Quantum order-by-disorder in ‘Kitaev model’ on a triangular lattice

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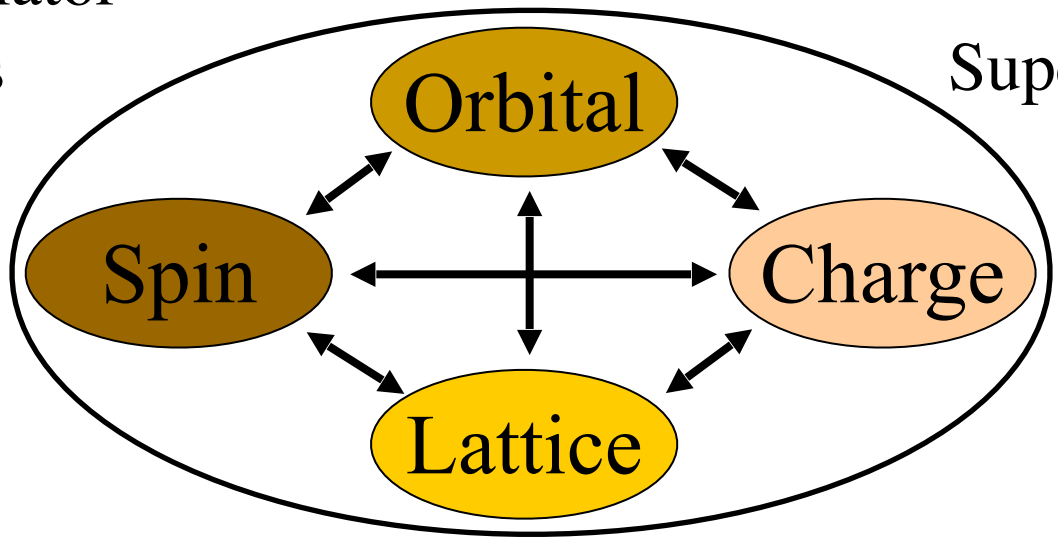
GJ & Avella, arXiv’15

