Lattice effects in spin-orbit Mott insulators

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IX TRIESTE WORKSHOP ON OPEN PROBLEMS IN STRONGLY CORRELATED SYSTEMS

14 - 25 July 1997

Trieste 1997

P.W. ANDERSON
Princeton University
Joseph Henry Laboratories of Physics
Princeton, New Jersey
U.S.A.

These are preliminary lecture notes, intended only for distribution to participants

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FUNDAMENTAL PROBLEMS IN THE HI Tc SYSTEM

Acknowledgements G. Baskaran

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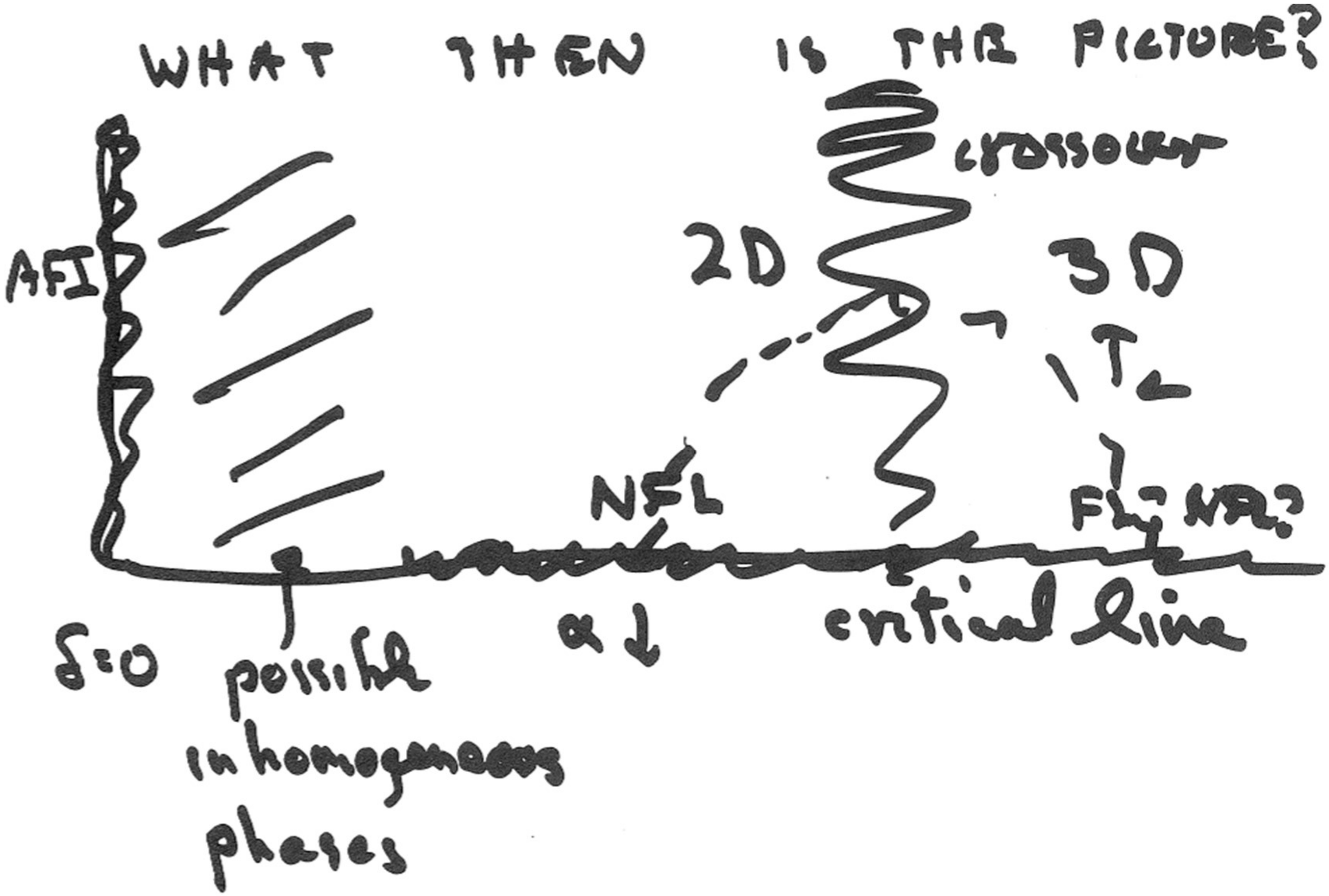
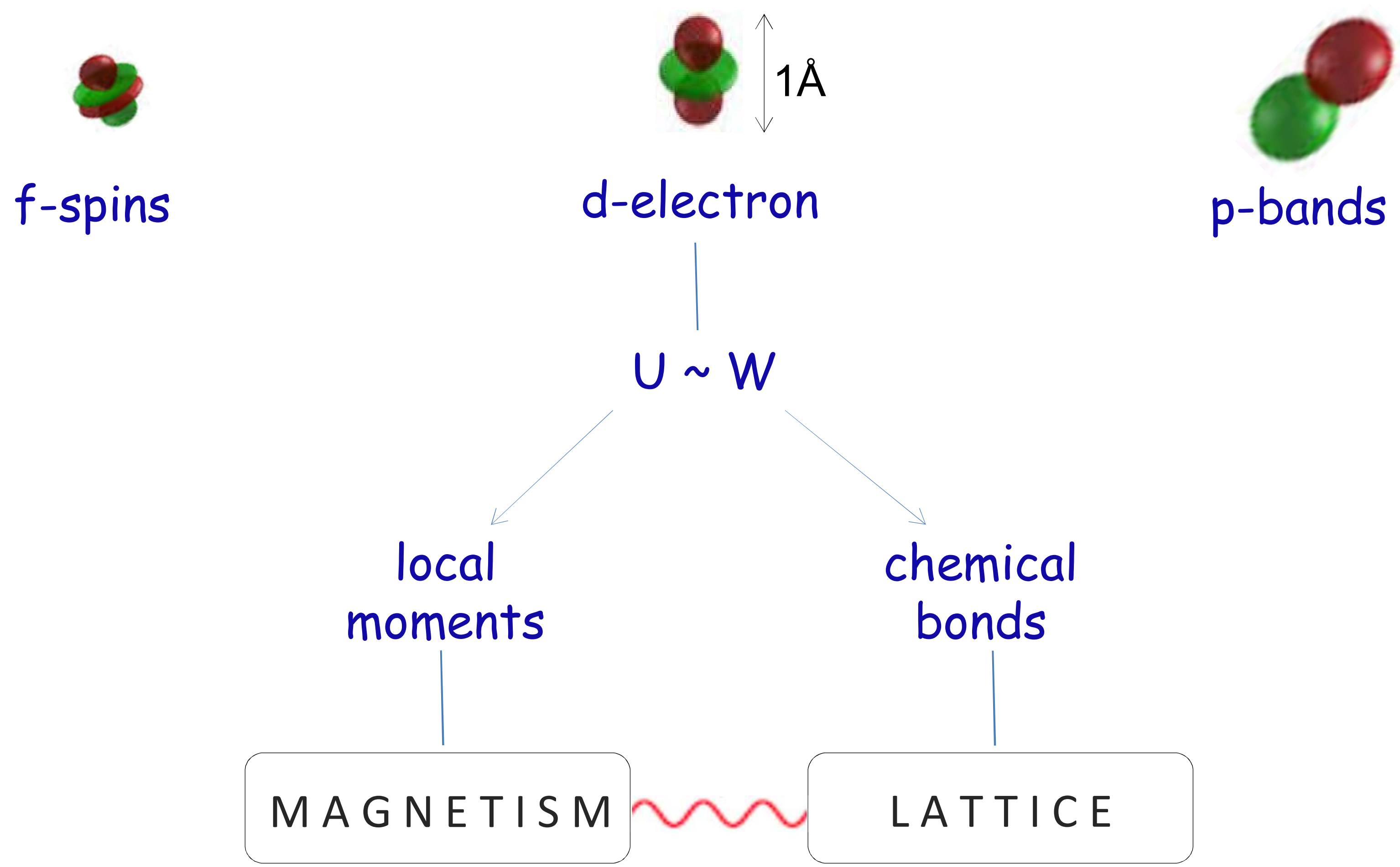


Lattice effects in spin-orbit Mott insulators

- Introduction
  - spin-lattice coupling

- Sr_2IrO_4
  - magnetic anisotropy
  - magnetoacoustic waves
  - spin nematic transition


1Å
f-spins
d-electron
p-bands
U ~ W
local moments
chemical bonds
MAGNETISM
LATTICE

NO ORBITAL DEGENERACY (e.g. cuprates)

Lattice vibrations modulate the exchange values J(R)

