Spatially anisotropic S=1/2 Heisenberg Kagome antiferromagnet

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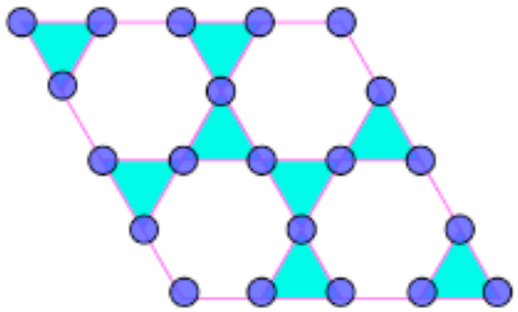
PRB 78, 174420 (2008)



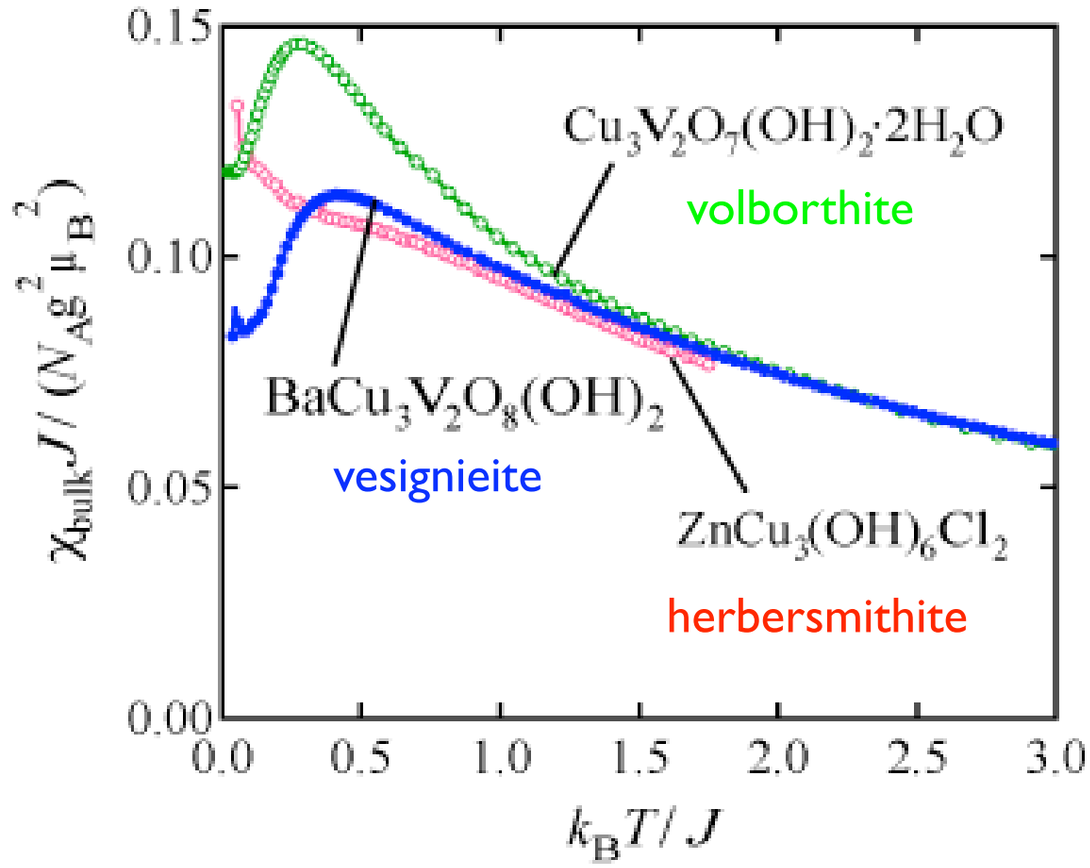
Thanks to J.-S. Caux for numerical data

Kagome spin-1/2 antiferromagnet: from model to experiments

archetype spin liquid for many years



no order for T << J

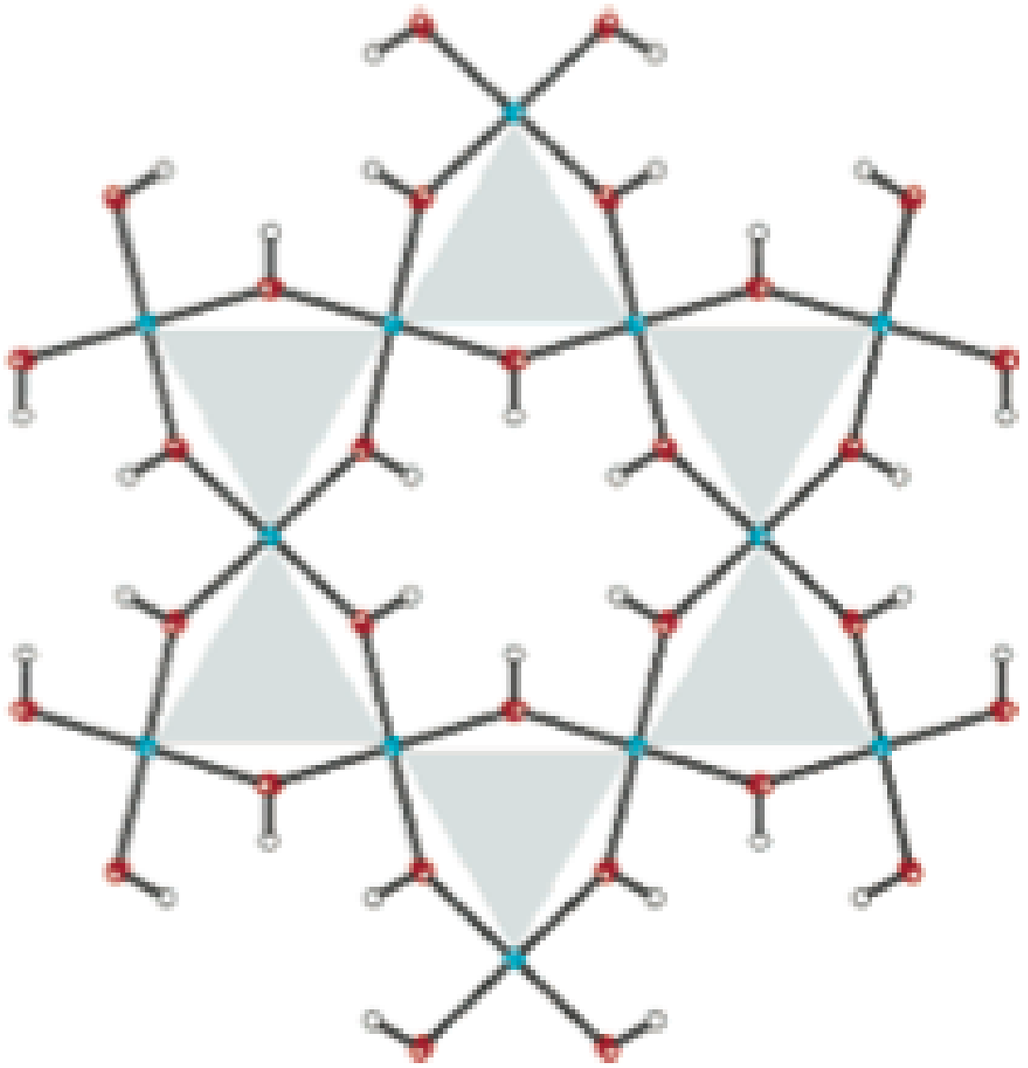


Hiroi et al. 2001, Shores et al. 2005, Okamoto et al. 2009

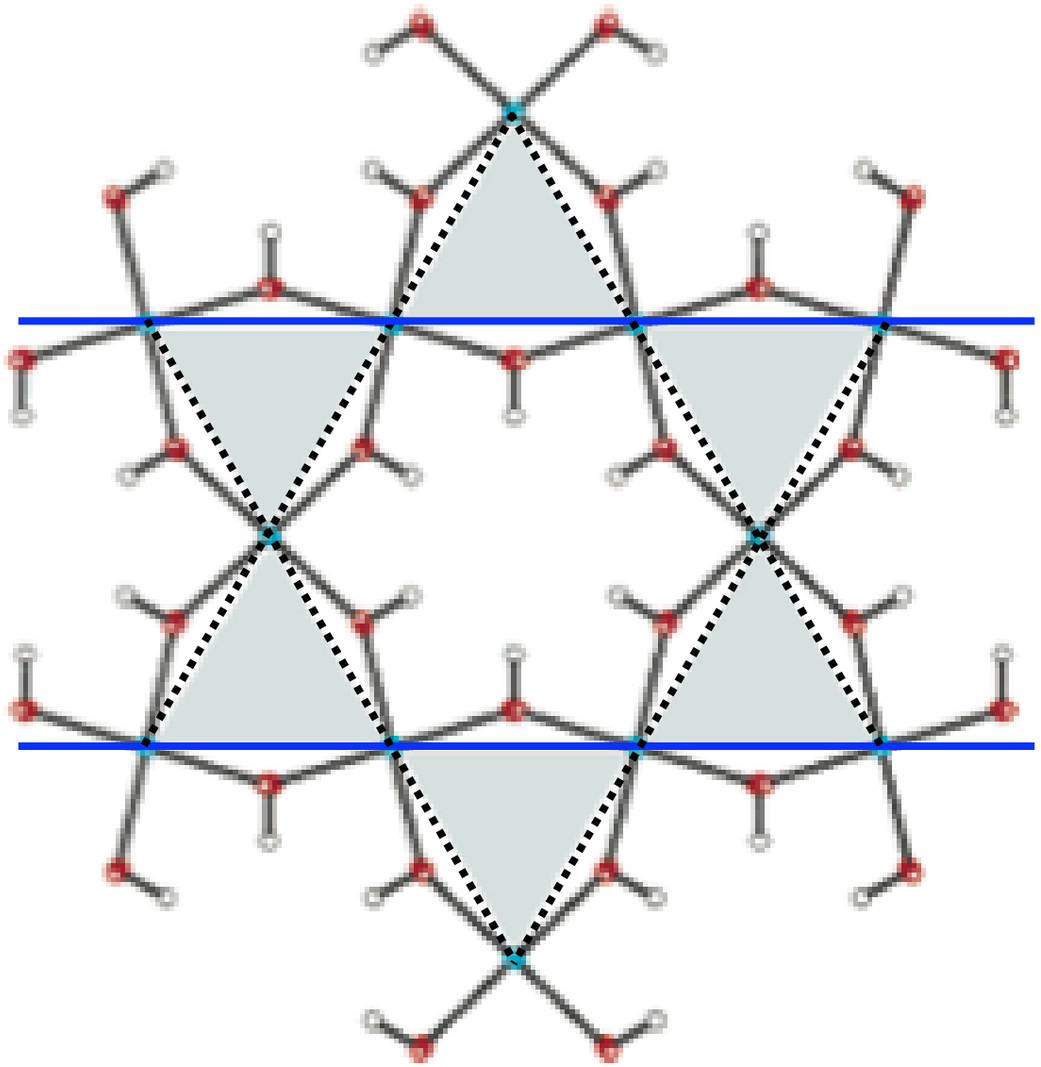
Outline

- Motivation
  - strong spatial anisotropy offers well controlled analysis
  - relevant experimentally
- Description of the J' << J limit
- Separation of scales
  - interstitial spins ordering via RKKY
  - subsequent order of chain spins
- Non-coplanar ordered state/coplanar ferrimagnetic
- Comparison and conclusions

