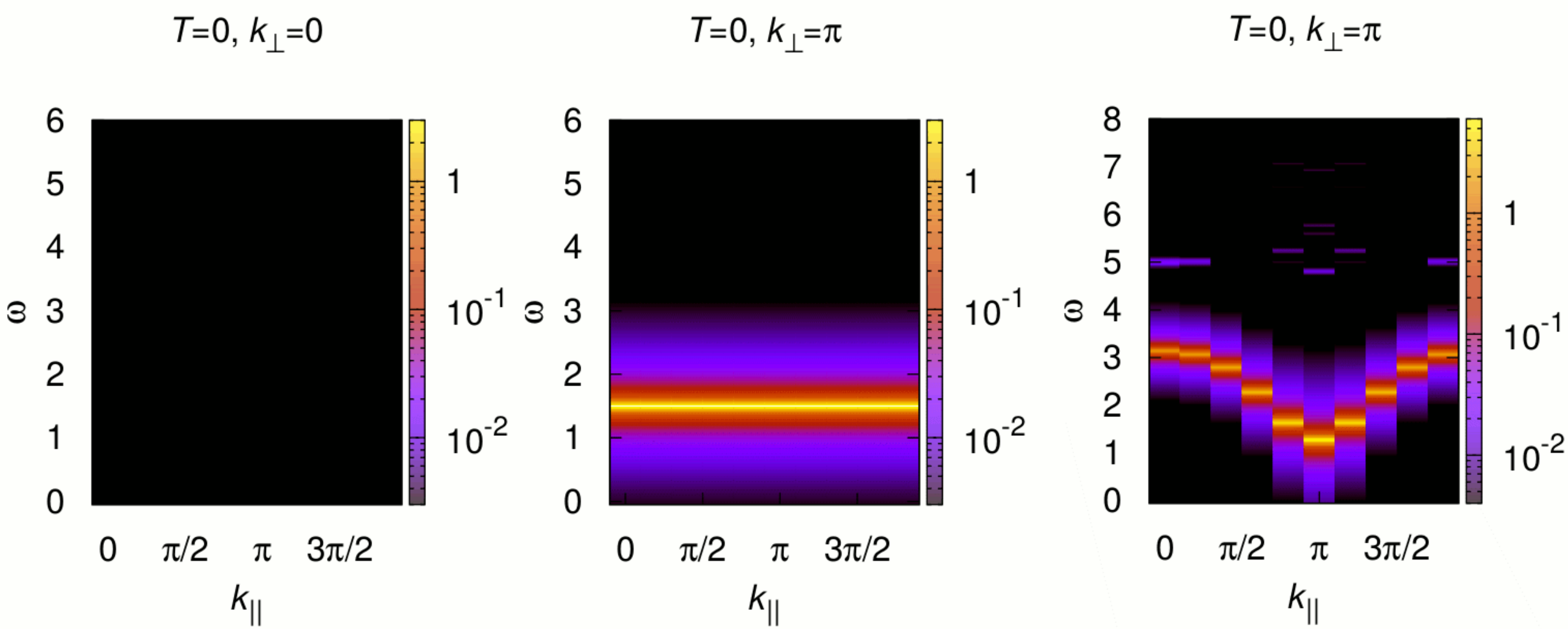
Finite-Temperature Dynamics of Highly Frustrated Quantum Spin Ladders

B. Normand

Renmin University of China, Beijing

with A. Honecker (LPTM Cergy-Pontoise) and F. Mila (EPF Lausanne)

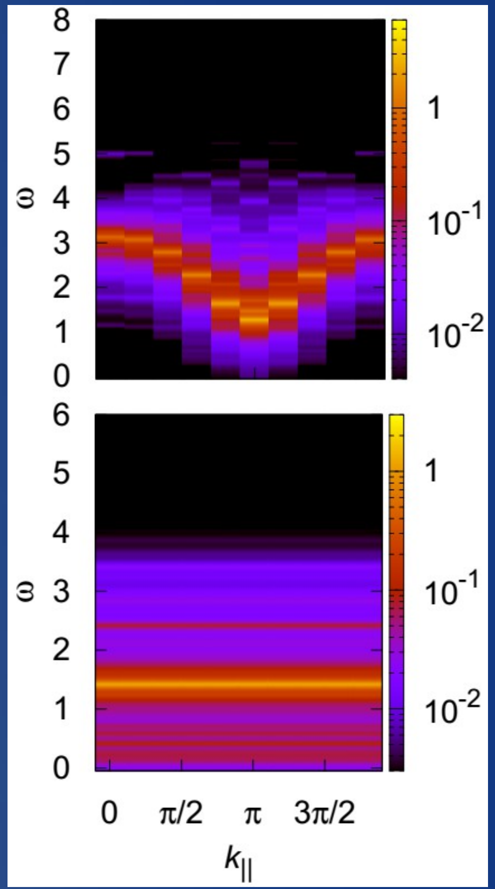


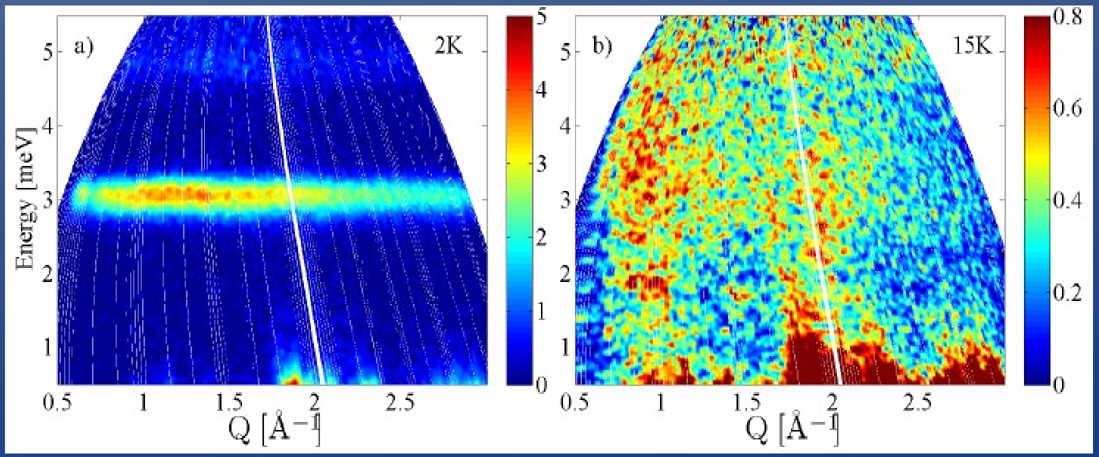
$J_\perp = 2,\ J_{||} = J_\times = 1$

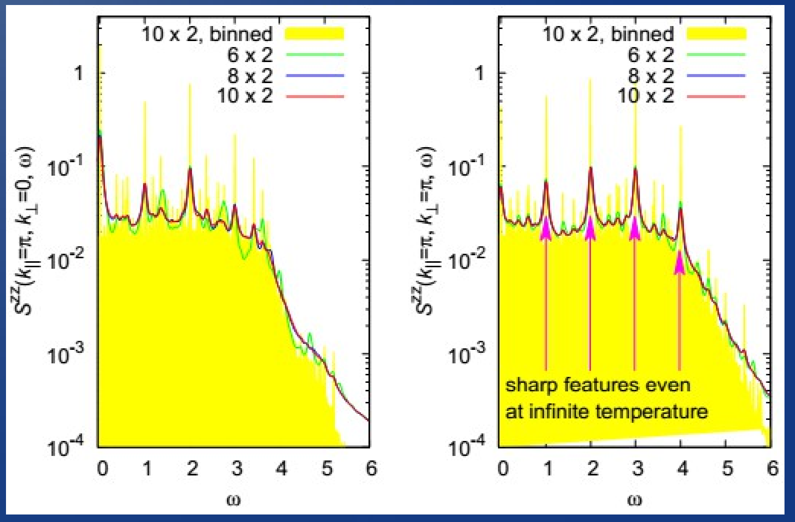
$J_\perp = 2,\ J_{||} = 1,\ J_\times = 0$

Road Map

- quantum vs. classical (thermal) fluctuations.
- unfrustrated vs. frustrated systems
  – highly anomalous thermal properties of SCBO.
- fully frustrated *S = 1/2* ladder model
  – exact bound states and QCP.
- thermodynamic properties
  – broadening, peak shifts and multi-triplet states.
- dynamical structure factor
  – contributions from bound states of many triplets,
  – anomalous spectral-weight shifts,
  – high-temperature spectral features.
- messages for experiment.

