Dimer Phases in Orbitally Degenerate Quantum Magnets

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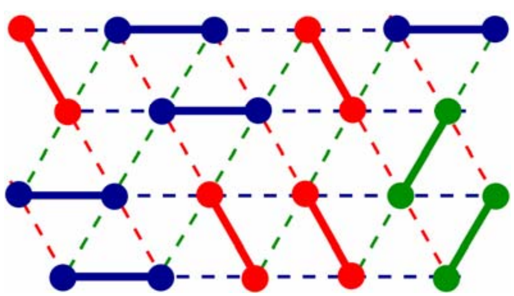


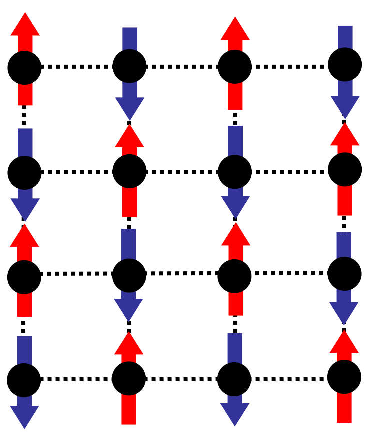
PRB 74, 132407 (2007)
PRB 72, 024431 (2005)
PRL 93, 077208 (2004)

Introduction

Isotropic quantum spin systems:
Two examples:

