Magnetism of a Frustrated Four-Spin-Tube

M. Arlego, WB, Phys. Rev. B **84**, 134426 (2011)
M. Arlego, et al. preprint

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Funding

nth nano school for contacts in nanosystems

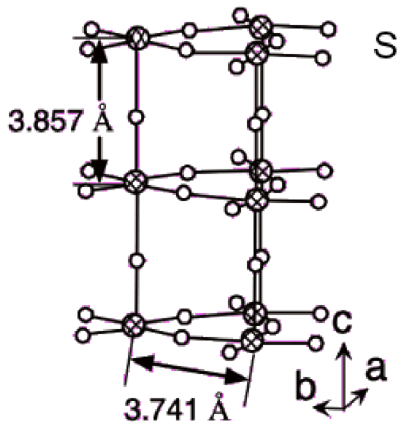
EU LOTHERM

DFG FOR 912

Spin Tubes

- N=3

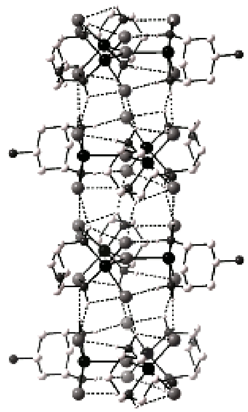
$CsCrF_4$



$S=\frac{3}{2}$

Manaka, et al.,
JPSJ 78, 93701 (09)

$[(CuCl_2tachH)_3Cl]Cl_2$



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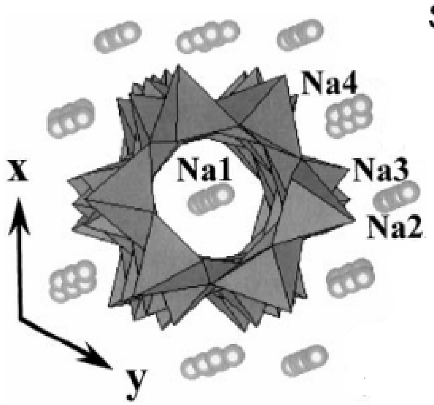
Schnack, et al.,
PRB 70, 17442 (04)

Geometric frustration

- N=9

$Na_2V_3O_7$



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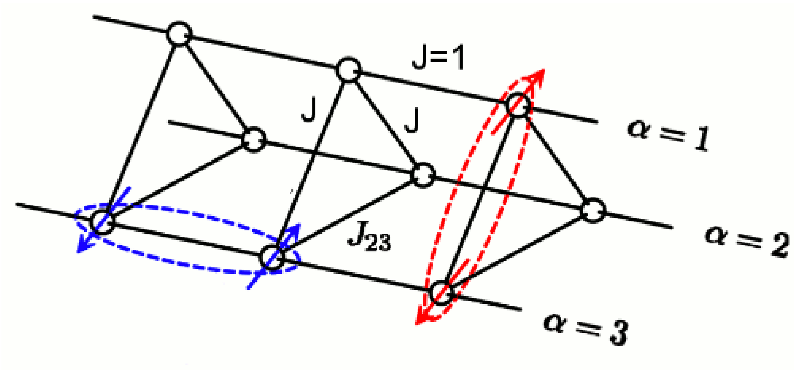
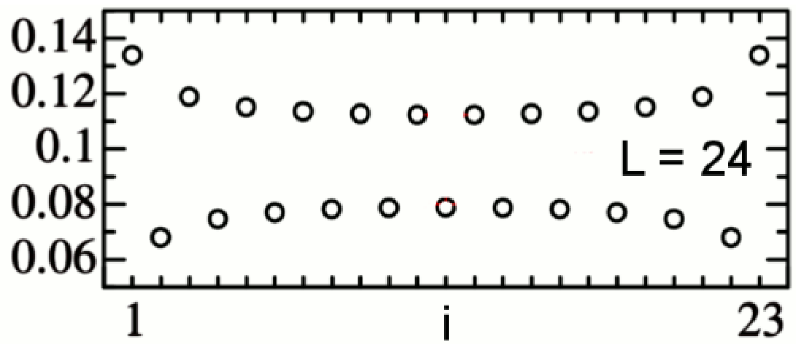
Millet, et al.,
JSSC 147, 676 (99)

- Three leg tube

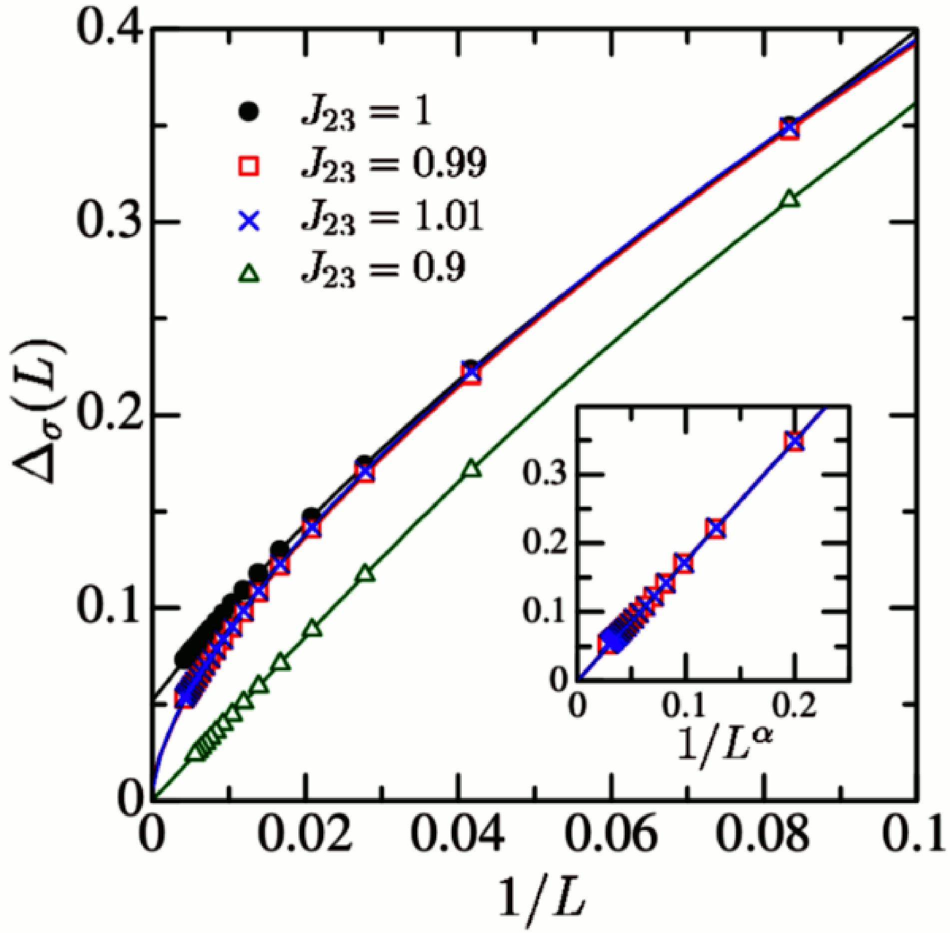


- consistent with LSM theorem

$$\left\langle \vec{S}_{\alpha,i}\cdot\vec{S}_{\alpha,i+1}\right\rangle$$



- … gapped at isotropic point



Kawano, Takahashi, JPSJ 66, 4001 (97)
Sakai, et al., Physica E 29, 633 (05)
Nishimoto, Arikawa, PRB 78, 054421 (08)

Sakai, et al., JPhys CondMat 22, 403201 (10)

Spin Tubes

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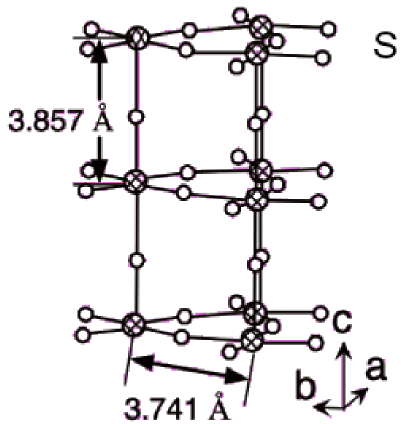

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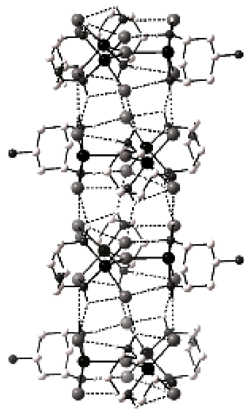


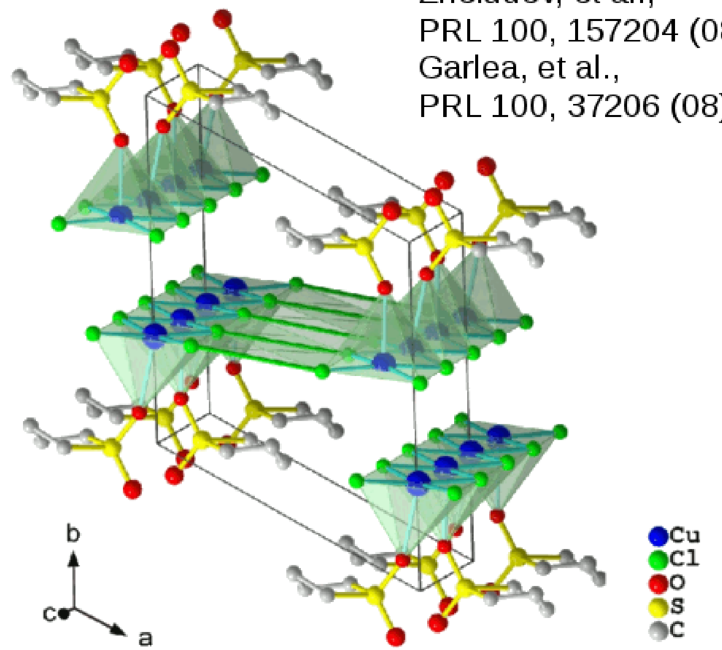
$S=\frac{1}{2}$

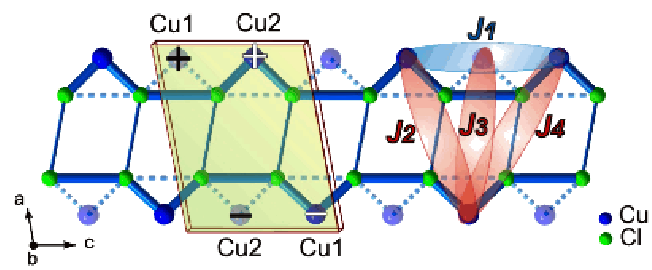
Schnack, et al.,
PRB 70, 17442 (04)

● N=4

$D_8C_4SO_2(Sul)\text{-}Cu_2Cl_4$

Zheludev, et al.,
PRL 100, 157204 (08)
Garlea, et al.,
PRL 100, 37206 (08)





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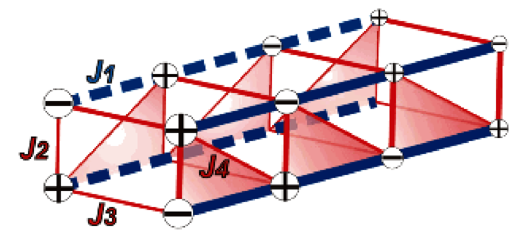

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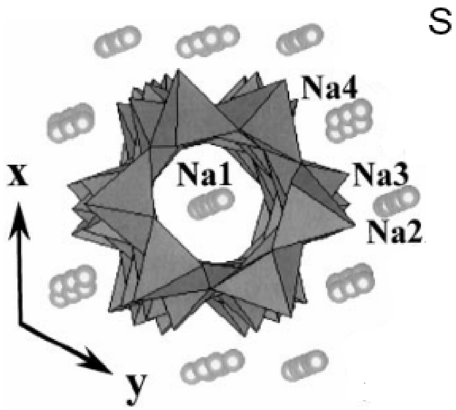
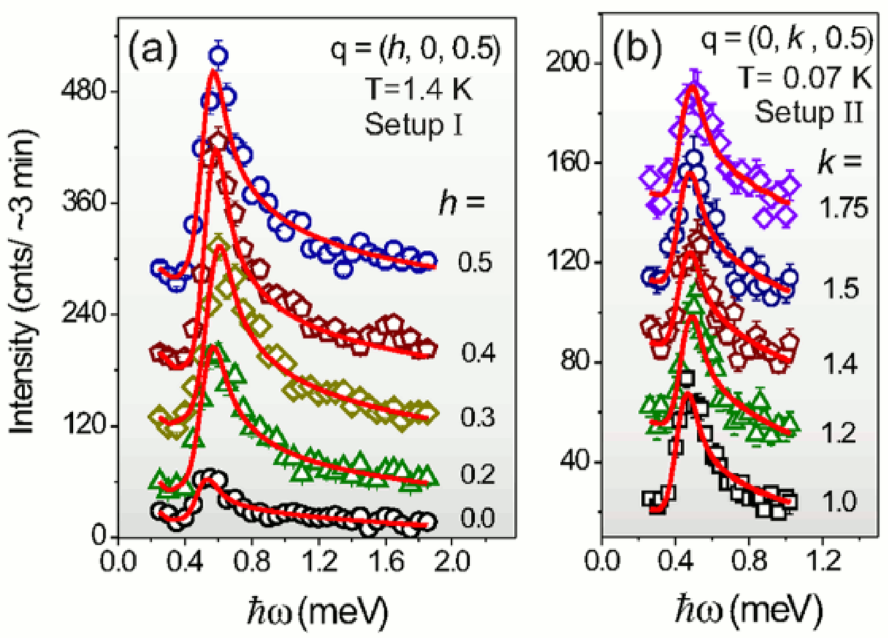


Millet, et al.,
JSSC 147, 676 (99)

Frustration

INS: strongly 1D



Sul-Cu_2Cl_4

Zheludev, et al., PRL 100, 157204 (08)
Garlea, et al., PRL 100, 37206 (08)

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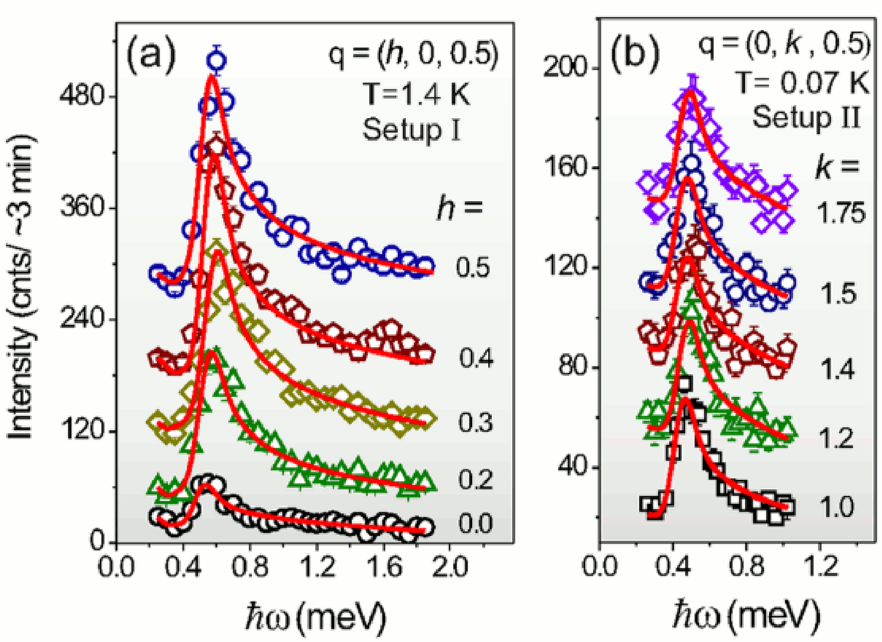
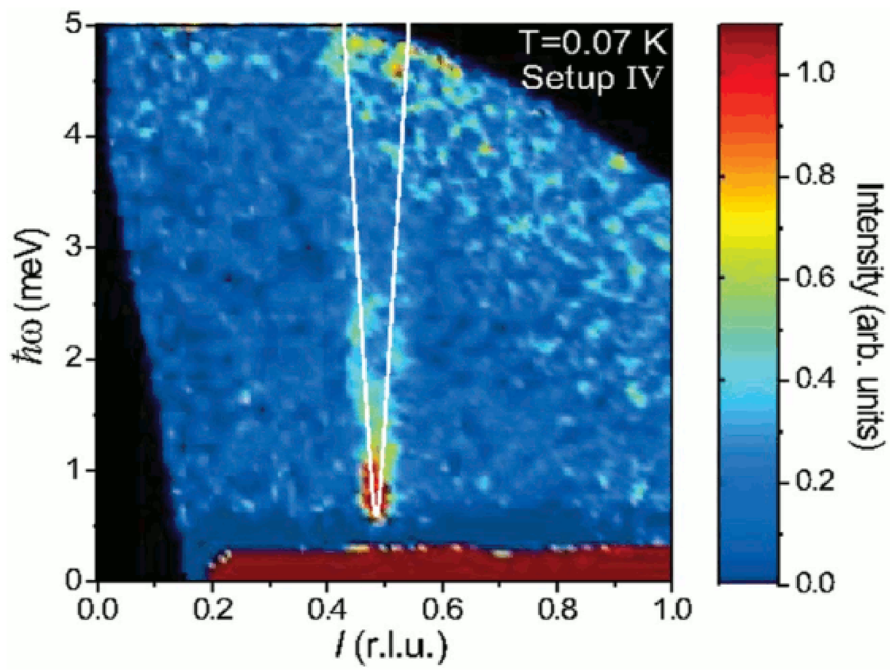
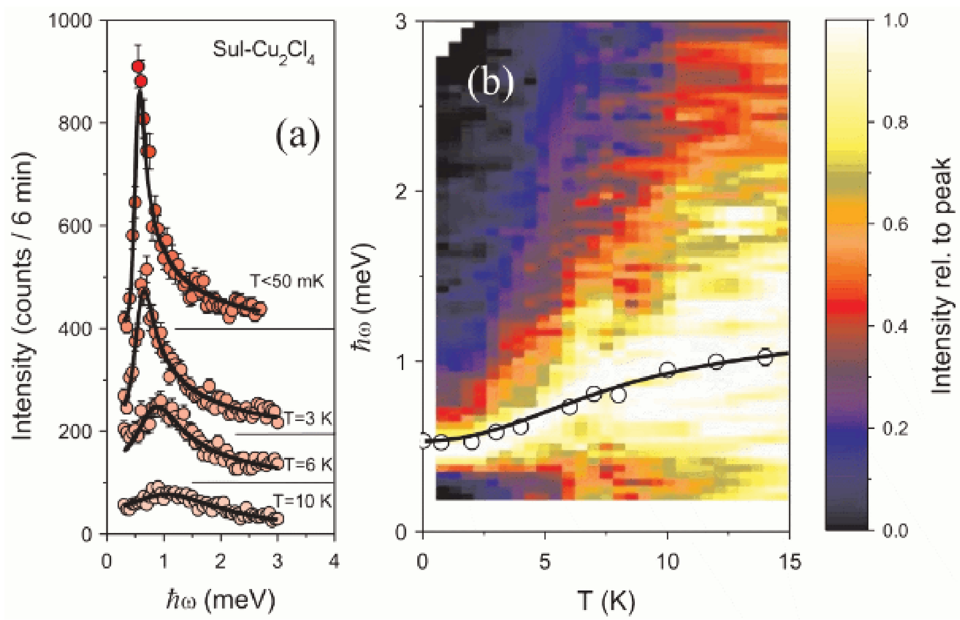