SPICE @Mainz , May 23 , 2015

Transition metal oxides: Plethora of Challenging Phenomena

Metall to Insulator transitions

High-Tc Superconductivity

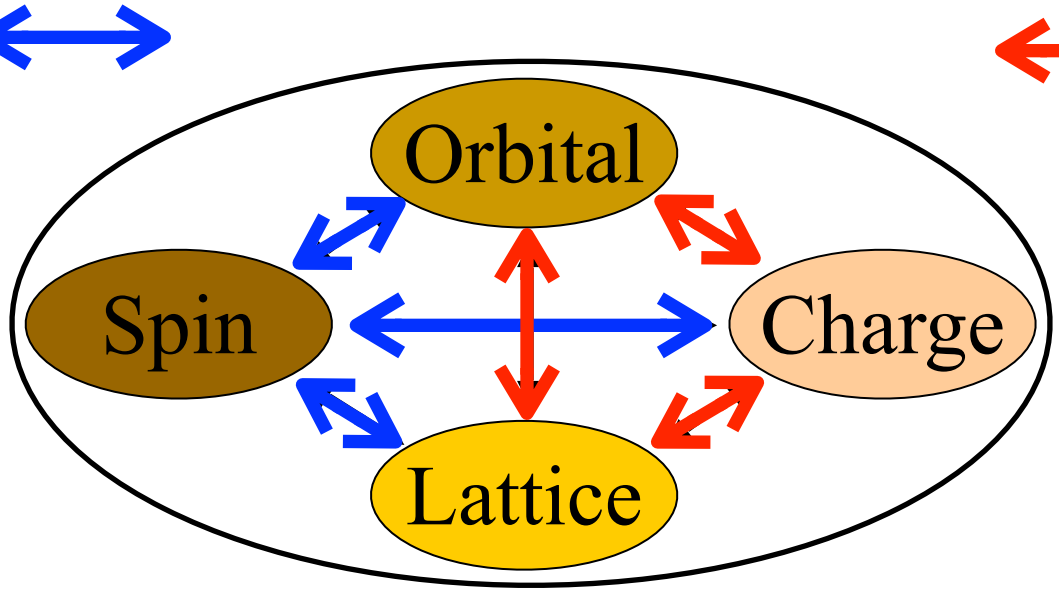


Colossal Magnetoresistance

Unexpected variety of phases and transitions between them

Relativistic in origin,
Spin-orbit coupling

Coulomb force



Enhance interplay by going to heavy TM elements

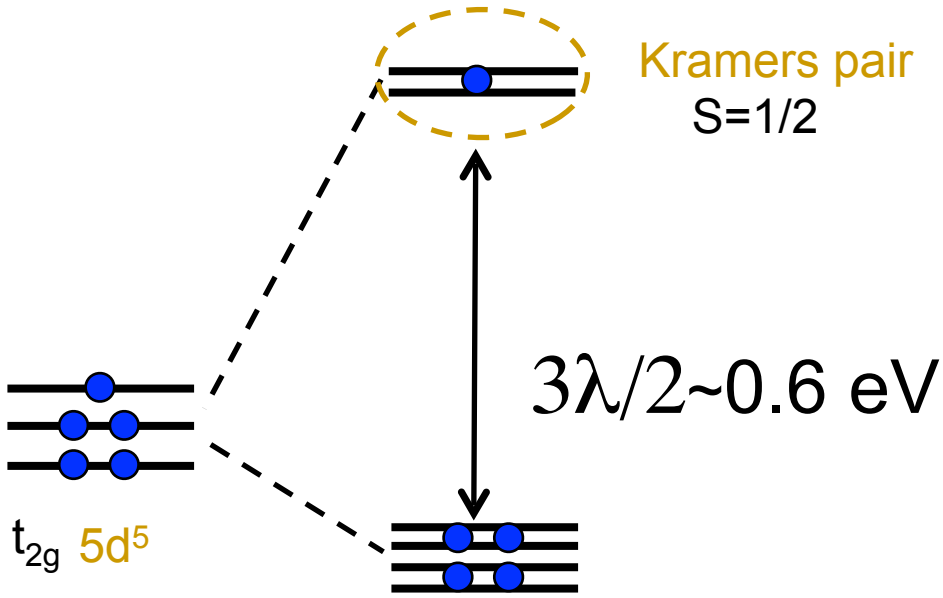
correlations

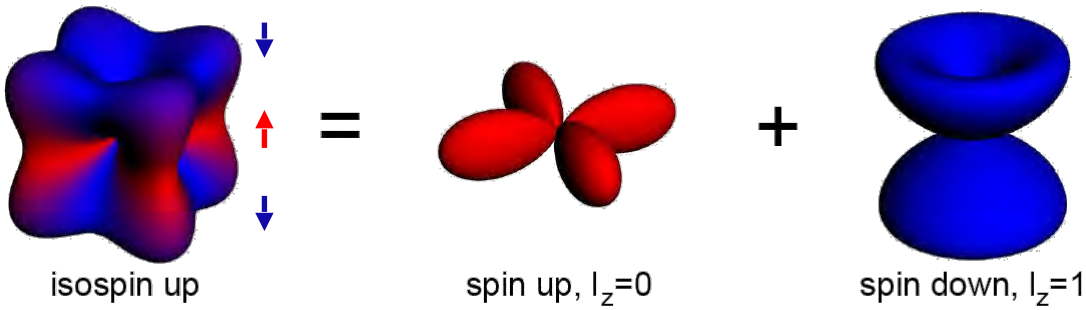
21	22	23	24	25	26	27	28	29	30
Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
44.9559	47.867	50.9415	51.9961	54.938	55.845	58.9332	58.6934	63.546	65.4089
Scandium	Titanium	Vanadium	Chromium	Manganese	Iron	Cobalt	Nickel	Copper	Zinc
39	40	41	42	43	44	45	46	47	48
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
88.9058	91.224	92.9064	85.94	98	101.07	102.9055	106.42	107.8682	112.411
Yttrium	Zirconium	Niobium	Molybdenum	Technetium	Ruthenium	Rhodium	Palladium	Silver	Cadmium
71	72	73	74	75	76	77	78	79	80
Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
174.967	178.49	180.9497	183.84	186.207	190.23	192.217	195.084	196.9666	200.59
Lutetium	Hafnium	Tantalum	Tungsten	Rhenium	Osmium	Iridium	Platinum	Gold	Mercury

spin-orbit

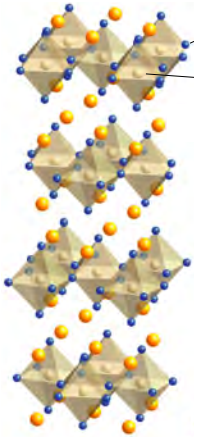
Kramers doublet of Ir^{4+}

A. Abragam and B. Bleaney, “EPR of Transition Ions”



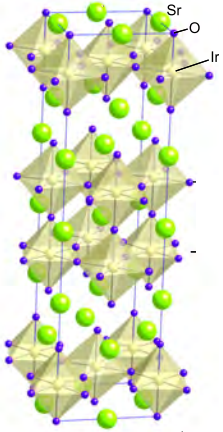


'Zoo' of Iridate compounds



Sr_2IrO_4

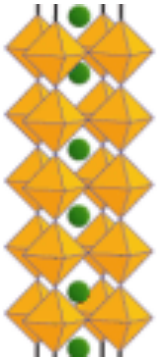
Heisenberg-like



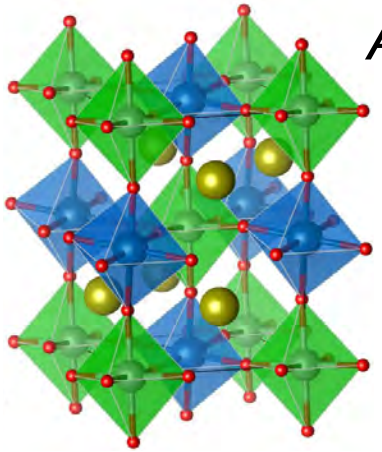
$Sr_3Ir_2O_7$

Ising-like

$SrIrO_3$

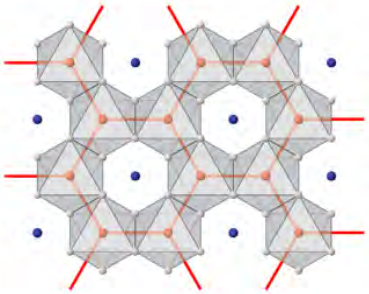


Semi-Metal,
Topological ?



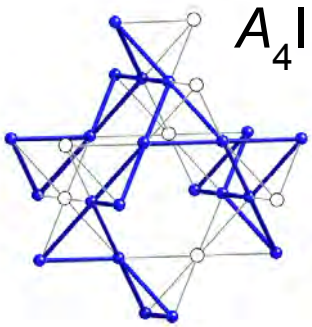
A_2BIrO_6

3d-5d Interplay



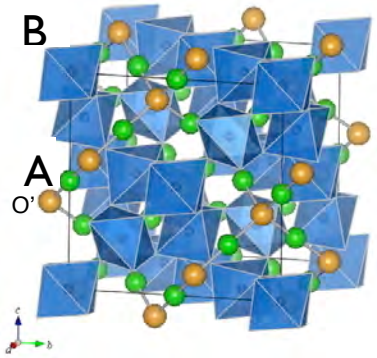
A_2IrO_3

Kitaev-like



$A_4Ir_3O_8$

QSL ?

