

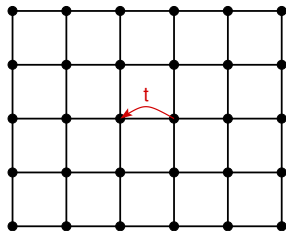
Quantum paramagnetic systems

Ricardo Luís Doretto
Instituto de Física Gleb Wataghin – Unicamp
São Carlos, May 2013

- Magnetic ordered phases
- Quantum paramagnetic phases
- Frustrated magnetic systems
- Theoretical tools for spin systems
- Triangular–lattice AFM Heisenberg model

From Hubbard to Heisenberg

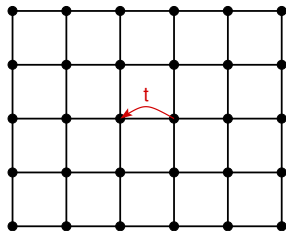
- electron spin: $\sigma = \uparrow\downarrow$
- half-filling:
 $n_{i\uparrow} + n_{i\downarrow} = 1$



$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})$$

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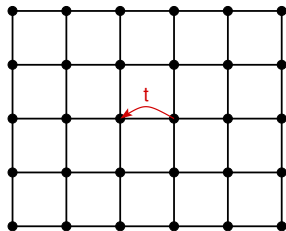


Hubbard model

$$H = -t \sum_{\langle ij \rangle \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad U > 0$$

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- $U \gg t$

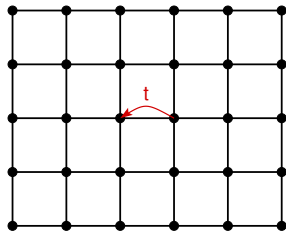


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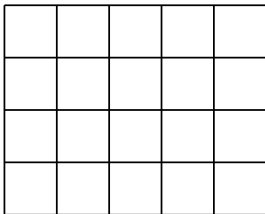
$$J = 4t^2/U \quad \text{exchange coupling}$$

$$S_i^k = \frac{1}{2} c_{i\alpha}^\dagger \sigma_{\alpha\beta}^k c_{i\beta}$$

$$k = x, y, z$$

Antiferromagnet (AFM) Heisenberg model

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Antiferromagnet (AFM) Heisenberg model

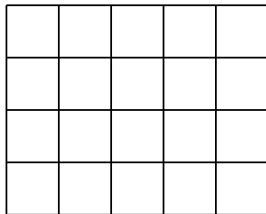
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Classical spins: $S \gg 1/2$

Ground state ($T = 0$):

Néel order $\xi_{\text{mag}} \rightarrow \infty$

$M = 0$ and $M_{\text{stagg}} = M_0$



Antiferromagnet (AFM) Heisenberg model

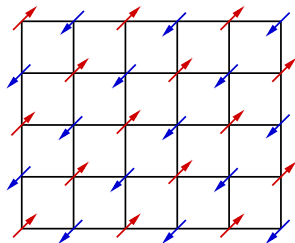
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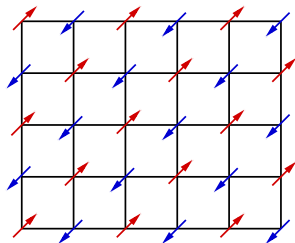
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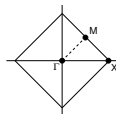
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Quantum case, $S = 1/2$: Néel + quantum fluctuations

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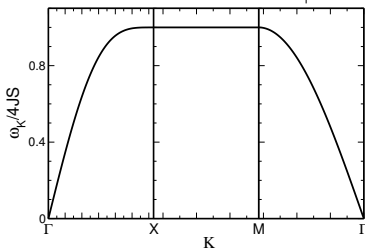


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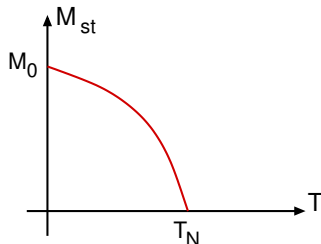
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2-D: paramagnetic (disorder) phase ($T \neq 0$)

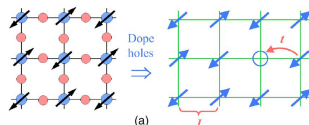
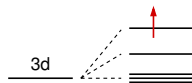
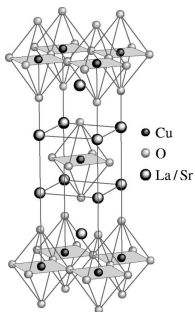
3-D: phase transition at finite temperature T_N (Néel)

Heisenberg model - antiferromagnetic (AFM)

Ex.: La_2CuO_4

$T_N \approx 300 \text{ K}$

$\text{Cu}^{+2}: [\text{Ar}]3d^9$



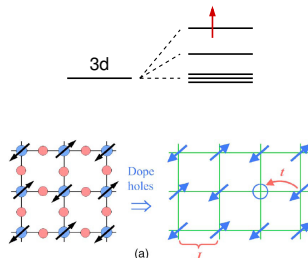
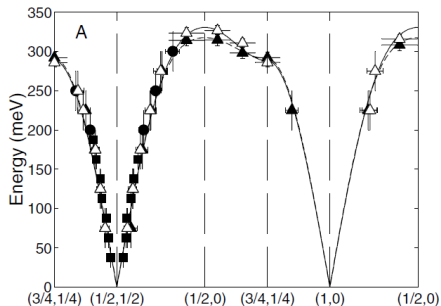
Coldea et al., 2001; Damascelli et al., 2003; Lee et al., 2006; Vojta, 2009

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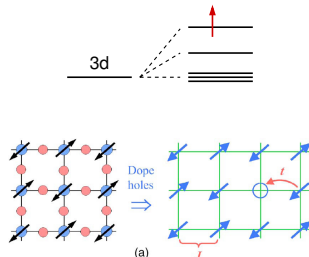
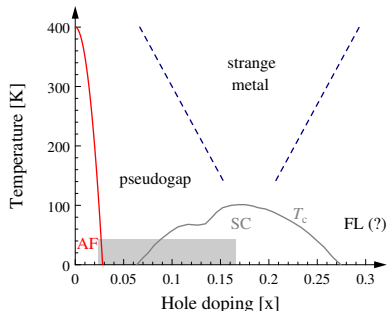
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$\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$: high-temperature superconductor