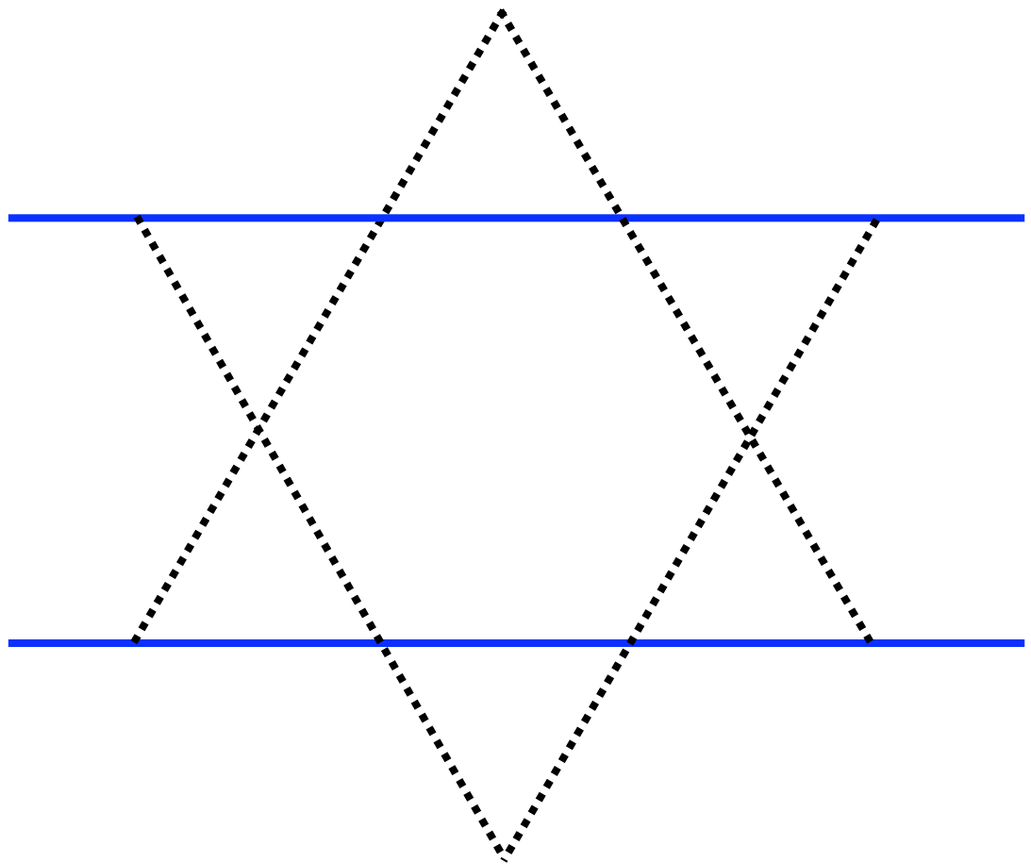
Volborthite $Cu_3V_2O_7(OH)_2\ 2H_2O$



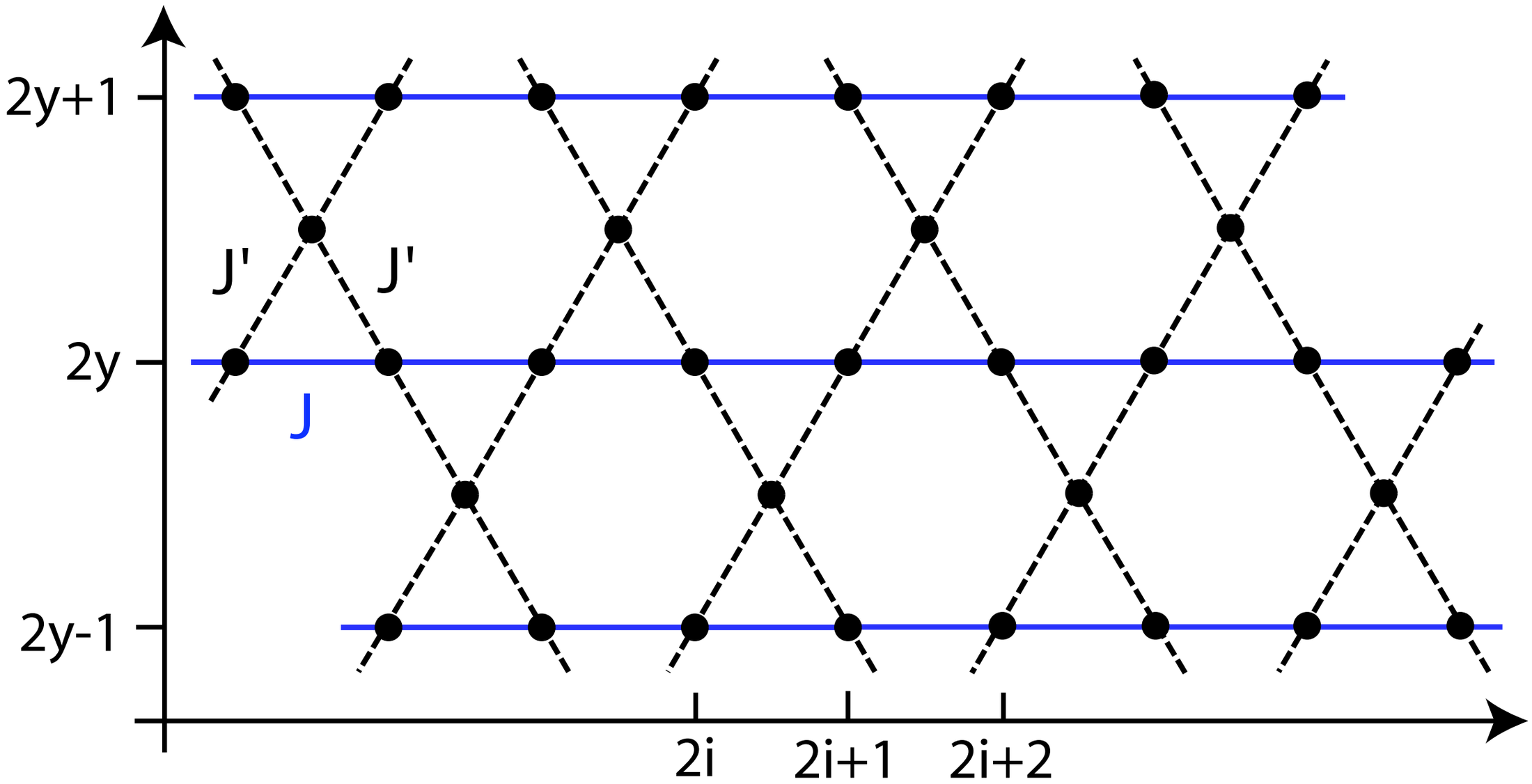
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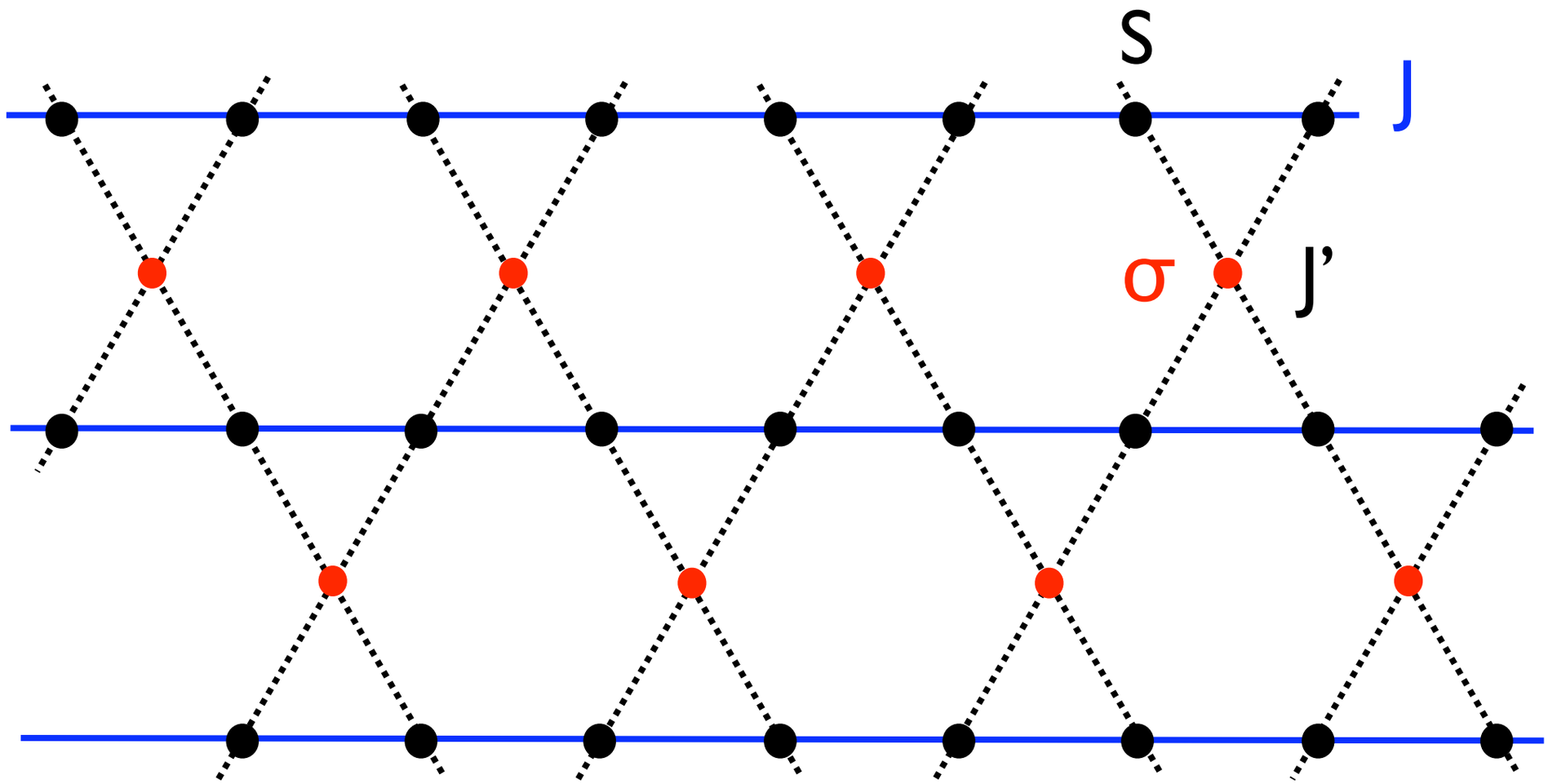
Volborthite $Cu_3V_2O_7(OH)_2\ 2H_2O$



Spatially anisotropic geometry



The model



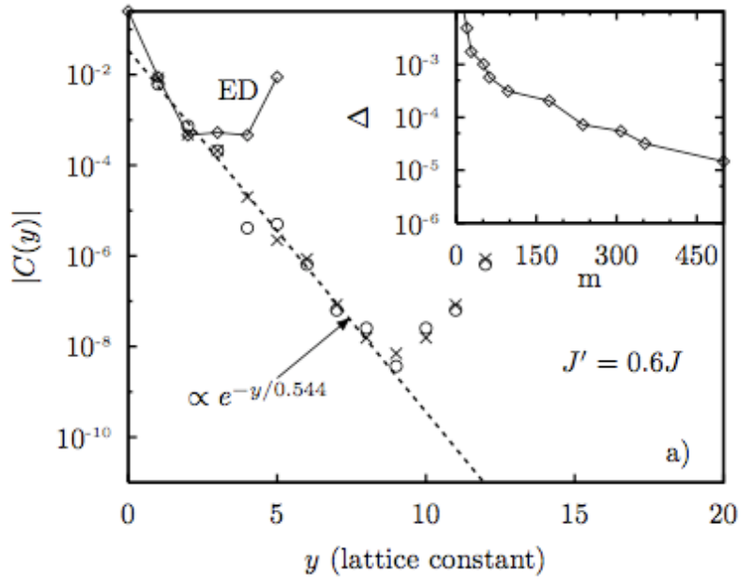
- Chain spins S (black dots), exchange interaction J (blue lines)
- Interstitial (interchain) spins σ (red dots), exchange J'
- Quasi-one-dimensional limit: J' << J

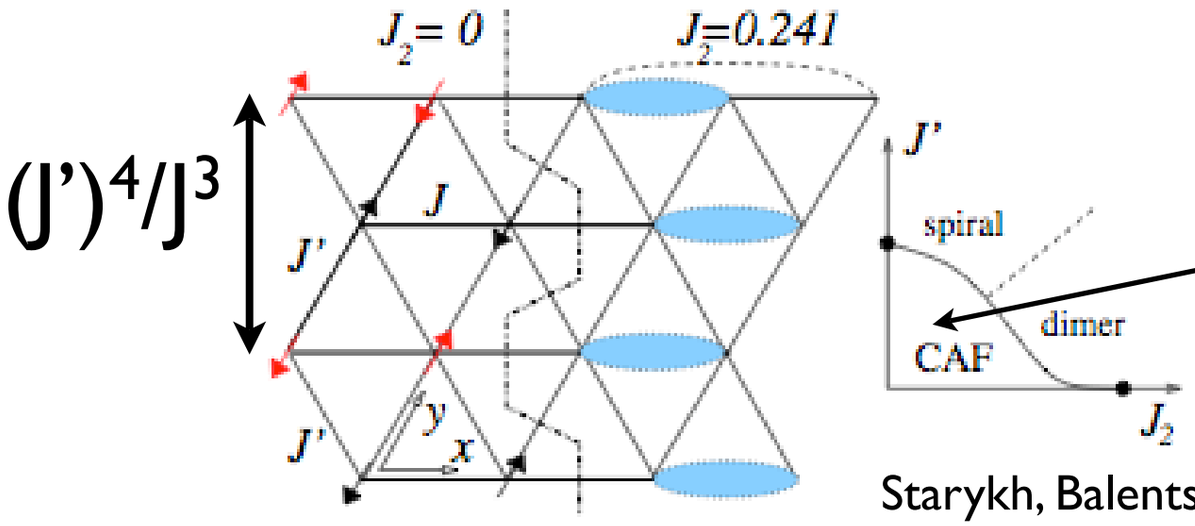
How small should J'/J be ?