INS: c-axis dispersion



Const. q-scan vs. T @ Q



gapped

incommensurate → frustration

$$Q=\pi(1-0.044)$$

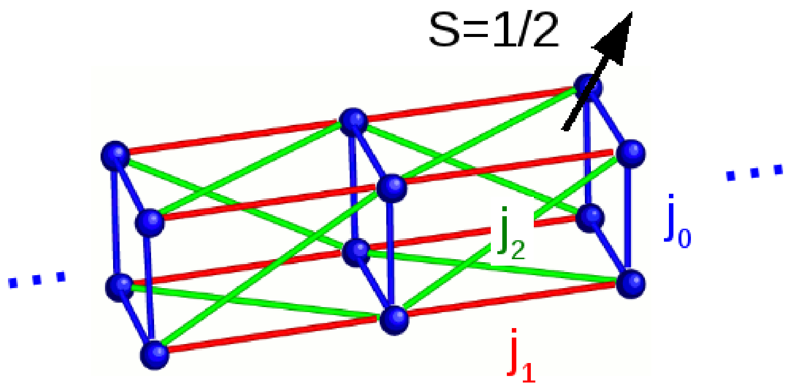
velocity

$$\partial\epsilon/\partial k \sim 100\,K \sim J_{avg}$$

Zheludev, et al., PRL 100, 157204 (08)
Garlea, et al., PRL 100, 37206 (08)

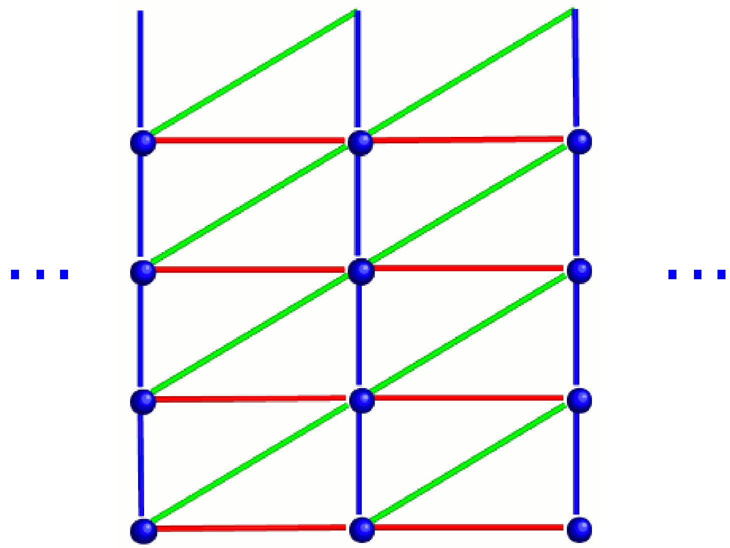
Tube Model

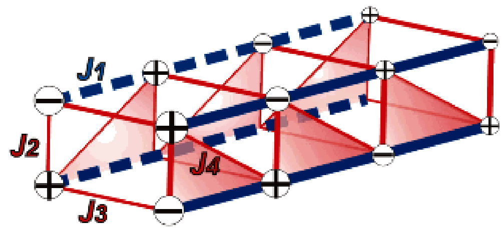
- Geometrically frustrated four-spin tube



$$H=\sum_{\langle lm \rangle} J_{lm}\,\vec{S}_l\cdot\vec{S}_m \qquad \text{all } j_i \text{ AFM}$$

- Anisotropic triangular lattice on a torus





1) Tube Materials & Model

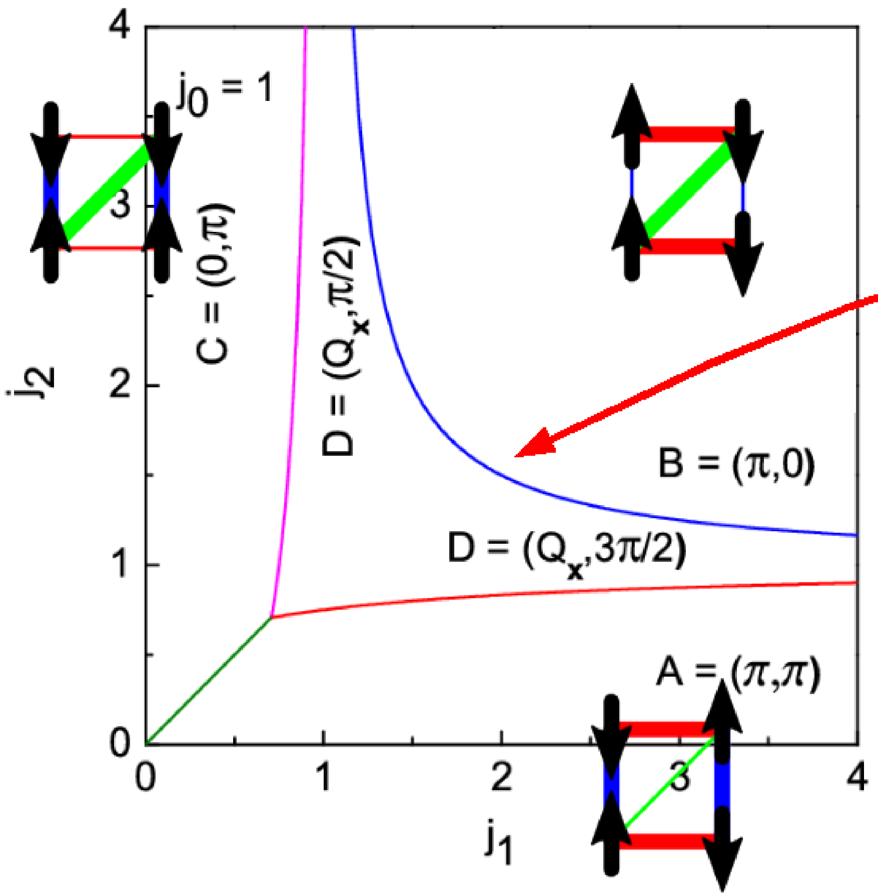
2) Phases and Static Correlations

3) Plaquette Regime

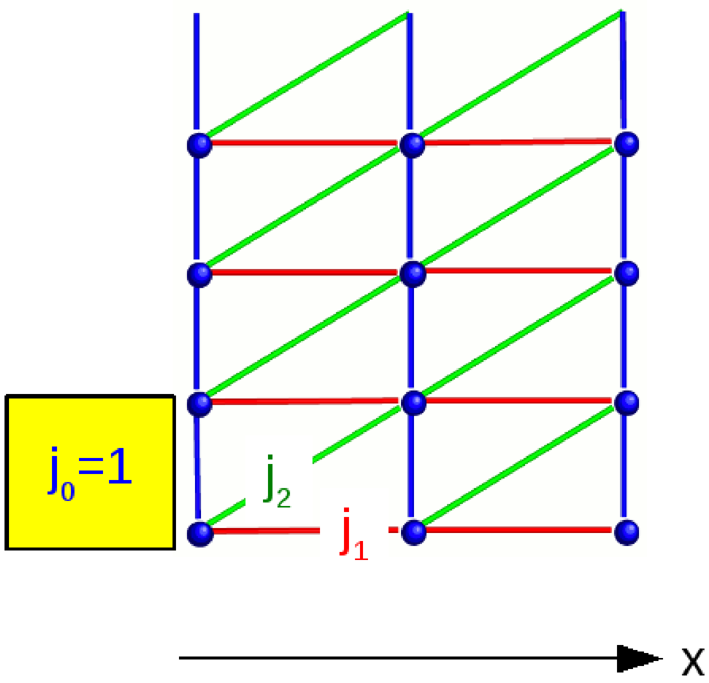
4) Strong Leg Coupling

Phases

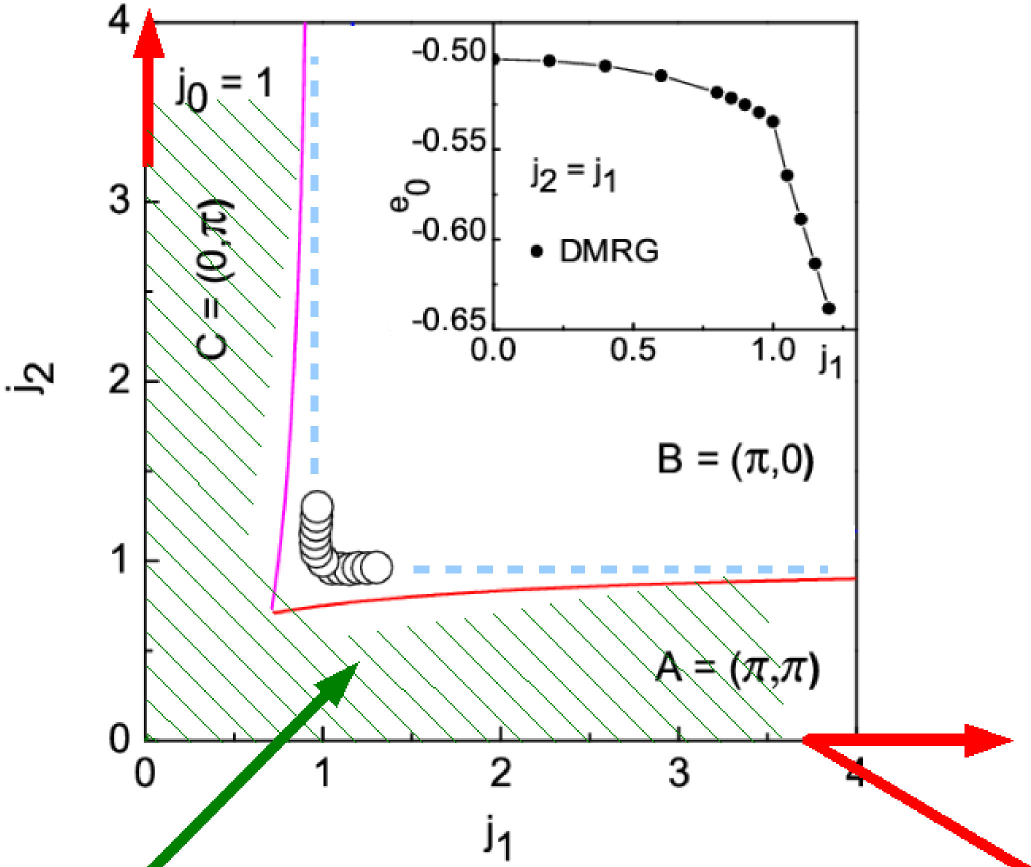
- Classical



- All 1[st] order



Phases



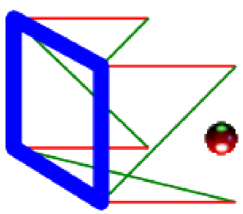
- DMRG L=50:

  One line of 1[st] order transitions terminating plaquette state

  Only moderate c→q renormalization

  Very weak beyond $j_1(j_2)$~1.5, $j_2(j_1)$~1

  No transition into (π,0) state



- coupled 4-spin singlet-plaquettes

  non-frustrated ladder-case j_2=0

  Cabra, Honecker,Pujol, PRB 58, 6241 (98)
  Kim and Sólyom, PRB 60, 15230 (99)

- $j_1=\infty$, j_2=0 Luttinger liquid
- $j_1 \leftrightarrow j_2$ symmetry

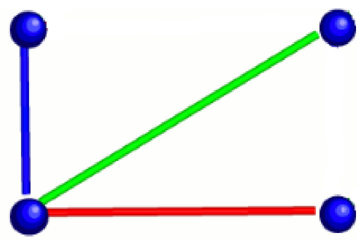
Phases: Schwinger Bosons

- SU(2) invariant decoupling

$$\mathbf{S}_l \cdot \mathbf{S}_m = :\hat{B}^+_{lm}\hat{B}_{lm}: - \hat{A}^+_{lm}\hat{A}_{lm}$$

FM $\quad \hat{B}^+_{lm} = \frac{1}{2}\sum_\sigma b^+_{l\sigma} b_{m\sigma}$

AFM $\quad \hat{A}_{lm} = \frac{1}{2}\sum_\sigma \sigma\, b_{l\sigma} b_{m-\sigma}$



$$A[B]_{lm} = \langle \hat{A}[\hat{B}]_{lm} \rangle$$

$$\sum_\sigma \langle b^+_{l\sigma} b_{l\sigma} \rangle - 2S = 0$$

6 bond mean fields
1 Lagrange params.

Ceccatto, Gazza, Trumper, PRB 47, 12329 (93)
Flint, Coleman, PRB 79, 014424 (09)

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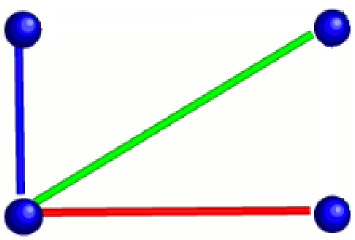