$H = J(R)\,(\mathbf{S}_i\,\mathbf{S}_j)$

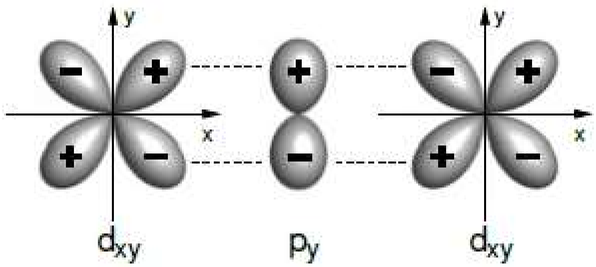
$J(R) = J(1 + \alpha\,\delta R)$

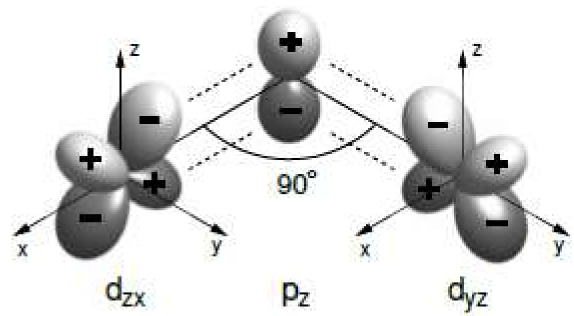
- Magnetostriction
- Spin-Peierls …

SPIN-ORBIT ENTANGLED MAGNETS:

Lattice affects very symmetry properties of the spin Hamiltonians

SPIN-ORBIT ENTANGLED MAGNETS





isotropic
Heisenberg

$$J\ \vec{S}_i \cdot \vec{S}_j$$

Magnetic order

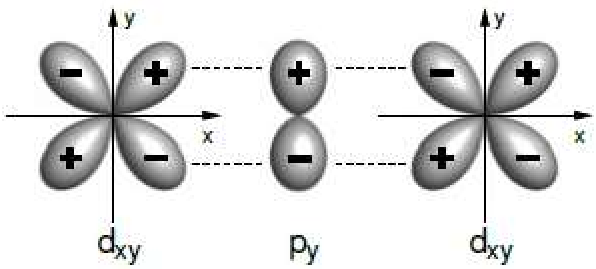
anisotropic
Ising

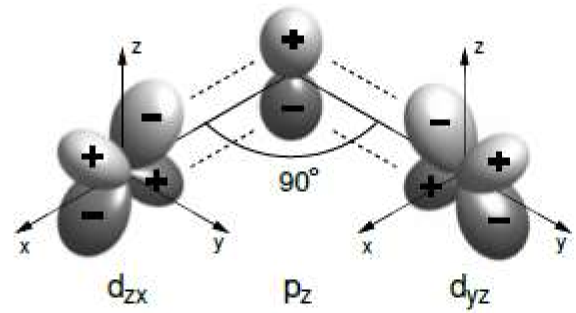
$$J S_i^{\gamma} S_j^{\gamma}$$

Kitaev spin liquid

Jackeli, GKh (2009)

