

Field Theory Approach to the Dynamics of Gapped Quantum Spin Chains

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Outline

1. Why low-D Quantum Spin Systems are interesting.
2. Some Gapped Quantum Spin Chains and their Quantum Field Theory Limits.
3. Integrable QFTs.
4. $T=0$ Dynamical Response Functions in integrable QFTs.
5. $T>0$ Dynamical Response Functions in integrable QFTs.
6. Nonequilibrium Dynamics.

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$$H = -t \sum_{\langle j,k \rangle, \sigma} c_{j,\sigma}^\dagger c_{k,\sigma} + \text{h.c.} \\ + U \sum_j n_{j,\uparrow} n_{j,\downarrow}$$

large U/t

$$H' = \frac{4t^2}{U} \sum_{\langle j,k \rangle} \mathbf{S}_j \cdot \mathbf{S}_k$$

Why (Low-D) Quantum Spin Systems are interesting:

Quantum Spin Systems are inherently **strong coupling** problems:



strong interactions are interesting as they are expected to lead to new **collective** behaviour

Dimensionality

D=3

“Conventional Behaviour”: Spontaneous Symmetry

Breaking of spin rotational symmetry at low T;
Physics of Long-Range Order (spinwaves)

Spinwaves determine physics over large range of T
and E (even far above T_N)

Basic physics is well understood.



Look at **Frustrated Systems** to
avoid simple SSB scenario; but
physics usually well described
classically.

Dimensionality

D=2

(layered materials)

Quantum Fluctuations are **stronger**: SSB only at T=0 (Mermin-Wagner).

Frustrated systems may realize new quantum states of matter: **Quantum Spin Liquids**

→ **very interesting**, but difficult to address theoretically by analytic or numeric means.

Dimensionality

D=1

(chain materials)

Quantum Fluctuations are **very strong**: SSB not even at $T=0$ (Mermin-Wagner).

Exotic Quantum Spin Liquid States are abundant in D=1.

- **Special techniques** (integrability, bosonization, DMRG, insert your favourite method here) **allow in depth analysis.**
- High-resolution experiments on **dynamical properties** for many materials.

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Paradigm 1: spin-1/2 Heisenberg Chain

- **Gapless spin liquid** (ground state disordered for all $T \geq 0$) Hulthen '38
- Excitations: fractionalized spin-1/2 objects "spinons" Faddeev&Takhtajan '84
- $T=0$: **quantum critical system** (power-law decays of correlations)
Luther&Peschel '75
Haldane '81
- low energy properties: **Luttinger Liquid**

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Extremely interesting! Remains object of much recent work (e.g. threshold singularities).

Glazman, Imambekov,
Pustilnik, Khodas,...
Affleck, Pereira, White,
Sirker...
Zvonarev, Cheianov,
Giamarchi
'06 - '11

A different talk !

Gapped Quantum Spin Chains & Ladders

A. Integer Spin Heisenberg Chains ($S=1,2,3,\dots$)

$$H = J \sum_n S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z, \quad S_j^2 = S(S+1).$$

Haldane '83, Affleck '90

Kenzelmann et. al. '01

Zaliznyak et. al. '01

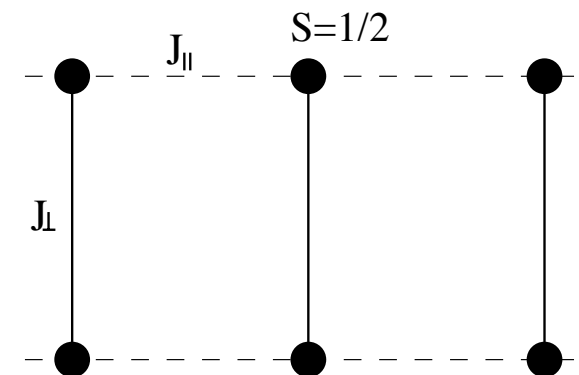
Zheludev et. al. '04

Xu et. al. '07

CsNiCl₃, NDMAP, YBaNiO₅...

B. 2-Leg Heisenberg Spin-1/2 Ladders

$$H = J_{\parallel} \sum_{a=1}^2 \sum_j S_{a,j} \cdot S_{a,j+1} + J_{\perp} \sum_j S_{1,j} \cdot S_{2,j}$$



Dagotto et. al. '92, Shelton et. al. '96,
Schmidt&Uhrig '05 ...

Notbohm et. al. '07; Ruegg et. al. '08,

Lake et. al. '10, Thielemann et. al. '09

Bouillot et. al. '11, Tennant et. al. '12,

Schmidiger et. al. '12 ...

CuNitrate, (C₅H₁₂N)₂CuBr₄, CaCu₂O₃, La₄Sr₁₀Cu₂₄O₄₁,
DIMPY ...

C. Field-Induced Gap spin-1/2 chain materials

$$\mathcal{H} = \sum_j JS_j \cdot S_{j+1} - HS_j^z - h(-1)^j S_j^x .$$

CuBenzoate, CDC, Cu-Pyrimidine, Yb₄As₃,...

Dender et al '97, Asano et al '00, '02,
Feyerherm et al '00, Kohgi et al '01,
Zvyagin et al '04, '05...

Oshikawa&Affleck '97, '02
Essler&Tsvetik '97, Essler '99, ...

