DQMP Department of Quantum Matter Physics

Quantum phase transitions in quantum spin systems

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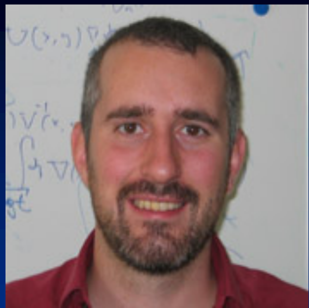
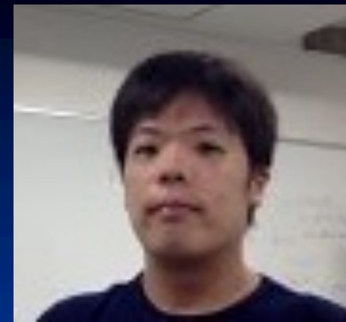


P. Bouillot

C. Kollath



S. Furuya

S. Takayoshi

E. Coira

N. Kestin

C. Berthier

C. Ruegg

A. Zheludev

V. Simonet

B. Grenier

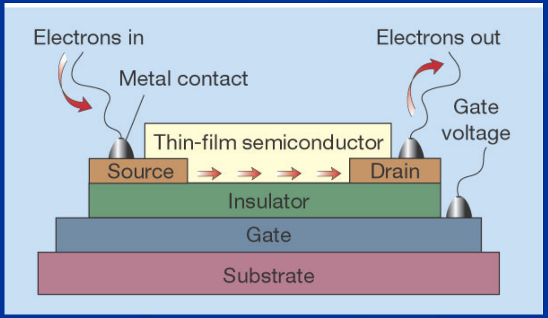
Why magnetic insulators

- Interesting problem in itself (spin liquid,…)
- Many materials; dimensions, interactions,….
- Microscopic interactions short range and thus well controled

Hard core bosons on a lattice

$$H = -\frac{J_{xy}}{2}\sum_{ij}[b_i^\dagger b_j + \mathrm{hc}] + J_z \sum_{ij}(n_z - \frac{1}{2})(n_j - \frac{1}{2})$$

- Magnetic field : chemical potential (gate voltage) for the bosons



Nature **428**, 269 (2004)

- In 3D !

- Go from 0 bosons/site to 1 boson/site

Probes

- Magnetization – number of bosons

$$m_z = \langle S_z \rangle$$

- Neutrons/NMR : dynamical correlations

$$\langle S_z(r,t) S_z(0,0) \rangle_{q,\omega} \to \langle \rho_z(r,t) \rho_z(0,0) \rangle$$

$$\langle S^-(r,t) S^+(0,0) \rangle_{q,\omega} \to \langle \psi(r,t) \psi^\dagger(0,0) \rangle$$

Quantum spin chains and ladders in the 21st century

- Small exchange constants J ~ 10 K
- Possibility to manipulate with magnetic field
- T, E, etc. ~J : field theory alone is not enough
- Need to develop essentially exact solutions

TG, C. Rend. Acad. Sci 17 322 (2017)

How to solve

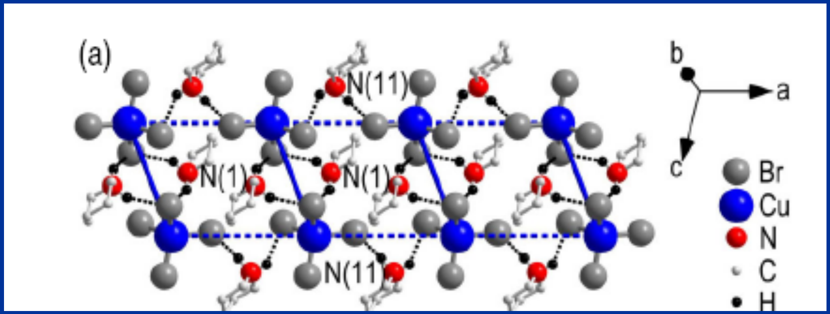
- Field theory:
  - Asymptotically true: (r >> a; t >> t0; T << J)
  - Amplitudes and TLL parameters unknown
- Numerics:
  - Efficient at short time, short distance
  - Takes into account the full microscopic model
- Best of both worlds: combine numerics (DMRG) or BA and field theory : essentially exact !

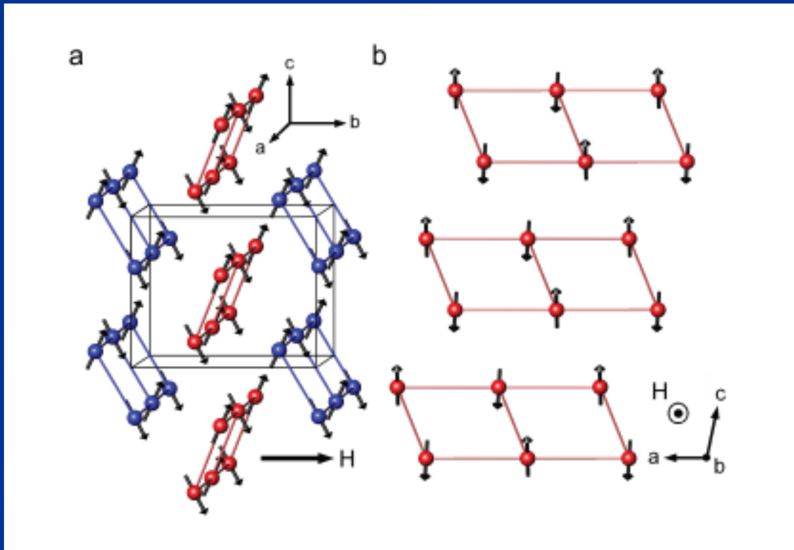
Some examples

Spin chains and ladder systems

BEC of dimers: TG, AM Tsvelik PRB 59 11398 (99)
TG, Ch. Rüegg, O. Tchernyshyov, Nat. Phys. 4 198 (08)

TLL Physics: M. Klanjsek et al., PRL 101 137207 (2008)

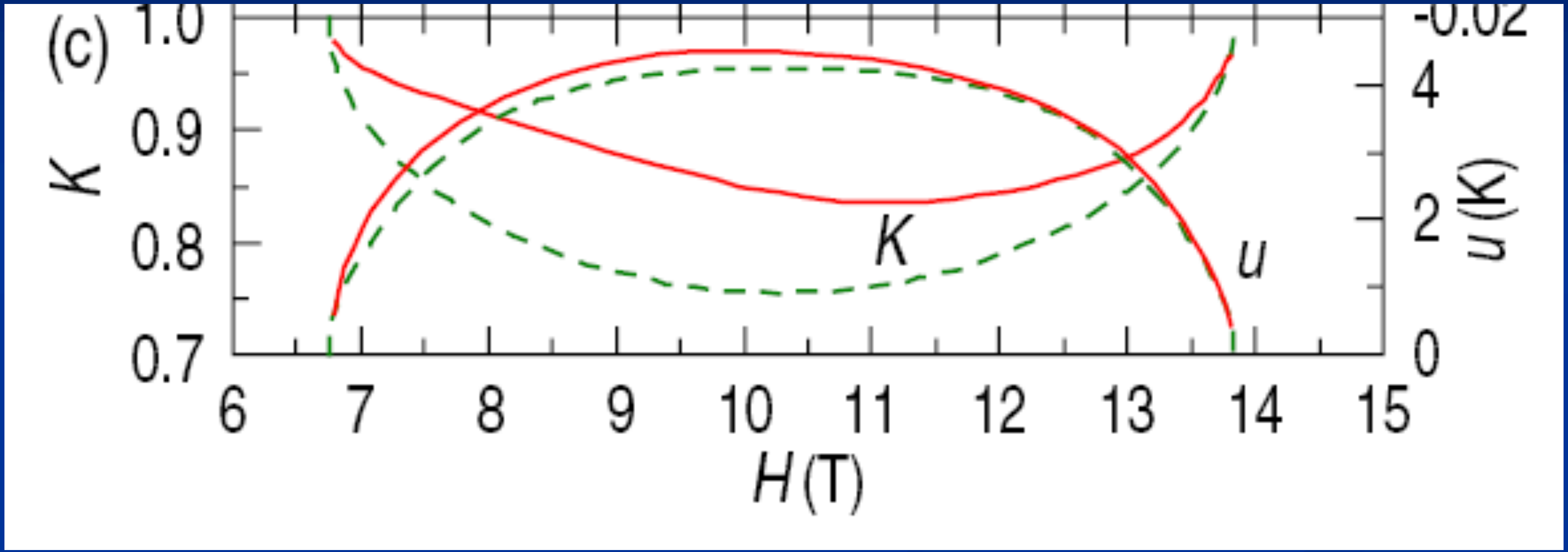




B. Thielemann et al.,

PRB **79**, 020408® 2009

Luttinger parameters



M. Klanjsek et al., PRL 101 137207 (2008)

Red : Ladder (DMRG)

Green: Strong coupling ($J_r \to \infty$) (BA)

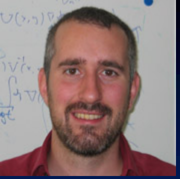
Correlation functions

M. Klanjsek et al., PRL 101 137207 (2008)

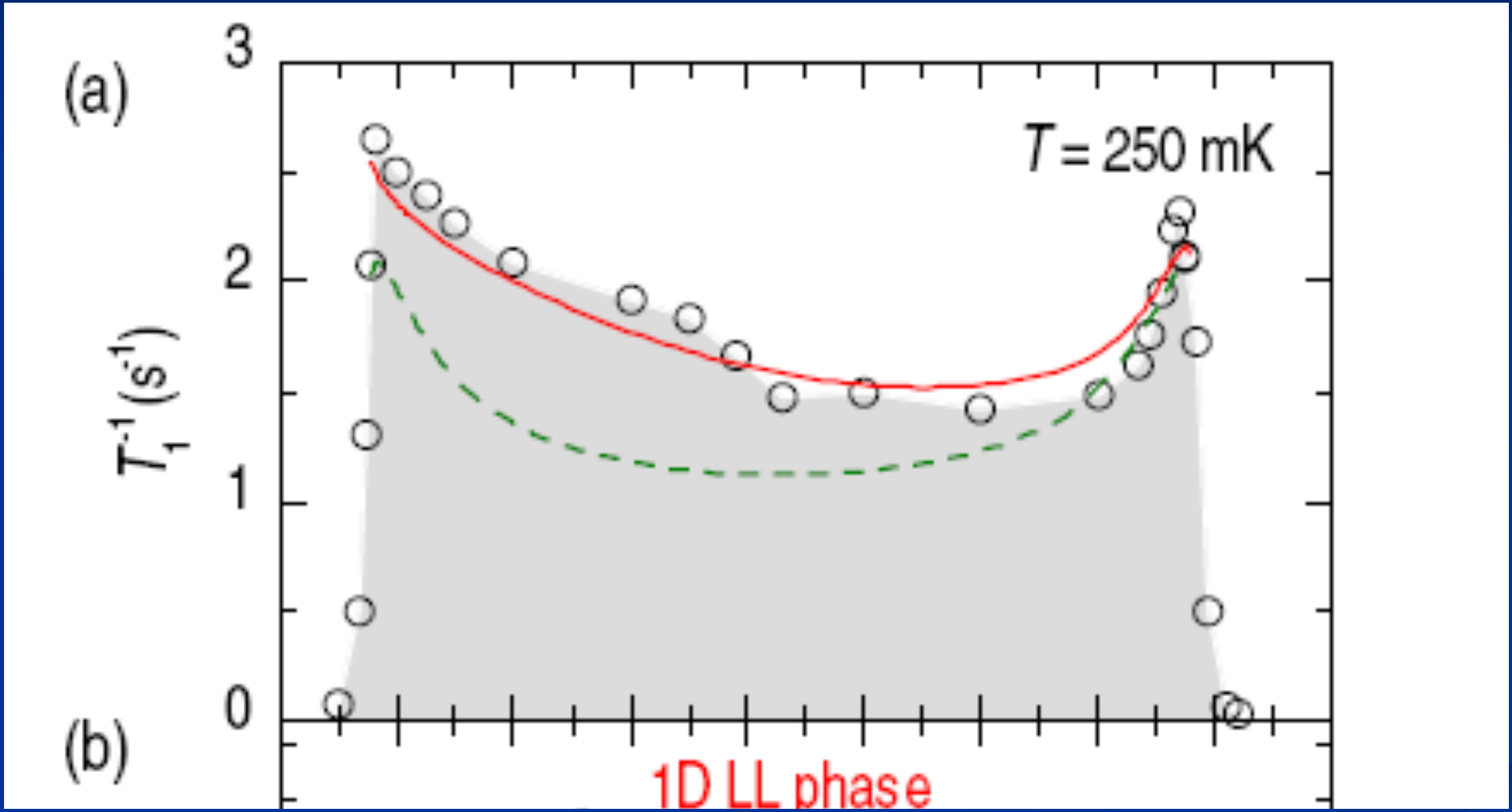
R. Chitra, TG PRB 55 5816 (97); TG, AM Tsvelik PRB 59 11398 (99)