Bond-directional nature of the orbital interactions



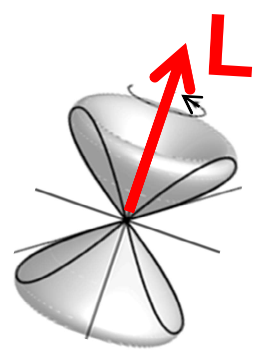


ORBITAL MAGNETISM

isotropic Heisenberg

$J \vec{S}_i \cdot \vec{S}_j$

Magnetic order

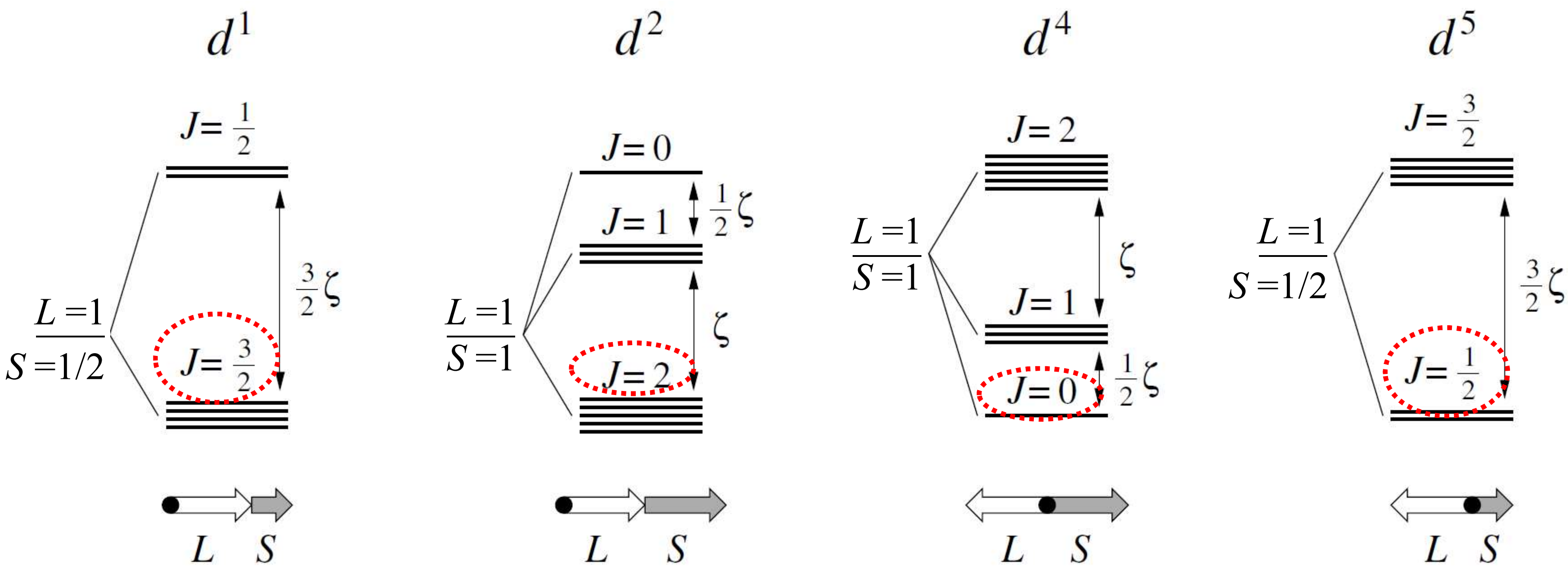


anisotropic Ising

$J S_i^{\gamma} S_j^{\gamma}$

Kitaev spin liquid

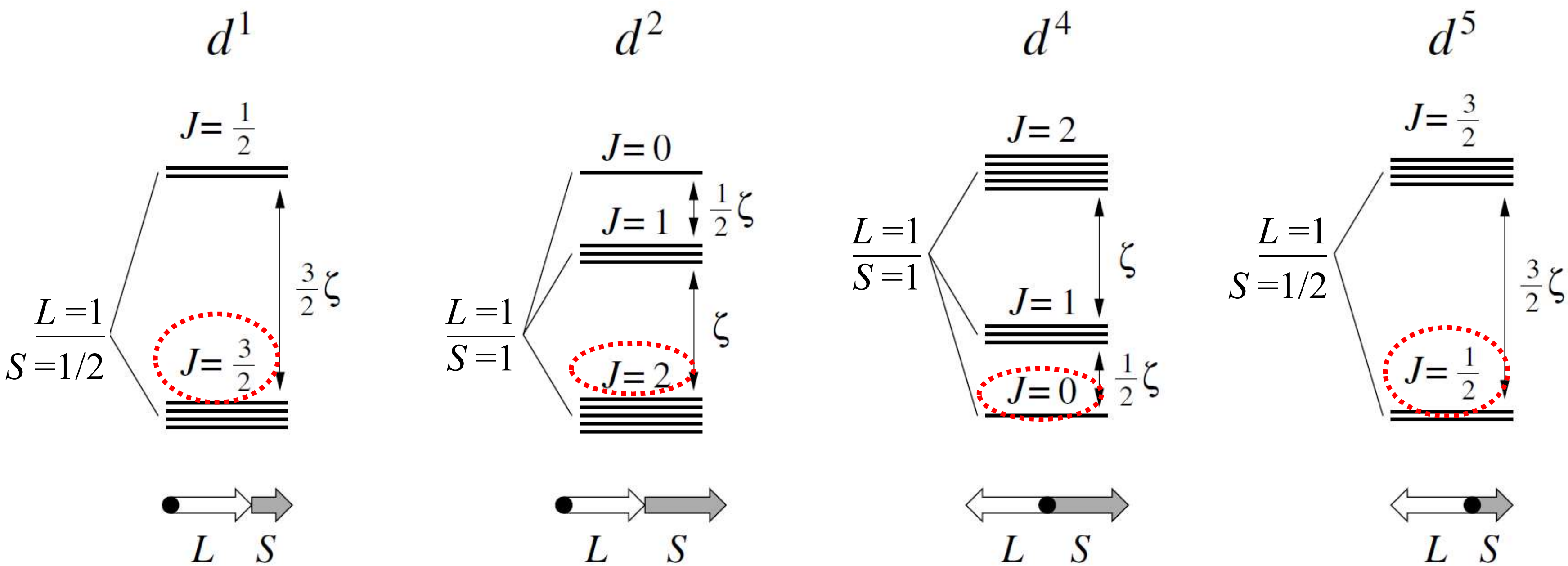
Spin-orbit multiplets of TM ions



V, Nb, Mo	Mo, Re, Os	Ru, Re, Os	Ru, Rh, Ir
g= 0	g= 1/2	g= 0	g= - 2

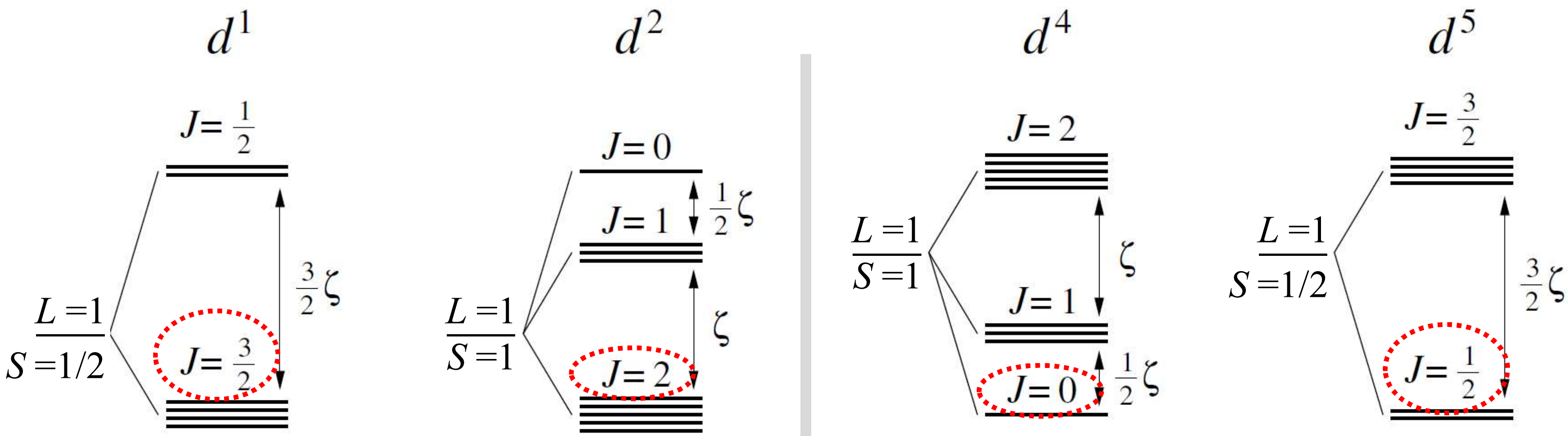
Large orbital contribution to magnetic moments

Spin-orbit multiplets of TM ions

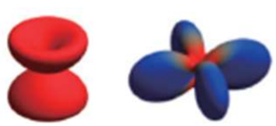


V, Nb, Mo	Mo, Re, Os	Ru, Re, Os	Ru, Rh, Ir
SU(4)	multipoles	triplons	Kitaev

Jahn-Teller *versus* spin-orbit

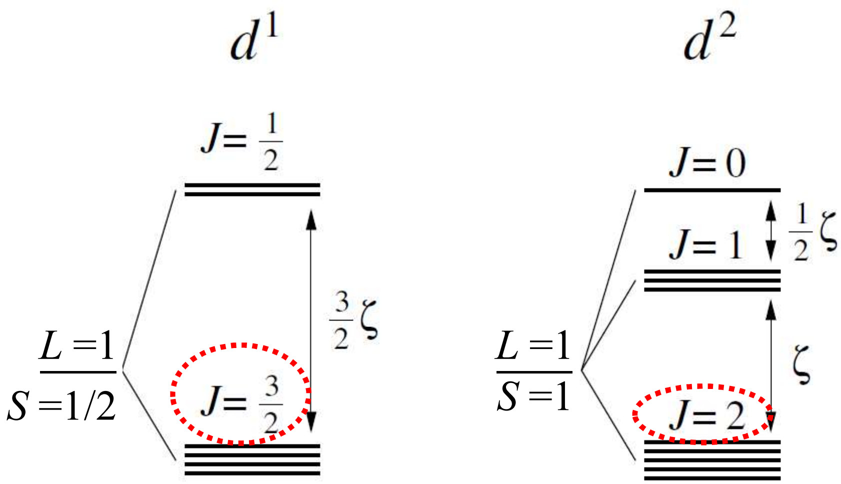


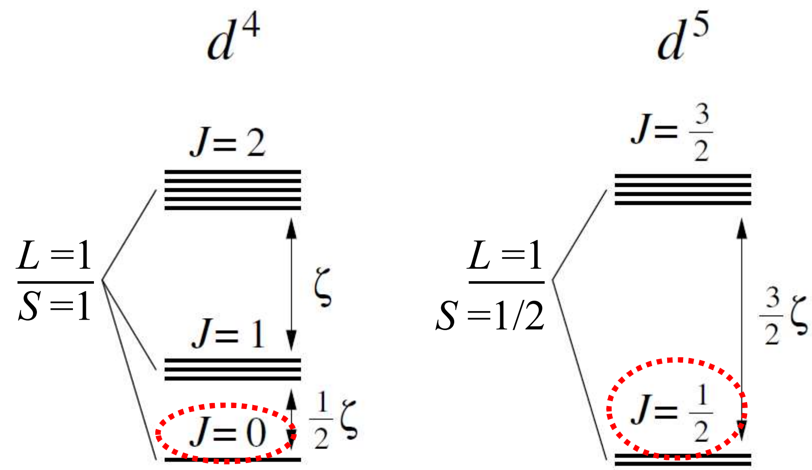
Two different orbital shapes involved



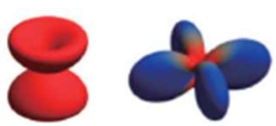
strong JT ions,
structural transition

Jahn-Teller *versus* spin-orbit



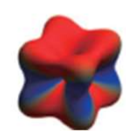


Two different orbital shapes involved



strong JT ions,
structural transition

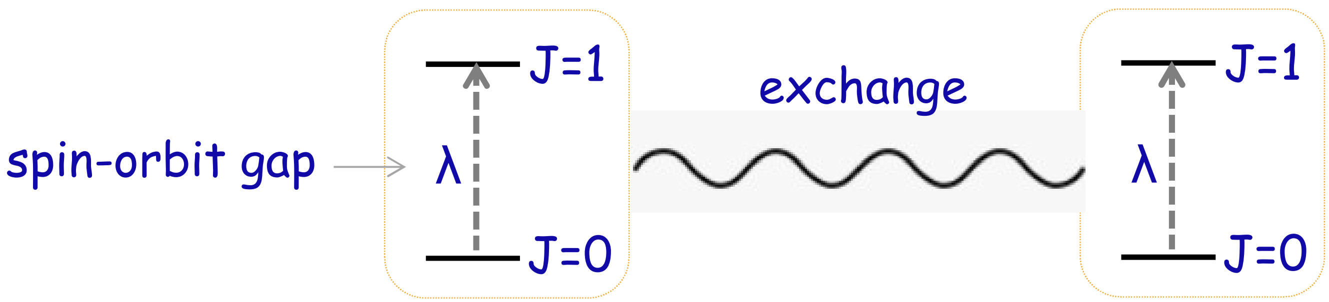
No orbital degeneracy left



shape modulation, new exchange terms + phonons

„pseudo-JT effect“

J=0 compounds (d^4 Ru)

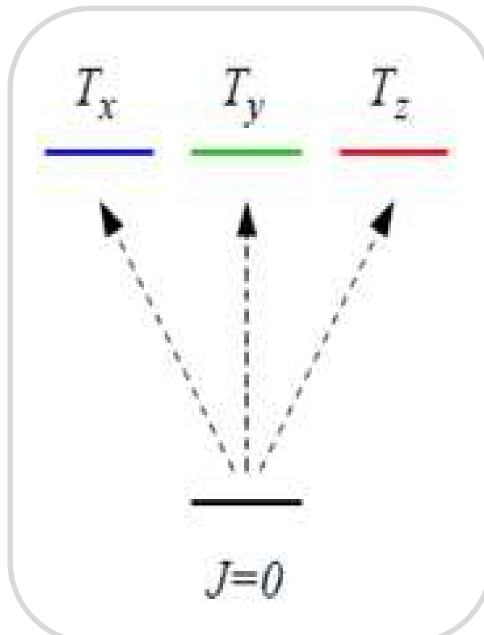


Interacting singlet-triplet models

BEC of spin-orbit excitons (J ~ λ)

GKh (PRL 2013)

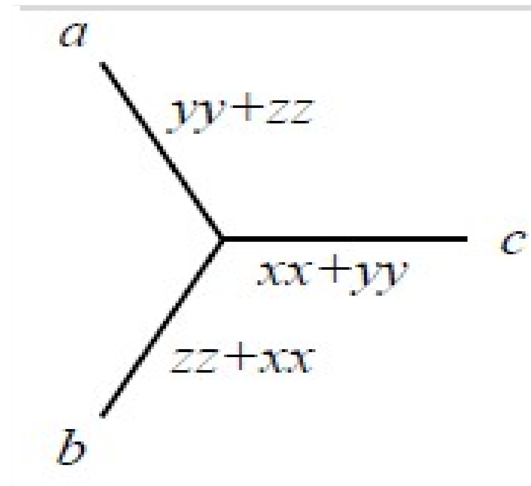
Spin-orbit triplons $T_{x/y/z}$ are „orbitally-colored"