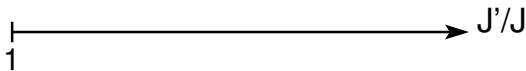
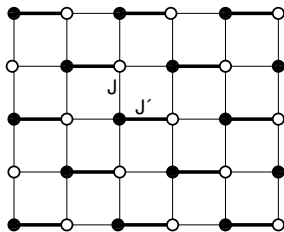
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Staggered dimerized AFM Heisenberg model

$$H = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$J_{ij} = J' \geq J > 0$$

$$S = 1/2 \quad T = 0$$

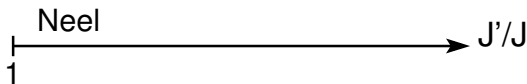
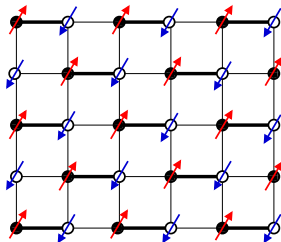


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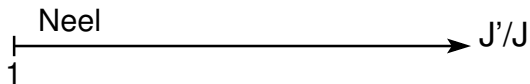
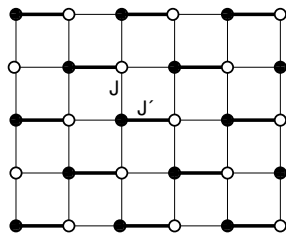


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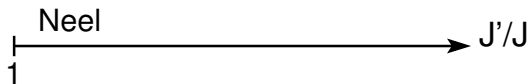
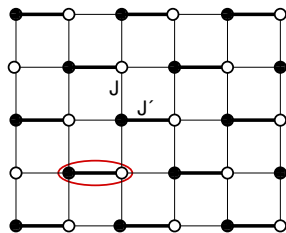


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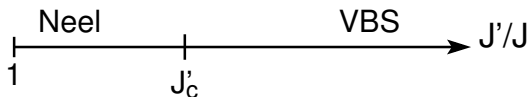
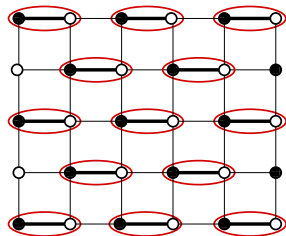


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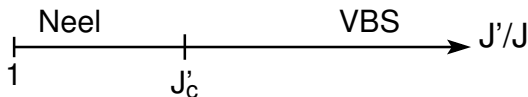
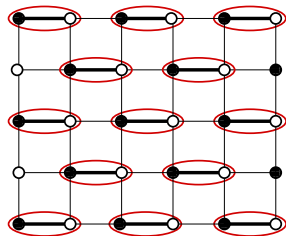


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VBS: Valence bond solid (quantum paramagnetic phase)

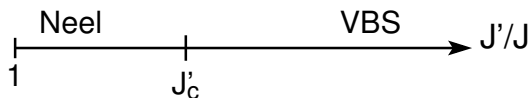
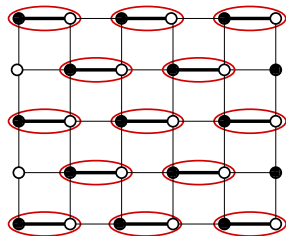
$$\xi_{\text{mag}} \sim 1$$

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Quantum Monte Carlo: $J'_c = 2.5186 J$

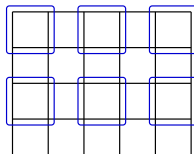
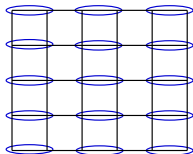
About quantum phase transition:

Wenzel et al., 2008

Fritz et al., 2011

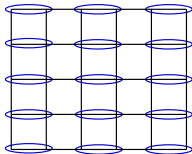
Quantum paramagnets: valence bond solid (VBS)

- VBS \sim crystal of singlets (valence bonds)
 $\xi_{\text{mag}} \sim 1$
- Spin-rotation symmetry preserved
- Columnar: **rotational** and **translational** symmetries spontaneously broken
- Plaquette: **translational** symmetries spontaneously broken



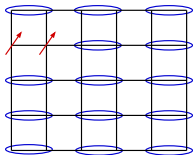
Quantum paramagnets: valence bond solid (VBS)

- Gapped excitations: triplons (spin-1) **confined phase**



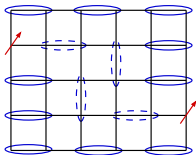
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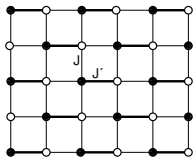
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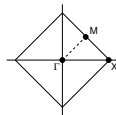
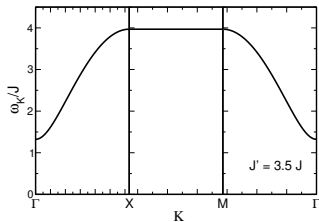
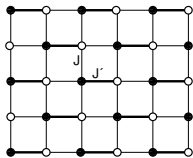
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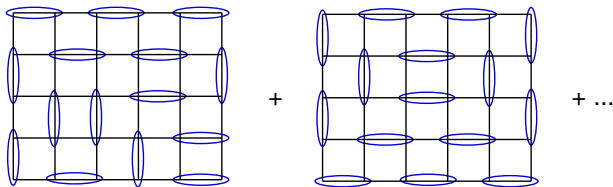
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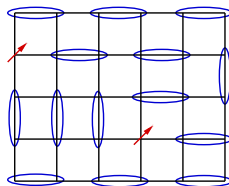
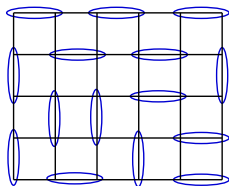
Quantum paramagnets: spin liquids

- Spin liquid \sim “liquid of singlets” (no long range order)
- Resonating Valence Bond (RVB)
- Spin-rotation and translational symmetries preserved
- Gapped/gapless excitations: spinons (spin-1/2, fractionalized)
- **Deconfined phase**