- Frustration greatly enhances region of "small" interchain J'
- Example: *spatially anisotropic triangular* AFM
- Numerics: *no* interchain correlations for J'/J < 0.6 - 0.7

Weng et al 2006, Hayashi Ogata 2007, Heidarian Sorella Becca 2009

interchain spin correlations,
J'=0.6 J;
exponential decay
Weng et al 2006



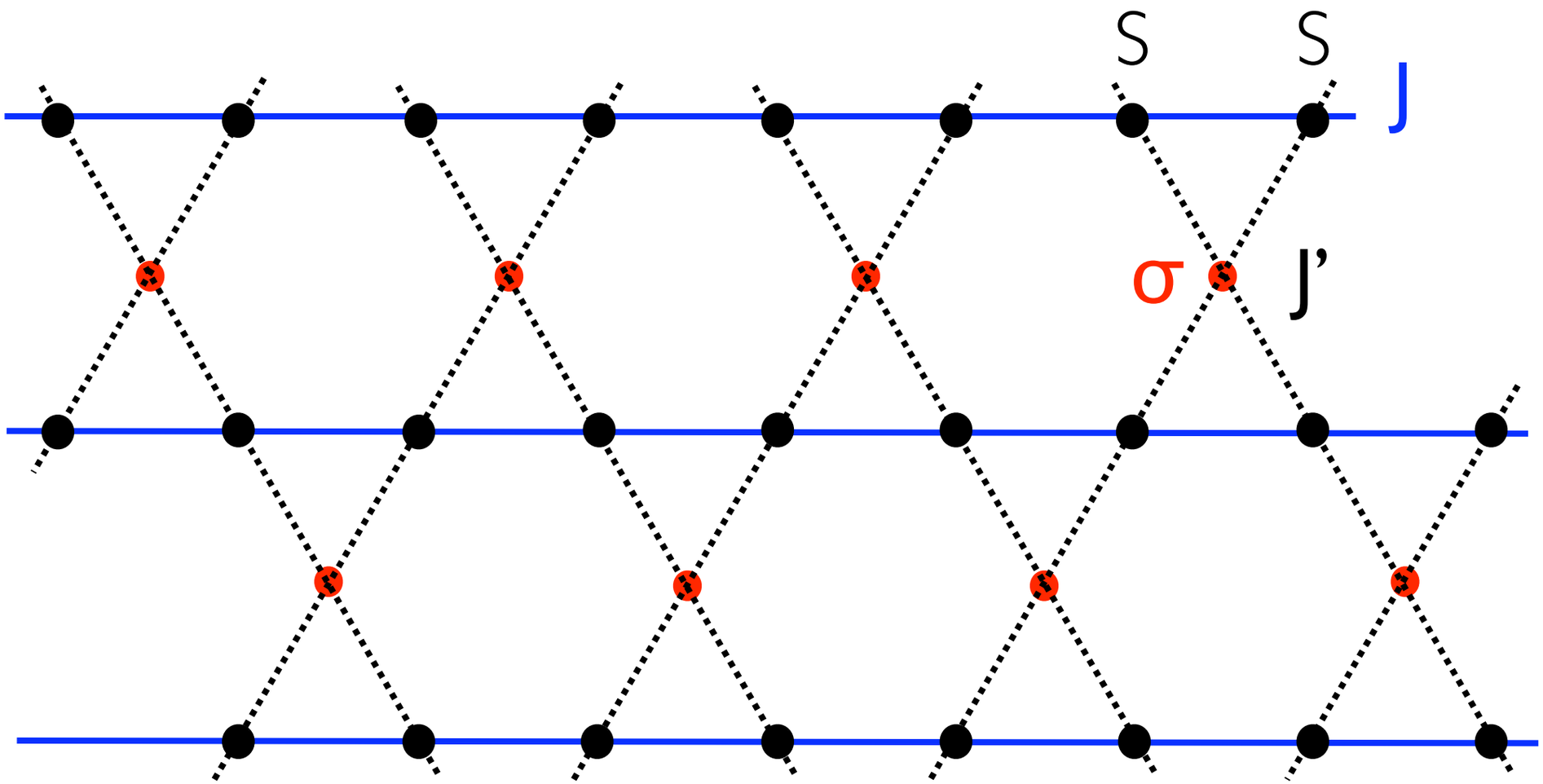


Starykh, Balents 2007

Collinear AFM state,
generated by quantum fluctuations,
coupling between NN chains $(J'/J)^4$

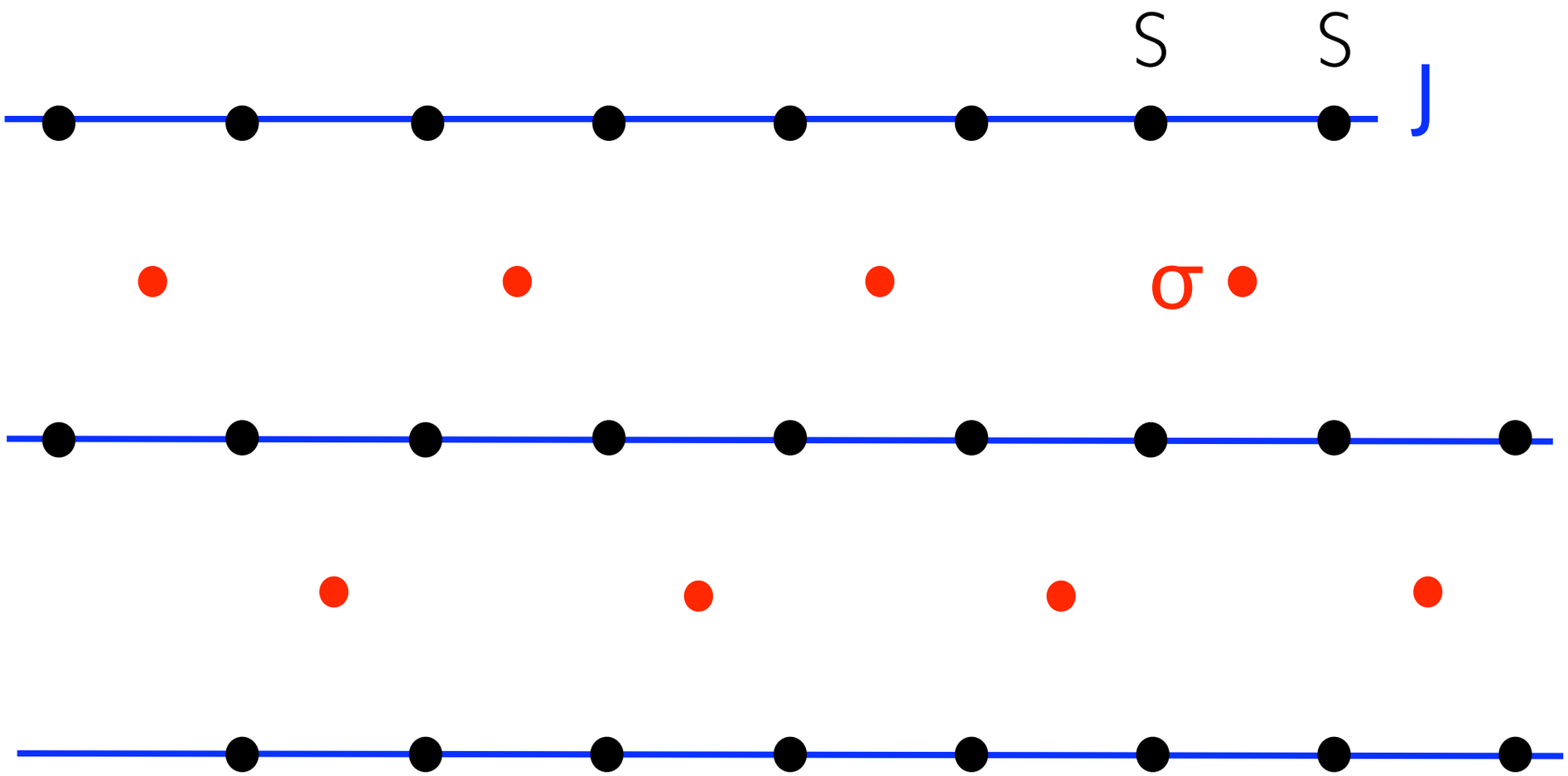
Pardini Singh 2008 - no; Bishop et al 2008 - yes

The decoupled limit, J'→0, is very singular



✴ collection of *independent* spin chains and interstitial spins

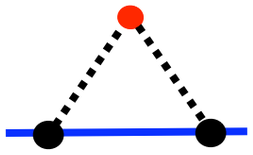
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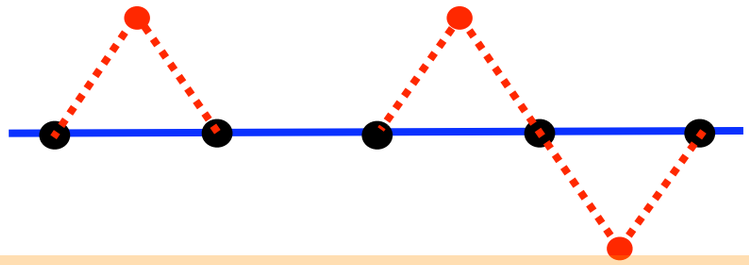
Separation of scales

- local Kondo coupling J' (marginal, $T_K \sim e^{-c\, J/J'}$)



- RKKY interaction between interstitial spins (via chains)

$T_{interstitial} \sim (J')^2/J$

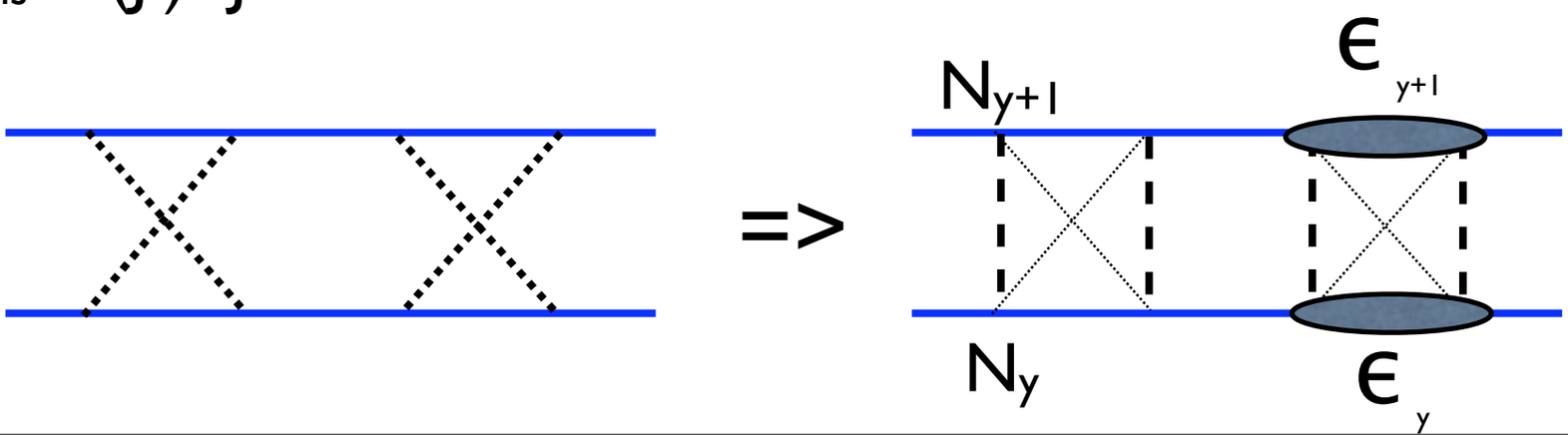


✦ The biggest non-frustrated interaction energy

$T_{interstitial} >> T_{chains} >> T_K$

- Interstitial-mediated coupling between spin chains

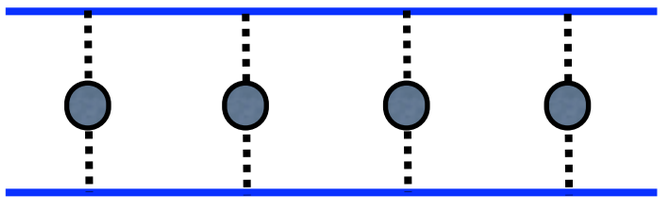
$T_{chains} \sim (J')^4/J^3$



Frustrated vs Non-Frustrated geometry

- Imagine non-frustrated *rectangular* geometry:

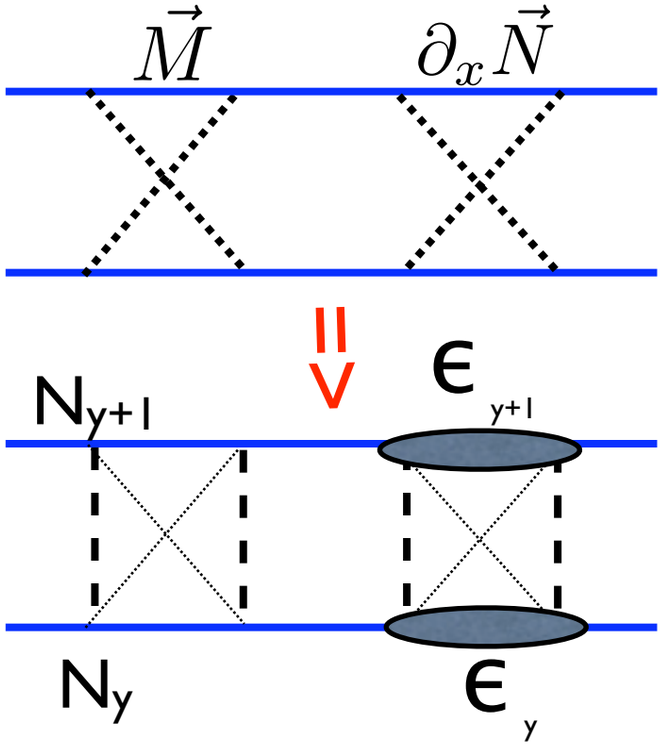
  then $T_{interstitial} \sim T_{chain} \sim (J')^2/J$



=>

no clear separation of energy scales,
difficult to analyze.
e.g. *Kondo necklace*, Essler Kuzmenko Zaliznyak 2007

