Rethinking α-$RuCl_3$

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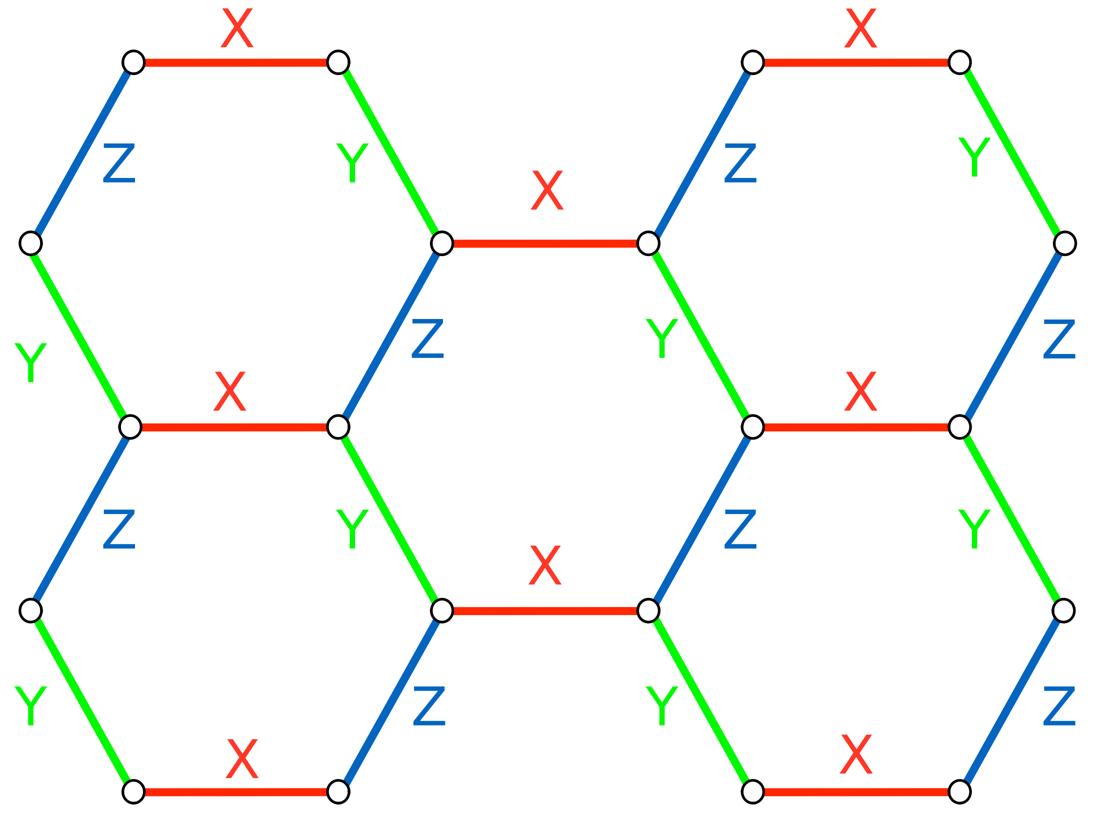
54th meeting of the PAC for Condensed Matter Physics

Honeycomb lattice Kitaev model

$$\mathcal{H} = K \sum_{\langle ij \rangle^\gamma} S_i^\gamma S_j^\gamma = K \sum_{\langle ij \rangle^\mathrm{x}} S_i^x S_j^x + K \sum_{\langle ij \rangle^\mathrm{y}} S_i^y S_j^y + K \sum_{\langle ij \rangle^\mathrm{z}} S_i^z S_j^z$$