- NMR relaxation rate:

$$T_1^{-1} = \frac{\hbar\gamma^2 A_\perp^2 A_0^x}{k_B u} \cos\left(\frac{\pi}{4K}\right) B\left(\frac{1}{4K}, 1 - \frac{1}{2K}\right)\left(\frac{2\pi T}{u}\right)^{(1/2K)-1},$$




Quantitative test of TLL

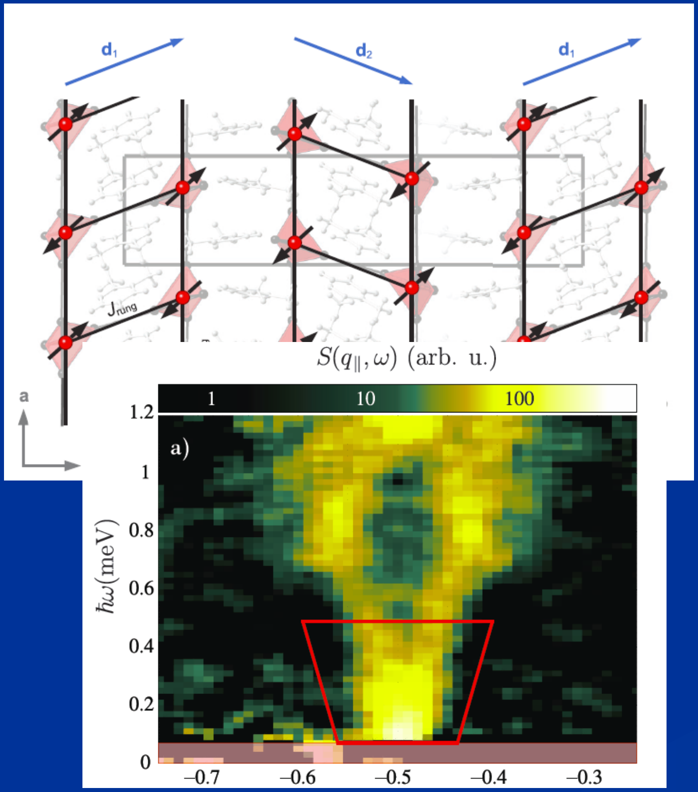
M. Klanjsek et al., PRL 101 137207 (2008)

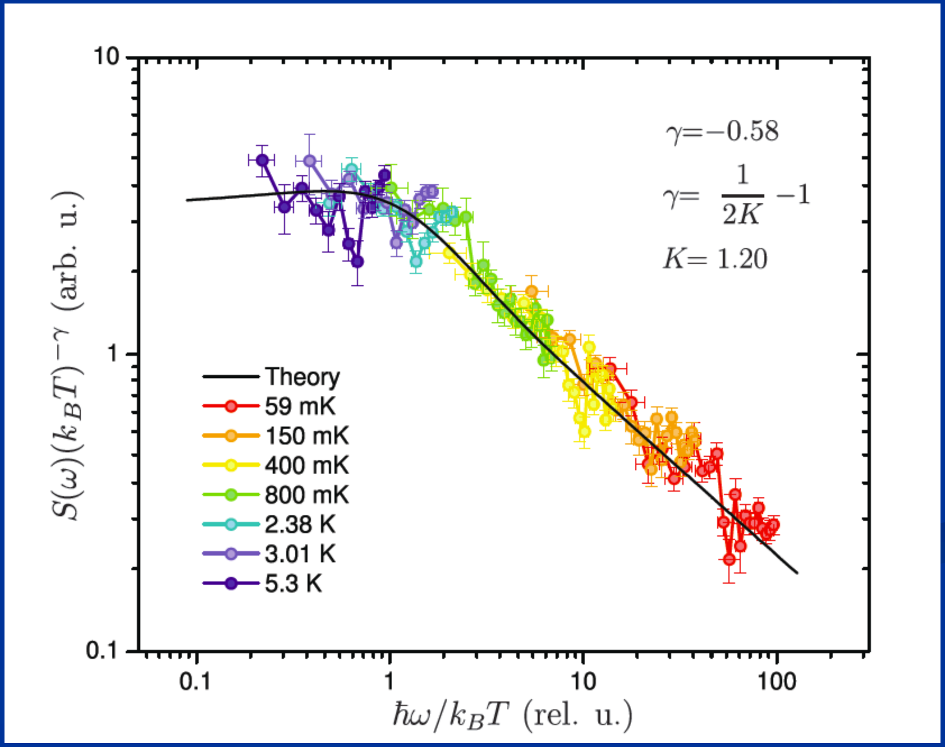
TLL scaling

D. Schmidiger et al. PRL 108 167201 (12):

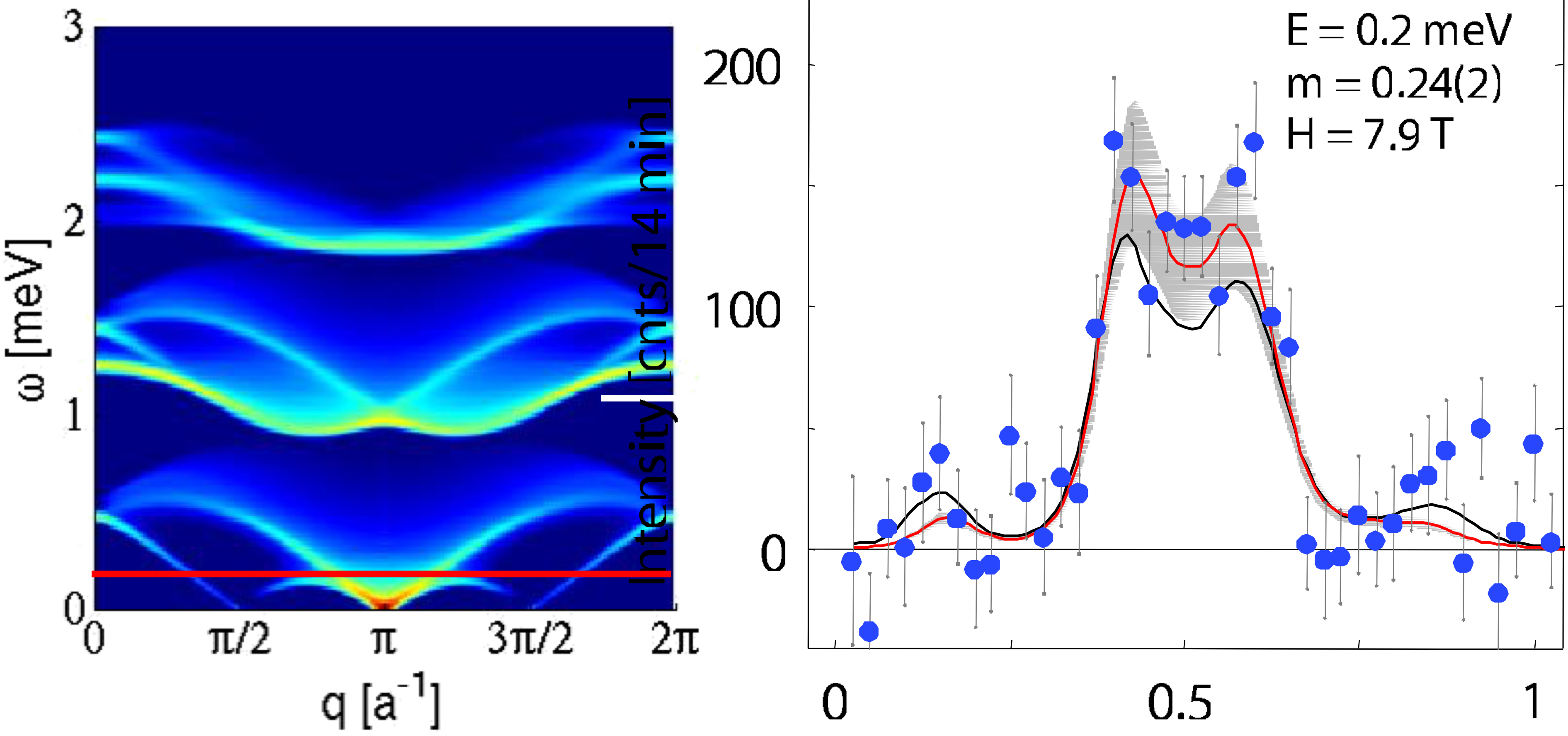
K. Yu et al. arxiv/1406.6876 (14)

$$\langle S^- S^+ \rangle_{q,\omega} = \langle \psi \psi^\dagger \rangle_{q,\omega}$$