- Frustrated Kagome geometry:



uniform magnetization

$$(\vec{S}_{2n} + \vec{S}_{2n+1})_y \sim \vec{M}_y + \partial_x \vec{N}_y$$

staggered magnetization

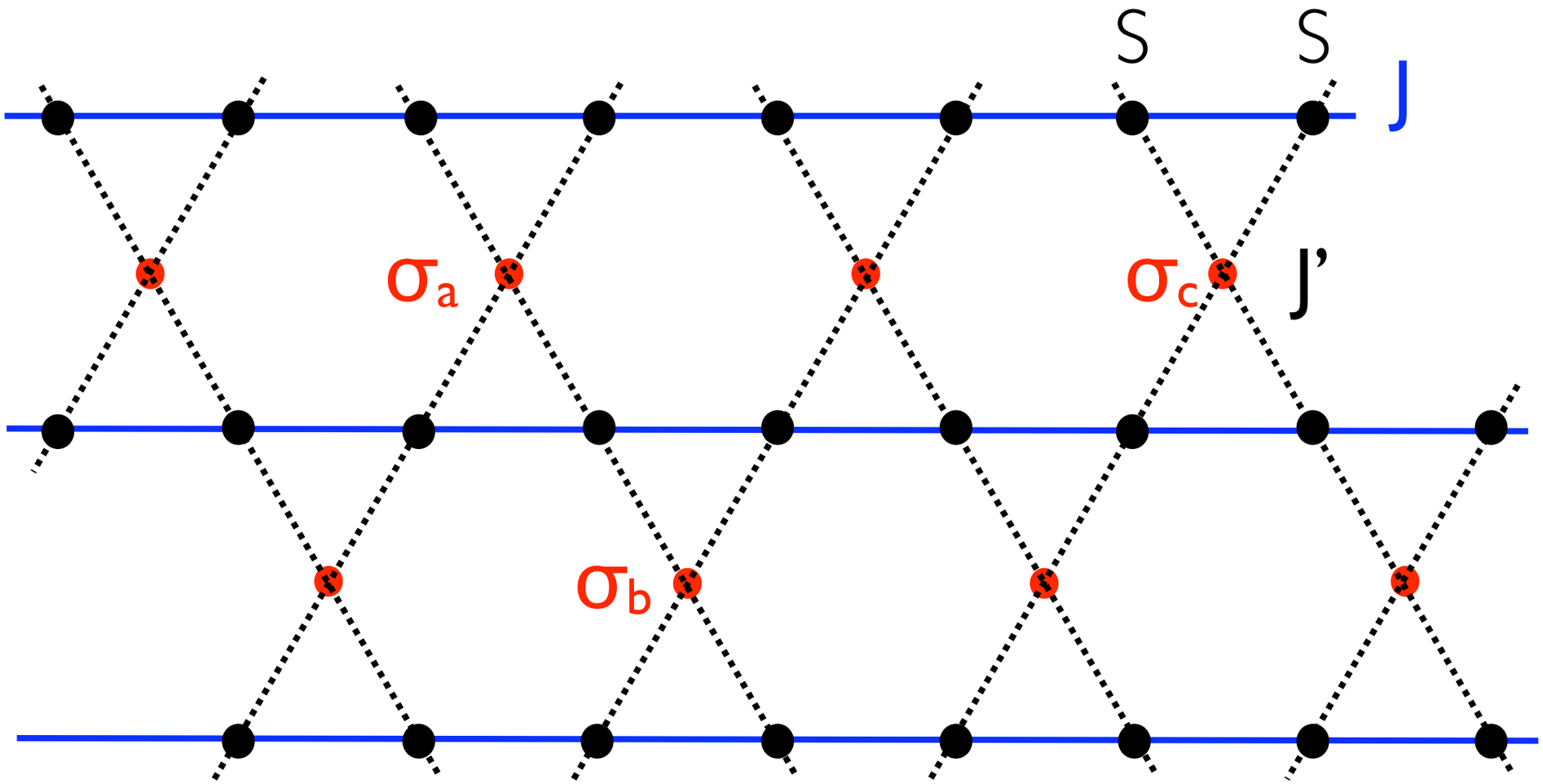
$(J')^2/J$ order: marginal coupling

$$V_{\rm ch}^{(1)} = \sum_y \int dx\ \gamma_{\partial N} \partial_x \vec{N}_y \cdot \partial_x \vec{N}_{y+1} + \gamma_M \vec{M}_y \cdot \vec{M}_{y+1}$$

$(J')^4/J$ order: relevant coupling

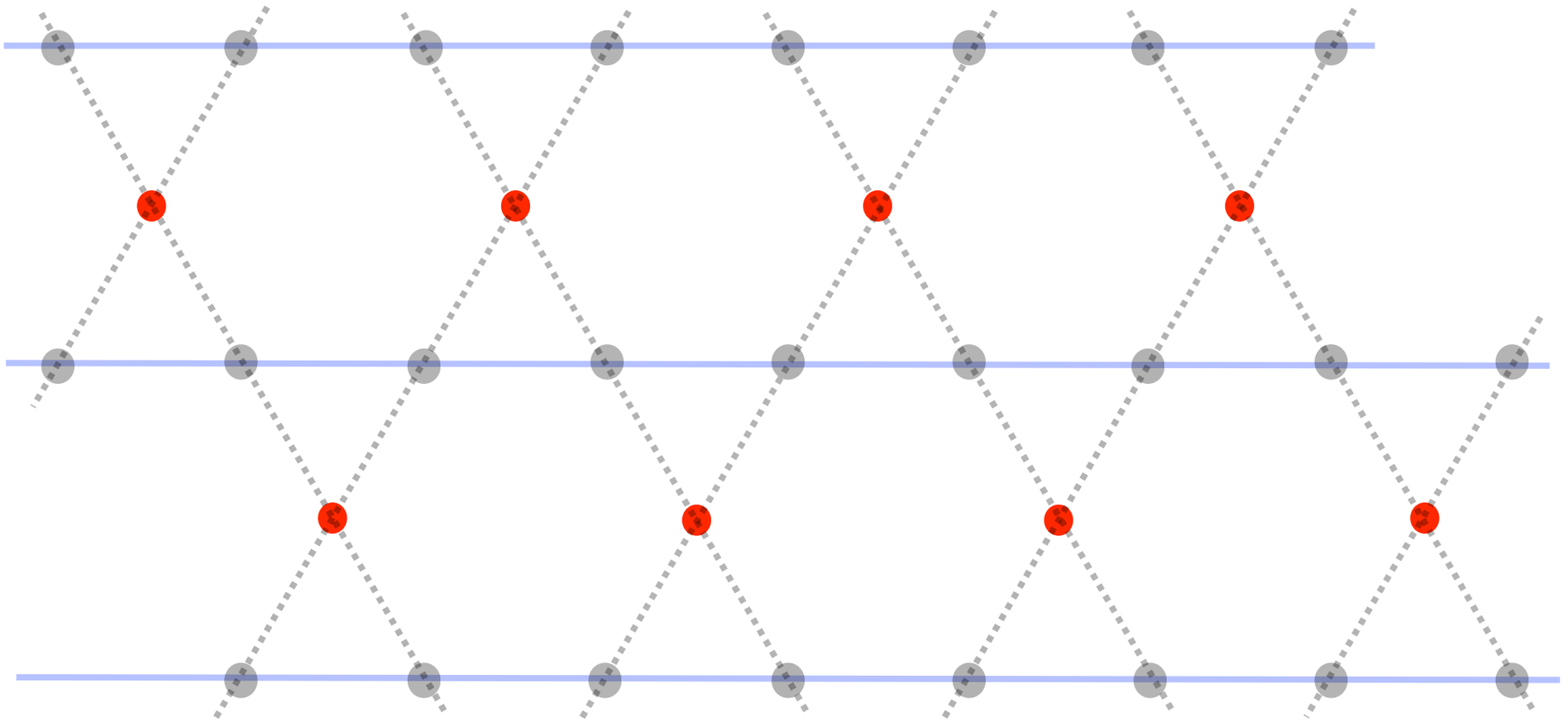
$$V_{\rm ch}^{(2)} = \sum_y \int dx\ \gamma_N \vec{N}_y \cdot \vec{N}_{y+1} + \gamma_\epsilon \epsilon_y \epsilon_{y+1}$$

RKKY interaction between interstitial spins



- σ_a polarizes spin chain, which in turn couples to $\sigma_{b,c}$: interaction between σ's connected to the same spin chain.

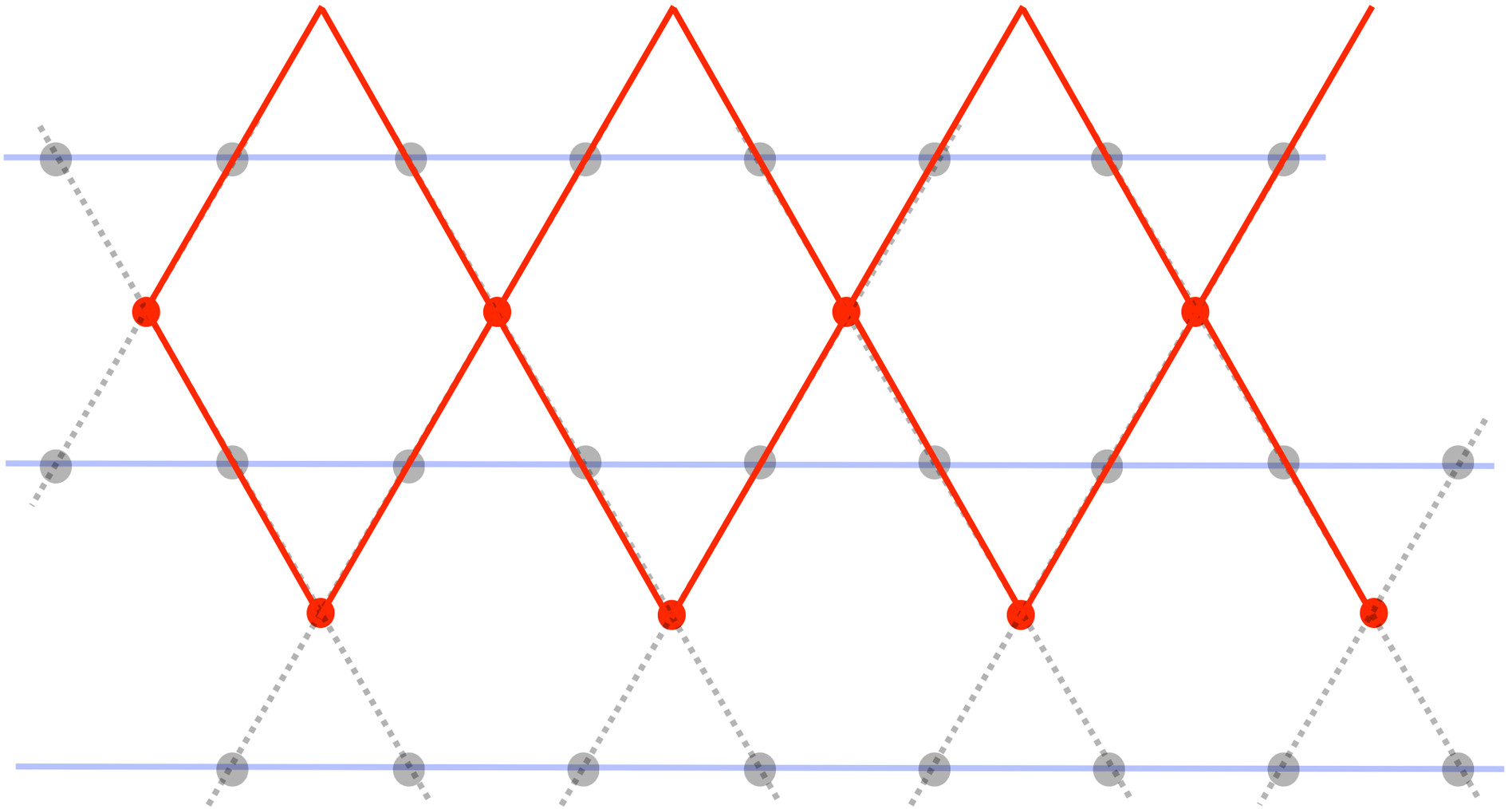
RKKY interaction between interstitial spins



- **Spatially anisotropic triangular lattice formed by K_1 and K_2 bonds**, with further-neighbor interactions $K_{3,4}$ etc.

