_{zz} = 0.026(3)$ meV, $J_{\pm\pm} = 0.048(2)$ meV,
$J_{\pm} = 0.074(2)$ meV, $J_{z\pm} = -0.159(2)$ meV,
$g_{\parallel} = 2.14(3)$, $g_{\perp} = 4.17(2)$.
J.D. Thompson *et al.*, PRL 2017

Two-magnon resonance

- Other parameter sets for $Yb_2Ti_2O_7$

Parameter set	J_1(meV)	J_2 (meV)	J_3 (meV)	J_4 (meV)	J_{zz} (meV)	$J_{\pm}$ (meV)	$J_{z\pm}$ (meV)	$J_{\pm\pm}$ (meV)	g_{xy}	g_z
Ross (10)	-0.09	-0.22	-0.29	+0.01	0.17	0.05	-0.14	0.05	4.32	1.8
Thompson (3)	-0.028	-0.326	-0.272	+0.049	0.026	0.074	-0.159	0.048	4.17	2.14
Robert (11)	-0.03	-0.32	-0.28	+0.02	0.07	0.085	-0.15	0.04	?	?
This study	-0.026(2)	-0.307(3)	-0.323(3)	+0.028(2)	0.094	0.087	-0.161	0.0611	4.17	2.14

Table S4. Spin Hamiltonian parameter sets used in the paper in two notations for $Yb_2Ti_2O_7$. The reported parameters from one notation were directly converted to the other notation (without accounting for error bars) unless already provided in the reference.

from A. Scheie *et al.*, PNAS **117,** 27245 (2020)

Ross *et al.*→ $\mu_0 H_c = 9.09$ (T)

Joubert et al., & Bowman *et al.*→ $\mu_0 H_c = 8.80$ (T)

Thompson *et al.*→ $\mu_0 H_c = 12.91$ (T)

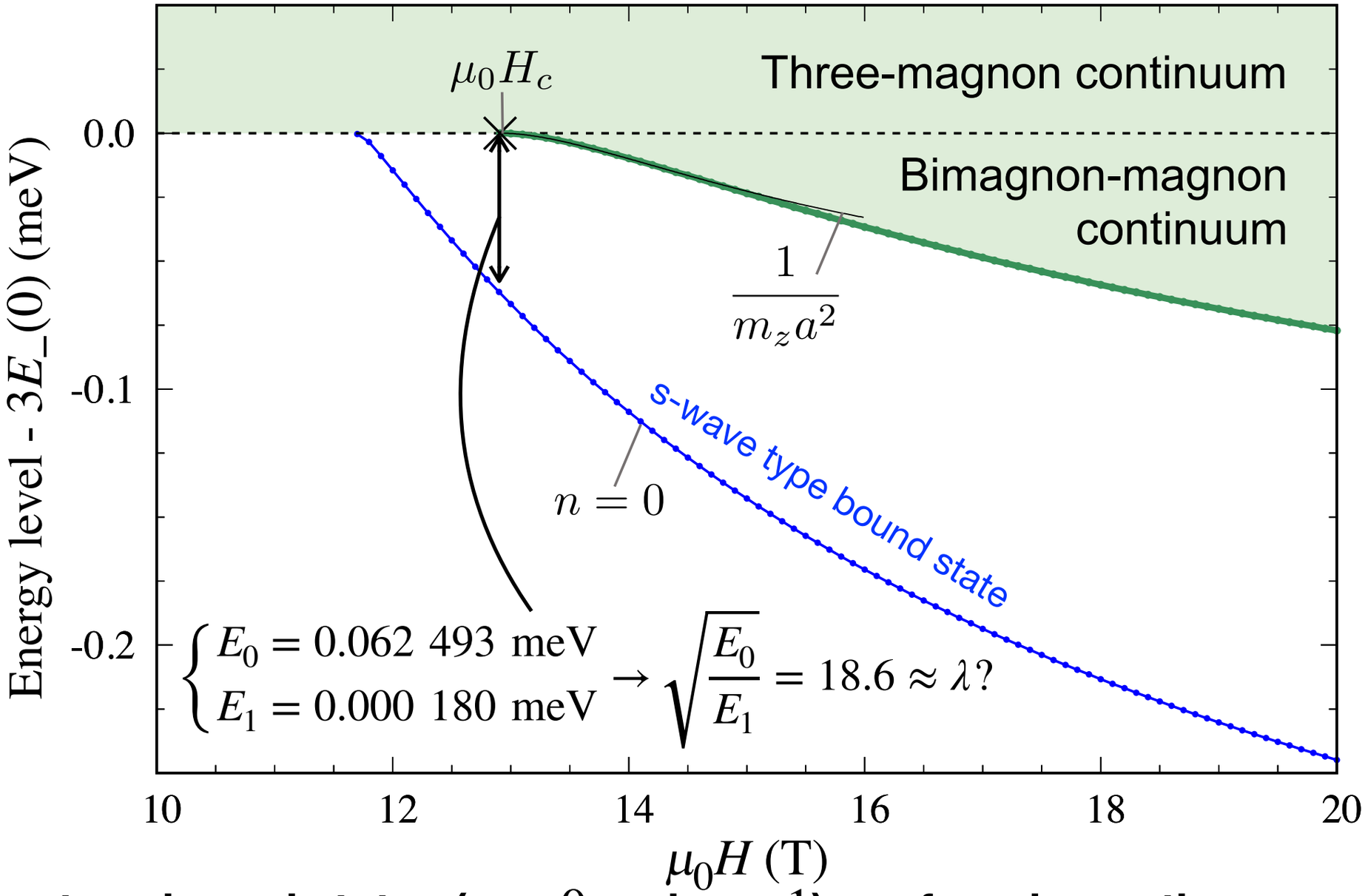
Robert *et al.*→ $\mu_0 H_c = 11.81$ (T)