$$S^x = ib^x c,\ \ S^y = ib^y c,\ \ S^z = ib^z c$$

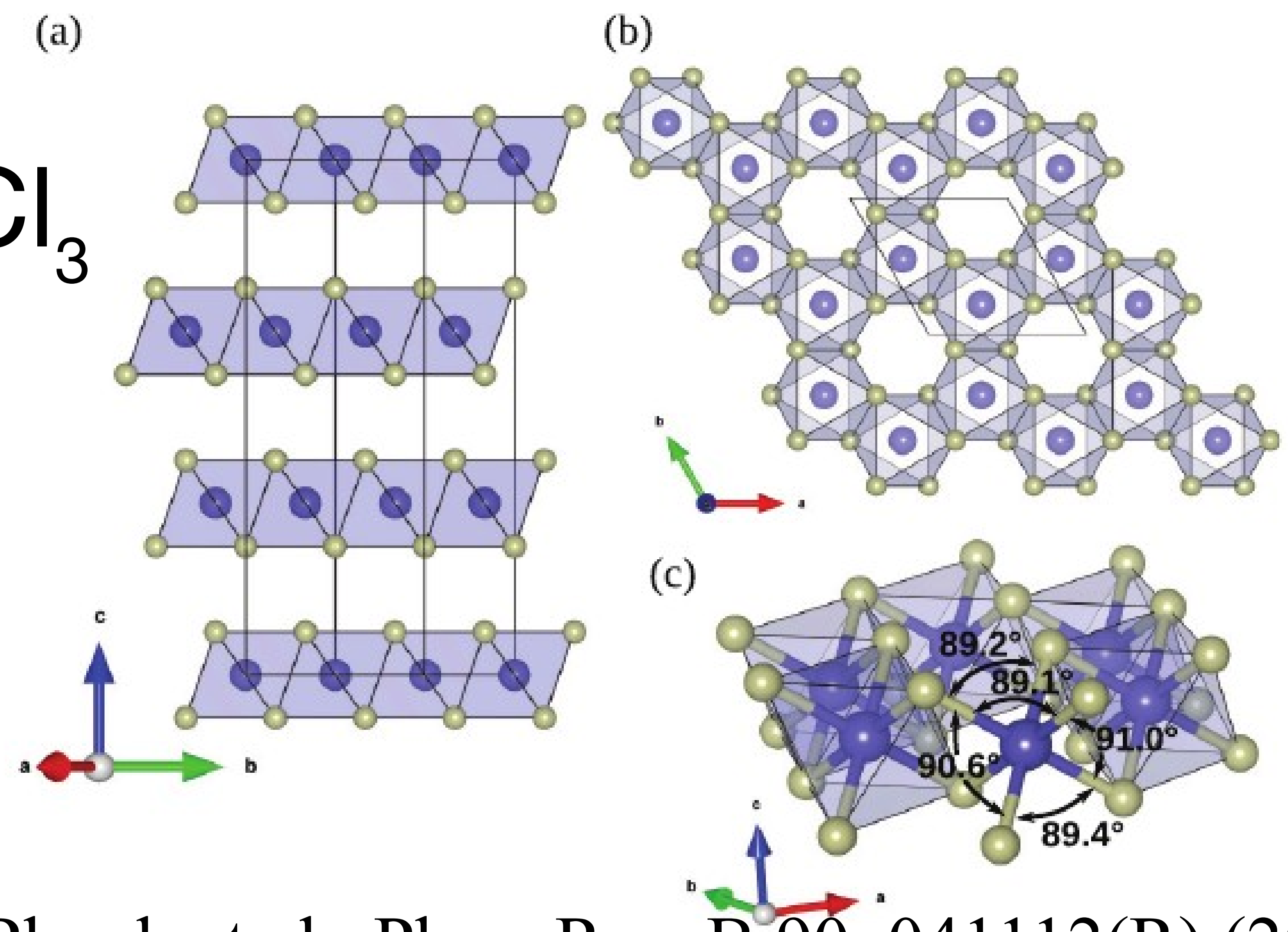
Majorana fermions:

$$c_j^2 = 1,\ c_i c_j = -c_j c_i,\ i \neq j$$

non-Abelian excitations in magnetic field!

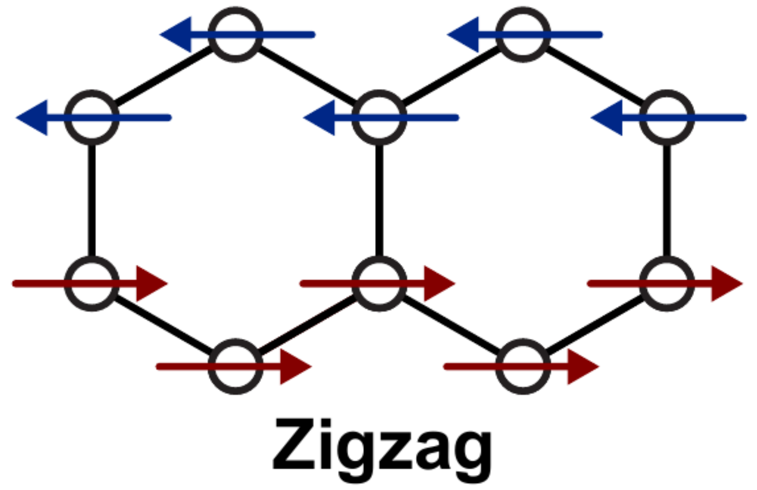
A. Kitaev (2006)