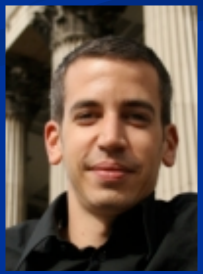


Direct calculation of correlations



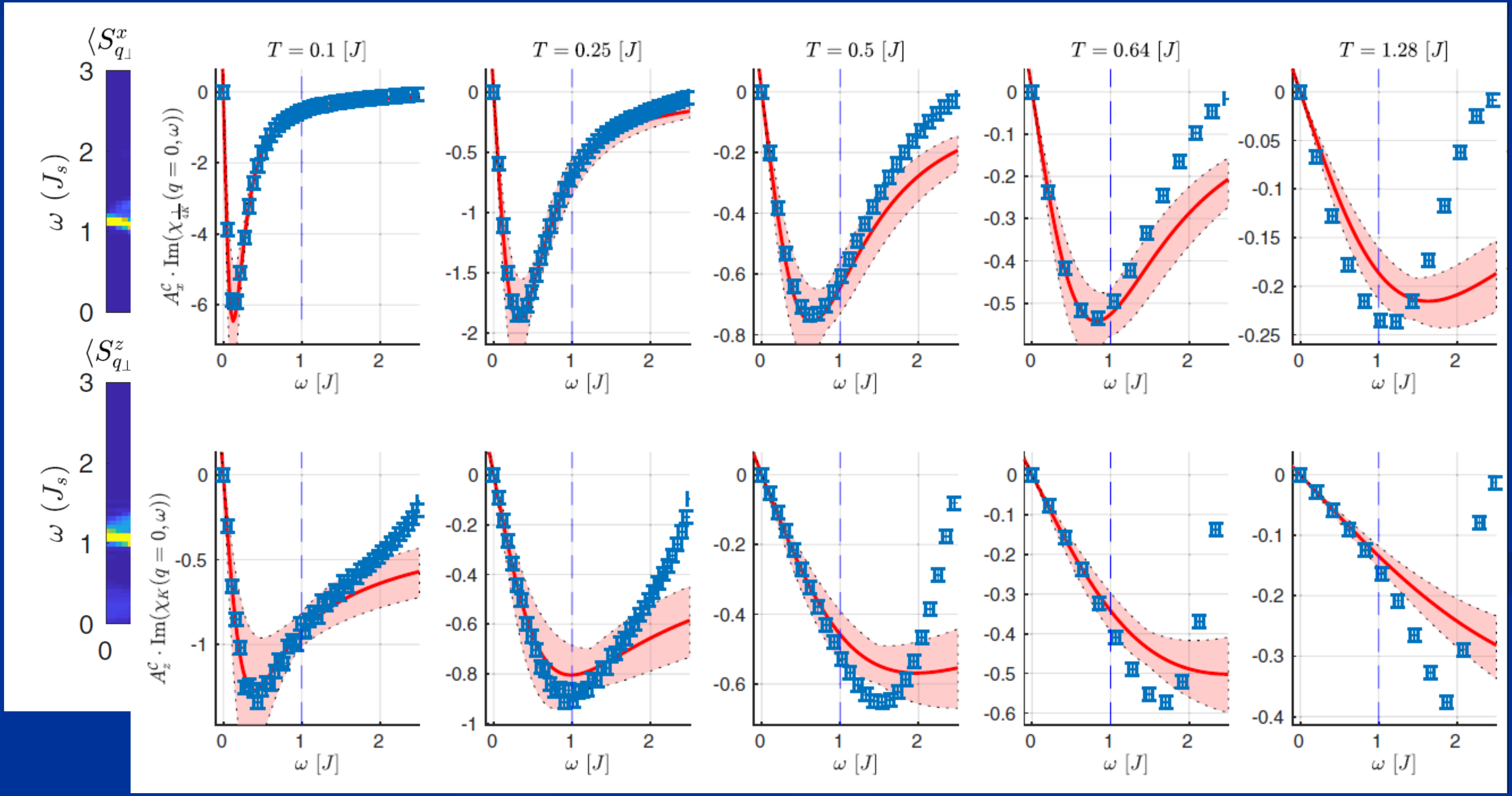
P. Bouillot et al.
PRB 83, 054407 (2011)





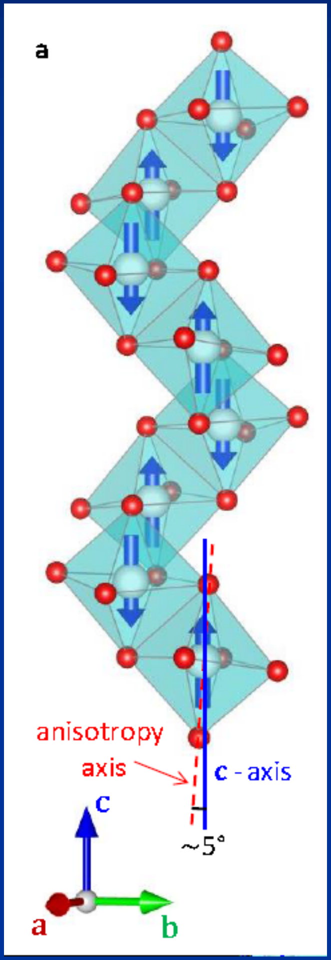
Neutron spectra, Finite T

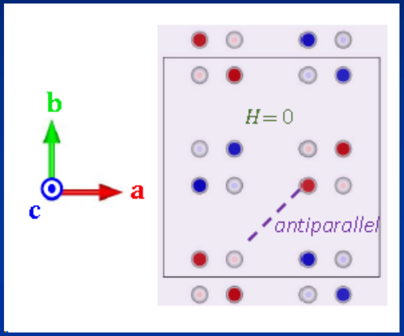
N. Kestin and T. Giamarchi, PRB 99, 195121 (2019)



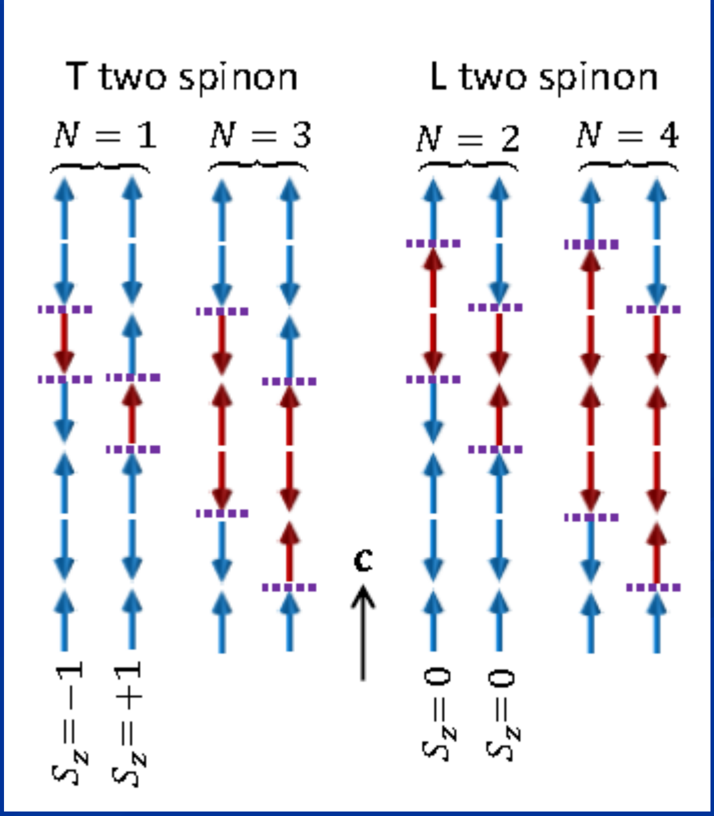
Power of such exact solutions

Ising-like chains: BaCoVO

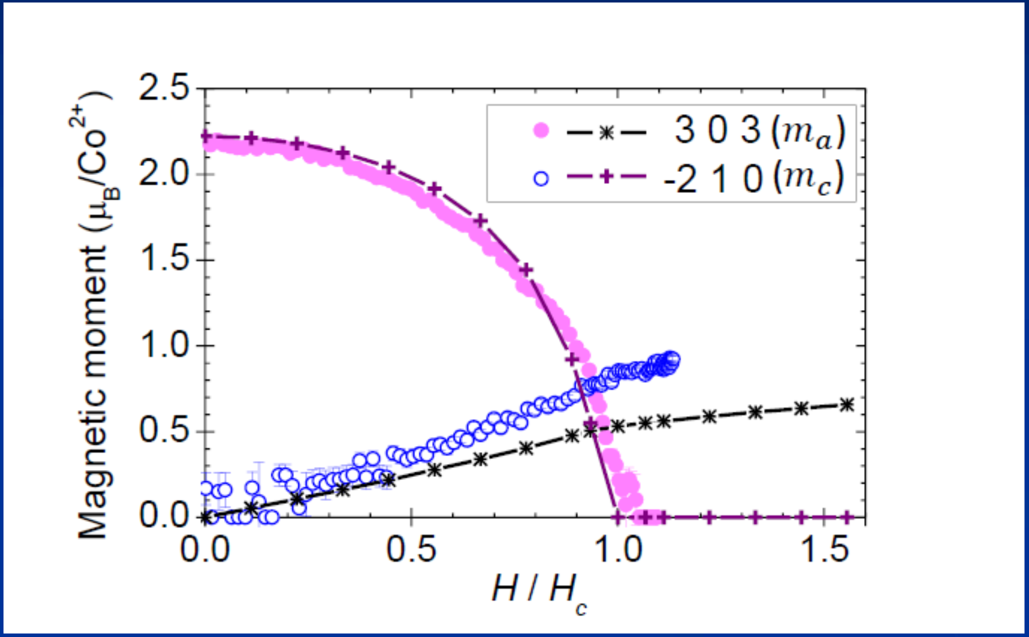




$$\mathcal{H}_{XXZ} = J \sum_{n,\mu} [\epsilon \left(S^x_{n,\mu} S^x_{n+1,\mu} + S^y_{n,\mu} S^y_{n+1,\mu} \right) + S^z_{n,\mu} S^z_{n+1,\mu}] - \sum_{n,\mu} \tilde{g} \mu_B \mathbf{H} \cdot \mathbf{S}_{n,\mu} + J' \sum_{n} \sum_{\mu,\nu(\mu \neq \nu)} S^z_{n,\mu} S^z_{n,\nu} \quad (1)$$



Transverse magnetic field



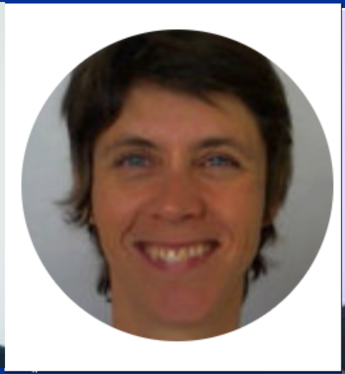
- Nature of the transition ?
- DMRG: not the transition in unif. field
- Effective staggered field hx (g- tensor)

Topological phase transitions

Topological quantum phase transition in the Ising-like antiferromagnetic spin chain BaCo2V2O8

Q. Faure, S. Takayoshi, et al

Nature Physics 14, 867 (2018)

