Phase transition induced by magnetic field in a two-leg spin ladder

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T. Sugimoto, *et al*, PRB 87, 155143 (2013).

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- Model: frustrated two-leg spin ladder
- Compound: $BiCu_2PO_6$
- Method: Dynamical DMRG
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Model

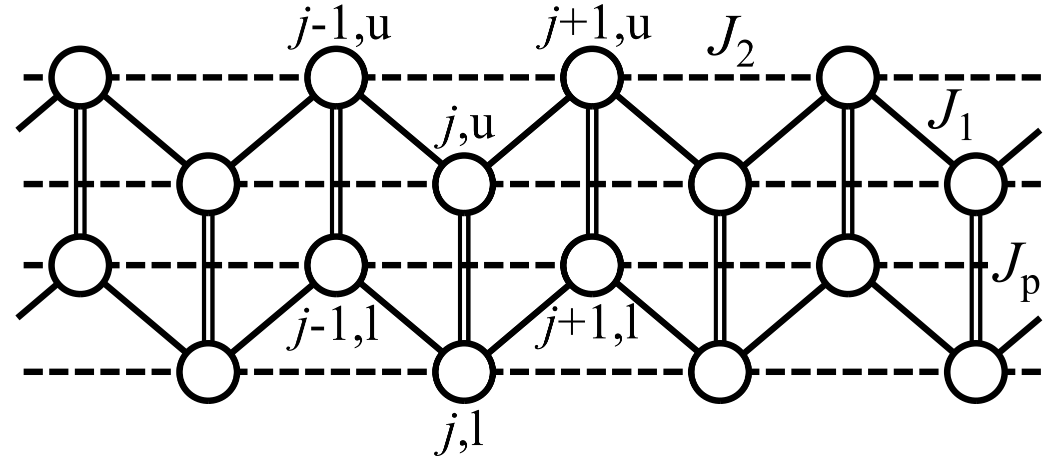
Frustrated two-leg spin-ladder system

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_p$$

$$\mathcal{H}_1 = J_1 \sum_j \left[\boldsymbol{S}_{j,\mathrm{u}} \cdot \boldsymbol{S}_{j+1,\mathrm{u}} + \boldsymbol{S}_{j,\mathrm{l}} \cdot \boldsymbol{S}_{j+1,\mathrm{l}} \right]$$

$$\mathcal{H}_2 = J_2 \sum_j \left[\boldsymbol{S}_{j,\mathrm{u}} \cdot \boldsymbol{S}_{j+2,\mathrm{u}} + \boldsymbol{S}_{j,\mathrm{l}} \cdot \boldsymbol{S}_{j+2,\mathrm{l}} \right]$$

$$\mathcal{H}_p = J_p \sum_j \boldsymbol{S}_{j,\mathrm{u}} \cdot \boldsymbol{S}_{j,\mathrm{l}}$$



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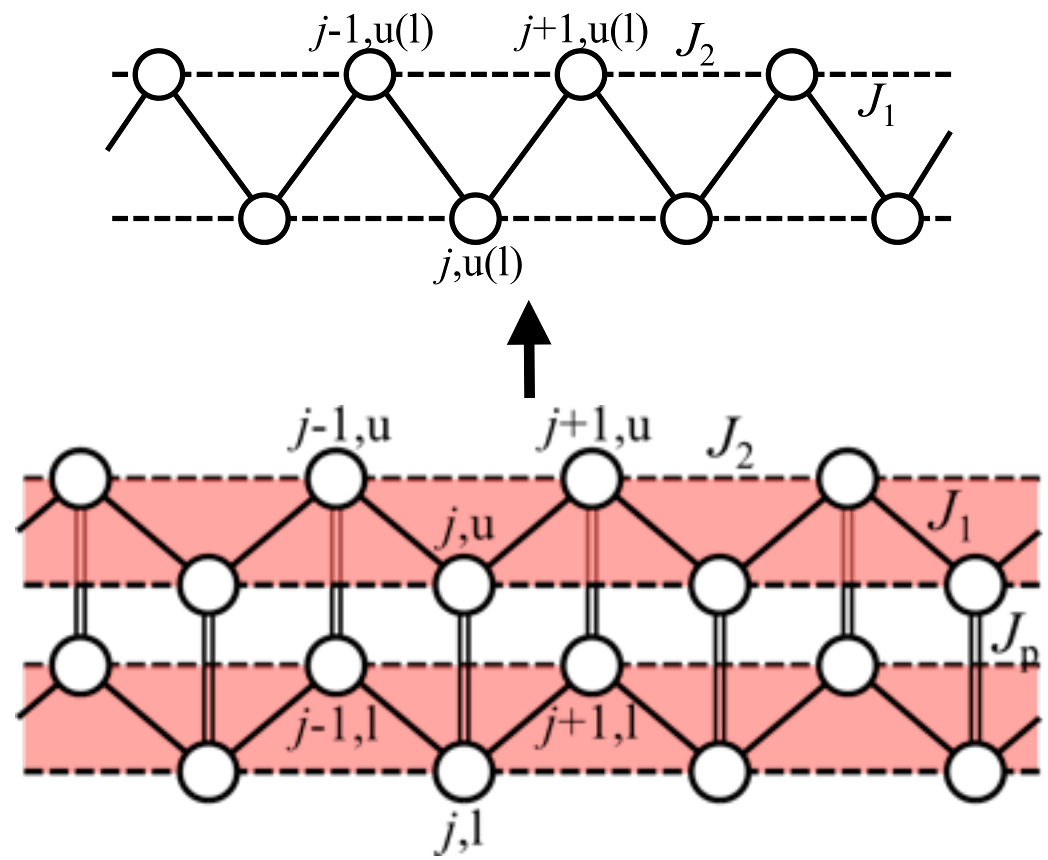
Frustrated spin-chain system



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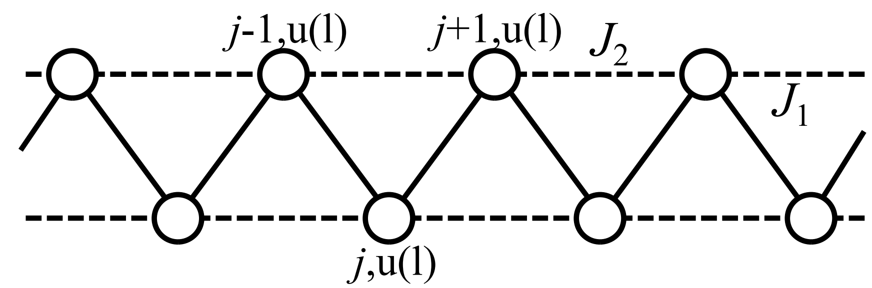
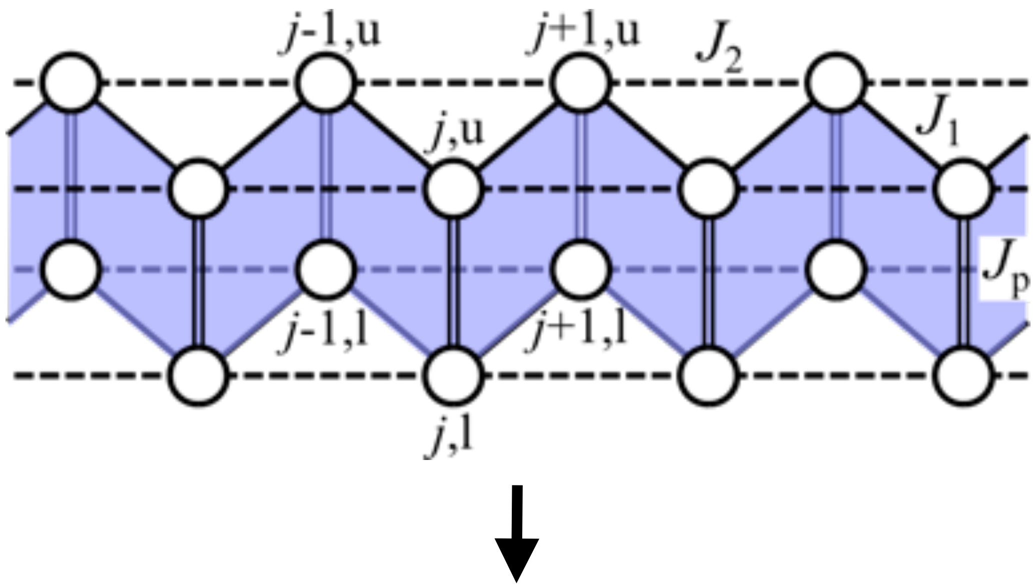
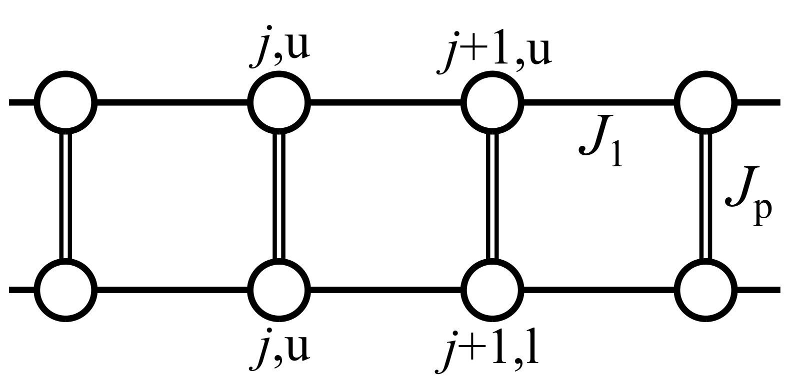




Non-frustrated spin-ladder system



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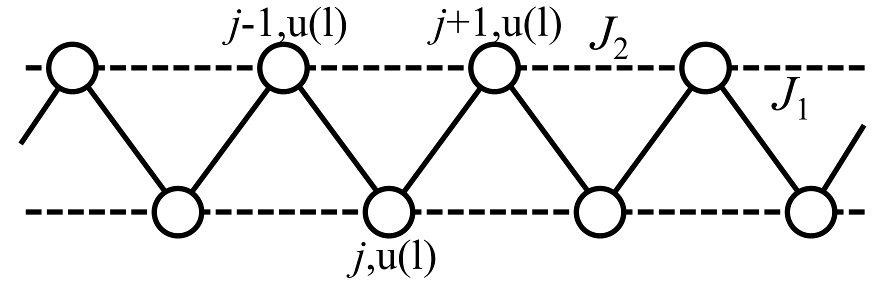
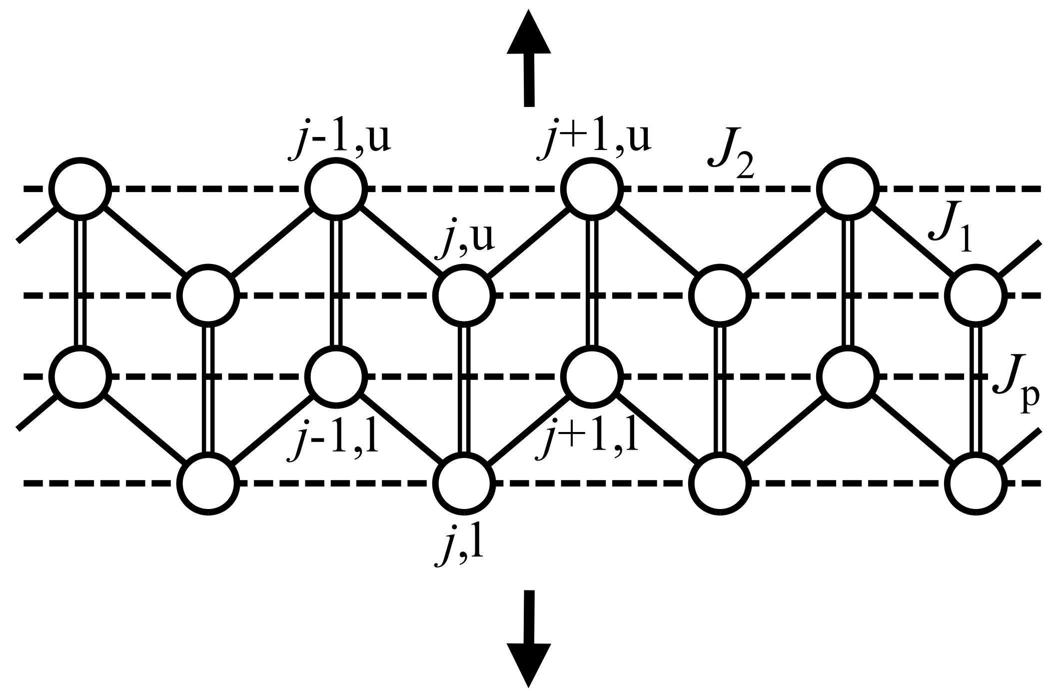
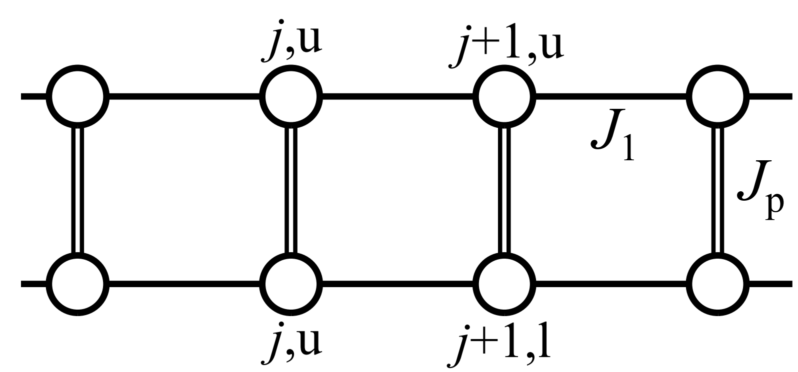
☛ This is a bridging model between the frustrated spin chain & non-frustrated spin ladder.

Frustrated spin-chain system (J_p=0)



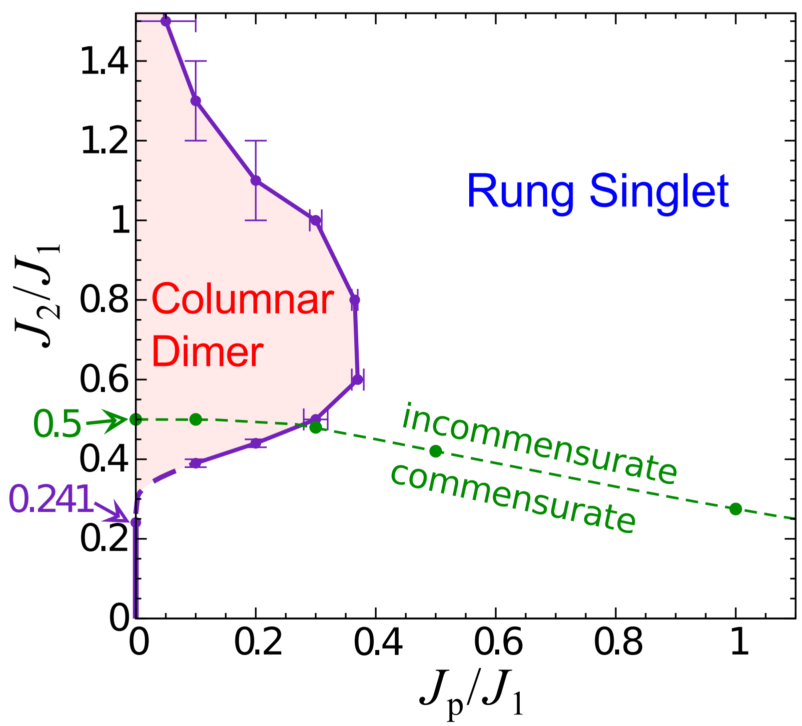


Non-frustrated spin-ladder system (J_2=0)



Model

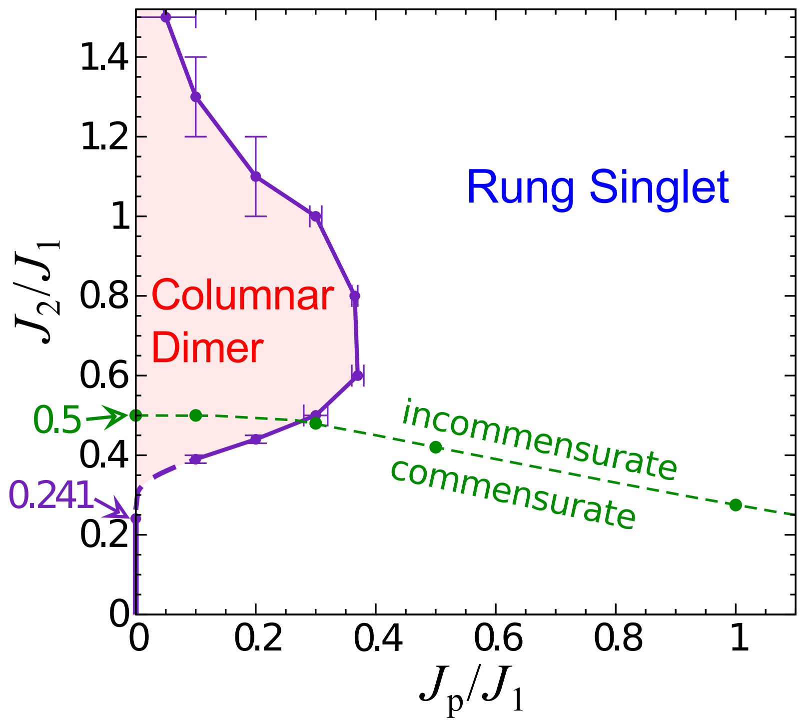
Ground-state phase diagram



A. Lavarélo, *et al*, PRB 84, 144407 (2011).

Model

Ground-state phase diagram



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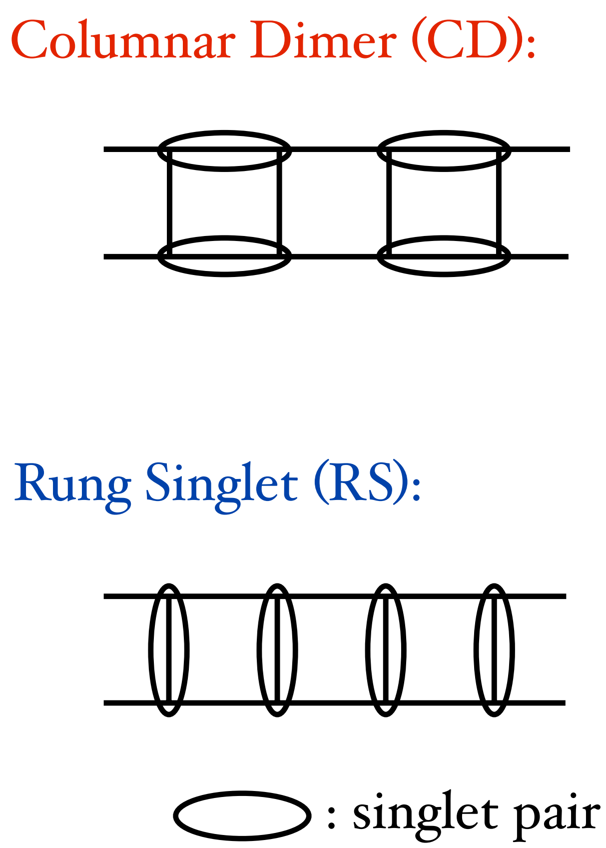
Ground state



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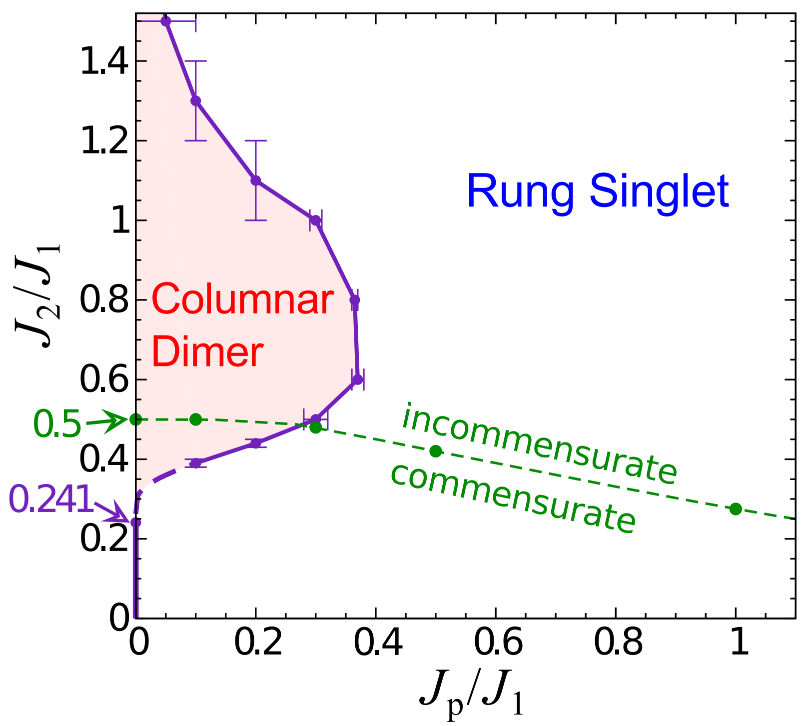

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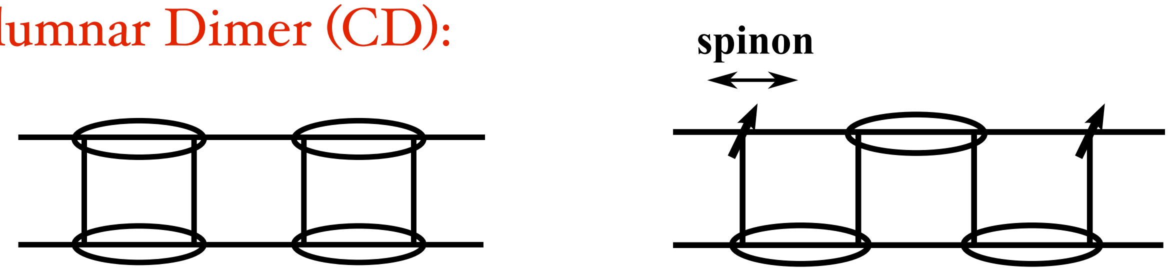
Ground state

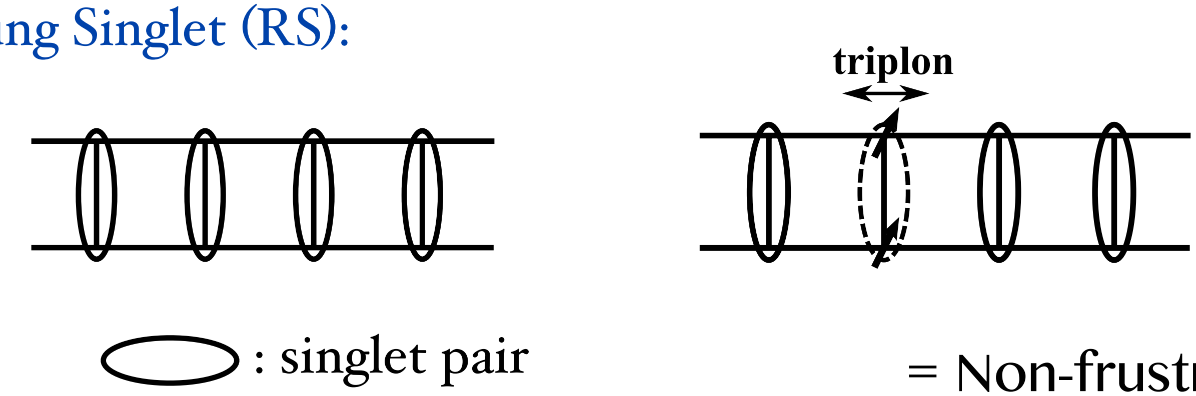
Elementary Excitation

Columnar Dimer (CD):