RKKY interaction between interstitial spins

K_1: nearest-neighbor interaction between σ's

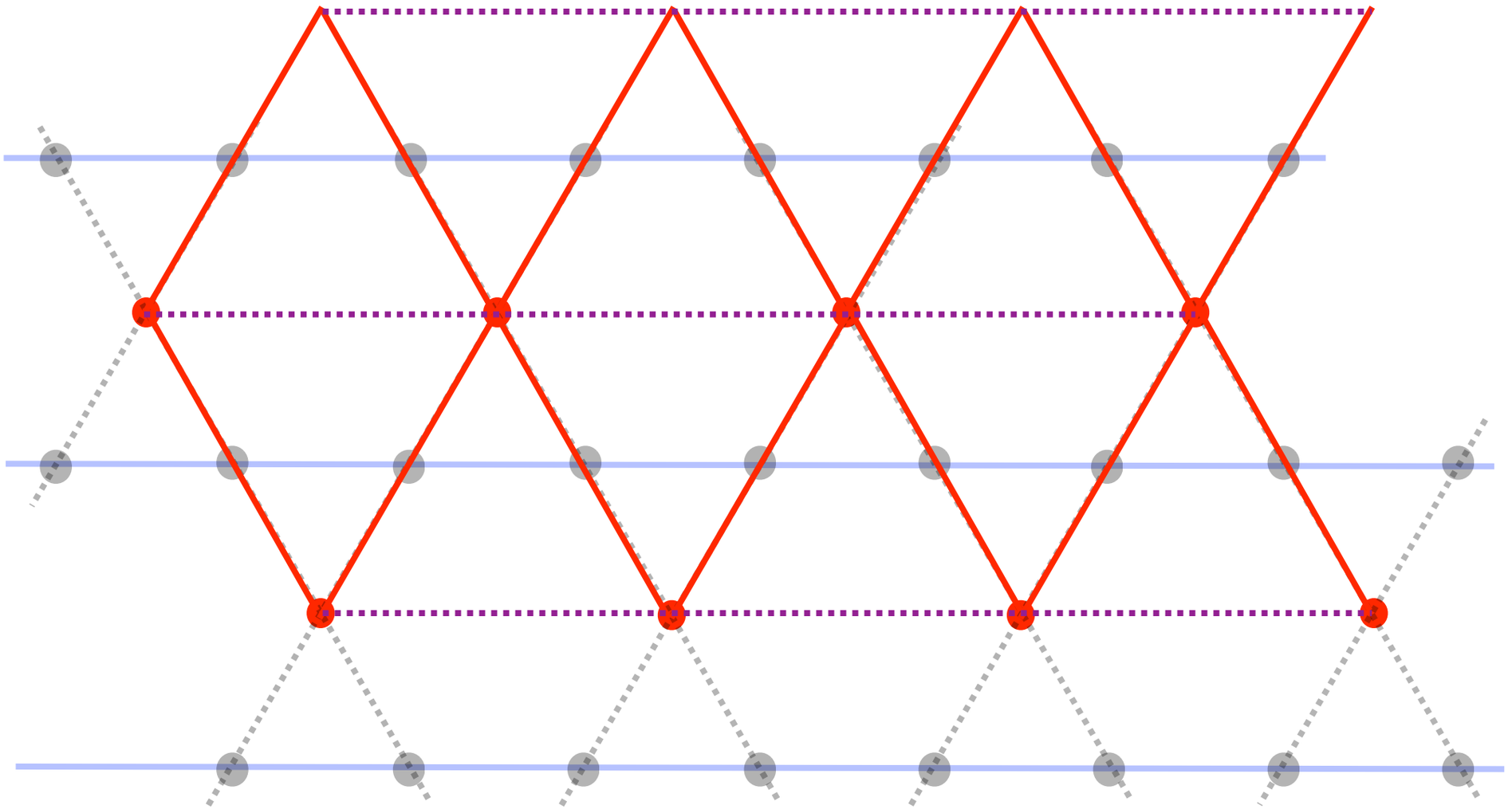


- **Spatially anisotropic triangular lattice formed by K_1 and K_2 bonds**, with further-neighbor interactions $K_{3,4}$ etc.

RKKY interaction between interstitial spins

K_1: nearest-neighbor interaction between σ's

K_2: next nearest-neighbor interaction

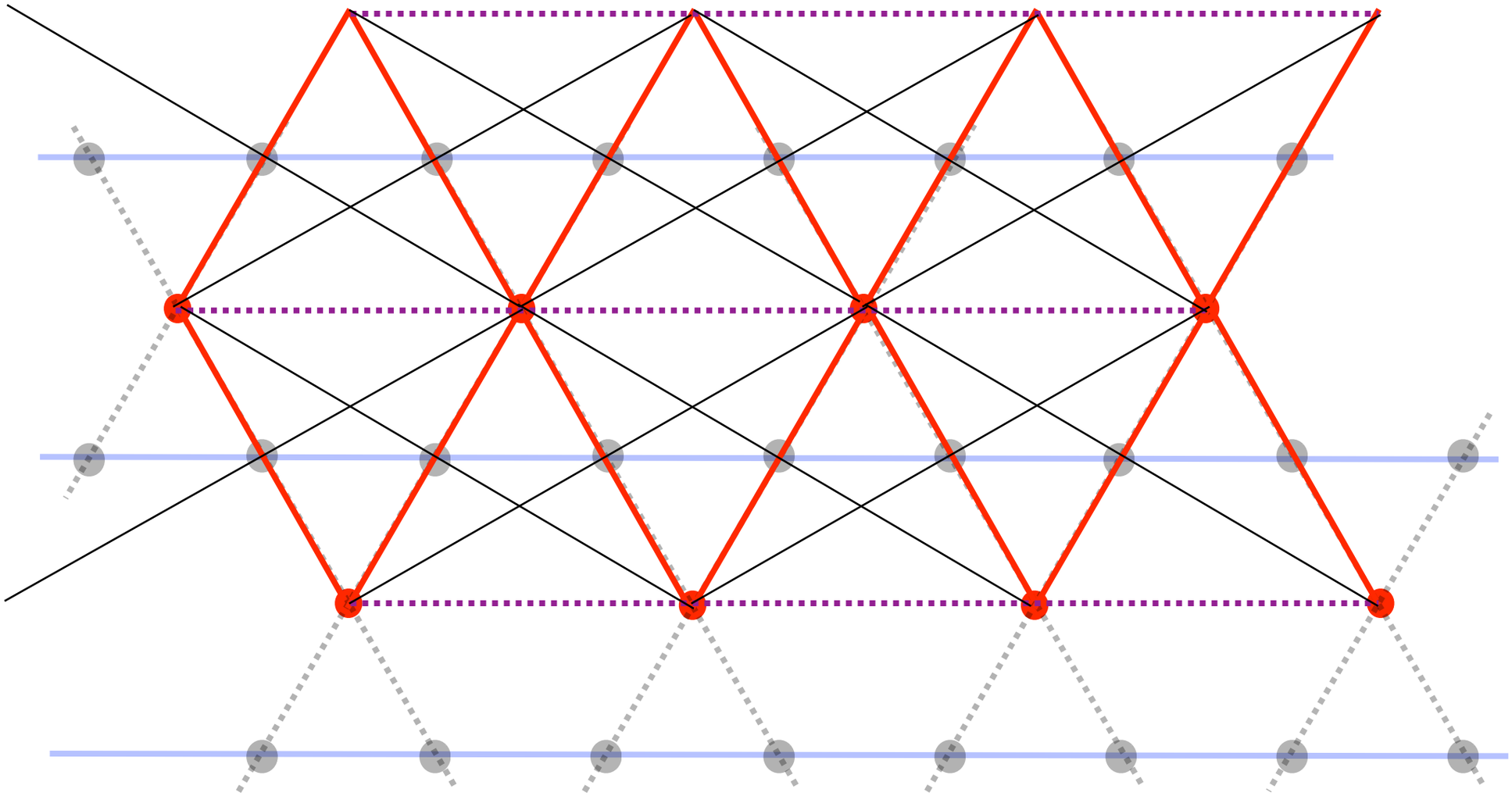


- **Spatially anisotropic triangular lattice formed by K_1 and K_2 bonds**, with further-neighbor interactions $K_{3,4}$ etc.

RKKY interaction between interstitial spins

K_1: nearest-neighbor interaction between σ's

K_2: next nearest-neighbor interaction



K_3: further-neighbor interactions

- **Spatially anisotropic triangular lattice formed by K_1 and K_2 bonds**, with further-neighbor interactions $K_{3,4}$ etc.

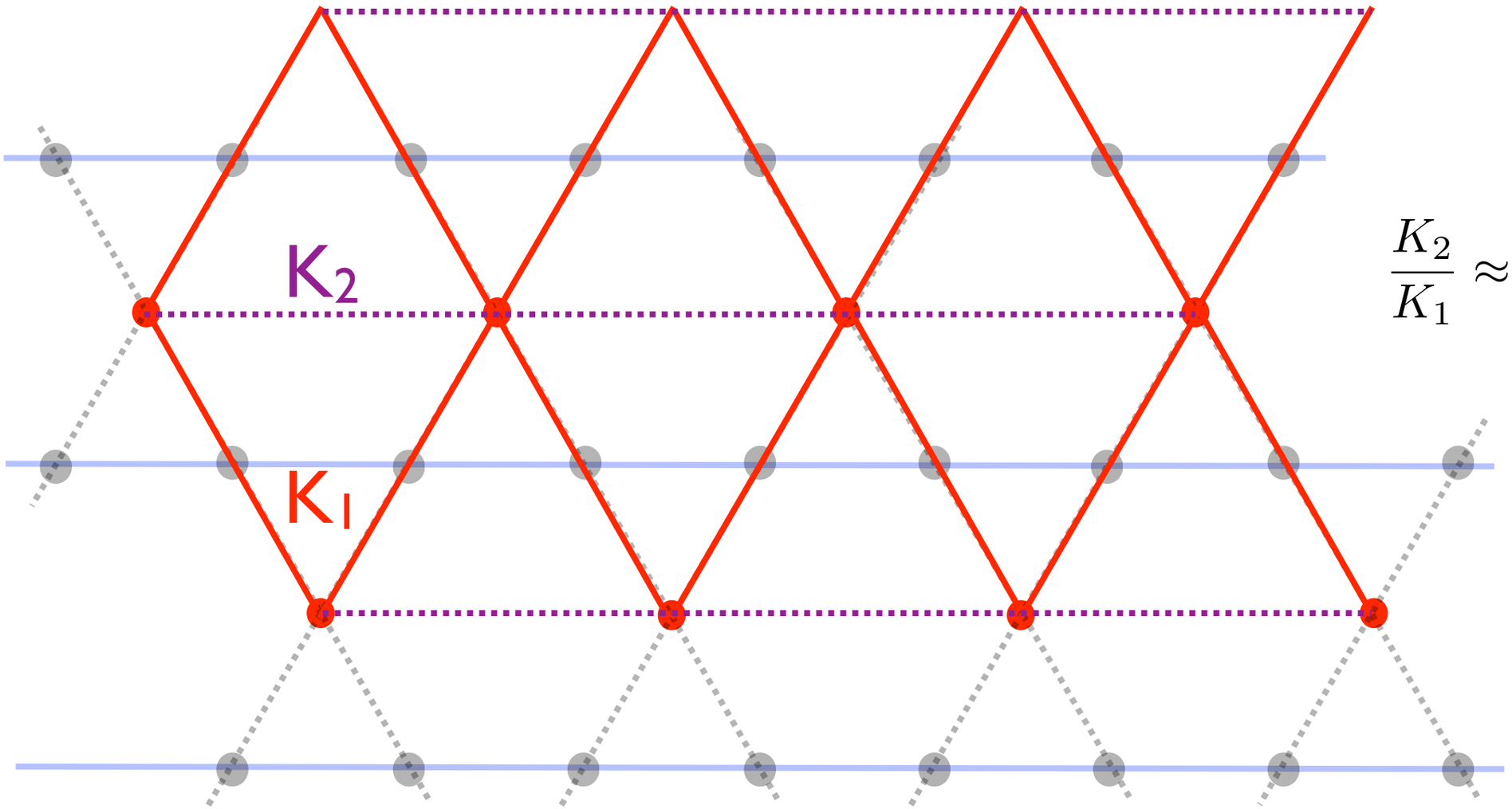
RKKY interaction between interstitial spins

K_1: nearest-neighbor interaction between σ's

K_2: next nearest-neighbor interaction

$$K_1 = 2(J')^2 A(1) \quad < 0 \text{ ferro}$$

$$K_2 = 4(J')^2 A(2) \quad > 0 \text{ antiferro}$$



$$\frac{K_2}{K_1} \approx -0.7$$

- Inter-σ interactions are determined by dynamical structure factor of critical spin-1/2 chain

$$A(\mathbf{r}) = \frac{8}{\pi} \int_0^\infty d\omega' \int_0^\pi dq \, \frac{S(q,\omega')}{\omega'} \cos^2(\frac{q}{2}) \cos(q\mathbf{r})$$

because $(J'/J)^4 << (J'/J)^2$

σ : Spatially anisotropic triangular lattice

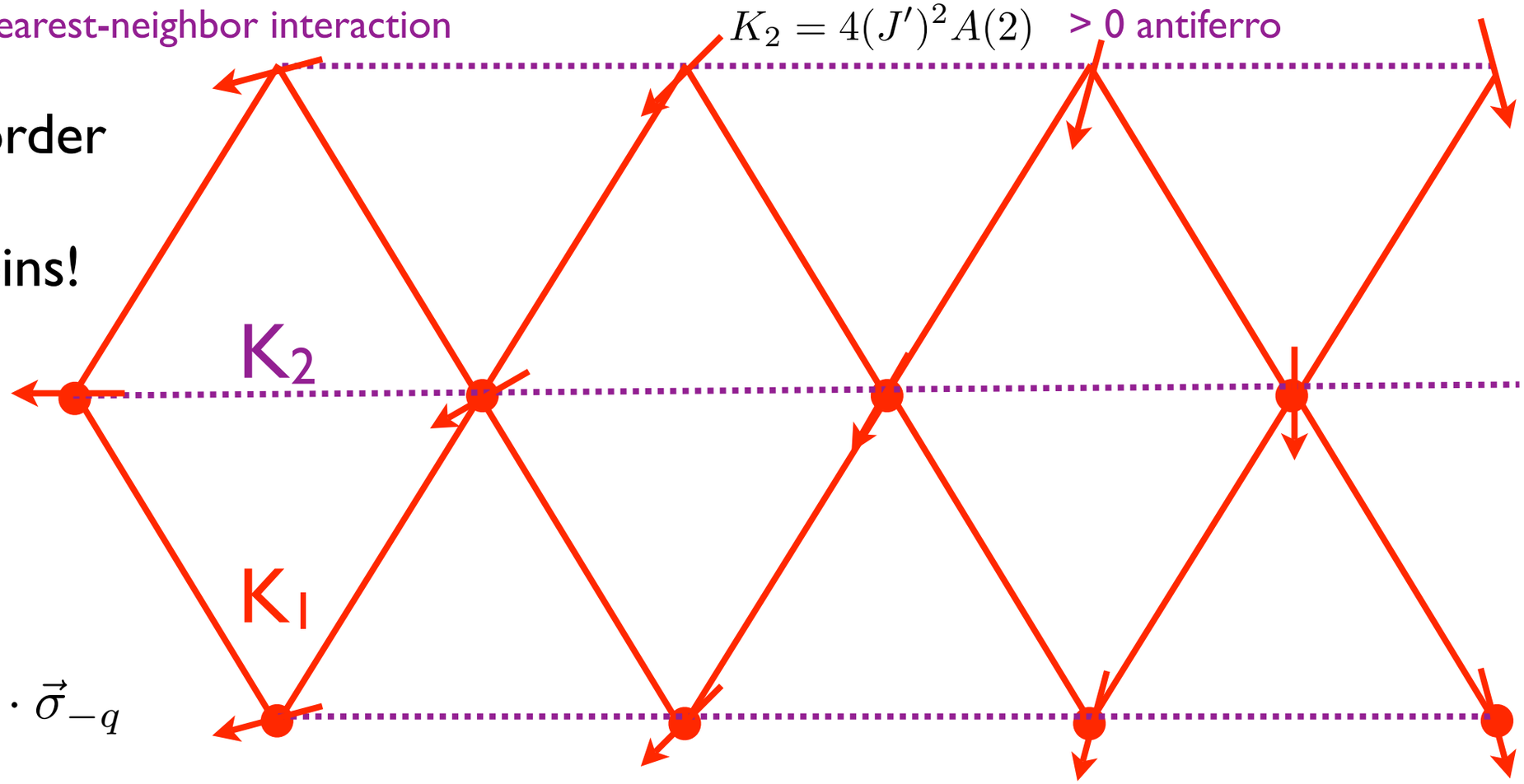
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$$K_1 = 2(J')^2 A(1) \quad < 0 \text{ ferro}$$

$$K_2 = 4(J')^2 A(2) \quad > 0 \text{ antiferro}$$

2d magnetic order amongst interstitial spins!