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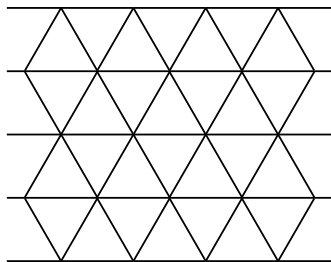
Excitations:

- particle-like
spin-1/2 and charge: $\pm e$
Ex.: metal (Fermi liquid).
- magnon-like
spin-1 and charge: 0
Ex.: spin-waves (FM and AFM), triplons (VBS),
- spinons
spin-1/2 and charge: 0 fractionalized excitations

Frustrated magnetic systems

AFM Heisenberg model on the triangular lattice

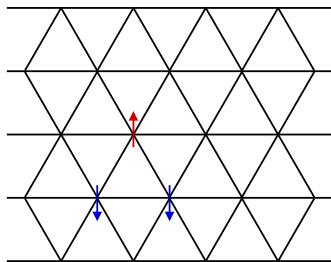
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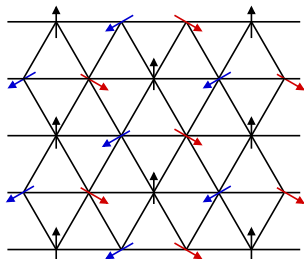
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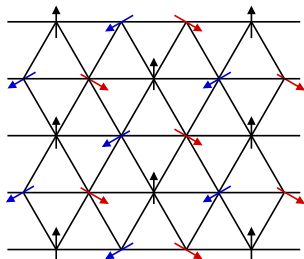


non-collinear 120° Néel order

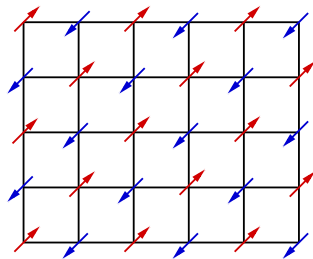
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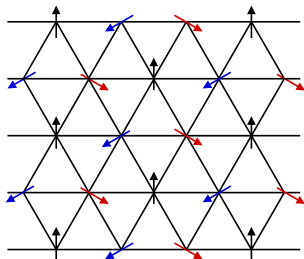


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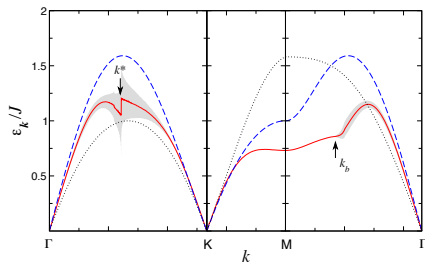
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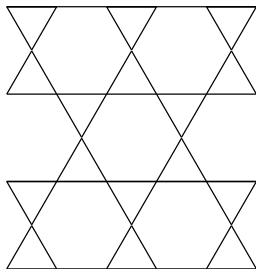


spin wave spectrum

Frustrated magnetic systems

AFM Heisenberg model on the kagome lattice

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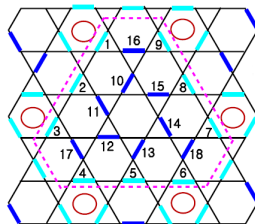
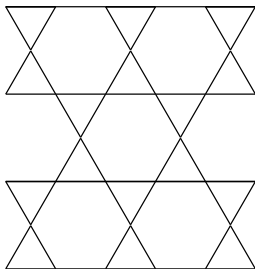
Ground state: spin liquid, VBS with 36-site unit cell

Yang et al., 2008; Han et al., 2012

Frustrated magnetic systems

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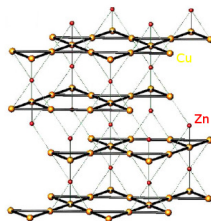
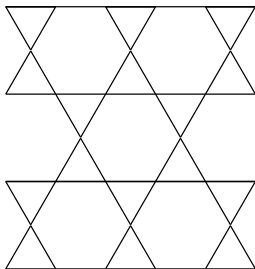
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ZnCu₃(OH)₆Cl₂

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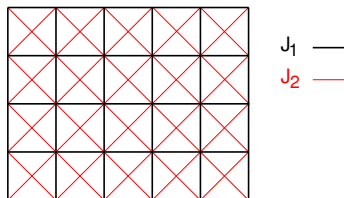
Frustrated magnetic systems

J_1 - J_2 AFM Heisenberg model

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$J_1, J_2 > 0$$

$$S = 1/2 \quad T = 0$$



Misguich and Lhuillier, 2003

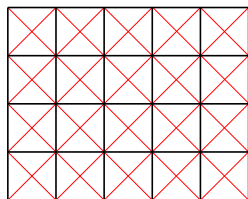
Frustrated magnetic systems

J_1 - J_2 AFM Heisenberg model

$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

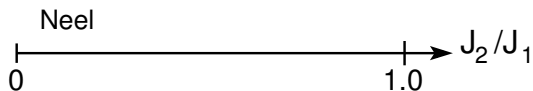
$$J_1, J_2 > 0$$

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J_1 —
 J_2 —

Classical phase diagram



Misguich and Lhuillier, 2003

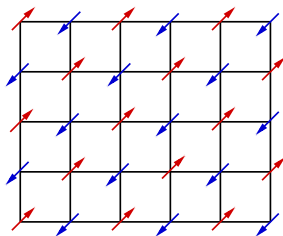
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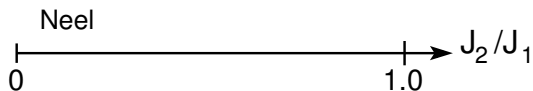
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Misguich and Lhuillier, 2003

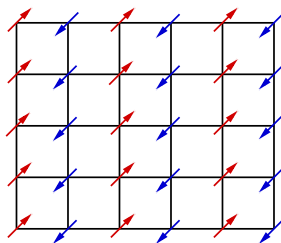
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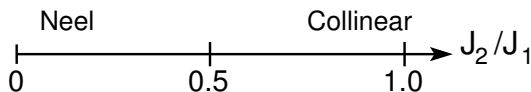
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Classical phase diagram