Long-range spin order

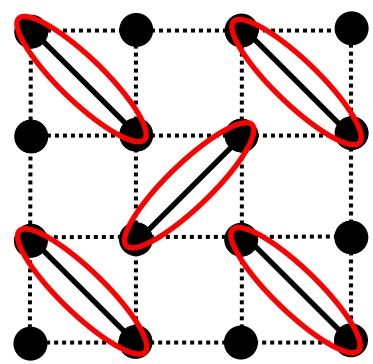
Square lattice HAFM



Goldstone mode:
Gapless spin waves

Valence-Bond Crystal

Shastry-Sutherland model



 $= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$

Gapped triplet excitations

Experimental examples

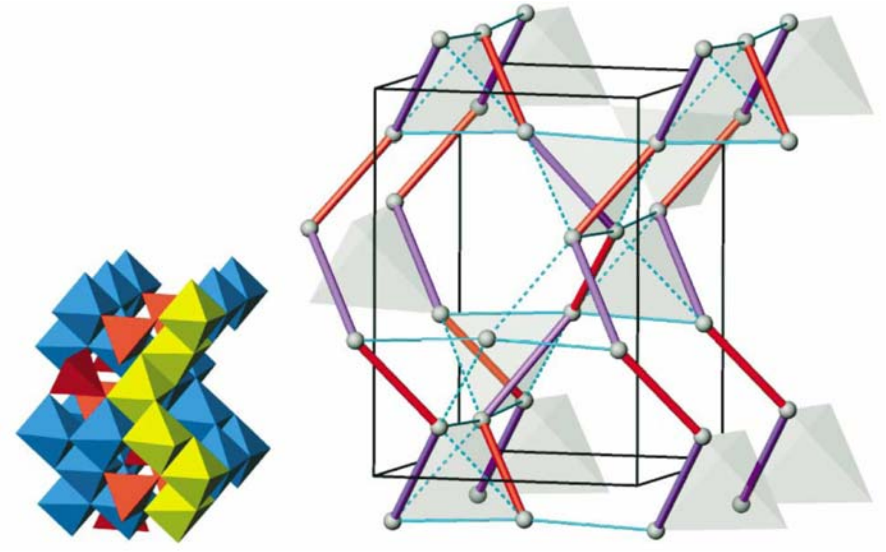
√ $MgTi_2O_4$--- Pyrochlore lattice

√ $NaTiO_2$ --- Triangular lattice

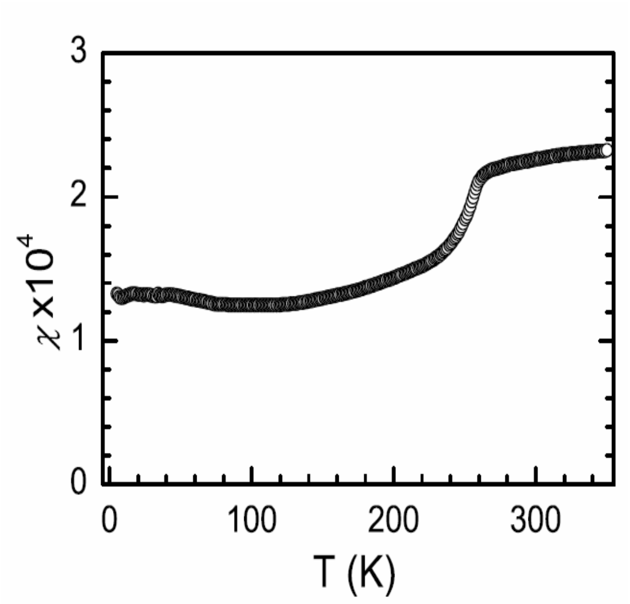
√ Sr_2VO_4 --- Square lattice