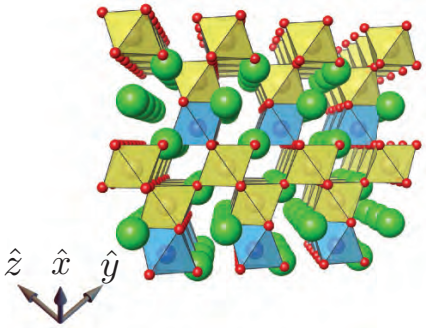


$A_2Ir_2O_7$

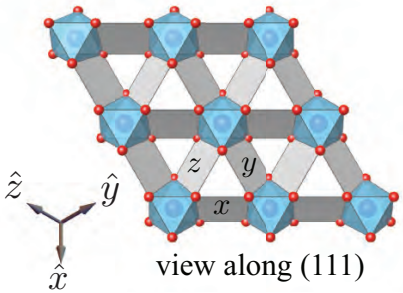
T-induced MIT,
Quantum critical metal

Trianglar lattice $Ba_3IrTi_2O_9$

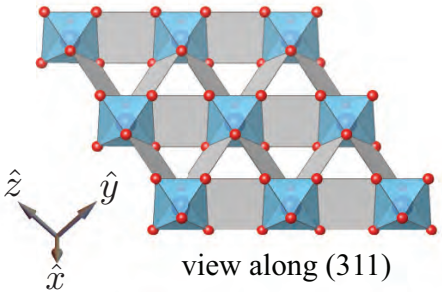
(a) crystal structure



(b) single Iridium layer

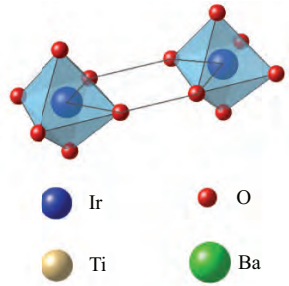


view along (111)



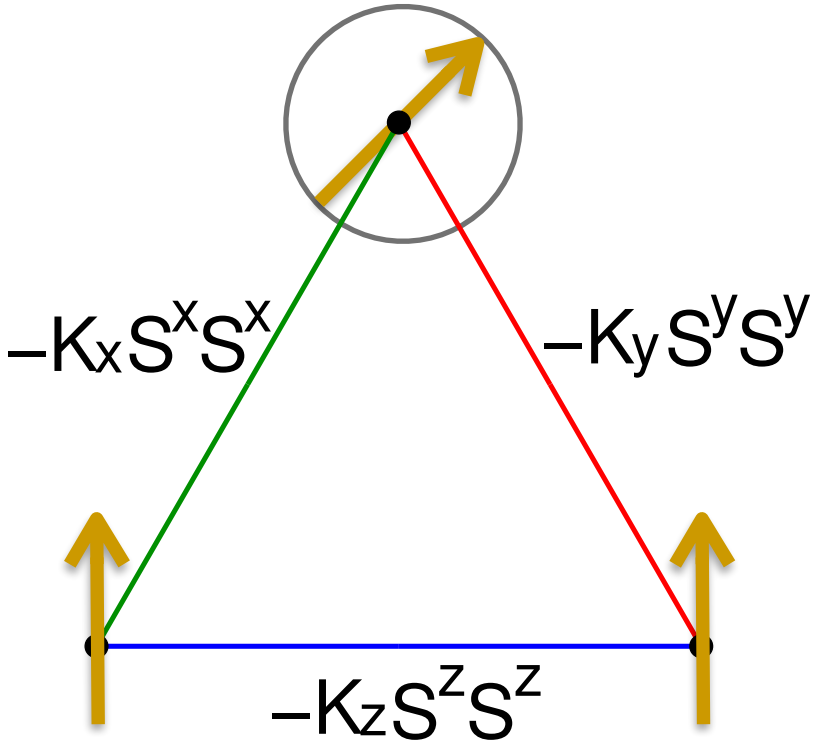
view along (311)