Misguich and Lhuillier, 2003

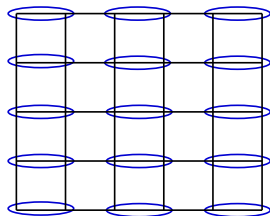
Frustrated magnetic systems

J_1 - J_2 AFM Heisenberg model

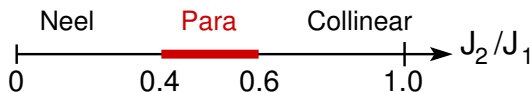
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Quantum phase diagram



Misguich and Lhuillier, 2003

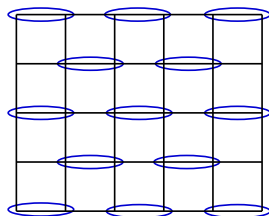
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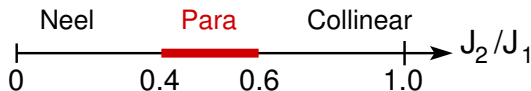
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Quantum phase diagram



Misguich and Lhuillier, 2003

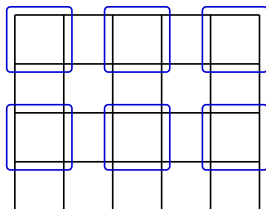
Frustrated magnetic systems

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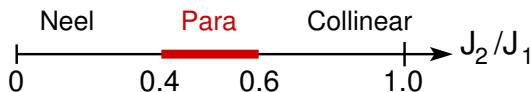
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Quantum phase diagram



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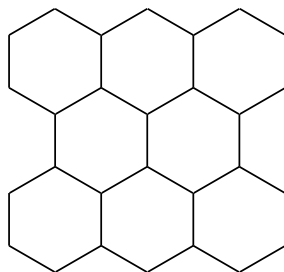
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Meng et al., 2010; Ganesh et al., 2013; Zhu et al., 2013

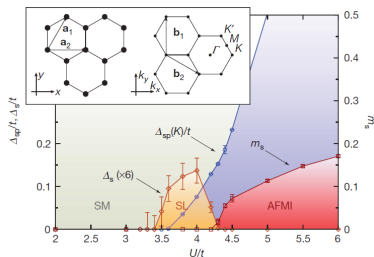
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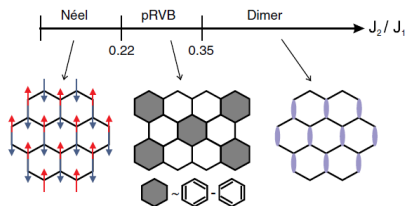
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Phase diagram:

density matrix renormalization group (DMRG)

Meng et al., 2010; Ganesh et al., 2013; Zhu et al., 2013

Spin-wave theory

Holstein-Primakoff representation

Auerbach, 1994

$$S^- = a^\dagger (2S - a^\dagger a)^{1/2}$$

$$S^+ = (2S - a^\dagger a)^{1/2} a$$

$$S^z = S - a^\dagger a$$

a_i^\dagger : boson

$$S_i^z |\uparrow\uparrow\uparrow \dots \uparrow\rangle = S |\uparrow\uparrow\uparrow \dots \uparrow\rangle$$

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Spin-wave theory

Holstein-Primakoff representation

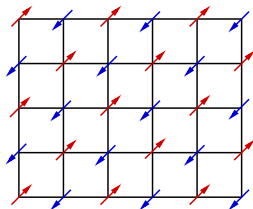
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$$S^- = a^\dagger (2S - a^\dagger a)^{1/2}$$

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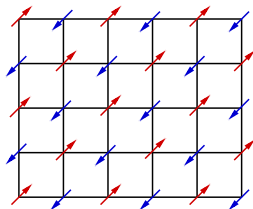
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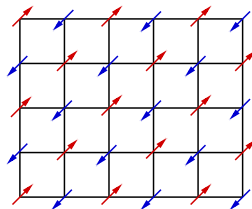
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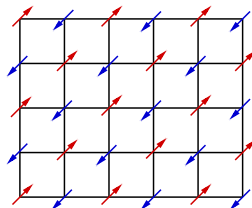
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$$\mathcal{H} = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad \rightarrow \quad \mathcal{H}_{\text{boson}} = \mathcal{H}_2 + \mathcal{H}_4$$

Spin-wave theory

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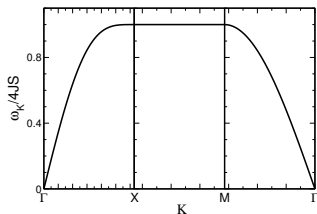
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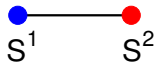


Bond operator representation

Hilbert space: 2 spins-1/2

$$|s\rangle \equiv s^\dagger |0\rangle$$

$$|\alpha\rangle \equiv t_\alpha^\dagger |0\rangle \quad \alpha = x, y, z$$



s^\dagger and t_α^\dagger : bosons

$$S_\alpha^{1/2} = \pm \frac{1}{2} \left(s^\dagger t_\alpha + t_\alpha^\dagger s - i \epsilon_{\alpha\beta\gamma} t_\beta^\dagger t_\gamma \right)$$

constraint: $s^\dagger s + \sum_\alpha t_\alpha^\dagger t_\alpha = 1$

generalization lattice \rightarrow description VBS

Sachdev and Bhatt, 1990

Slave bosons/fermions

Spin operator

$$\mathbf{S} = \frac{1}{2} b_{\alpha}^{\dagger} \hat{\sigma}_{\alpha, \beta} b_{\beta} \quad b_{\alpha}^{\dagger} : \text{spinon}$$

- spinon: fermion
- spinon: boson (Schwinger bosons)

Slave bosons/fermions

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Mean-field approximation: Z_2 , $U(1)$ spin liquids

Slave bosons/fermions

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Mean-field approximation: Z_2 , $U(1)$ spin liquids

Several labels: $b_{j\sigma} \rightarrow e^{i\phi_j} b_{j\sigma}$

Fluctuations: phase mean-field ansatz \sim gauge fields

Valence bond solid in frustrated antiferromagnets

Idea: Frustration effects on valence bond solid

- triplon (spin) gap at incommensurate momentum
- finite lifetime high energy triplon excitations