Experimental examples - $MgTi_2O_4$

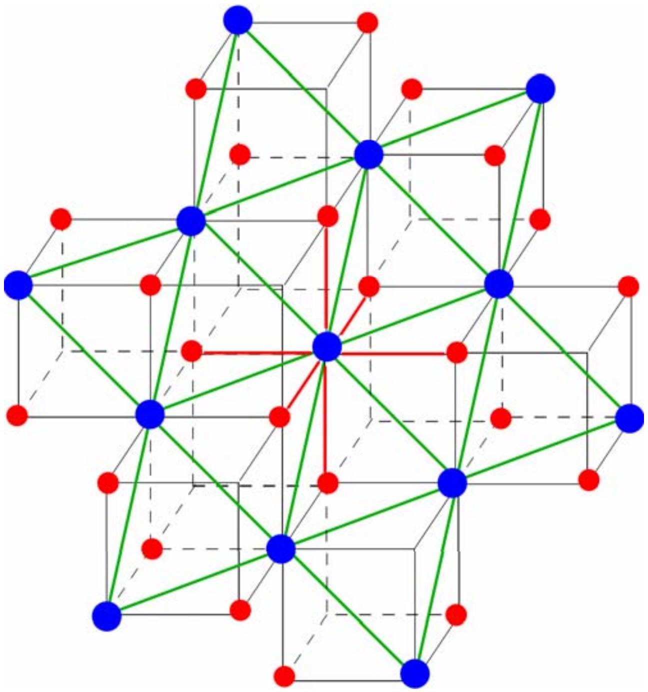
Schmidt et al. PRL'04



Isobe and Ueda JPSJ'02

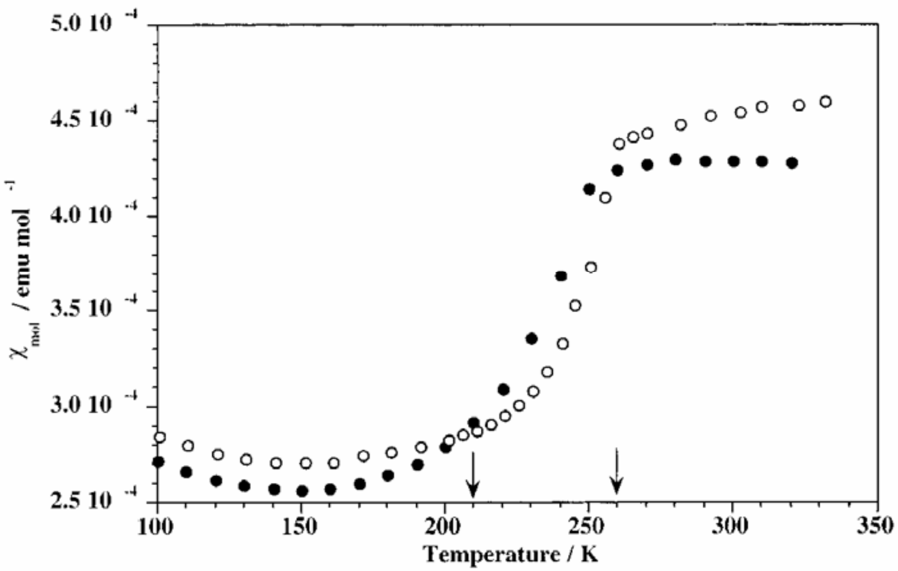


Experimental examples - $NaTiO_2$

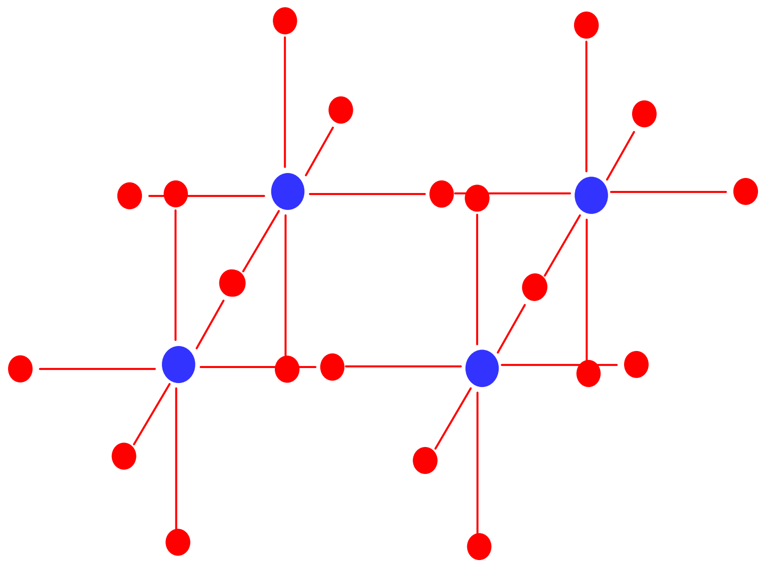


Takeda et al JPSJ'92

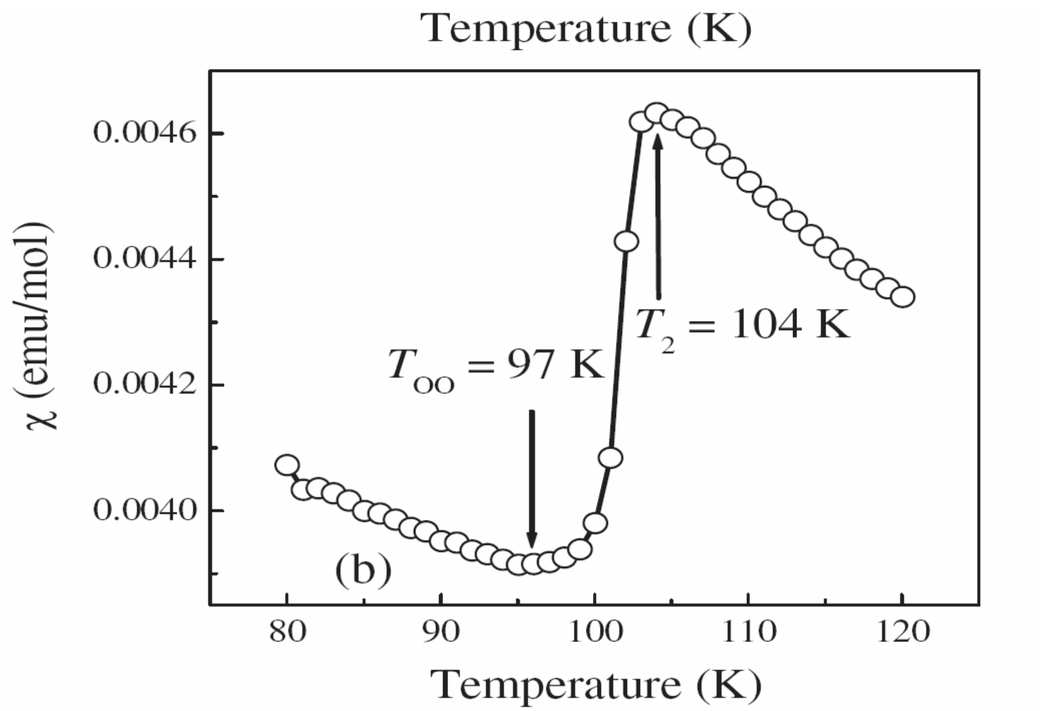
Clarke et al Chem.Mat.'98



Experimental examples - Sr_2VO_4

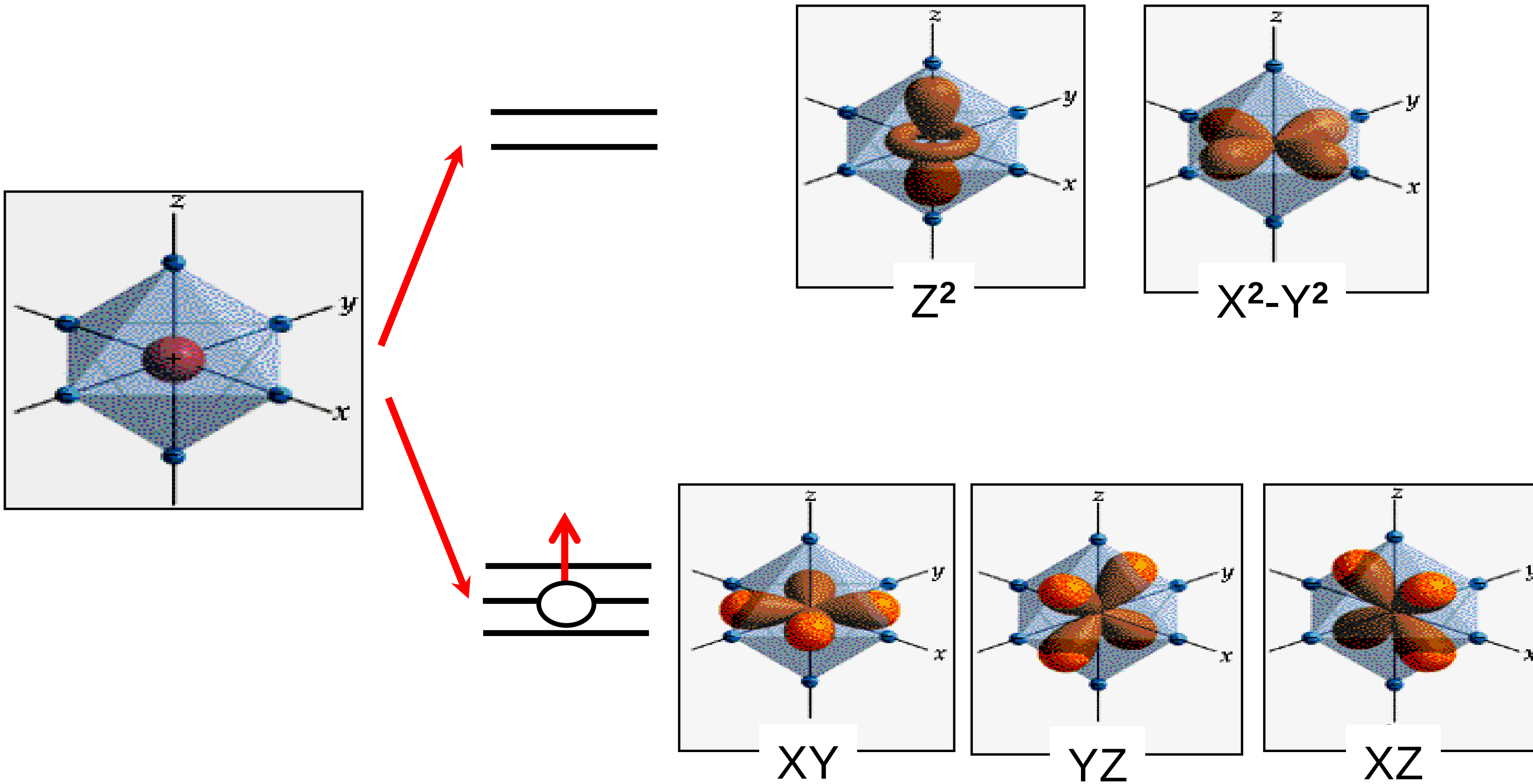


Zhou et al PRL'07



What these systems have in common?

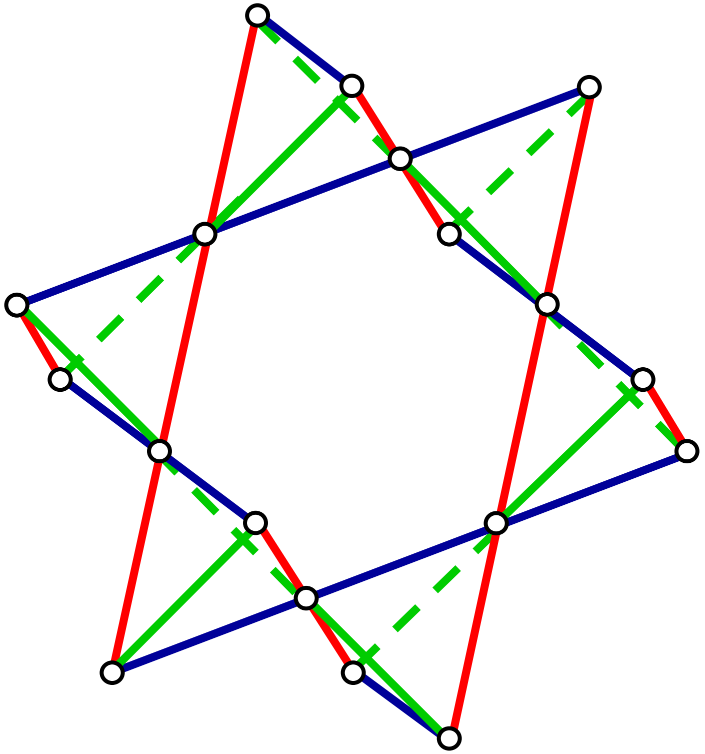