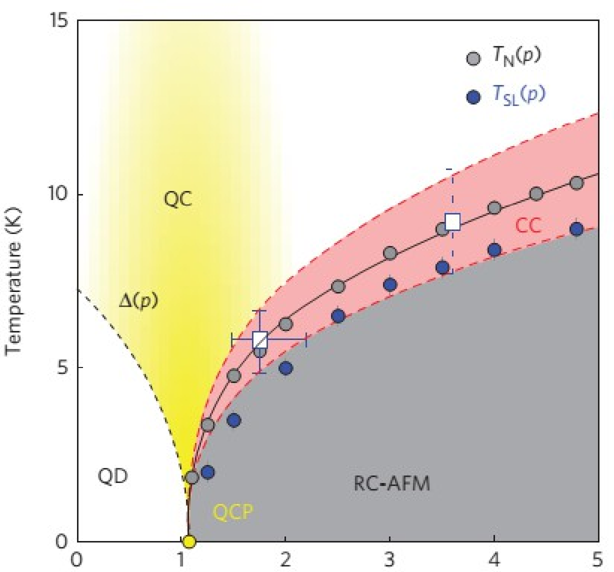




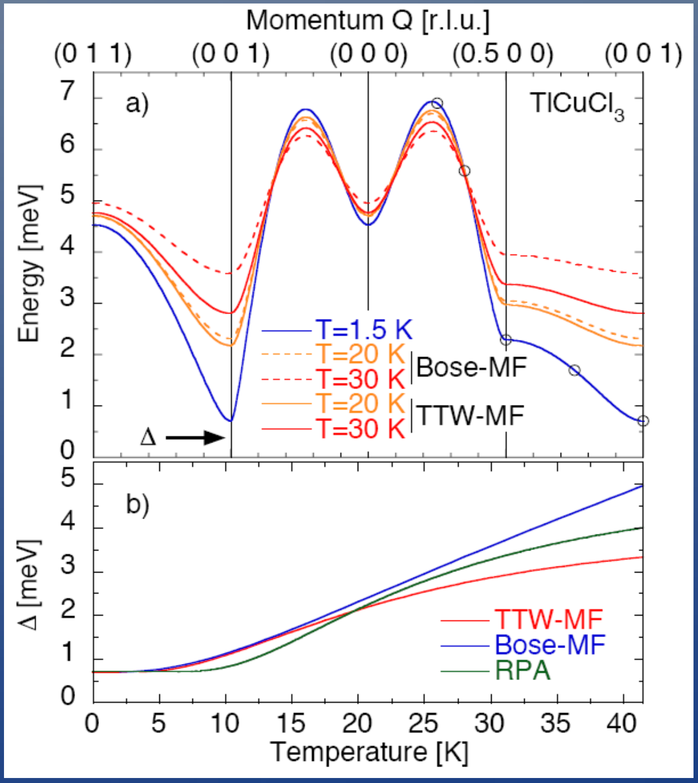


Quantum and Classical Fluctuations

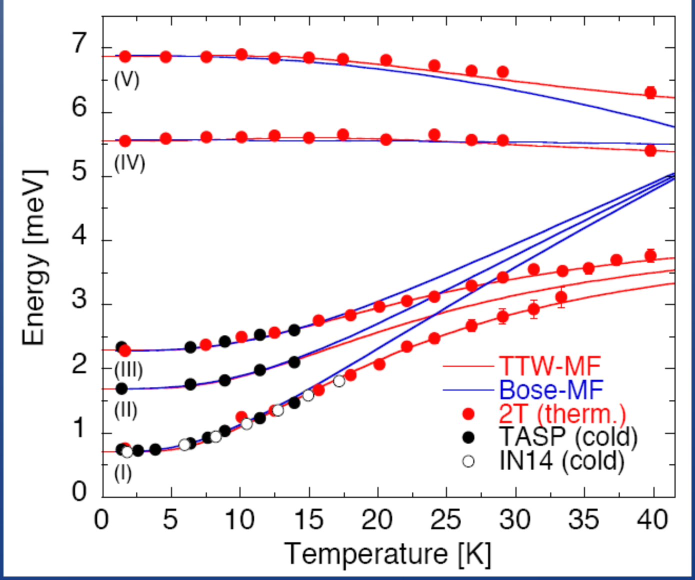
Some of the most fundamental phenomena in physics are a consequence of the interplay between quantum and thermal fluctuations. Key examples include **quantum and classical criticality** (next talk) [1].



How quantum and thermal fluctuations combine in a **restricted phase space**, where the two *cannot be independent*, ranks as a **fundamental unsolved problem**.



The effect of thermal fluctuations on the excitation spectrum [2]



depends on:

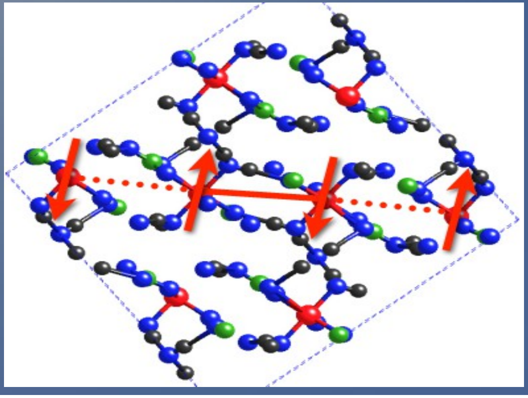
- dimensionality (independence)
- frustration (bandwidths).

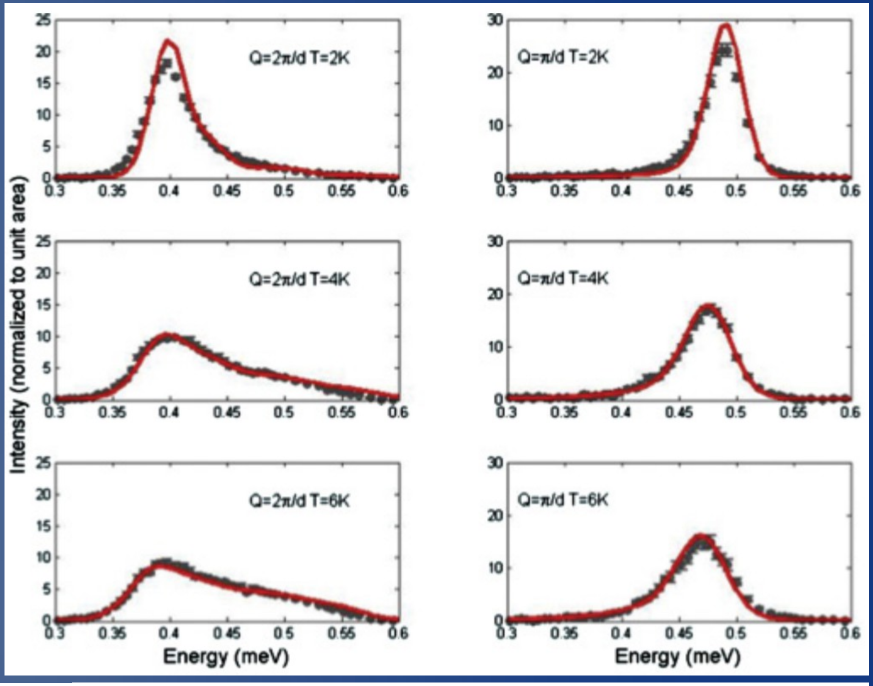
[1] P. Merchant *et al.*, Nature Phys. **10**, 373 (2014).

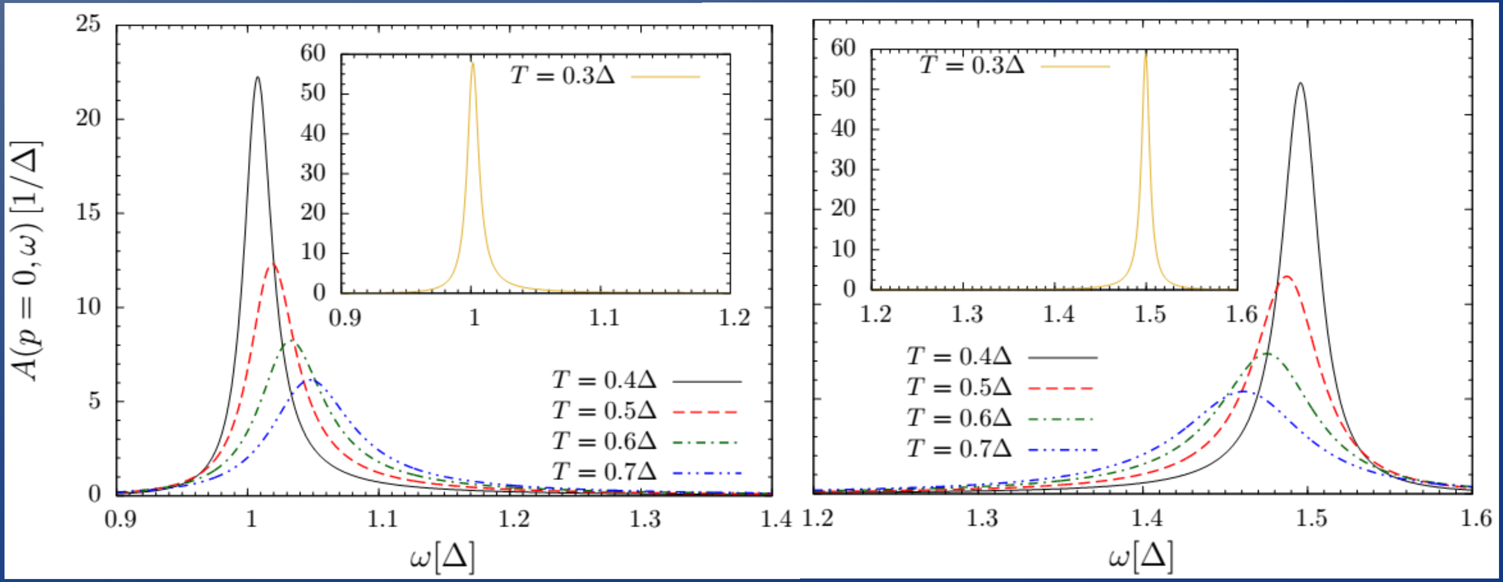
[2] Ch. Rüegg *et al.*, PRL **95**, 267201 (2005).

High- and Low-Dimensional Systems

Unfrustrated systems in high dimensions show coherent shifts of spectral weight; in low dimensions, mixing of states within the one-triplet band causes characteristic asymmetrical lineshapes [1], as observed [2] in $Cu(NO_3)_2.2.5H_2O$, an alternating-chain material.