α-$RuCl_3$



K. W. Plumb et al., Phys. Rev. B 90, 041112(R) (2014)

Long-range
order at 7K



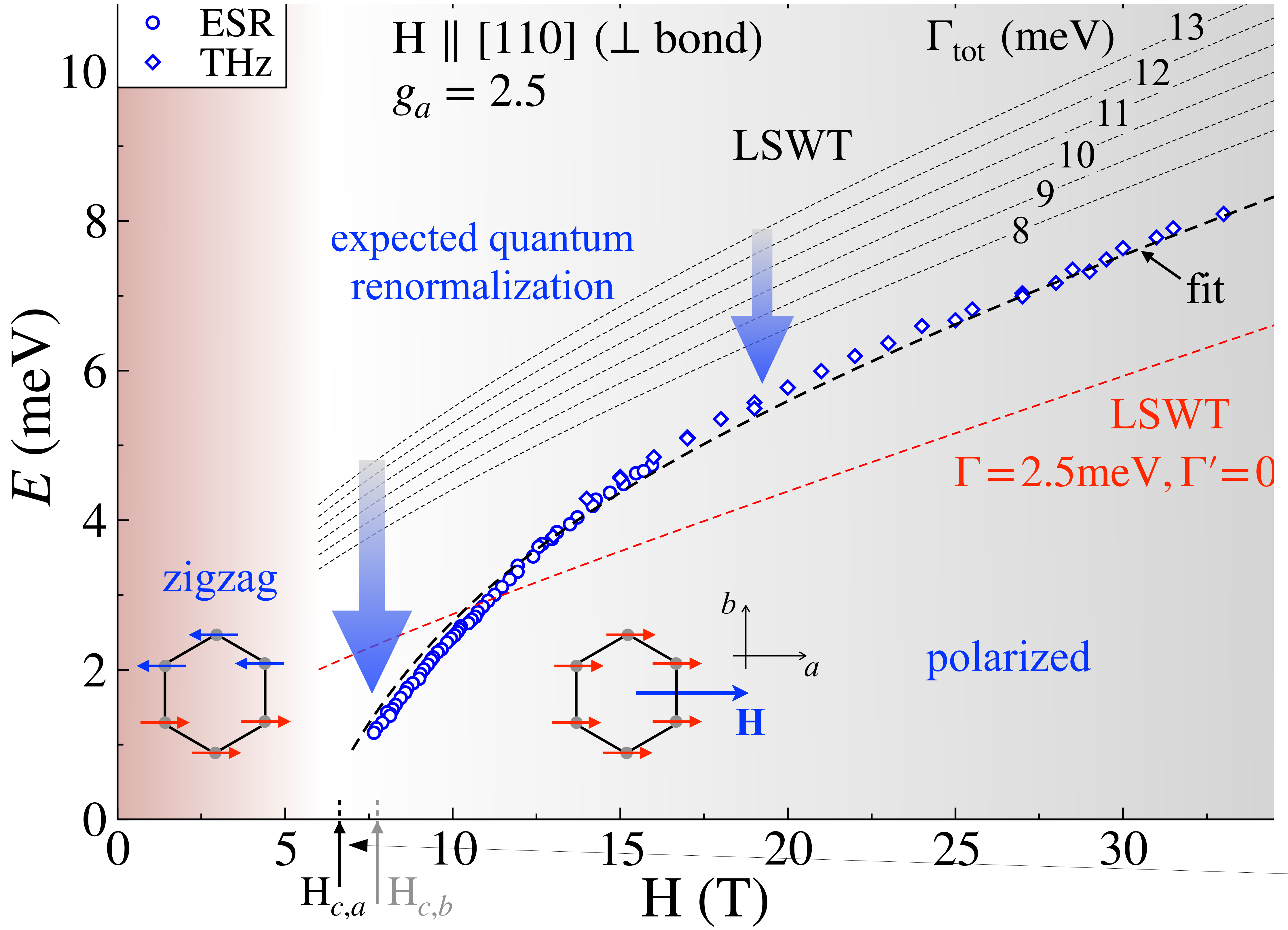
Extended Kitaev-Heisenberg model:

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

Material parameters and polarized phase spectrum

Magnon at the BZ center:

$$\varepsilon_{\mathbf{k}=0} = \sqrt{g\mu_B H \left(g\mu_B H + 3S\left(\Gamma + 2\Gamma'\right)\right)}$$