Two competing topological excitations: DFDSG

- XXZ anisotropy $J_z \cos(4\phi)$

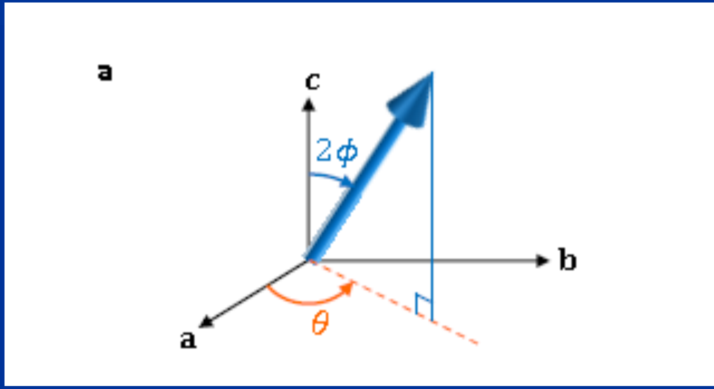
Relevant for K < 1/2

- Staggered magnetic field $h_x \cos(\theta)$

Relevant for K > 1/8

Effective Hamiltonian

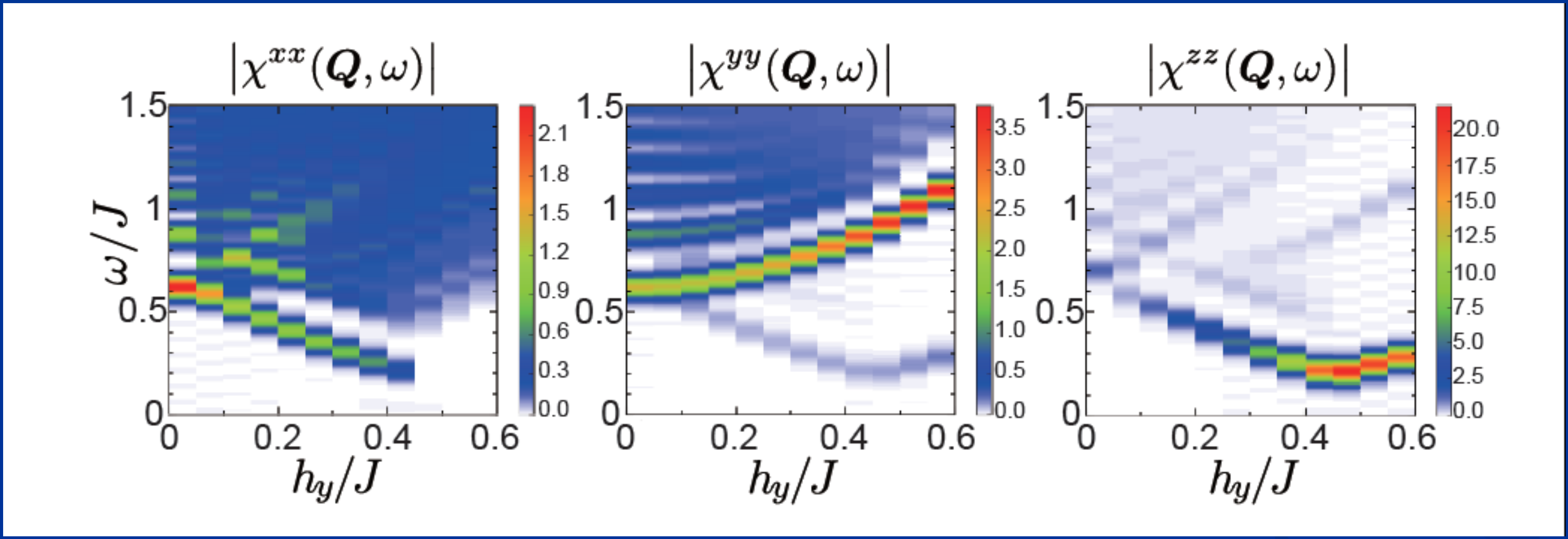
- Bosonization of the spin chain



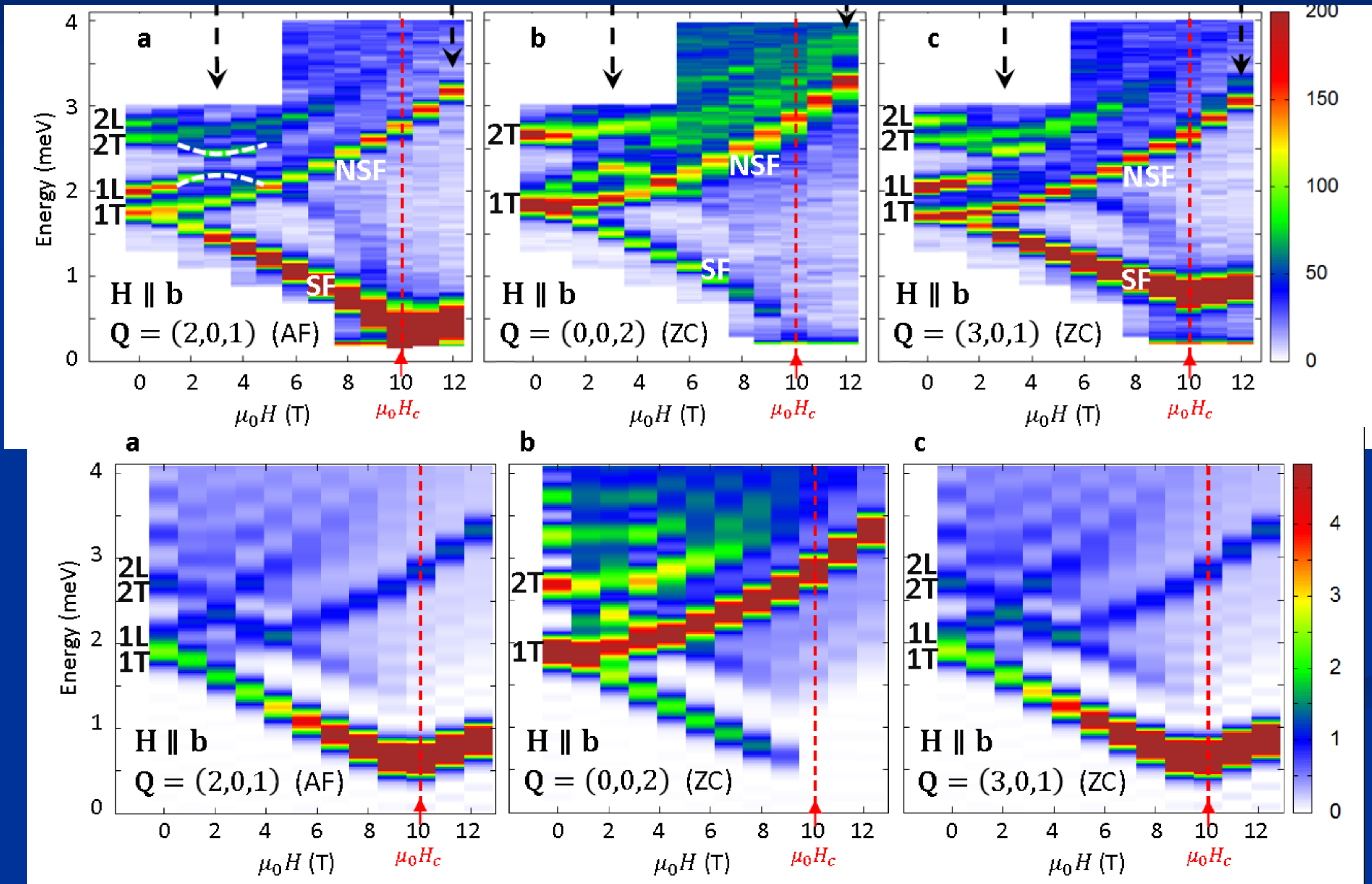
$$\mathcal{H}^{\text{eff}} = \frac{v}{2\pi}\int dz \Big[\frac{1}{K}\Big(\frac{d\phi(z)}{dz}\Big)^2 + K\Big(\frac{d\theta(z)}{dz}\Big)^2\Big]$$

$$-\frac{2g}{(2\pi\alpha)^2}\int dz \cos 4\phi(z) - \frac{g_{yx}\mu_B H}{\sqrt{2\pi\alpha}}\int dz \cos\theta(z), \quad (3)$$

Spin-Spin correlations



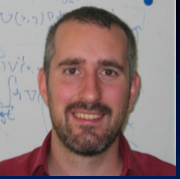
Neutrons (un-pol. and polarized)



Open problems

- More complex 1D transitions
- Disorder
- Out of equilibrium situations
- Coupled chains/ladders ....

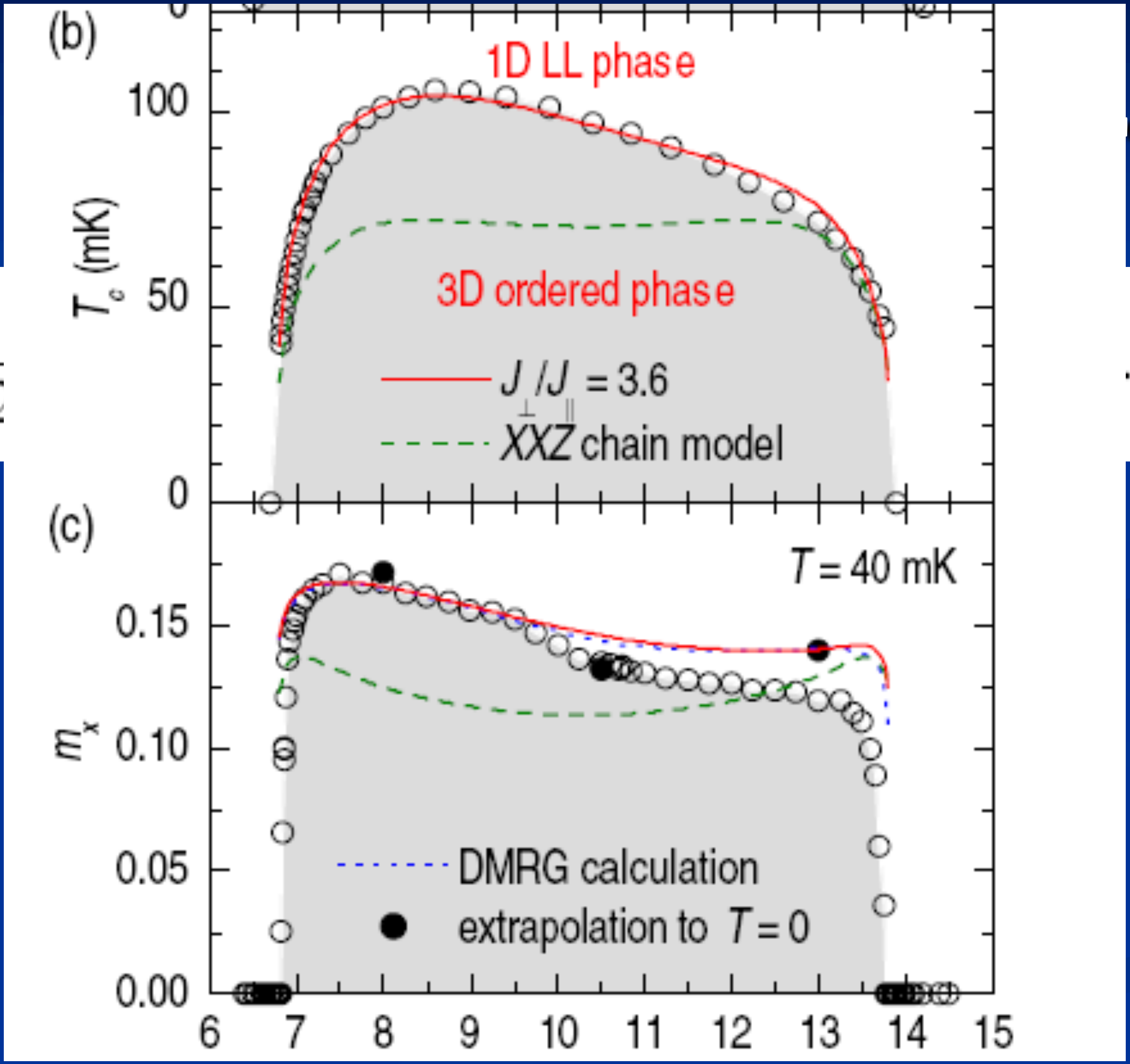
Mean field (RPA) works....