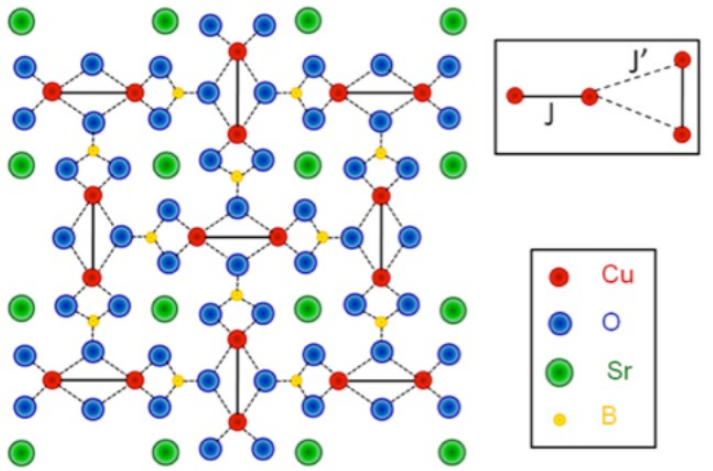


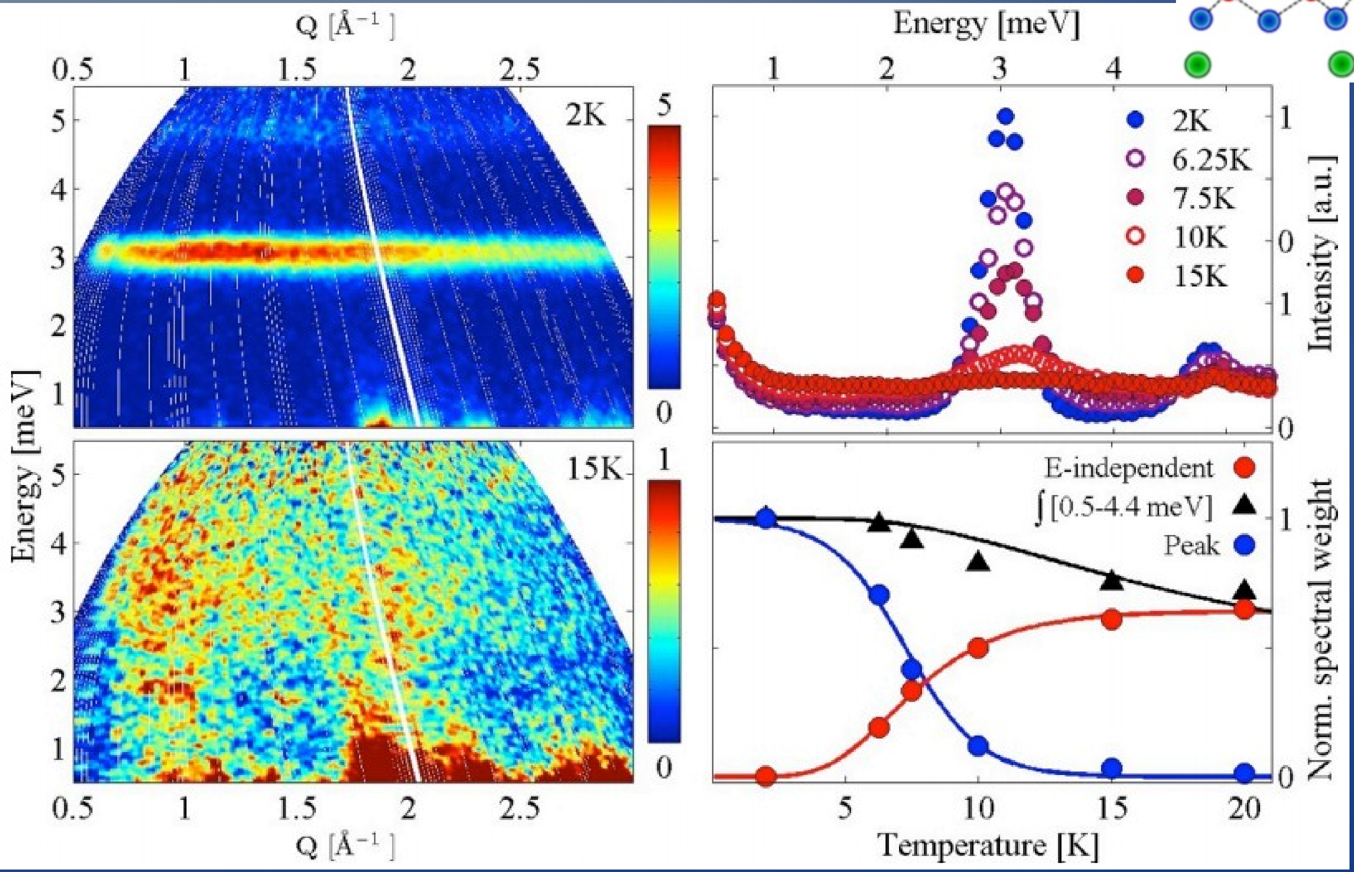


[1] B. Fauseweh, J. Stolze and G. S. Uhrig, PRB **90**, 024408 (2014).
[2] D. A. Tennant *et al.*, PRB **85**, 014402 (2012).

Unfrustrated and Frustrated Systems

Systems with *strong magnetic frustration* have **flat excitation bands**. The thermal evolution of the spectral weight in the Shastry-Sutherland material $SrCu_2(BO_3)_2$ is **highly anomalous**: the one-triplet band is lost at $T = \Delta/3$ [1,2].





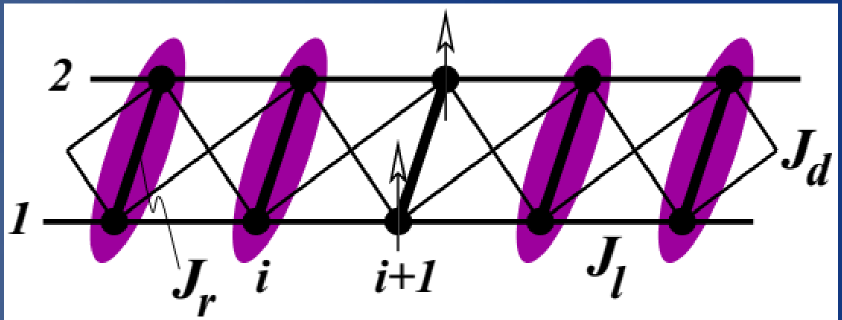
Unfrustrated: strong shifts of spectral weight possible without loss of coherence.

Frustrated: complete loss of coherent excitations ?

[1] B. D. Gaulin *et al*., PRL **93**, 267202 (2004).
[2] M. E. Zayed *et al*., PRL **113**, 067201 (2014).

Fully Frustrated Ladder

Model: consider a S = ½ ladder with equal leg and diagonal couplings [1,2,3].



$$H = \sum_i J_r \vec{S}_i^1 . \vec{S}_i^2 + \sum_{i,m=1,2} \left[J_l \vec{S}_i^m . \vec{S}_{i+1}^m + J_d \vec{S}_i^m . \vec{S}_{i+1}^{\bar{m}} \right]$$

- no net triplet hopping, *i.e.* flat magnetic excitation bands (as in $SrCu_2(BO_3)_2$).
- there is a first-order quantum phase transition between an all-singlet ground state and an all-triplet state, which occurs at *J'/J = 0.7135, J/J' = 1.40148*.

Mathematically, the Hamiltonian has two essential properties:

$$\mathcal{H} = J_{||} \sum_i \vec{T}_i \cdot \vec{T}_{i+1} + J_{\perp} \sum_i \frac{1}{2} \left(\vec{T}_i^2 - \frac{3}{2} \right)$$

- **exact triplet bound states**;
  an n-triplet bound state has exactly the spectrum of an n-site Haldane chain.
- S_z is conserved on every rung,
  leading to an infinite number of locally conserved quantities.

$J_r = J = J_{perp}$

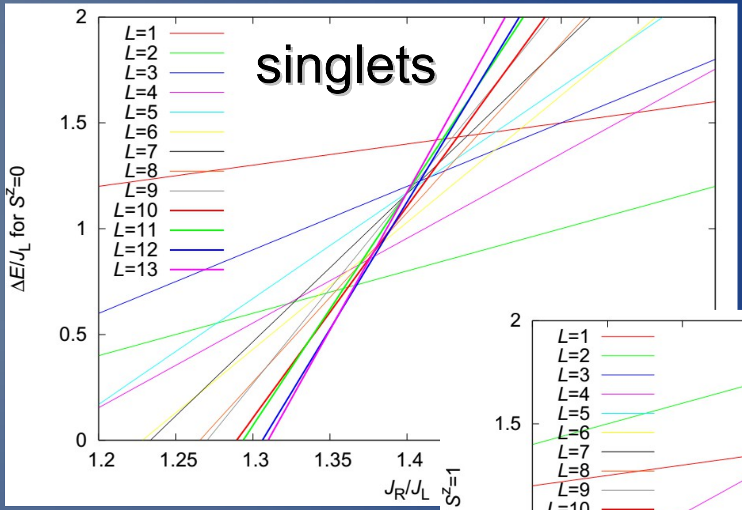
$J_l = J_d = J' = J_{||}$

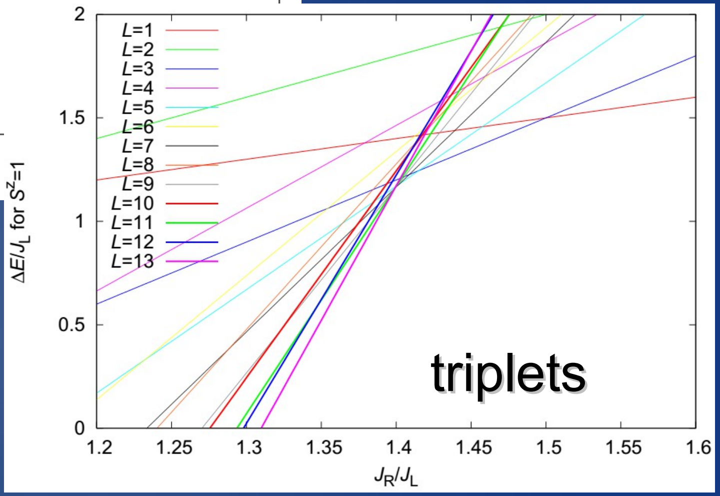
Numerical methods: this is a 1D system with a *very short correlation length* so exact diagonalisation (ED) should be particularly suitable; DMRG is to date not appropriate ...

[1] M. P. Gelfand, PRB **43**, 8644 (1991).
[2] Y. Xian, PRB **52**, 12485 (1995).
[3] A .Honecker, F. Mila and M. Troyer, EPJB **15**, 227 (2000).

Multi-Triplet Bound States

The key to the physics of the fully frustrated ladder is found in the **spectra** of multi-triplet bound states of all lengths. An analytical understanding of the bound-state spectra is found from finite Haldane chains.





Example: the 2-triplet bound state has

- one quintet at $E_{2q} = 2J + J'$
- one triplet at $E_{2t} = 2J - J'$
- one singlet at $E_{2s} = 2J - 2J'$.