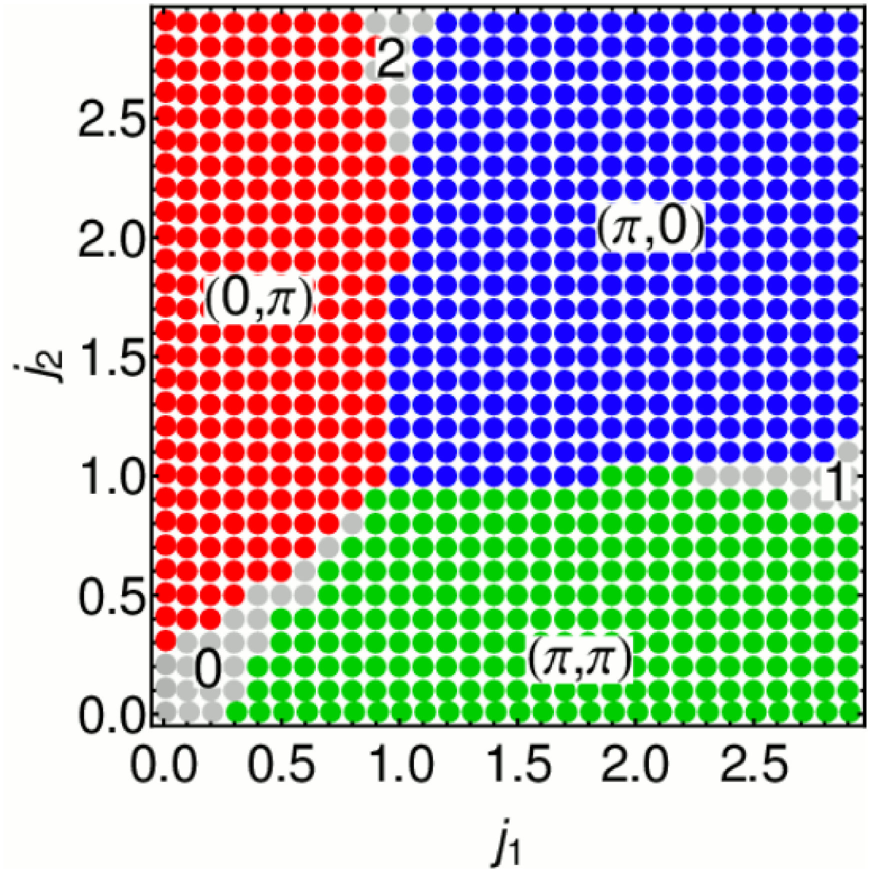

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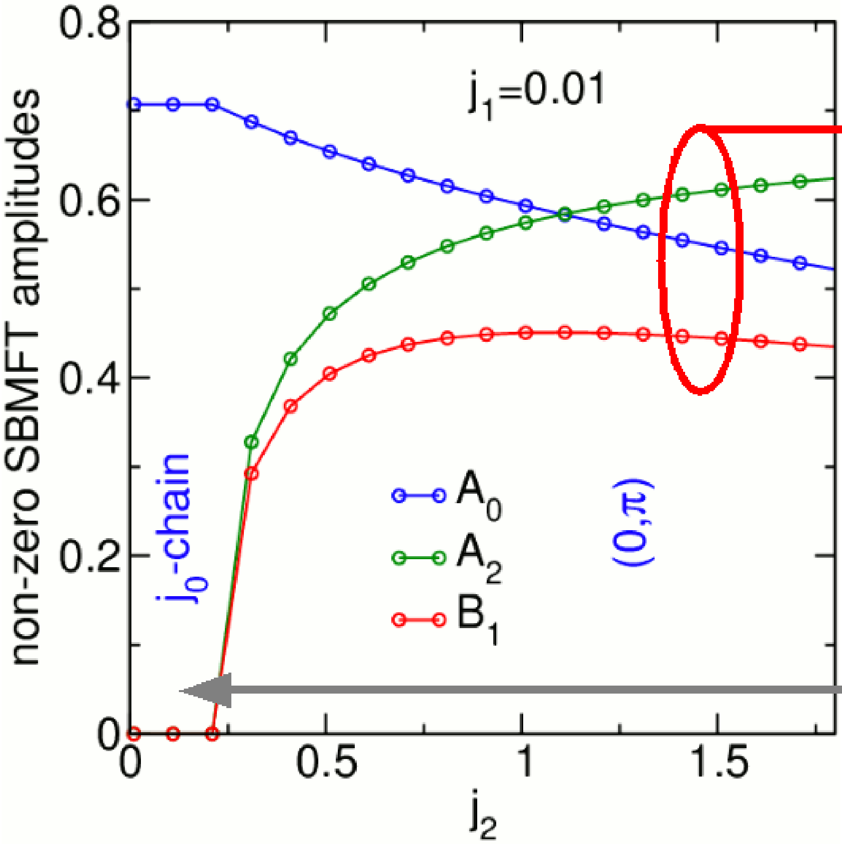
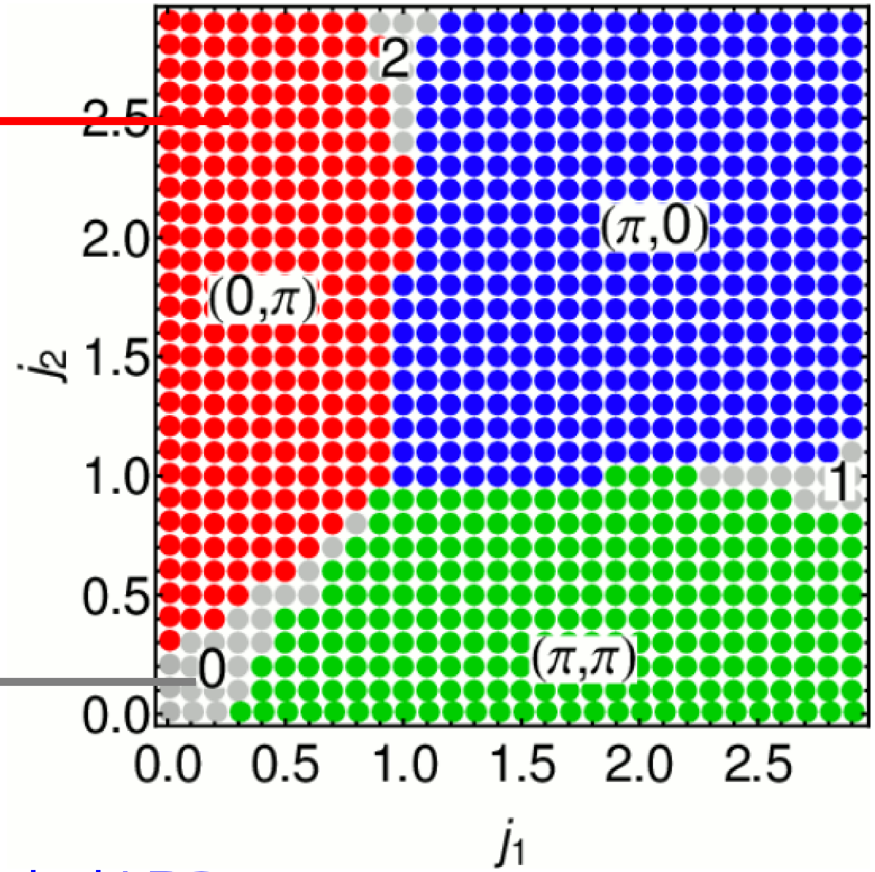
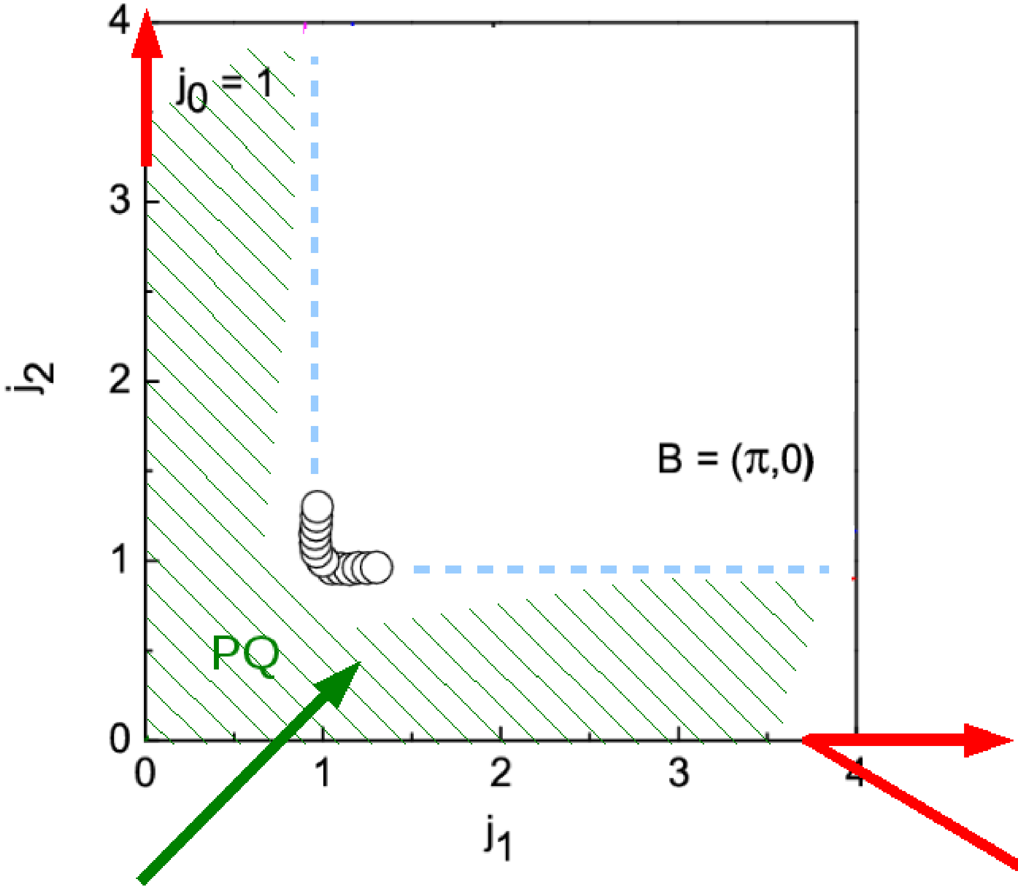


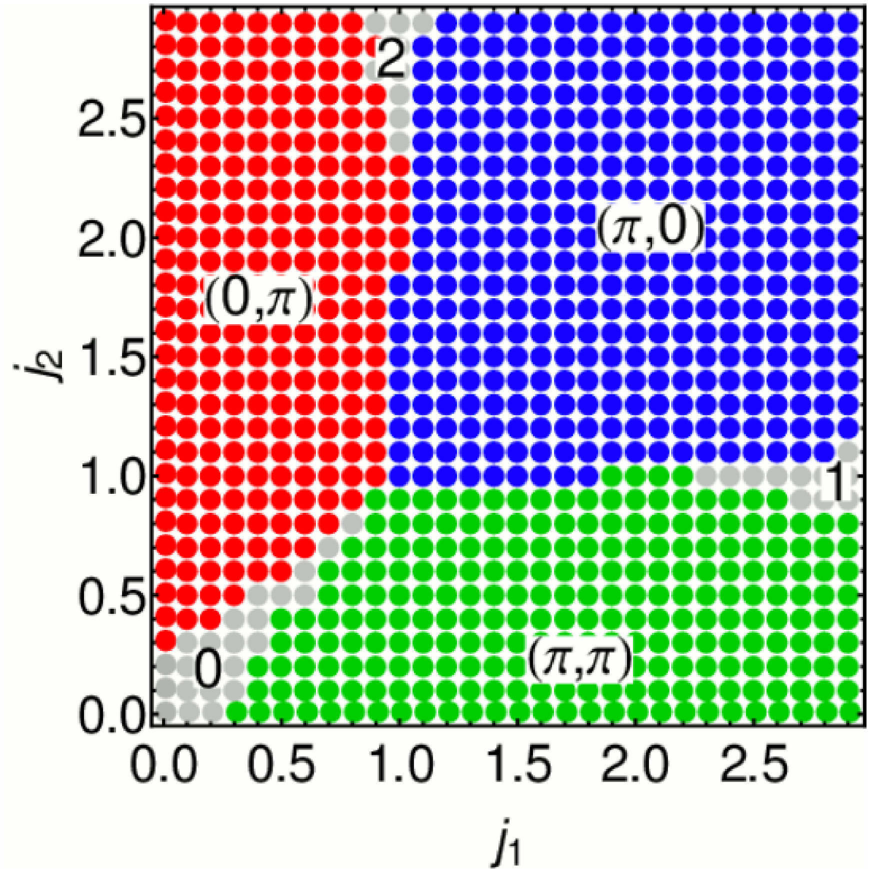


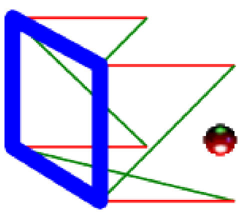
- SR0 similar to classical LRO but no boson condensate
- no IC phase
- red↔green↔blue: 1st order
- RGB↔gray: 2nd order
- gray = unphysical

Phases

- Schwinger Bosons

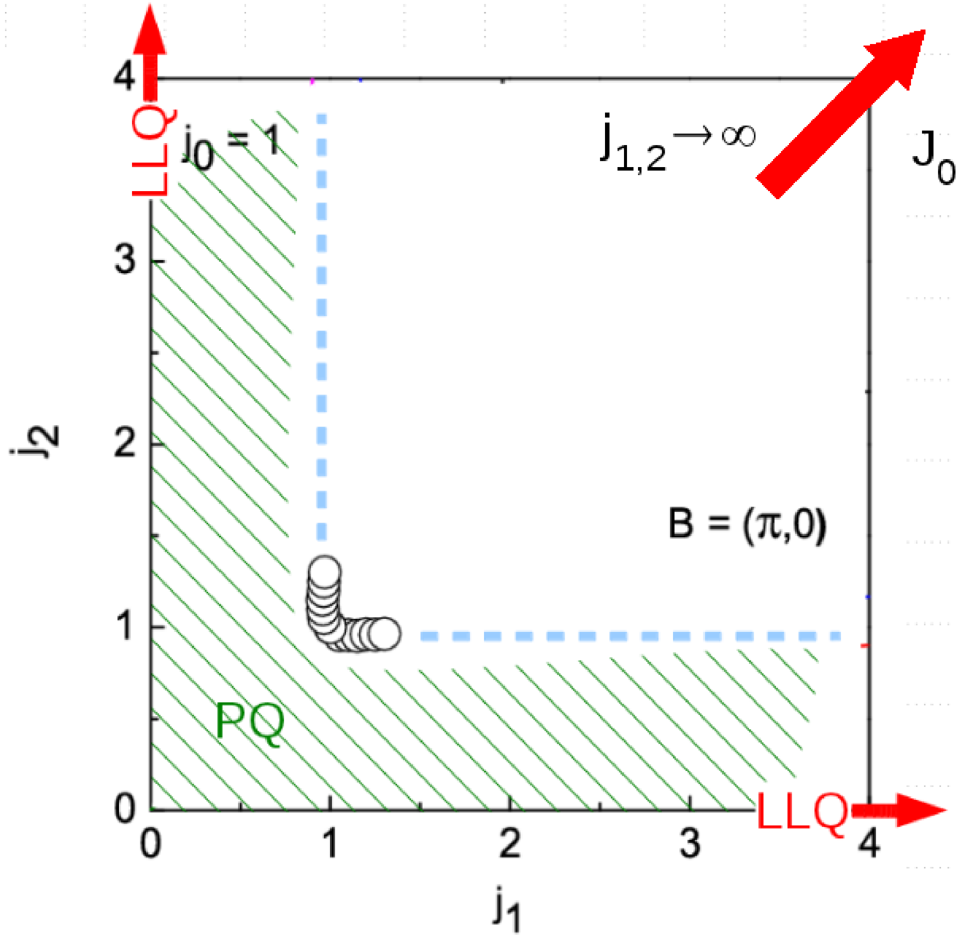






- coupled 4-spin plaquettes
- $j_1=\infty$, $j_2=0$ Luttinger liquid

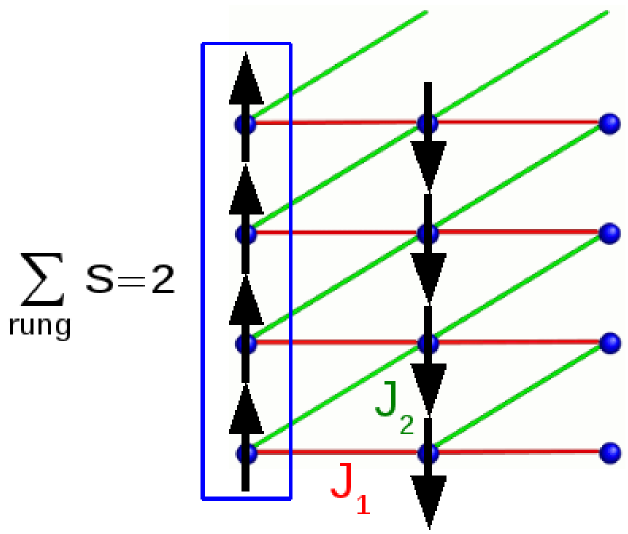
Phases: AFM 'Spin-2 Chain' Limit $J_0=0$



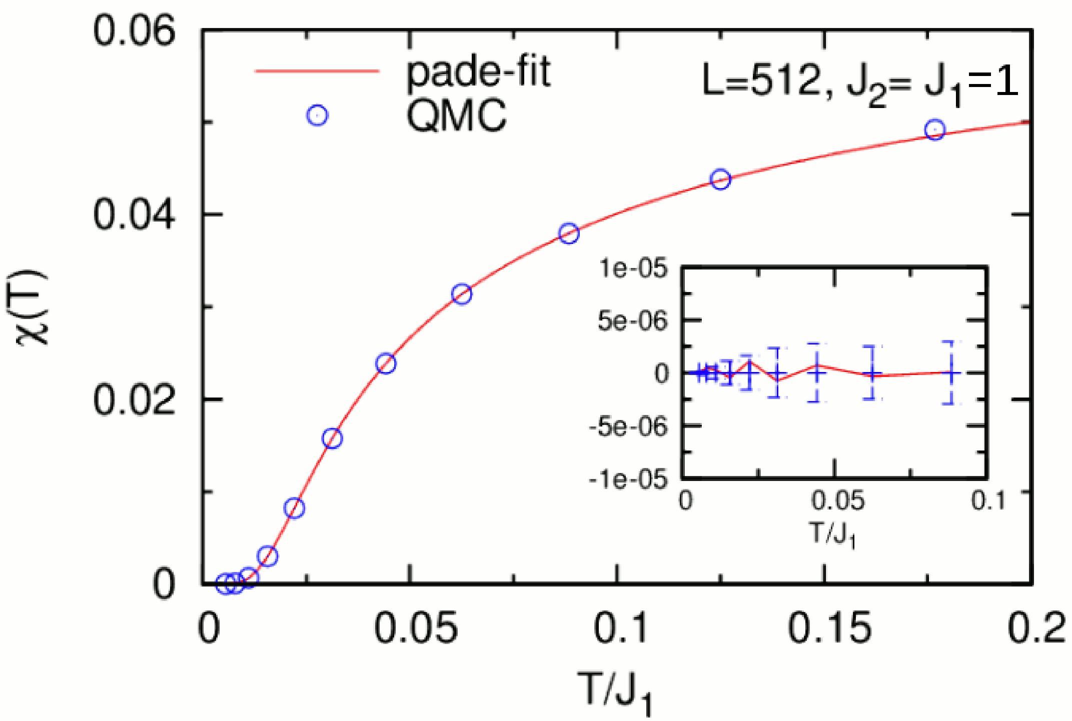
$J_0 = 0, J_2/J_1$

Phases: AFM 'Spin-2 Chain' Limit J_0=0

- Unfrustrated. Classical: 1D S=2 AFM



- QMC uniform susceptibility: spin gap



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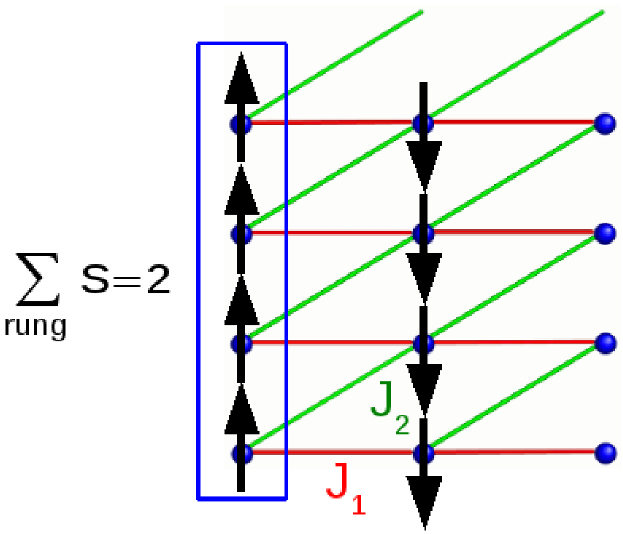