Interladder coupling

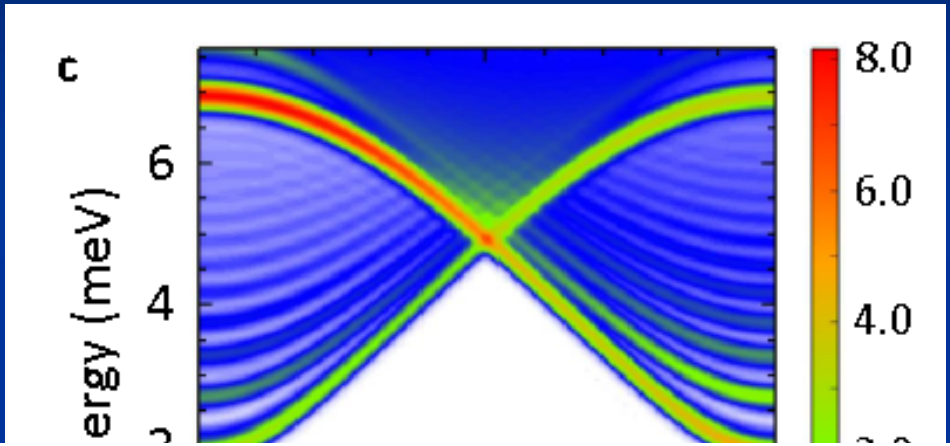
- Tc to c)

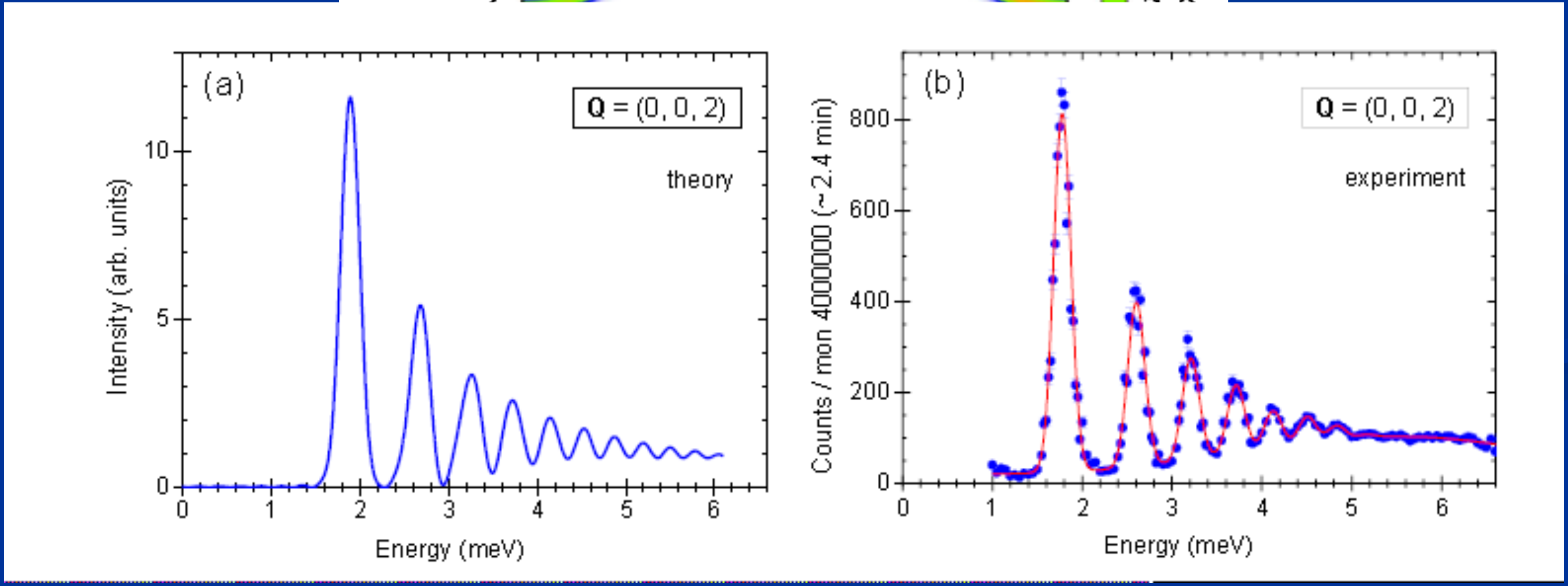
$$T_c =$$



M. Klanjsek et al., PRL 101 137207 (2008)

Confinement of spinons BaCoVO



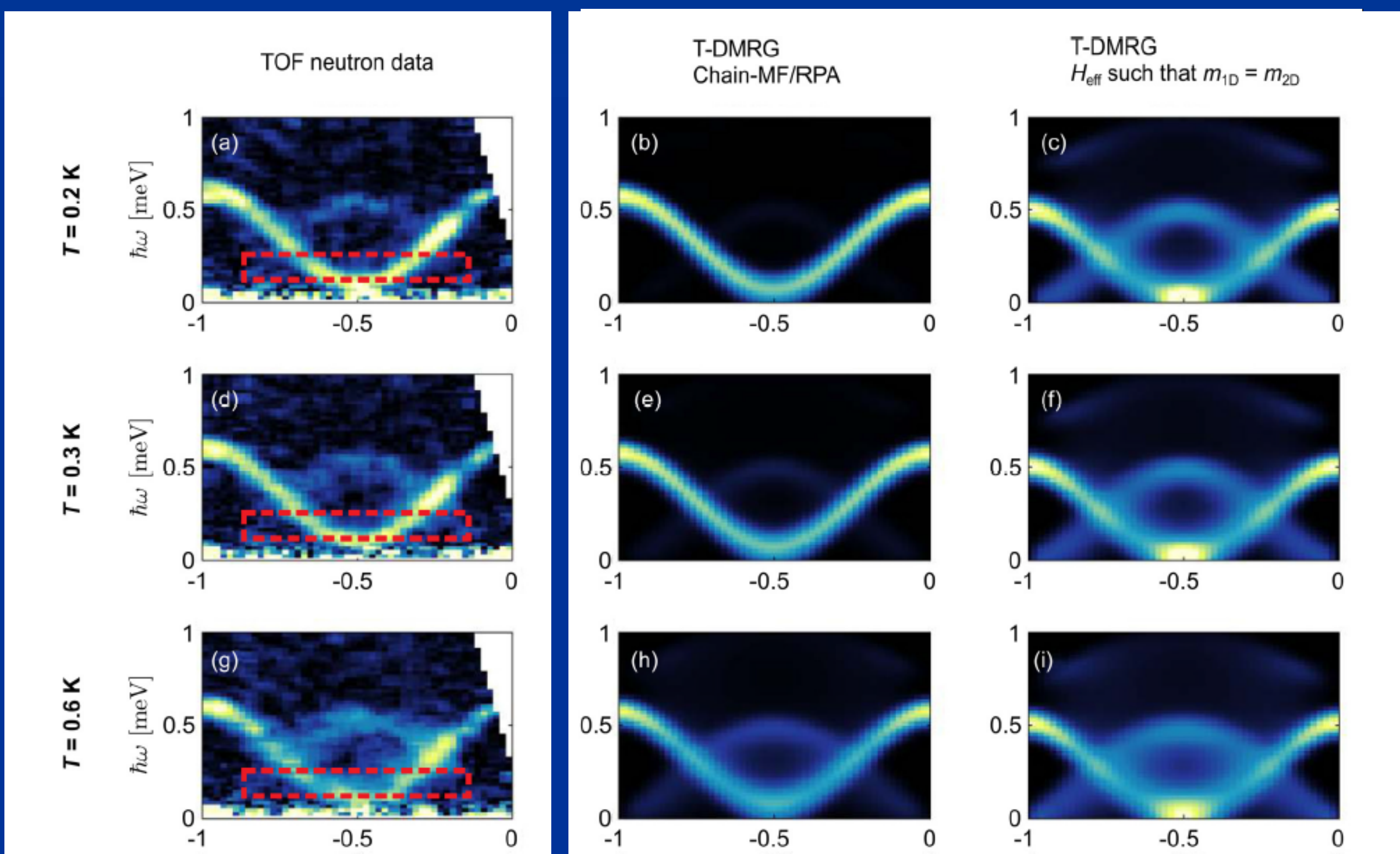


But not so well in some cases…

PHYSICAL REVIEW B **96**, 134406 (2017)

Finite-temperature correlations in a quantum spin chain near saturation

D. Blosser,[1,*] N. Kestin,[2] K. Yu. Povarov,[1] R. Bewley,[3] E. Coira,[2] T. Giamarchi,[2] and A. Zheludev[1,†]



Calculation with $m_{2D} = m_{1D}$	
m	h^z_{eff} (K)
0.429	5.81
0.426	5.86
0.405	5.94
0.384	5.98
0.348	6.04
0.298	6.08

Conclusions

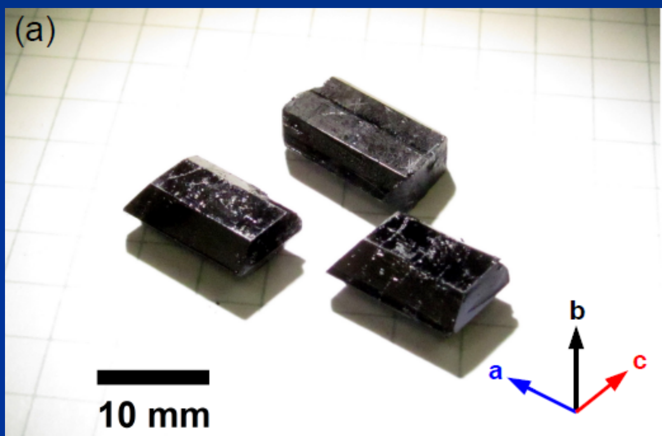
- Efficicient and precise methods for simple 1D systems: finite T, real time, spatial correlations
- Possibility to combine numerics and analytics methods to get an essentially exact method
- Quantum spin systems: very rich physics for 1D and quasi-1D systems.
- Quantitative test of Tomonaga-Luttinger theory
- Novel Topological phase transitions in Q. spin systems

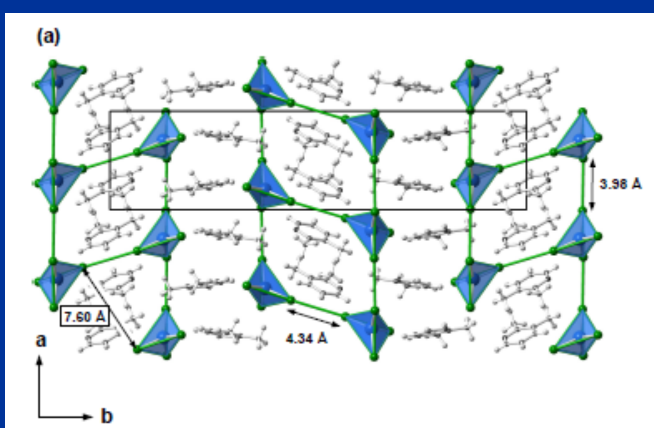
For the future..