Scheie *et al.*→ $\mu_0 H_c = 11.48$ (T)

- $Yb_2Ge_2O_7$ [C.L. Sarkis *et al.*, Phys. Rev. B **102**, 134418 (2020)] → $\mu_0 H_c = 14.80$ (T)

The two-magnon resonance is expected to be realized at experimentally reachable magnetic field.

Three-magnon Efimov states



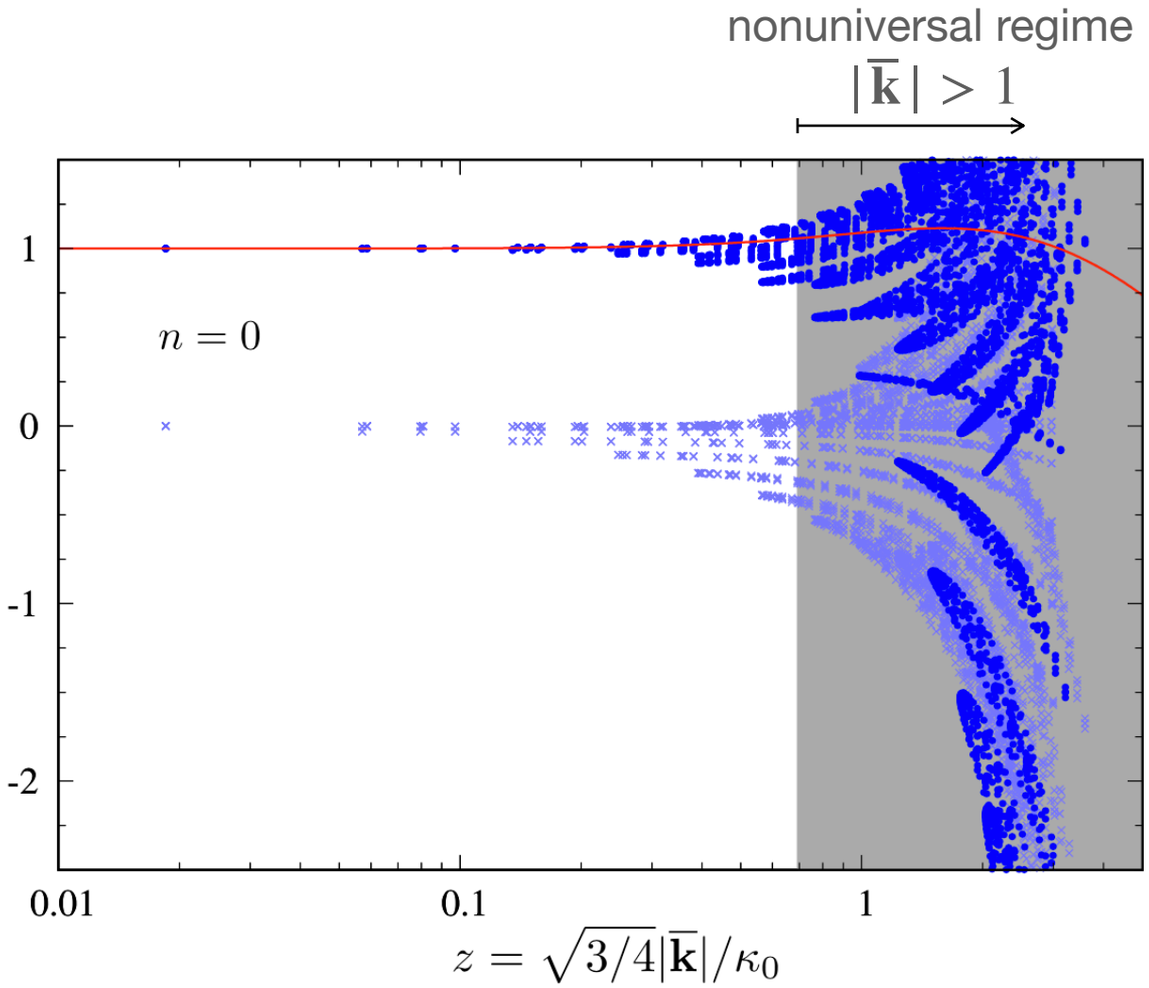
The s-wave type bound states ($n = 0$ and $n = 1$) are found near the resonance.