Collaborator: Matthias Vojta (TU Dresden)

Details: Phys. Rev. B **85**, 104416 (2012)

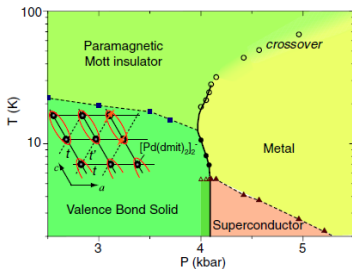
Financial support: Fapesp and DFG - SFB 608 (Köln)

Experimental data: $\text{EtMe}_3\text{P}[\text{Pd}(\text{dmit})_2]_2$

Organic material

Triangular lattice, $J = 250 \text{ K}$ (mag. susceptibility, high- T)

P - T phase diagram (resistivity measurements)



VBS borders SC, contrast high- T_c : Néel borders SC

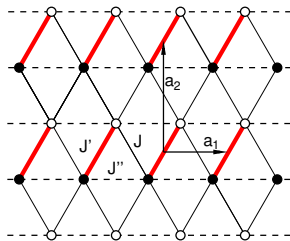
Shimizu et al., 2007

Anisotropic and dimerized AFM Heisenberg model

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

spin-1/2

$$J_{ij} = J = 1, J', J''$$

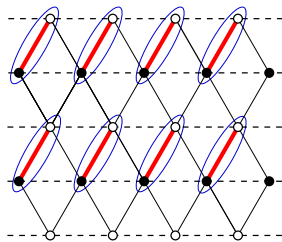


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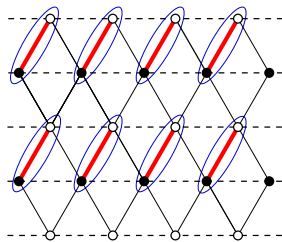


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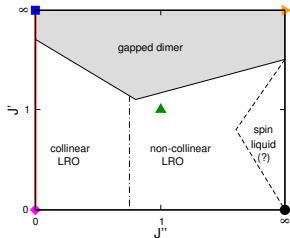
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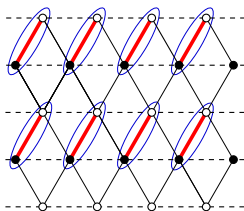
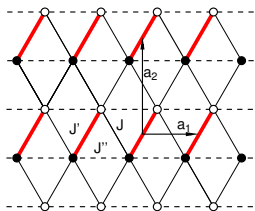
Phase diagram $T = 0$:



Effective triplon model

Bond operator formalism: $S_\alpha^{1/2} \sim \pm \left(s^\dagger t_\alpha + t_\alpha^\dagger s - i \epsilon_{\alpha\beta\gamma} t_\beta^\dagger t_\gamma \right)$

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad \rightarrow \quad \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4$$



Reference state: columnar VBS

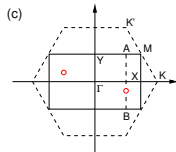
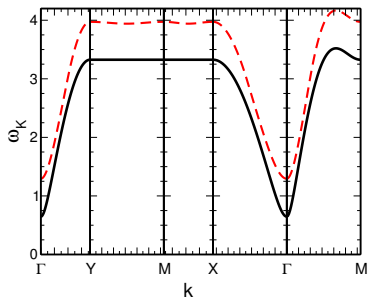
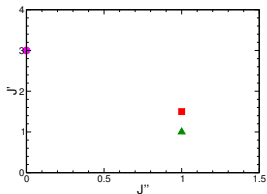
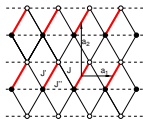
$$s_i^\dagger = s_i = \langle s_i^\dagger \rangle = \langle s_i \rangle \rightarrow \sqrt{N_0}$$

Triplon dispersion relation – harmonic approximation

$$J' = 3.0 \quad J'' = 0.0$$

nonfrustrated

commensurate (C)



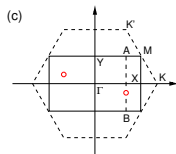
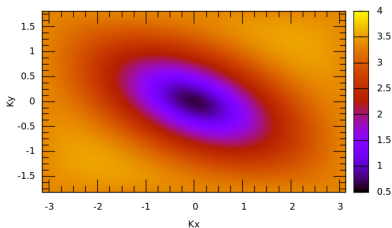
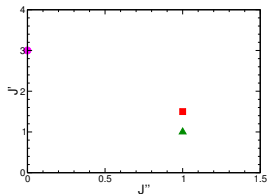
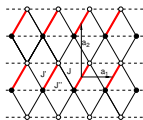
$$E_p = \min(\epsilon_{p-k} + \epsilon_k)$$

Triplon dispersion relation – harmonic approximation

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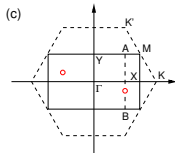
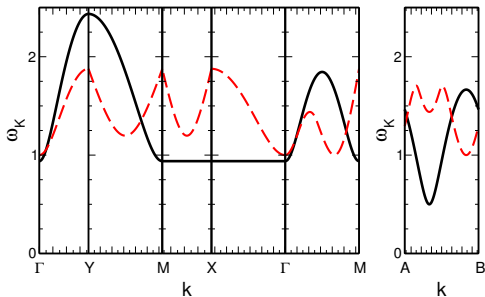
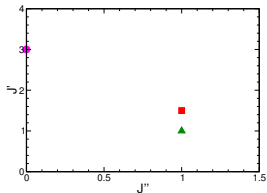
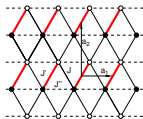
$$E_p = \min(\epsilon_{p-k} + \epsilon_k)$$

Triplon dispersion relation – harmonic approximation

$$J' = 1.5 \quad J'' = 1.0$$

frustrated

incommensurate (INC)