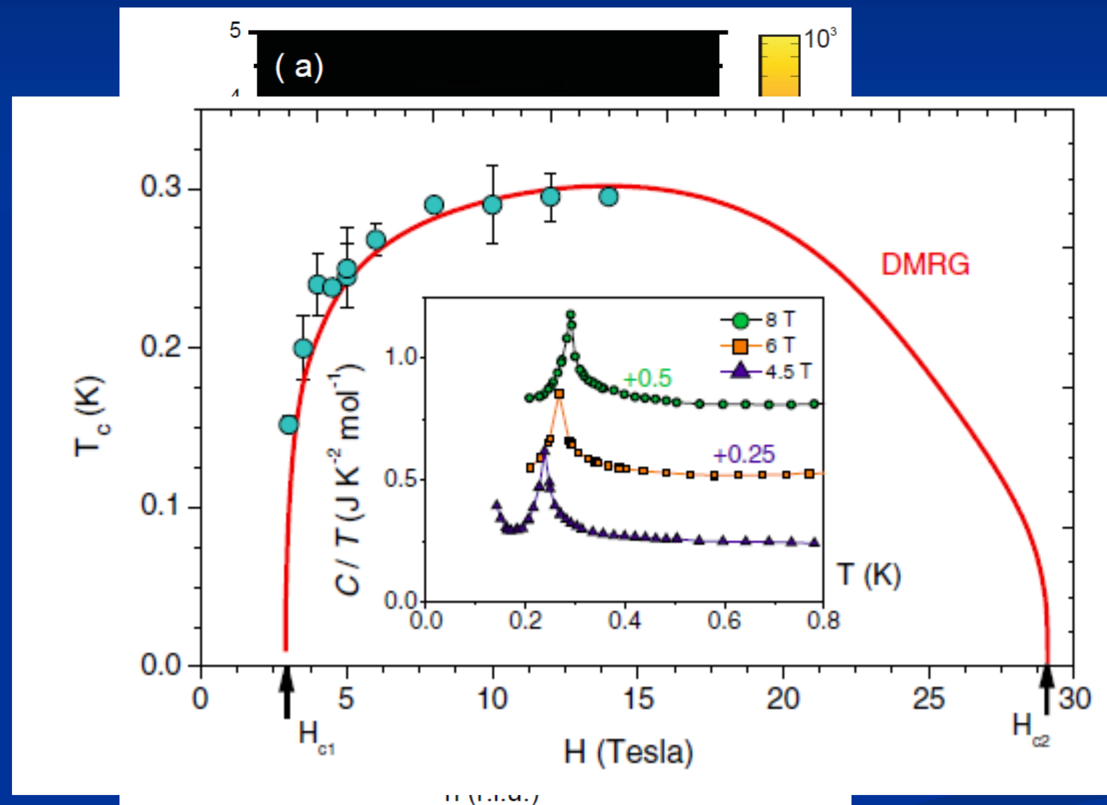
- Other systems with the DSG toological phase transitions (cold atoms ?)
- More involved 1D systems (e.g. Disorder, DM terms etc.)
- Effects of finite temperature
- Out of equilibrium phenomena
- Need to treat quasi-1D systems beyond mean-field theory /RPA

Hamiltonian reconstruction

D. Schmidiger et al. PRL 108 167201 (2012)



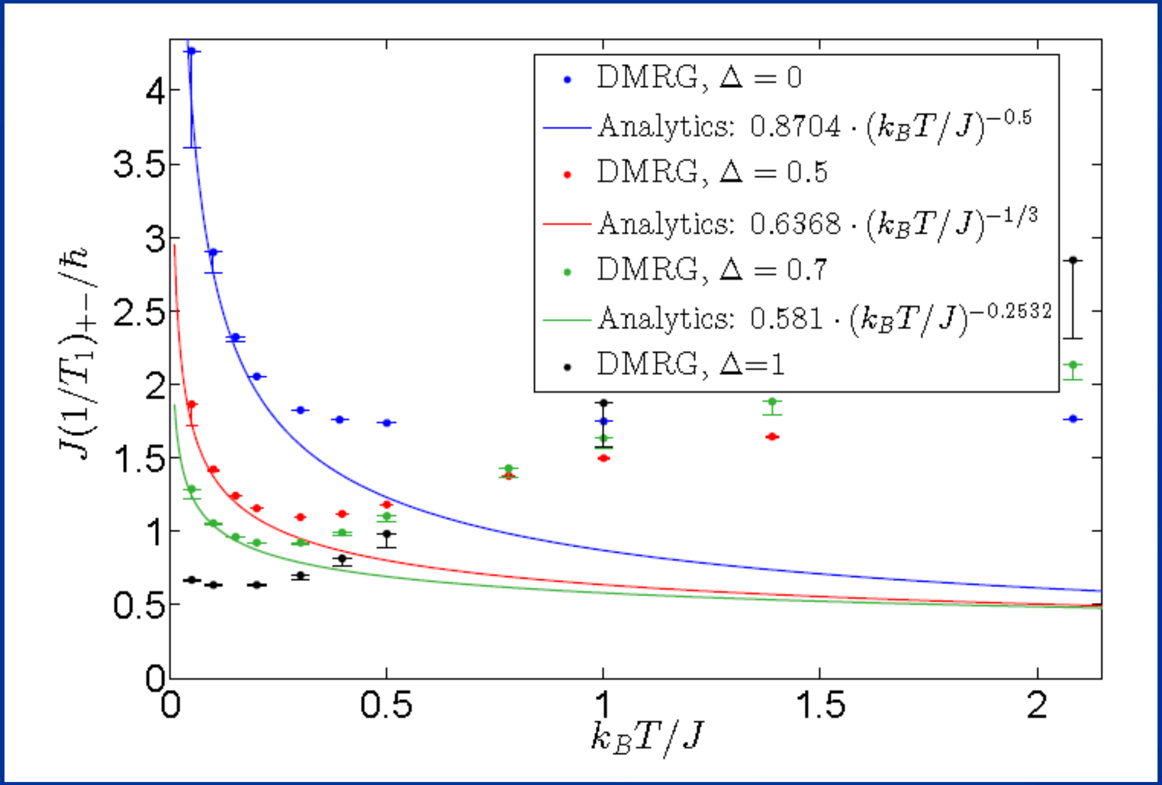




$$\mathcal{H} = J_{\text{leg}} \sum_{l,j} \mathbf{S}_{l,j} \cdot \mathbf{S}_{l+1,j} + J_{\text{rung}} \sum_{l} \mathbf{S}_{l,1} \cdot \mathbf{S}_{l,2} - g\mu_B H \sum_{l,j} S^z_{l,j}.$$

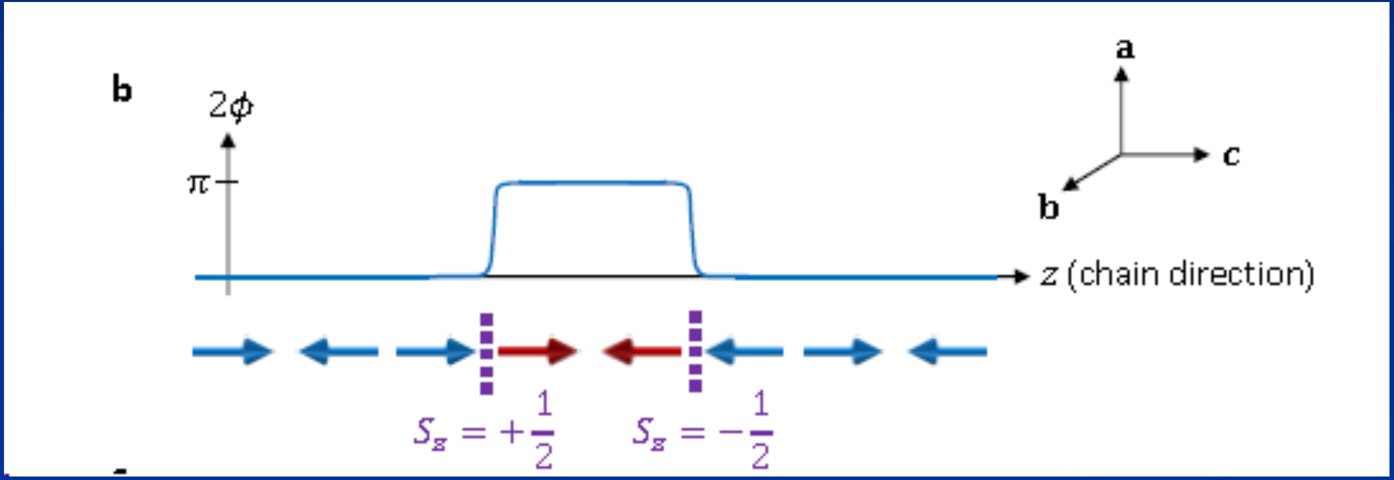
NMR

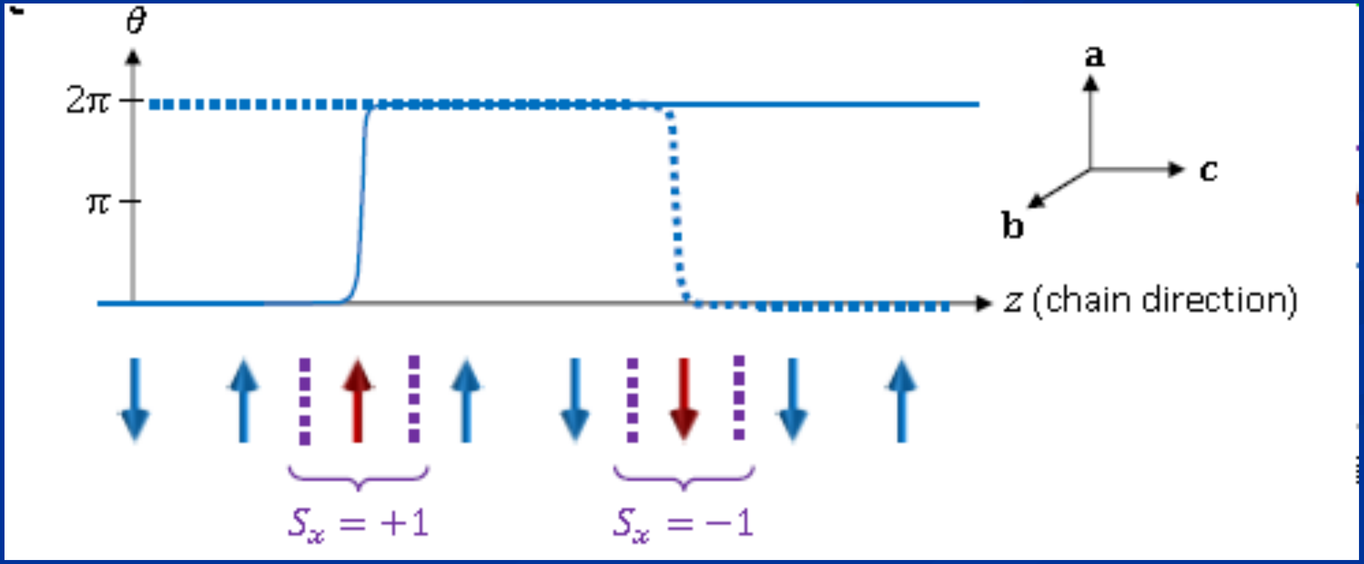
$$1/T_1 = \lim_{\omega \to 0} \frac{T}{\omega} Im \sum_q \langle [S^+(q,\omega), S^-(q,\omega)] \rangle$$