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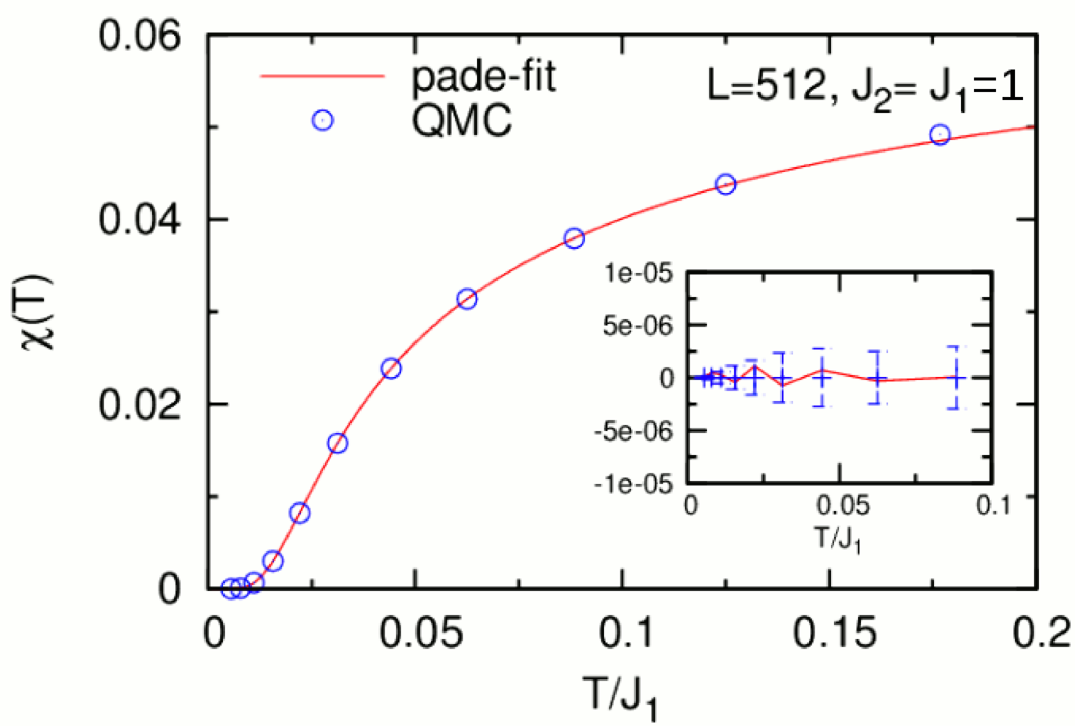
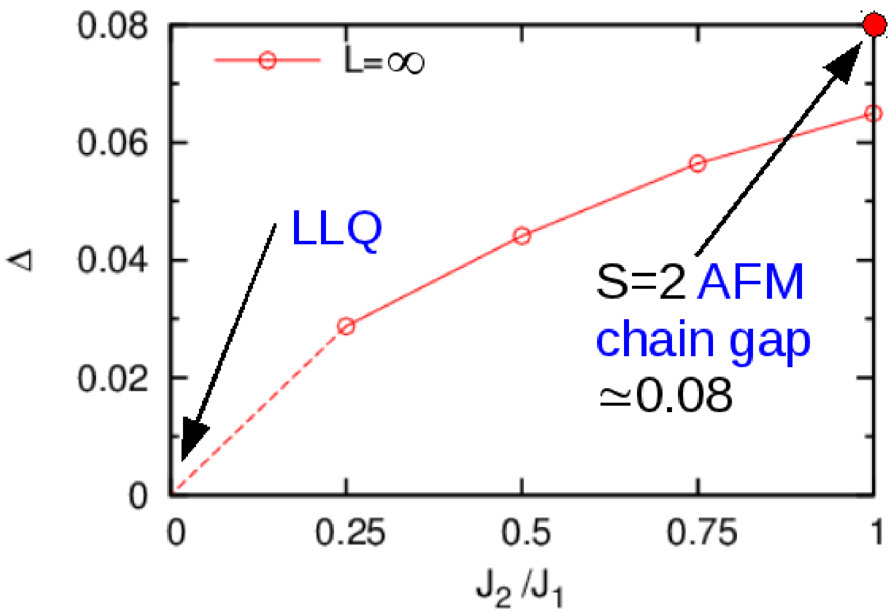
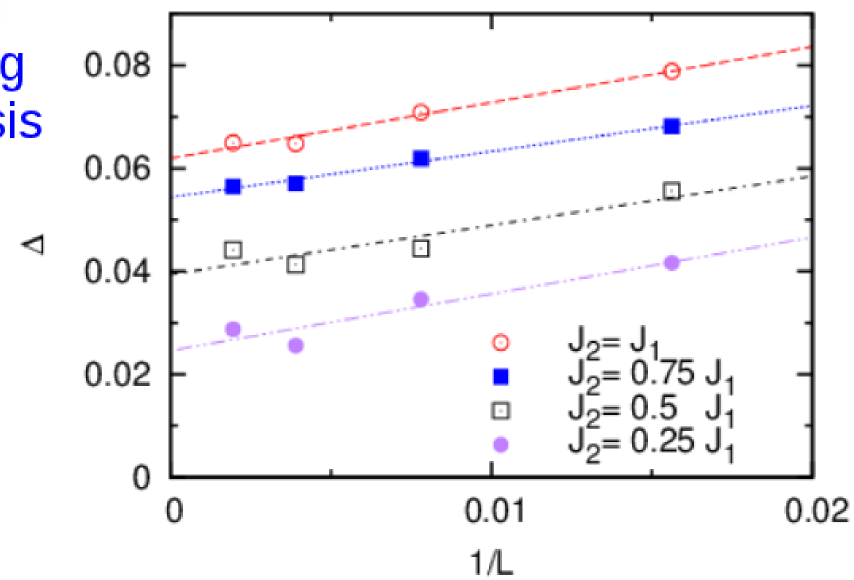


- Gap vs. J_2/J_1

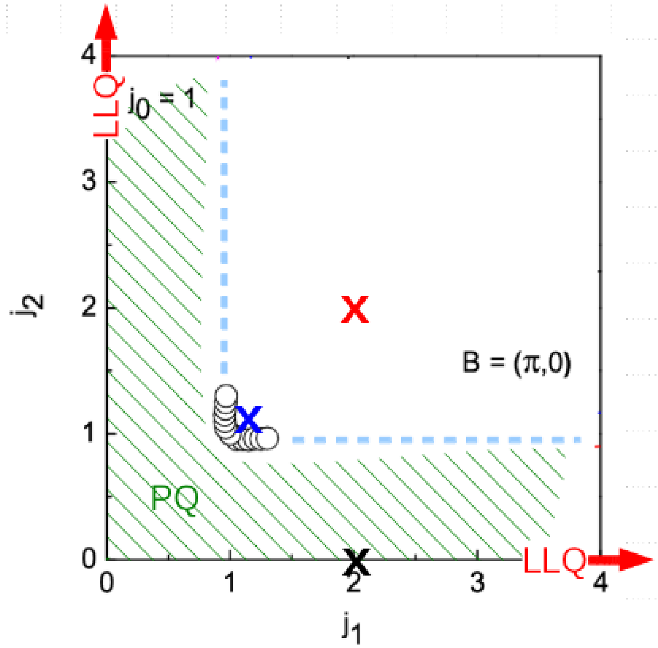


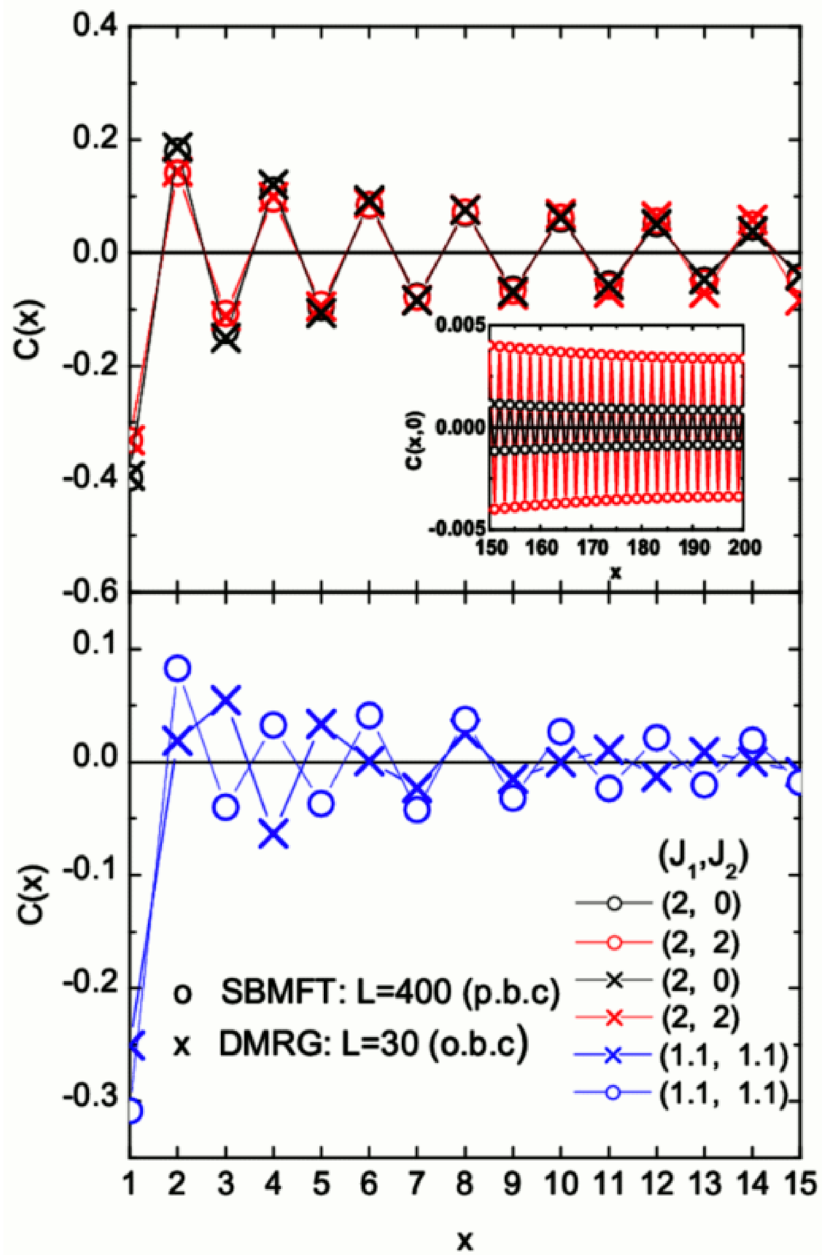
- Scaling analysis



Static Correlation Functions & Structure Factor

- $C(x)=\langle S^z_{r=(x,0)} S^z_{(0,0)}\rangle$ from DMRG & SBMFT

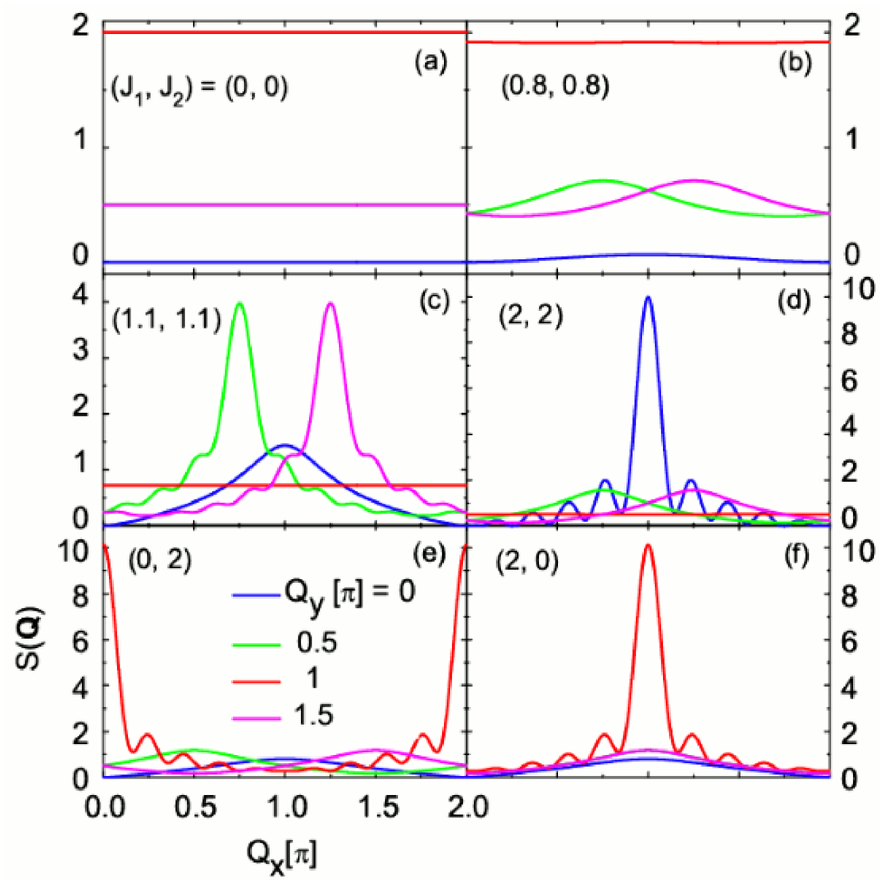


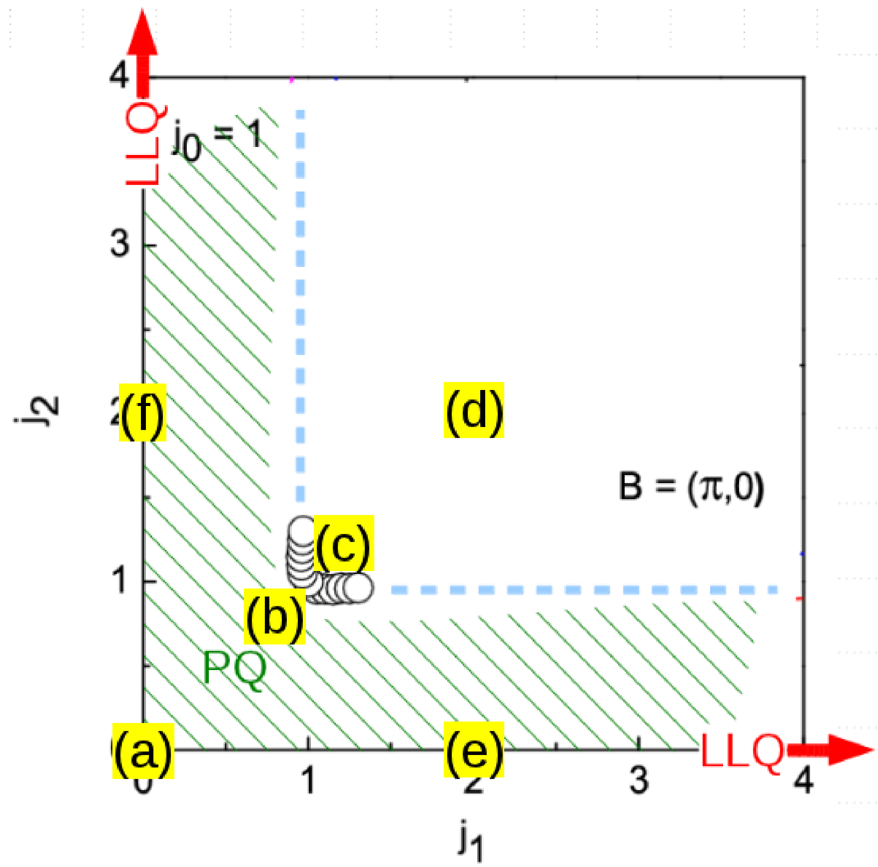


- commensurate cases DMRG and SBMFT agree ✔
- however: incommensurate region in DMRG beyond 1st order transition
- $C(x) \sim \exp(-x/l)$ with $l \to 0$ as $j_{1,2} \to 0$