A) Orbital Degeneracy

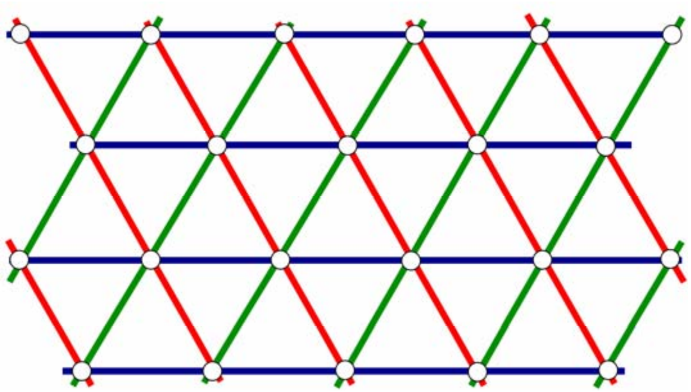


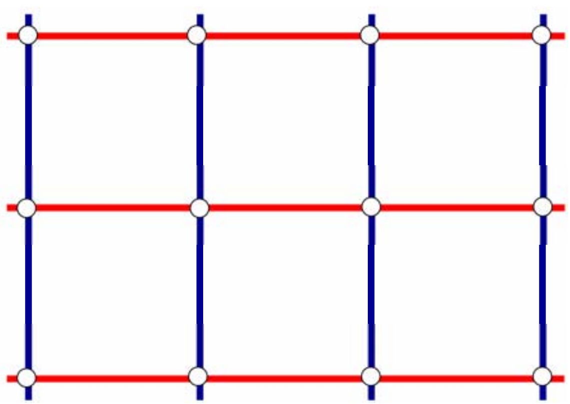
What these systems have in common?

B) Directional hopping of orbitals

XY XZ YZ



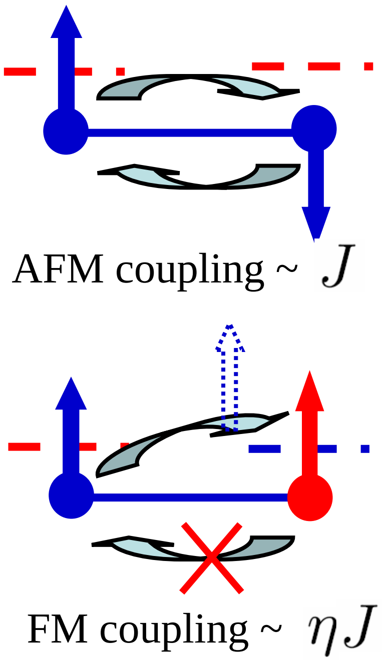




Coupled spin-orbital model

$$H = J_{\rm AF} \sum_{\langle ij \rangle} [\vec{S}_i \cdot \vec{S}_j / S^2 - 1] O_{ij}^{\rm OF}$$

$$- \sum_{\langle ij \rangle} [J_{\rm O} + J_{\rm F} \vec{S}_i \cdot \vec{S}_j] O_{ij}^{\rm OAF}$$