$$H_\sigma = \sum_q K(q)\vec{\sigma}_q \cdot \vec{\sigma}_{-q}$$

$$K(q) = 2K_1 \cos q_x \cos q_y + K_2 \cos(2q_x) + 2K_3 \cos(3q_x)\cos q_y + K_4 \cos(4q_x)$$

$$\langle \vec{\sigma} \rangle = s_0[\hat{\mathbf{x}} \cos(qx) + \hat{\mathbf{y}} \sin(qx)]$$

Note: s_0 ~ O(1)

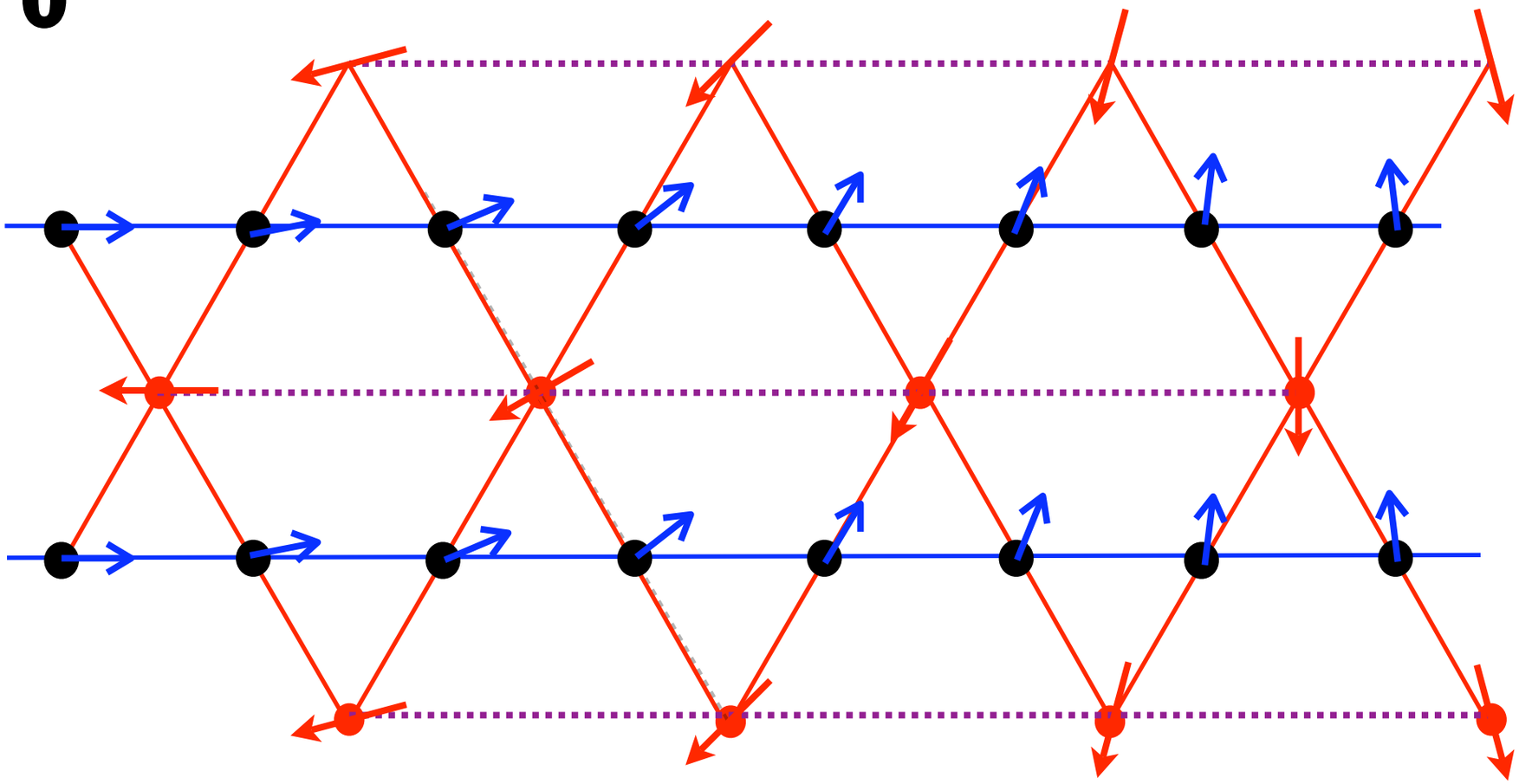
- 2-spinon approximation for A(r) : **rotating spiral** ground state, **q=2π(0.08,0)**
- ABACUS database (N=500 site chain): **ferromagnetic** ground state, **q=0**

consider both cases!

✴ J.S.Caux, U Amsterdam

Ordering of chain spins I

q > 0



- Chain spins are subject to:
  - ➡ external rotating field due to ordered σ 's: $\mathbf{h}_x = 2s_0 \cos(q/2)\mathbf{J}'[\hat{\mathbf{x}}\cos(qx) + \hat{\mathbf{y}}\sin(qx)]$
  - ➡ marginal "backscattering" term in every chain $H_{\rm bs} = g_{\rm bs}\int dx\ \vec{M}_R \cdot \vec{M}_L$
  - ➡ (J'/J)^4 fluctuation-generated interchain interactions $V_{\rm ch}^{(2)} = \sum_y \int dx\ \gamma_N \vec{N}_y \cdot \vec{N}_{y+1} + \gamma_\epsilon \epsilon_y \epsilon_{y+1}$
- Expect response to h_x : static magnetization in **x-y** plane, of magnitude O(J'/J)

Ordering of chain spins II

q > 0 *details of the ordering require more technical consideration*

- To accommodate rotating field h_x , transform into comoving frame: $S_{x,y} \rightarrow R_x S_{x,y}$

$$\mathbf{h}_x = 2s_0 \cos(q/2)\mathbf{J}'[\hat{\mathbf{x}}\cos(qx) + \hat{\mathbf{y}}\sin(qx)] \qquad H_S = \sum_{x,y} \vec{h}_x \cdot \vec{S}_{x+1/2,y} \rightarrow -4s_0 \cos(q/2) J' \sum_{x,y} S^z_{x+1/2,y}$$

  - Under this transformation, chain Hamiltonian H_0 transforms into $H_0 + H_{DM}$

$$H_0 = J\sum_{x,y} \vec{S}_{x-1/2,y} \cdot \vec{S}_{x+1/2,y} \rightarrow H_0 + Jq\sum_{x,y}[S^y_{x-1/2}S^z_{x+1/2} - S^z_{x-1/2}S^y_{x+1/2}]_y \quad +\ldots$$

Effective Dzyaloshinskii-Moriya (DM) term

- Low-energy description

$$H_{\text{chains}} = \sum_y v \int dx \{\vec{M}_R \cdot \vec{M}_R + \vec{M}_L \cdot \vec{M}_L\}_y + H_{\text{field}} + H_{\text{bs}} + V^{(2)}_{\text{ch}}$$

perturbations

the free Hamiltonian possess remarkable extended symmetry:
independent SU(2) rotations of right- and left- spin-currents $M_{R/L}$

- H_{field} includes *both* rotating (h_x) and DM terms ($d = q\,J$, $h \sim s_0 J'$)

$$H_{\text{field}} = \sum_y \int dx \{d(M^x_R - M^x_L) - h(M^z_R + M^z_L)\}_y$$

Use extended symmetry to
rotate left/right currents separately!

Ordering of chain spins III

q > 0

- Chiral rotation, followed by abelian bosonization *shift*

$$H_{\rm field} = -\sum_y \int dx\ \sqrt{h^2+d^2}\{M^z_R + M^z_L\}_y \rightarrow -\sum_y \int dx\ \sqrt{h^2+d^2}\ \partial_x \varphi_y$$

$$\mathbf{M}_{R/L} \rightarrow \mathcal{R}(\pm\theta)\mathbf{M}_{R/L}$$

$$\mathcal{R}(\theta) = \begin{pmatrix} \cos[\theta] & 0 & -\sin[\theta] \\ 0 & 1 & 0 \\ \sin[\theta] & 0 & \cos[\theta] \end{pmatrix}$$

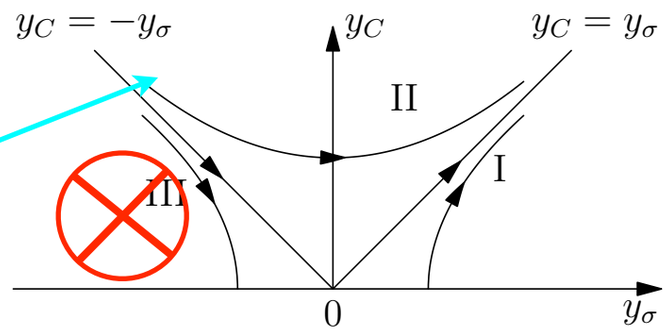
$$\tan(\theta) = d/h$$

$$\varphi_y \rightarrow \varphi_y + \frac{\sqrt{h^2+d^2}}{\sqrt{2\pi}v} x$$

The field-term is completely incorporated now!

- Momentum-conserving perturbations

chain $$H_{\rm bs} = \sum_{x,y}\{\frac{y_C}{2}(M^+_R M^+_L + M^-_R M^-_L) + y_\sigma M^z_R M^z_L\}_y$$



always flow to strong coupling,
feeds inter-chain couplings $\gamma_{x,y,+}$

inter-chain $$V^{(2)}_{\rm ch} = \sum_{x,y}\{\gamma_y N^y_y N^y_{y+1} + \gamma_x N^x_y N^x_{y+1} + \gamma_+(N^z_y N^z_{y+1} + \epsilon_y \epsilon_{y+1})\}$$

also appears in a quantum wire with spin-orbit problem: Gangadharaiah, Sun, Starykh 2008

RG $$\frac{d}{d\ell}\ln[\frac{\gamma_x}{\gamma_y}] = \frac{y_c}{\pi v}$$ > 0, γ_x is the leading inter-chain instability (in a rotated basis!)