= Frustrated spin chain

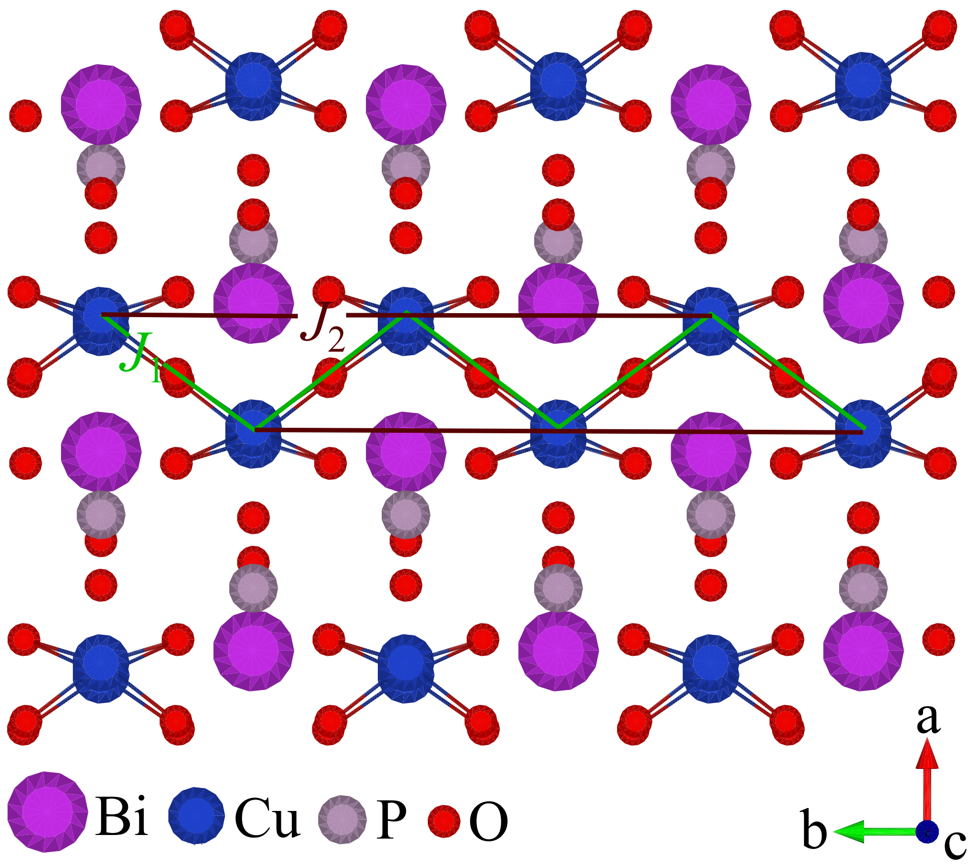
Rung Singlet (RS):

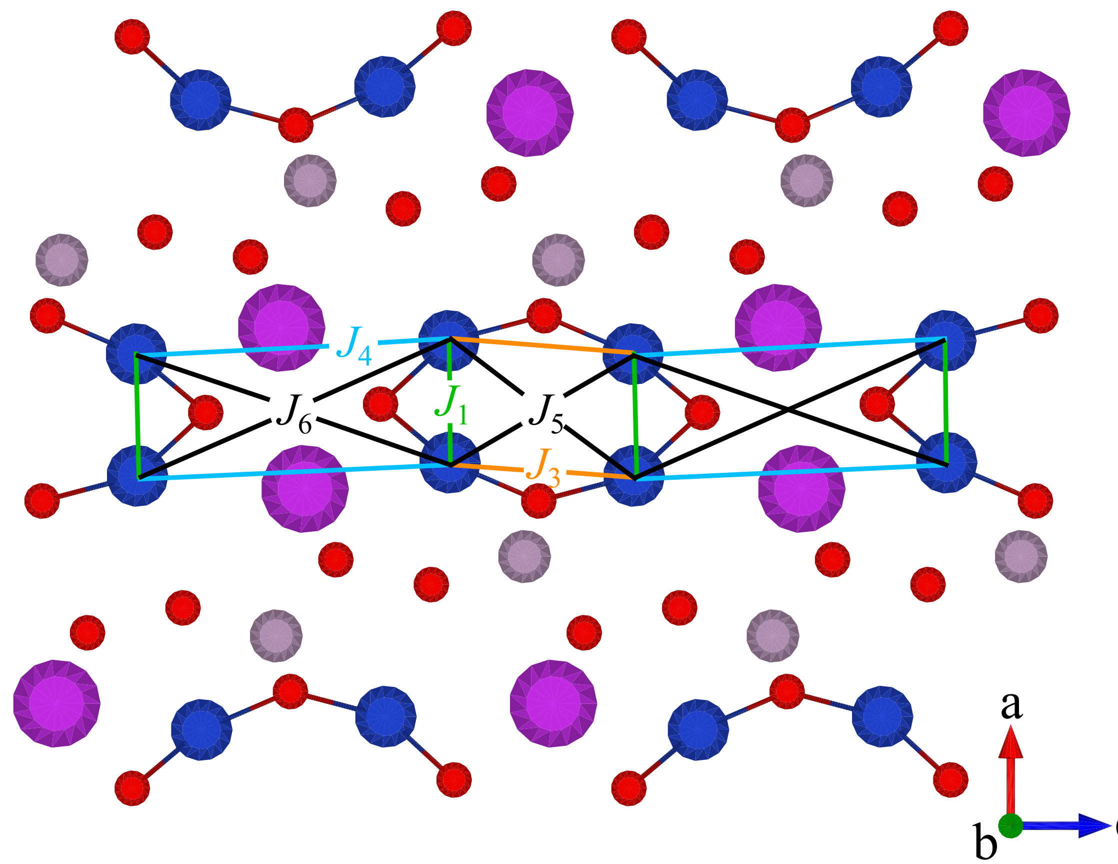


= Non-frustrated spin ladder

Real compound

- Crystal Structure of $BiCu_2PO_6$





- Exchange energy by DFT calculation

Ref.	J_1	J_2	J_3	J_4	J_5	J_6
1	1	$0.67 \sim 0.79$	$0.41 \sim 0.69$	$1.0 \sim 1.2$	$-2.5 \sim 2.9 \times 10^{-3}$	$-9.0 \sim 9.7 \times 10^{-3}$
2	1	$0.88 \sim 0.97$	$-0.14 \sim 0.13$	$0.78 \sim 0.88$	-	-

☛ J_5 & J_6 are much smaller than others.

☛ J_2 (NNN in leg) may be comparable to J_1.

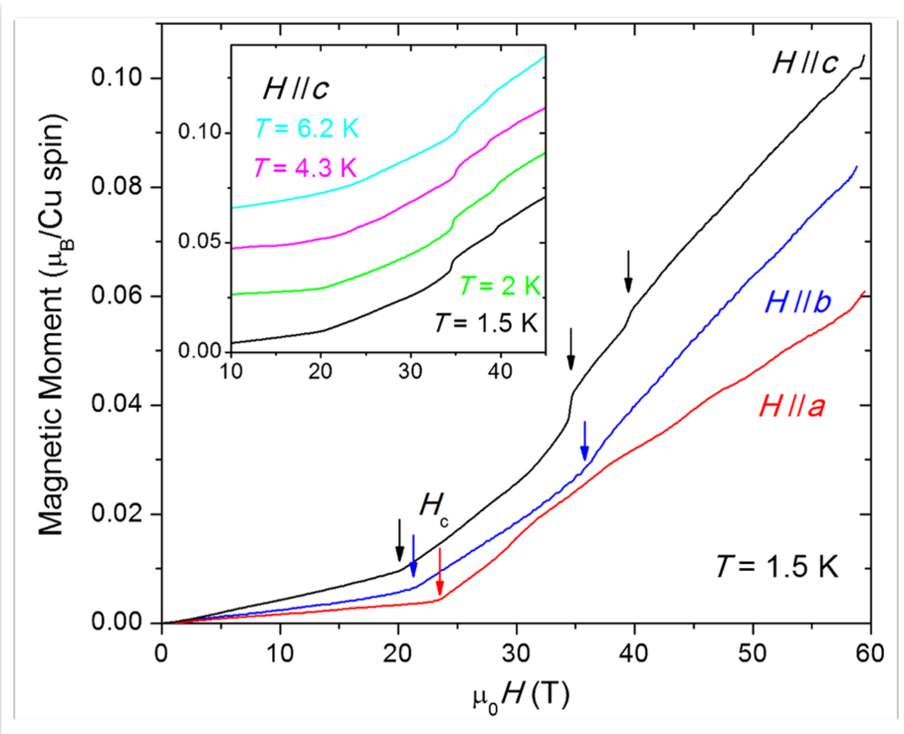
☛ Effective model corresponds to J_1-J_2-J_4 model.

[1] O. Mentré, *et al*, PRB 80, 180413(R) (2009).

[2] A. A. Tsirlin, *et al*, PRB 82, 144426 (2010).

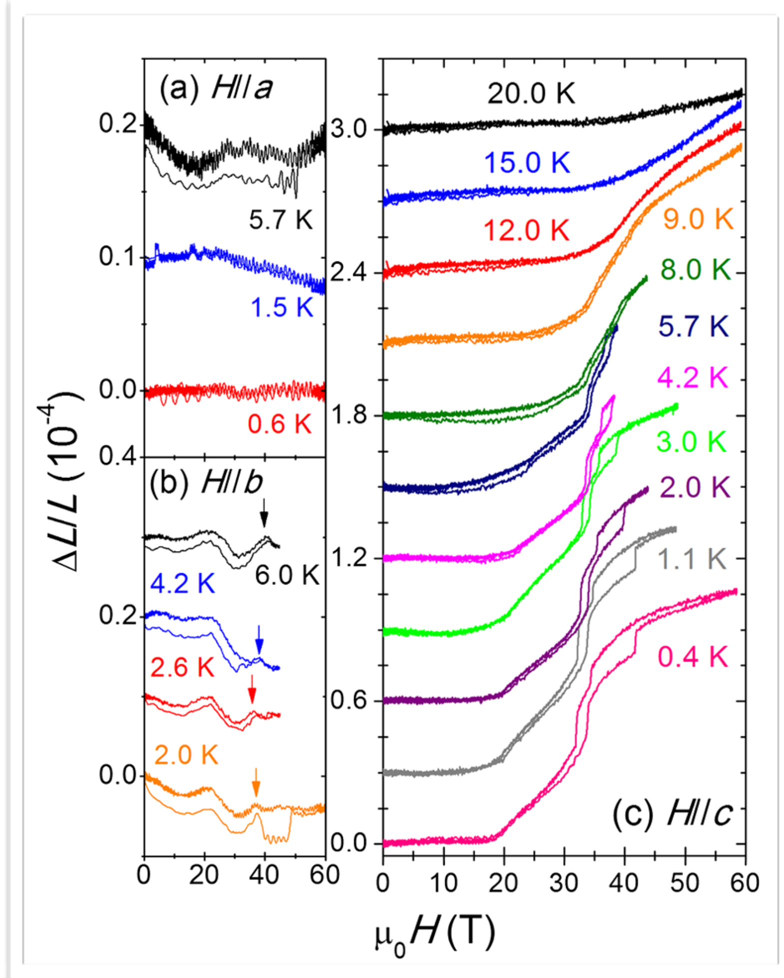
Real compound

M-H curve

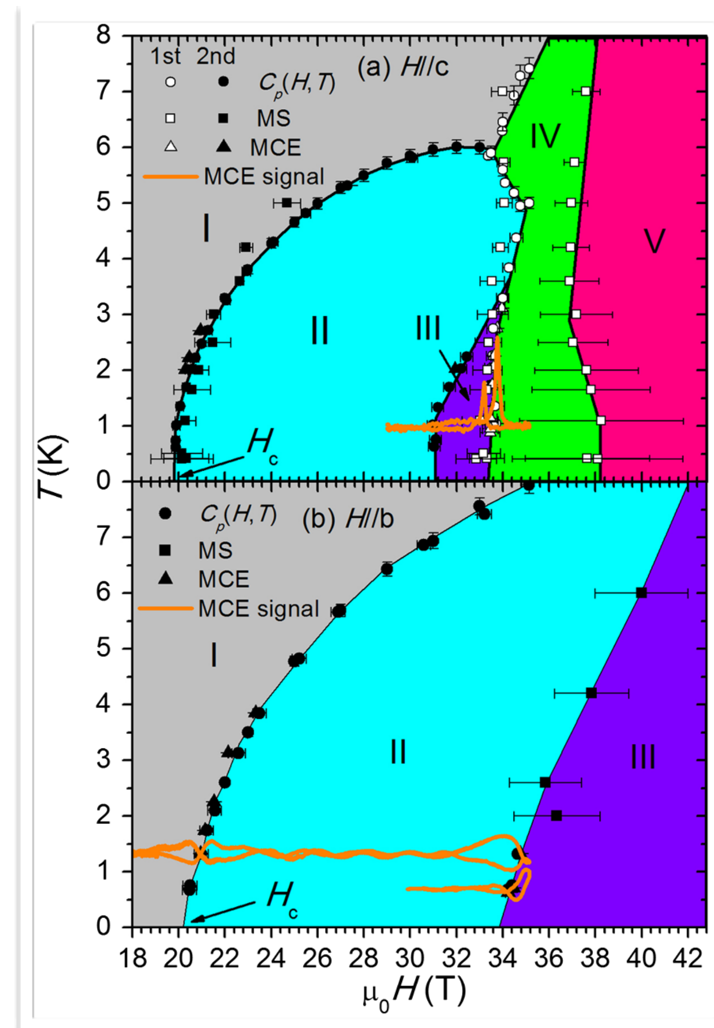


Y. Kohama, *et al*, PRL **109**, 167204 (2012).

Magnetostriction



Phase diagram



☛ M-H curve along c-axis is quite different from those along a- and b-axis.

☛ Phase IV & V may occur caused by spin-lattice coupling.

☛ Phase II & III may be spin-liquid phases.

However, the transition between two different spin-liquid phases does not appear in non-frustrated two-leg spin ladder.

Purpose

Our purposes are

to determine the ground-state phase of $BiCu_2PO_6$,
and to clarify the phase transition induced by magnetic field.

☛ To determine the ground-state phase of $BiCu_2PO_6$, we use the magnetic excitation, which can be addressed by inelastic neutron scattering.

☛ The dynamical spin correlation function (DSCF):

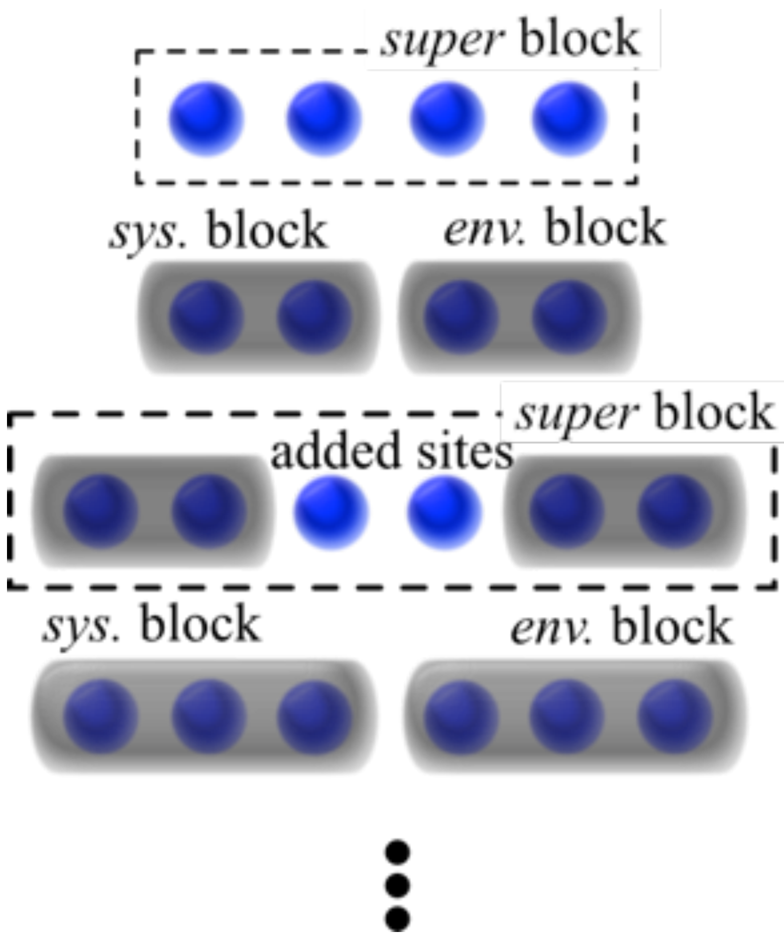
$$\chi(\boldsymbol{q},\omega) = -\frac{1}{\pi}\Im \int_0^\infty dt e^{i\omega t} \langle 0 | S^{z\dagger}(\boldsymbol{q},t) S^z(\boldsymbol{q},0) | 0 \rangle$$

☛ To clarify the phase transition, we can use the bond-operator transform. Then, boson-like quasi-particle “triplon” is important to understand the phase transition.

Method

DMRG method:

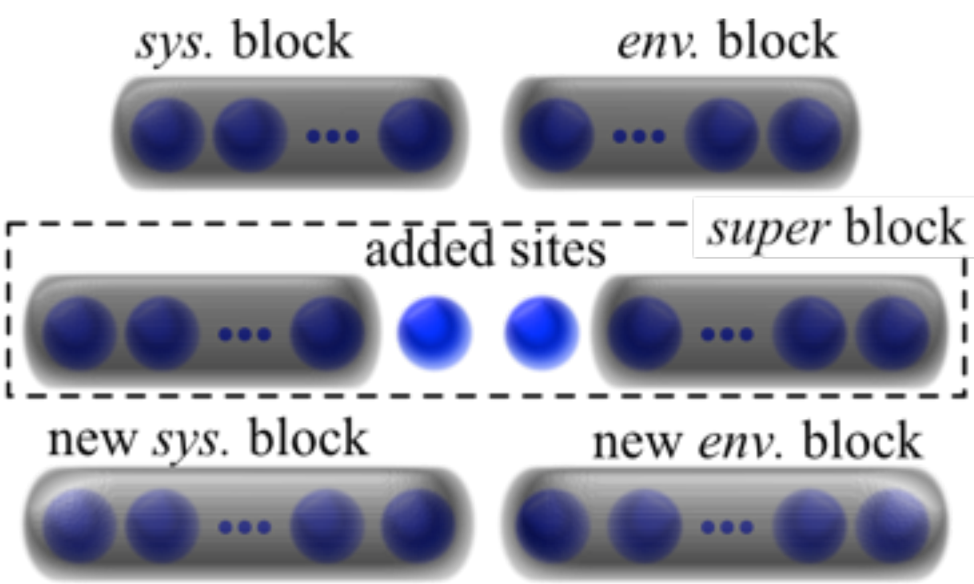
- This is a variational method to optimize the basis for the best description of physical quantities of interest.
- The main idea of the DMRG method is a systematic selection of kept states after diagonalization of the reduced density matrix.
- The reduced density matrix is made with proper target states.



Method

Variational procedure of DMRG:

1. Target states are obtained for the super block.
2. Reduced density matrix is obtained by using the target states.
3. Diagonalization of the reduced density matrix is used to select kept states.
4. Basis of new sys. block is given by orthonormal matrix obtained by the diagnoralization.



Target state (e.g. the ground state):

$$|\psi\rangle = \sum_{i,j} \psi_{ij} |i\rangle_s |j\rangle_e.$$

$|i\rangle_s$: the basis of the sys. block and the left added site.

$|j\rangle_e$:the basis of the env. block and the right added site.

Reduced density matrix:

$$\rho^r_{il} = \sum_j \psi_{ij}\psi^*_{jl}.$$

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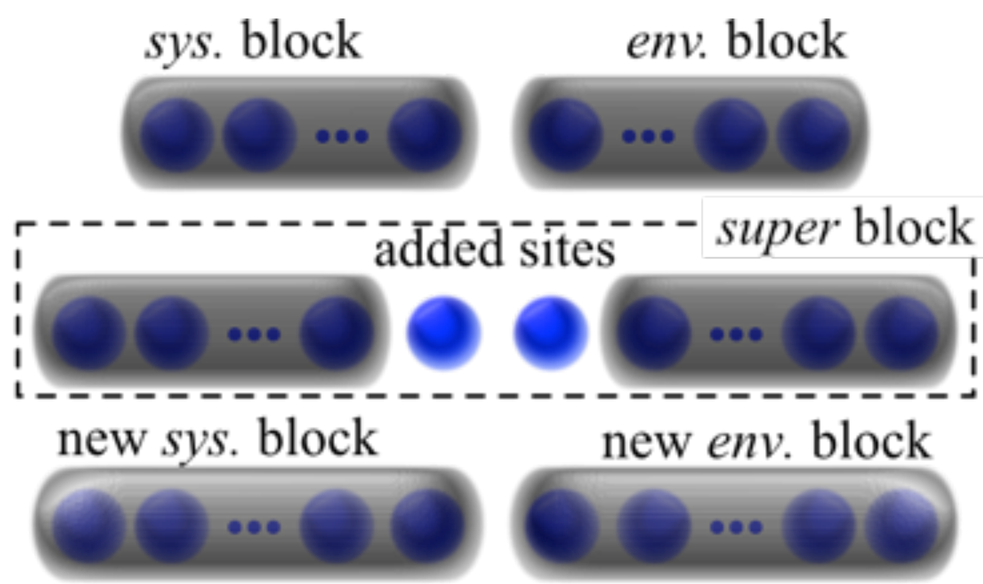

Diagonalization of RDM:

$$\rho^r_{il} = \sum_k U^*_{ik} \Lambda^2_{kk} U_{kl}.$$

Λ_{kk} : diagonal matrix.

U_{kl} : unitary matrix.

Basis of new sys. block:

$$|u^\alpha\rangle_s = \sum_i U^*_{i\alpha} |i\rangle_s.$$

$\alpha = 1, 2, \ldots, M.$

M : truncation number of DMRG.

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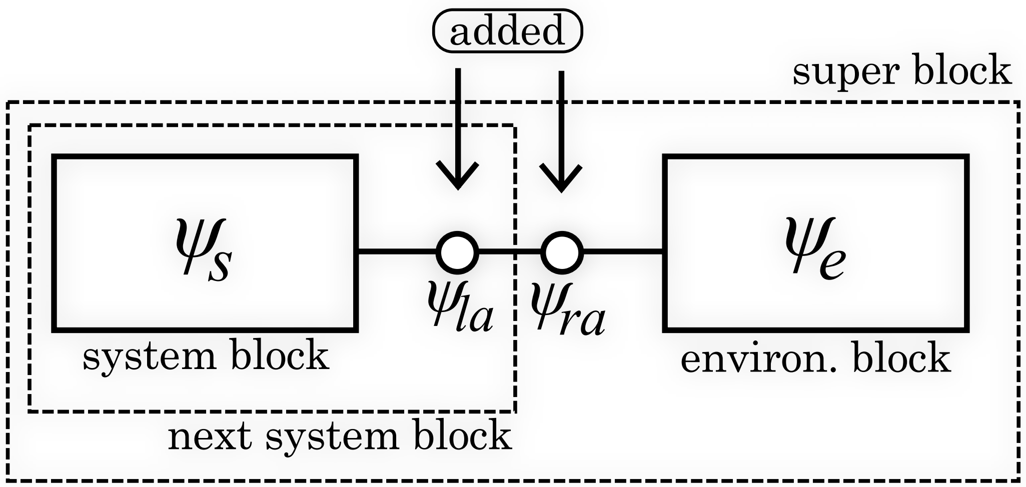
Method

- Density-matrix renormalization-group method



- Dynamical spin correlation function

$$\chi(\boldsymbol{q},\omega) = -\frac{1}{\pi}\Im\int_0^\infty dt\, e^{i(\omega+i\gamma)t}\langle 0|\boldsymbol{S}^\dagger(\boldsymbol{q},t)\cdot\boldsymbol{S}(\boldsymbol{q},0)|0\rangle$$

$$= -\frac{1}{\pi}\Im\langle 0|\boldsymbol{S}^\dagger(\boldsymbol{q})\frac{1}{\omega-\mathcal{H}+E_0+i\gamma}\boldsymbol{S}(\boldsymbol{q})|0\rangle.$$

- Target states

$$|0\rangle,\ \boldsymbol{S}(\boldsymbol{q})|0\rangle,\ \text{and}\ \frac{1}{\omega-\mathcal{H}+E_0+i\gamma}\boldsymbol{S}(\boldsymbol{q})|0\rangle.$$

☛ We use the DMRG method to obtain the DSCF numerically.
☛ We calculate the DSCF in 32*2 sites ladder.