(c) Ir-O-O-Ir exchange path



from Becker et al PRB'15

Frustration from anisotropy

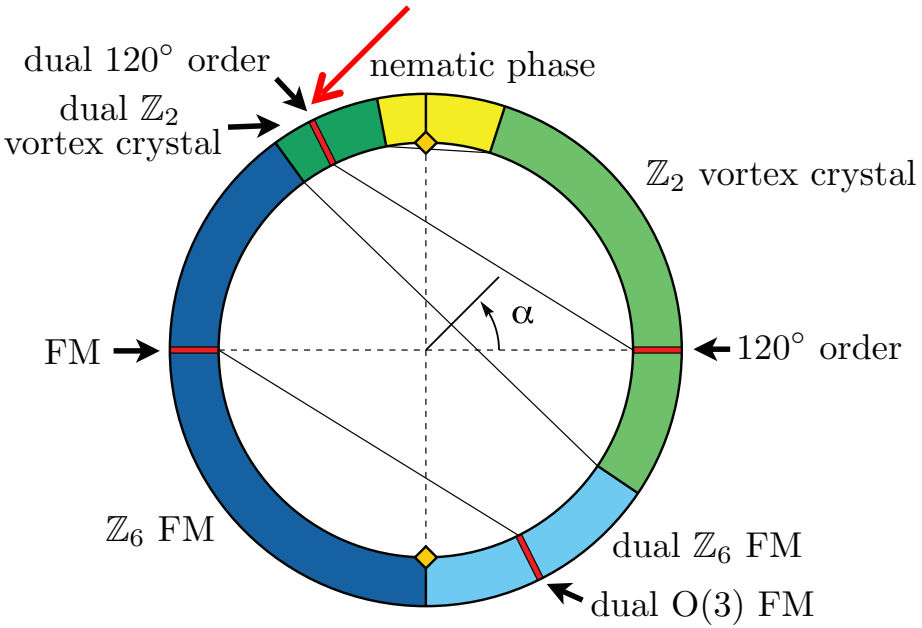


Impossible to satisfy simultaneously every pairwise interactions

⇨

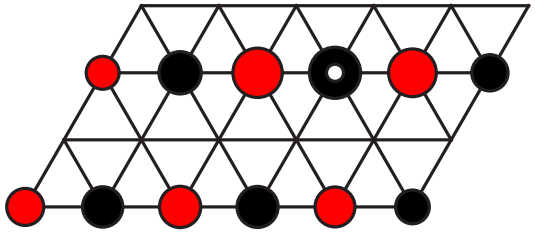
Infinitely many classical ground states

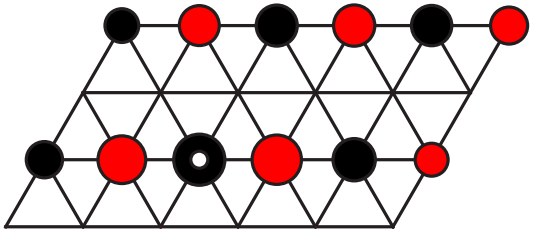
G. Khaliullin, PTPS'05



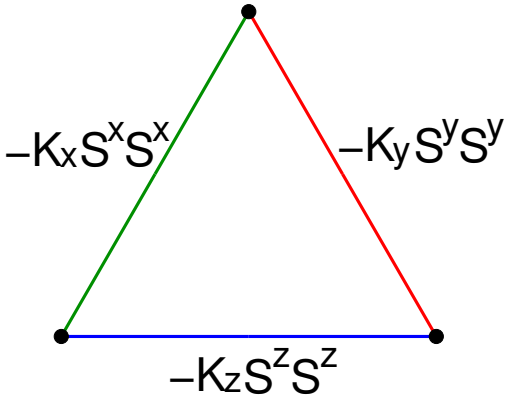
CMC simulations on Classical model:
Rousochatzakis et al, arXiv'14

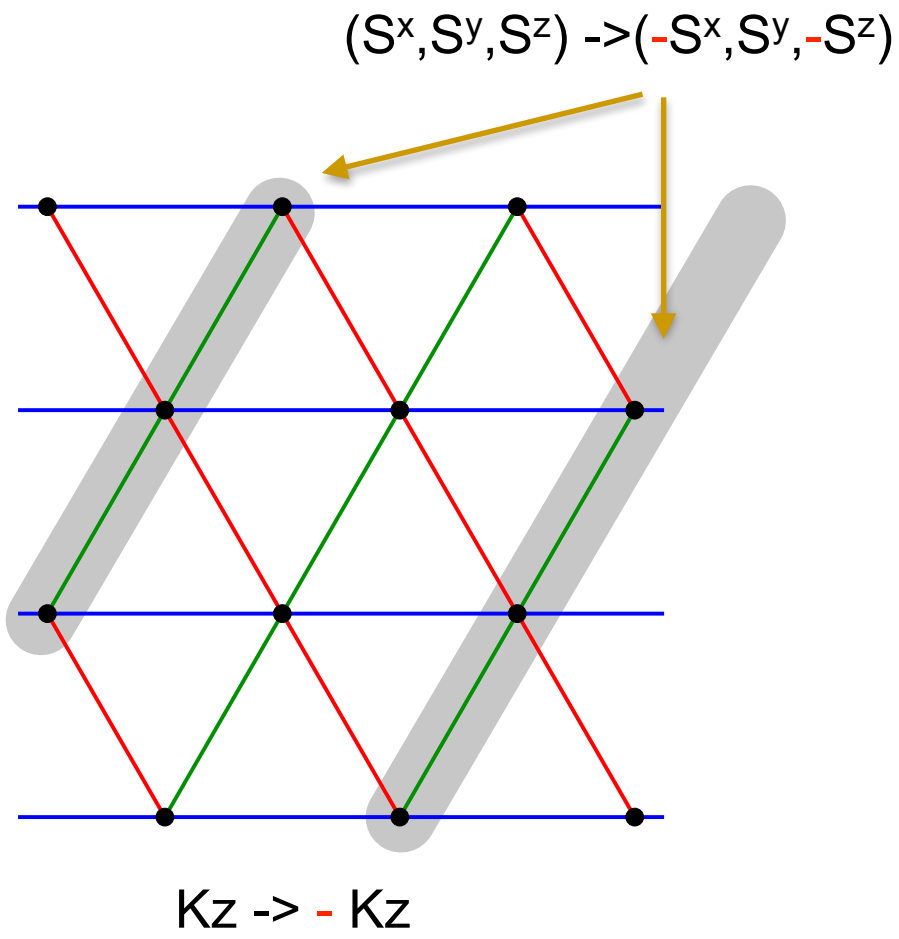
DMRG and ED on Quantum model:
Becker et al, PRB'15