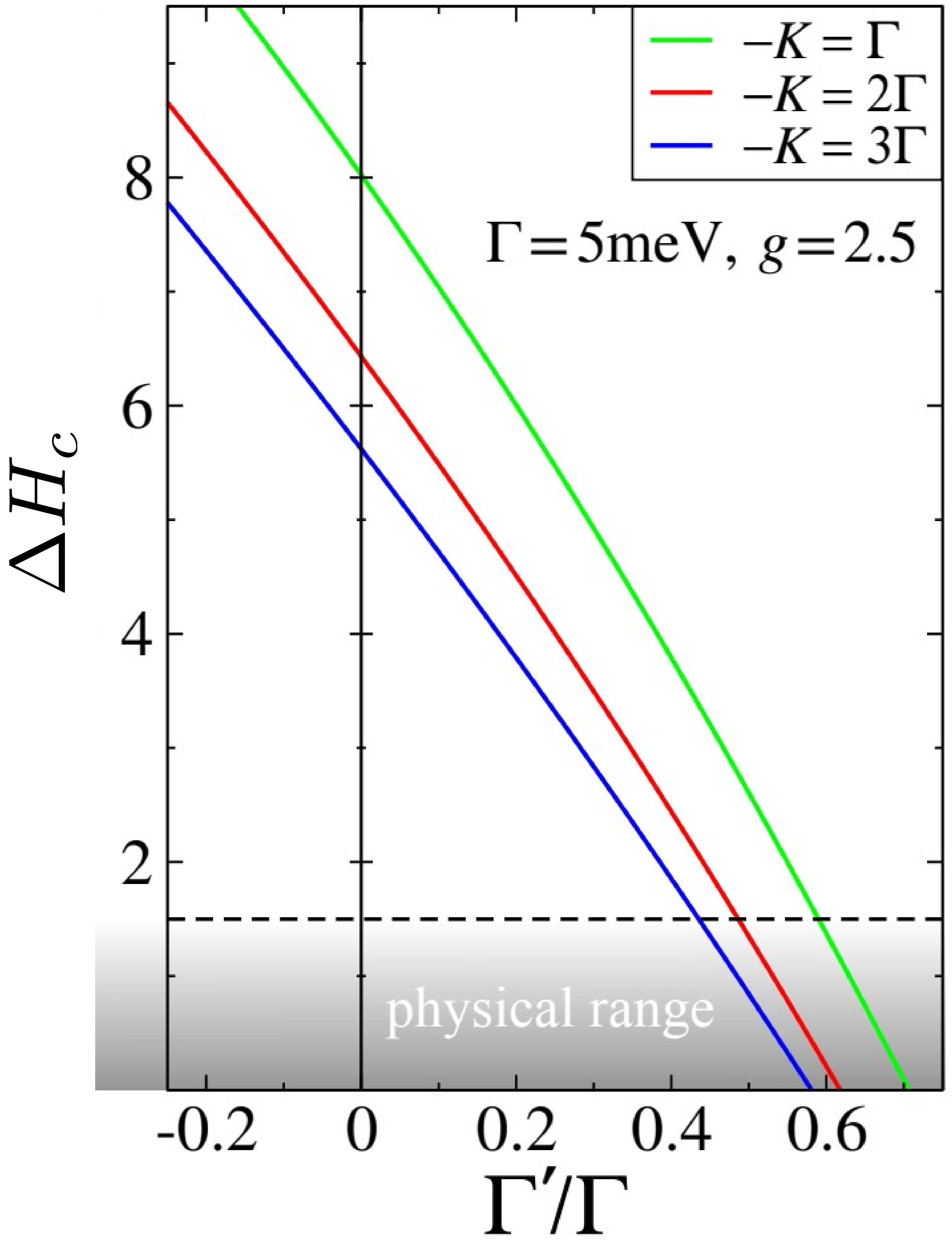


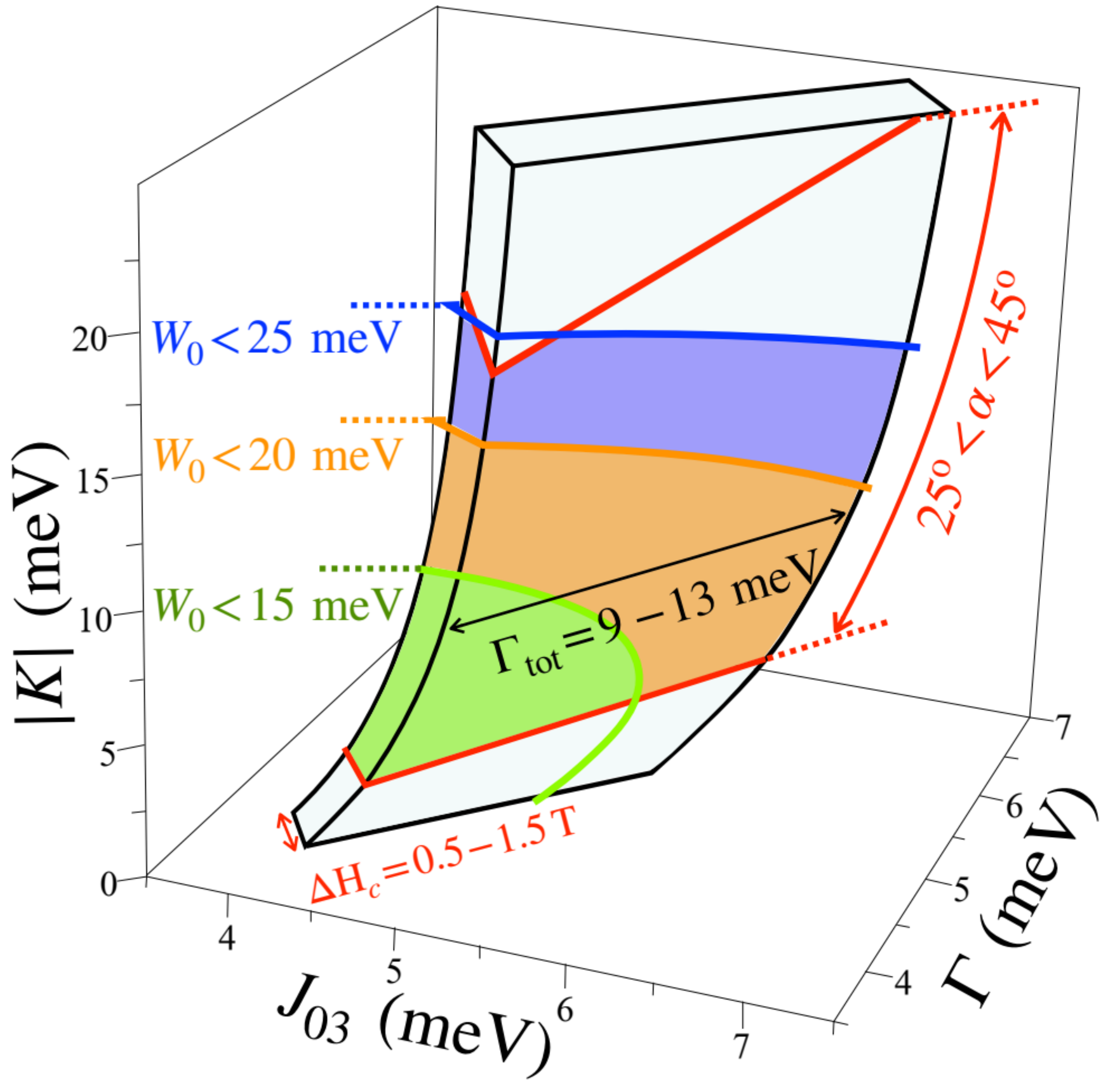
Reference	Method	K	Γ	Γ'	J	J_3	$\Gamma+2\Gamma'$	$J+3J_3$
Banerjee et al. [22]	LSWT, INS fit	+7.0			**-4.6**			-4.6
Kim et al. [29]	DFT+t/U, $P3$	**-6.55**	**5.25**	-0.95	**-1.53**		3.35	-1.53
	DFT+SOC+t/U	**-8.21**	**4.16**	-0.93	-0.97		2.3	-0.97
	same+fixed lattice	-3.55	7.08	-0.54	**-2.76**		6.01	-2.76
	same+U+zigzag	+4.6	**6.42**	-0.04	**-3.5**		6.34	-3.5
Winter et al. [30]	DFT+ED, $C2$	**-6.67**	**6.6**	-0.87	**-1.67**	**2.8**	4.87	**6.73**
	same, $P3$	+7.6	8.4	+0.2	-5.5	**2.3**	**8.8**	+1.4
Yadav et al. [24]	Quantum chemistry	**-5.6**	-0.87		+1.2		-0.87	+1.2
Ran et al. [34]	LSWT, INS fit	**-6.8**	9.5				**9.5**	
Hou et al. [31]	DFT+t/U, $U=2.5$eV	**-14.43**	**6.43**		**-2.23**	**2.07**	6.43	+3.97
	same, $U=3.0$eV	**-12.23**	**4.83**		**-1.93**	1.6	4.83	+2.87
	same, $U=3.5$eV	**-10.67**	**3.8**		**-1.73**	1.27	3.8	+2.07
Wang et al. [32]	DFT+t/U, $P3$	**-10.9**	**6.1**		-0.3	0.03	6.1	-0.21
	same, $C2$	**-5.5**	7.6		+0.1	0.1	7.6	+0.4