Bond-dependent triplon T_x , T_y , T_z interactions

(A) hopping via oxygen

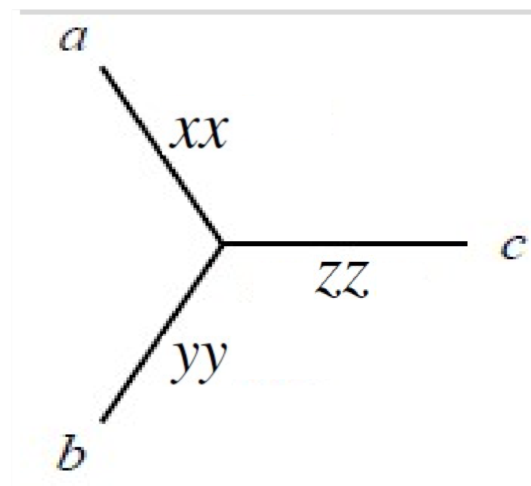
bond-dependent „XY“



(B) direct overlap

bond-dependent „ISING“

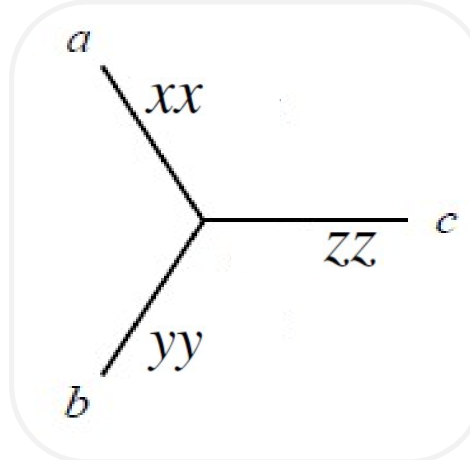
„triplon Kitaev model“



Bosonic Kitaev model

x-bond: $T_{ix}^{\dagger} T_{jx} + T_{ix}^{\dagger} T_{jx}^{\dagger}$

hopping   pair-generation



Chaloupka, GKh (2019)

1) *Extensive number of conserved quantities*

2) *Nonmagnetic ground state, no BEC*

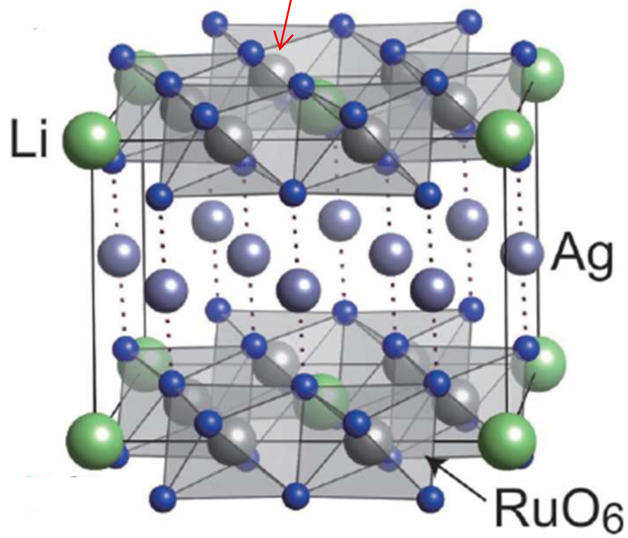
3) *NN-only spin correlations, finite spin gap*

} *as in Kitaev model*

4) *However, no gapless Majoranas*

5) *Magnetic field: topological triplon bands* *(Daghofer et al. 2019)*

$J = 0$ Ru honeycomb lattice



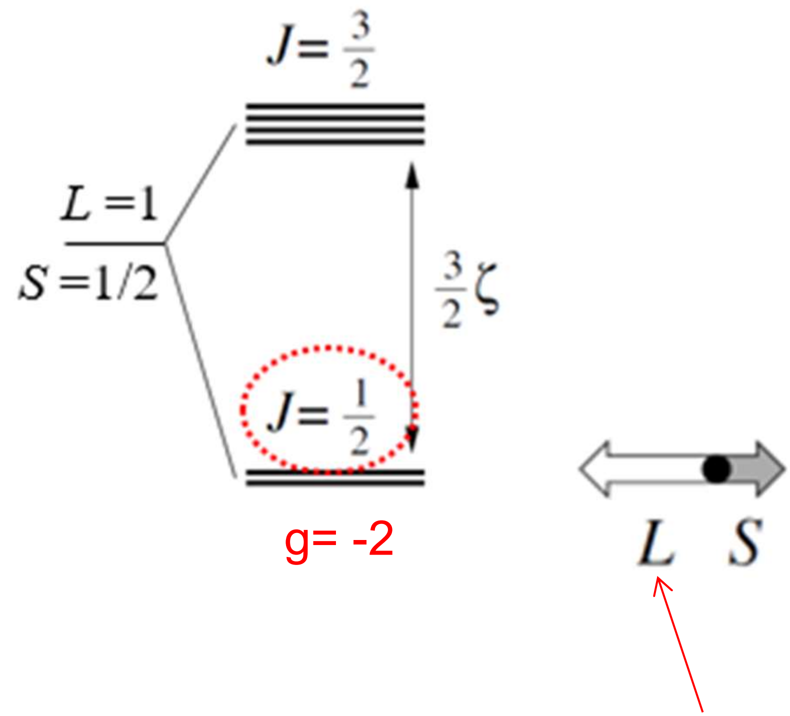
Takayama *et al.* (2022)

- No magnetic LRO
- Spin gap
- Structural transition under pressure

triplon gap *versus* spin-lattice

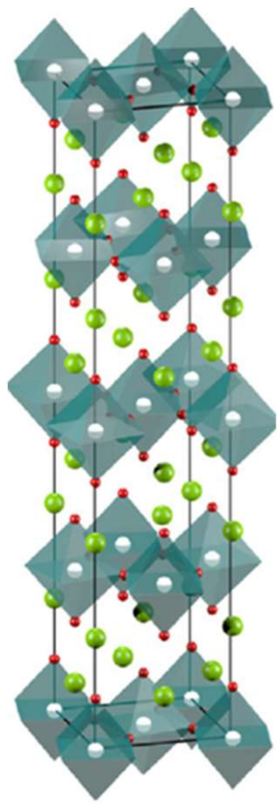
Critical coupling ⇨ dimerisation

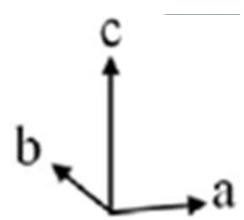
Kramers J=1/2 ions (d^5 Ir)