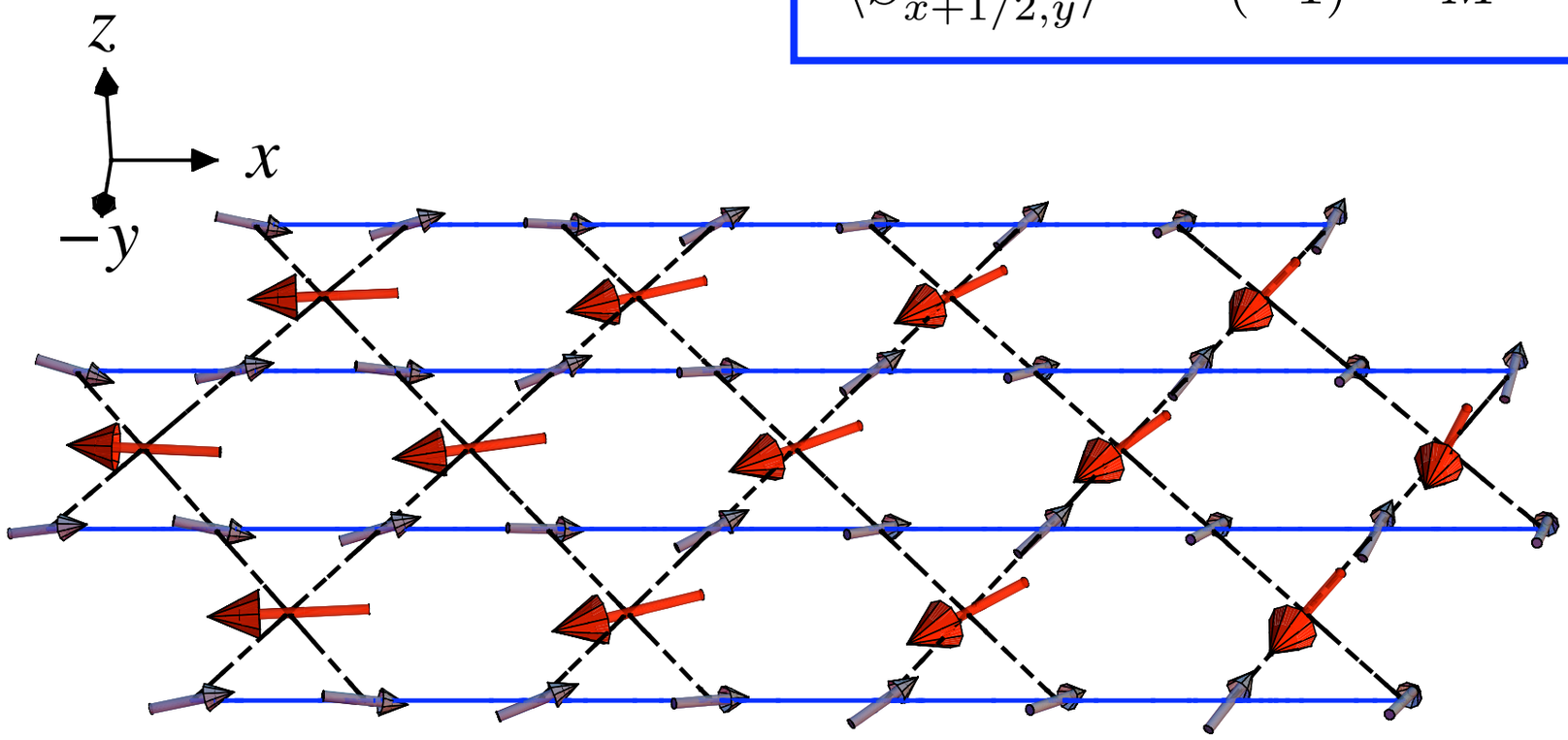
q > 0 Ordering of chain spins IV

- Order in a "rotated" basis:

$$\langle N_y^x \rangle = (-1)^y M \ , \ M = c(J'/J)^2$$
$$\langle M_{R/L}^a \rangle = \langle \epsilon_y \rangle = 0$$

- Order in the original basis:

$$\langle S^+_{x+1/2,y} \rangle = -\frac{\sqrt{h^2+d^2}}{2\pi v} \cos\theta \ e^{iqx} \quad \sim \mathbf{J'/J}$$
$$\langle S^z_{x+1/2,y} \rangle = -(-1)^{x+y} M \quad \sim \mathbf{(J'/J)^2}$$



Non-coplanar order (q > 0)

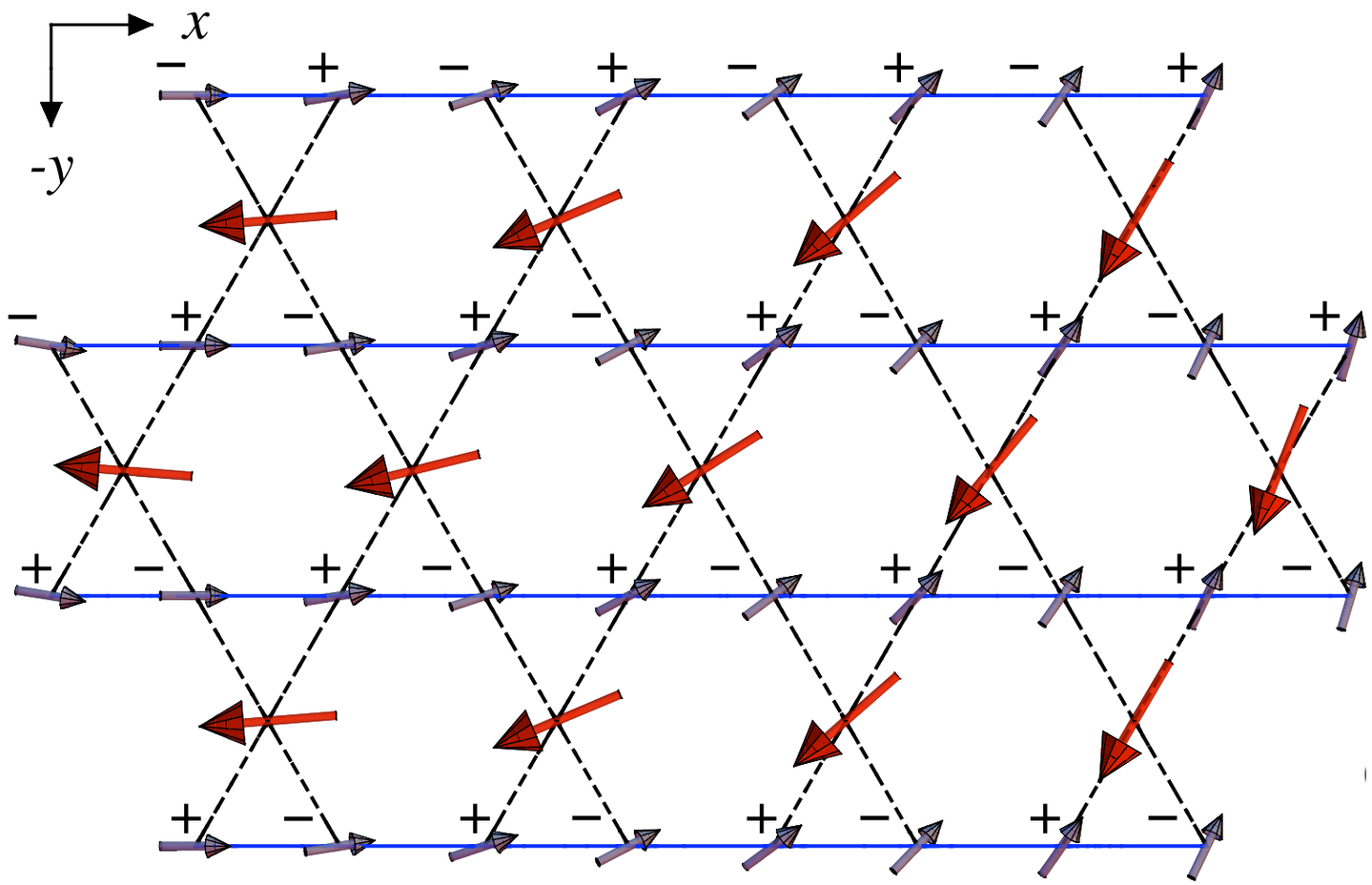
$$\langle \sigma^{x,y} \rangle \sim O(1) \gg \langle S^{x,y} \rangle \sim O(J'/J) \gg \langle S^z \rangle \sim O(J'/J)^2$$

Ordering of chain spins: top view

interstitial spins form **spiral**,

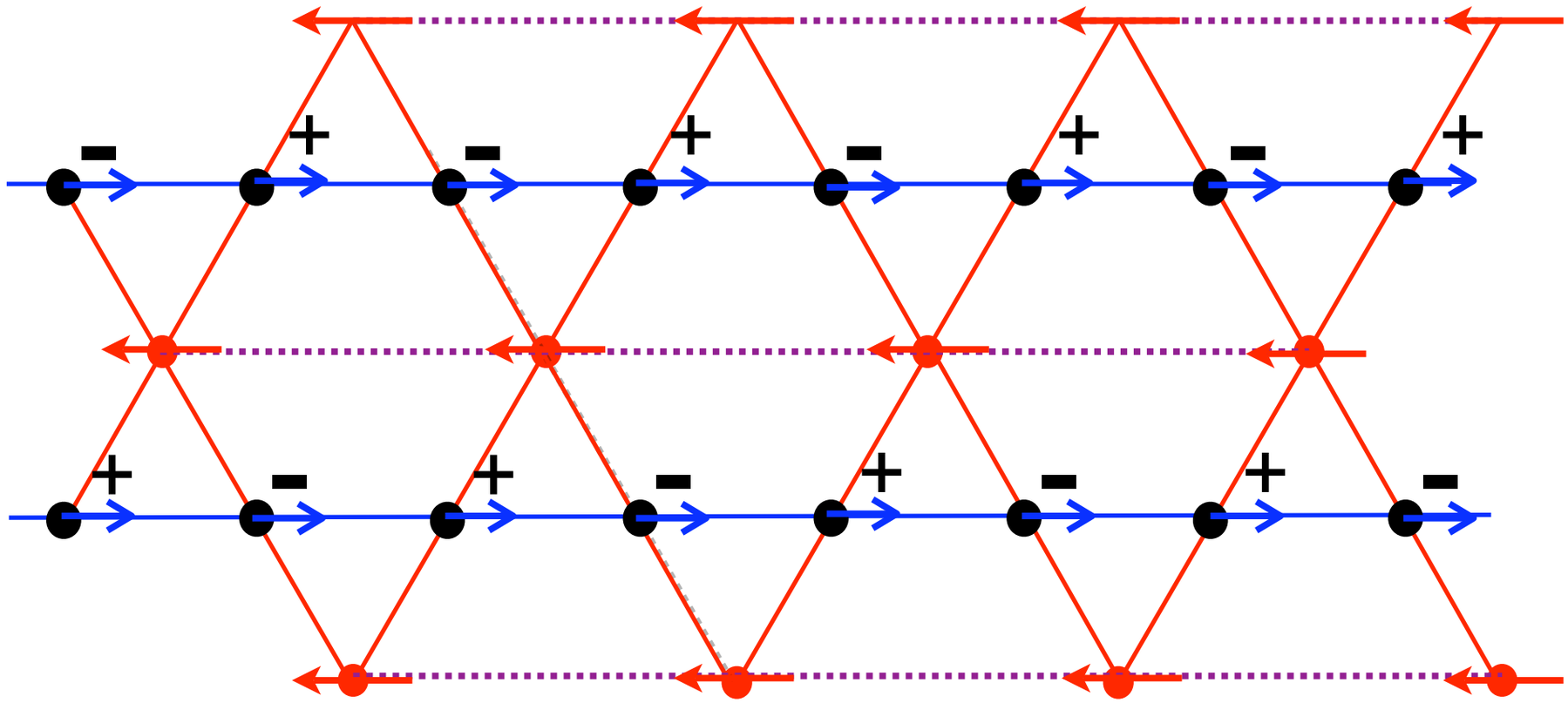
chain spins are locally **anti-parallel** to it,

with small **staggered** component **normal** to **the spiral** plane



basic physics: s=1/2 chain subject to magnetic field -
components orthogonal to the field are most relevant

Ordering of chain spins: **q=0** case

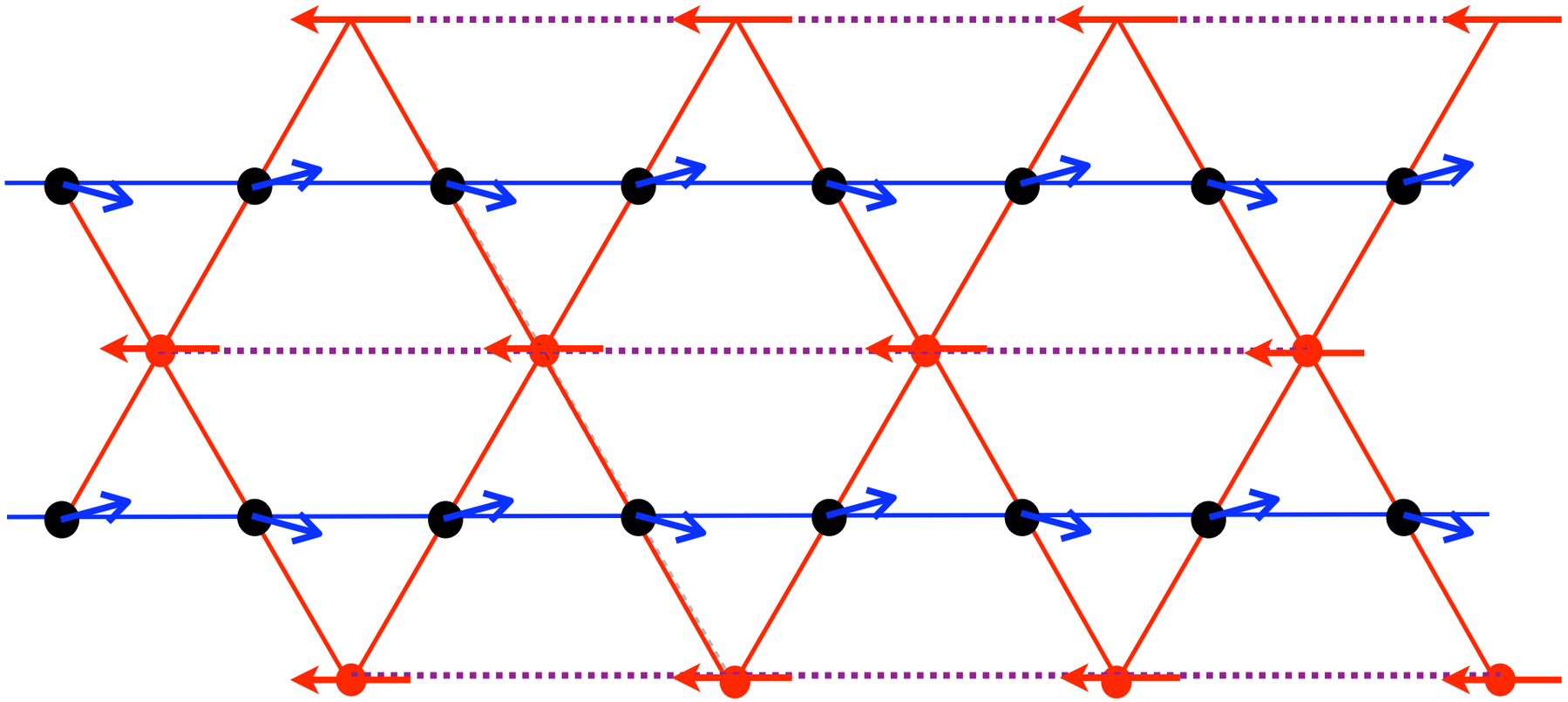


Ferromagnetic order among interstitial spins,
predominantly ferromagnetic ordering among chain spins,
with weaker antiferromagnetic order along, and between, chains:
coplanar state, ferrimagnet.