Model on Triangular Lattice: Symmetry

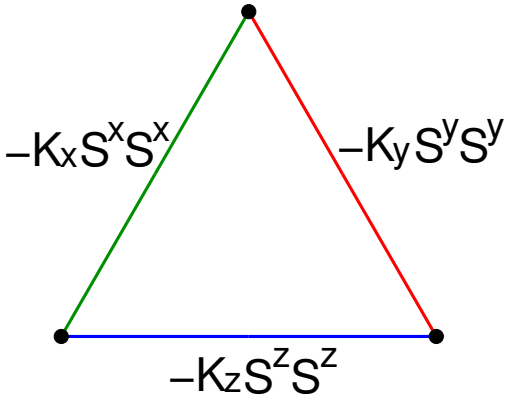


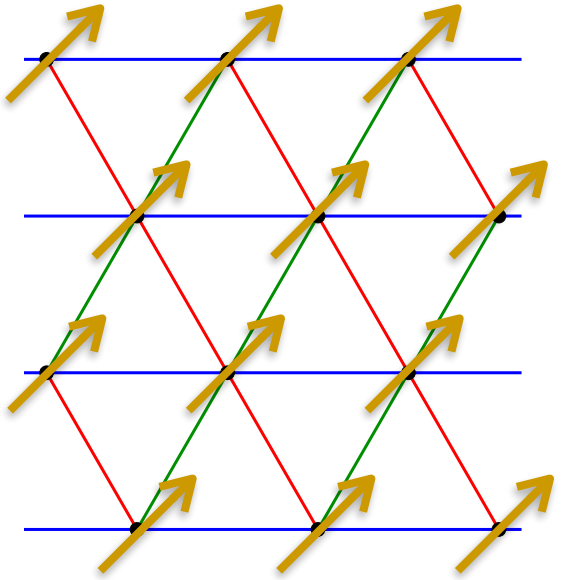


We can thus focus on the case all couplings being FM

Classical Ground State Manifold

$K_x=K_y=K_z>0$





In FM state Classical energy

$E=-(M^xM^x+M^yM^y+M^zM^z)=-M^2$

Global moment M can be freely rotated: accidental symmetry

Classical Ground State Manifold

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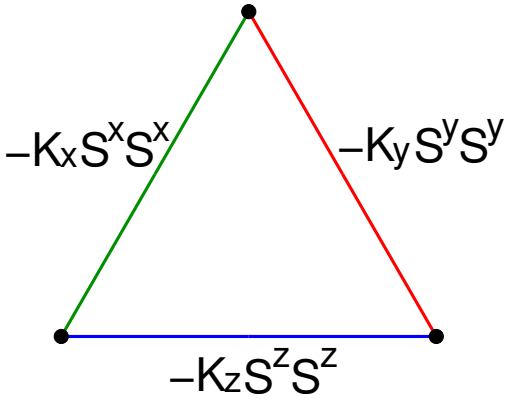
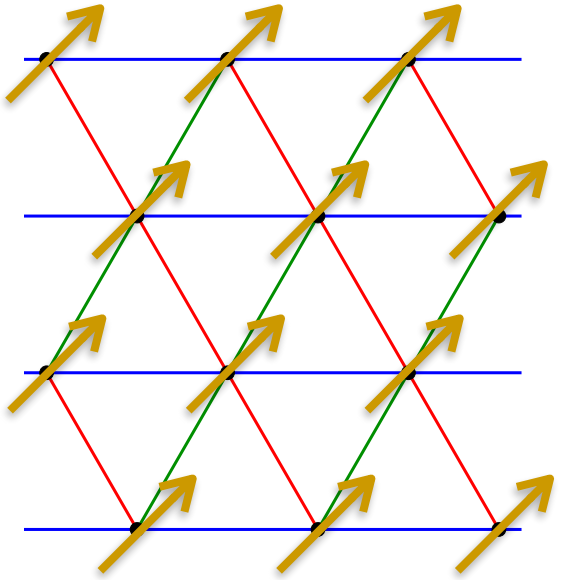