Winter et al. [35]	*Ab initio*+INS fit	**-5.0**	2.5		-0.5	0.5	2.5	+1.0
Suzuki et al. [36]	ED, C_p fit	-24.41	**5.25**	-0.95	**-1.53**		3.35	-1.53
Cookmeyer et al. [37]	thermal Hall fit	**-5.0**	2.5		-0.5	0.11	2.5	-0.16
Wu et al. [38]	LSWT, THz fit	-2.8	2.4		-0.35	0.34	2.4	+0.67
Ozel et al. [39]	same, $K>0$	+1.15	2.92	+1.27	-0.95		5.45	-0.95
	same, $K<0$	-3.5	2.35		+0.46		2.35	+0.46
Eichstaedt et al. [33]	DFT+Wannier+t/U	**-14.3**	9.8	-2.23	-1.4	0.97	5.33	+1.5
Sahasrabudhe et al. [42]	ED, Raman fit	**-10.0**	3.75		-0.75	0.75	3.75	1.5
Sears et al. [40]	Magnetization fit	**-10.0**	10.6	-0.9	**-2.7**		**8.8**	-2.7
Laurell et al. [41]	ED, Cp fit	**-15.1**	10.1	-0.12	-1.3	0.9	**9.86**	+1.4
This work	**range**	[-19,-3.8]	[3.9,6.5]	[2.0,3.6]	[-6.5,-1.6]	[2.1,4.3]	[9.0,13.0]	[4.4,6.8]
	point 1	**-4.8**	**4.08**	**2.5**	**-2.56**	**2.42**	**9.08**	**4.7**
	point 2	**-10.8**	**5.2**	**2.9**	**-4.0**	**3.26**	**11.0**	**5.78**
	point 3	**-14.8**	**6.12**	**3.28**	**-4.48**	**3.66**	**12.7**	**6.5**