Numerical Results

DSCF for three points:

a, b) Incomm. CD phase (★)

J_2/J_1=0.6, J_p/J_1=0.2

c, d) Comm. RS phase (★)

J_2/J_1=0.1, J_p/J_1=1.0

e, f) Incomm. RS phase (★)

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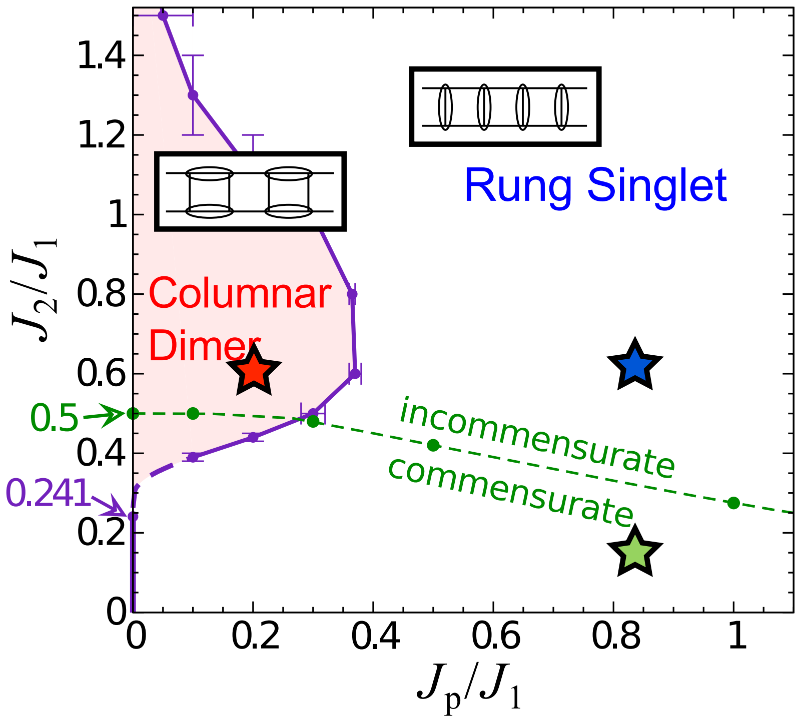

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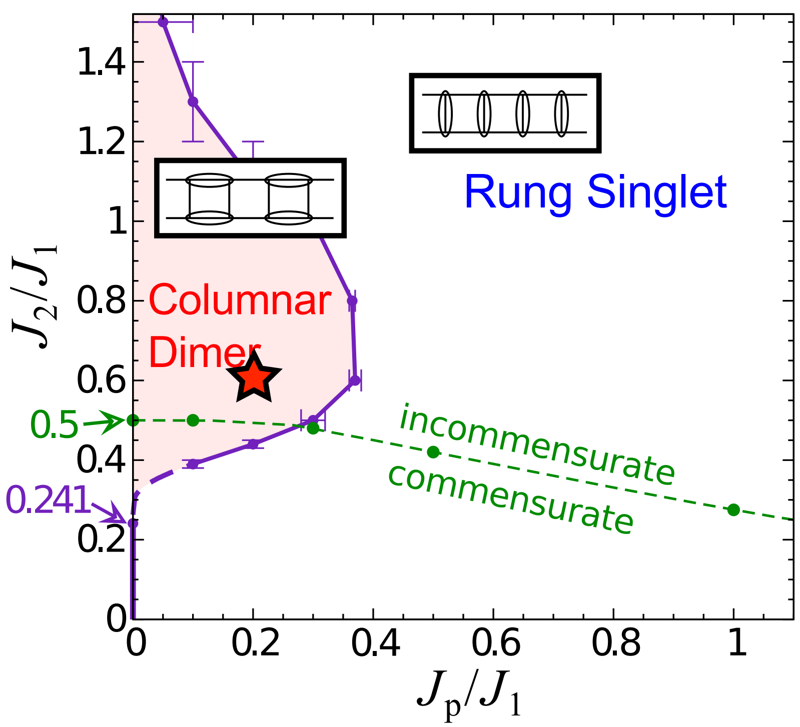

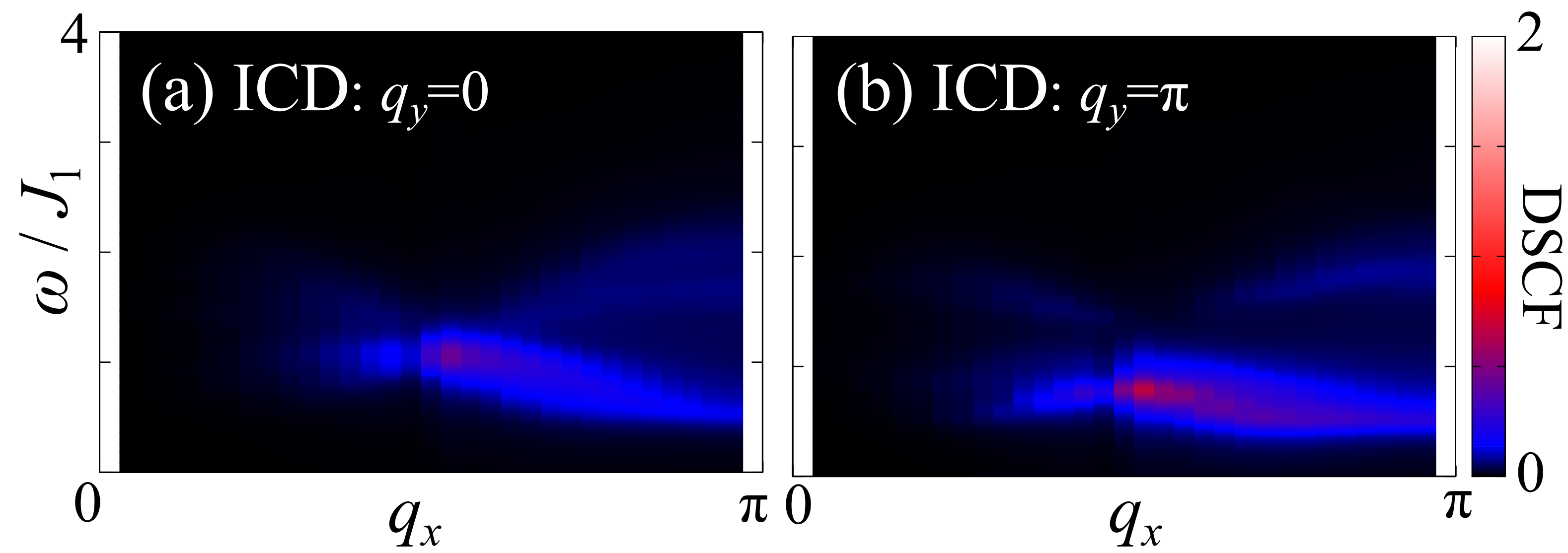

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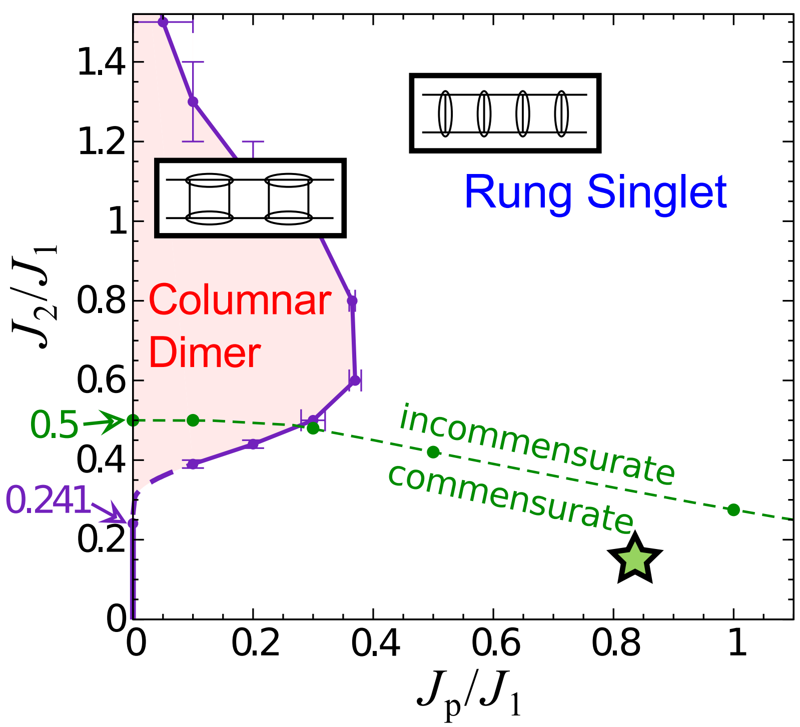

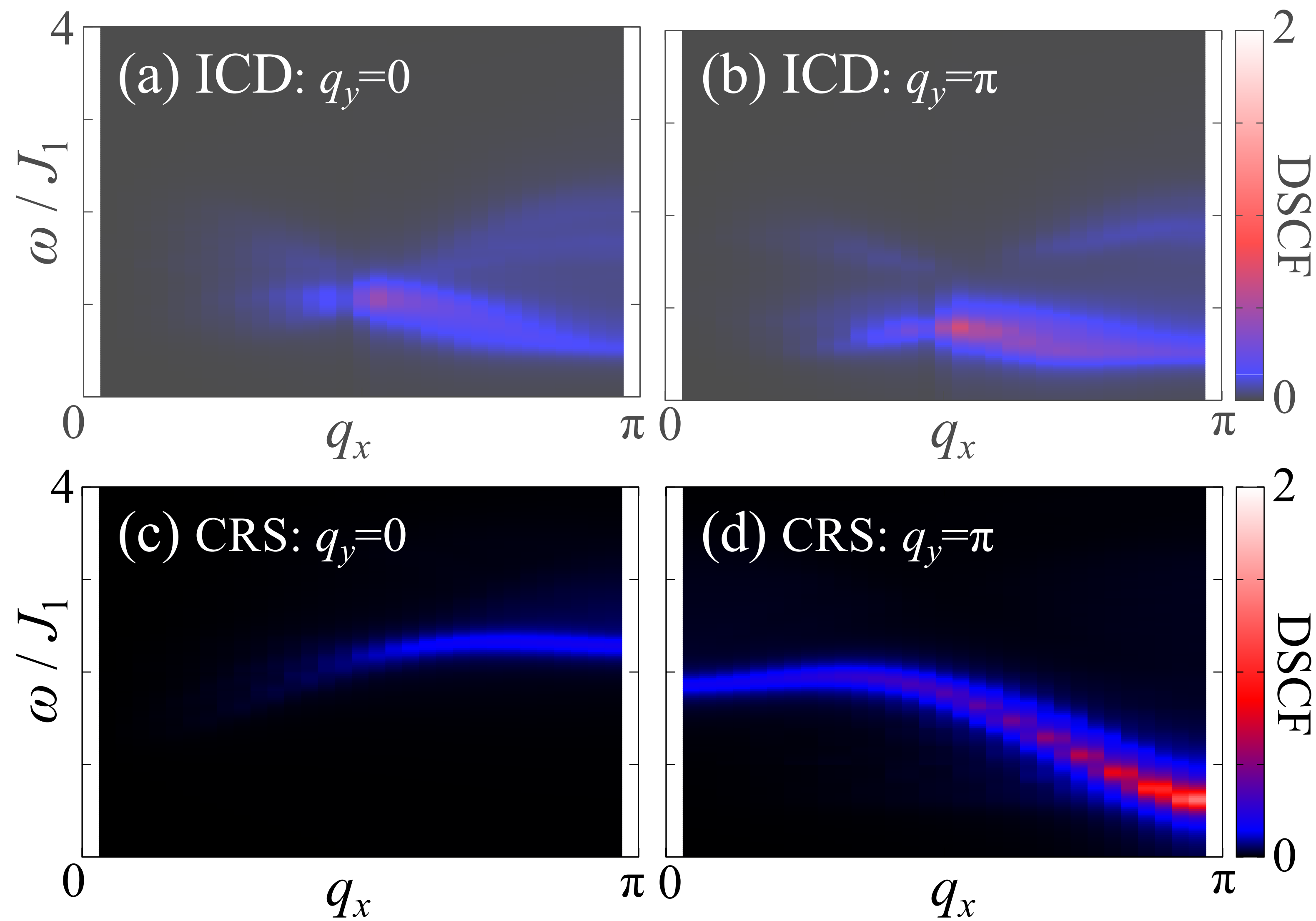

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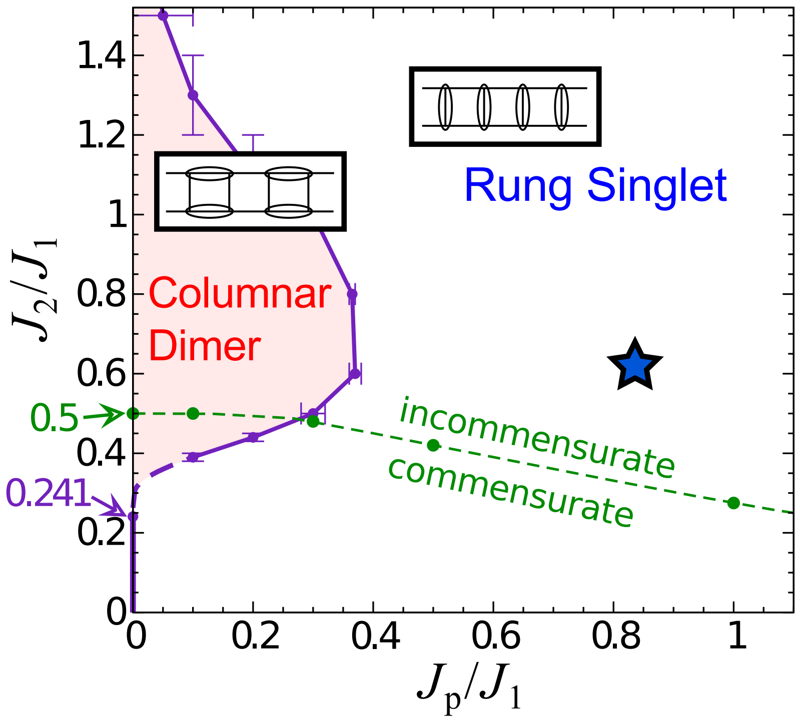

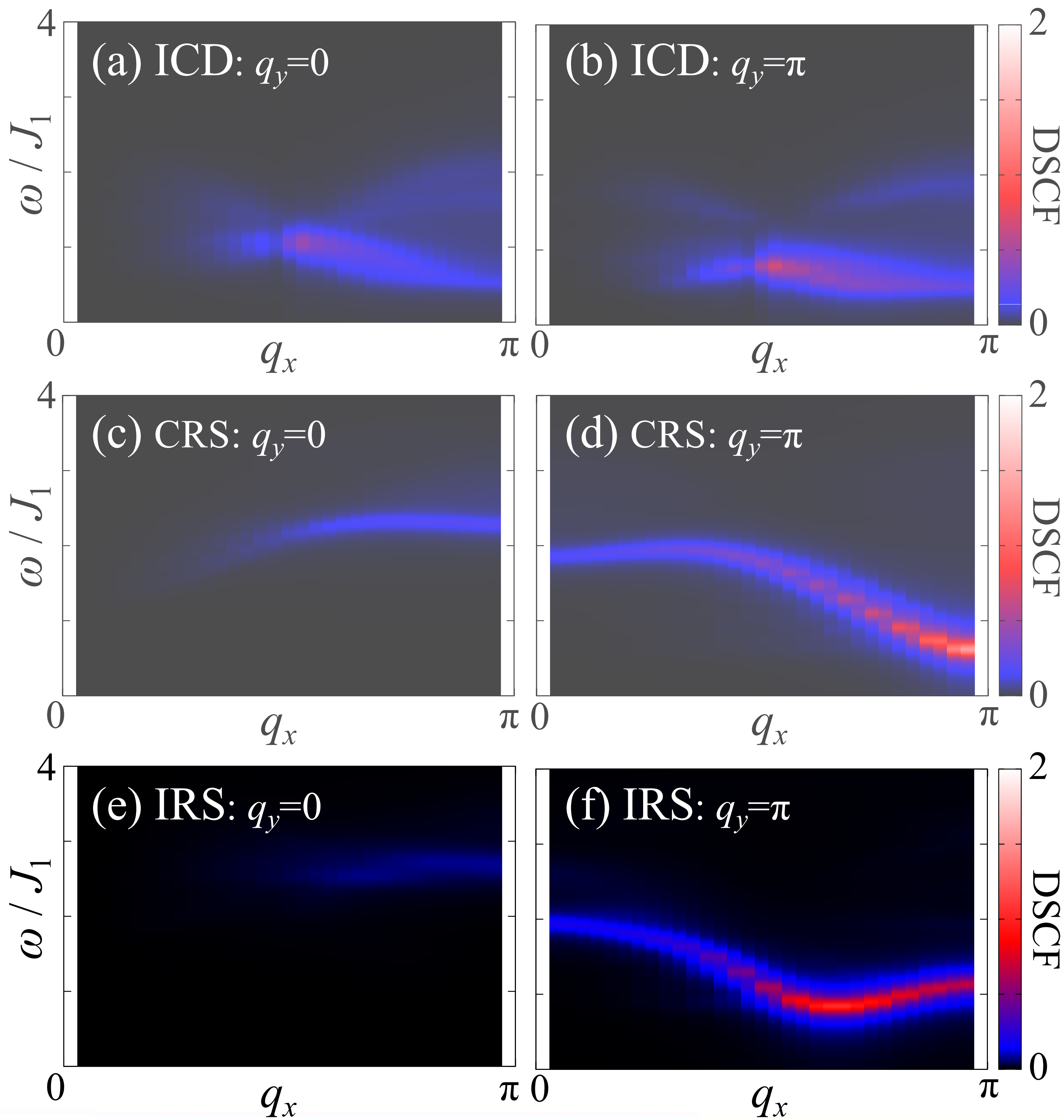

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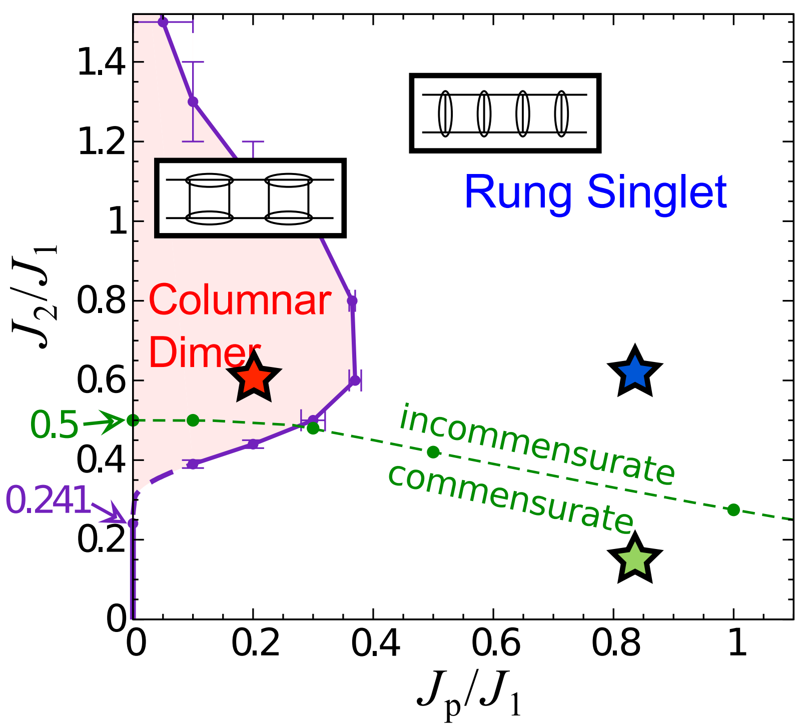
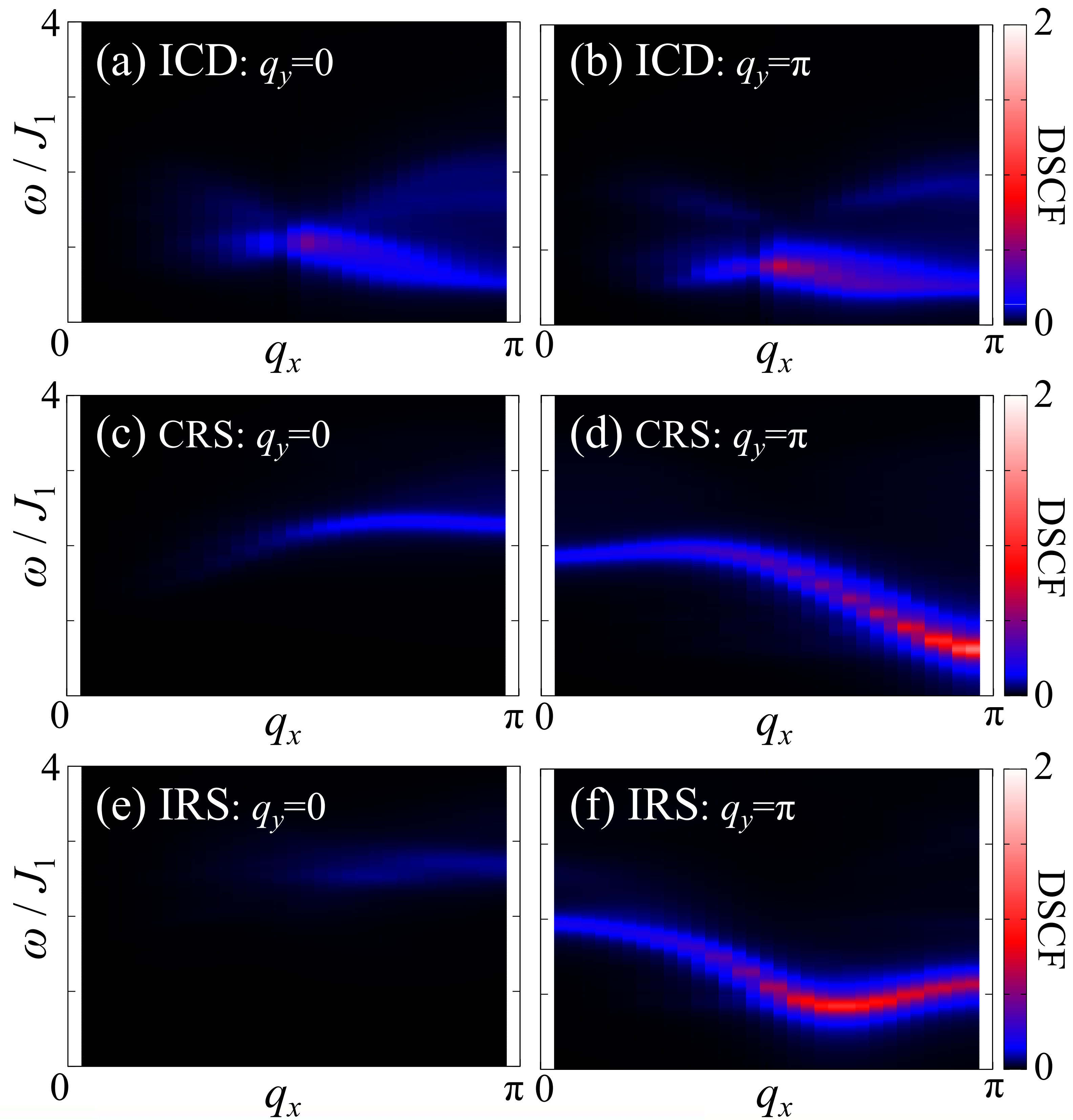


☛ We can distinguish CD and RS phases by comparing the spectral weight in q_y=0 plane with that of q_y=π.