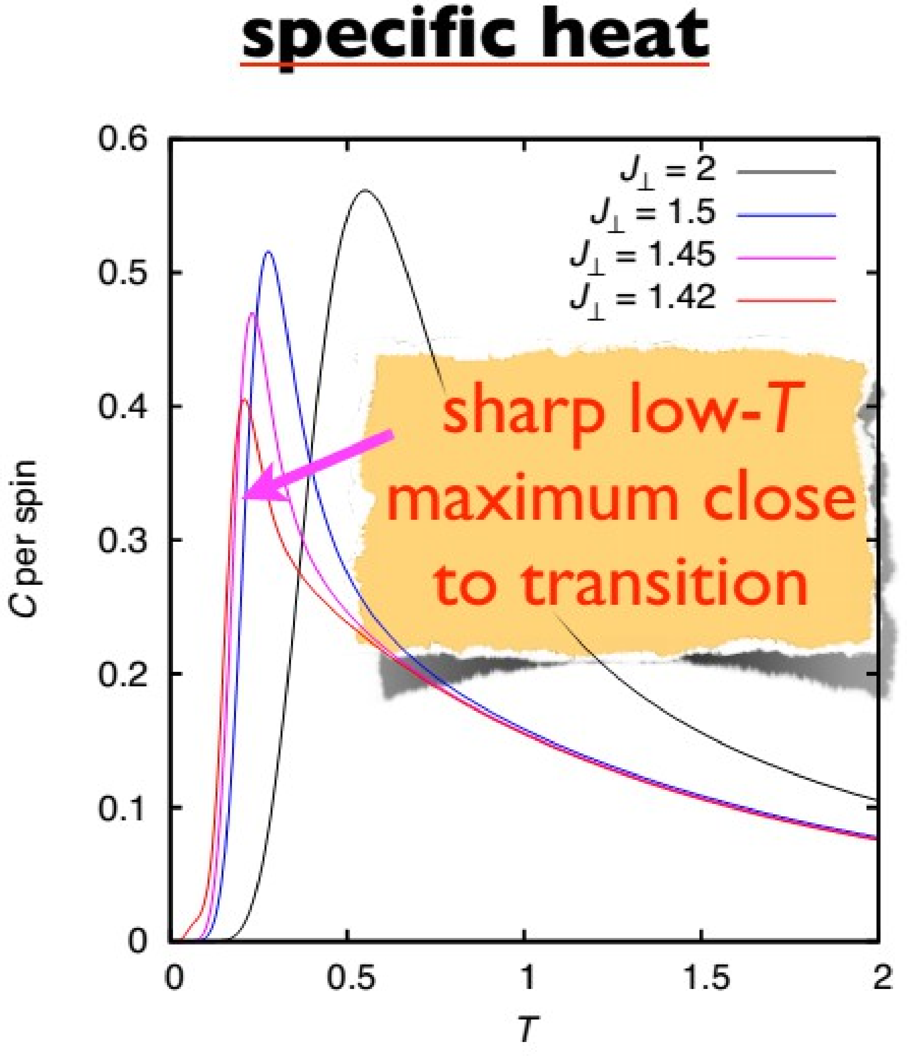
The 3-triplet bound state has $E_{3h} = 3J + 2J'$, $E_{3qa} = 3J + J'$, $E_{3ta} = 3J$, $E_{3qb} = E_{3tb} = 3J - J'$, $E_{3s} = 3J - 2J'$, $E_{3tc} = 3J - 3J'$.

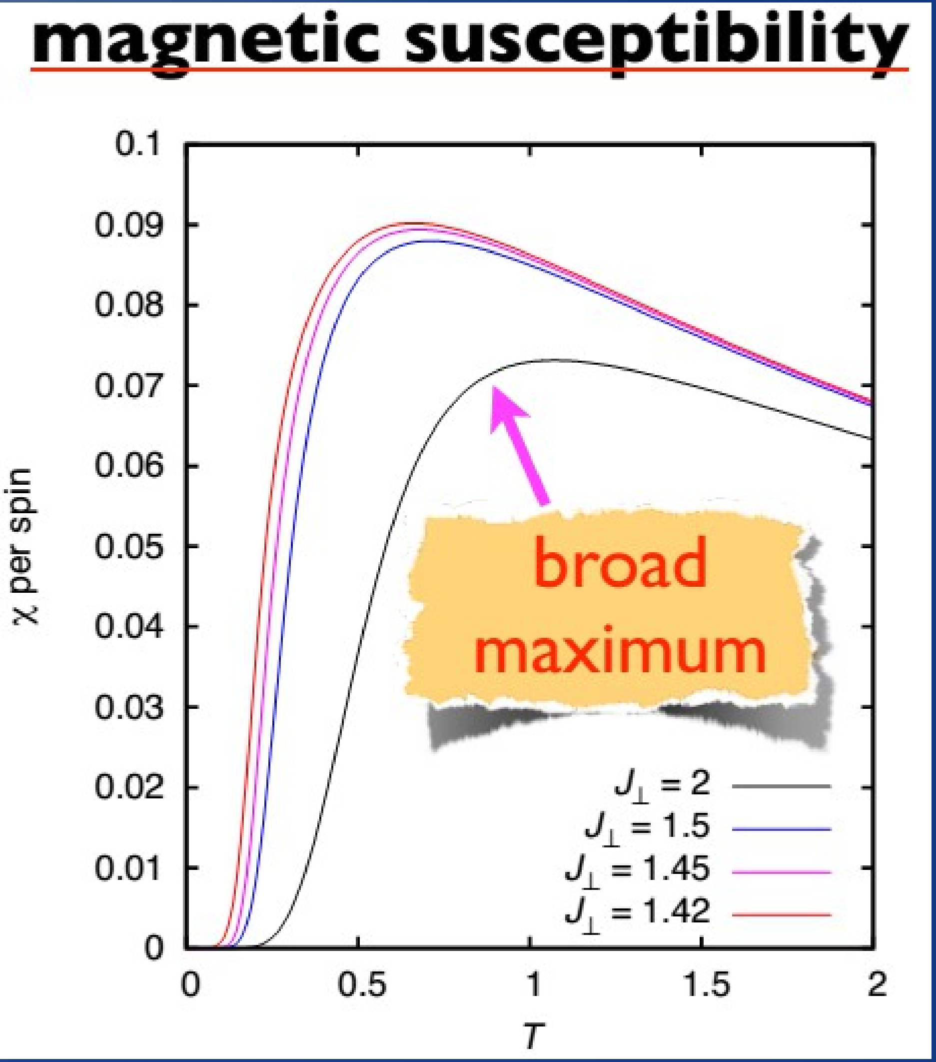
$$S^{zz}(\vec{k},\omega) = \frac{1}{\pi Z}\sum_{n,m} \mathrm{Im} \frac{\mathrm{e}^{-E_n/T} \left| \langle n | S^z(\vec{k}) | m \rangle \right|^2}{\omega - (E_m - E_n + i\,\eta)}$$

These results are used to interpret the **thermodynamic response**, $C_m(T)$ and $\chi(T)$ computed by ED and QMC, as well as the **dynamical structure factor** $S(q,\omega,T)$ computed by finite-T ED.

Thermodynamics I: Gaps

Exact diagonalisation calculations performed for ladders of *14* x *2* spins.





Measure of singlet spectrum.

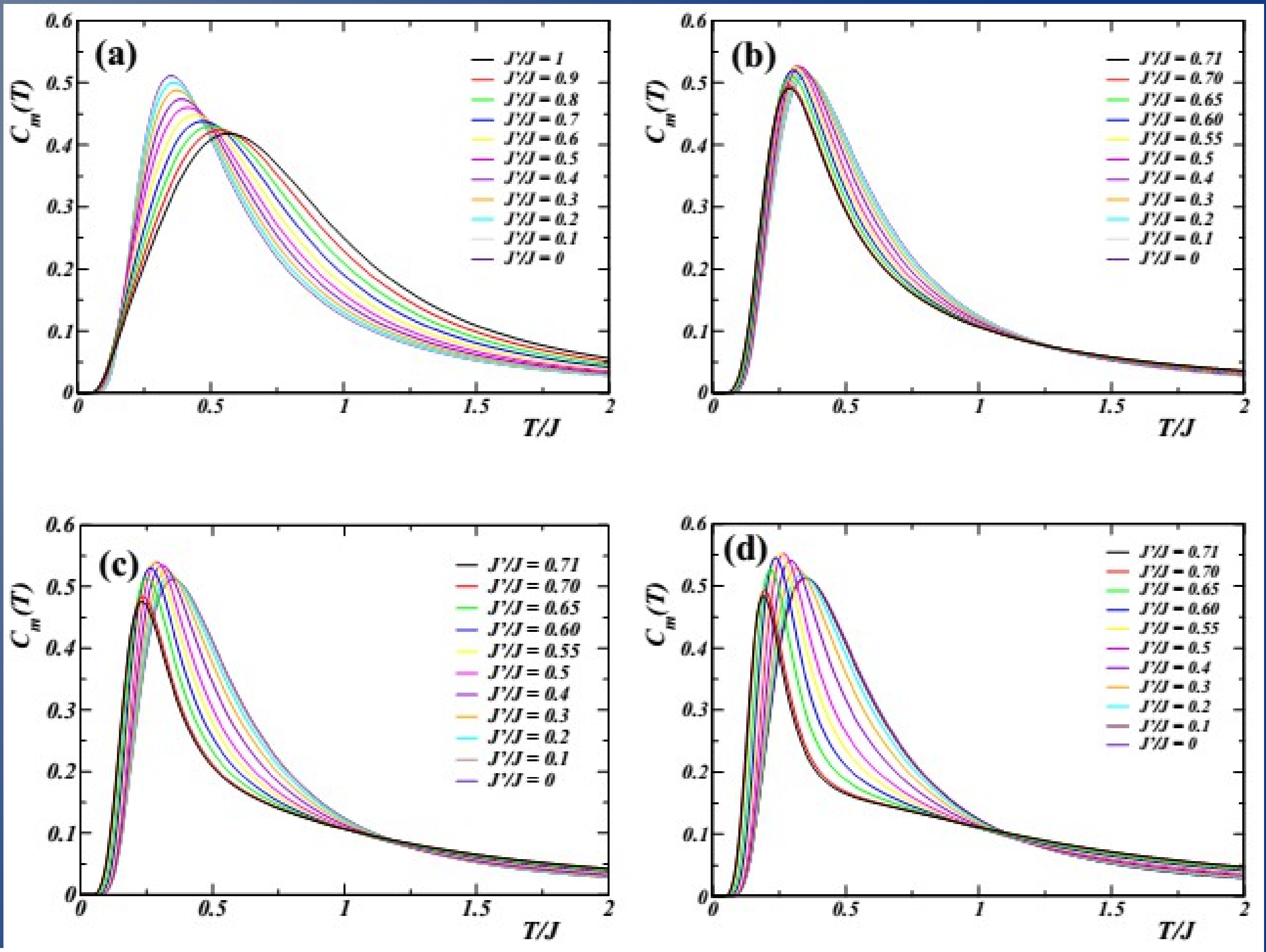
Measure of triplet spectrum.