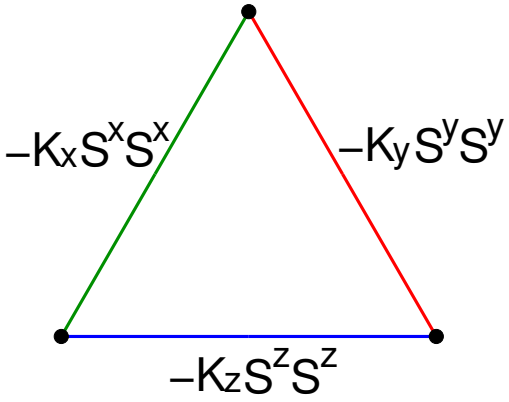


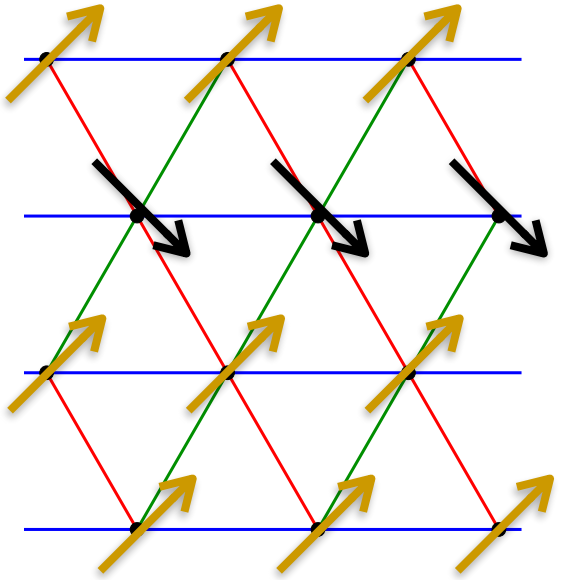
Coupling between NN chains

$E_{12}=-(M_1^xM_2^x+M_1^yM_2^y)$

Classical Ground State Manifold

$K_x=K_y=K_z>0$





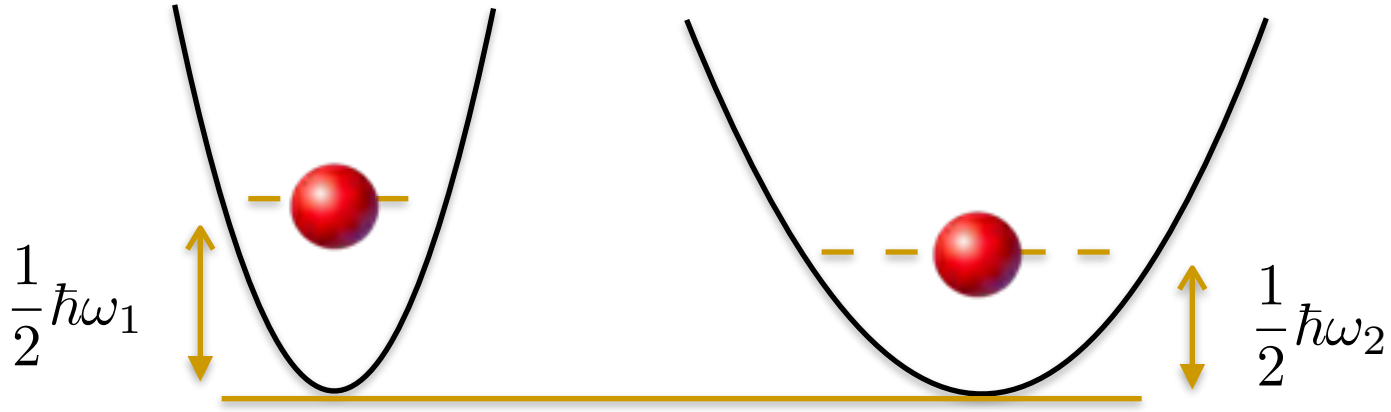
Coupling between NN chains

$E_{12}=-(M_1^xM_2^x+M_1^yM_2^y)$

M^z of each chain can be individually flipped

Classical Ground State Manifold

Accidental degeneracies - not related to symmetry: can be lifted by fluctuations



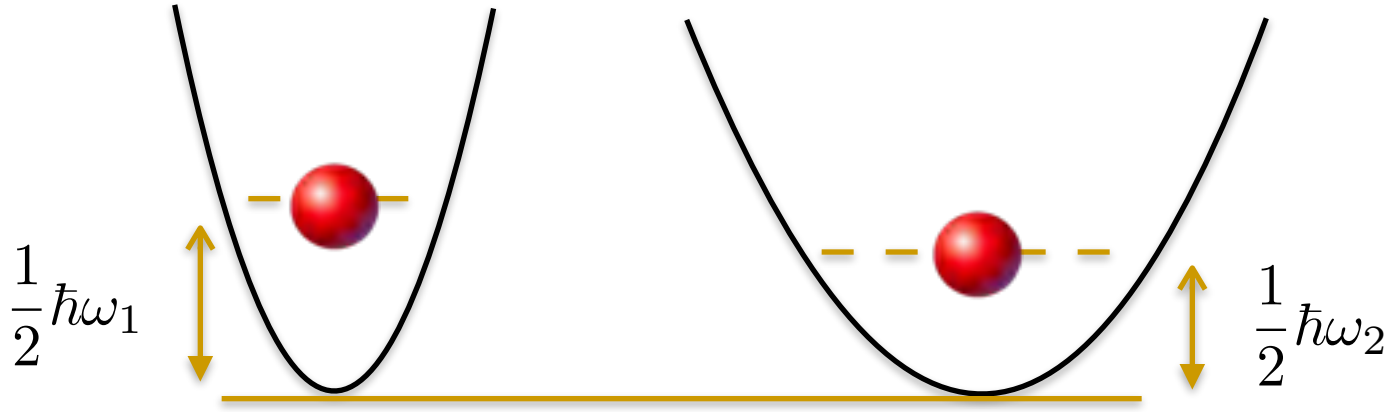
For magnets we need to calculate SW spectra for each Classical state and compare

$$\frac{1}{2}\sum \hbar\omega_n(k)$$

Not always possible!

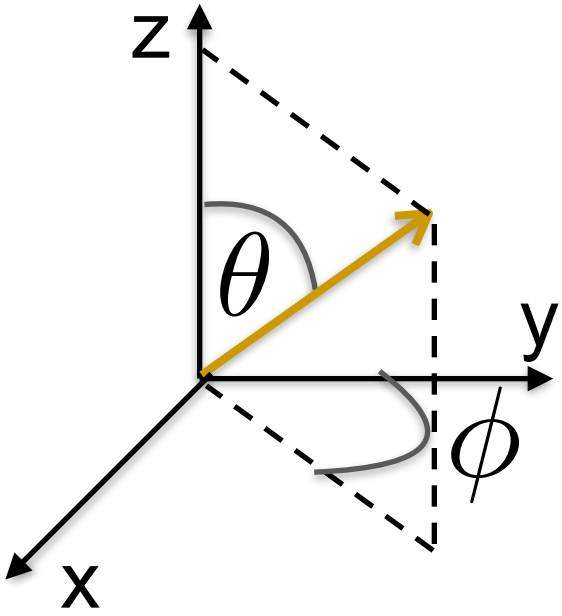
Classical Ground State Manifold

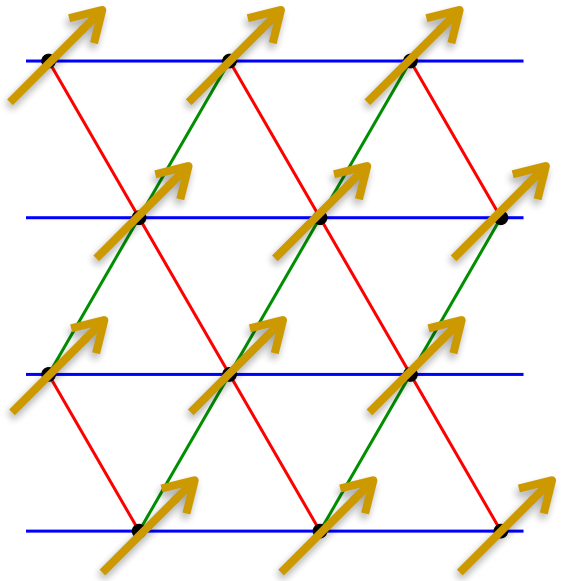
Accidental degeneracies - not related to symmetry:
can be lifted by fluctuations



Linked cluster expansion:
calculate corrections from short wave-length fluctuations