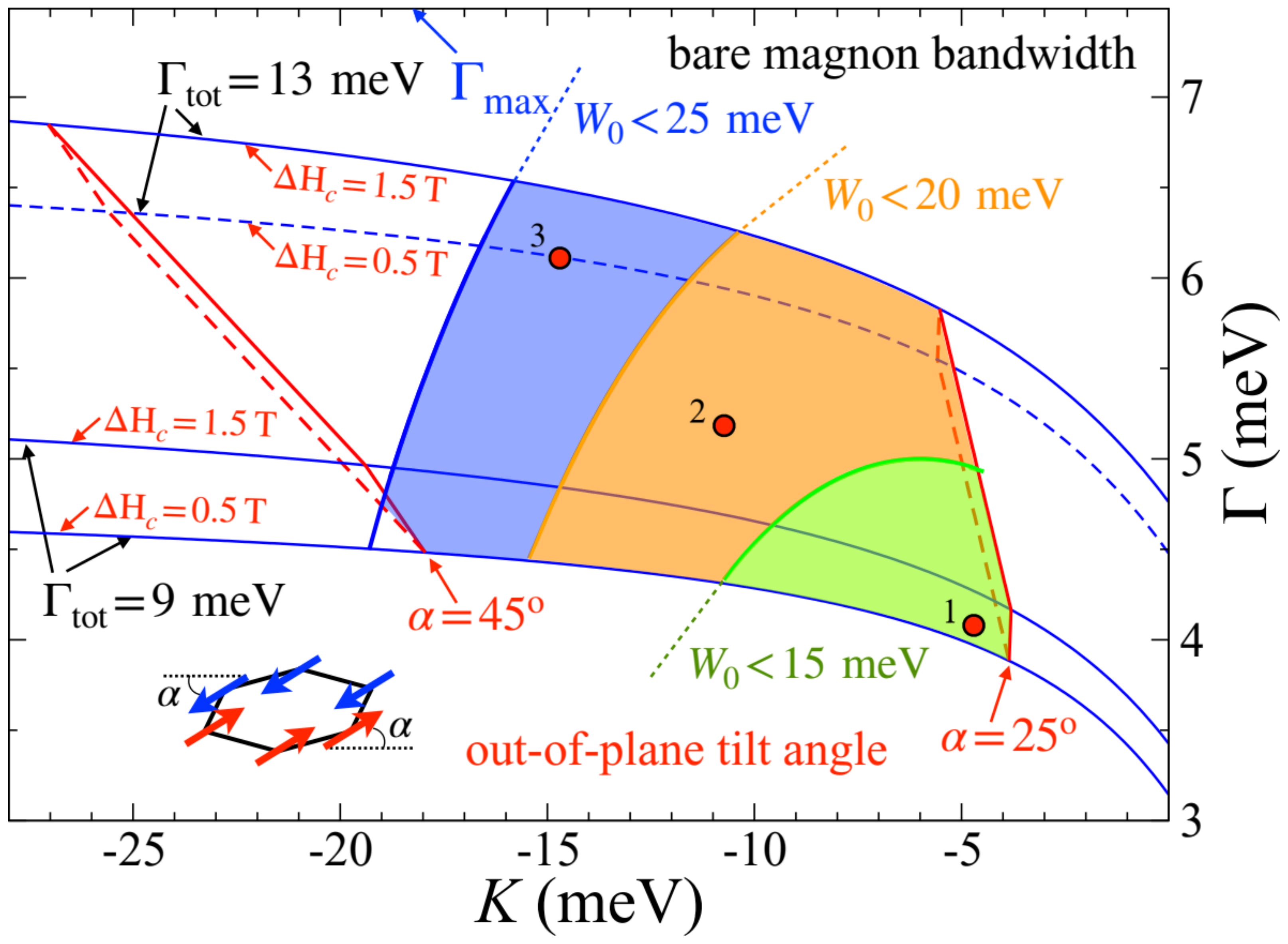
Critical fields for *a* and *b* field directions are very close