Thermodynamics II: Cluster Model

Interpretation: (a) shows the specific heat of an unfrustrated system, (b-d) of fully frustrated ones.

For (b-d), the gap decreases below $J_r = 2$ (above $J'/J = 0.5$) and **the maximum moves to lower T**.

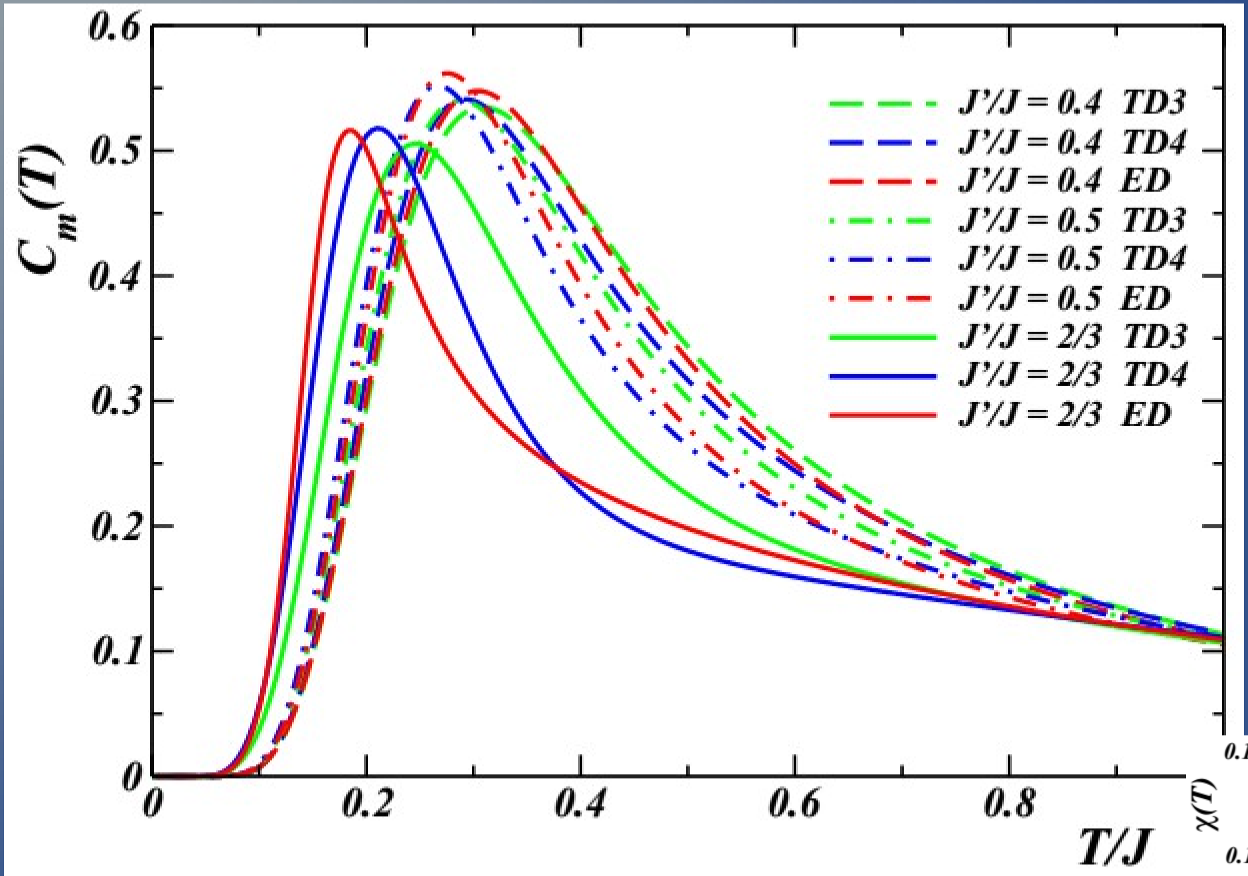
The position of the maximum can be reproduced in a simple model for the thermo-dynamic response of



$$
\begin{aligned}
Z_1(\beta) &= 1 + 3e^{-\beta J}, \\
Z_2(\beta) &= 1 + 6e^{-\beta J} + \sum_m g_{2m} e^{-\beta E_{2m}}, \qquad (3) \\
Z_3(\beta) &= 1 + 9e^{-\beta J} + 3\sum_m g_{2m} e^{-\beta E_{2m}} + \sum_m g_{3m} e^{-\beta E_{3m}},
\end{aligned}
$$

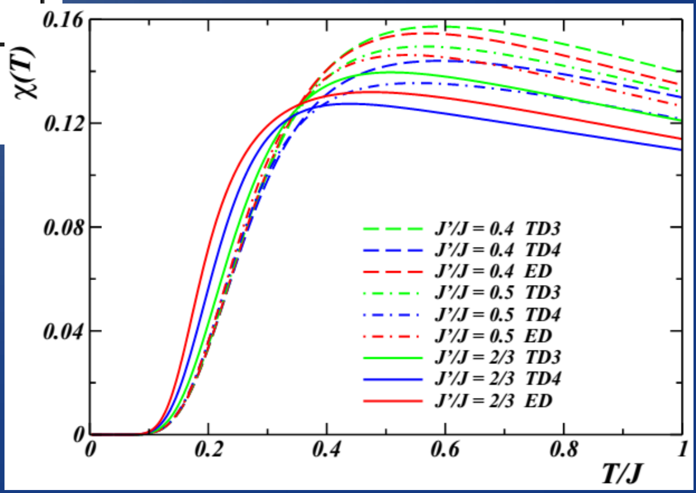
one-, two-, three- … dimer clusters, which represent the energies of bound states up to the same maximum sizes.

Thermodynamics III: Multi-Triplet Bound States



Even-length clusters contain low-lying singlets close to the gap energy and provide a more accurate account of the magnetic specific heat. However, for coupling ratios near the QCP they fail to reproduce the **anomalously low peak position.**

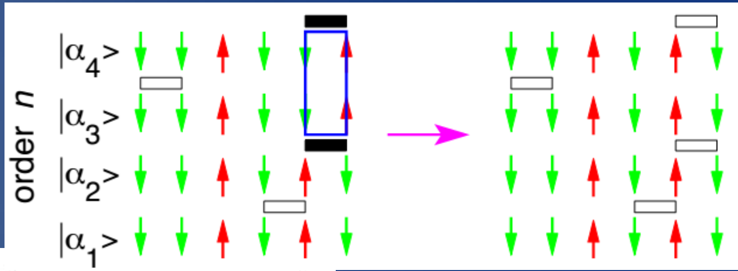
Odd-length clusters contain low-lying triplets close to the gap energy and provide the most accurate account of the magnetic susceptibility, although this broad function is less sensitive to details of the spectrum.

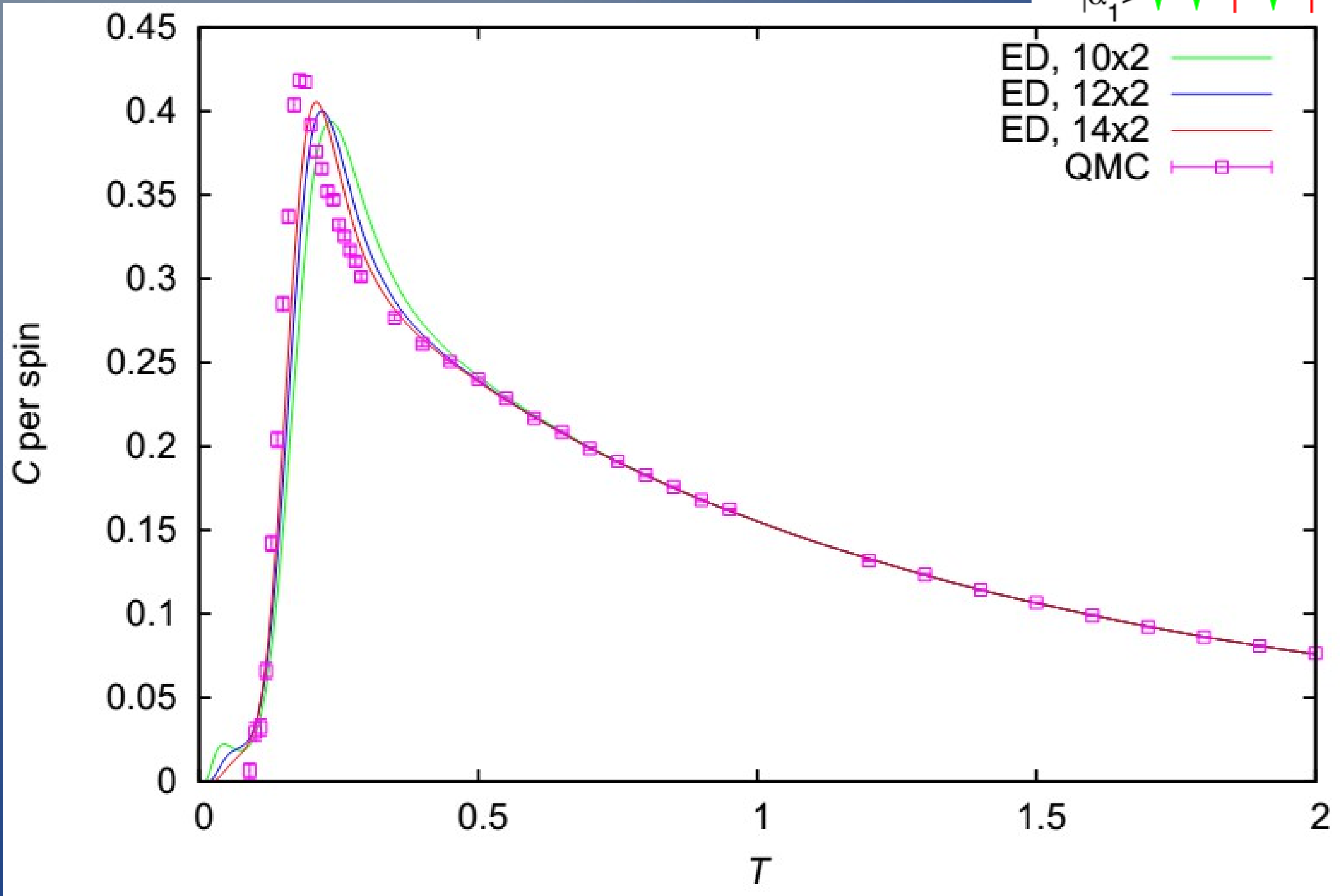


Thermodynamics IV: QMC

with R. Kerkdyk, S.Wessel and T. Pruschke

The fully frustrated ladder can be coded as a sign-problem-free system and hence its thermodynamic properties can be calculated by Stochastic Series Expansion Quantum