Selection of quantum easy axes





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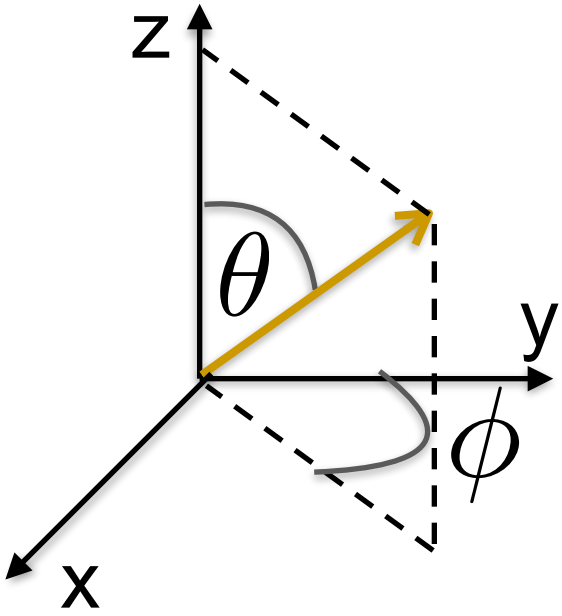
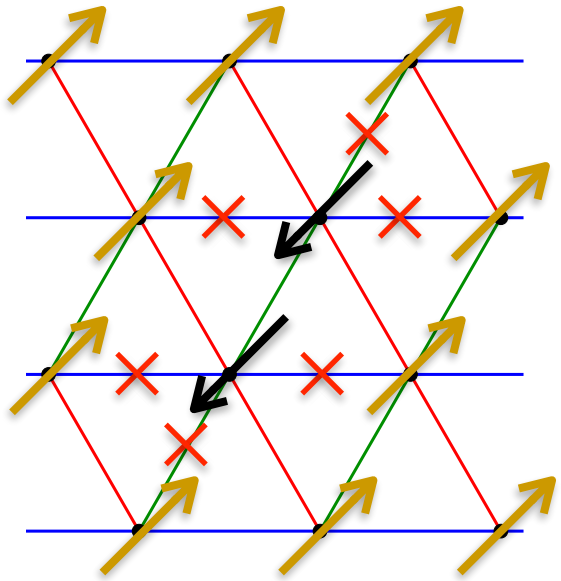
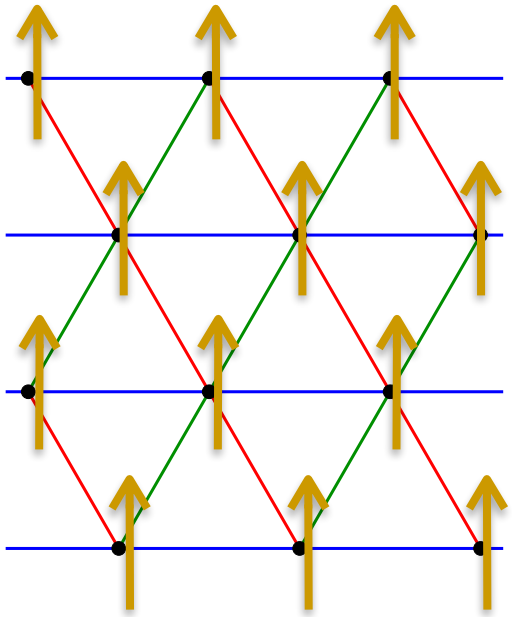
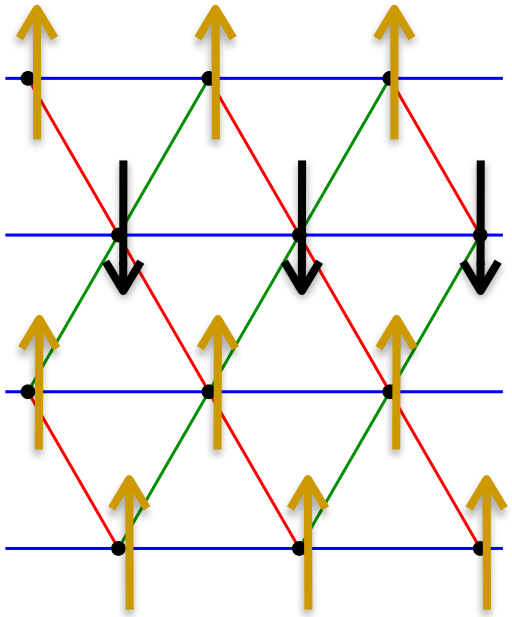




$$\delta E^{(2)}(\mathbf{m}) = -\sum_{\gamma} \frac{T_\gamma^2}{\Delta_\gamma} \simeq -\frac{3}{64}\left(1 + \frac{1}{6}\sum_{\gamma} m_\gamma^4\right)$$