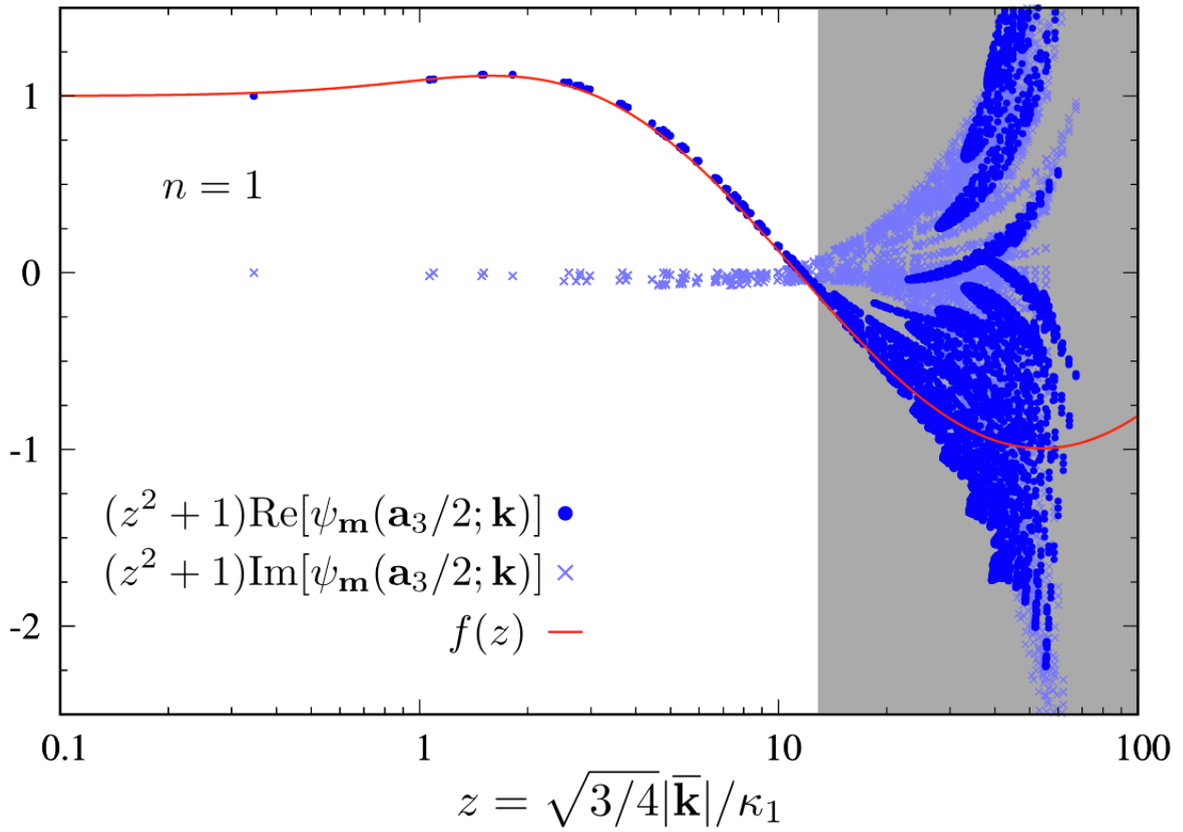
Analysis of the wave functions

Three-magnon Efimov states

Comparison with the universal function $f(z)$ at H_c

$$\kappa_n = \sqrt{m_z E_n}$$





The excellent agreement in the long wavelength region ($|\mathbf{k}| < 1$)

Although the $n = 0$ state may not, the $n = 1$state is identified as the Efimov state.

Experimental realization

- Raman scattering is the ideal technique for observing two-magnon bound states [M.F. Thorpe, PRB(1971), B.S. Shastry & B.I. Shraiman, PRL(1990)].

→ The resonance condition can be identified.

- The number non-conserved terms proportional to $na^\dagger$ exit in the hard core boson model before the approximation based on the perturbation theory.

→ Two-magnon states are mixed to the three-magnon bound states as an $\mathcal{O}(J/H)$ perturbation.

→ Three-magnon bound states could be also observed via Raman spectroscopy.

Summary

- The magnetic field acts as a knob to tune the *s*-wave scattering length of magnons in $Yb_2Ti_2O_7$ (**counterpart of Feshbach resonance**).

- A two-magnon resonance condition is achieved at an experimentally reachable magnetic field strength of $H_c \sim 13$ T along the [110] direction.

- In our calculations, a couple of three-magnon bound states with the *s*-wave wave function were found just below the three-magnon continuum of the excitation spectrum near H_c.

- While the ground state ($n = 0$) exhibits some deviations from the universal character due to lattice effects, the first excited state ($n = 1$) is indeed an Efimov state.

Publication:

Y. Kato, S.-S. Zhang, Y. Nishida, and C.D. Batista, Phys. Rev. Research **2**, 033024 (2020).