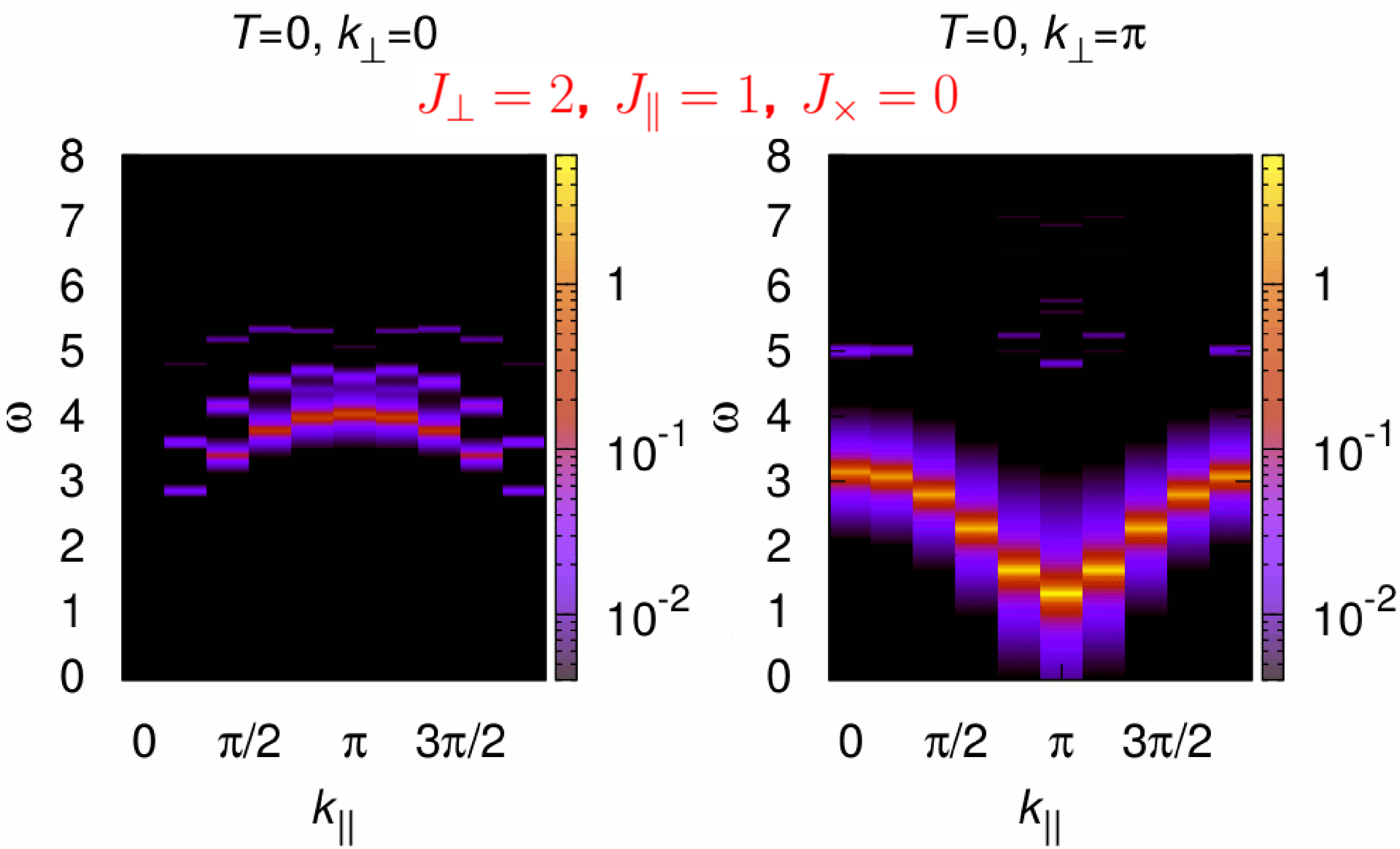




Monte Carlo methods. The large system sizes (*L = 100* x *2* spins) made accessible by this technique allow a complete elimination of the finite-size effects visible in the ED results close to the QCP.

Dynamical Structure Factor I: Unfrustrated

Unfrustrated ladder: dispersive bands and spreading of spectral weight equally to all energies at high temperatures.



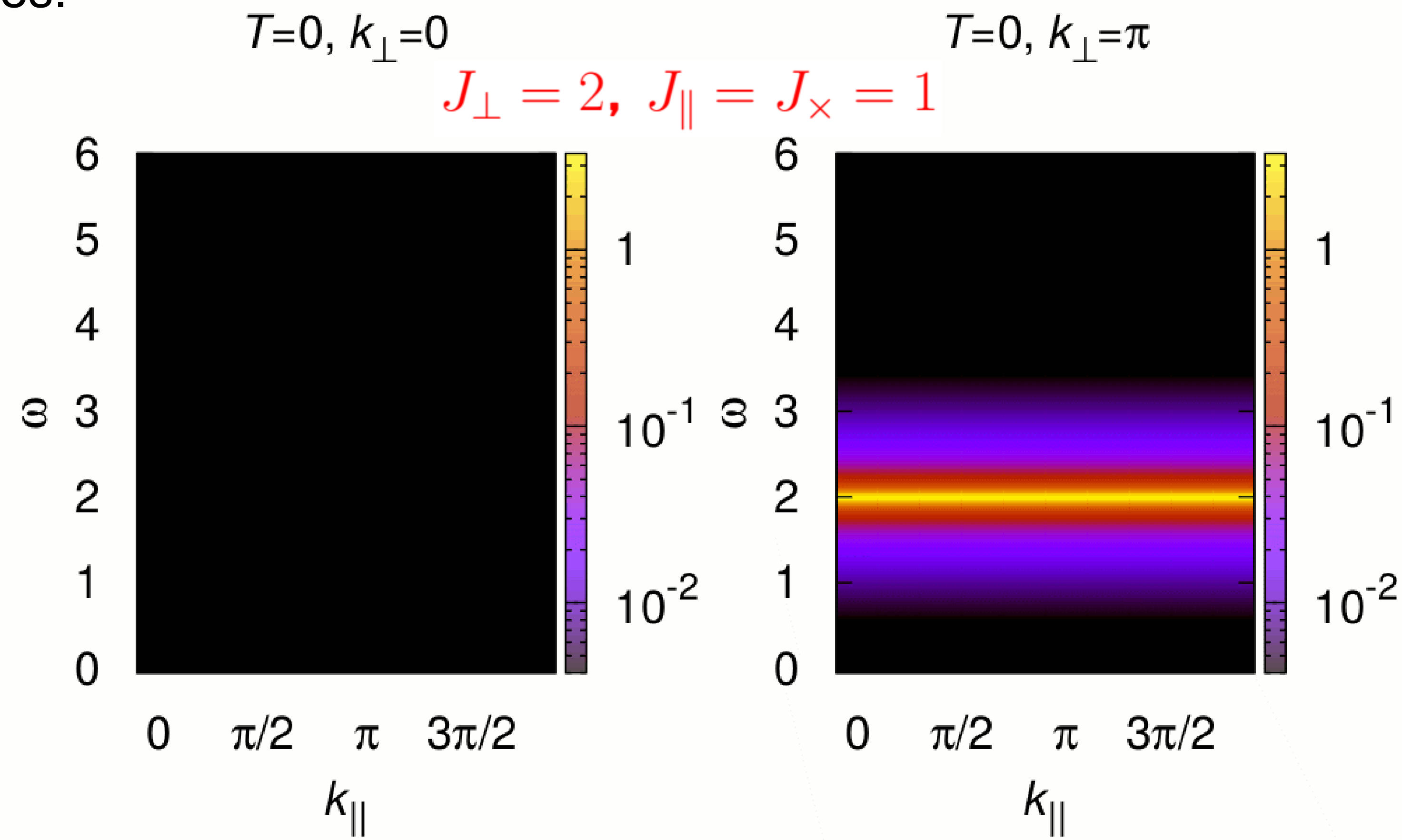
Symmetric channel: two-magnon excitations

Antisymmetric channel: one-magnon excitations

Here the system size is *L* = *10* rungs; although finite-size effects may be significant, these spectra benchmark the behaviour of a typical system with dispersive excitations.

Dynamical Structure Factor II: Fully Frustrated

Generic fully frustrated ladder situation: a number of flat bands contribute significantly due to the presence of multi-triplet bound states.