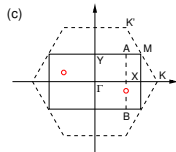
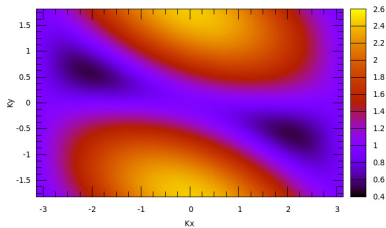
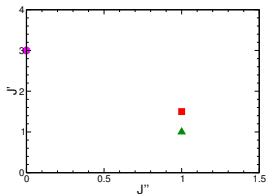
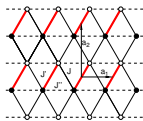
$$E_p = \min(\epsilon_{p-k} + \epsilon_k)$$

Triplon dispersion relation – harmonic approximation

$$J' = 1.5 \quad J'' = 1.0$$

frustrated

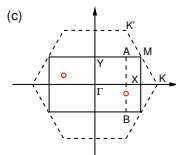
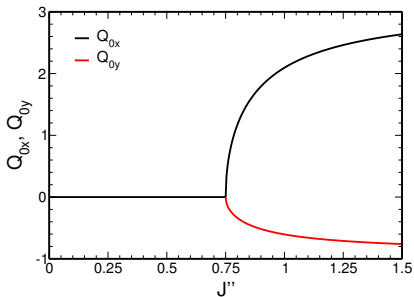
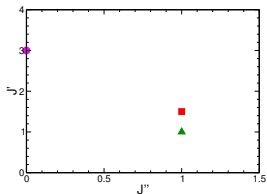
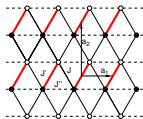
incommensurate (INC)



$$E_p = \min(\epsilon_{p-k} + \epsilon_k)$$

Triplon dispersion relation – harmonic approximation

\mathbf{Q}_0 : momentum \sim gap Δ



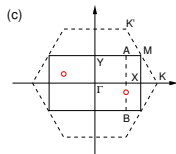
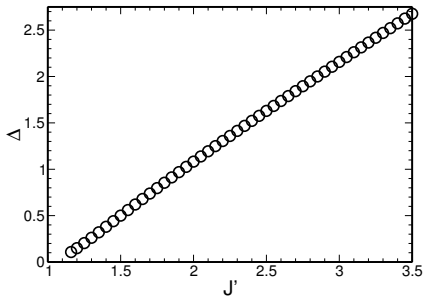
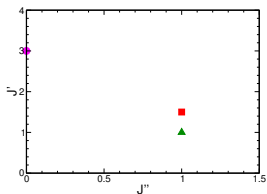
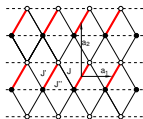
Triplon dispersion relation – harmonic approximation

Gap $\Delta \times J'$

line $J'' = 1.0$

$\Delta = 0$:

continuous phase transition



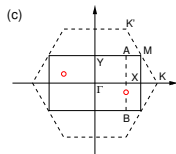
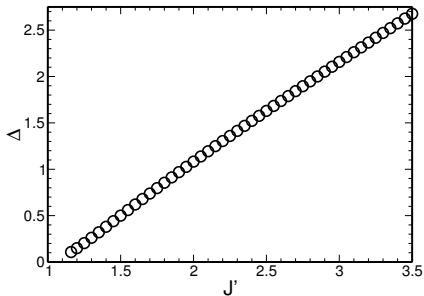
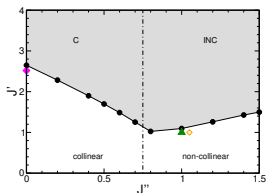
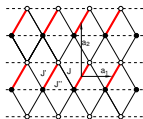
Triplon dispersion relation – harmonic approximation

Gap $\Delta \times J'$

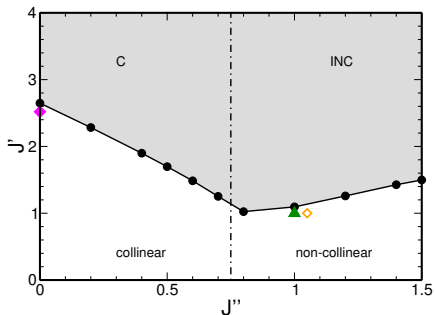
line $J'' = 1.0$

$\Delta = 0$:

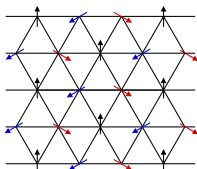
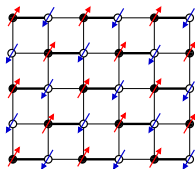
continuous phase transition



Harmonic approximation – phase diagram



- ◆ QMC stagger dimer
- ▲ isotropic model
- ◇ Pd(dmit)



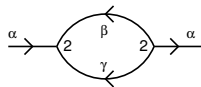
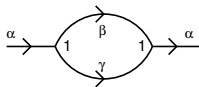
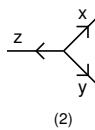
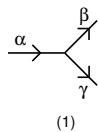
Beyond harmonic approximation

Quartic term \mathcal{H}_4 :

self-consistent Hartree–Fock approximation

Cubic term \mathcal{H}_3 :

lowest-order perturbation theory

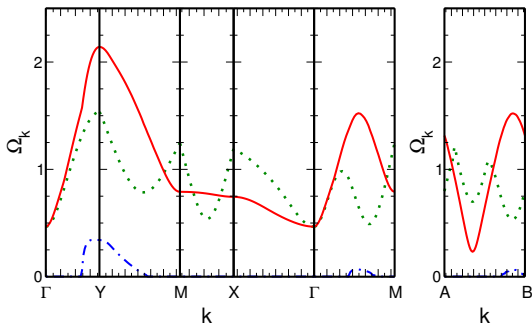
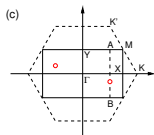