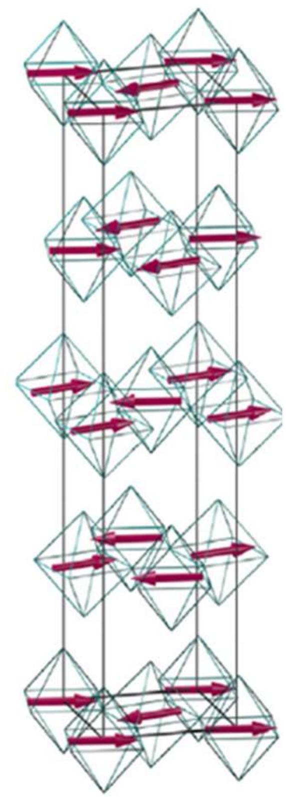


Magnetism: predominantly of orbital origin

Sr_2IrO_4



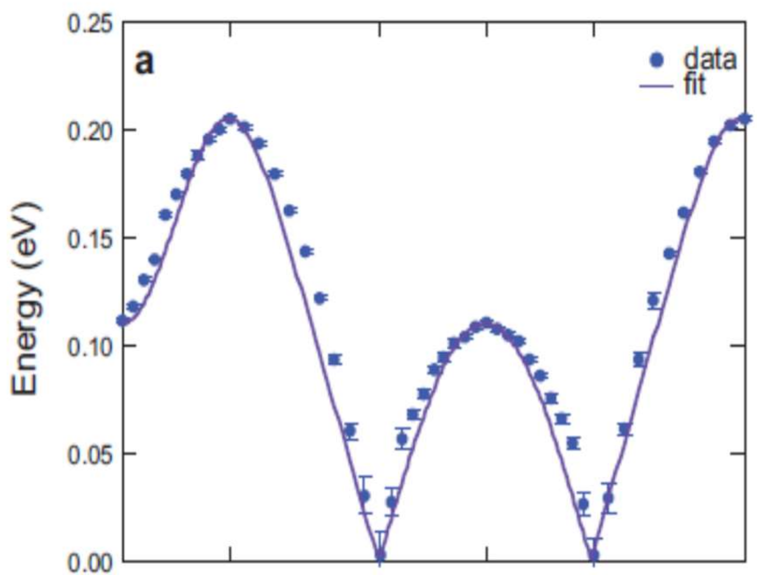




Layered perovskite, tetragonal

Quasi-2D, $J_{ab} \sim 10000\ J_c$

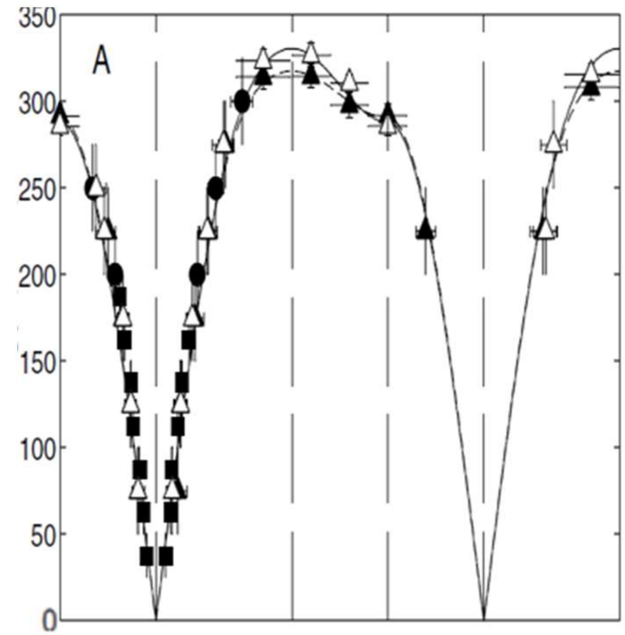
Spin-waves: iridates vs cuprates



Sr_2IrO_4

T_N~240 K

J. Kim et al. (2012)

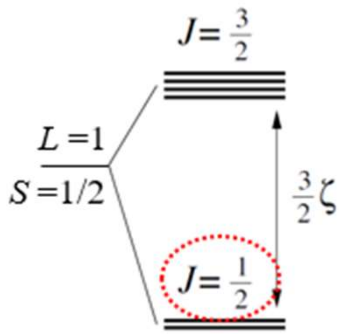


La_2CuO_4

T_N~320 K

Coldea et al.(2001)

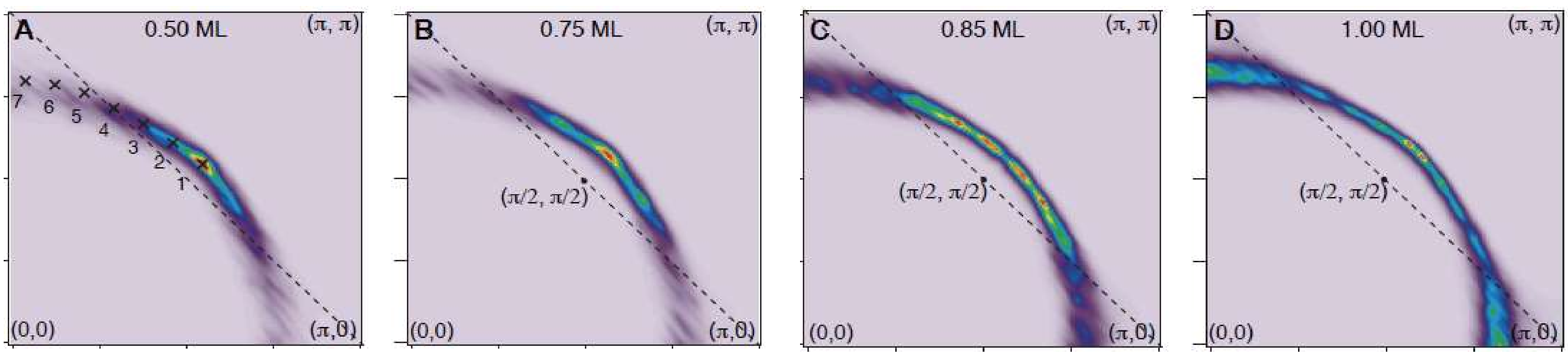
Quasi-2D spin one-half Heisenberg



Doped Sr_2IrO_4 : single-band FS

„Fermi-arcs“ low doping

„normal“ FS



B.J. Kim et al. (2014)

Sr_2IrO_4

- *quantum spins 1/2*
- *single-band FS*
- *strong AF*

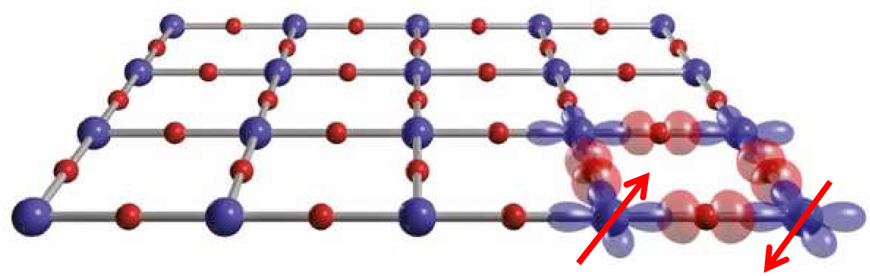
~ two D

P.W. Anderson (1987)

RVB theory for high T_c

- *quantum spins 1/2*
- *single-band FS*
- *strong AF*

~ *two D*



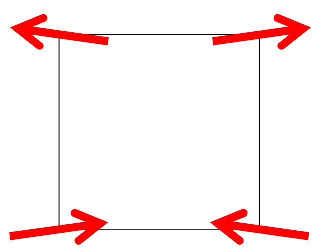
Sr_2IrO_4 possesses all these ingredients…

Problems with magnetism . . .

Symmetry dictated spin Hamiltonian:

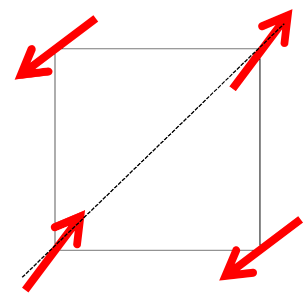
$$J\vec{S}_i\cdot\vec{S}_j + J_z S_i^z S_j^z + \vec{D}\cdot[\vec{S}_i\times\vec{S}_j] + K(\vec{S}_i\cdot\vec{r}_{ij})(\vec{S}_j\cdot\vec{r}_{ij})$$

1. **Predicts wrong magnetic pattern**

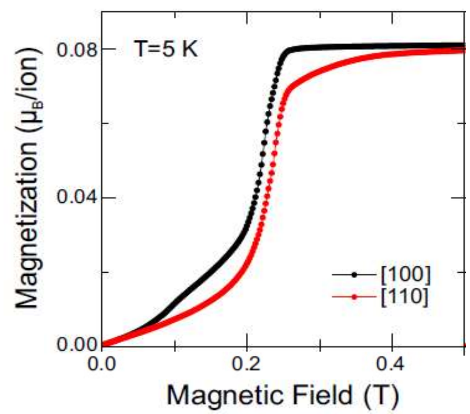


moments along Ir-Ir bond

Experiment



moments along diagonal



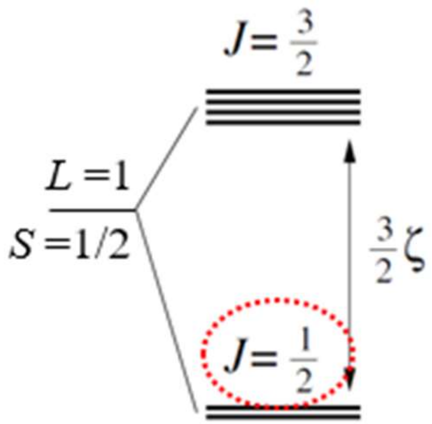
2. **Fails to explain metamagnetic tr.**

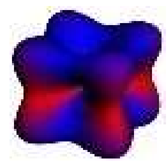
3. **Fails to explain the magnon gaps …**