Static Correlation Functions & Structure Factor

$$S(\mathbf{Q}) = \sum_{\mathbf{r}} \exp(i\mathbf{Q}\cdot\mathbf{r})$$





- $j_{1,2} \ll 1$: plaquette regime, $Q_y \to \pi$, $Q_x \to$ const
- $j_{1,2} >\sim 1$: incommensurate, $Q_y, Q_x \cong$ classical

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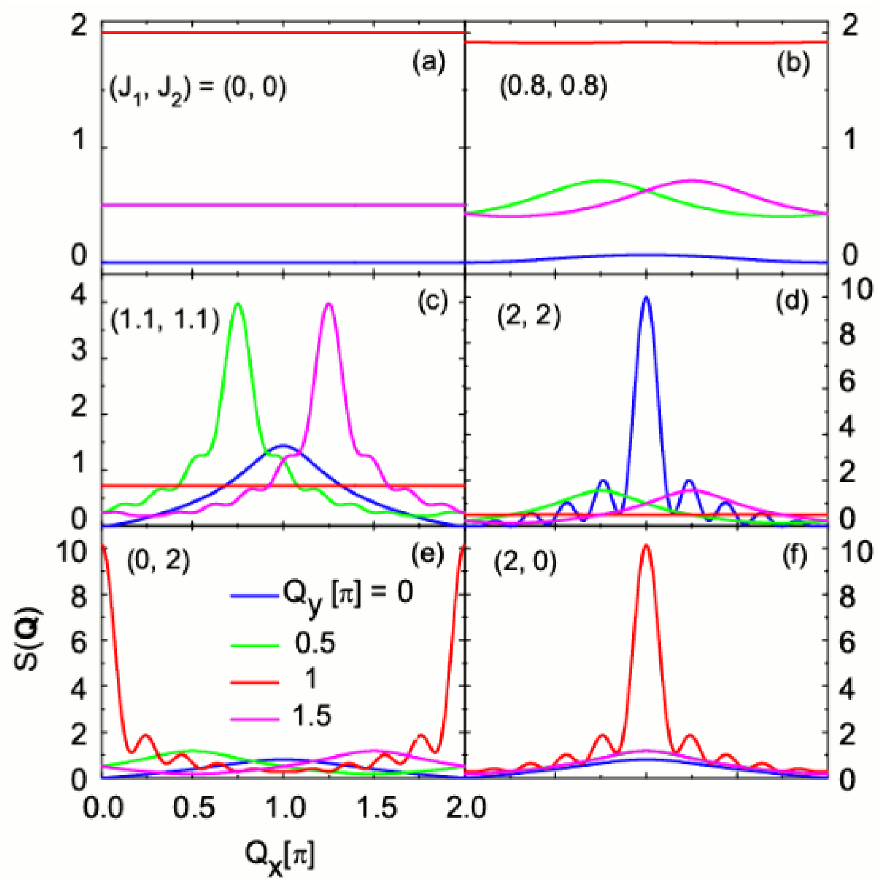

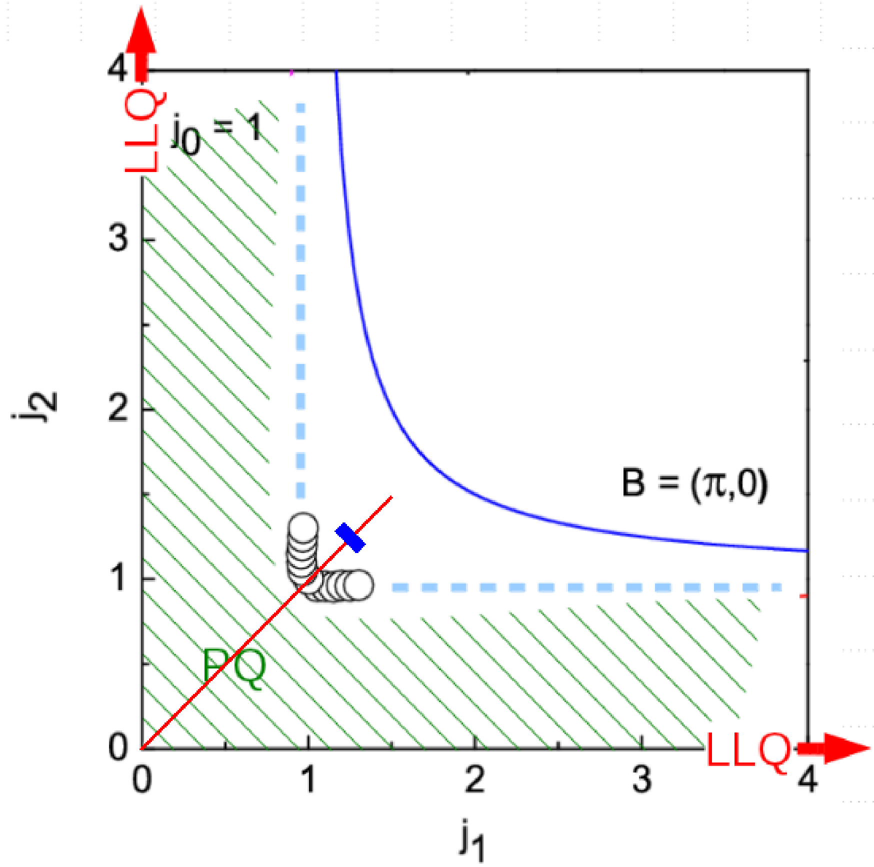

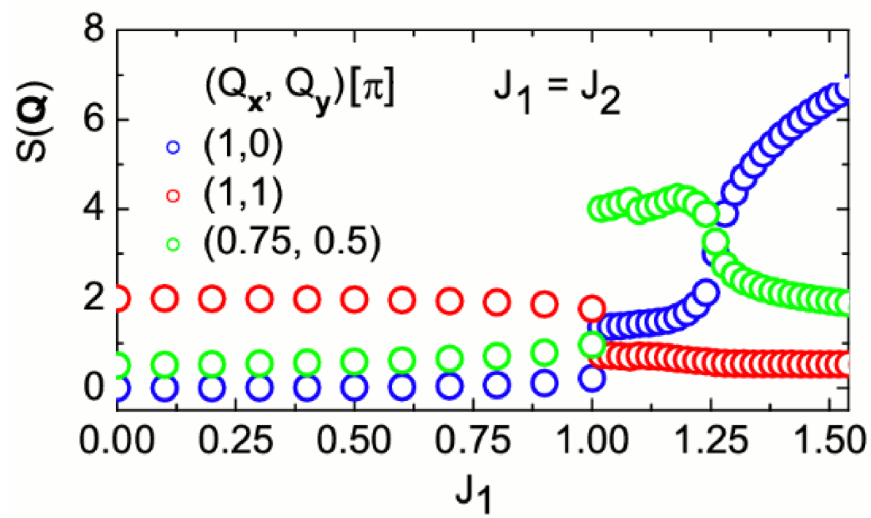

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- small IC region likely

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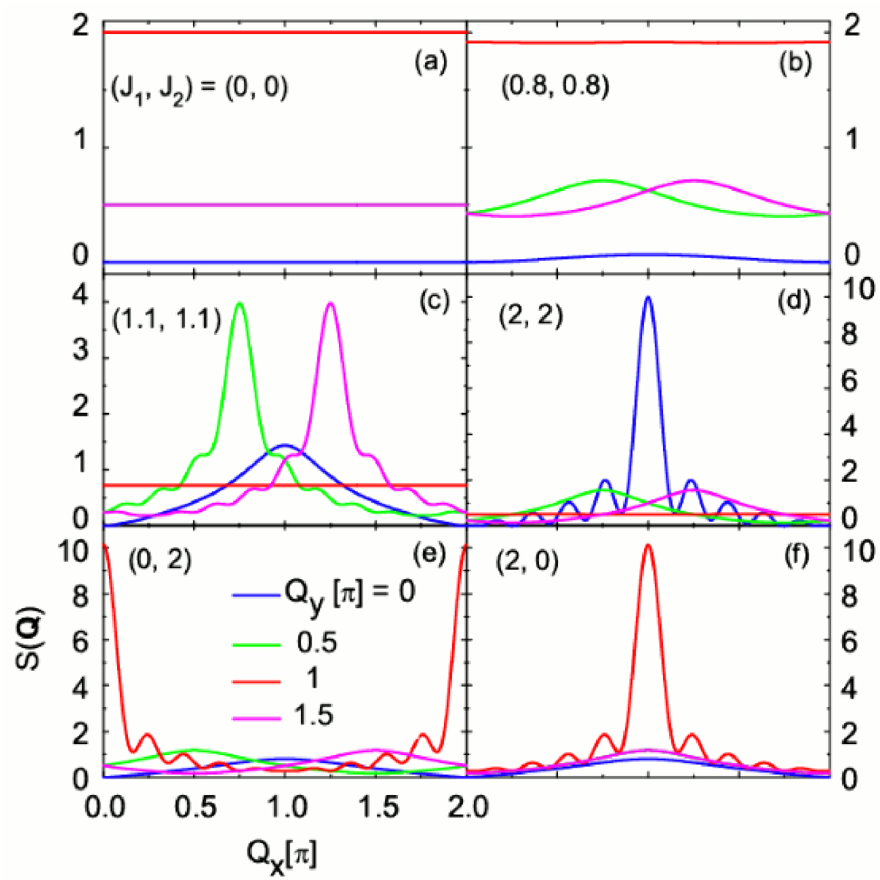

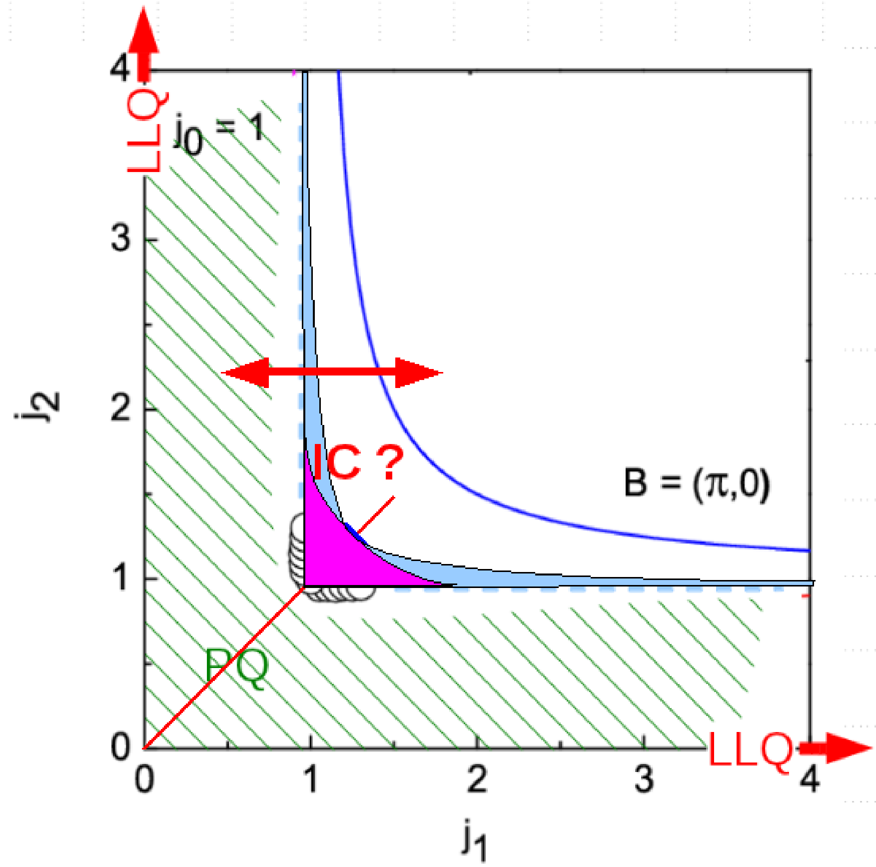

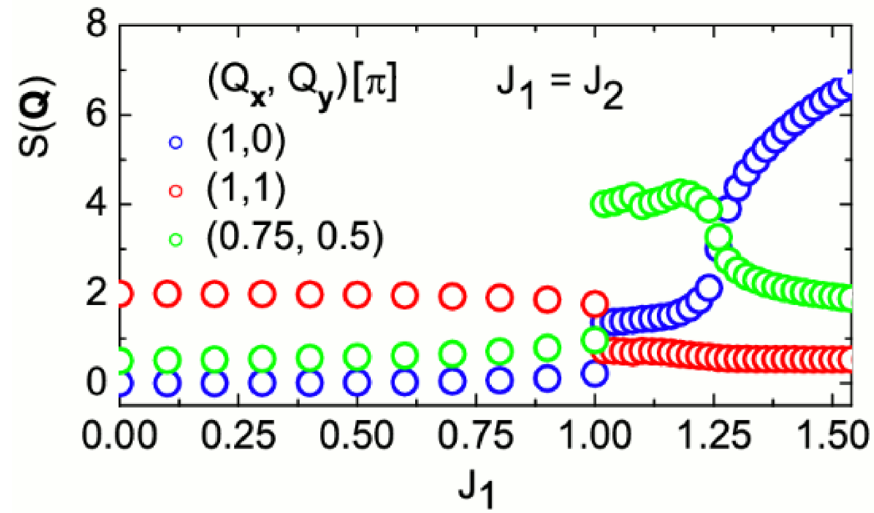

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1) Tube Materials & Model

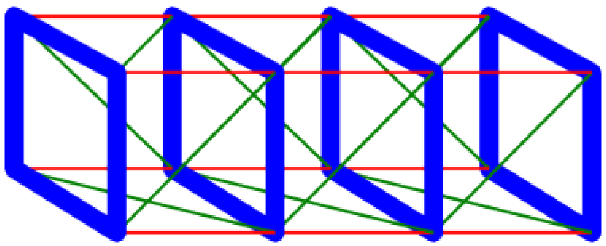
2) Phases and Static Correlations

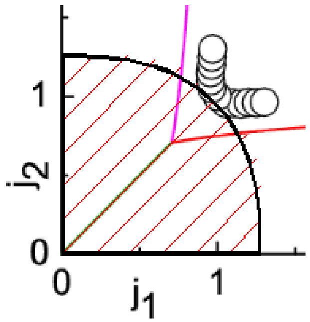
3) Plaquette Regime

4) Strong Leg Coupling

Spectrum in the Plaquette Regime: Series expansion analysis

- Plaquette basis





plaquette spectrum

E	S	q_l
1	2	3
0	0⊕1⊕1	2
-1	1	1
-2	0	0

quanta

equidistant

- Continuous unitary trafo $H_{eff} = e^{-\eta(l)} H e^{\eta(l)}$

Wegner, Ann. Phys. (94)
Knetter, et al., EPJB (00)

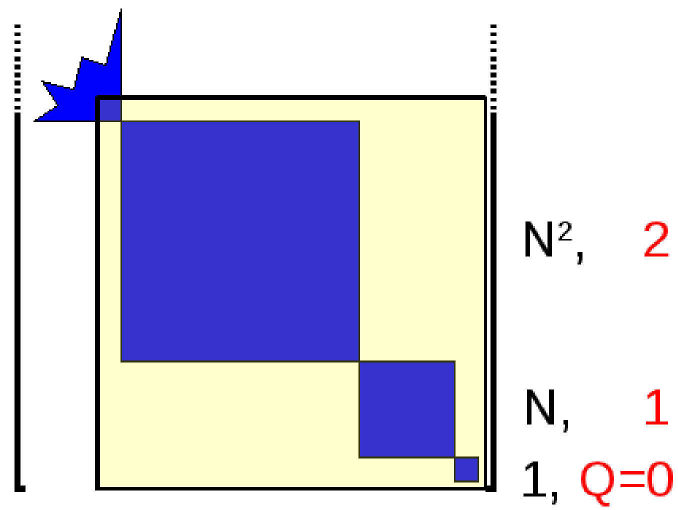
$$H = H_0 + \sum_{i=1}^{2} \sum_{n=-N}^{N} j_i T_{i,n}$$

$$\left[H_{eff}\big|_{l\to\infty}, \Sigma_l q_l \right] = 0$$

$$H_{eff} = H_0 + \sum_{ij} \boxed{j_1^i j_2^j} \left(\sum \prod \boxed{C}_{\dots} T_{\dots} \right)$$

from DEQN

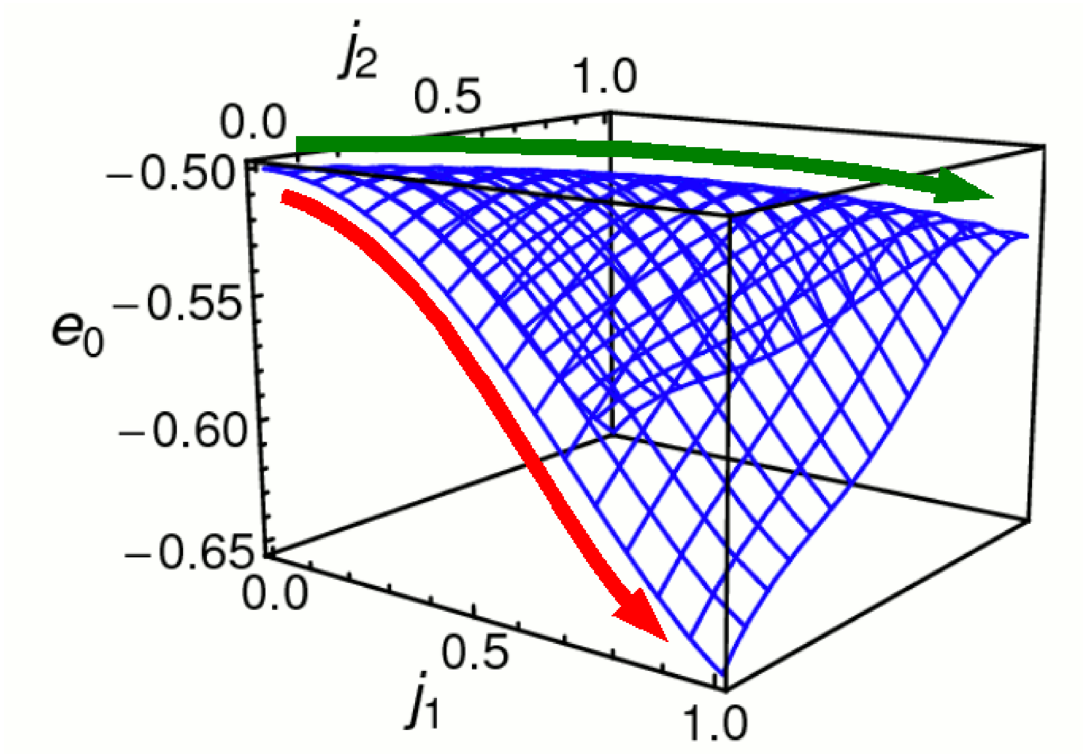
$H_{eff} =$



Arlego, WB PRB (11); Reuther, WB, et al. PRB (10); Arlego, WB, PRB (08); Arlego, WB, PRB (07); Arlego, WB, EPJB (06); WB, Grzeschik, MMM (04); WB, Grzeschik, PRB (04); WB PRB (03); WB, Honecker, PRB (02)