Beyond harmonic approximation

Triplon dispersion relation

$$\omega = \Omega_{\mathbf{k}} - i\tilde{\Gamma}_{\mathbf{k}}$$

$\tilde{\Gamma}_{\mathbf{k}}^{-1}$: lifetime



$$J' = 1.5 \quad J'' = 1.0$$

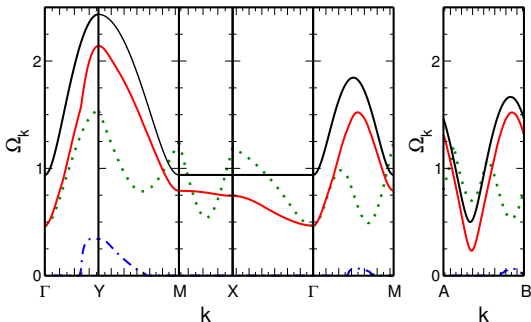
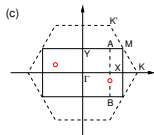
$$E_p = \min(\epsilon_{p-k} + \epsilon_k)$$

Beyond harmonic approximation

Triplon dispersion relation

$$\omega = \Omega_{\mathbf{k}} - i\tilde{\Gamma}_{\mathbf{k}}$$

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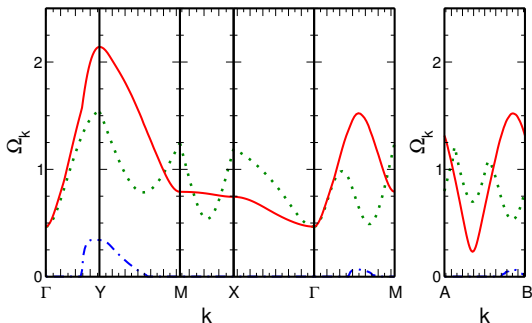
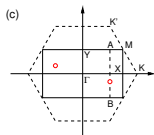
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Beyond harmonic approximation

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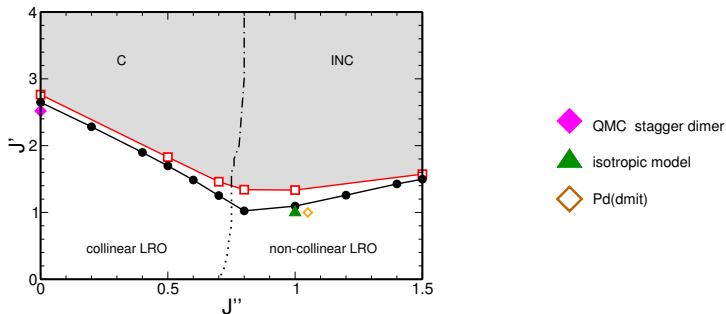
$\tilde{\Gamma}_{\mathbf{k}}^{-1}$: lifetime



$$J' = 1.5 \quad J'' = 1.0$$

$$E_p = \min(\epsilon_{p-k} + \epsilon_k)$$

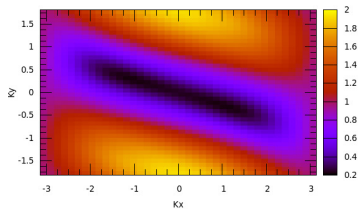
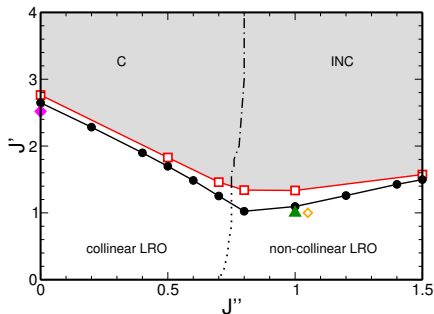
Beyond harmonic approximation – phase diagram



neutron scattering measurements $P[\text{Pd}(\text{dmit})_2]_2$:

- triplon (spin) gap at incommensurate momentum
- finite lifetime high energy triplon excitations

Beyond harmonic approximation – phase diagram

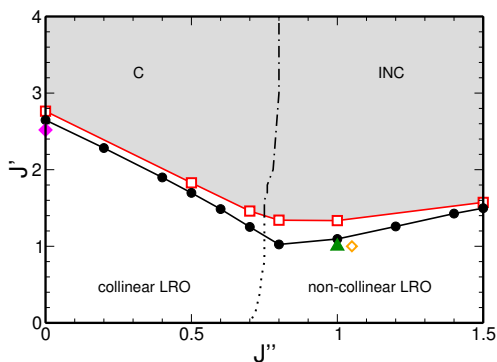


- Commensurate–incommensurate transition
- multicritical (Lifshitz) point: 3 phases

$$G^{-1}(\mathbf{k}, \omega) \sim \omega^2 - \Delta^2 + ck_{\perp}^2 + dk_{\parallel}^4$$

Summary

- Valence bond phase triangular lattice AFM Heisenberg model:
bond operator formalism



- Details: Phys. Rev. B **85**, 104416 (2012)

Effective triplon model

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4$$

where

$$\mathcal{H}_0 = -3J'N/8 - \mu N(N_0 - 1)/2$$

$$\mathcal{H}_2 = \sum_{\mathbf{k}} \left[A_{\mathbf{k}} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{1}{2} B_{\mathbf{k}} \left(t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + \text{H.c.} \right) \right]$$

Effective triplon model

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$$\mathcal{H}_3 = \frac{1}{2\sqrt{N'}} \epsilon_{\alpha\beta\lambda} \sum_{\mathbf{p}, \mathbf{k}} \xi_{\mathbf{k}-\mathbf{p}} t_{\mathbf{k}-\mathbf{p}\alpha}^\dagger t_{\mathbf{p}\beta}^\dagger t_{\mathbf{k}\lambda} + \text{H.c.}$$

Effective triplon model

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_3 + \mathcal{H}_4$$

where

$$\mathcal{H}_0 = -3J'N/8 - \mu N(N_0 - 1)/2$$

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$$\mathcal{H}_3 = \frac{1}{2\sqrt{N'}} \epsilon_{\alpha\beta\lambda} \sum_{\mathbf{p}, \mathbf{k}} \xi_{\mathbf{k}-\mathbf{p}} t_{\mathbf{k}-\mathbf{p}\alpha}^\dagger t_{\mathbf{p}\beta}^\dagger t_{\mathbf{k}\lambda} + \text{H.c.}$$

$$\mathcal{H}_4 = \frac{1}{2N'} \epsilon_{\alpha\beta\lambda} \epsilon_{\alpha\mu\nu} \sum_{\mathbf{q}, \mathbf{p}, \mathbf{k}} \gamma_{\mathbf{k}} t_{\mathbf{p}+\mathbf{k}\beta}^\dagger t_{\mathbf{q}-\mathbf{k}\mu}^\dagger t_{\mathbf{q}\nu} t_{\mathbf{p}\lambda}$$