Spin-only Hamiltonian description of Sr_2IrO_4 is insufficient

Pseudospin-lattice coupling

Huimei Liu, GKh (2019)





$$= |xy\uparrow\rangle + |yz\downarrow\rangle + i|zx\downarrow\rangle$$

Phonons modulate the orbital
shape of the Kramers doublet

⇓

New terms in the Hamiltonian

Spin-lattice coupling Hamiltonian

$$\mathcal{H}^{ij}_{\mathrm{sp-lat}} = g_1\varepsilon_1(S_i^x S_j^y + S_i^y S_j^x) + g_2\varepsilon_2(S_i^x S_j^x - S_i^y S_j^y)$$

xy-distortion　　*xy*-quadrupole　　x^2-y^2

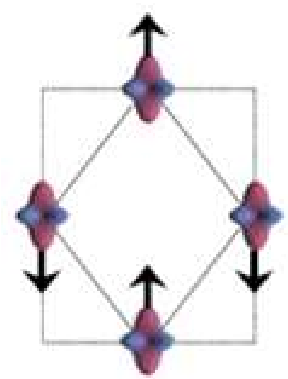
Linear coupling to distortions

⇩

Tetra-to-ortho transition

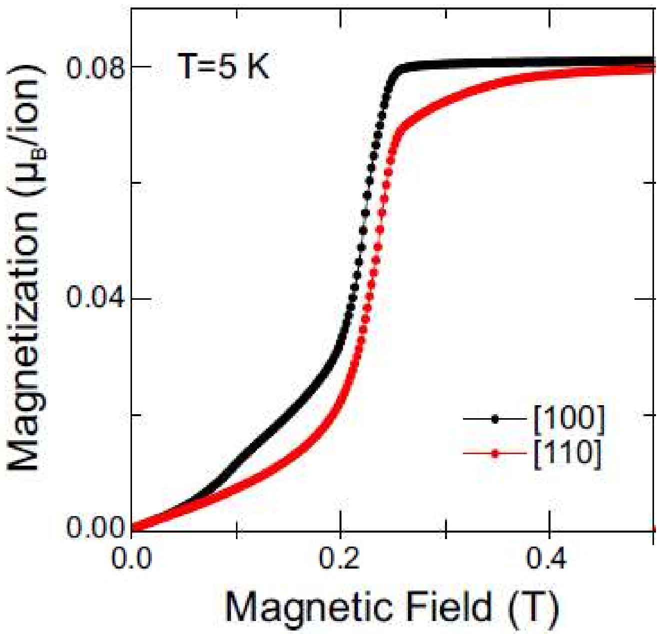
⇩

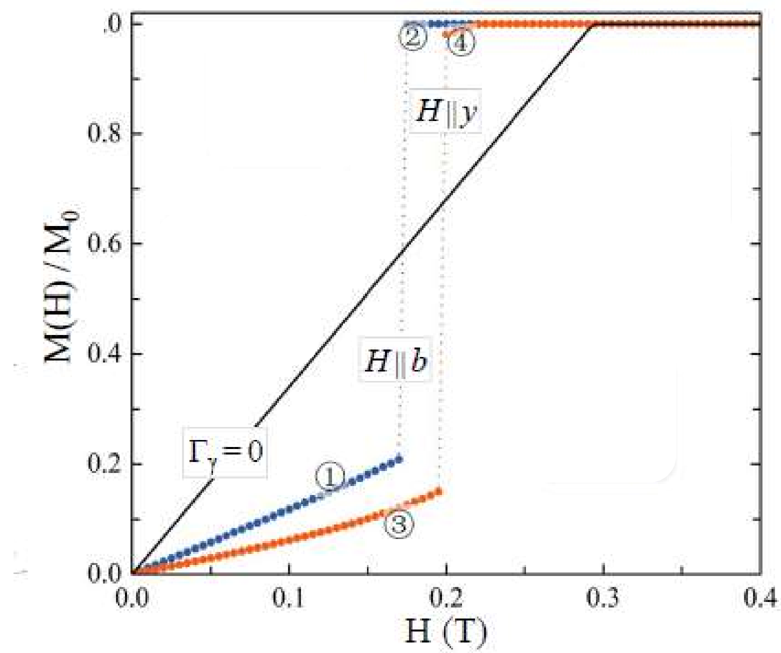
Easy axis along ***b*** axis as observed



$b > a$

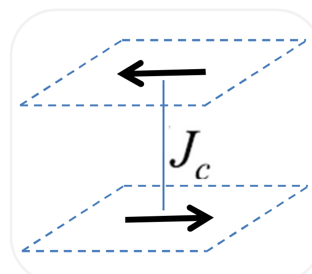
Spin-lattice coupling ⇨ spin-flop transition





metamagnetic transition,
in-plane anisotropy

Porras et al. (2019)



spin-flop transition

Huimei Liu, GKh (2019)

In-plane magnon gap in Sr_2IrO_4

Raman data: $\omega_{ab} \sim 2.3 \text{ meV}$

Cooper *et al.* (2016)
Gretarsson *et al.* (2017)

Theory: $\omega_{ab} = 8S\sqrt{J\Gamma_1}$

$\sim 3\ \mu\text{eV}$

$\Gamma_1 = g_1\varepsilon_1^0$

$\sim 10^{-4}$

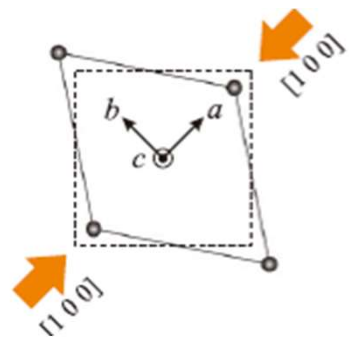
expected orthorhombic distortion

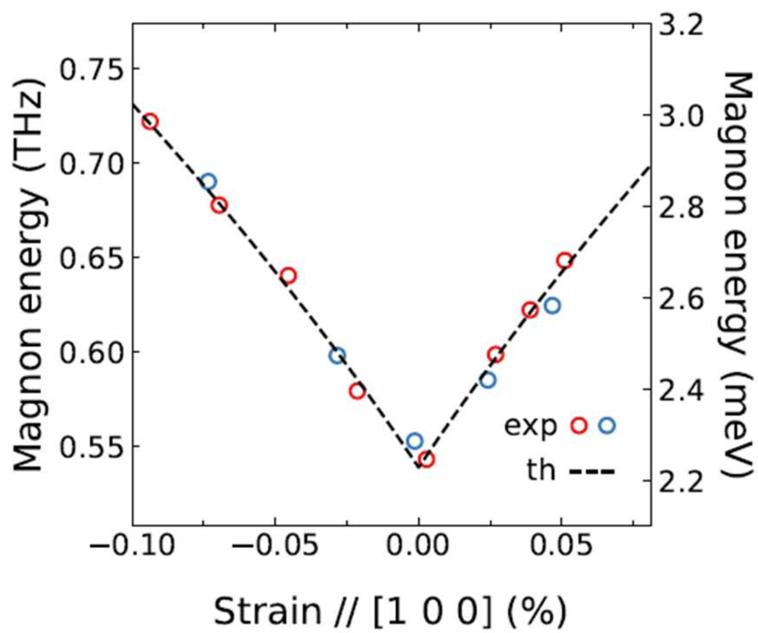
Giant stress response of terahertz magnons in a spin-orbit Mott insulator

Hun-Ho Kim[1], Kentaro Ueda[1,2], Suguru Nakata[1], Peter Wochner[1], Andrew Mackenzie[3,4], Clifford Hicks[3,5], Giniyat Khaliullin[1], Huimei Liu[1,6], Bernhard Keimer[1] & Matteo Minola[1]

nature communications

Apply uniaxial strain:

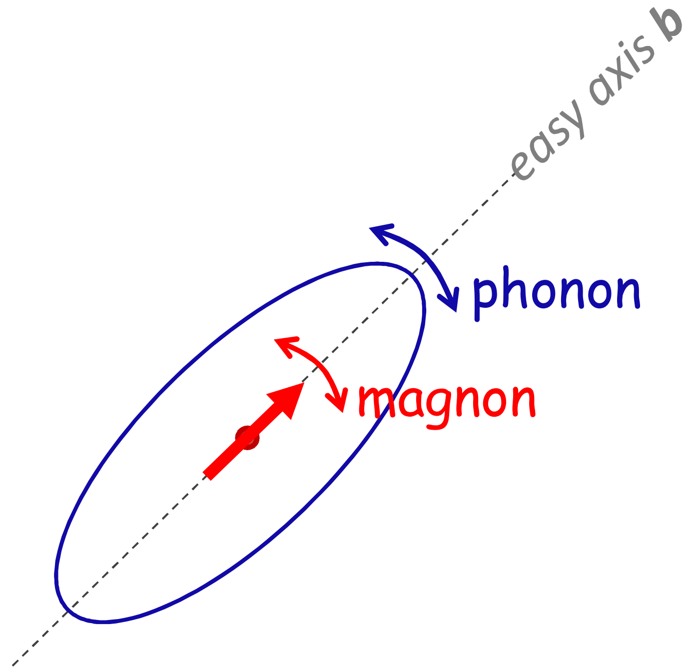




...magnon gap increases

Magnetoacoustic waves:

Elementary excitations with mixed magnon-phonon character



Spin-lattice coupling

$$\mathcal{H}^{ij}_{\text{sp-lat}} = g_1 \varepsilon_1 \, (S^b_i S^b_j - S^a_i S^a_j) + g_2 \varepsilon_2 \, (S^a_i S^b_j + S^b_i S^a_j)$$