Critical fields for *a* and *b* directions

$$\Delta H_c = H_c^{(b)} - H_c^{(a)} = \Delta H_c(K, \Gamma, \Gamma')$$







- Zigzag ground state
- Magnon bandwidth
- Tilt angle

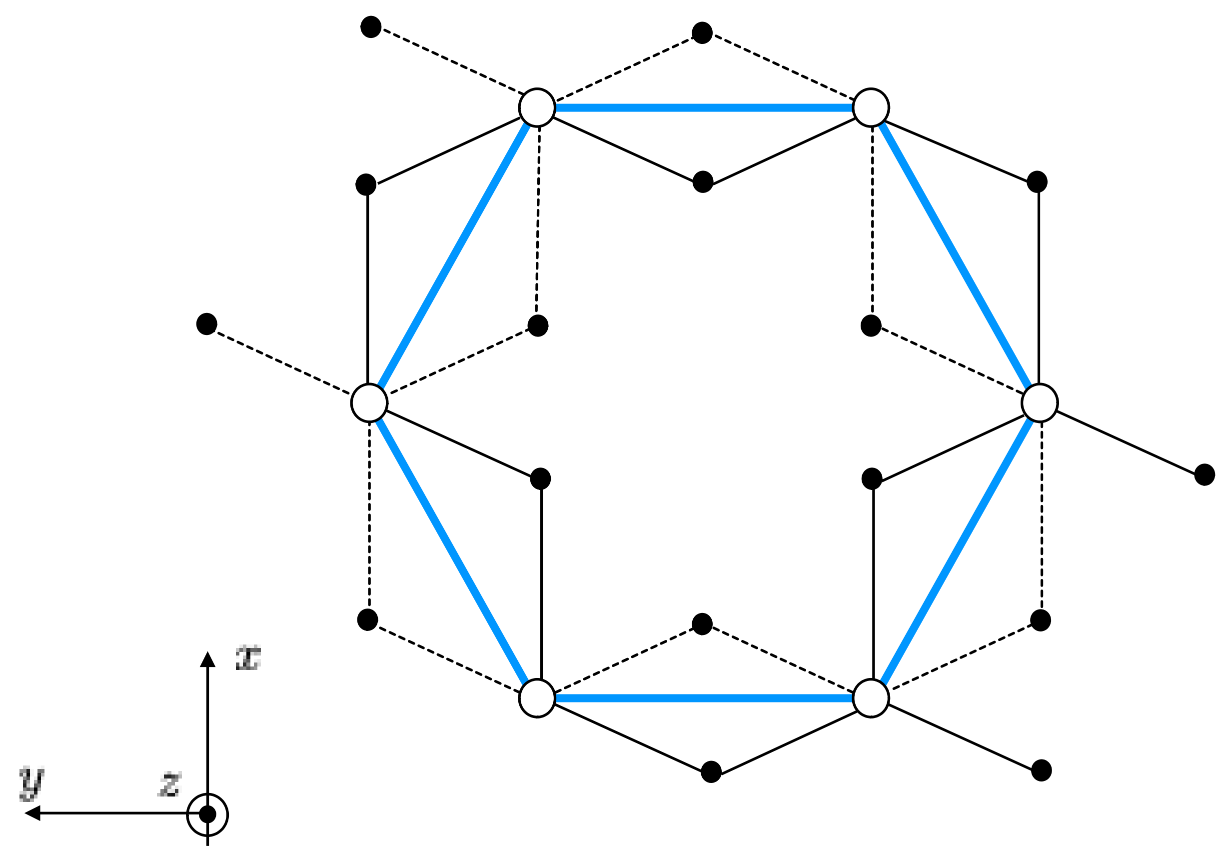
$$(J, K, \Gamma, \Gamma', J_3)$$

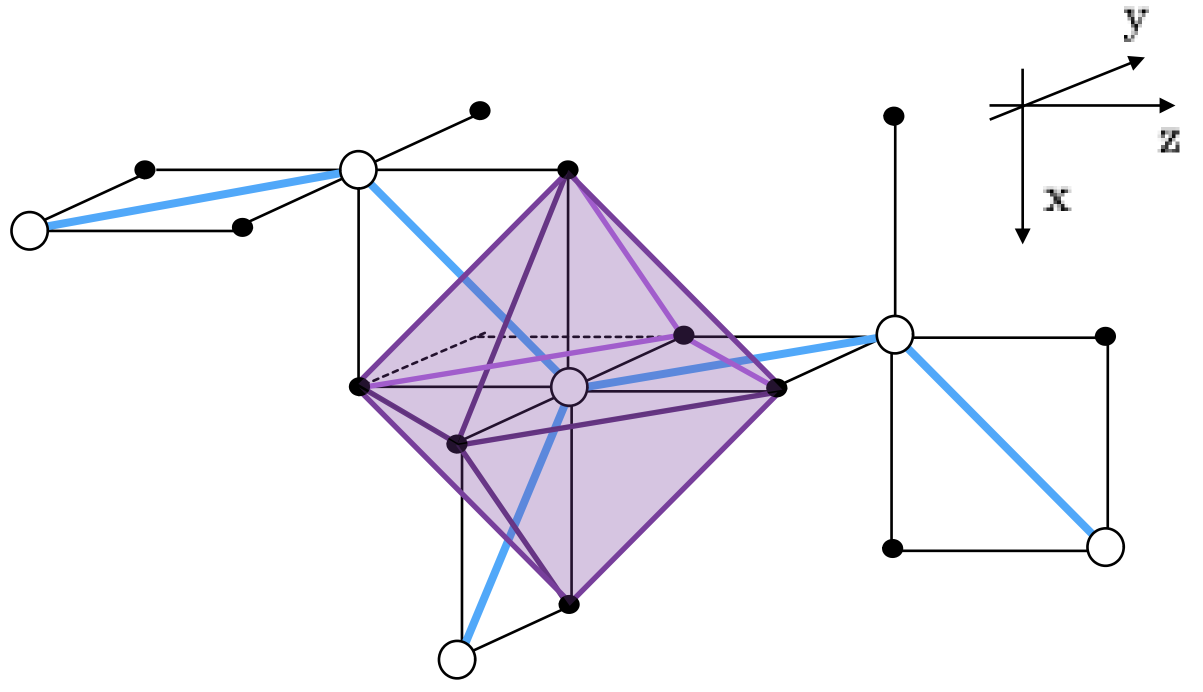
Point 1: $(-2.56, -4.8, 4.08, 2.5, 2.42)$

Point 2: $(-4.0, -10.8, 5.2, 2.9, 3.26)$

Point 3: $(-4.48, -14.8, 6.12, 3.28, 3.66)$,

Axes transformation





Crystallographic axes

$$\mathcal{H} = \sum_{\langle ij\rangle} \mathrm{J}_{\pm}\left(S_i^x S_j^x + S_i^y S_j^y\right) + \mathrm{J}_z S_i^z S_j^z$$
$$-2\mathrm{J}_{\pm\pm}\left(\left(S_i^x S_j^x - S_i^y S_j^y\right)\cos\tilde{\varphi}_\alpha - \left(S_i^x S_j^y + S_i^y S_j^x\right)\sin\tilde{\varphi}_\alpha\right)$$
$$-\mathrm{J}_{z\pm}\left(\left(S_i^x S_j^z + S_i^z S_j^x\right)\cos\tilde{\varphi}_\alpha + \left(S_i^y S_j^z + S_i^z S_j^y\right)\sin\tilde{\varphi}_\alpha\right)$$
$$+\sum_{\langle ij\rangle_3} J_3\left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z\right), \qquad \text{(A1)}$$