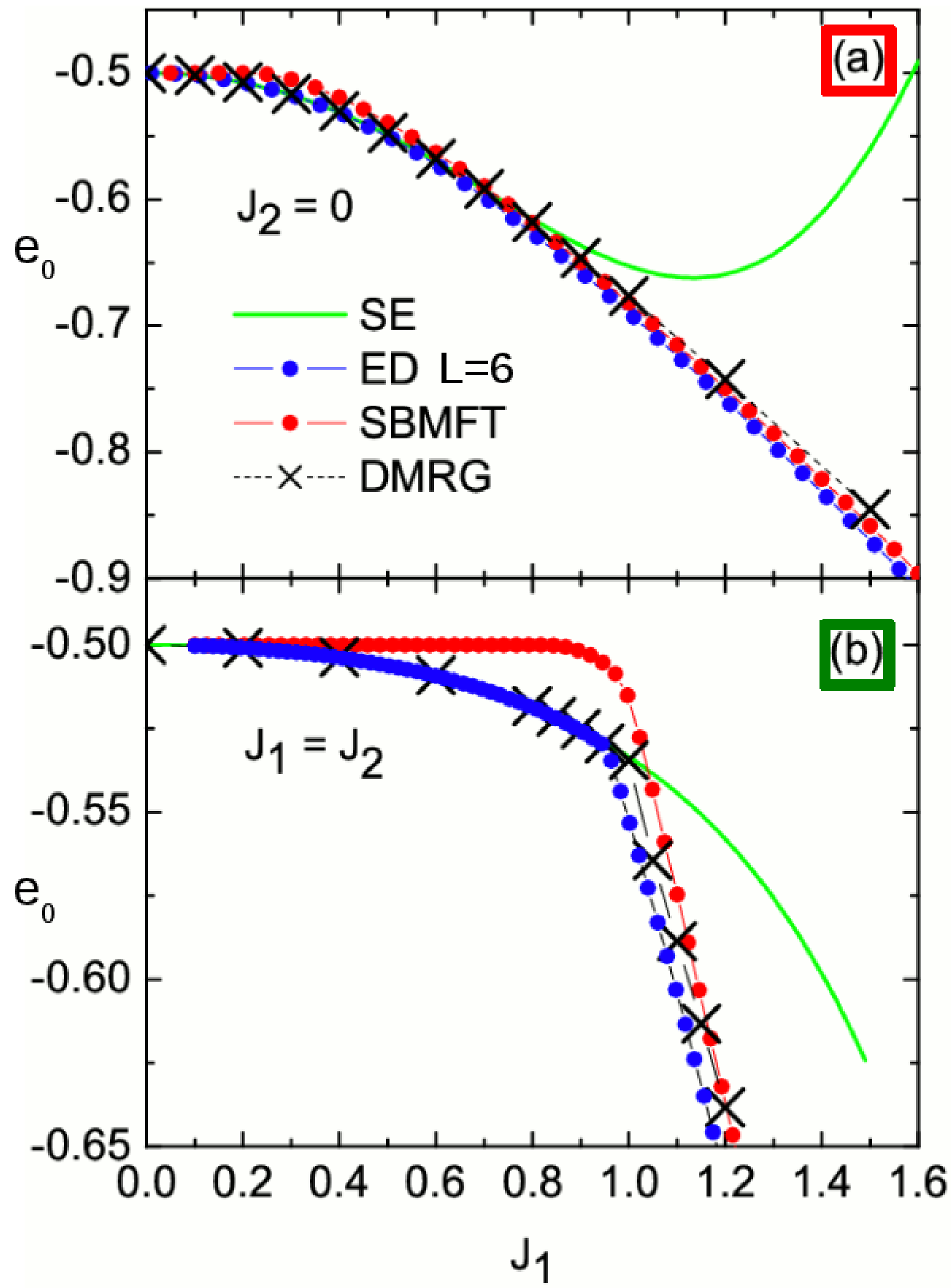
Ground State Energy

- $e_0 = \langle Q=0 | H_{eff} | Q=0 \rangle_0 / L$ up to O(7) in $j_{1,2}$



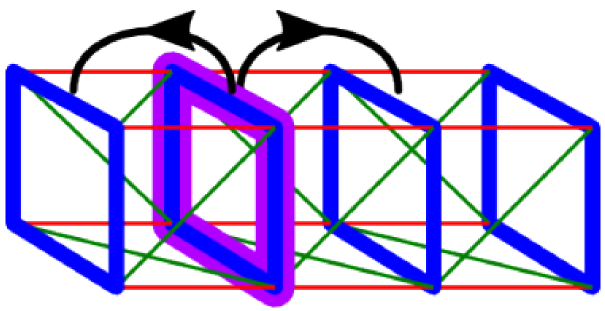
- frustration ↑ energy gain ↓
- up to 1st order QPT agrees with DMRG ✔
- convergence radius ~ 1

- contrast ...



Elementary One-Particle Excitations

t_{eff} to O(7) in j_1, j_2



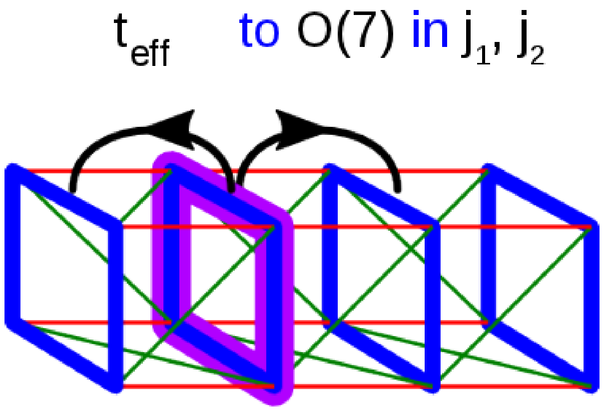
- From Q=1 sector

$$H_{eff}|Q=1,r=0\rangle_0=\sum_l t_l|Q=1,r=l\rangle_0 \quad \text{to } O(7)$$

- From Q=2 sector?

$$\langle Q=2,2pt|H_{eff}|Q=2,1pt\rangle_0 = 0 \quad \text{to } O(7)$$

Elementary One-Particle Excitations



- From Q=1 sector

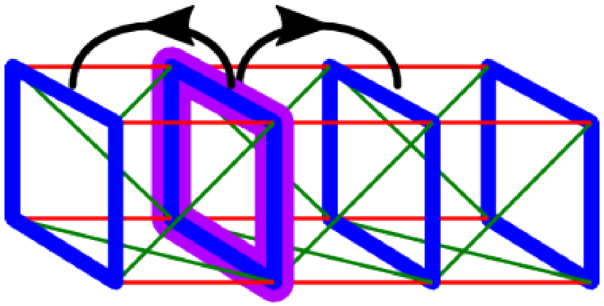
$$H_{eff}|Q=1, r=0\rangle_0 = \sum_l t_l |Q=1, r=l\rangle_0 \quad \text{to } O(7)$$

- From Q=2 sector?

$$H_{eff}|Q=2, 1pt, r=0\rangle_0 = \sum_l t_l |Q=2, 1pt, r=l\rangle_0 \quad \text{to } O(7)$$

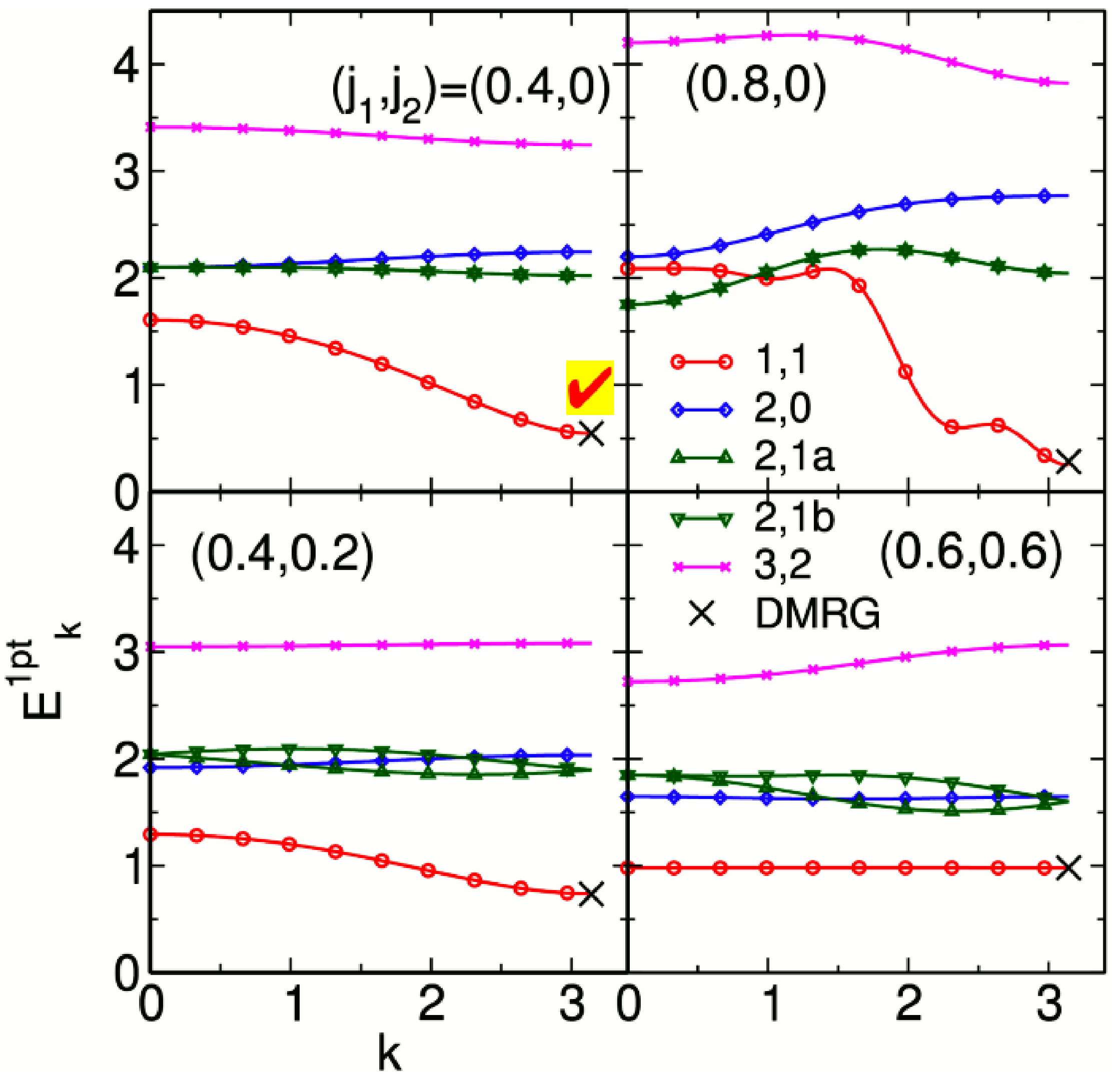
Elementary One-Particle Excitations

t_{eff} to O(7) in j_1, j_2



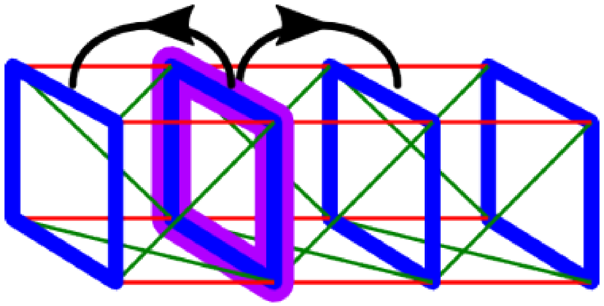
Q	
Q=1	1 triplon
2	2 triplons + 1 singlon
3	1 quinton (?)

un-protected



Elementary One-Particle Excitations

t_{eff} to O(7) in j_1, j_2



Q=1	1 triplon	
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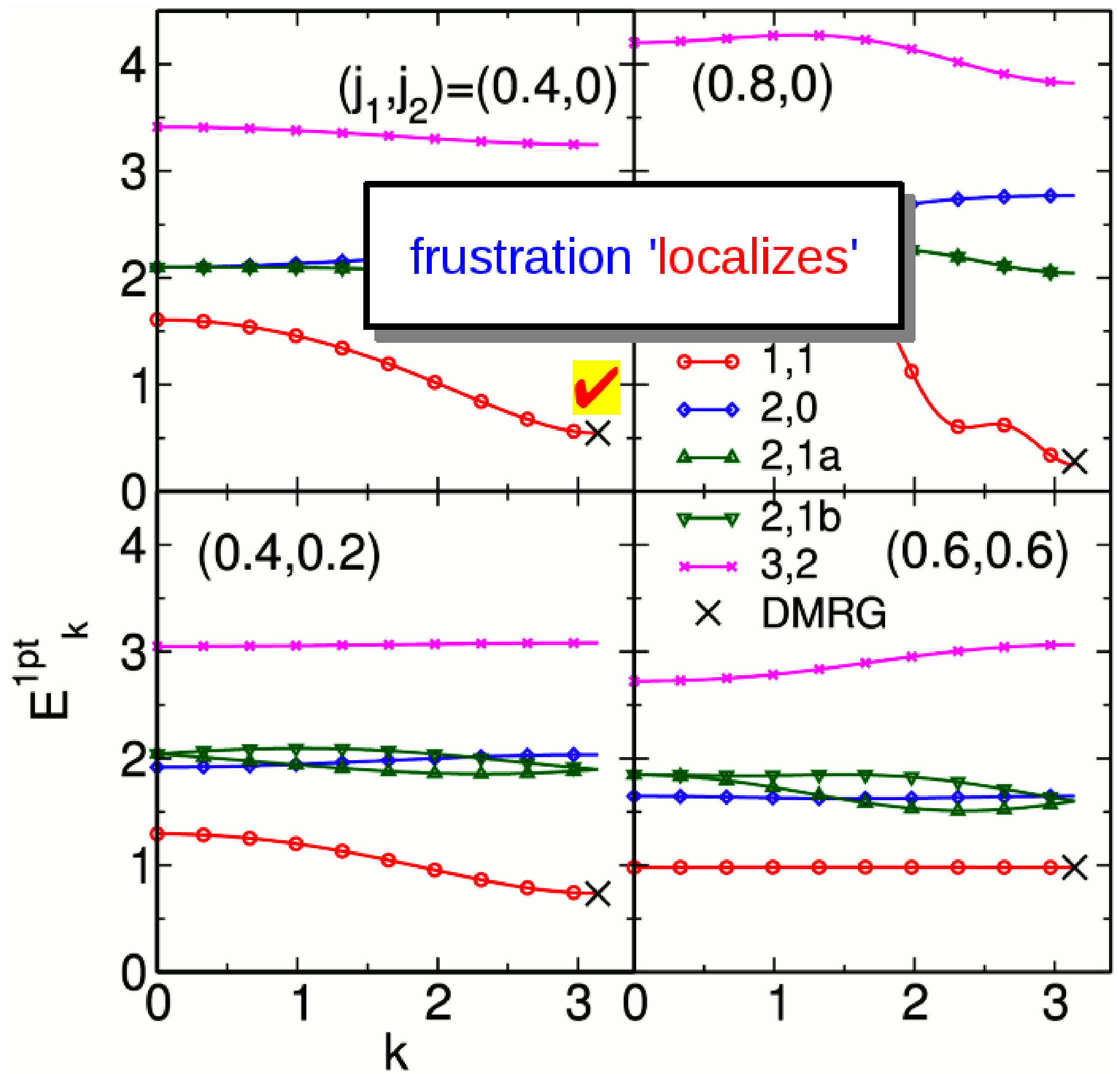