E. Coira, P. Barmettler, TG, C. Kollath, PRB **94**, 144408 (2016)

Dual topological excitations





Other DFDSG

- m=4, n=1 : XXZ + staggered magnetic field

$$-J_z \cos(4\phi) - h_x \cos(\theta)$$ K = ½ ; K = 1/8

K=1/4 $$-J_z \psi_R^\dagger \psi_L - h_x \psi_R^\dagger \psi_L^\dagger + \text{h.c.}$$

Ising-like transition (c=1/2)

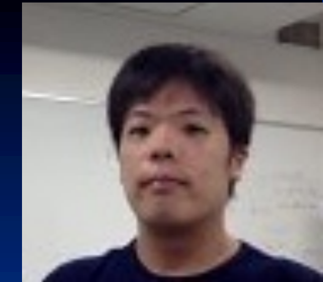
- m=4, n=2 : XXZ + XY anistropy

TG + H.J Schulz J. Physique 49 819 (88)

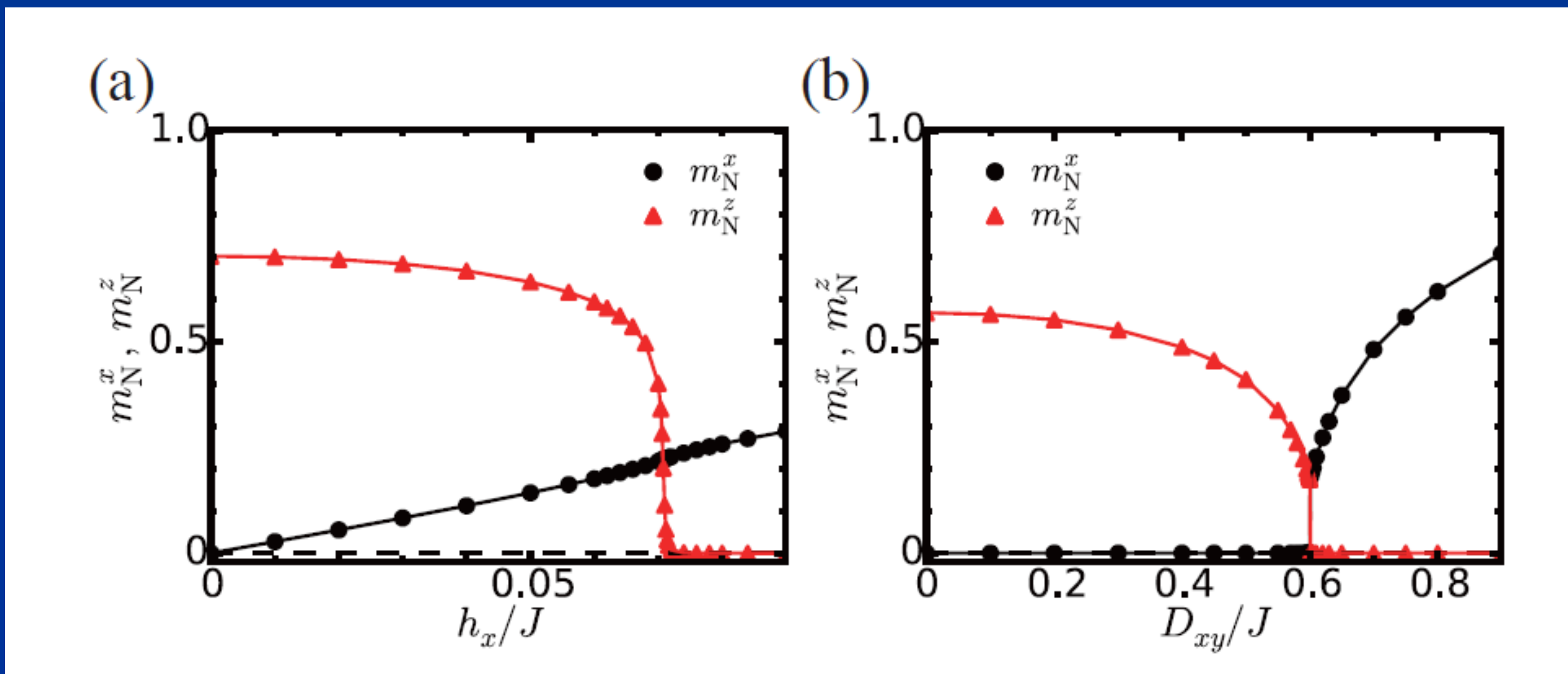
$$-J_z \cos(4\phi) - h_x \cos(2\theta)$$ K = ½ ; K = ½

BKT-like transition (c=1)

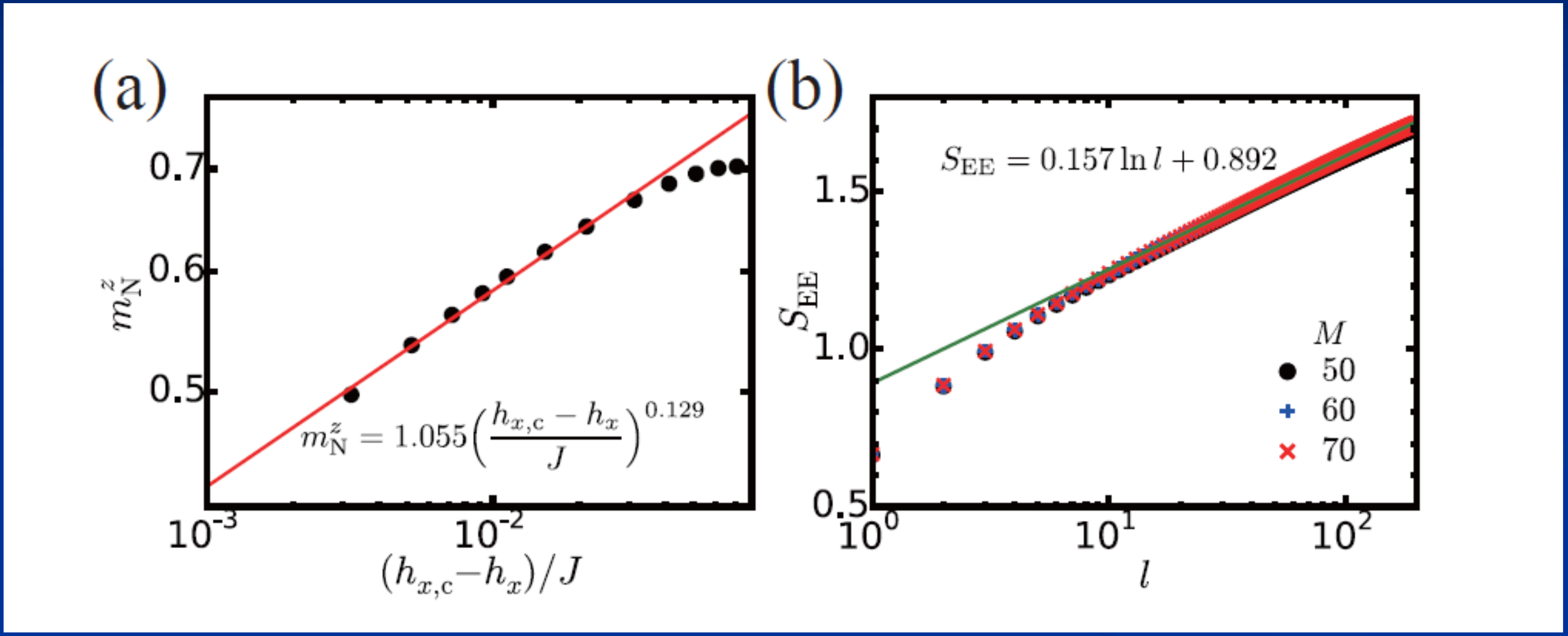
Two types of transition



S. Takayoshi, S. Furuya, TG, PRB 98 184429 (2018)



M=4, N=1 (BACOVO)



$$S_{EE} = \frac{c}{3}\log(l) + Cste \qquad \beta = 0.129 \quad c = 0.471$$

Longitudinal magnetic field H //c

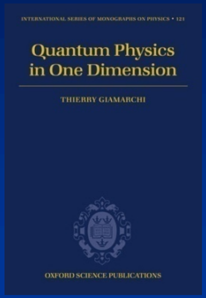
PHYSICAL REVIEW LETTERS **123,** 027204 (2019)

Tomonaga-Luttinger Liquid Spin Dynamics in the Quasi-One-Dimensional Ising-Like Antiferromagnet $BaCo_2V_2O_8$

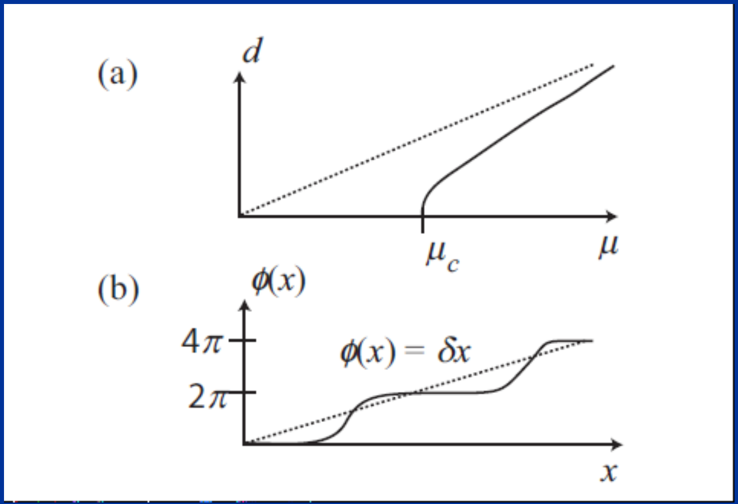
Quentin Faure,[1,2] Shintaro Takayoshi,[3,4,*] Virginie Simonet,[2] Béatrice Grenier,[1,†] Martin Månsson,[5,6] Jonathan S. White,[5] Gregory S. Tucker,[5,7] Christian Rüegg,[5,4,8] Pascal Lejay,[2] Thierry Giamarchi,[4] and Sylvain Petit[9]