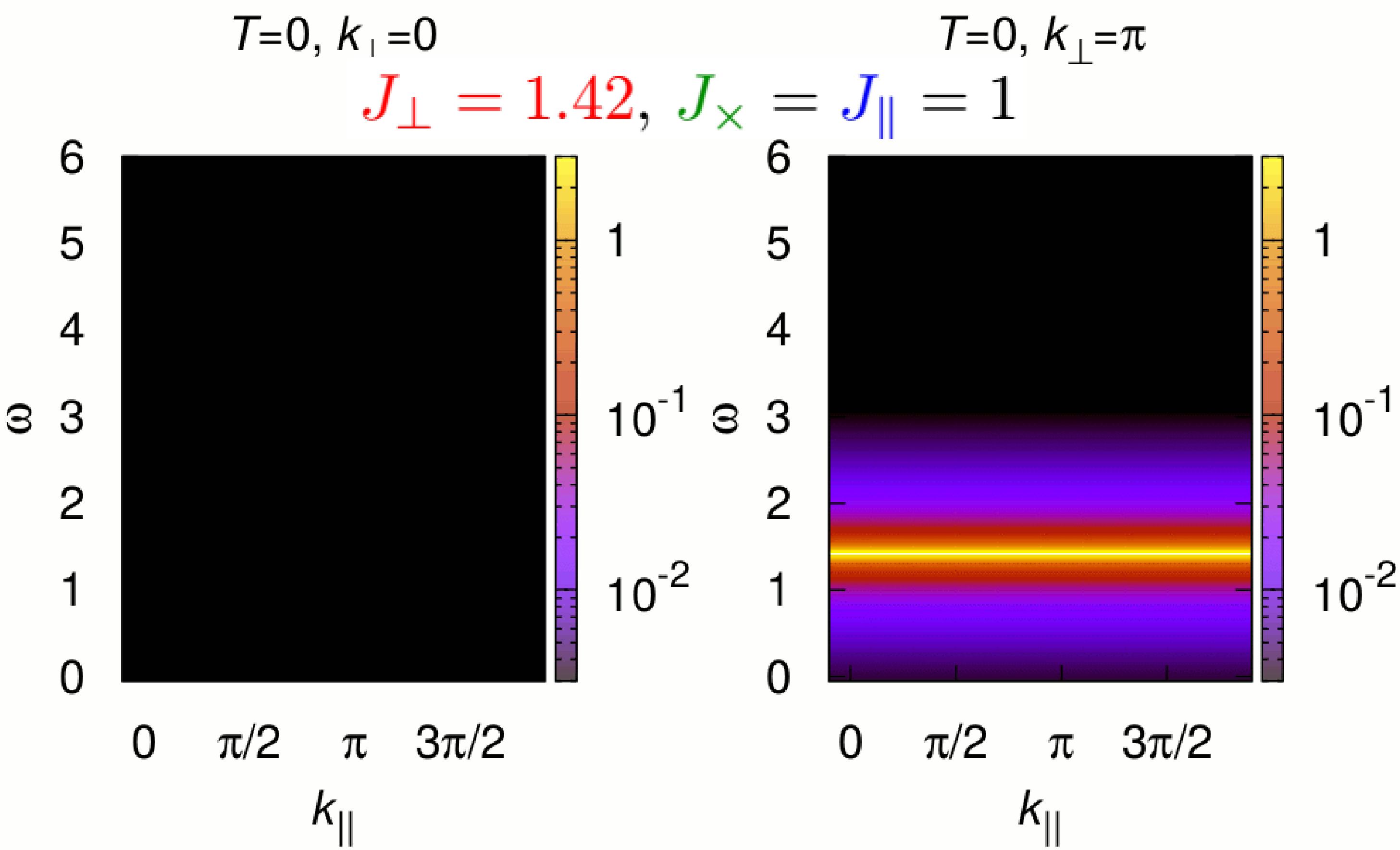


Energies and relative intensities may be deduced from couplings and splittings in two-, three-, four- … triplet bound states.

Here finite-size effects are negligible due to the very short correlation length in the fully frustrated ladder. These spectra show the behaviour of a typical system with flat triplet bands.

Dynamical Structure Factor III: QCP

Close to the QCP, the spectral weight is spread over a wide range of energies even at very low temperatures.



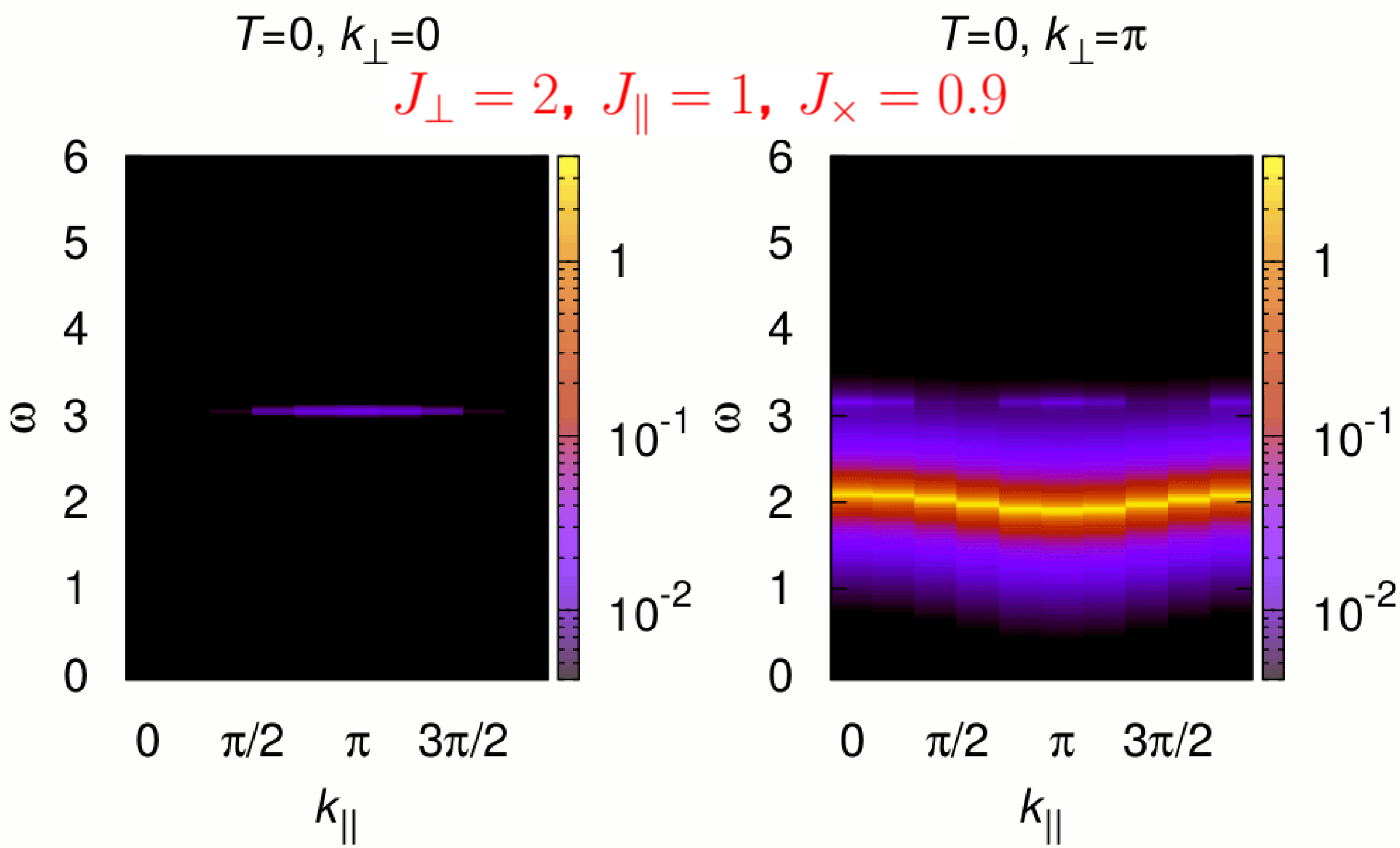
This occurs due to presence of many multi-triplet bound states at energies near the gap.

Here finite-size effects are once again important, because the many-triplet bound states are extended objects, but the calcula-tions remain a good qualitative description of $S(q,\omega,T)$.

Dynamical Structure Factor IV: Partial Frustration

If the fully frustrated ladder is "detuned" from the flat-band situation, the bound states are no longer exact.

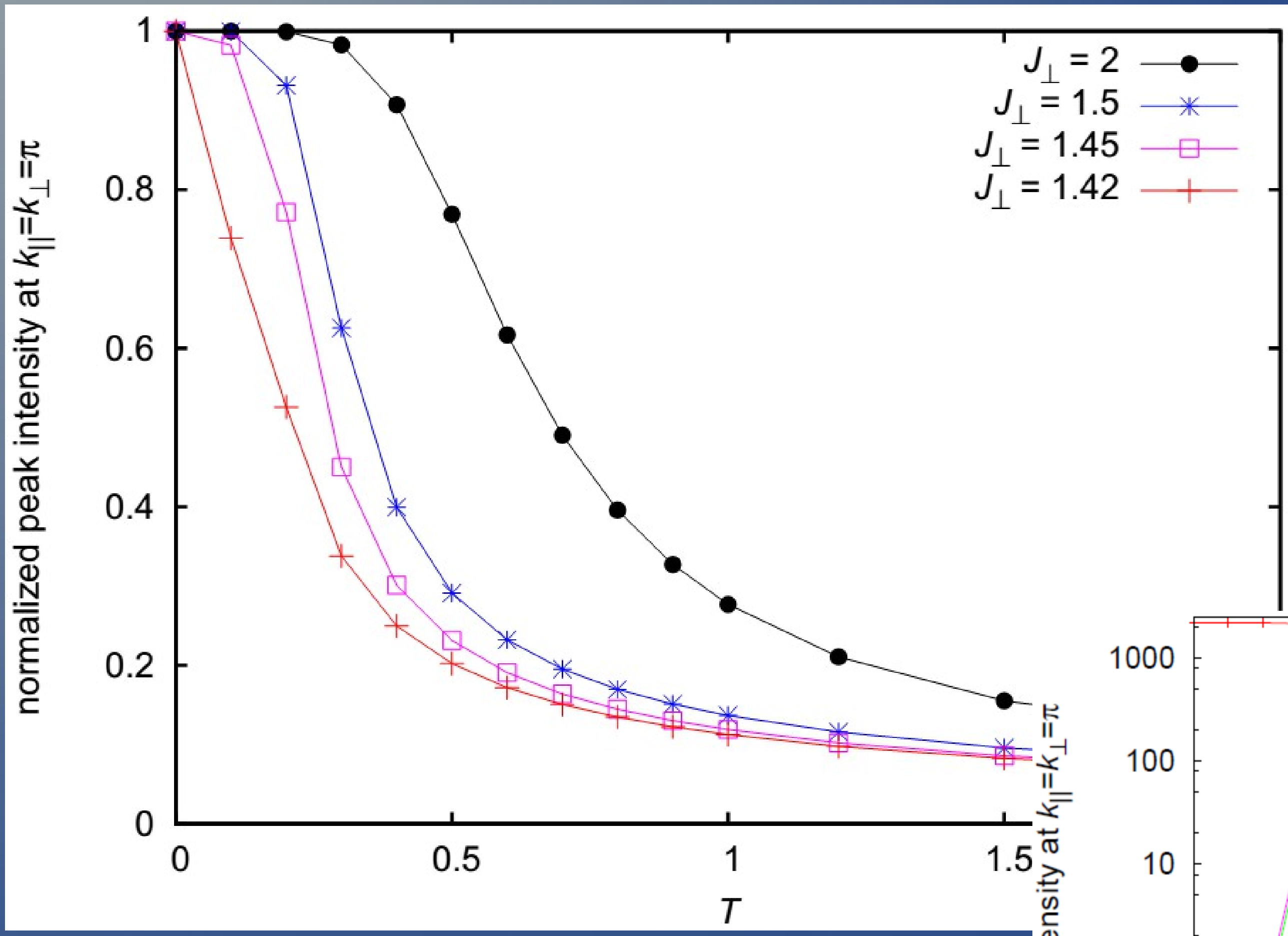
$J_\perp = 2, \; J_\parallel = 1, \; J_\times = 0.9$