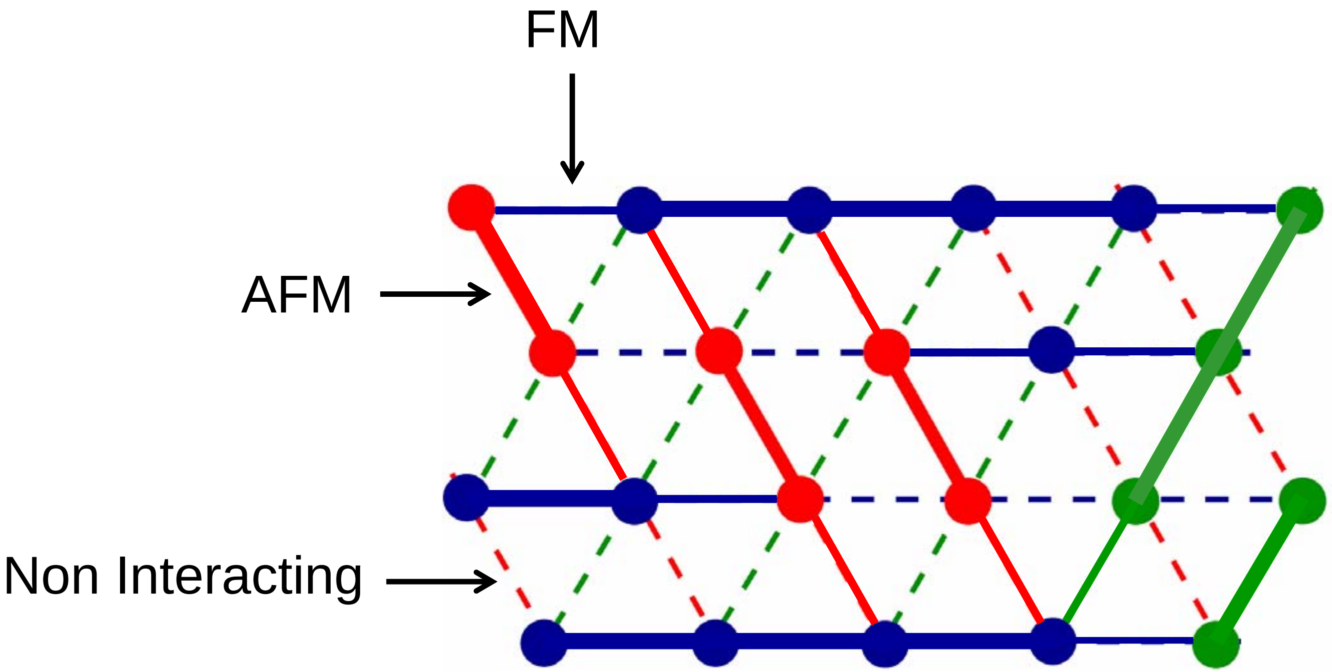
Couplings:

$$J_{\rm AF} \simeq J_{\rm O} \sim J = t^2/U$$

$$J_{\rm F} \sim \eta J, \quad \eta = J_{\rm H}/U \ll 1$$

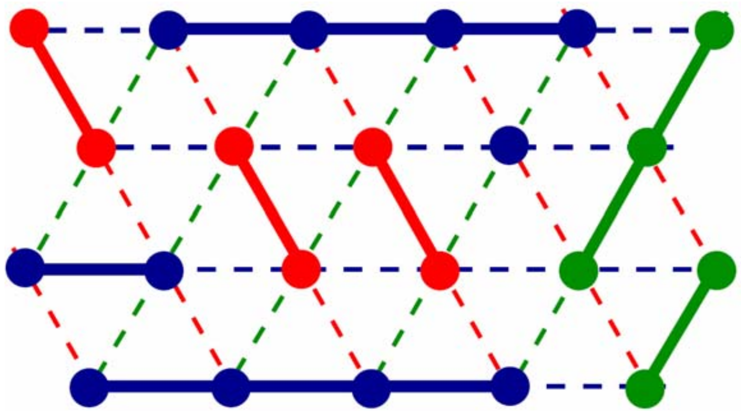
Orbital degrees are static Pott's-like!