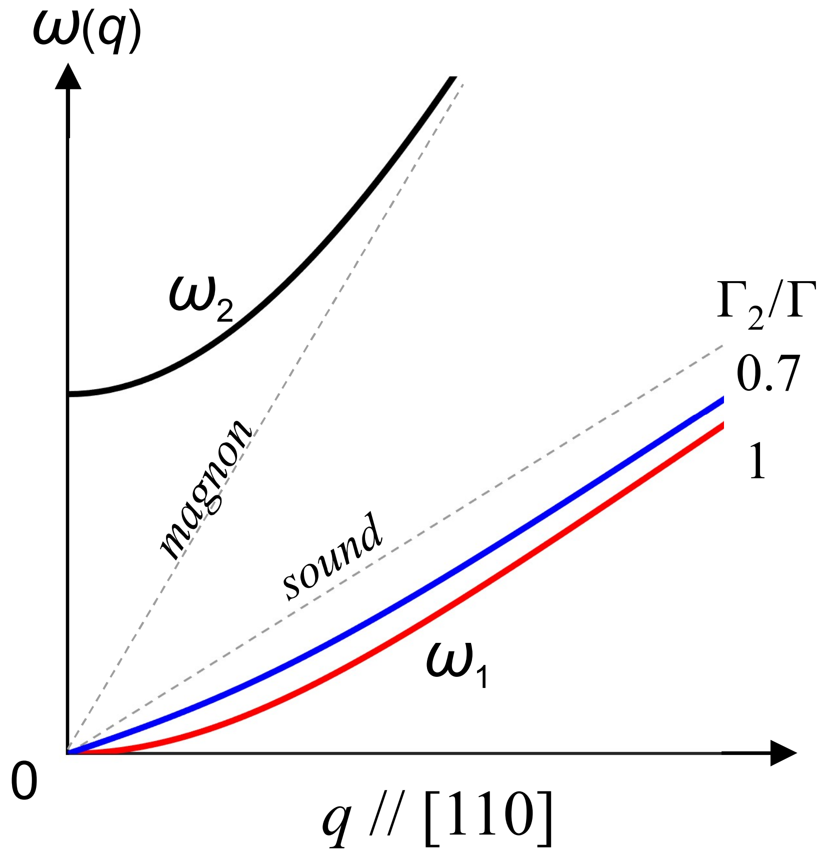
condensed

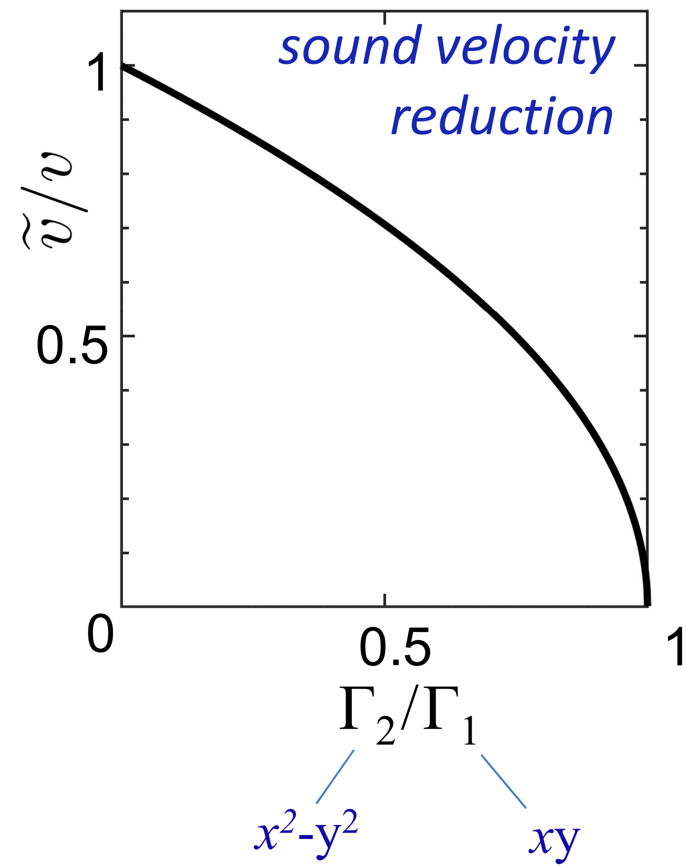
phonon

magnon

linear magnon-phonon coupling

Magnon-phonon mixing in Sr_2IrO_4

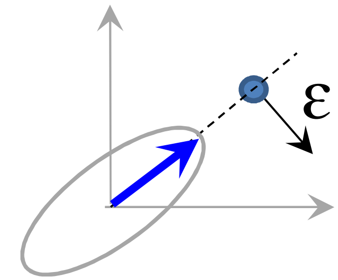


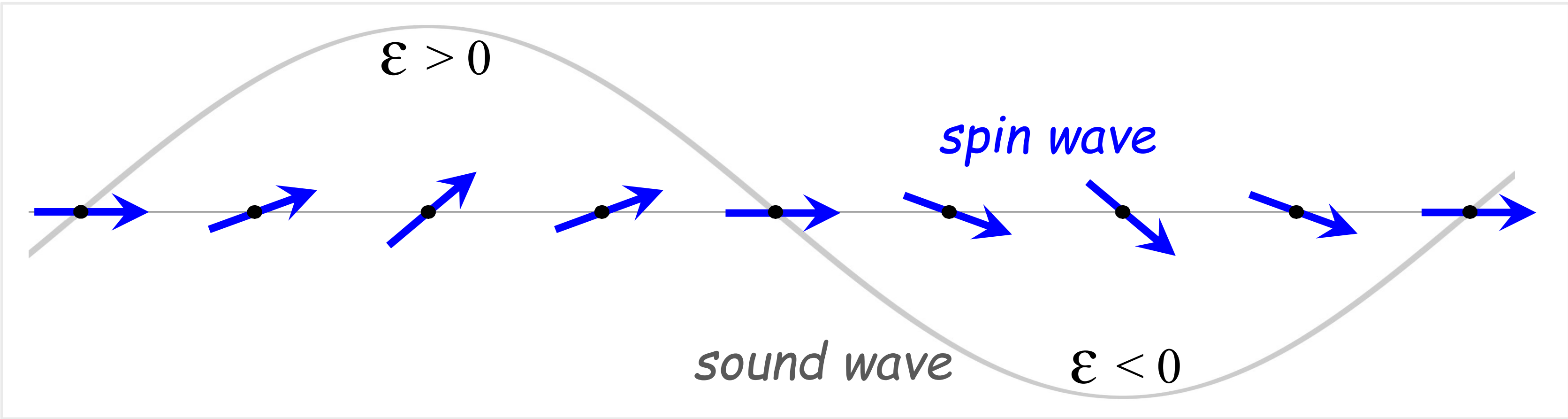


$$v \sim \sqrt{(C_{11} - C_{12})/\rho}$$

elastic constants

Magnetoacoustic wave



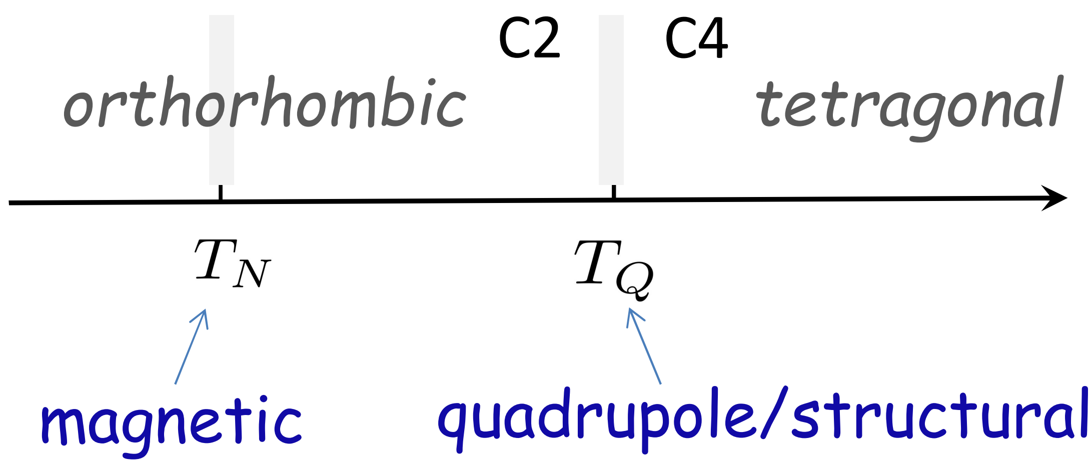


Exciting AF magnons by ultrasound or vice versa

Terahertz magnonics

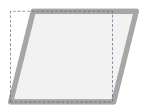
Life above T_N

Spin-quadrupole („nematic") transition



$$\mathcal{H}^{ij}_{\mathrm{sp-lat}} = g_1 \varepsilon_1 (S^x_i S^y_j + S^y_i S^x_j)$$

xy-type distortion — *xy*-quadrupole



$$Q_q = \sum_k (\gamma_k + \gamma_{k+q}) S^x_{k+q} S^y_{-k}$$

Elastic constant C_{66} is reduced:

$$\tilde{C}/C = \alpha(T) = 1 - \frac{2}{S^2} \cdot \Gamma_1 \chi_Q(T)$$

Quadrupole suscep. (← χ_Q)