J. Chaloupka and G. Khaliullin, Phys. Rev. B 92, 024413 (2015)

Cubic axes

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

$$\mathrm{J}_{\pm} = J + \frac{1}{3}\left(K - \Gamma - 2\Gamma'\right),$$
$$\mathrm{J}_z = J + \frac{1}{3}\left(K + 2\Gamma + 4\Gamma'\right),$$
$$2\mathrm{J}_{\pm\pm} = \frac{1}{3}\left(-K - 2\Gamma + 2\Gamma'\right),$$
$$\sqrt{2}\mathrm{J}_{z\pm} = \frac{1}{3}\left(2K - 2\Gamma + 2\Gamma'\right),$$

$$(J, \Delta, J_{\pm\pm}, J_{z\pm}, J_3)$$

Point 1: $(-7.20, -0.26, 0.3, -3.0, 2.42)$
Point 2: $(-11.3, 0.02, 1.0, -3.3, 3.26)$
Point 3: $(-13.6, 0.07, 1.5, -8.3, 3.66)$.

XY J-$J_{z\pm}$-J_3 model(!)

Conclusions

- α-$RuCl_3$ is a magnetic insulator with sizeable anisotropic Kitaev interactions
- Some experimental observations can only be explained with large Γ and Γ', which are usually neglected
- Combination of other criteria form a region of allowed parameters
- The transformation of axes shows that α-$RuCl_3$ can be described as a simple three-parameter XY J-$J_{z\pm}$-J_3 model