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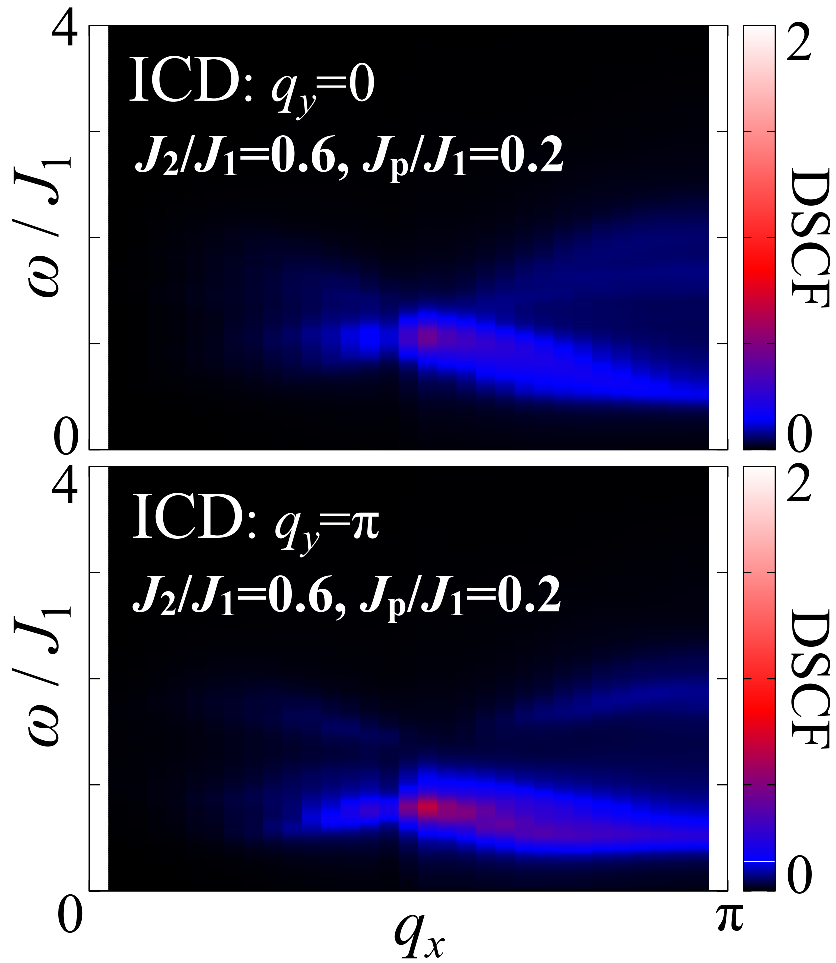
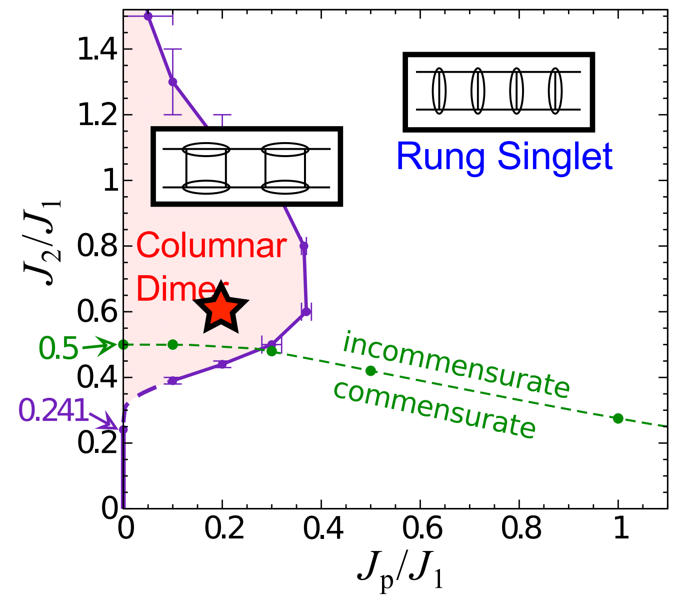
Result: Columnar-Dimer phase

DSCF in Incomm. CD phase:





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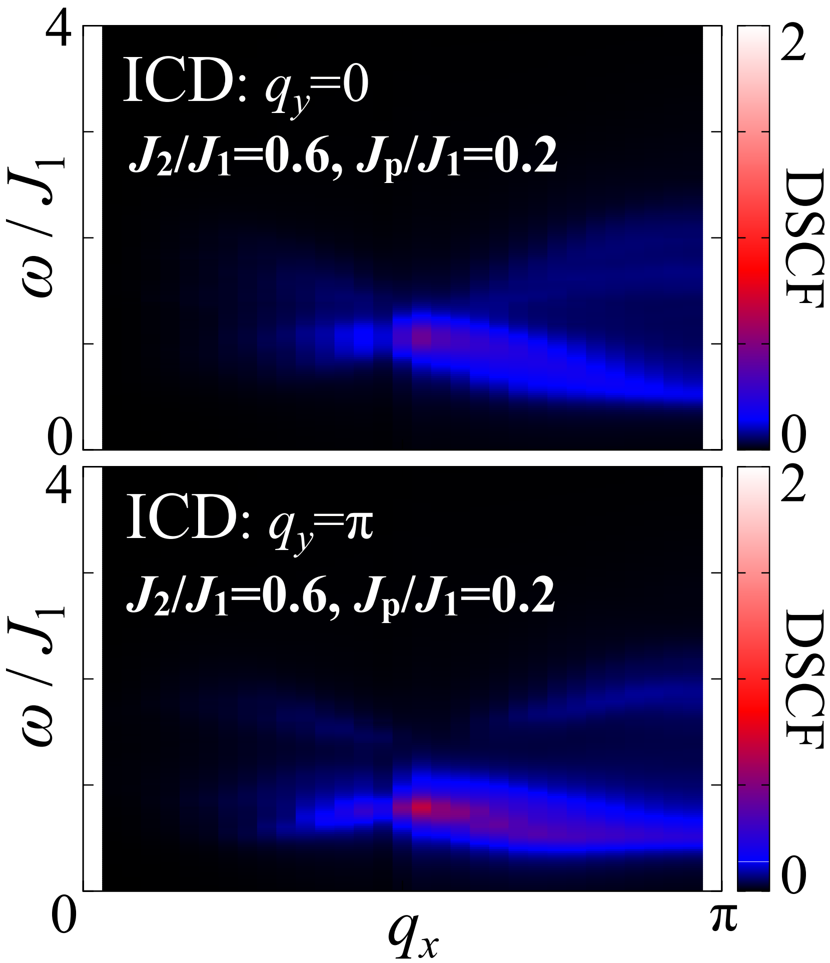

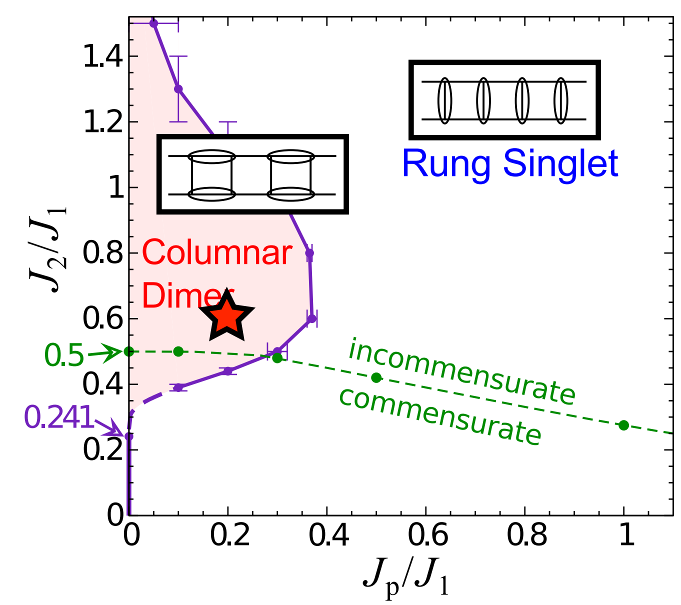

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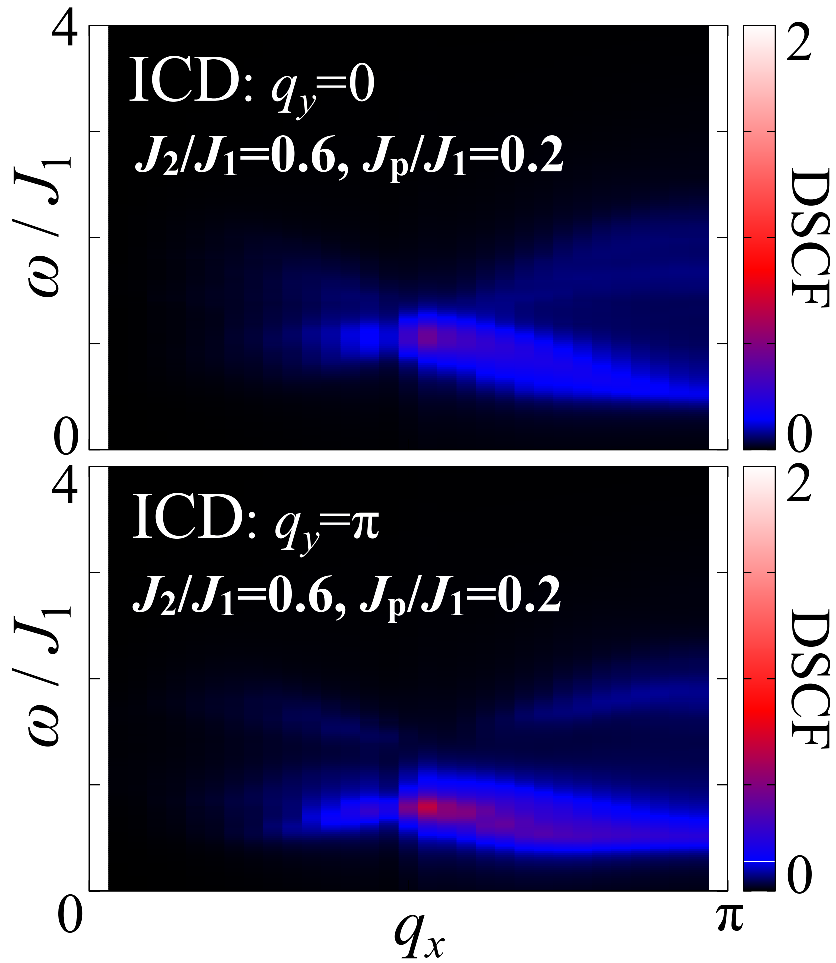
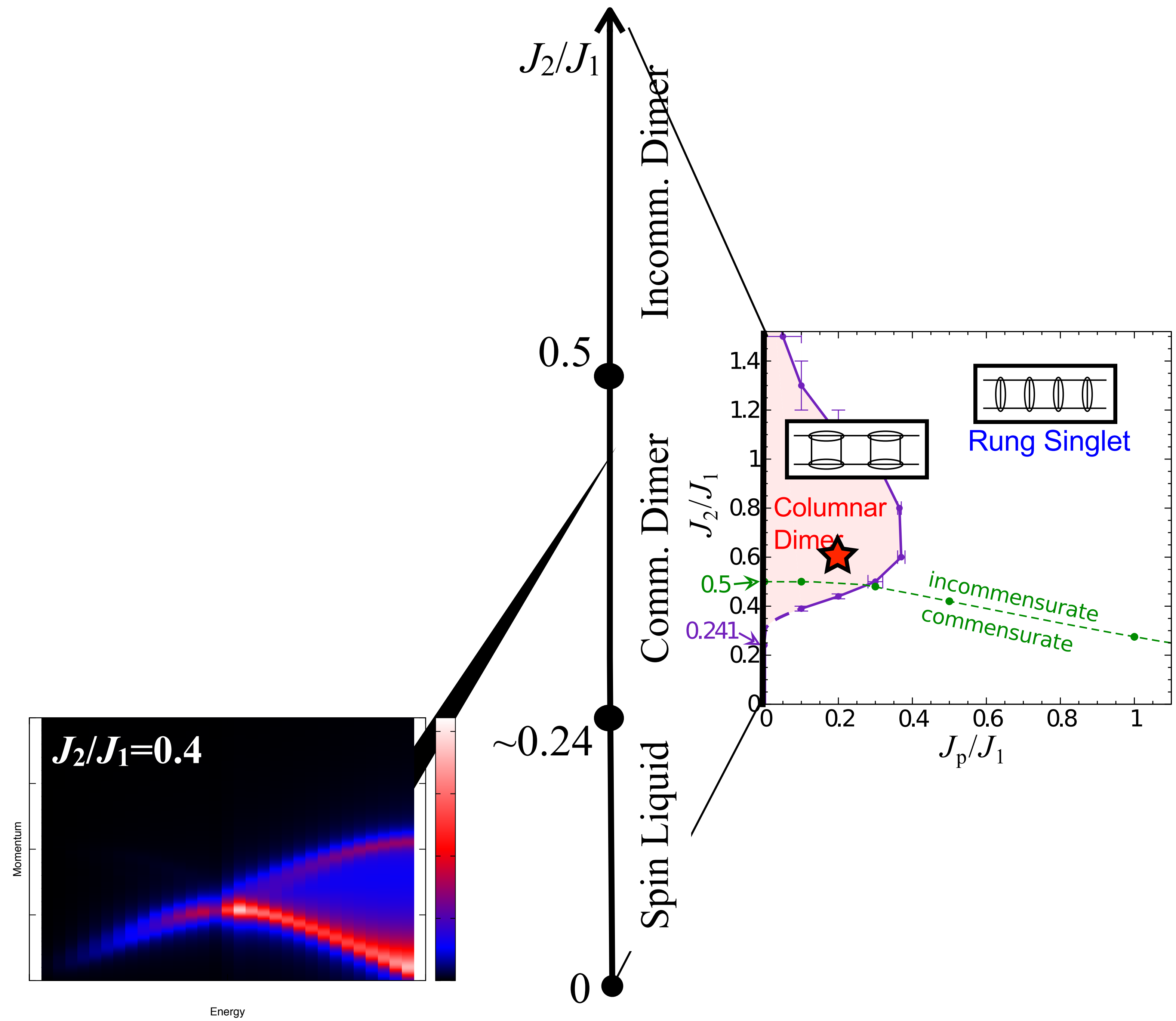


DSCF for Frustrated spin chain (J_p=0)



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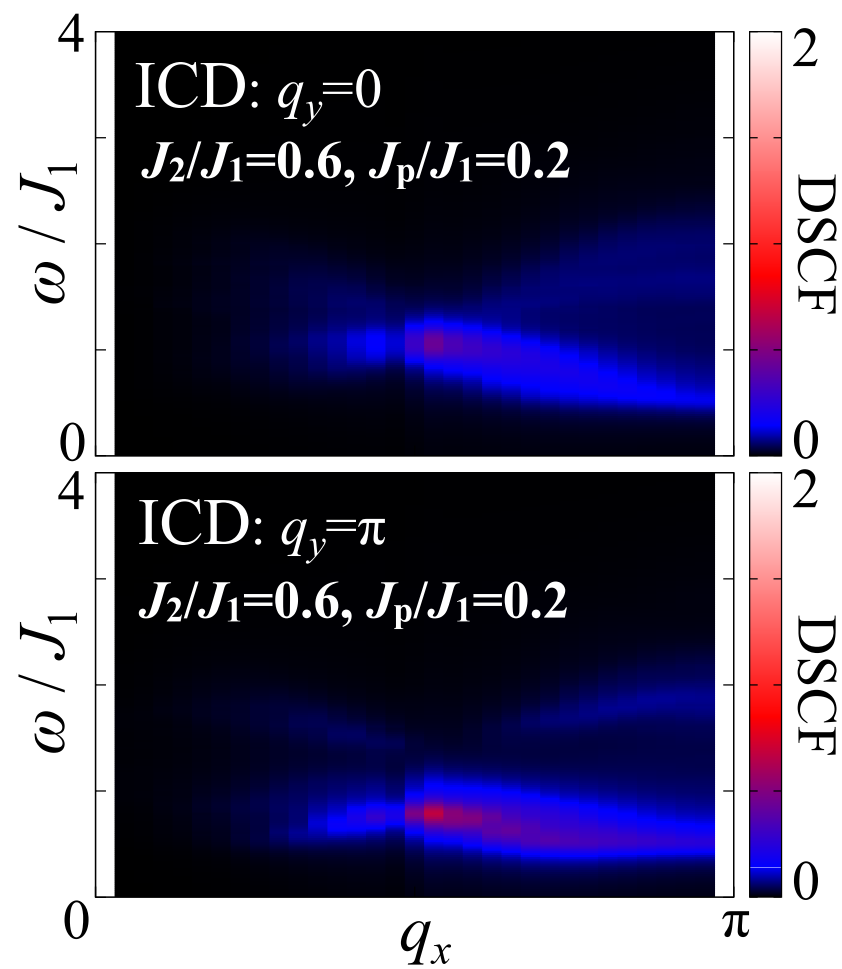

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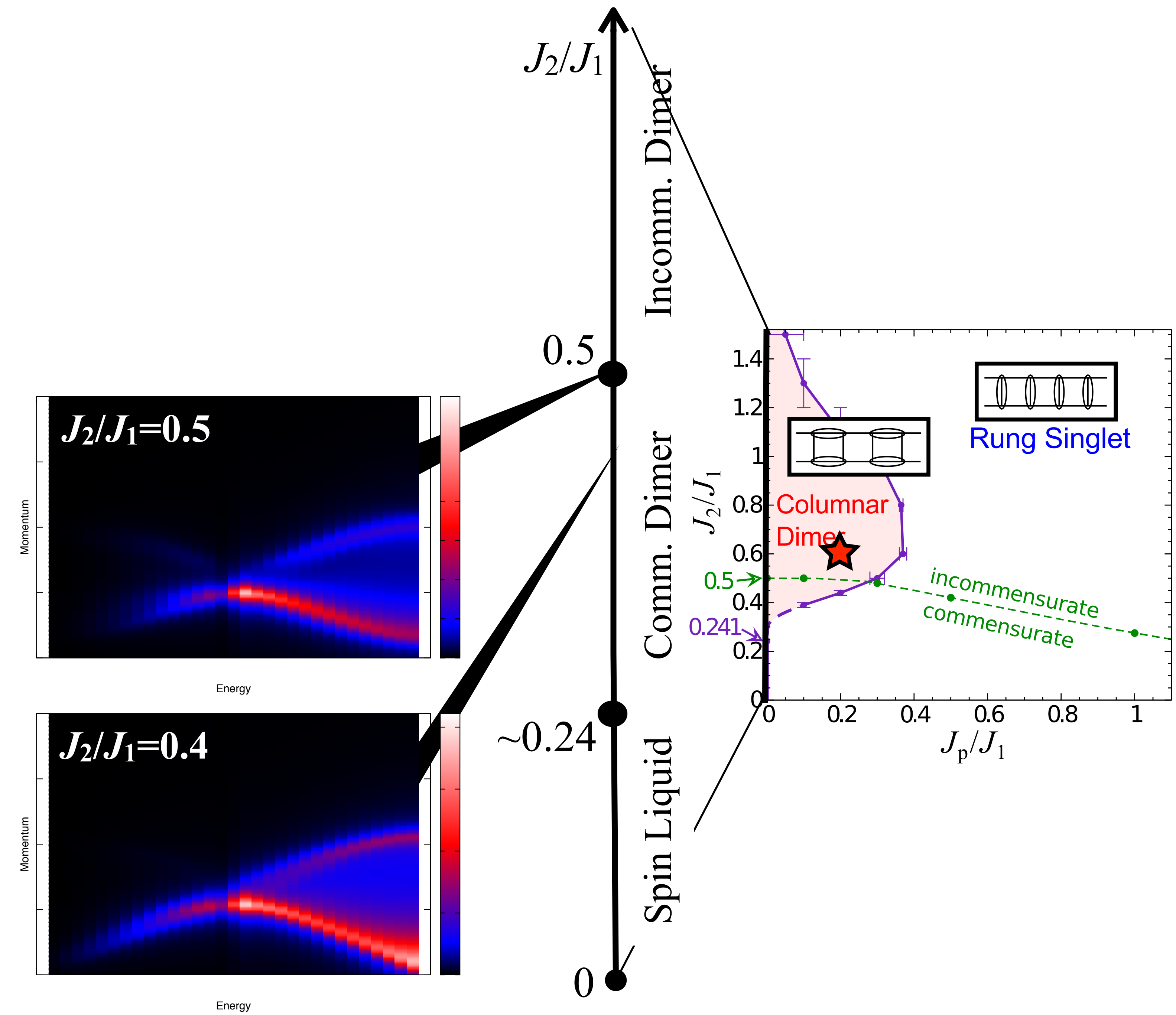

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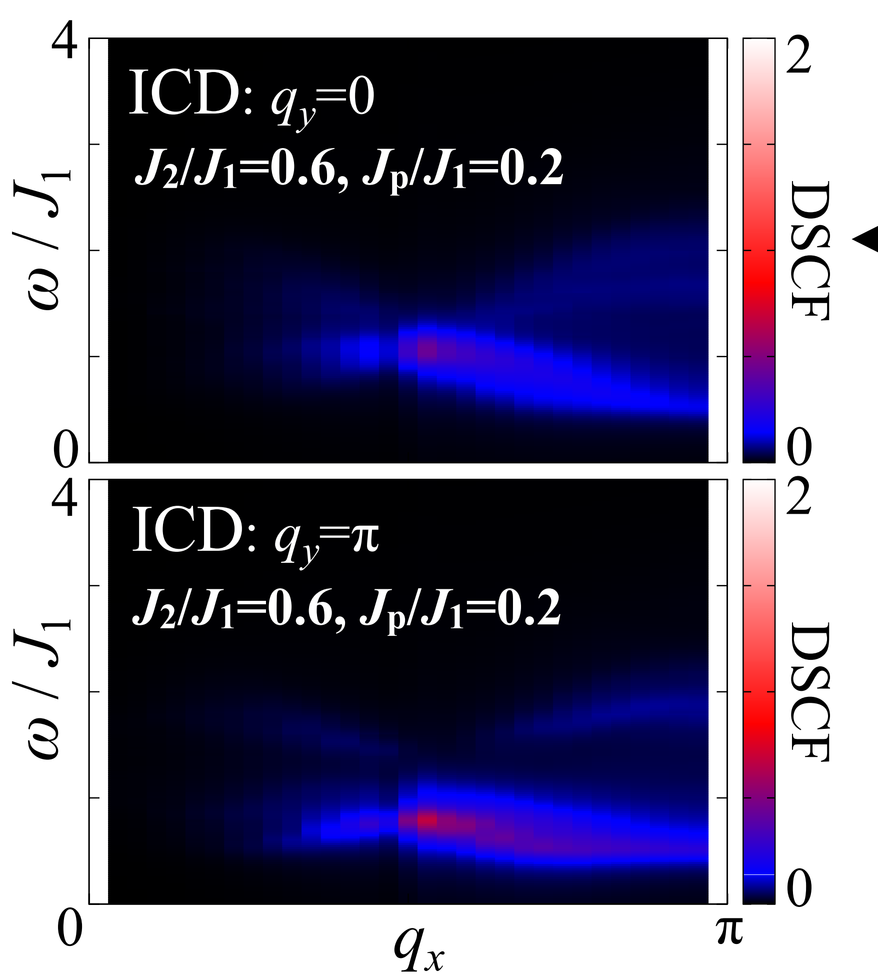
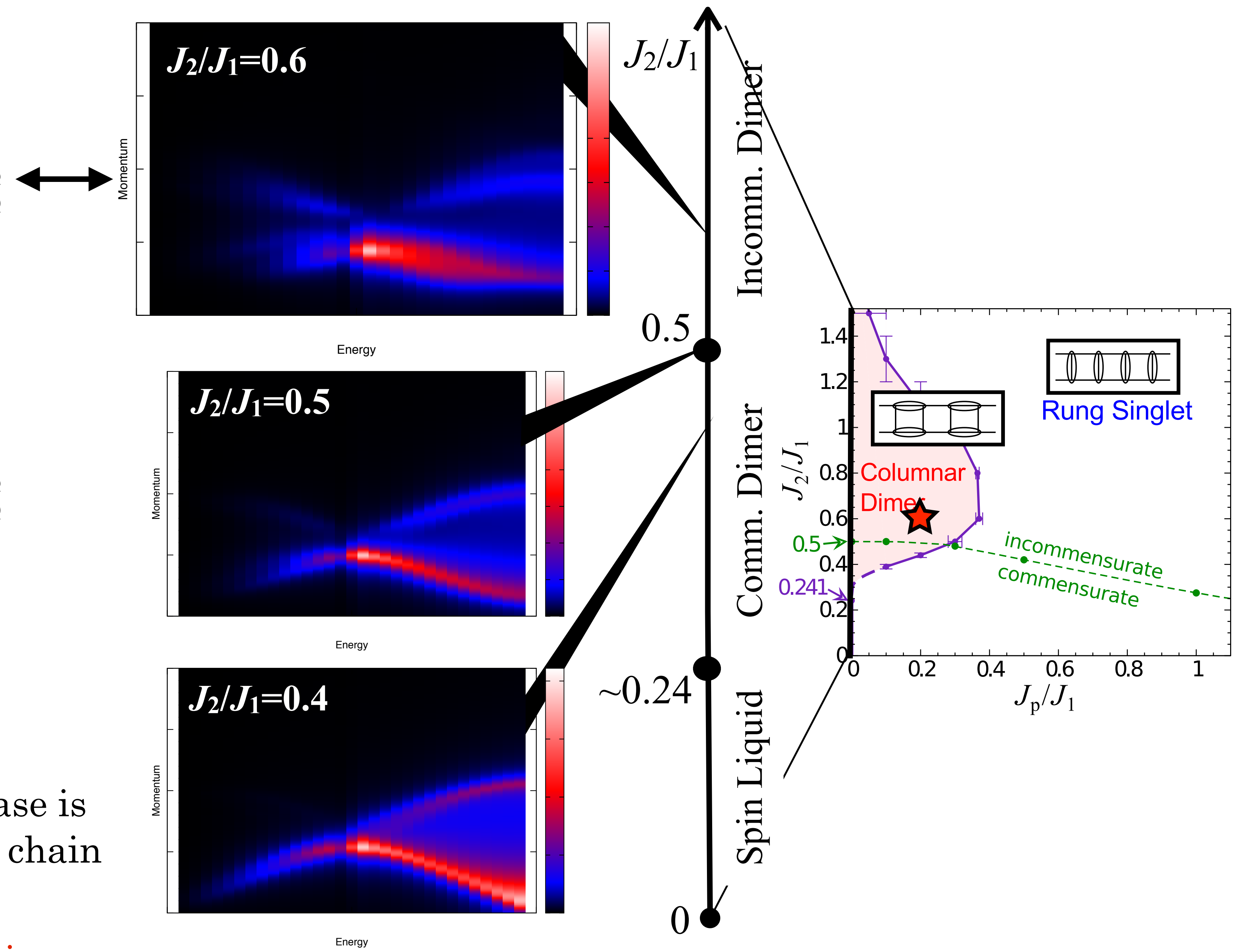
DSCF in Incomm. CD phase:



DSCF for Frustrated spin chain (J_p=0)



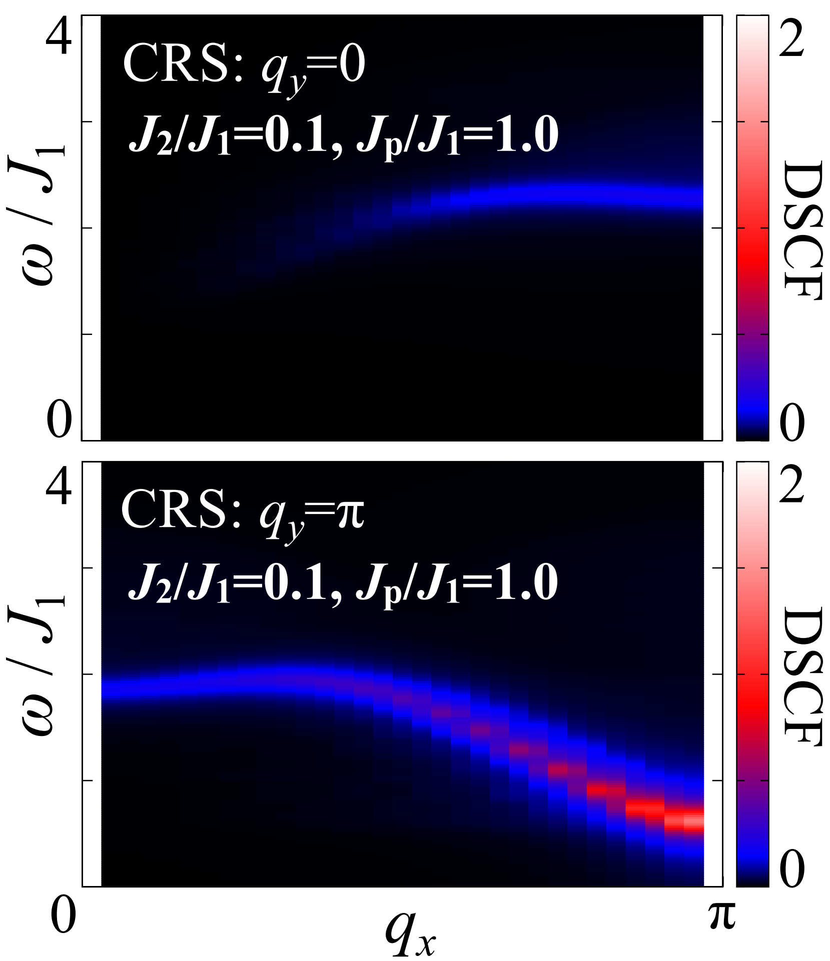
☛ The DSCF in incomm. CD phase is quite similar to that for the spin chain with frustration.

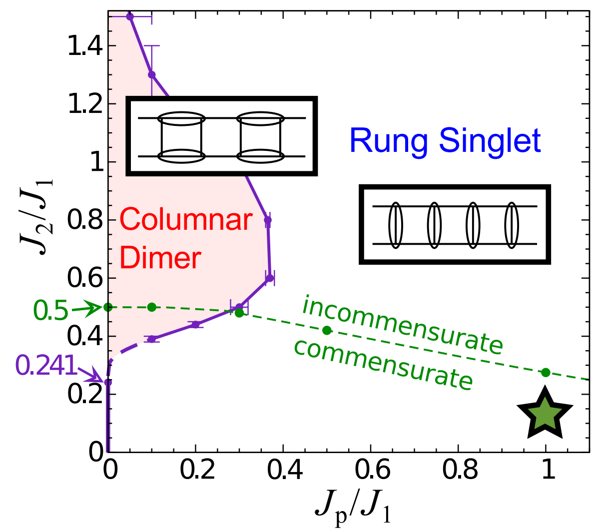
☛ Elementary excitations are spinons, which are not bounded on rung bond.

"Phase transition induced by magnetic field in a TLSL" T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

Result: Rung-Singlet phase

DSCF in Comm. RS phase:

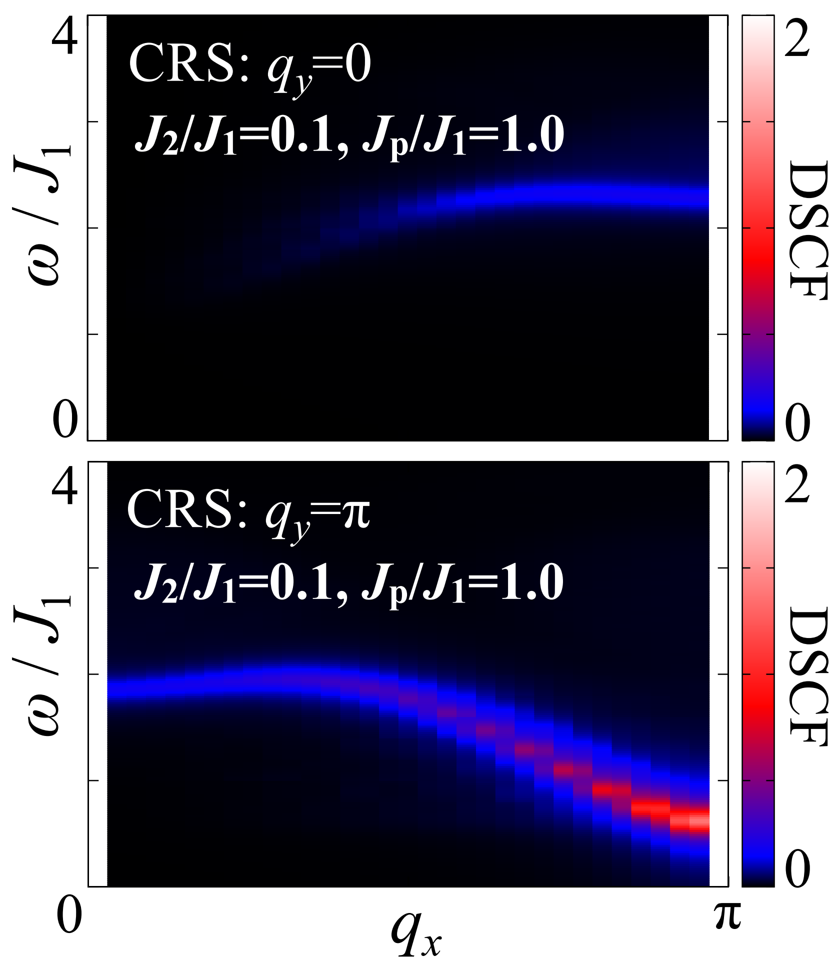


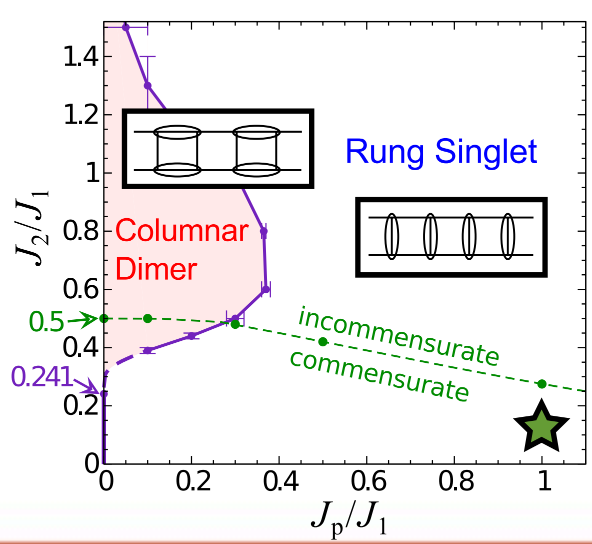


“Phase transition induced by magnetic field in a TLSL” T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

Result: Rung-Singlet phase

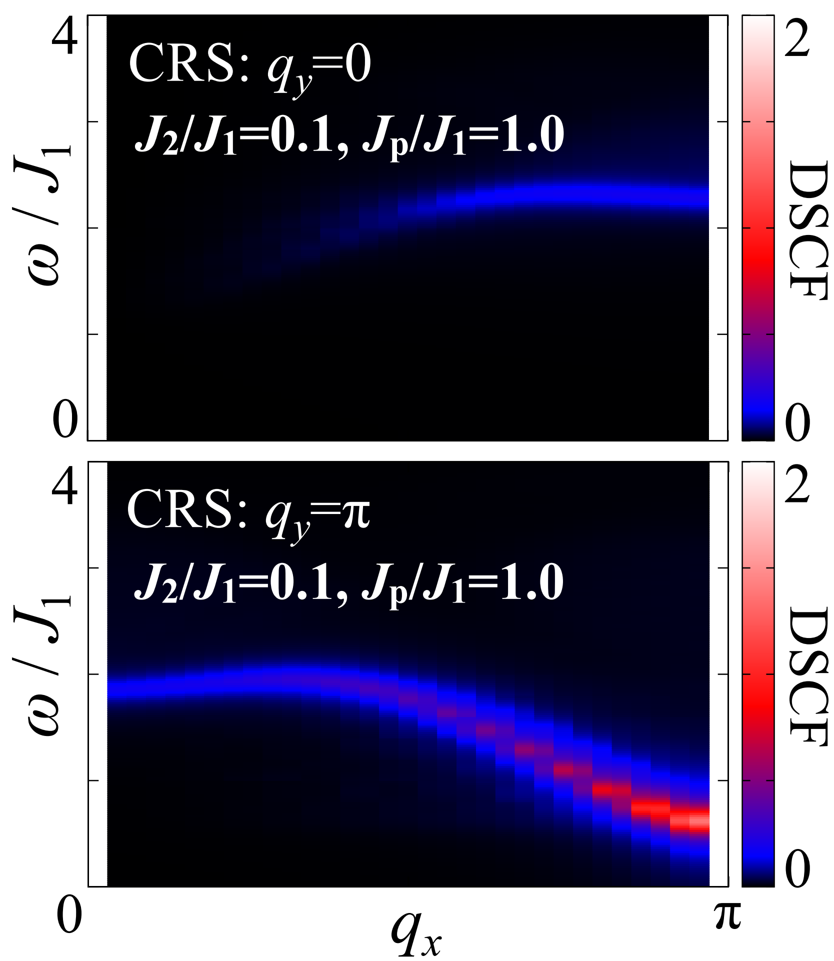
DSCF in Comm. RS phase:

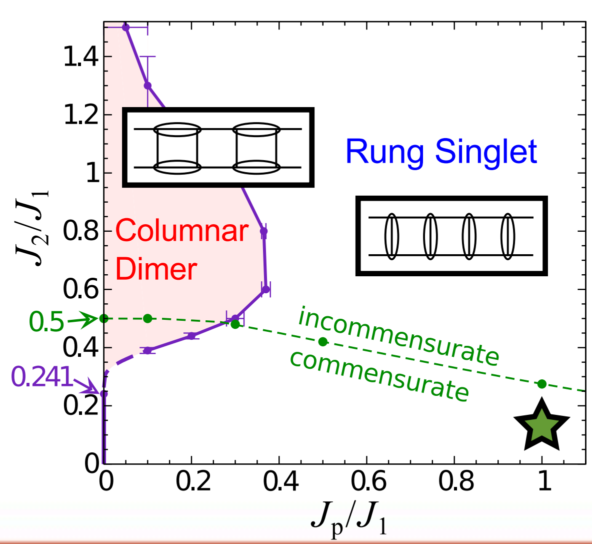




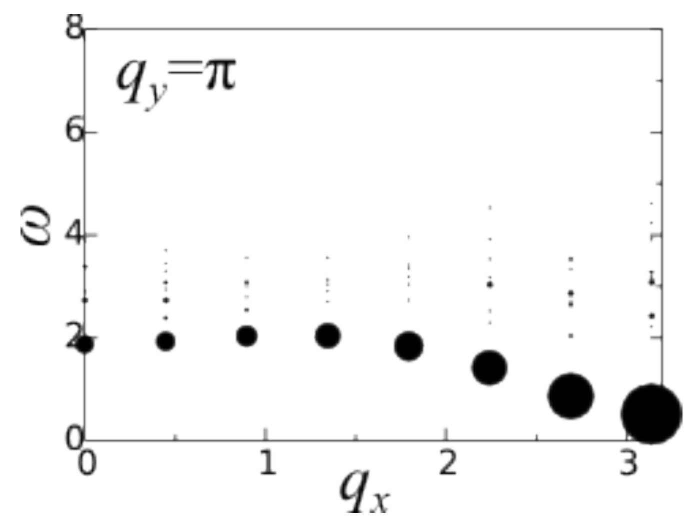
Result: Rung-Singlet phase

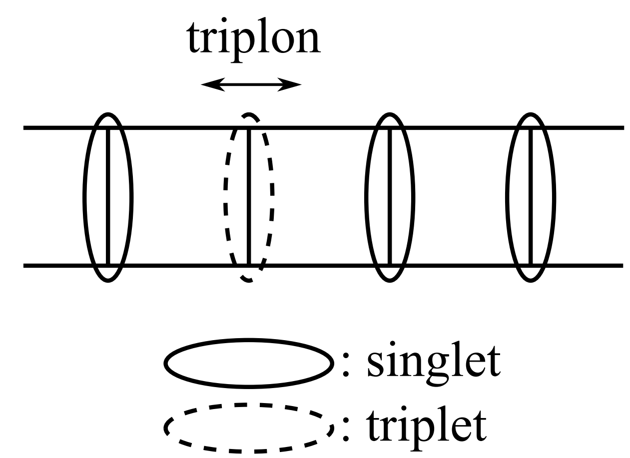
<u>DSCF in Comm. RS phase:</u>





DSCF for Non-frustrated spin ladder





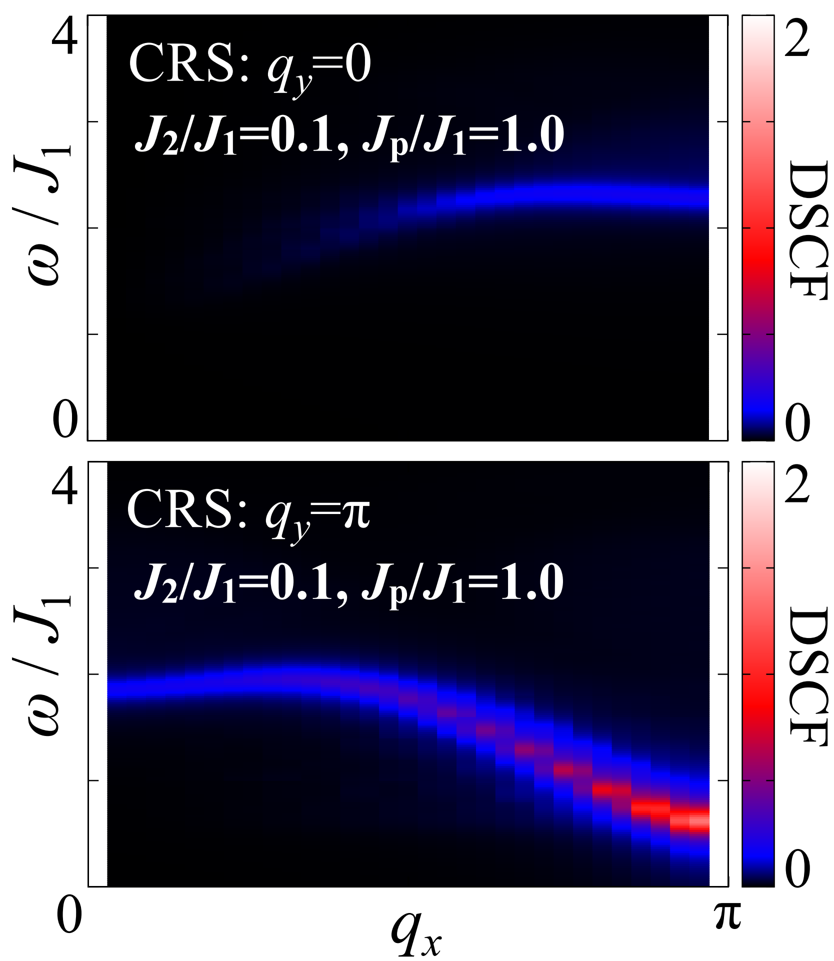
N. Haga and S. Suga, PRB **66**,132415 (2002).

☛ In comm. RS phase, anti-bonding mode ($q_y=\pi$) can be understood as triplon mode for non-frustrated spin ladder.

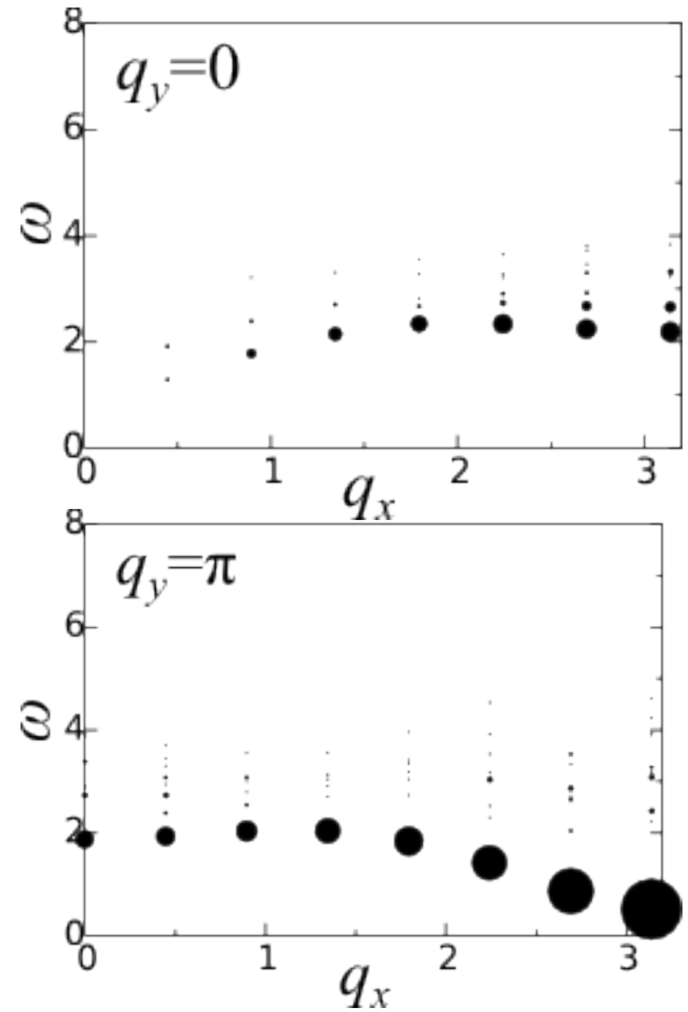
13年6月17日月曜日

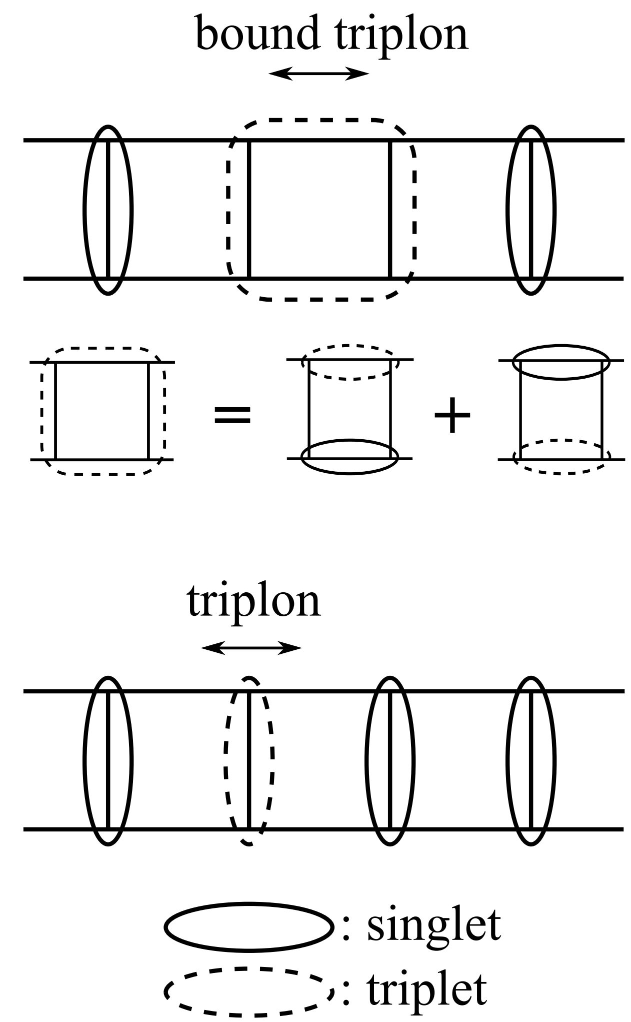
Result: Rung-Singlet phase

DSCF in Comm. RS phase:

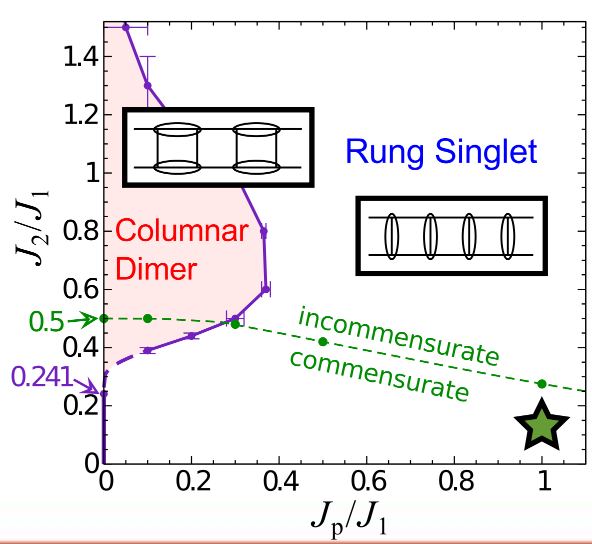


DSCF for Non-frustrated spin ladder





N. Haga and S. Suga, PRB **66**,132415 (2002).

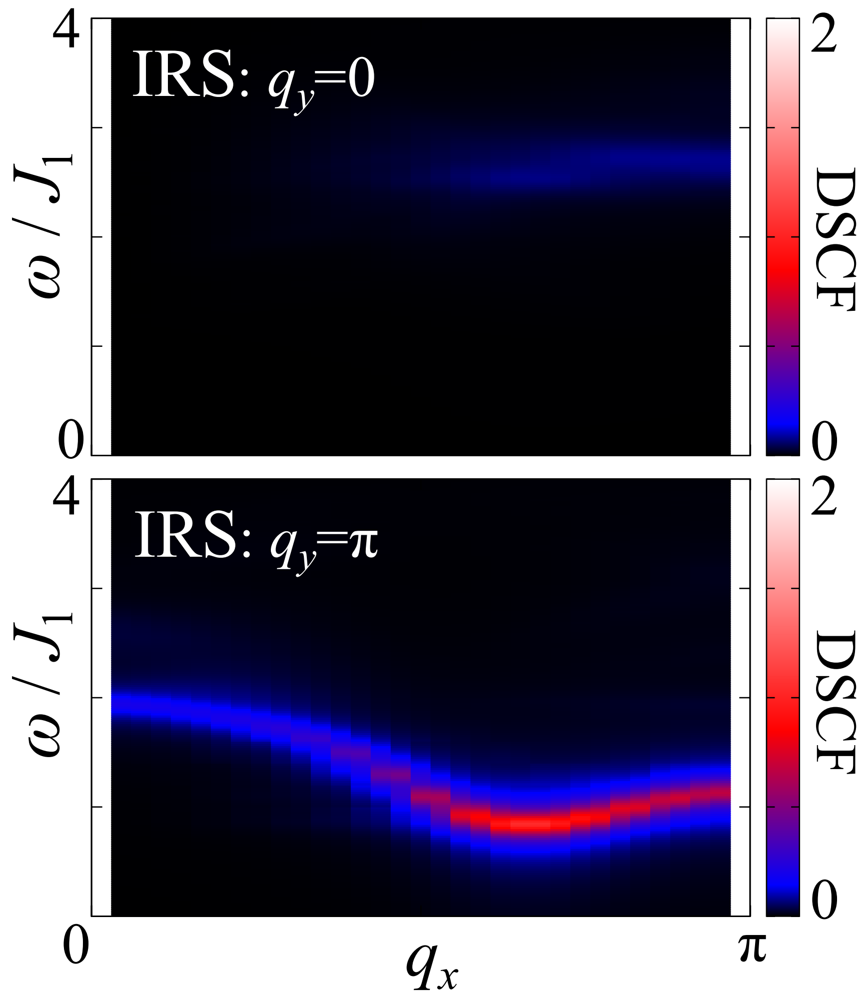


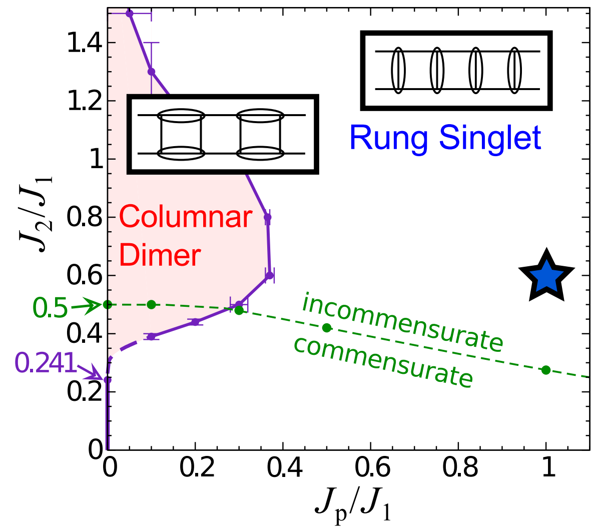
☛ In comm. RS phase, anti-bonding mode (q_y=π) can be understood as triplon mode for non-frustrated spin ladder.

☛ Bonding mode (q_y=0) can be understood as the mode of bound triplon.

Result: Frustration Effects

DSCF in Incomm. RS phase:

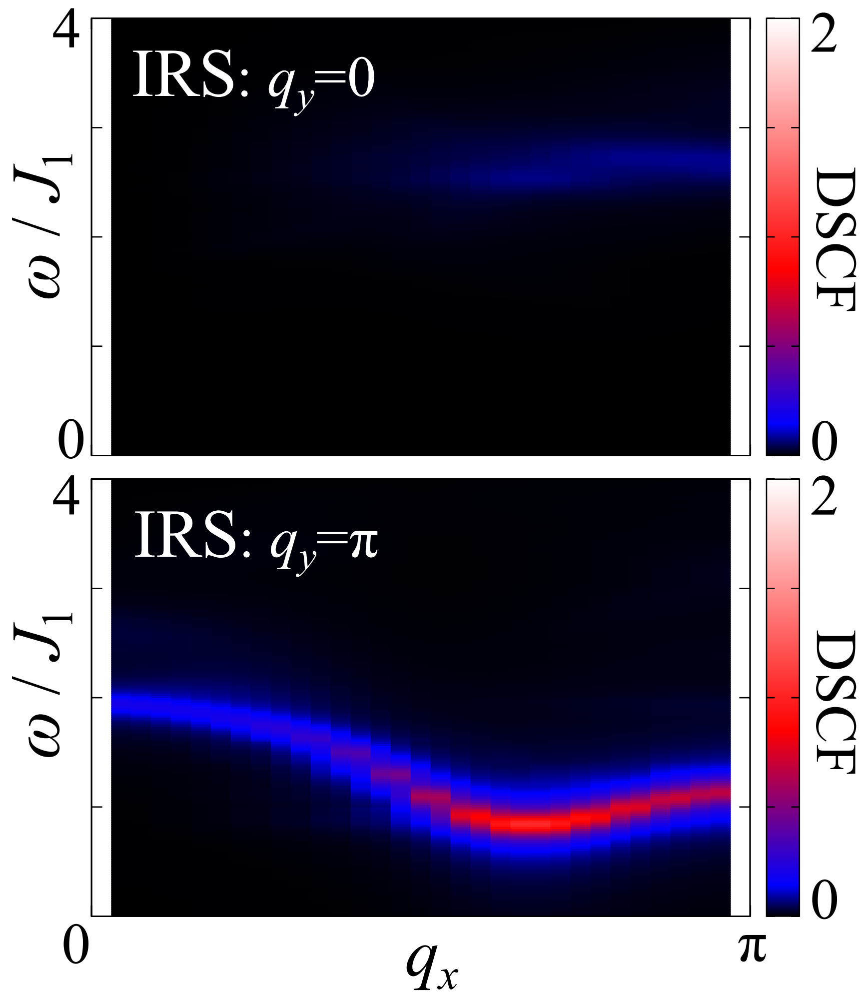


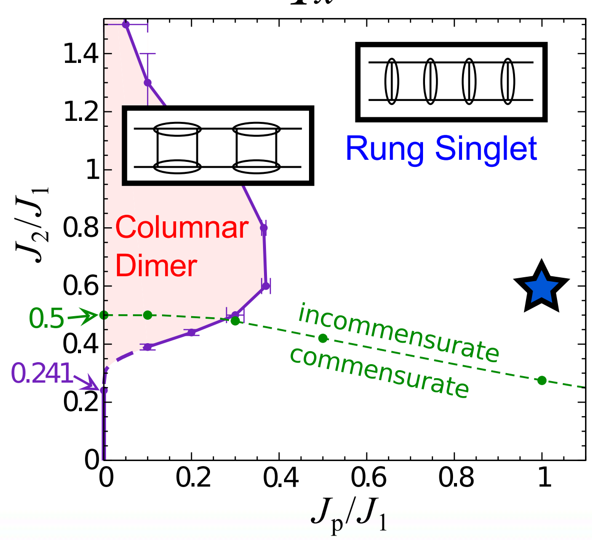


"Phase transition induced by magnetic field in a TLSL" T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

Result: Frustration Effects

DSCF in Incomm. RS phase:

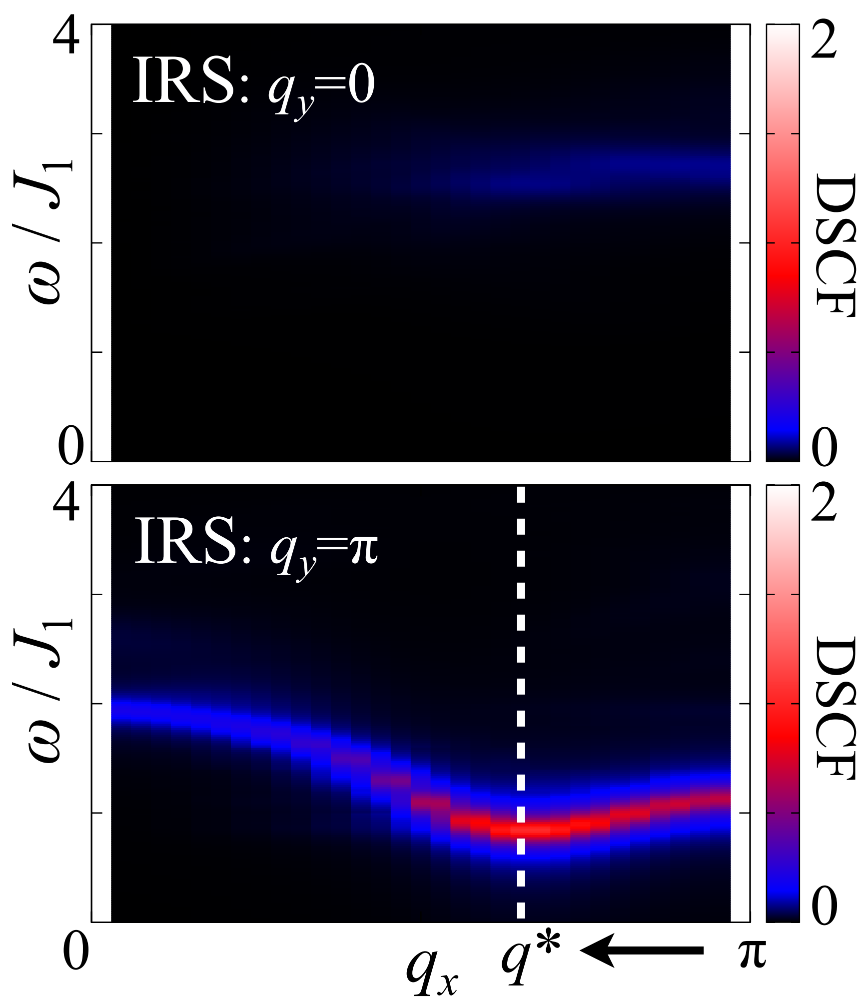


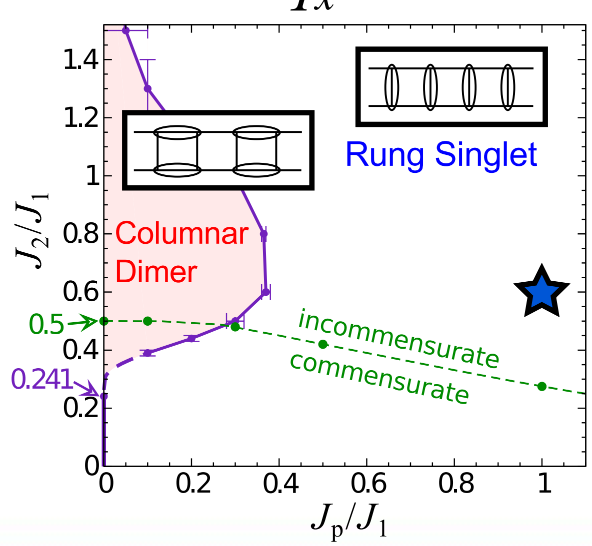


"Phase transition induced by magnetic field in a TLSL" T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

Result: Frustration Effects

DSCF in Incomm. RS phase:





Strong rung-coupling limit ($J_1, J_2 \ll J_p$)

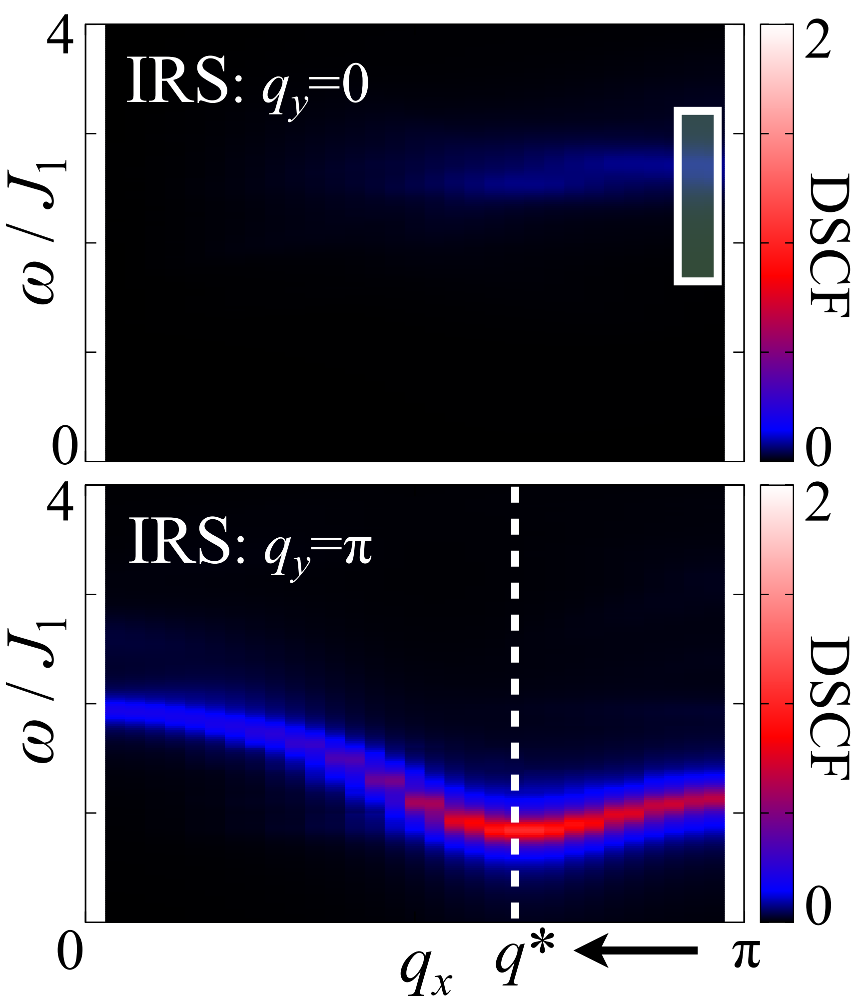
$$\epsilon_{\rm T}(q_x) \cong J_p + J_1\cos(q_x) + J_2\cos(2q_x) + \frac{3}{4}\left(\frac{J_1^2}{J_p} + \frac{J_2^2}{J_p}\right)$$

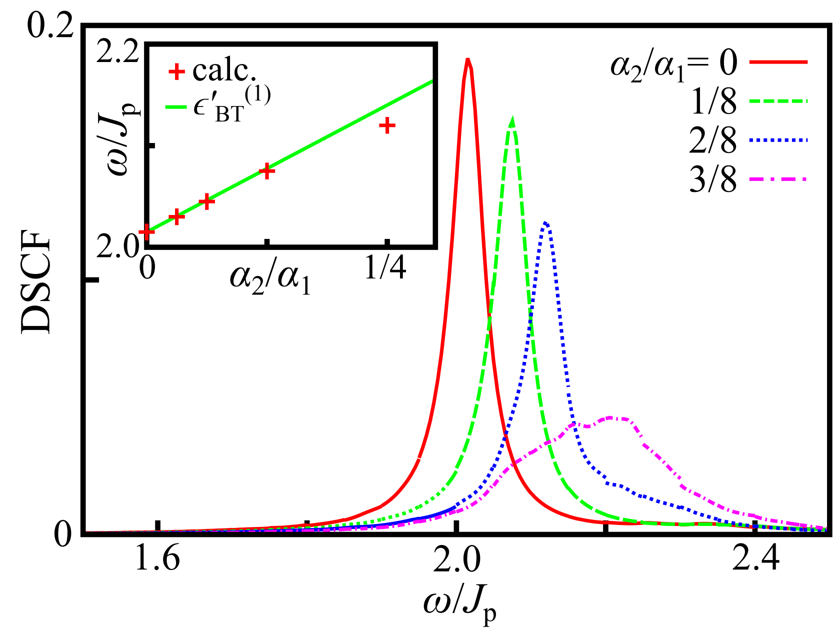
$$q^* \cong \cos^{-1}\left(-\frac{J_1}{4J_2}\right)$$

☛ Frustration affects the wave number of the lowest excitation, and change it from π to incommensurate one.

Result: Frustration Effects

DSCF in Incomm. RS phase:





☛ With large frustration, the bound triplon is smeared over the continuum.

Strong rung-coupling limit (J_1, $J_2 \ll J_p$)

$$\epsilon_{\mathrm{T}}(q_x) \cong J_p + J_1 \cos(q_x) + J_2 \cos(2q_x) + \frac{3}{4}\left(\frac{J_1^2}{J_p} + \frac{J_2^2}{J_p}\right)$$

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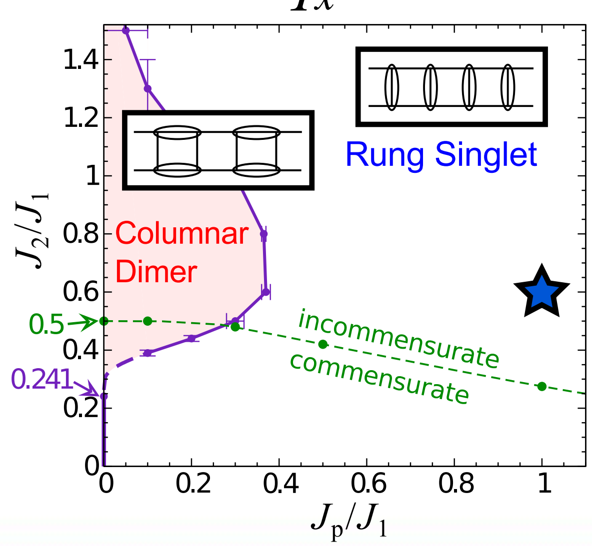
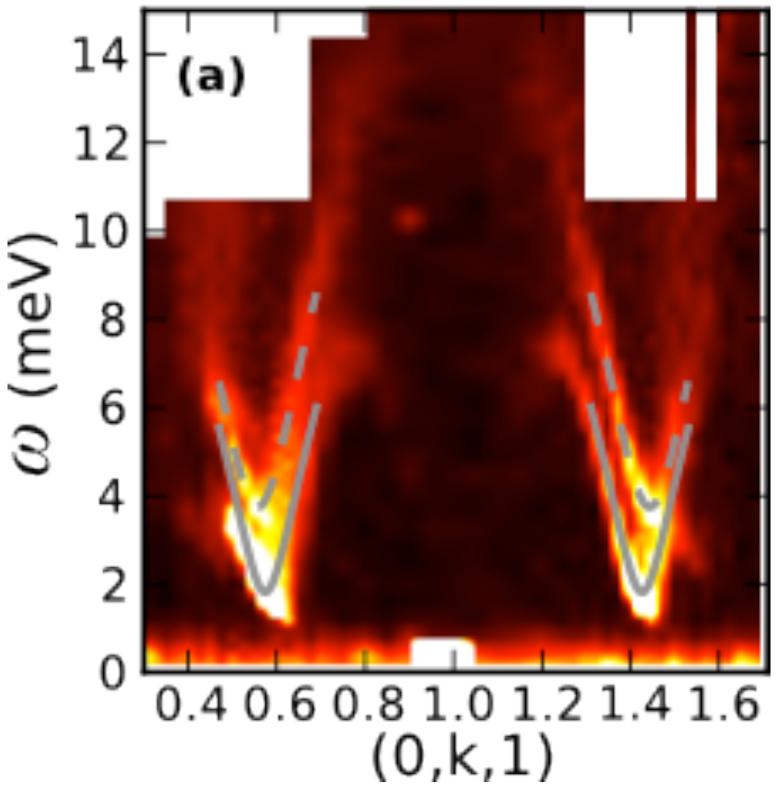


☛ Frustration affects the wave number of the lowest excitation, and change it from π to incommensurate one.

Experiment: inelastic neutron scattering

Grand-state phase:

Inelastic neutron scattering for $BiCu_2PO_6$



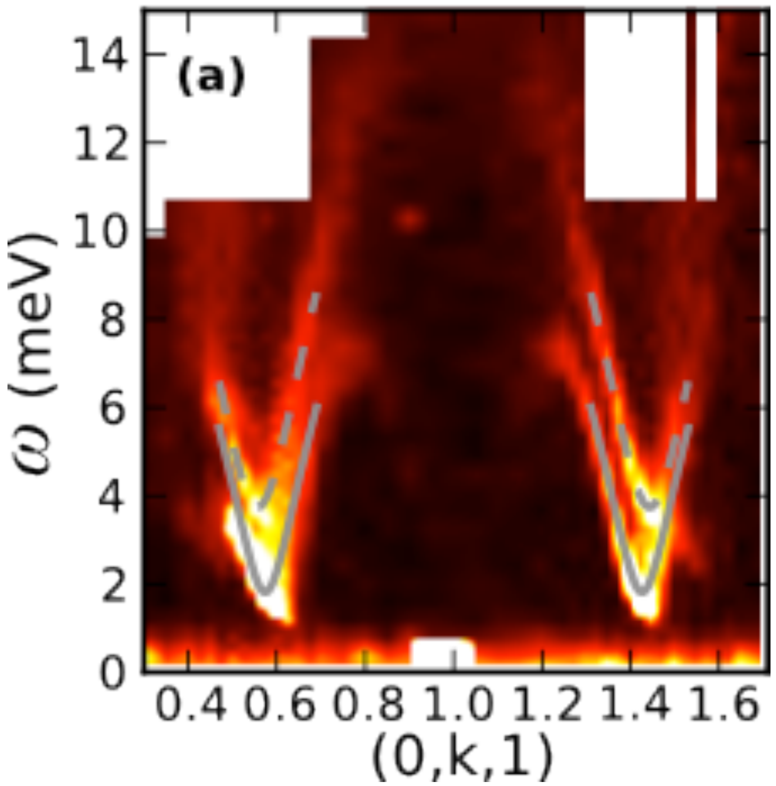
K.W. Plumb, *et al*, arXiv:1301.5324.

Triplon excitation with an incomm. wave number is observed.

Experiment: inelastic neutron scattering

Grand-state phase:

Inelastic neutron scattering for $BiCu_2PO_6$



K.W. Plumb, *et al*, arXiv:1301.5324.

Triplon excitation with an incomm. wave number is observed.

☛ BiCu2PO6 is located in the incomm. rung-singlet phase.

☛ The triplon dispersion relation indicates comparable magnitudes of exchange energies, $J_1 \sim J_2 \sim J_p$.