Linked cluster expansion:
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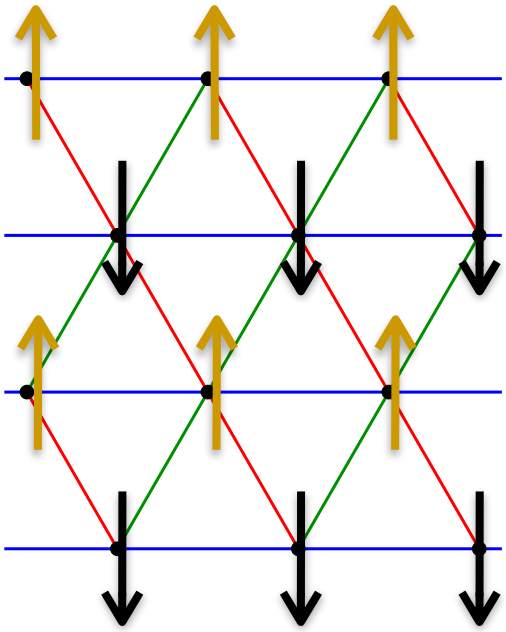
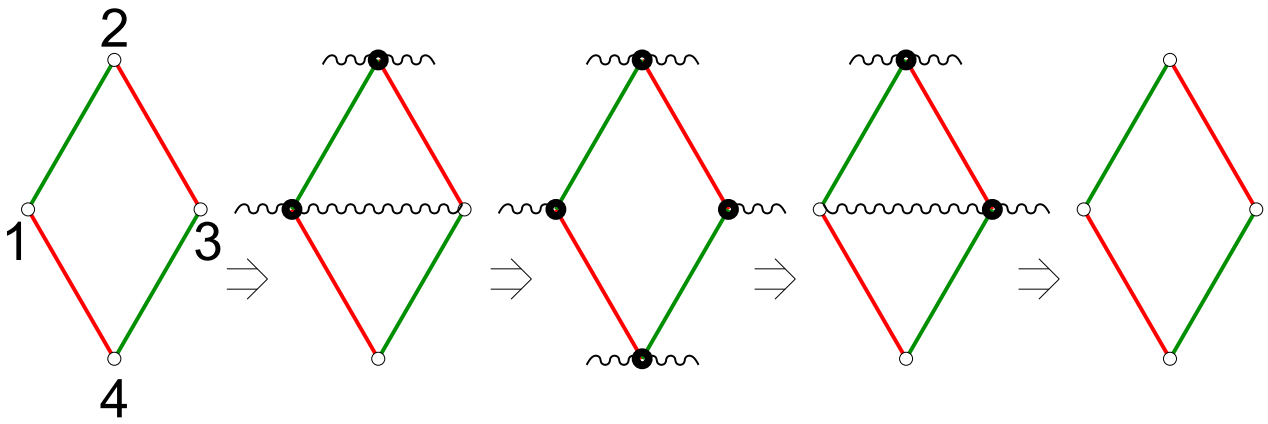
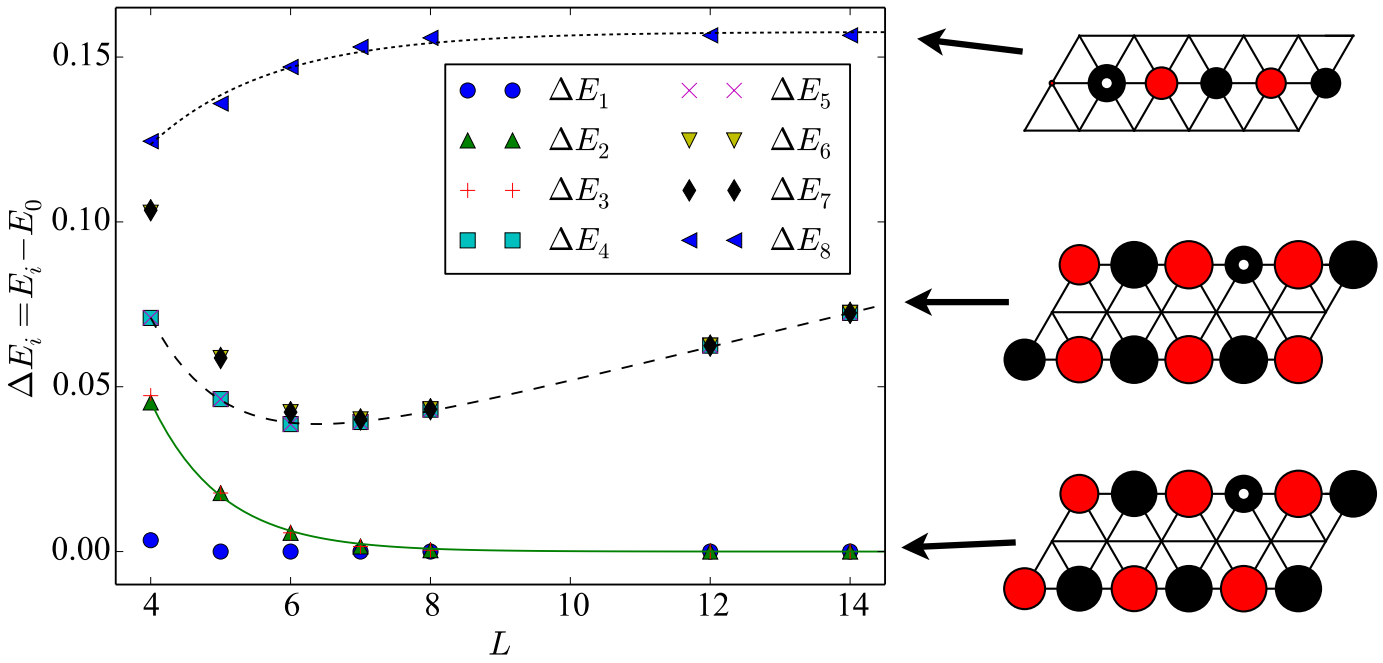




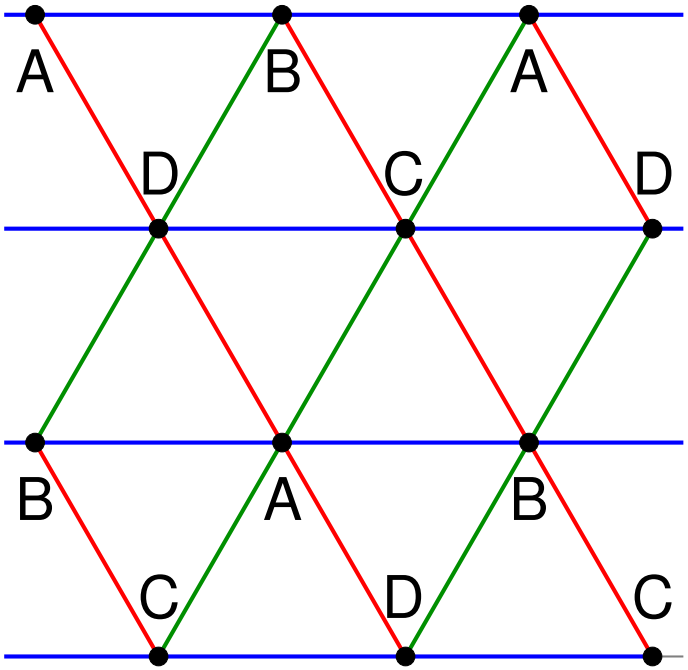
$$\delta\mathcal{H} = -D(S_1^z S_3^z) S_2^z S_4^z$$

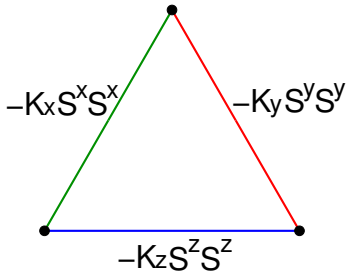
Gives the coupling between NNN chains,
forming two sub-lattices decoupled from each other



from Becker et al PRB'15

Symmetry protected degeneracy





Canonical transformation:

A: (x,y,z) B: (-x,-y,z)

C:(x,-y,-z) D:(-x,y,-z)

Hamiltonian remains unchanged,

but

z-comp. every 2nd chain gets flipped.

No correlations of z-comp

between NN chains