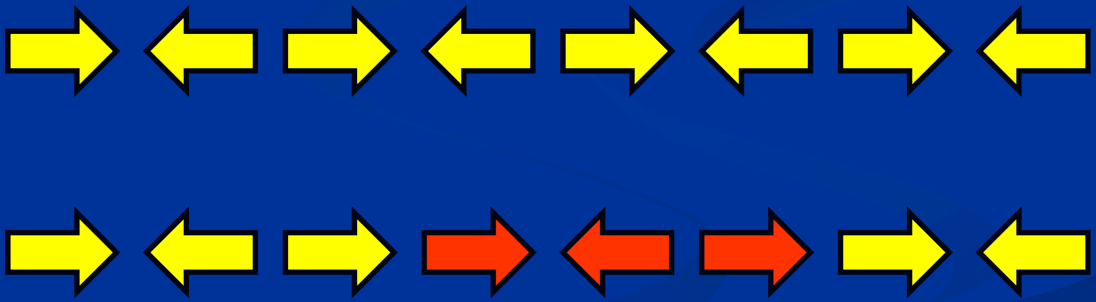
Pokrovsky-Talapov (C-IC) transition

R. Chitra, TG PRB 55 5816 (97); TG, AM Tsvelik PRB 59 11398 (99)

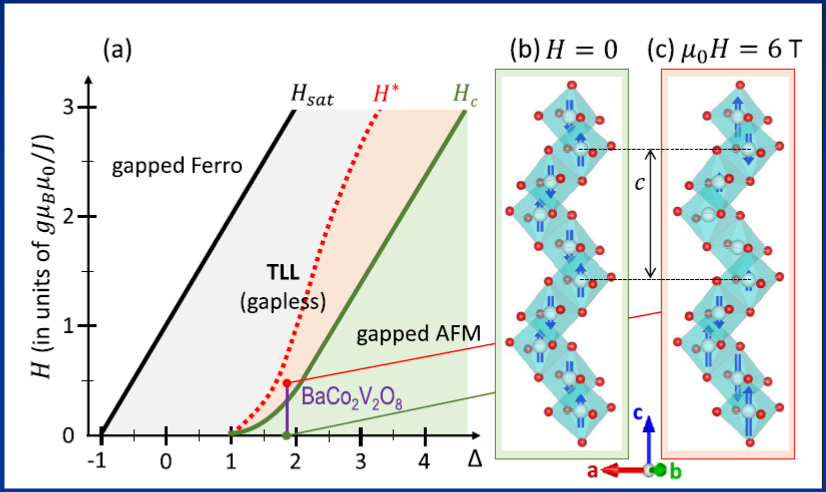


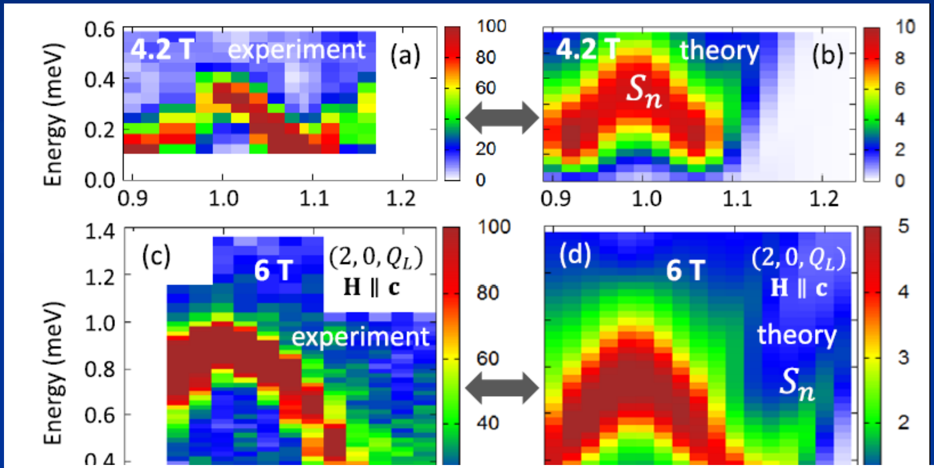
$$H = \frac{1}{2\pi}\int dx[K(\Pi_\phi)^2 + \frac{1}{K}(\nabla_x\phi)^2] - g\int dx\cos(4\phi) - h\int dx\nabla_x\phi$$

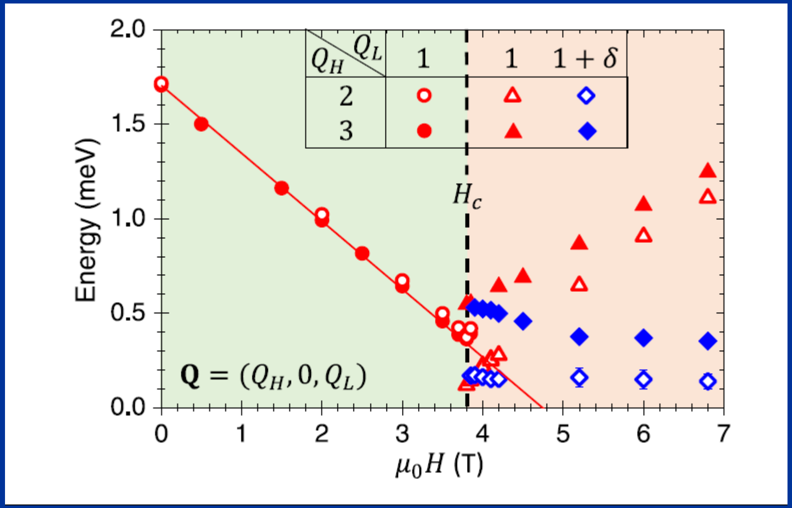


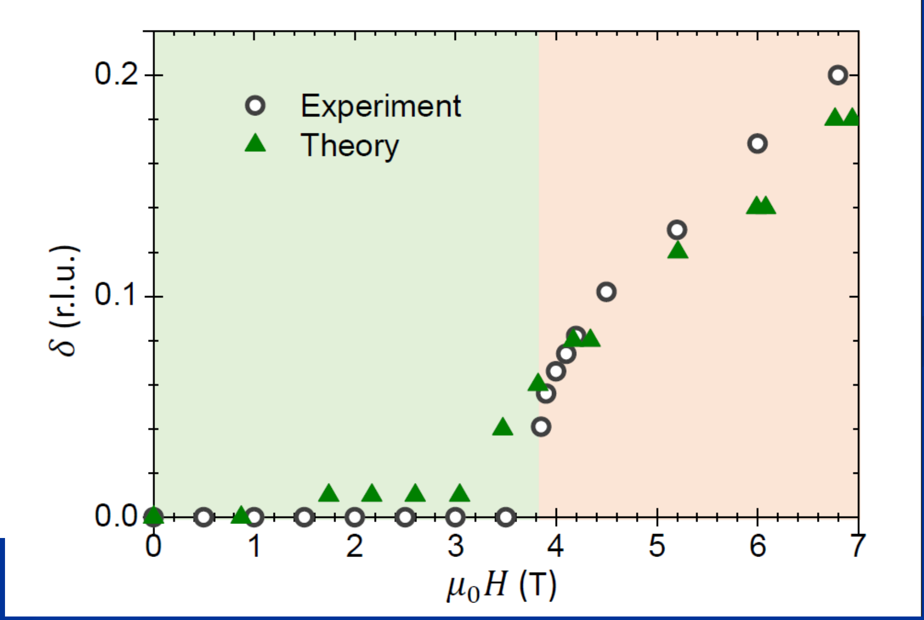


Neutrons and DMRG calculation

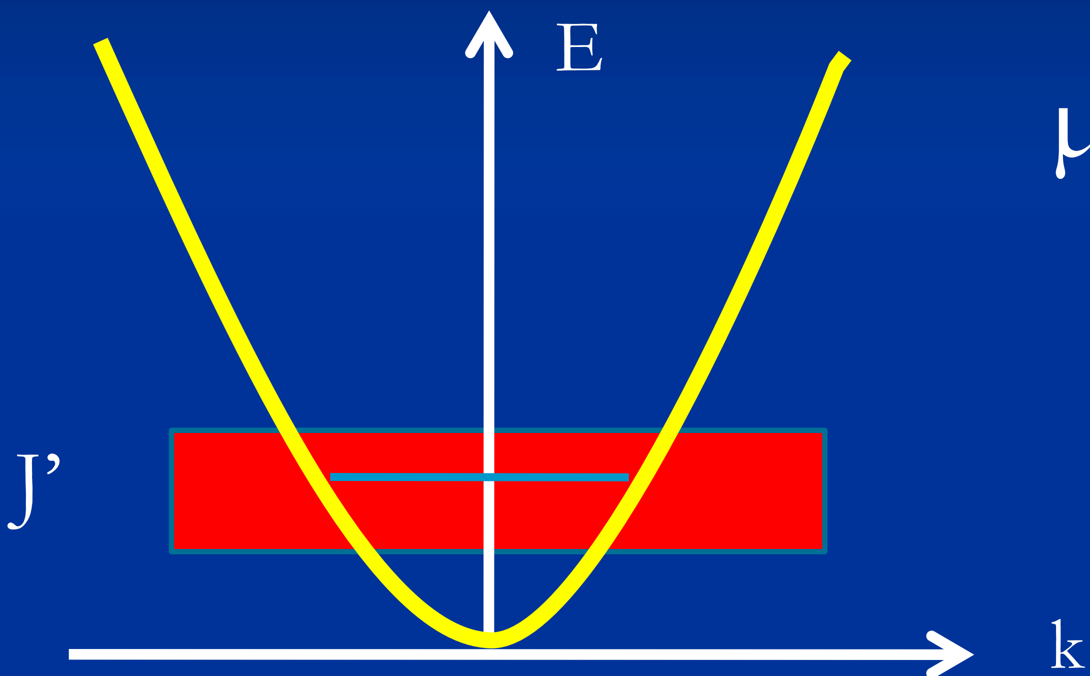








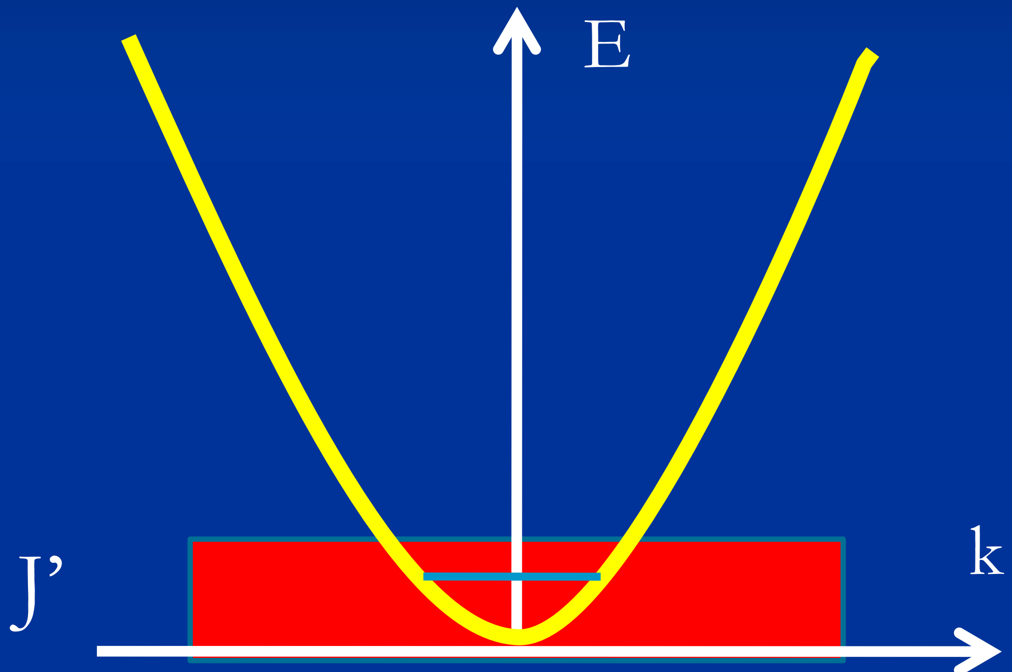
Weakly coupled 1D systems



$$\mu = h - h_{c1}$$

Quasi-1D ; Luttinger liquid approach

Close to QCP: Dimensional crossover



$\mu = h - h_{c1}$

J’ > μ:
3D
behavior

Always 3D close to QCP !