Example of orbital and spin-coupling pattern



The limit of zero Hund's coupling

Reduction of Dimensionality:
Factorization in non interacting clusters of open 1D chains



$$H = E_0 + 4J \sum_{\langle ij \rangle} [\vec{S}_i \cdot \vec{S}_j + S^2] O_{ij}^{\mathrm{OF}}$$

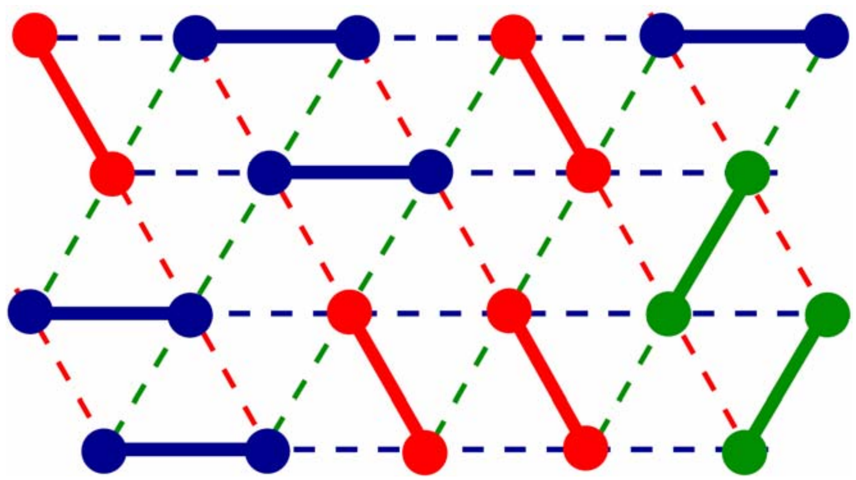
Extensive degeneracy of classical Neel type states ($S_i S_j + S^2 = 0$)

This is a feature of the Model but not of the underling lattice

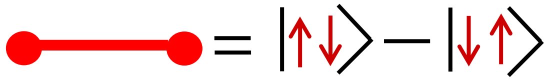
The ground state manifold

<u>Conclusion:</u> The ground state manifold is generated by hard-core dimer coverings with additional “no-chain” constraint.

Extensive orientational degeneracy



Each spin is bound into spin-singlet



Spin Gap

The Dimer GS is a feature of the Model but not of the underling lattice

Lifting the orientational degeneracy of dimers

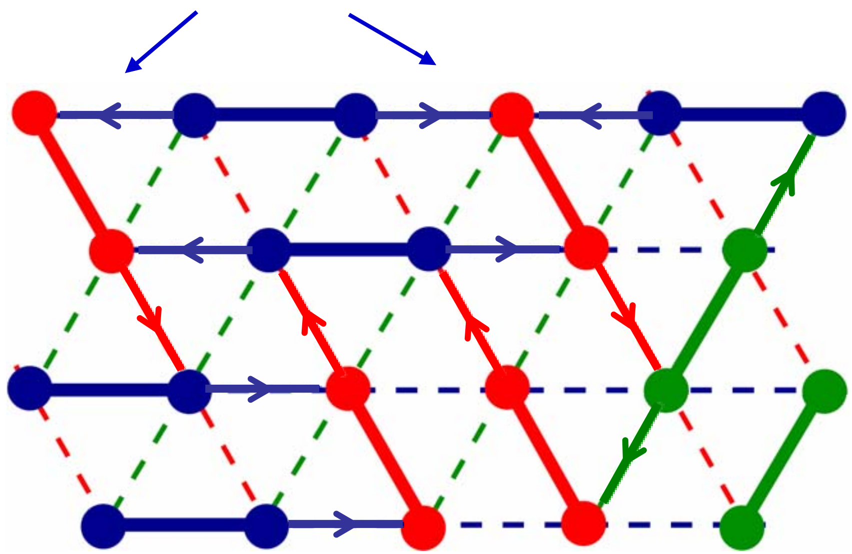
Possible scenarios:

- ✓ By weak Interdimer coupling ($\eta \neq 0$):
  Order-out-of disorder by triplet fluctuations

- ✓ By other interactions:
  Spin-Peierls like mechanism
  (relevant for MgTi2O4)

Order-out-of- disorder by triplet fluctuations

Weak FM interdimer coupling $\sim\eta$



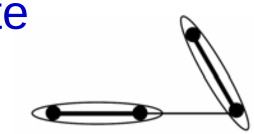
Different dimer coverings => different pattern of interdimer coupling:
Thus different zero point energy due to quantum fluctuations

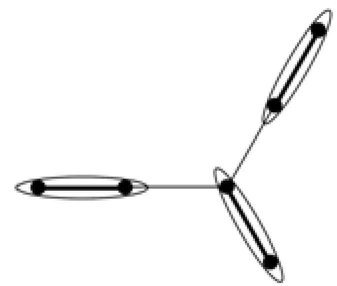
Order-out-of- disorder by triplet fluctuations

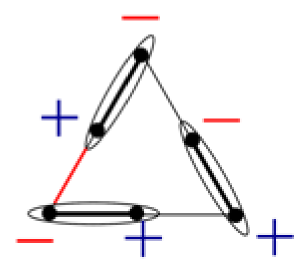
- Bond operator formalism: Mapping to hardcore bosons
- Linked graph expansion $E[\{N_c\}]=\sum_{\{c\}} E_c N_c$