Experiment: inelastic neutron scattering

Grand-state phase:

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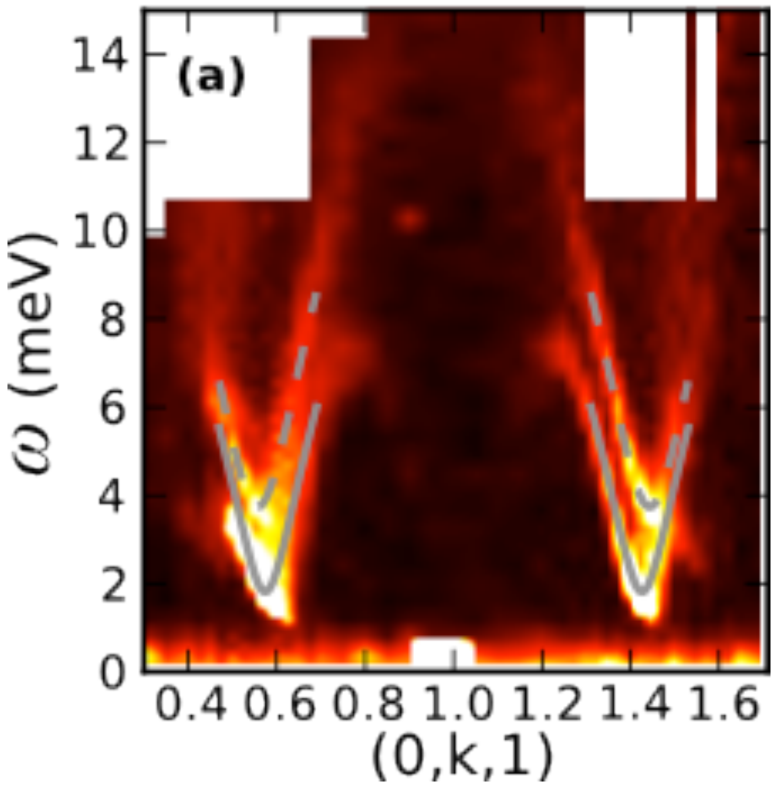

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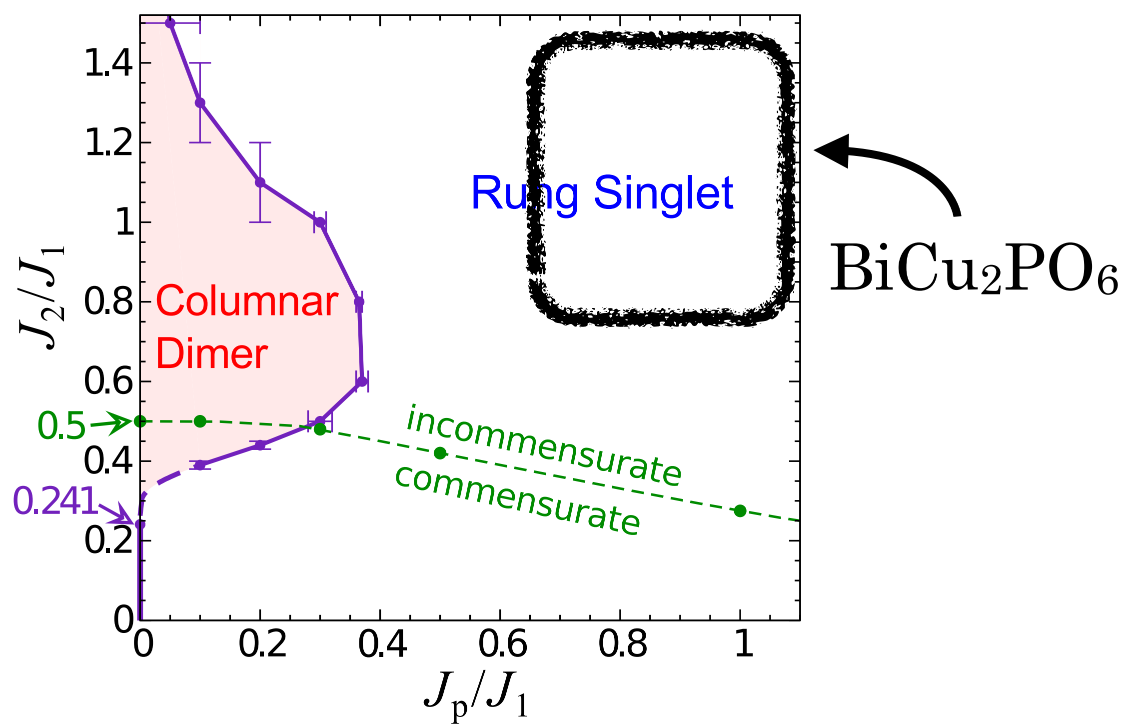


A. Lavarélo, *et al*, PRB 84, 144407 (2011).

Field effect

Frustrated two-leg spin ladder

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_p + \mathcal{H}_Z$$

$$\mathcal{H}_1 = J_1 \sum_j \left[\boldsymbol{S}_{j,\mathrm{u}} \cdot \boldsymbol{S}_{j+1,\mathrm{u}} + \boldsymbol{S}_{j,\mathrm{l}} \cdot \boldsymbol{S}_{j+1,\mathrm{l}} \right]$$

$$\mathcal{H}_2 = J_2 \sum_j \left[\boldsymbol{S}_{j,\mathrm{u}} \cdot \boldsymbol{S}_{j+2,\mathrm{u}} + \boldsymbol{S}_{j,\mathrm{l}} \cdot \boldsymbol{S}_{j+2,\mathrm{l}} \right]$$

$$\mathcal{H}_p = J_p \sum_j \boldsymbol{S}_{j,\mathrm{u}} \cdot \boldsymbol{S}_{j,\mathrm{l}}$$

$$\mathcal{H}_Z = h^z \sum_j (S^z_{j,\mathrm{u}} + S^z_{j,\mathrm{l}})$$

Bond-operator transform & Mean-field approx.

$$s_j^\dagger |0\rangle = |s\rangle_j = \frac{1}{\sqrt{2}}(|\uparrow\rangle_{j,\mathrm{u}} |\downarrow\rangle_{j,\mathrm{l}} - |\downarrow\rangle_{j,\mathrm{u}} |\uparrow\rangle_{j,\mathrm{l}})$$

$$t_j^{+\,\dagger} |0\rangle = |t^+\rangle_j = |\uparrow\rangle_{j,\mathrm{u}} |\uparrow\rangle_{j,\mathrm{l}}$$

$$t_j^{0\,\dagger} |0\rangle = |t^0\rangle_j = \frac{1}{\sqrt{2}}(|\uparrow\rangle_{j,\mathrm{u}} |\downarrow\rangle_{j,\mathrm{l}} + |\downarrow\rangle_{j,\mathrm{u}} |\uparrow\rangle_{j,\mathrm{l}})$$

$$t_j^{-\,\dagger} |0\rangle = |t^-\rangle_j = |\downarrow\rangle_{j,\mathrm{u}} |\downarrow\rangle_{j,\mathrm{l}}$$

Non-interacting triplon (NIT)

$$\mathcal{H}_{\mathrm{eff}} = \sum_{q,\alpha} \omega(q) n_q^\alpha + \mathrm{sgn}(\alpha) h^z n_q^\alpha$$

$$\omega(q) = J_1 \cos(q) + J_2 \cos(2q) + J_p$$

$$n^\alpha = t^{\alpha\,\dagger} t^\alpha \ (\alpha = +, 0, -)$$

☛ Triplon is a hard-core boson.

☛ Bose-Einstein condensation is expected induced by magnetic field.

"Phase transition induced by magnetic field in a TLSL" T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

Bose-Einstein condensation

Non-interacting triplon (NIT)

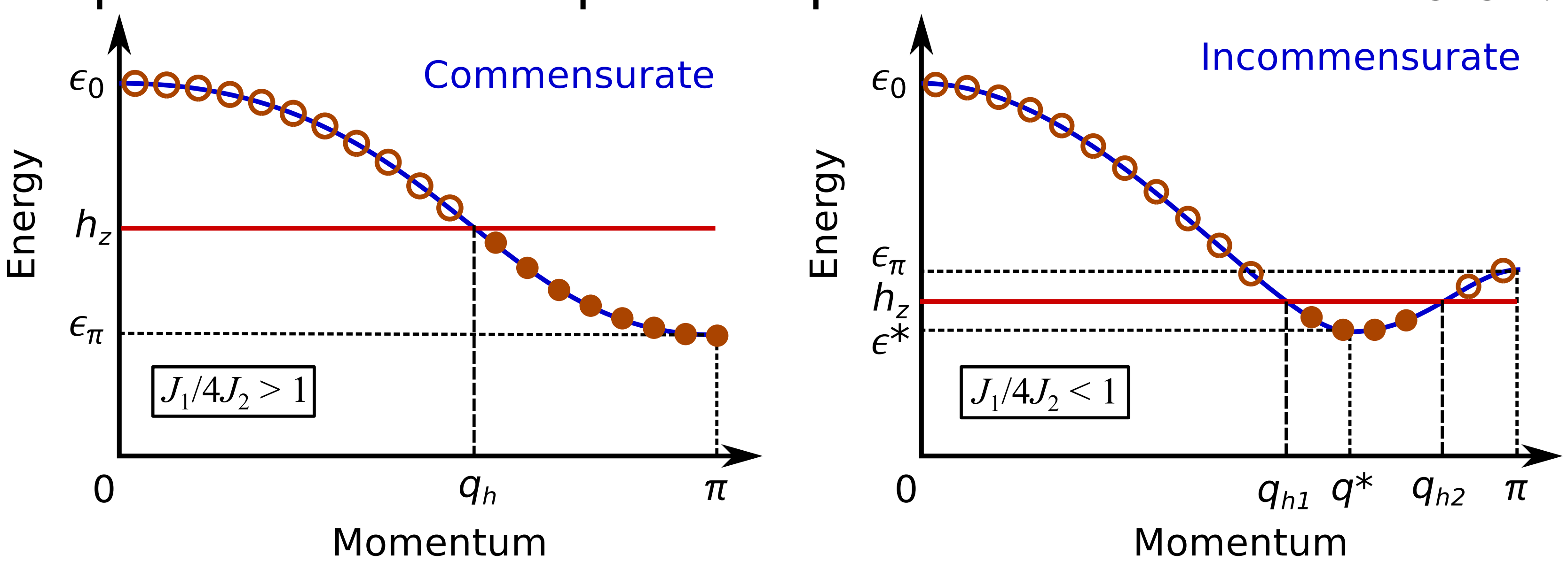
$$\mathcal{H}_{\rm eff}^{(-)} = \sum_q \omega(q) n_q^- - h^z n_q^-$$

$$\omega(q) = J_1 \cos(q) + J_2 \cos(2q) + J_p$$

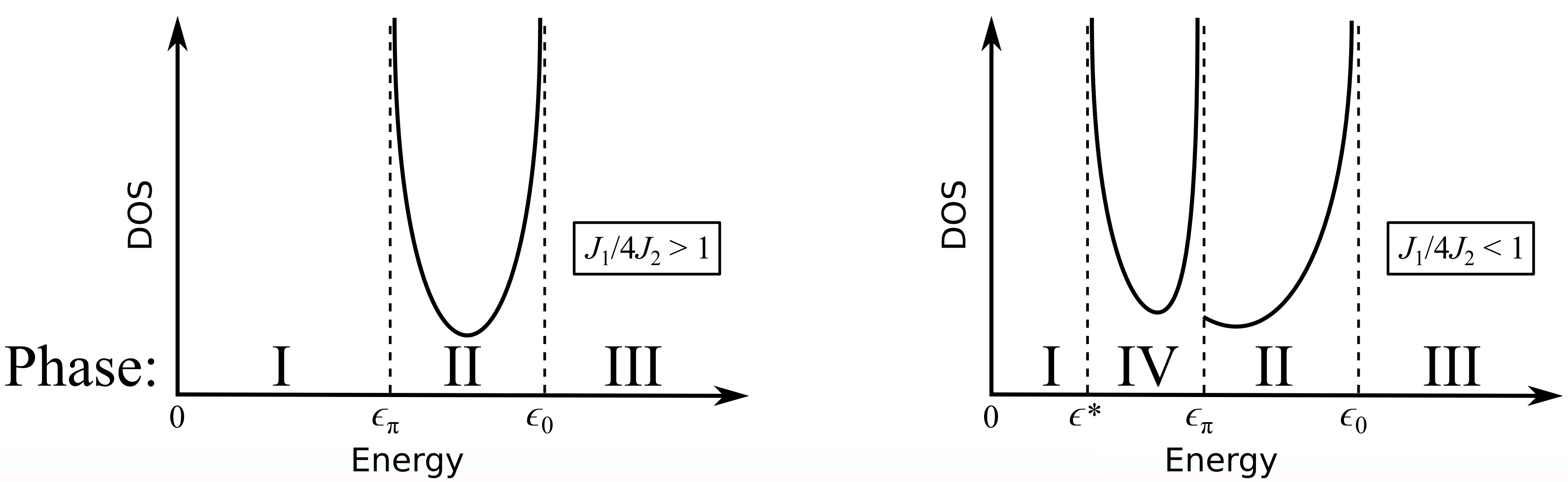
Bose-Einstein condensation

Bose gas	**NIT**
boson particle	triplon
boson num. (N)	magnetization (M)
chem. potential (μ)	magnetic field (h^z)

Dispersion relation & triplon occupation



Density of states



☛ Without frustration , there are three phases:

Phase I: $h^z < \epsilon_\pi$, $M = 0$, gapped.

Phase II: $\epsilon_\pi < h^z < \epsilon_0$, $0 < M < 1$, gapless.

Phase III: $\epsilon_0 < h^z$, $M = 1$, gapped.

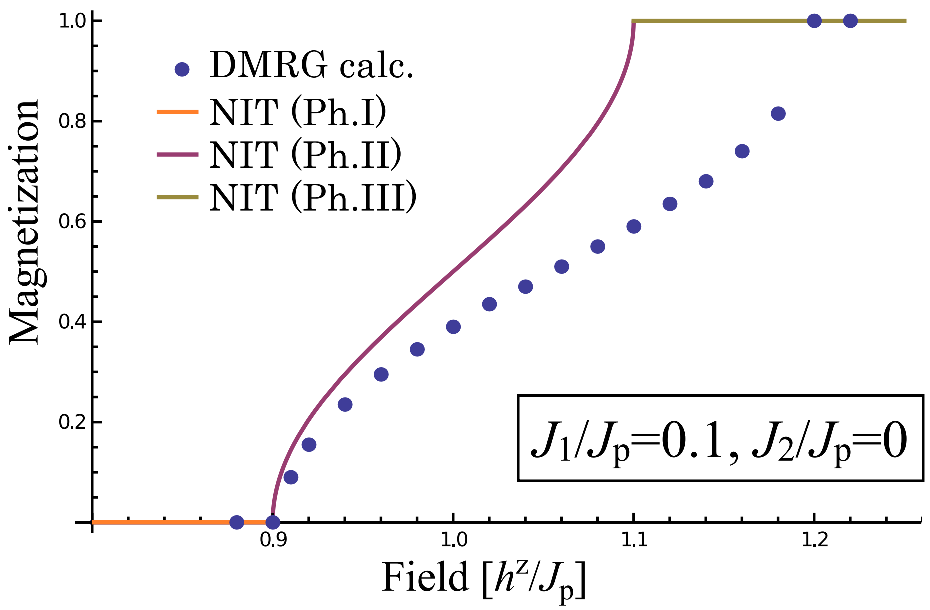
☛ With frustration, a new gapless phase appears,

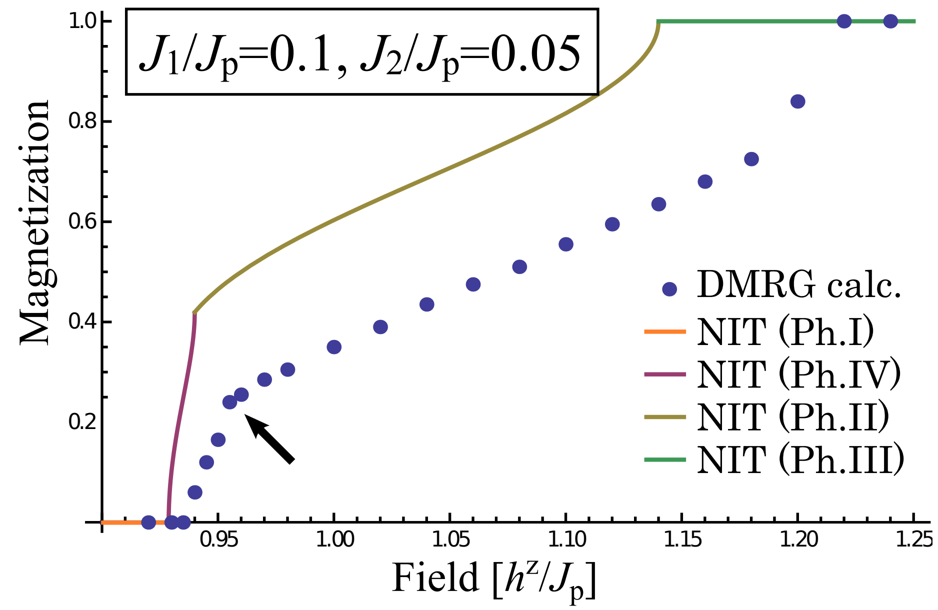
Phase IV: $\epsilon^* < h^z < \epsilon_\pi$, $0 < M < 1$, gapless.

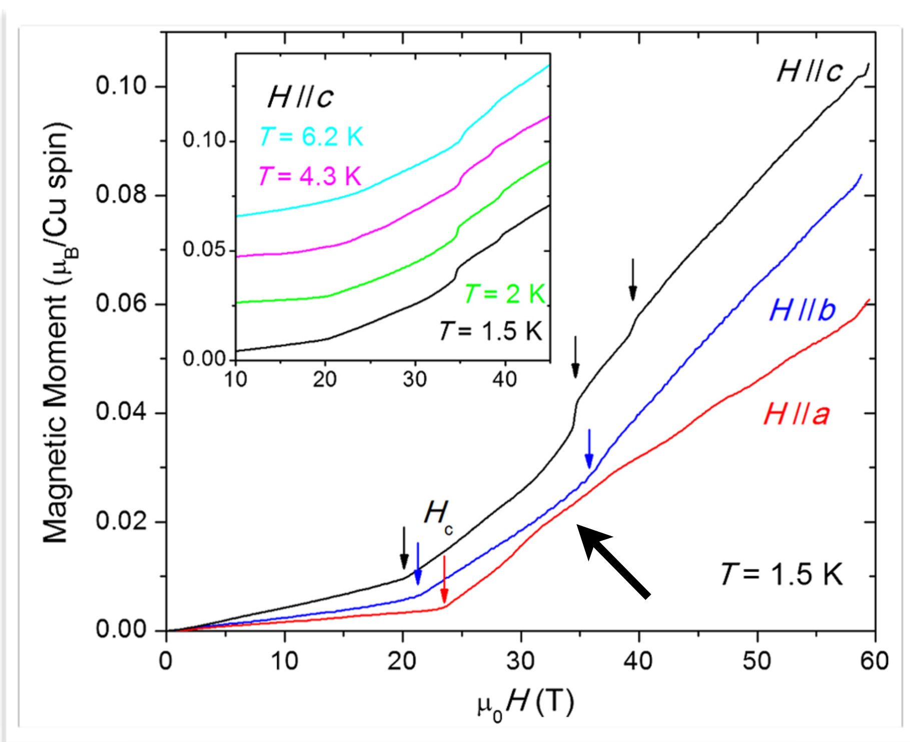
“Phase transition induced by magnetic field in a TLSL” T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

M-H curve

M-H curve







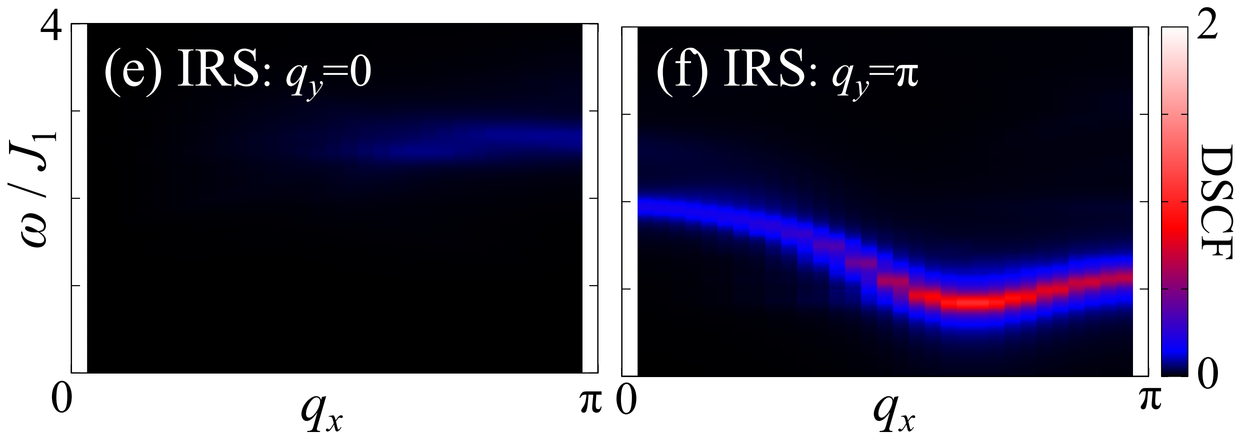
Y. Kohama, *et al*, PRL **109**, 167204 (2012).

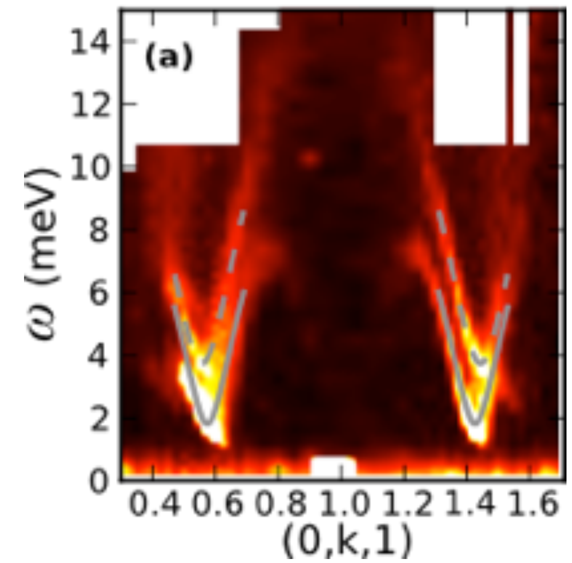
☛ With frustration, the cusp-like singularity appears in M-H curve.

☛ The phase transition in the compound BiCu2PO6 can be understood using triplon picture with frustration.

Summary

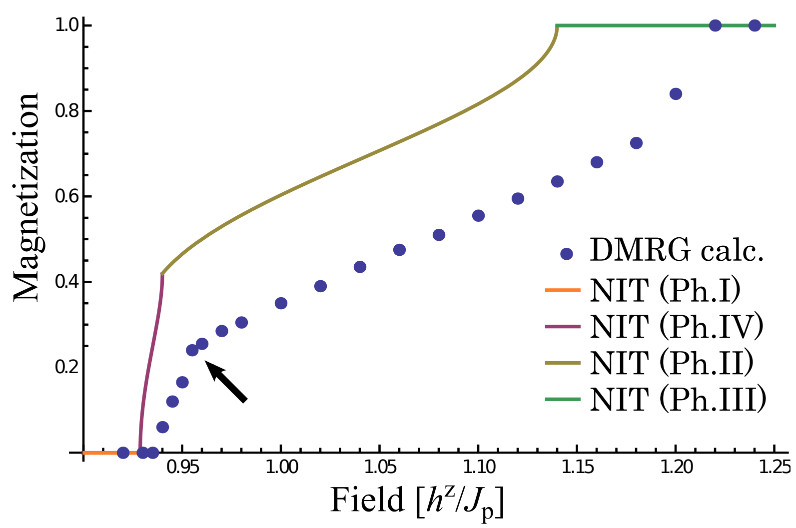
We determine the ground-state phase of $BiCu_2PO_6$, with excitation spectra obtained by DDMRG calculation and INS experiment.

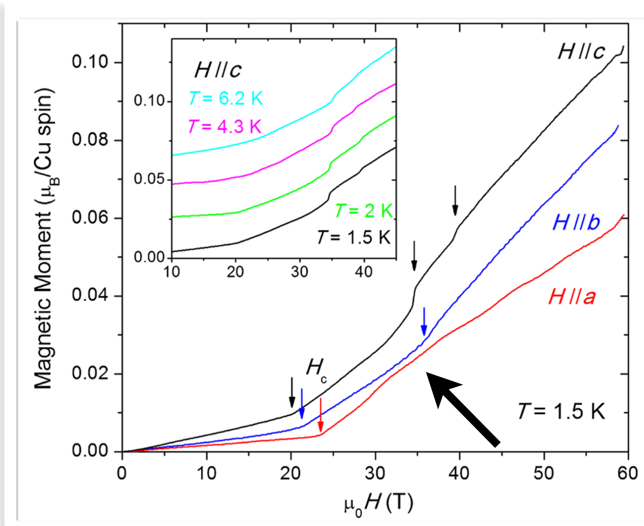




K.W. Plumb, *et al*, arXiv:1301.5324.