Effective triplon model

Harmonic approximation:

$$\mathcal{H} \approx \mathcal{H}_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{1}{2} B_{\mathbf{k}} \left(t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + \text{H.c.} \right) \right]$$

Effective triplon model

Harmonic approximation:

$$\mathcal{H} \approx \mathcal{H}_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{1}{2} B_{\mathbf{k}} \left(t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + \text{H.c.} \right) \right]$$

Bogoliubov transformation: $t_{\mathbf{k}\alpha}^\dagger = u_{\mathbf{k}} b_{\mathbf{k}\alpha}^\dagger - v_{\mathbf{k}} b_{-\mathbf{k}\alpha}$

Effective triplon model

Harmonic approximation:

$$\mathcal{H} \approx \mathcal{H}_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{1}{2} B_{\mathbf{k}} \left(t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + \text{H.c.} \right) \right]$$

Bogoliubov transformation: $t_{\mathbf{k}\alpha}^\dagger = u_{\mathbf{k}} b_{\mathbf{k}\alpha}^\dagger - v_{\mathbf{k}} b_{-\mathbf{k}\alpha}$

$$\mathcal{H} = \bar{E}_0 + \sum_{\mathbf{k}\alpha} \omega_{\mathbf{k}} b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha} \quad \omega_{\mathbf{k}}(N_0, \mu) = \sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}$$

Effective triplon model

Harmonic approximation:

$$\mathcal{H} \approx \mathcal{H}_0 + \sum_{\mathbf{k}} \left[A_{\mathbf{k}} t_{\mathbf{k}\alpha}^\dagger t_{\mathbf{k}\alpha} + \frac{1}{2} B_{\mathbf{k}} \left(t_{\mathbf{k}\alpha}^\dagger t_{-\mathbf{k}\alpha}^\dagger + \text{H.c.} \right) \right]$$

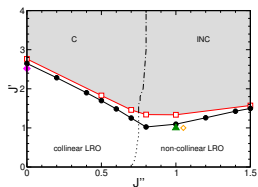
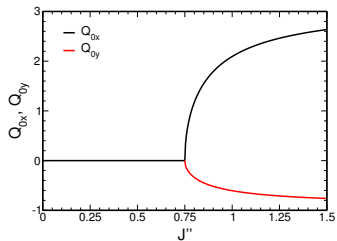
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Saddle point conditions: $\partial \bar{E}_0 / \partial N_0 = 0$ and $\partial \bar{E}_0 / \partial \mu = 0$
 \Rightarrow self-consistent equations

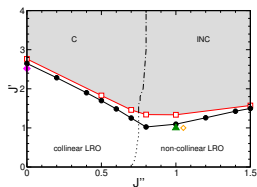
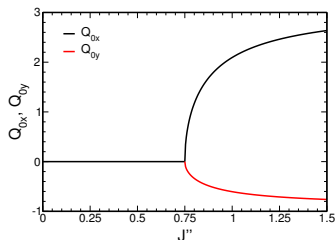
Commensurate–incommensurate transition

bond operator formalism



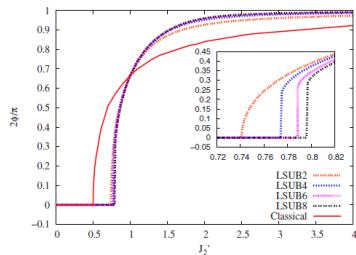
Commensurate–incommensurate transition

bond operator formalism



Coupled cluster method
(numerical)

line $J' = 1.0$

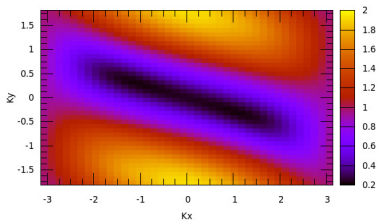


Bishop et al., 2009

Commensurate–incommensurate transition

Triplon dispersion relation

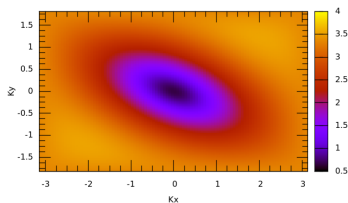
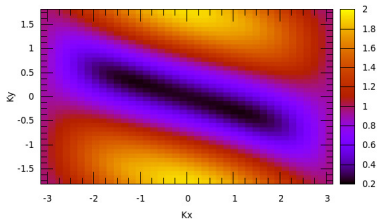
$$J' = 1.5 \quad J'' = 0.8$$



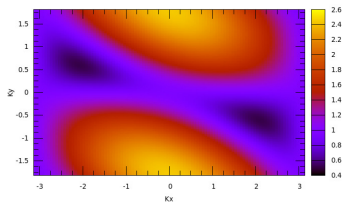
Commensurate–incommensurate transition

Triplon dispersion relation

$$J' = 1.5 \quad J'' = 0.8$$



$J' = 3.0 \quad J'' = 0.0$
commensurate (C)



$J' = 1.5 \quad J'' = 1.0$
incommensurate (INC)

Effective triplon model – coefficients

$$A_{\mathbf{k}} = \frac{J'}{4} - \mu + B_{\mathbf{k}}$$

$$B_{\mathbf{k}} = \frac{1}{2} N_0 \left[(2J'' - 1) \cos(k_x) - \cos(\sqrt{3}k_y) - \cos(k_x + \sqrt{3}k_y) \right]$$

$$\xi_{\mathbf{k}} = -\sqrt{N_0} \left[\sin(k_x) + \sin(\sqrt{3}k_y) + \sin(k_x + \sqrt{3}k_y) \right]$$

$$\gamma_{\mathbf{k}} = -\frac{1}{2} \left[(2J'' + 1) \cos(k_x) + \cos(\sqrt{3}k_y) + \cos(k_x + \sqrt{3}k_y) \right]$$