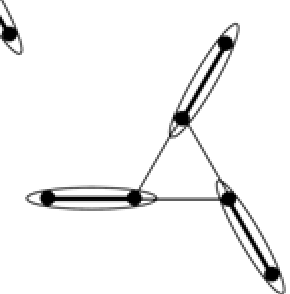
Tree-like graphs with n links contribute

to the leading order as η^{2n}



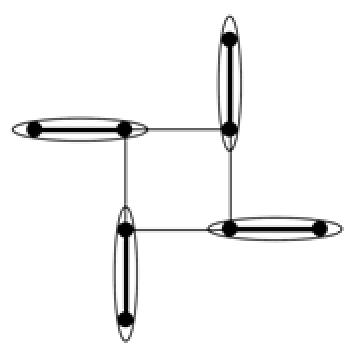


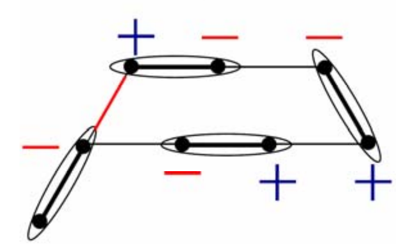




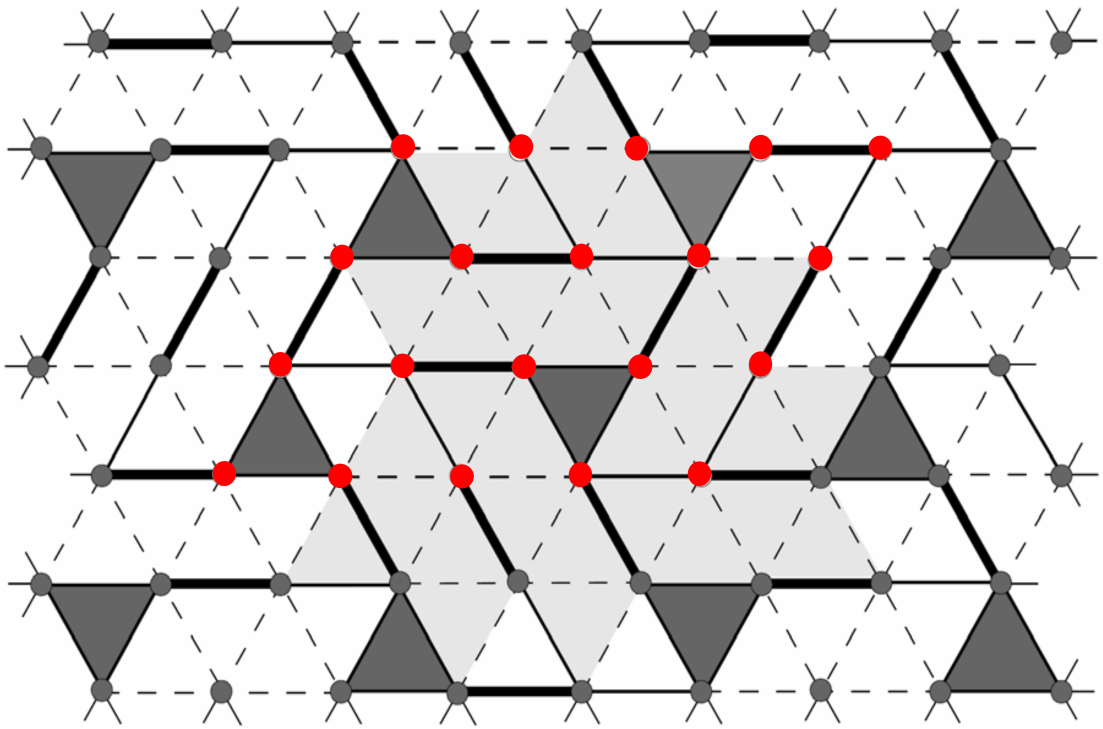
Loop-like graphs with n links contribute

to the leading order as η^{n}

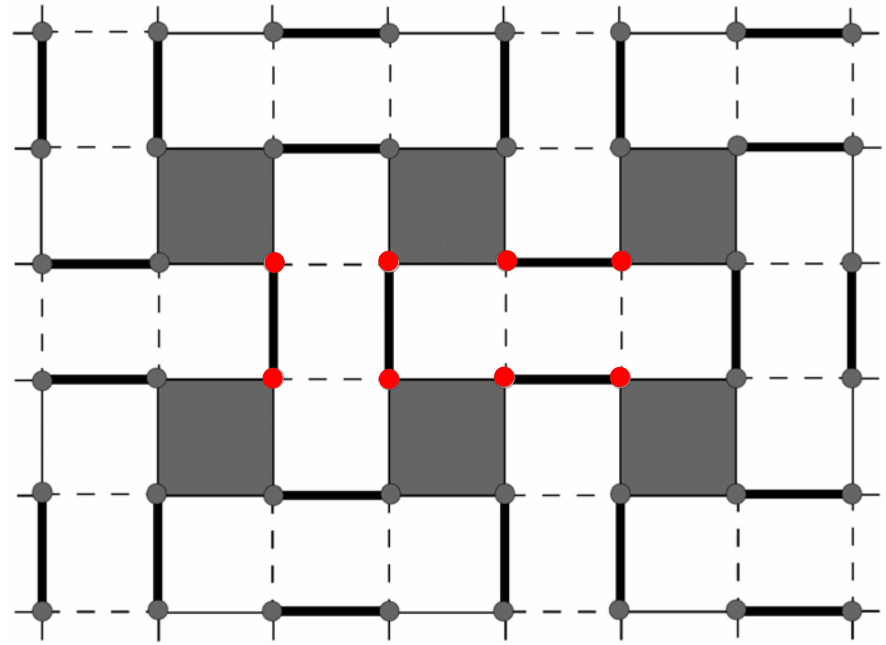




VBC on Triangular lattice



VBC on Square lattice



Lifting of degeneracy by magneto elastic coupling

Magnetoelastic coupling

$$\Delta E_{ij}^{mag} = \left[\frac{\partial J(d)}{\partial d} \right]_{d=d_0} \delta d_{ij} (\vec{S}_i \cdot \vec{S}_j)$$