We clarify the phase transition in $BiCu_2PO_6$, with M-H curve of DMRG calculation, non-interacting triplon analysis, and the experiment.



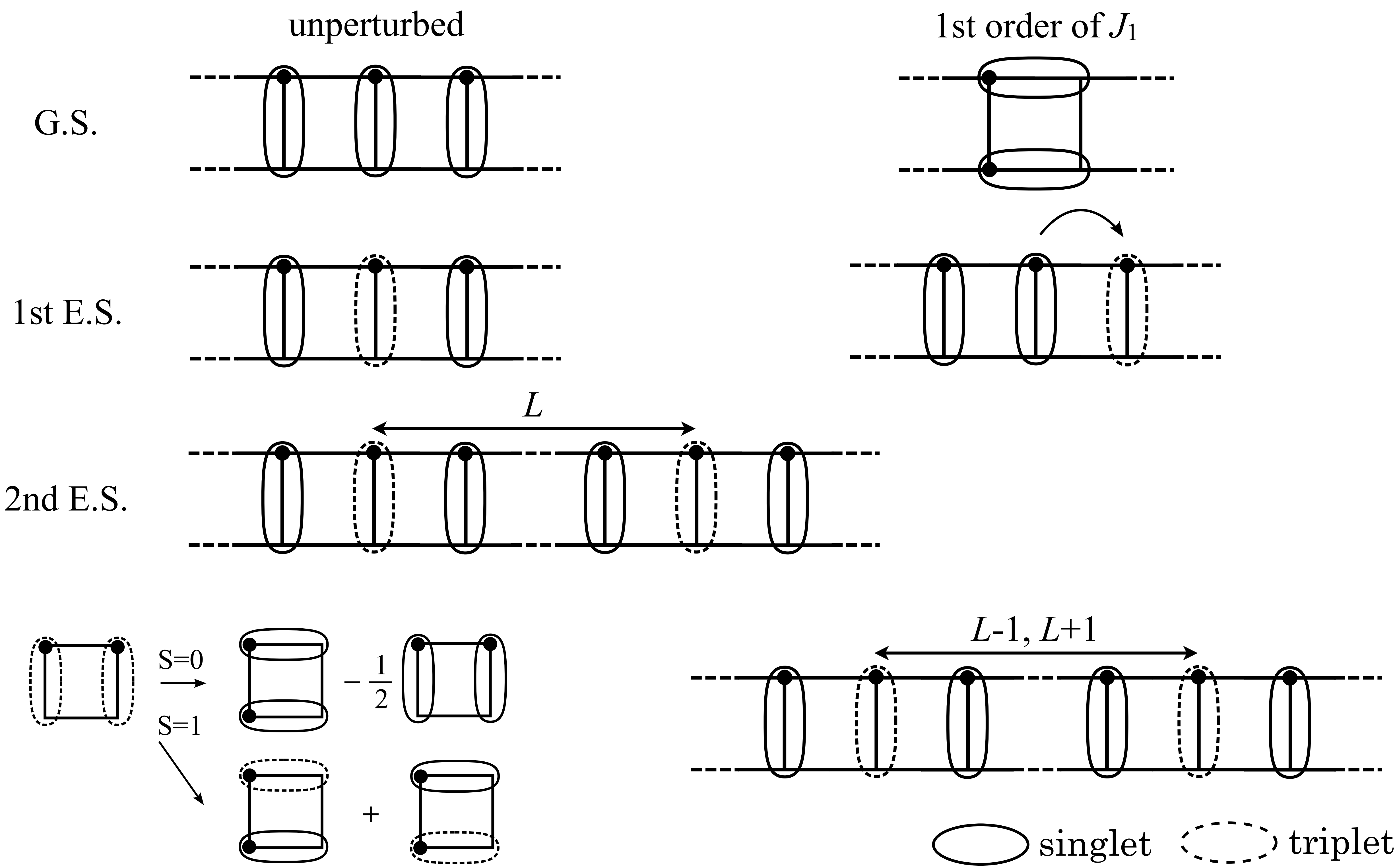


Y. Kohama, *et al*, PRL **109**, 167204 (2012).

Appendix

Purbation analysis

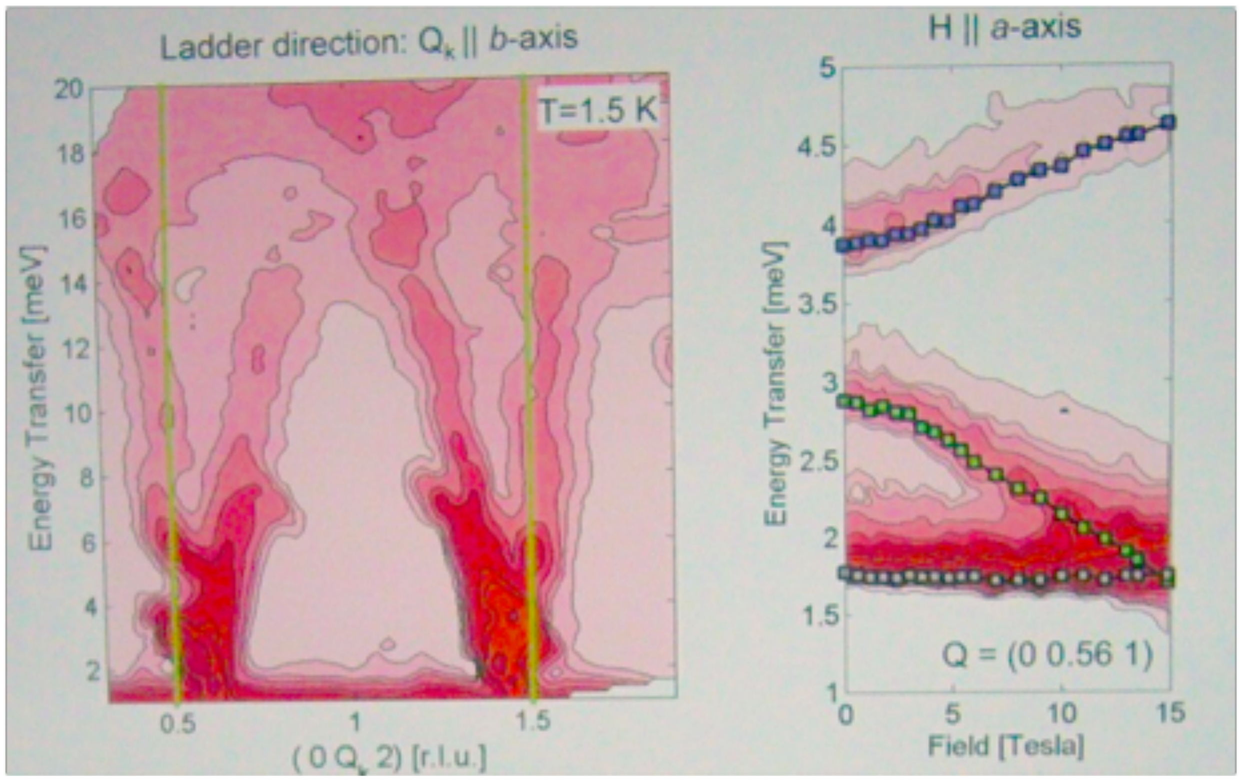
Strong rung-coupling limit



"Phase transition induced by magnetic field in a TLSL" T. Sugimoto *et. al.*, EQPCM13 @ ISSP, June 17, 2013.

Zeeman splitting

- Field dependence (experiment) ref. ICM poster



☛ Field effects on lowest excitations seems Zeeman splitting of triplet.

- 2 spins Hamiltonian with anisotropy

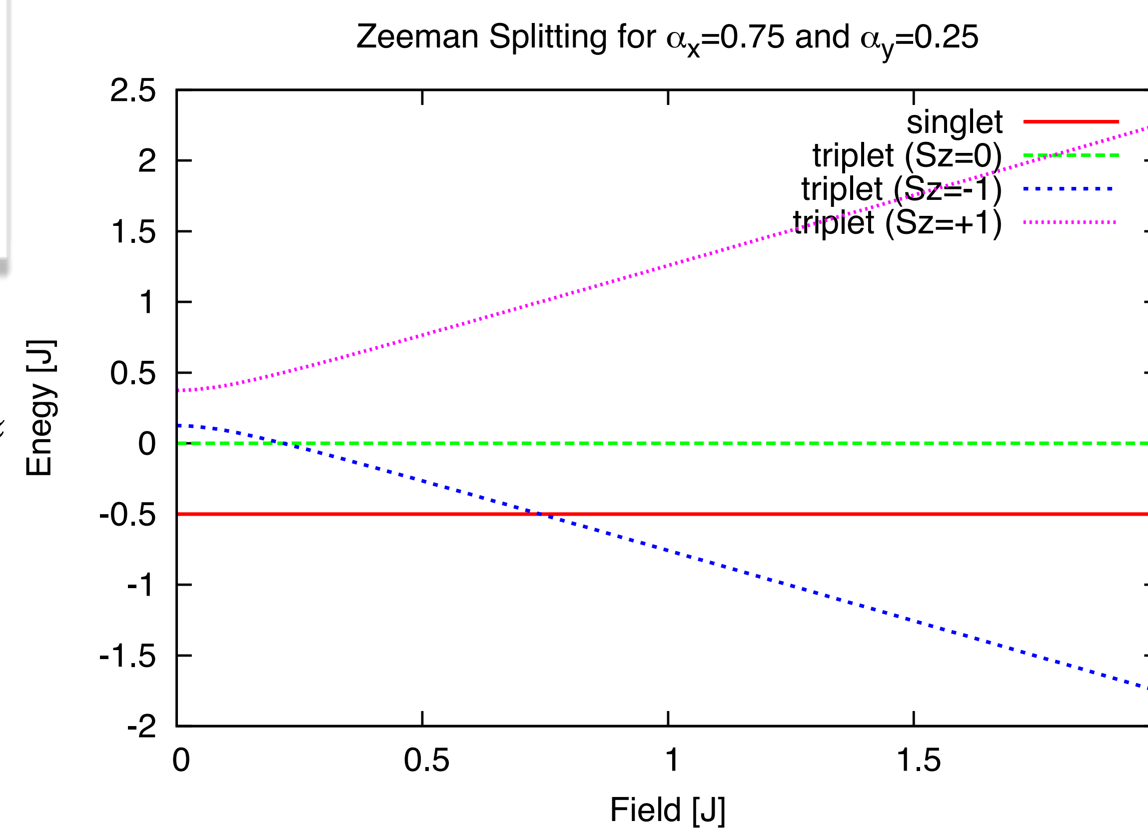
$$\mathcal{H} = J(\alpha_x S_1^x S_2^x + \alpha_y S_1^y S_2^y + S_1^z S_2^z) + (S_1^z + S_2^z)H_z$$

$$E^s = -\frac{J}{4}\left(1 + |\alpha_x + \alpha_y|\right),$$

$$E_0^t = \frac{J}{4}\left(-1 + |\alpha_x + \alpha_y|\right),$$

$$E_{-1}^t = \frac{J}{4}\left[1 - \sqrt{\frac{16H_z^2}{J^2} + (\alpha_x - \alpha_y)^2}\right],$$

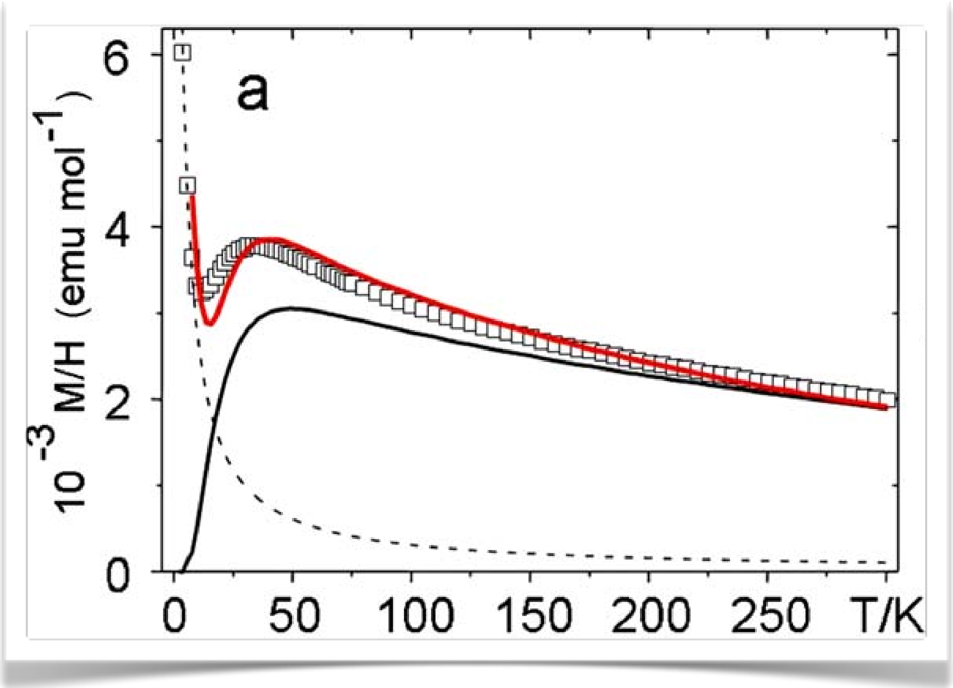
$$E_1^t = \frac{J}{4}\left[1 + \sqrt{\frac{16H_z^2}{J^2} + (\alpha_x - \alpha_y)^2}\right].$$



☛ Spin interaction between two spins forming triplet has anisotropy.

Real compound

- Susceptibility



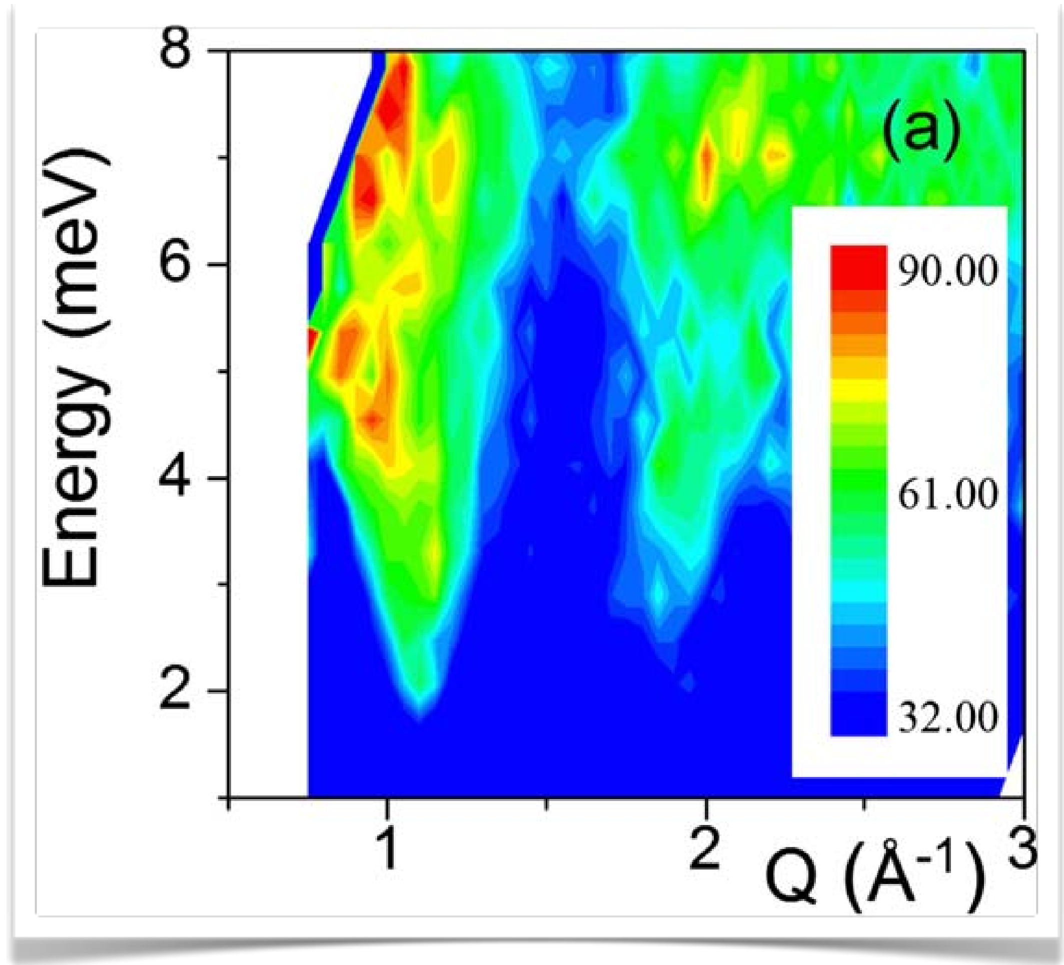
☛ Fitting (paramag. impurity + frustrated ladder) gives better coincidence, than fitting by using the ladder model.

Here, fitting function is as follows,

$$\chi_{\rm fit}(T) = C/T + \chi_{1-2-4}(T).$$

$$\rightarrow J_1/k_B = 137\,\mathrm{K},\ J_2/k_B = 73\,\mathrm{K},\ J_4/k_B = 58\,\mathrm{K}.$$

- Inelastic neutron scattering for powder

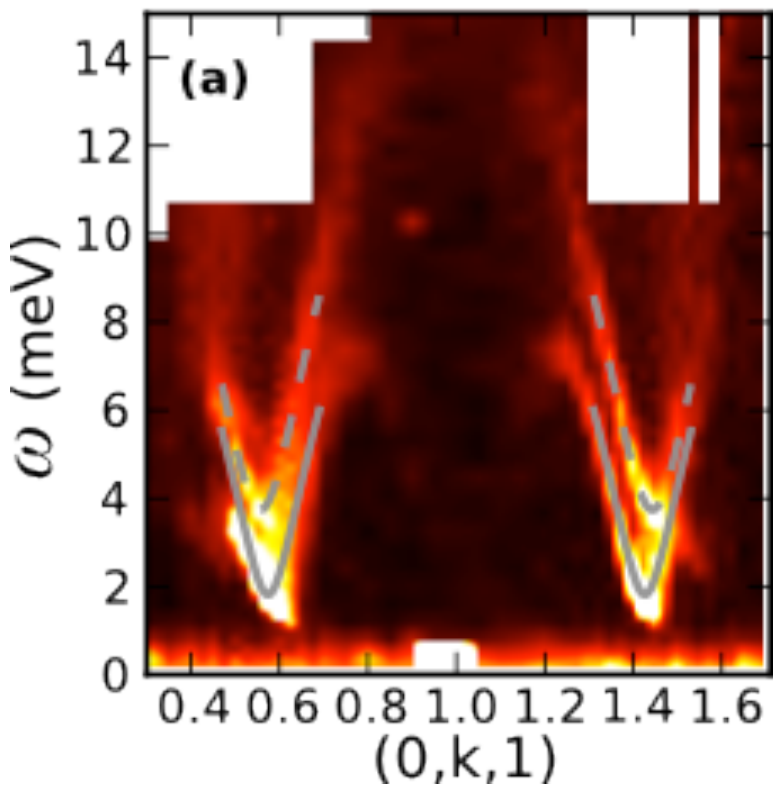


☛ Inelastic Neutron scattering is done for powder sample. The gap is estimated at 4 meV (46 K).

☛ Experimental results are consistent for the J_1-J_2-J_4 model, but exchange ratios J_2/J_1 & J_4/J_1 are not determined precisely.

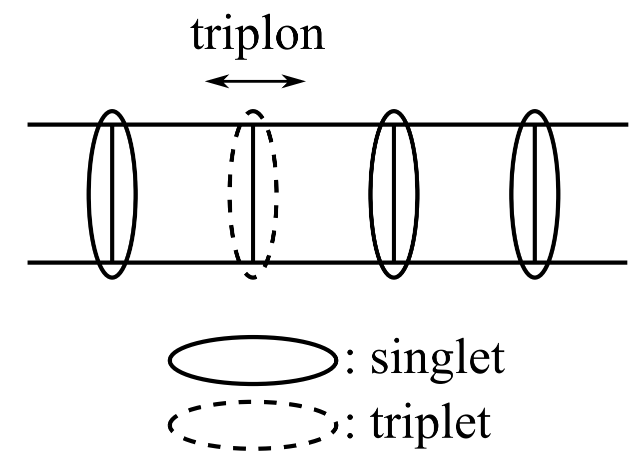
O. Mentré, *et al*, PRB 80, 180413(R) (2009).

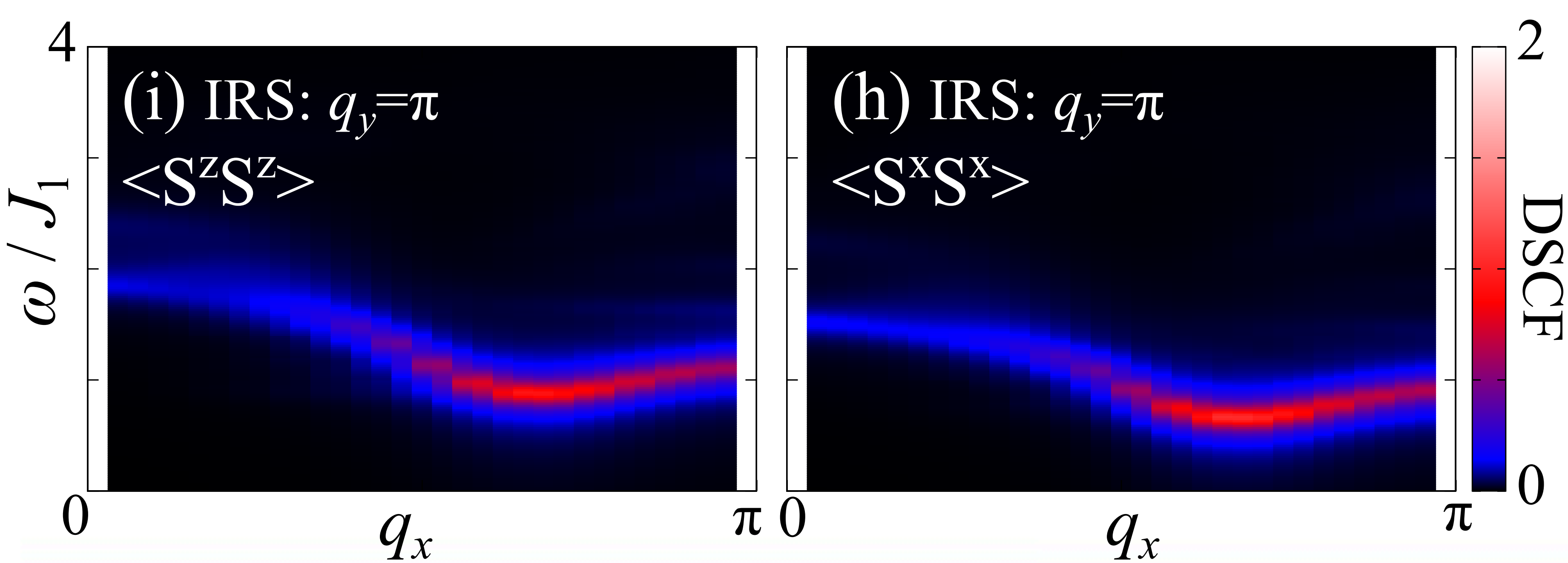
Inelastic neutron scattering



K.W. Plumb, *et al*, arXiv:1301.5324.

→ Splitting of triplon mode





$$E^s = -\frac{J}{4}\left(1 + 2|\alpha_{\rm Ising}|\right),$$

$$E^t_0 = \frac{J}{4}\left(-1 + 2|\alpha_{\rm Ising}|\right),$$

$$E^t_{-1} = \frac{J}{4}\left[1 - \left|\frac{4H_z}{J}\right|\right],$$

$$E^t_1 = \frac{J}{4}\left[1 + \left|\frac{4H_z}{J}\right|\right].$$