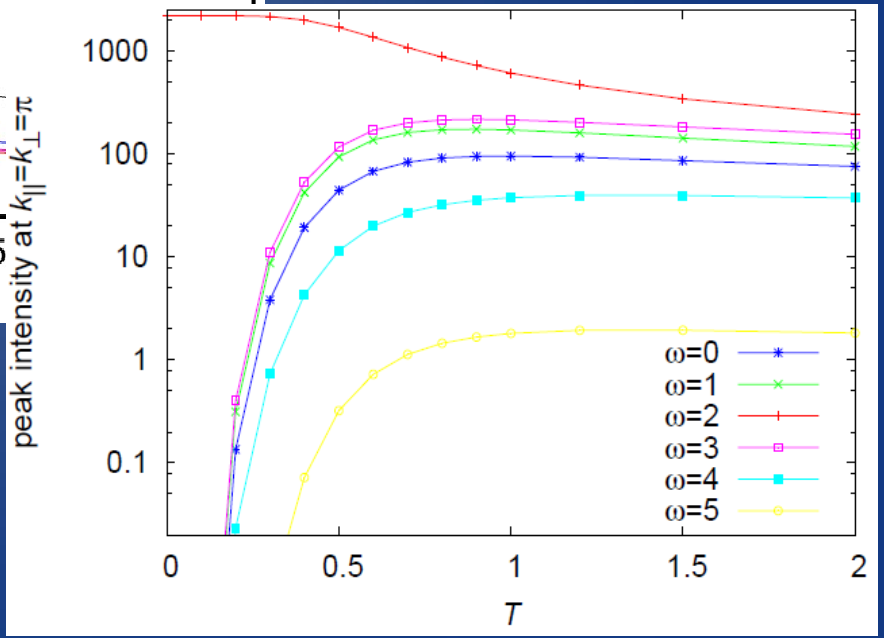
As these multiplets begin to disperse in *k*, continuum spreading of the spectral weight appears over narrow regions of ω.

In this case finite-size effects are once again small. These spectra show limited dispersive behaviour and line-broadening in a system with nearly-flat triplet bands.

Dynamics V: Spectral-Weight Shifts

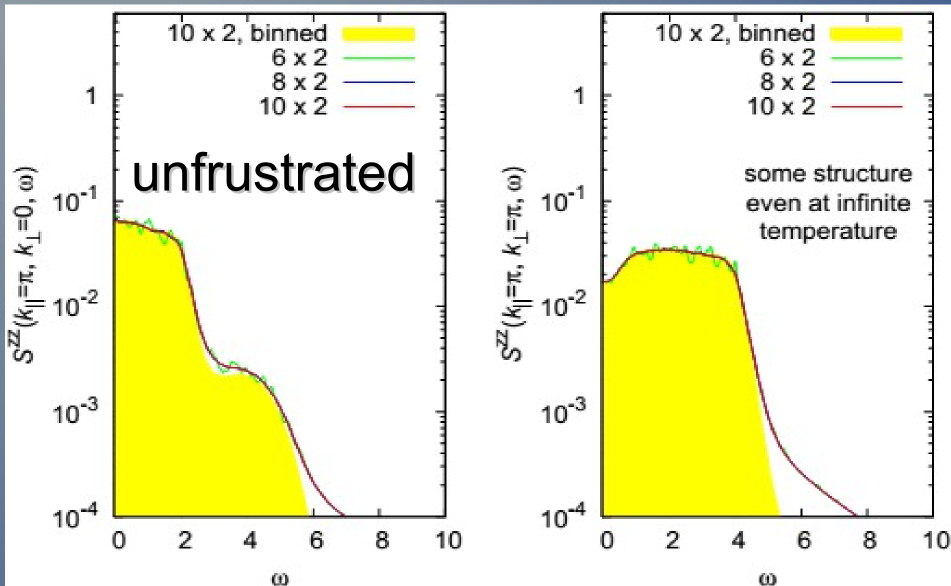


The spectral weight remaining in one-triplet band for the fully frustrated ladder falls with increasing T; this decrease is very abrupt near the QCP due to the **proliferation of many-triplet bound states.**

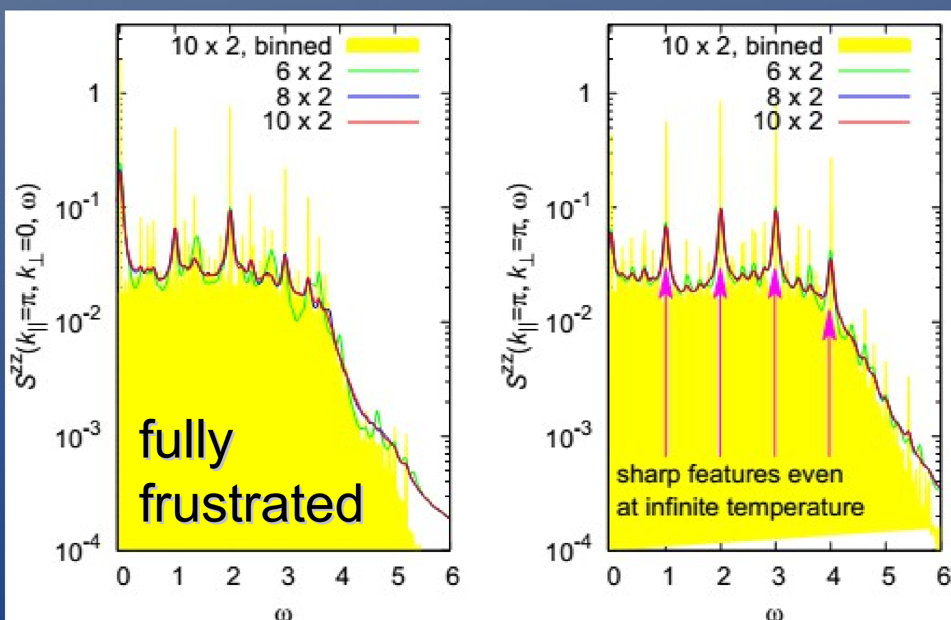


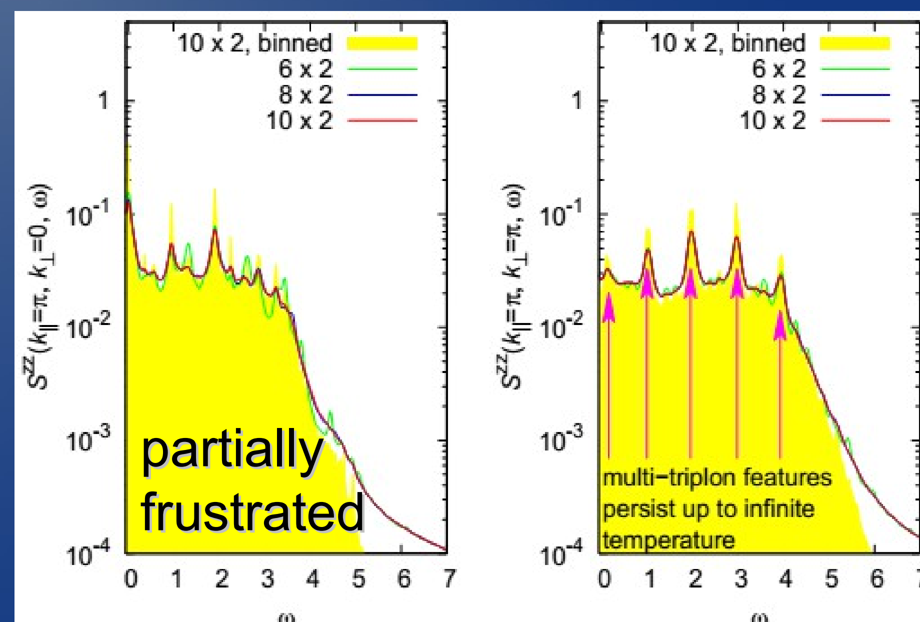
The bound states with the strongest spectral weights correspond to the leading low-lying triplet states of the smaller (odd-length) multi-triplet clusters.

Dynamics VI: Infinite Temperature



Sharp spectral features remain present in the fully frustrated system **at the highest temperatures**. *This is a consequence of the discrete support.* It contrasts strongly with the flat spectrum of the unfrustrated ladder, which shows only separate triplet sectors. Nearly-flat bands give finite peak widths at infinite temperature.





Summary

- interplay of quantum and thermal fluctuations
- frustrated systems: flat bands and bound states
- quantum critical proliferation of bound states
  – extended states of many triplets at gap energy
- thermodynamics: broadening and peak shifts
- dynamical spectral function $S(q,\omega,T)$:
  – discrete support determined by bound-states,
  – anomalously strong weight shifts near QCP,
  – well-defined features at infinite *T*.
- experiment: thermal evolution is interesting …
  frustrated systems are cool …
  especially near a QCP …