$\alpha(T) \Rightarrow 0$: structural transition

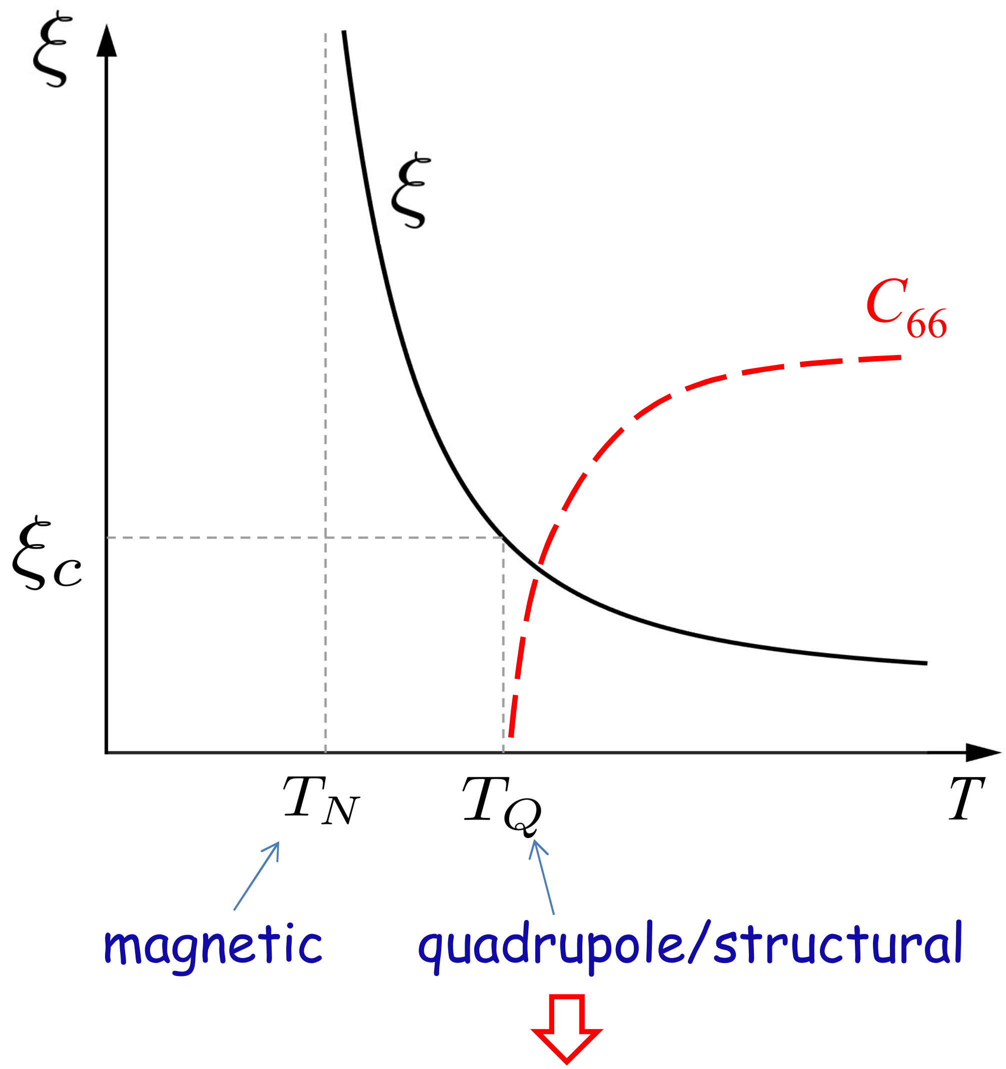
Quadrupole (bare) suscept.: $\chi_Q \simeq \frac{4}{9\pi} \frac{T_N}{J} \frac{(\xi/a)^2}{J}$

spin correl. length

Tetra-to-ortho transition at spin corr. length value:

$$\xi_c(Sr_2IrO_4) \simeq \sqrt{\frac{9\pi}{32} \cdot \frac{J}{T_N} \cdot \frac{J}{\Gamma_1}} \sim 160\,(a_0)$$

Two distinct phase transitions are expected



- *Anomalies in elastic properties, sound velocity*
- *Spin quadrupole response: central peak (Raman)*

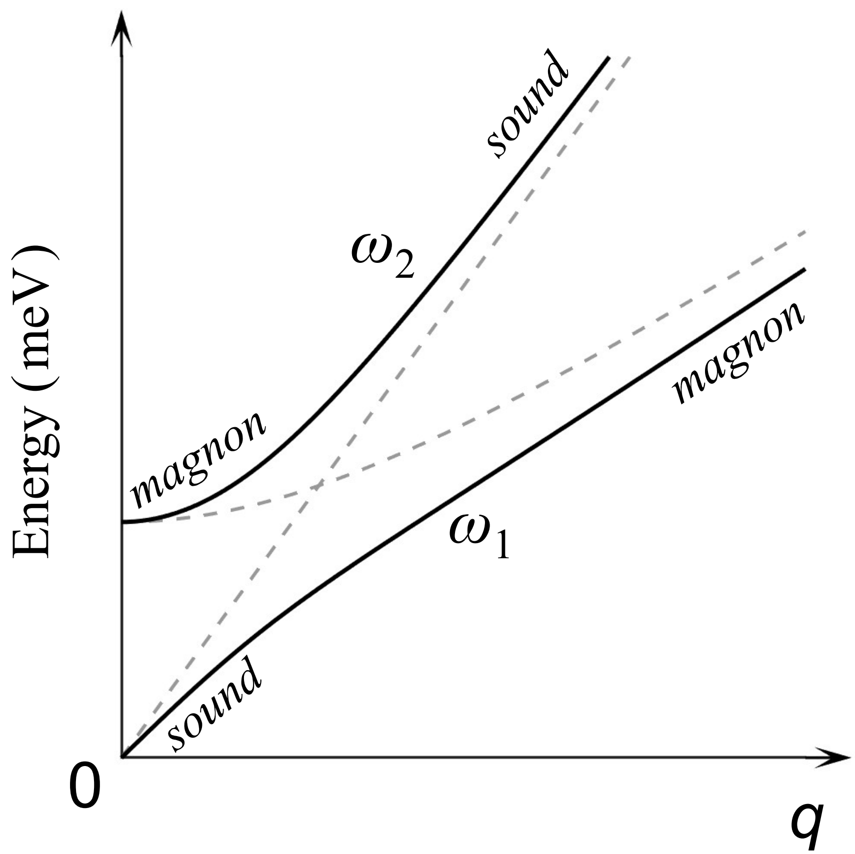
$v_{mag} >> v_{ph}$

Beyond Sr_2IrO_4:

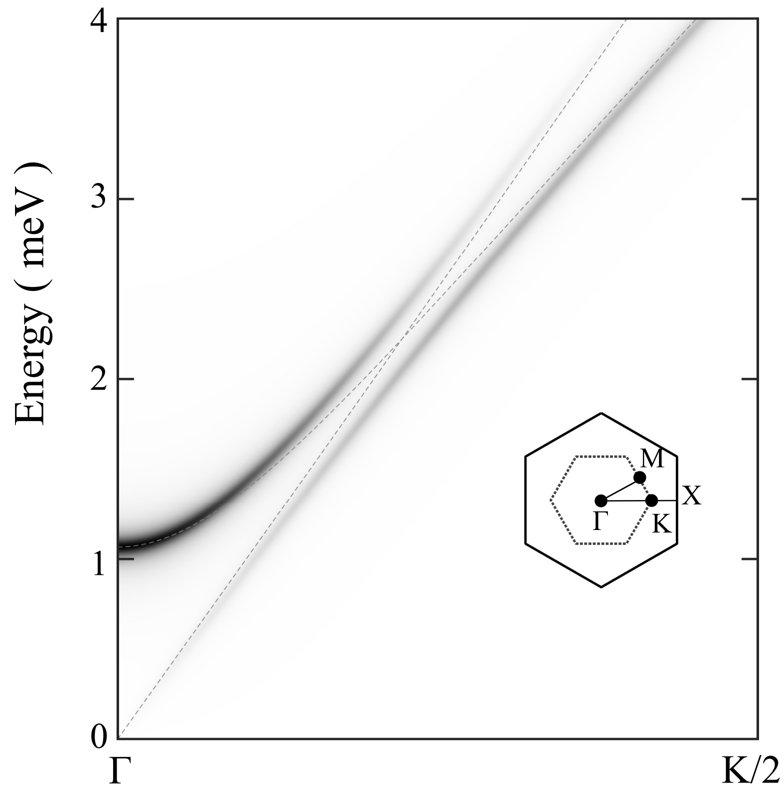
e.g. Kitaev materials

$v_{mag} \sim v_{ph}$

Magnon-phonon anticrossing



Magnetic intensity of the magnetoelastic waves



SPIN-ORBIT ENTANGLED MAGNETS

Direct link between magnetic moments and lattice

⇩

- *Lattice control of magnetic order and excitations*
- *Excitations with mixed spin and phonon character*

⇨ implications for spin & heat transport

Spin-only models are insufficient to describe the data

⇨ implications for „spin-liquid“ materials?

Kitaev + phonons: *Perkins et al.*
Hermanns et al.
Seifert et al.