- $j_1 \leftrightarrow j_2$ from symmetries eg.:

$$E^{1pt}_{1,1}(k, j_1, j_2) = E^{1pt}_{1,1}(k+\pi, j_2, j_1), \ldots$$

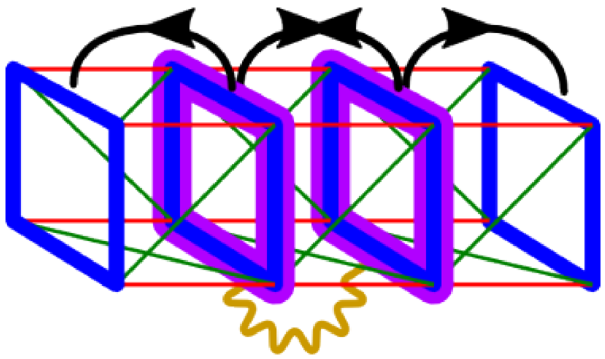
- Gap @ j_2=0

$$E^{1pt}_{1,1}(\pi, j_1, 0) = 1 - \frac{4}{3}j_1 + \frac{41}{108}j_1^2 + \frac{349}{1296}j_1^3 + \frac{4596401}{39191040}j_1^4 - \frac{169497997}{4702924800}j_1^5 - \frac{689874137639377}{2986545364992000}j_1^6 - \frac{843016534549843272 1}{451565659186790400 00}j_1^7$$

Cabra, et al. PRB 58, 6241 (98)

Two-Particle Excitations

t_{eff} to O(7) in j_1, j_2



V_{eff} to O(6)

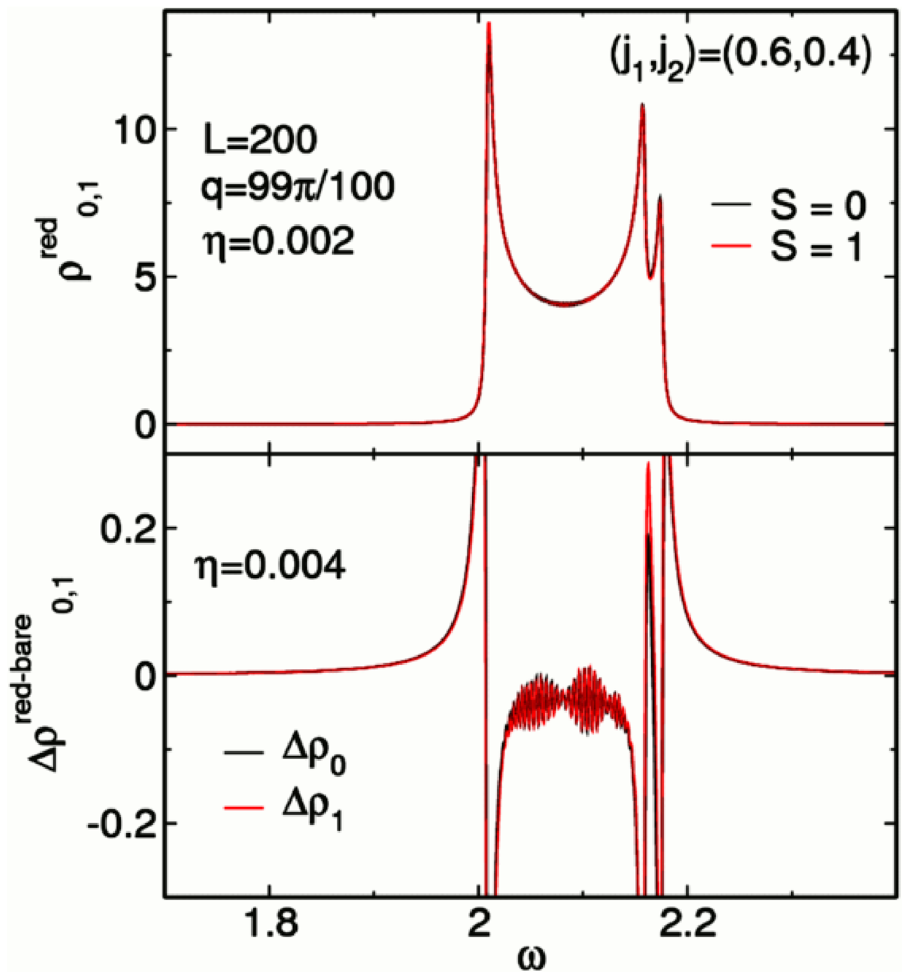
$$|q,d\rangle^{Sm} = \frac{1}{\sqrt{L}} \sum_r e^{iq(r+d/2)} |Q=2, r, r+d\rangle^{Sm}$$

- ${}^{Sm}\langle q,d|H_1 + H_2|q,d\rangle^{Sm}$ on finite L

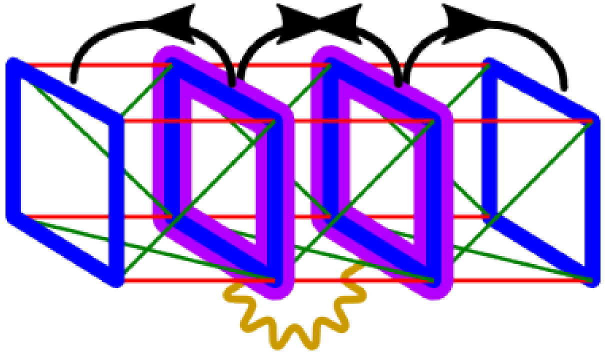
one- kinetic erg. hard-core (H_1)

two-particle irreducible 'real' interactions (H_2)

- one-particle irreducible



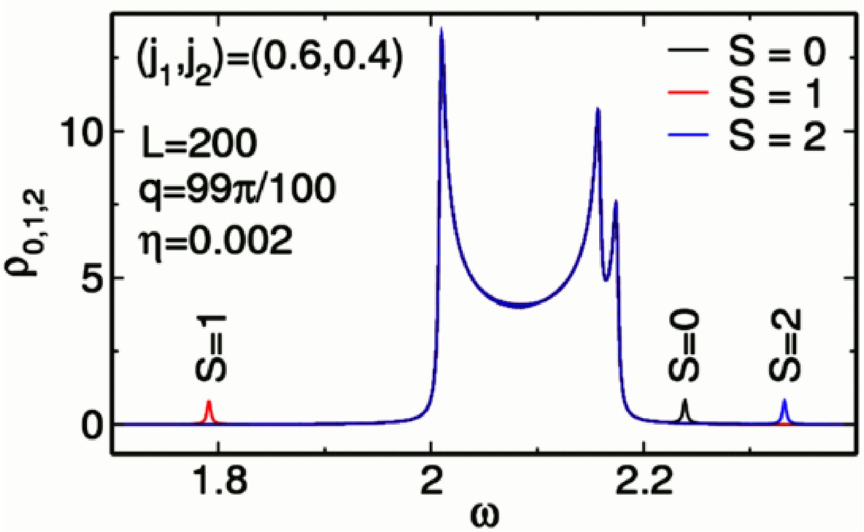
Two-Particle Excitations

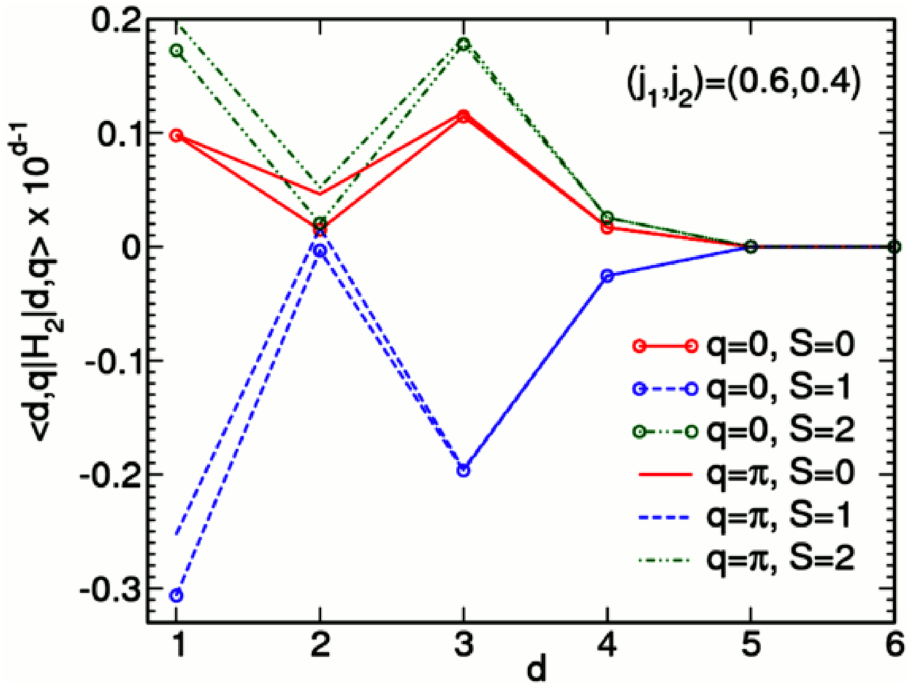


- Scattering continua +
  bound triplet +
  anti-bound singlet + quintet

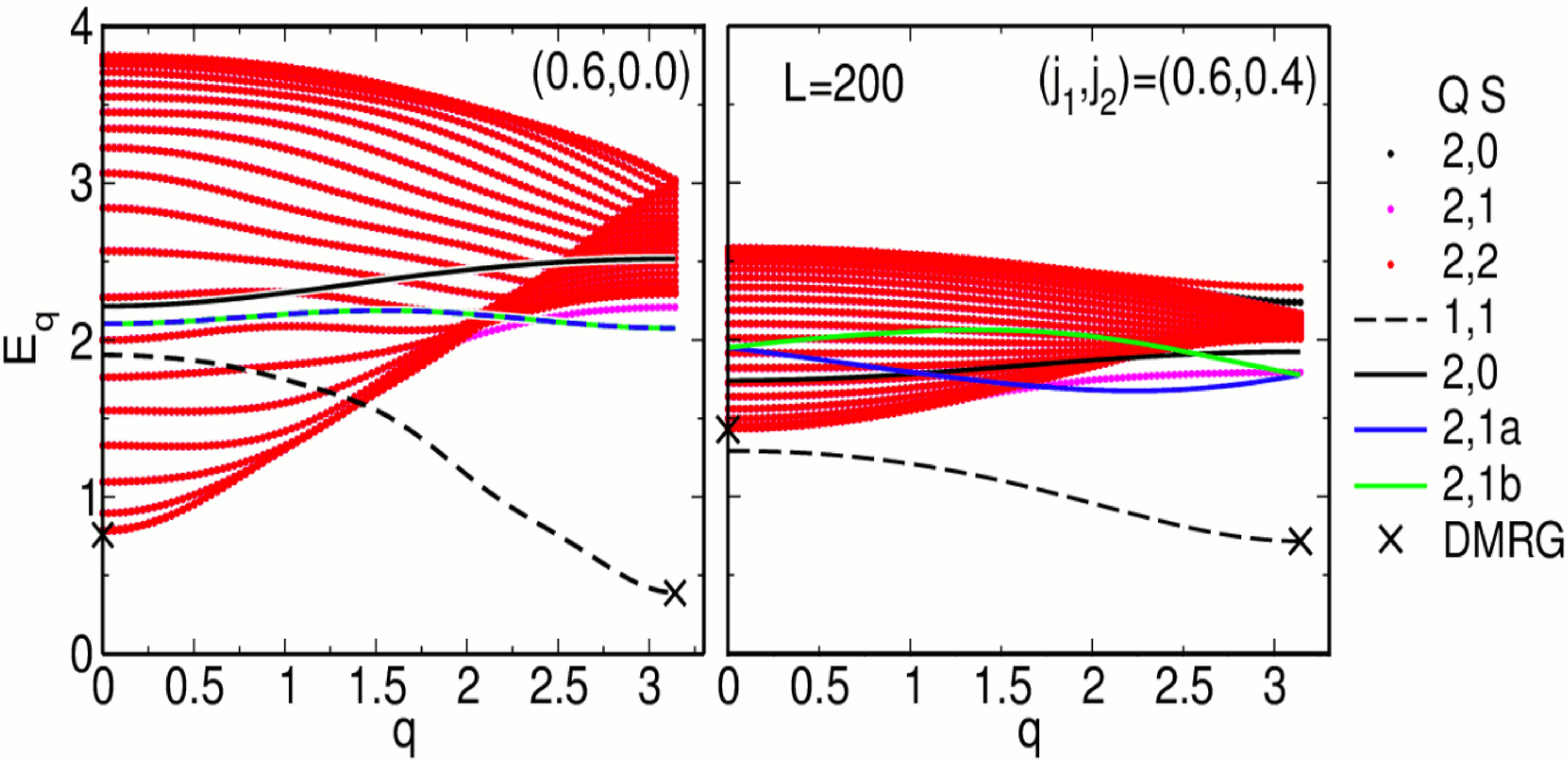
- two-particle potential as f(d)
  rapidly decaying

- one- and two-particle irreducible



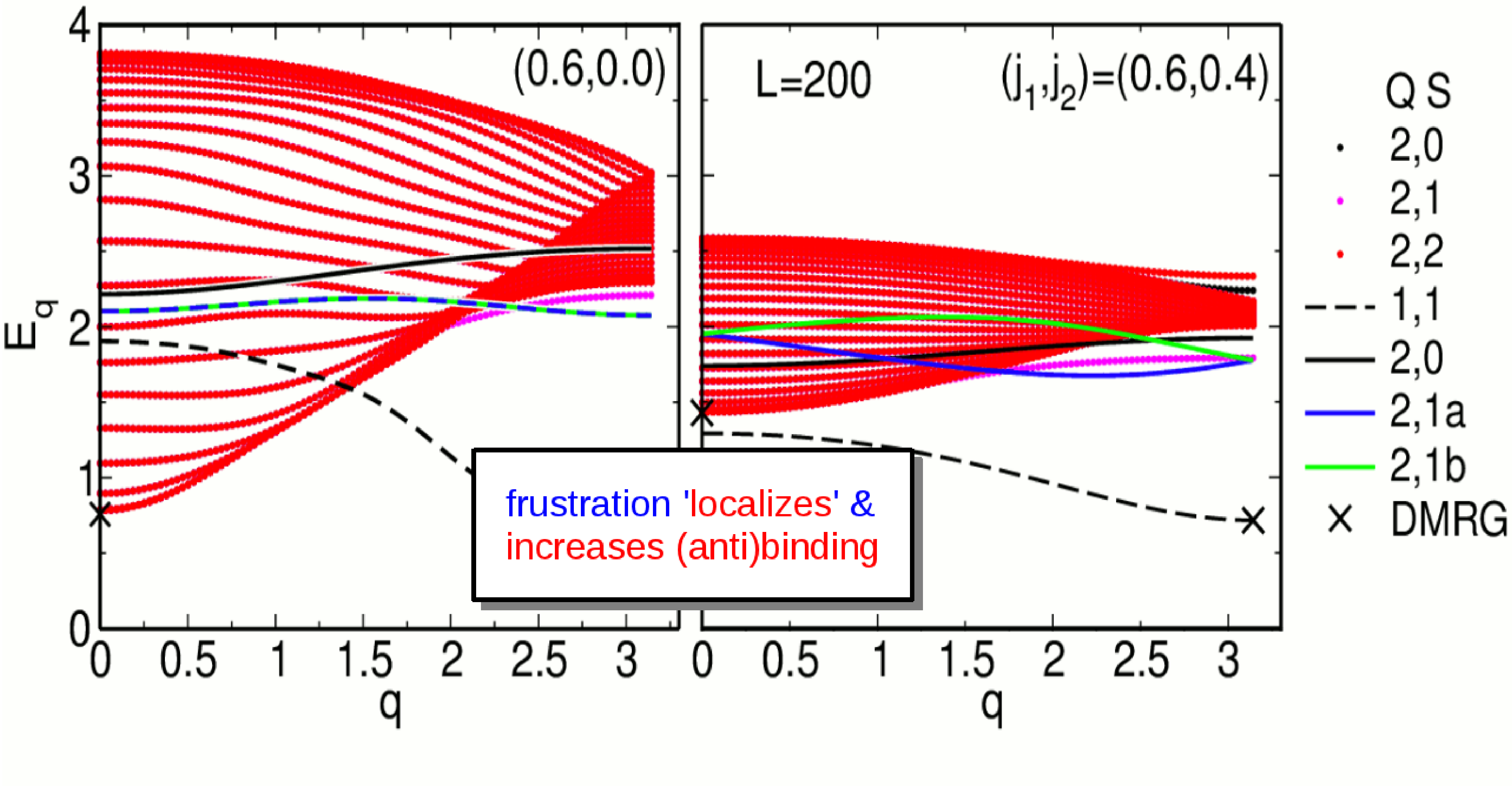


One- & Two-Particle Dispersion



- several one-particle sates within the two-particle continuum
- three collective (anti)bound states
- excellent agreement with DMRG

One- & Two-Particle Dispersion



- several one-particle sates within the two-particle continuum
- three collective (anti)bound states
- excellent agreement with DMRG