Shortening of the strong bond
=Gain of magnetic energy

Elastic energy

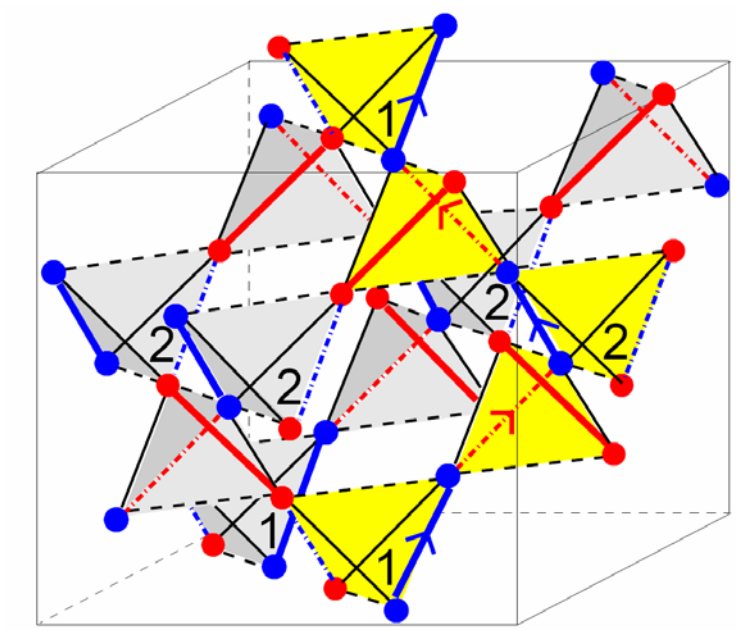
$$\Delta E_{ij}^{el} = \frac{C_0}{2} \frac{(\delta d_{ij})^2}{d_0^2}$$

Different distortion pattern
Costs different elastic energy

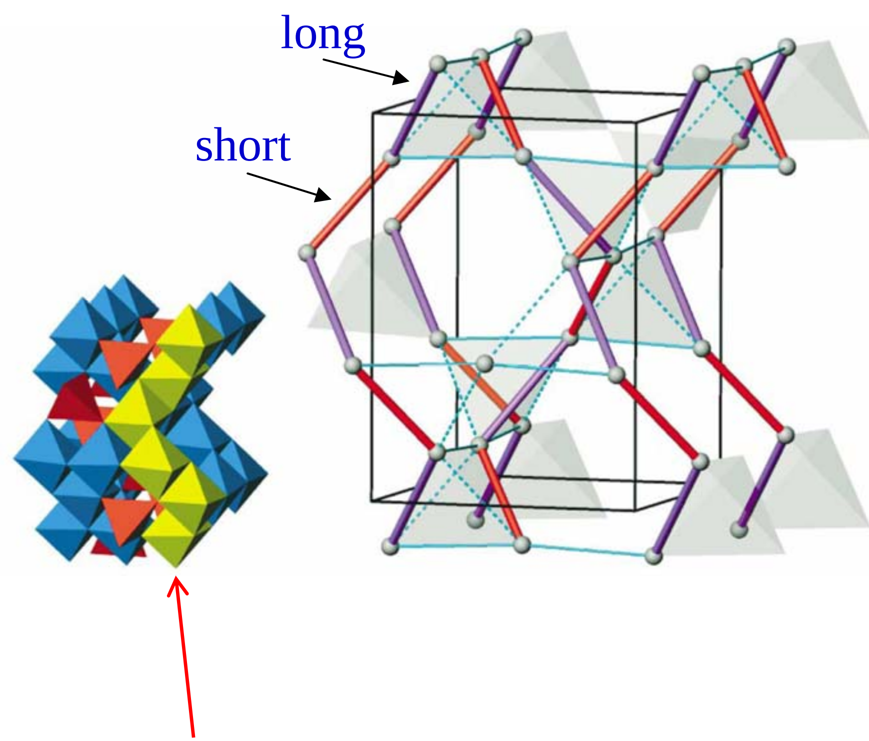
Selection of ground state

Lifting of degeneracy by magneto elastic coupling

Application to a pyrochlore lattice



Schmidt et al. PRL'04



- Dimers condense in Valence Bond crystal forming a helical pattern

- Orbital order is Ferro-type along helix and Antiferro between them

Dimerized helical pattern

Conclusions & Outlook

- Orbital induced frustration of spins
  - ⇨ Spin gap formation and spontaneous dimerization in D>1
- Exact realization of classical dimer problems
- Degeneracy lifting by perturbations
  - ⇨ Formation of different types of VBC

Open Issues:

- Finite temperature properties:
  - ⇨ Susceptibility, thermodynamics, VBC melting
- Role of quantum fluctuations of orbitals
  - ⇨ Quantum dynamics of dimers