Ordering of chain spins: **q=0** case

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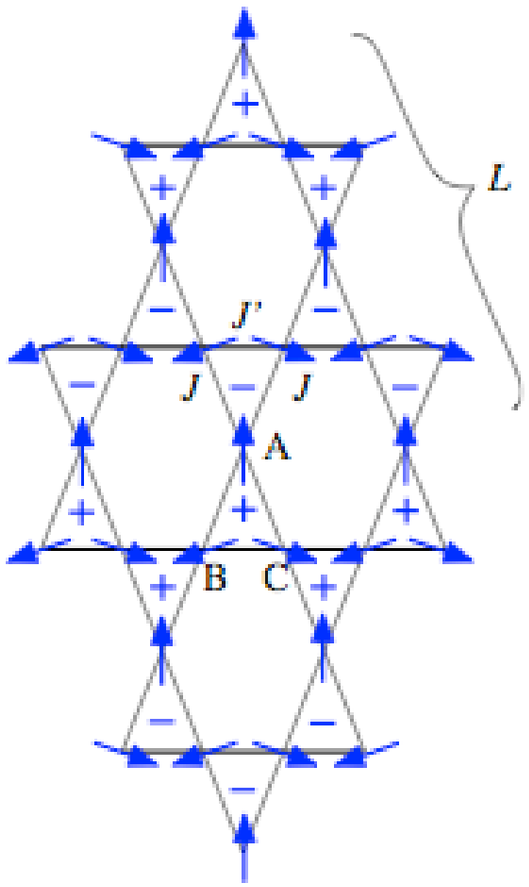
Ordering of chain spins: **q=0** case



Ferromagnetic order among interstitial spins,
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Comparison

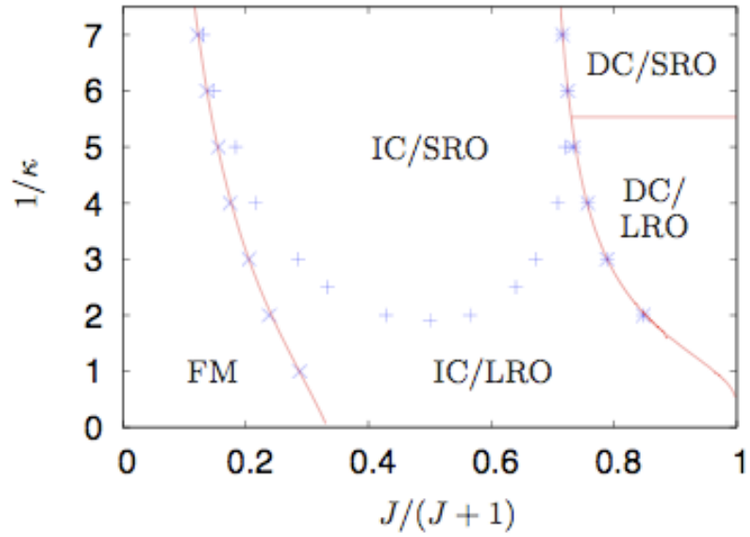
large-S semiclassical analysis



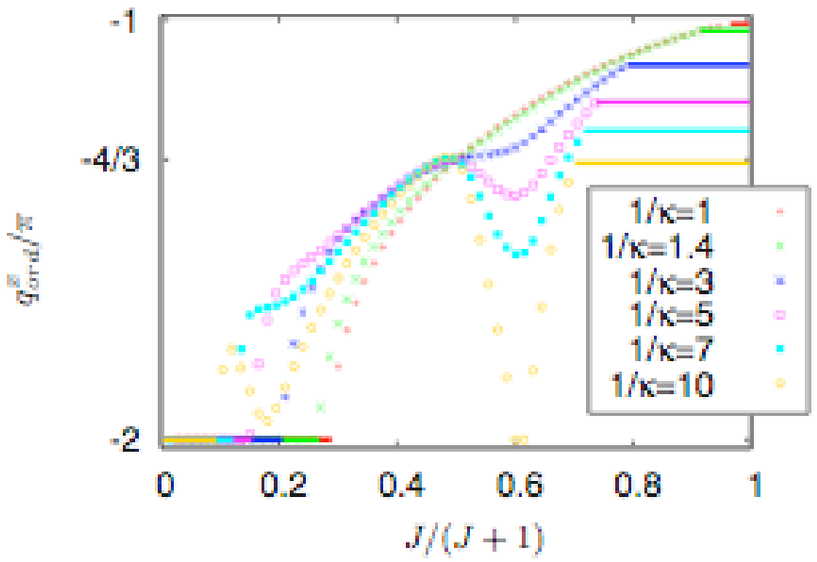
Wang, Vishwanath, Kim 2007:
q=0 state

very similar to our q=0 state

large-N Sp(N)



1d limit: J'=1, J>>1



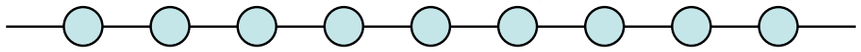
Yavorskii, Apel, Everts 2007:
extended region of incommensurate order **q>0**
among inter-chain spins, disordered chains

Conclusions

- Surprise: spatially anisotropic kagome antiferromagnet is magnetically ordered
- The order is non-coplanar (q > 0)
  - coplanar with q=0 is possible (ferrimagnetic state)
- Interesting hierarchy of scales
  - interstitial spins order at $T_{interstitial} \sim (J')^2/J$
  - chain spins order at $T_{chain} \sim (J')^4/J^3 << T_{interstitial}$
- some open questions:
  - ground state at higher J'/J ?
  - magnetization process Stoudenmire Balents 2008, steps?
  - dynamic structure factor?

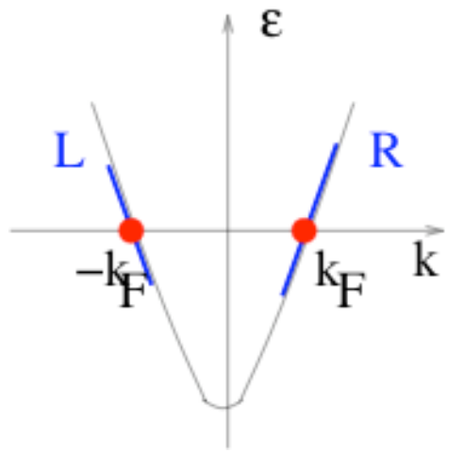
Heisenberg spin chain via free Dirac fermions

- Spin-1/2 AFM chain = half-filled (1 electron per site, $k_F=\pi/2a$) fermion chain



- Spin-charge separation

$$H_{\text{dirac}} = iv \int dx \sum_{s=\uparrow,\downarrow} (\Psi^+_{L,s}\partial_x\Psi_{L,s} - \Psi^+_{R,s}\partial_x\Psi_{R,s})$$



- *q=0 fluctuations: right- and left- spin currents*

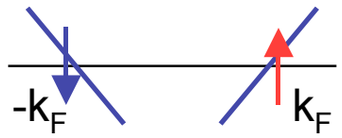
$$\vec{J}_R = \Psi^+_{Rs}\frac{\vec{\sigma}_{ss'}}{2}\Psi_{Rs'} \ , \ \vec{J}_L = \Psi^+_{Ls}\frac{\vec{\sigma}_{ss'}}{2}\Psi_{Ls'}$$

- *$2k_F$ (= π/a) fluctuations: charge density wave ε , spin density wave N*

Staggered Magnetization N

$$N^+ \sim \Psi^+_{R\uparrow}\Psi_{L\downarrow} + \text{h.c.}$$
$$N^z \sim \Psi^+_{R\uparrow}\Psi_{L\uparrow} - \Psi^+_{R\downarrow}\Psi_{L\downarrow} + \text{h.c.}$$

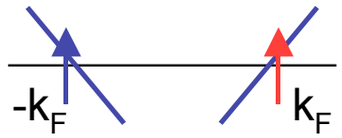
Spin flip $\Delta S=1$



Staggered Dimerization

$$\varepsilon \sim i\left(\Psi^\dagger_{R\uparrow}\Psi_{L\uparrow} + \Psi^\dagger_{R\downarrow}\Psi_{L\downarrow} - \text{h.c.}\right)$$

$\Delta S=0$



Susceptibility

1/q $\quad \chi_{1d}(q)$

1/q

1/q

ε = $(-1)^x$ S_x S_{x+a}

Low-energy degrees of freedom

• Quantum triad: uniform magnetization **M** = $\mathbf{J_R} + \mathbf{J_L}$,
staggered magnetization **N** and staggered dimerization $\varepsilon = (-1)^x S_x S_{x+1}$

✓Components of Wess-Zumino-Witten-Novikov SU(2) matrix $G = \varepsilon + i\vec{N}\cdot\vec{\sigma}$

• Hamiltonian H ~ $\mathbf{J_R J_R} + \mathbf{J_L J_L} + \gamma_{bs}\, \mathbf{J_R J_L}$

marginal perturbation

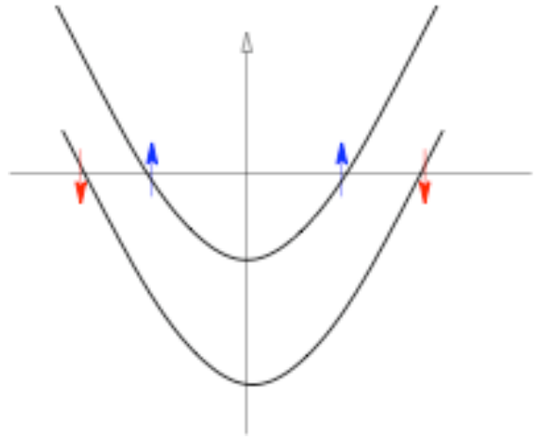
• Operator product expansion $z = v\,\tau - ix$ (similar to commutation relations)

$$\begin{cases} J_R^a(x,\tau)J_R^b(0,0) = \dfrac{\delta^{ab}}{8\pi^2 z^2} + \dfrac{i\varepsilon^{abc}J_R^c(x,\tau)}{2\pi z} \\ J_R^a(x,\tau)N^b(0,0) = \dfrac{-i\delta^{ab}\varepsilon(x,\tau) + i\varepsilon^{abc}N^c(x,\tau)}{4\pi z}\,,\; J_R^a(x,\tau)\varepsilon(0,0) = \dfrac{iN^a(x,\tau)}{4\pi z} \end{cases}$$

• Scaling dimension 1/2 (relevant) $\langle N^a(x,\tau)N^a(0,0)\rangle \sim \dfrac{1}{\sqrt{v^2\tau^2+x^2}} \sim \langle \varepsilon(x,\tau)\varepsilon(0,0)\rangle$

• Scaling dimension 1 (marginal) $\langle M^a(x,\tau)M^a(0,0)\rangle \sim \dfrac{1}{z^2} + \dfrac{1}{\bar{z}^2}$

S=1/2 AFM Chain in a Field



- Field-split Fermi momenta: $k_{F\uparrow} = \frac{\pi}{2} - \delta \, , \; k_{F\downarrow} = \frac{\pi}{2} + \delta$
  - ✓ Uniform magnetization $M = \frac{k_{F\uparrow} - k_{F\downarrow}}{2\pi} \rightarrow \delta = \pi M$
  - ✓ Half-filled condition $n = \frac{1}{2} = \frac{k_{F\uparrow} + k_{F\downarrow}}{2\pi} \rightarrow k_{F\uparrow} + k_{F\downarrow} = \pi$

- S^z component ($\Delta S=0$) peaked at $\pi \pm 2\delta$ scaling dimension $1/4\pi R^2$ **increases**

$S^z_{\pi \pm 2\delta}$

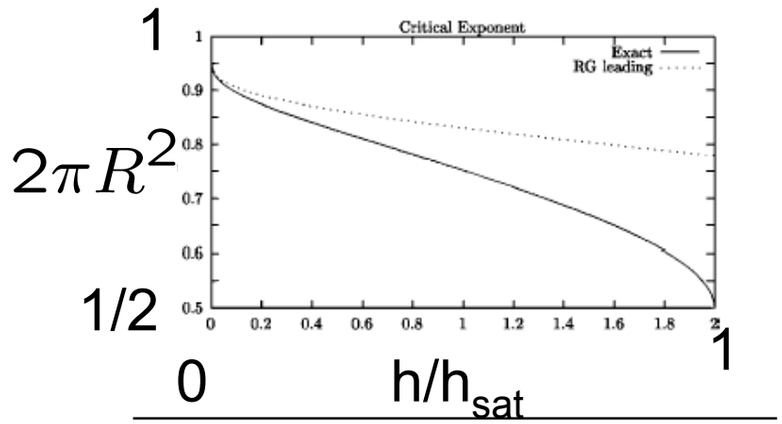
- $S^{x,y}$ components ($\Delta S=1$) remain at π scaling dimension πR^2 **decreases**

$S^{\pm}_{\pi}$

- Derived for free electrons but correct always - *Luttinger Theorem*

1

Affleck and Oshikawa, 1999



- XY AF correlations grow with h *and remain commensurate*
- Ising "SDW" correlations decrease with h and shift from π