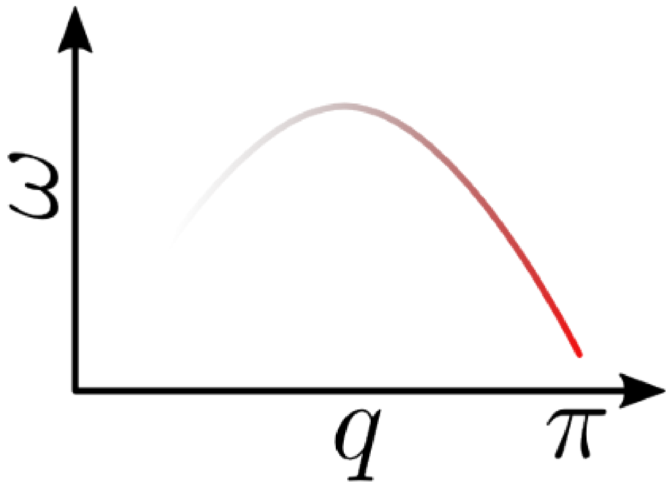
1) Tube Materials & Model

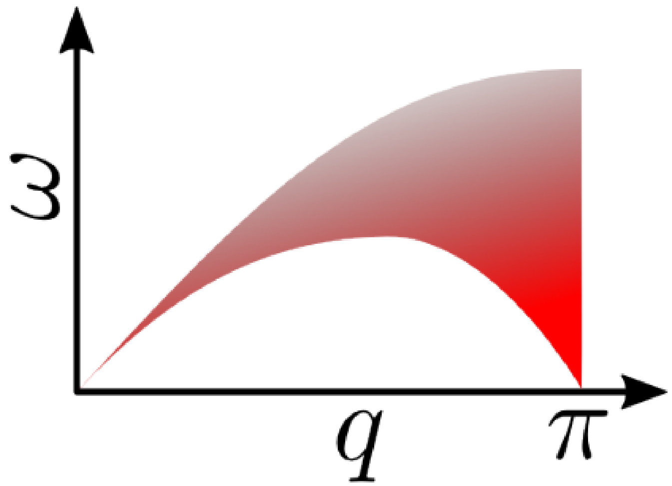
2) Phases and Static Correlations

3) Plaquette Regime

4) Strong Leg Coupling

Spinon-Magnon Crossover





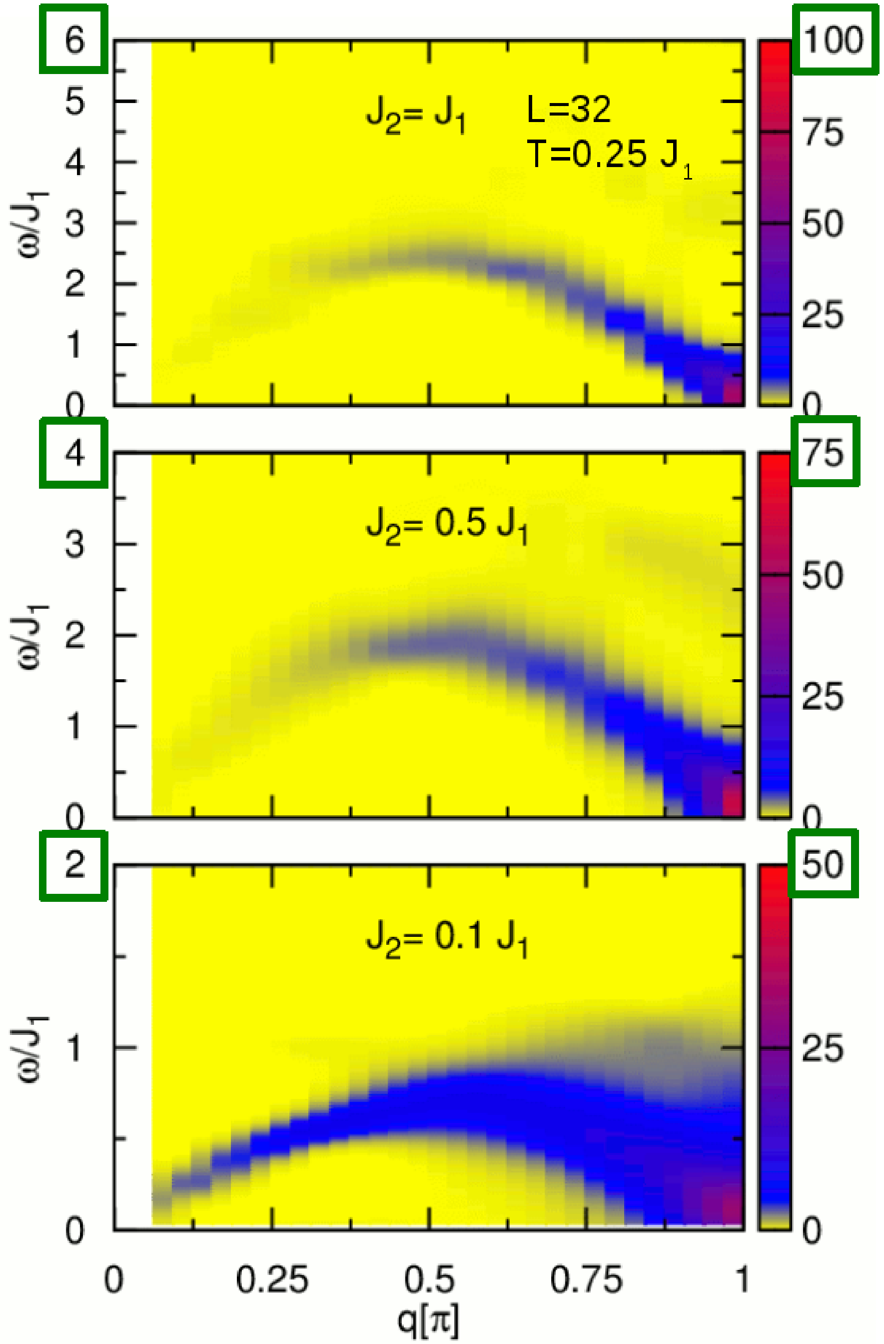
$J_0=0$

$J_2/J_1=1$, $(\pi,0)$ S~2-chain: magnons

$J_2/J_1=0$, 4 S-1/2-chain: spinons

Spinon-Magnon Crossover

- Dynamic structure factor vs J_2/J_1

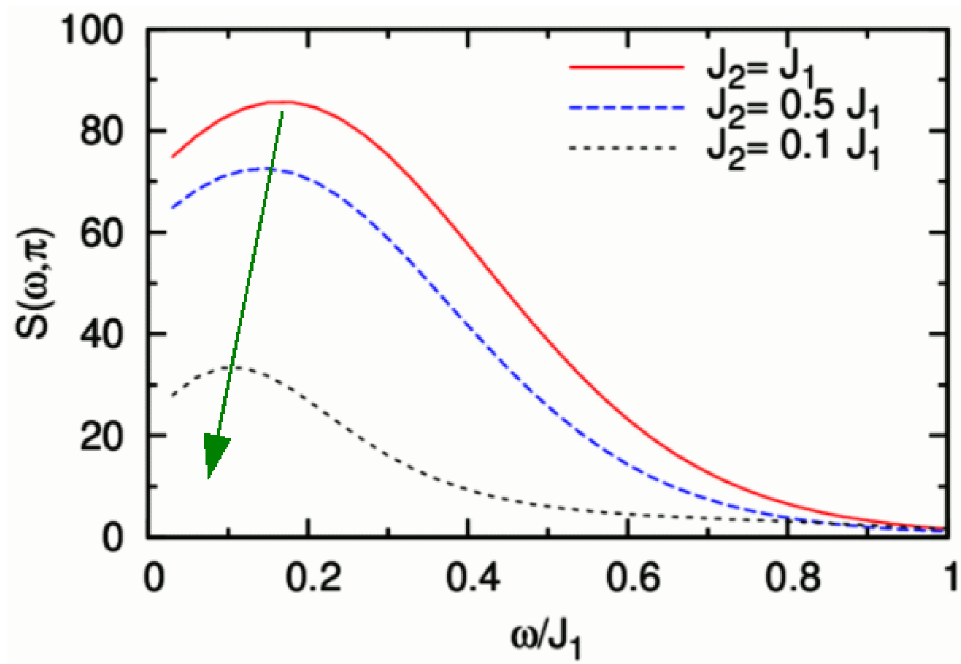


$J_0=0$

$J_2/J_1=1$, $(\pi,0)$ S~2-chain: magnons

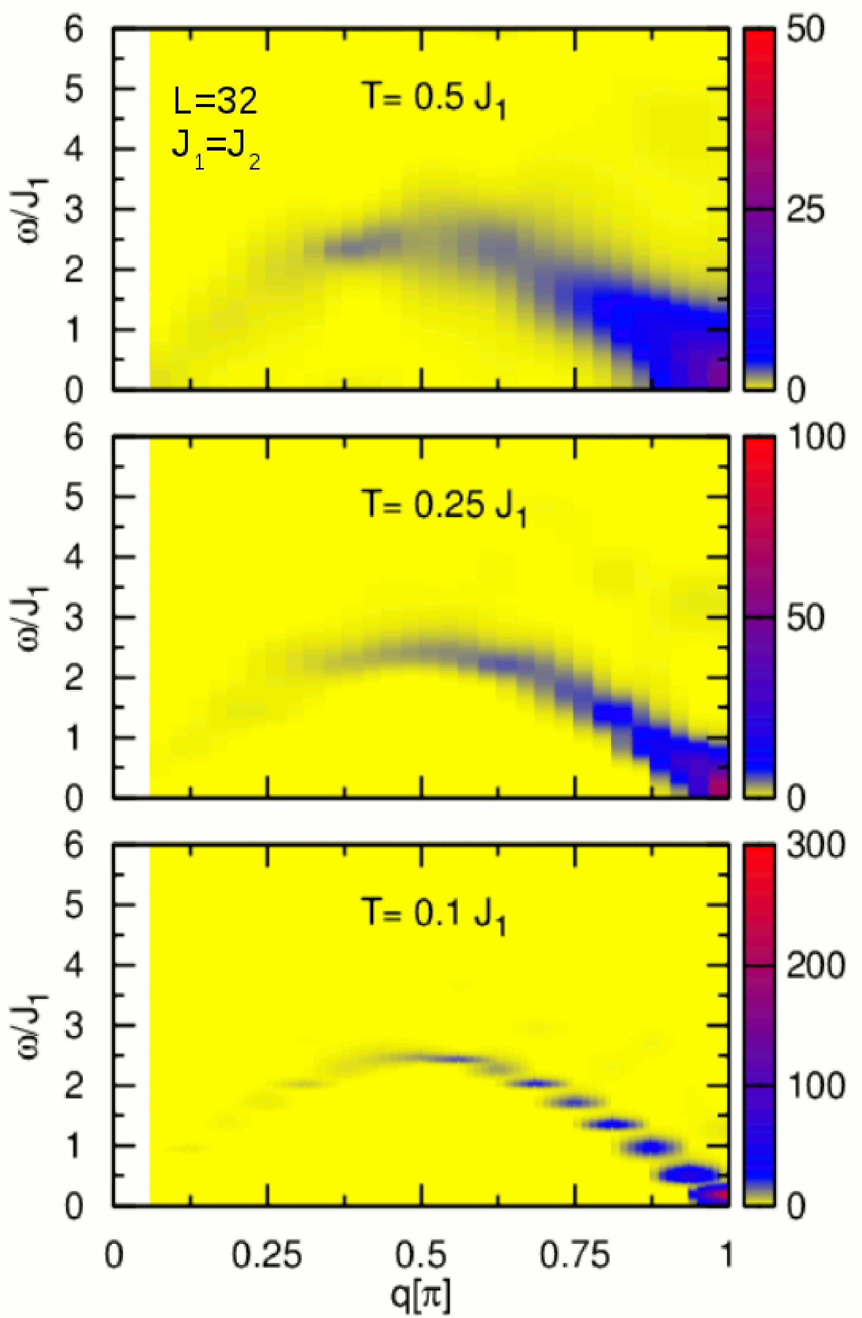
$J_2/J_1=0$, 4 S-1/2-chain: spinons

- Peak shift ~ gap closure

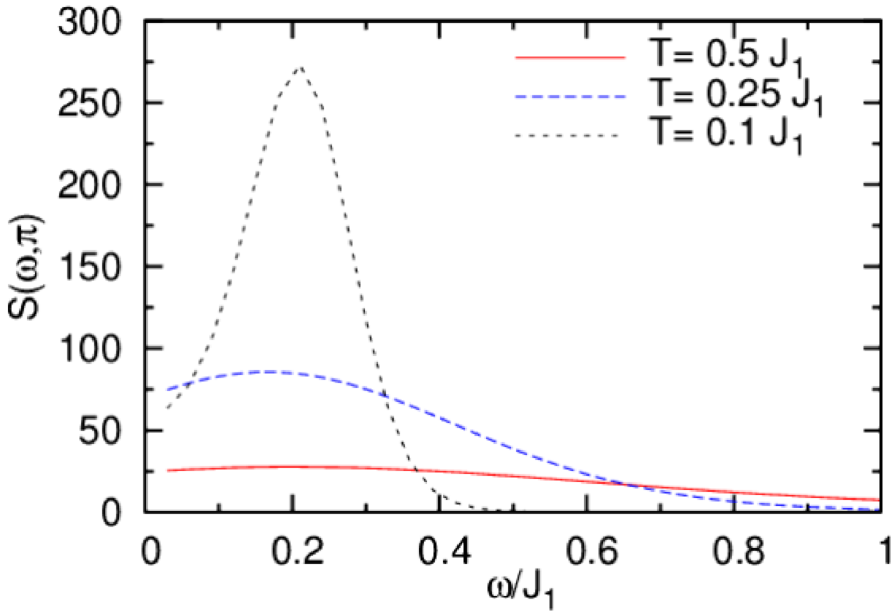


Lineshape vs Temperature

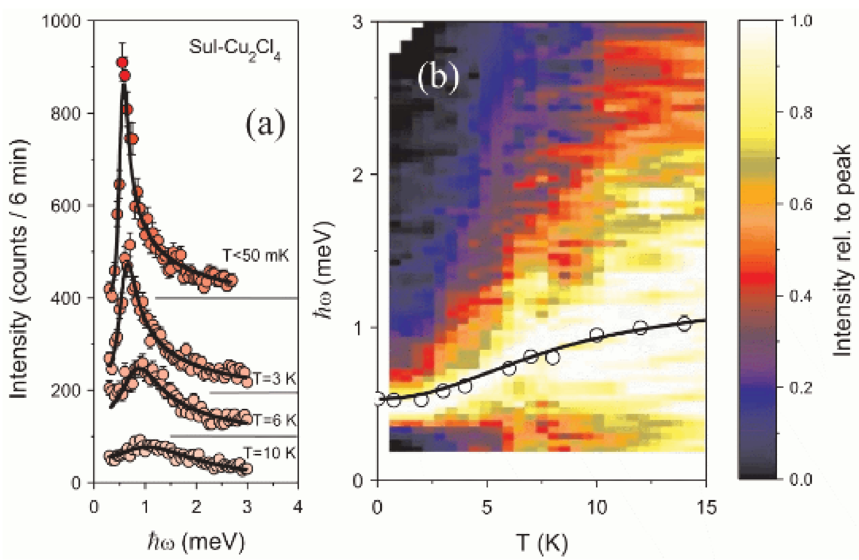
- Dynamic structure



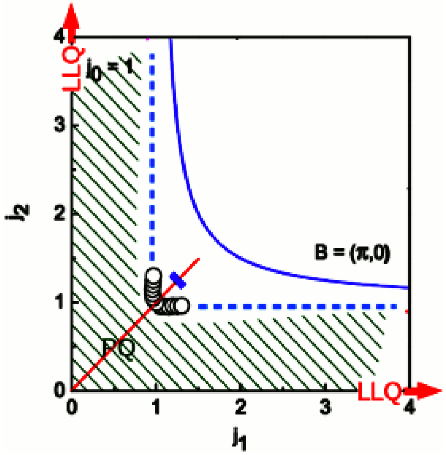
- Cut at q=π



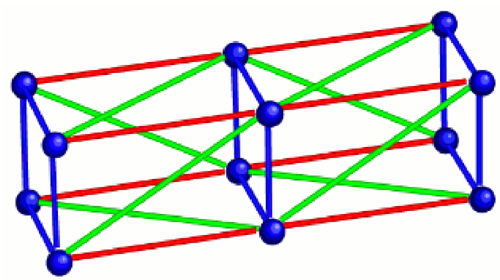
- … tempting



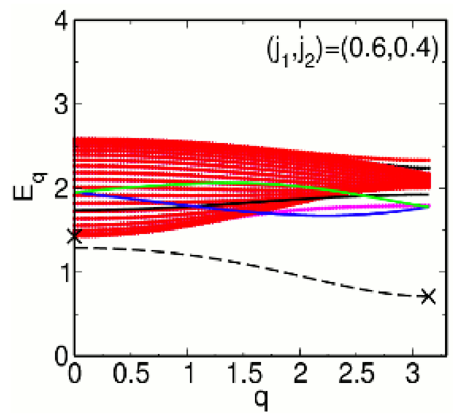
Conclusions



- Plaquette, incommensurate, Luttinger, and Haldane phases



- Novel elementary excitations and bound states



- Spinon-magnon crossover