D. Transverse Field Spin-1/2 Chain

$$\mathcal{H} = \sum_j J[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \delta S_j^z S_{j+1}^z] - HS_j^x .$$

Cs₂CoCl₄, CsCoBr₃, CsCoCl₃, TlCoCl₃, ...

Nagler et al '82; Kenzelmann et al '02;
Oosawa et al '06

Dmitriev, Krivnov&Ovchinnikov '02
Caux, Essler&Loew '03
Coldea et al (unpublished)

E. J_1 - J_2 Model a.k.a. 2-leg zigzag ladder

$$\mathcal{H} = J_1 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+2} \quad J_2 > 0.2411 J_1 > 0$$

Haldane '82, White&Affleck '96,
Eggert '96, Nersesyan et al '98, ...

SrCuO₂, LiCuVO₄ (ferromagnetic J_1),...

F. Dimerized Spin-1/2 Chain

$$\mathcal{H} = J \sum_n [1 - (-1)^n \delta] \mathbf{S}_n \cdot \mathbf{S}_{n+1}$$

Uhrig&Schulz '96, Essler, Tsvetlik&Delfino '96
Knetter&Uhrig '00, Orignac '04,...

CuGeO₃

G. Transverse Field Ising Chain

$$\mathcal{H} = -J \sum_j S_j^x S_{j+1}^x + h S_j^z$$

Coldea et al '10

Pfeuty '70, Wu et al '76, Vaidya&Tracy '78
Cardy&Mussardo '90, Yurov&Zamolodchikov '91

CoNb₂O₆

Field Theory Limit of Quantum Spin chains

Spin- S Heisenberg model with $S \gg 1$.

Haldane '83,
Affleck '89

staggered component: $n_{2i+1/2}^a = (S_{2i+1}^a - S_{2i}^a)/2S$,

smooth component: $M_{2i+1/2}^a = (S_{2i+1}^a + S_{2i}^a)/2$.

Constraint:

$$\mathbf{n} \cdot \mathbf{n} = 1 + \frac{1}{s} - \frac{\mathbf{M} \cdot \mathbf{M}}{s^2} \approx 1, \quad \mathbf{n} \cdot \mathbf{M} = 0.$$

Naive Continuum Limit: $n_{2i+1/2}^a \rightarrow n^a(x), M_{2i+1/2}^a \rightarrow a_0 M^a(x),$

$$H = \frac{v}{2} \int dx \left[g \left(\mathbf{M} + \frac{\theta}{4\pi} \partial_x \mathbf{n} \right)^2 + \frac{1}{g} (\partial_x \mathbf{n})^2 \right], \quad \theta = 2\pi S, \quad g = 2/S, \quad v = JSa_0.$$

Commutators:

$$\begin{aligned} [M^a(x), M^b(y)] &= i\epsilon^{abc} M^c(x) \delta(x-y) , \\ [M^a(x), n^b(y)] &= i\epsilon^{abc} n^c(x) \delta(x-y) , \\ [n^a(x), n^b(y)] &= \frac{1}{S^2} i\epsilon^{abc} M^c(x) \delta(x-y) \simeq 0. \end{aligned}$$

solved by

$$M^a(x) = \frac{1}{vg} \mathbf{n}(x) \times \frac{\partial \mathbf{n}(x)}{\partial t}.$$



O(3) nonlinear
sigma model

$$\mathcal{L} = \frac{v}{2g} \partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n}$$

Constraint: $\mathbf{n} \cdot \mathbf{n} = 1$

$$\begin{aligned} v &= JSa_0. \\ g &= 2/S \end{aligned}$$

When does this QFT describe the lattice model ?

- large distances, late times (for dynamics)
- low energies: $\omega \ll J$
- gap much less than cutoff $\rightarrow \Delta \ll J$

C. Field-Induced Gap spin-1/2 chain materials

$$\mathcal{H} = \sum_j JS_j \cdot \mathbf{S}_{j+1} - HS_j^z - h(-1)^j S_j^x .$$



$$\mathcal{H} = \frac{v}{16\pi} \int dx \left[(\partial_x \Phi)^2 + (\partial_x \Theta)^2 \right] - \mu(h) \int dx \cos(\beta\Theta).$$

Sine-Gordon model

$$\partial_x \Theta = -\partial_t \Phi$$

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$$\beta = \beta(H)$$

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C.N. Sine



R. Gordon

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$$H = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[\frac{iv}{2} (\bar{\psi} \partial_x \bar{\psi} - \psi \partial_x \psi) - i\Delta \psi \bar{\psi} \right]$$

Majorana (real) fermion

B. 2-Leg Heisenberg Spin-1/2 Ladders

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$$\mathcal{H} = \sum_{a=1}^4 \int \frac{dx}{2\pi} \left[\frac{iv}{2} (\bar{\psi}_a \partial_x \bar{\psi}_a - \psi_a \partial_x \psi_a) - i\Delta_a \psi_a \bar{\psi}_a \right]$$

$$\Delta_1 = \Delta_2 = \Delta_3 = -\frac{\Delta_4}{\sqrt{3}}$$

4 "Ising models"

These relativistic QFTs are **integrable** (the lattice models are not!)



use integrability to determine
dynamical
correlation functions

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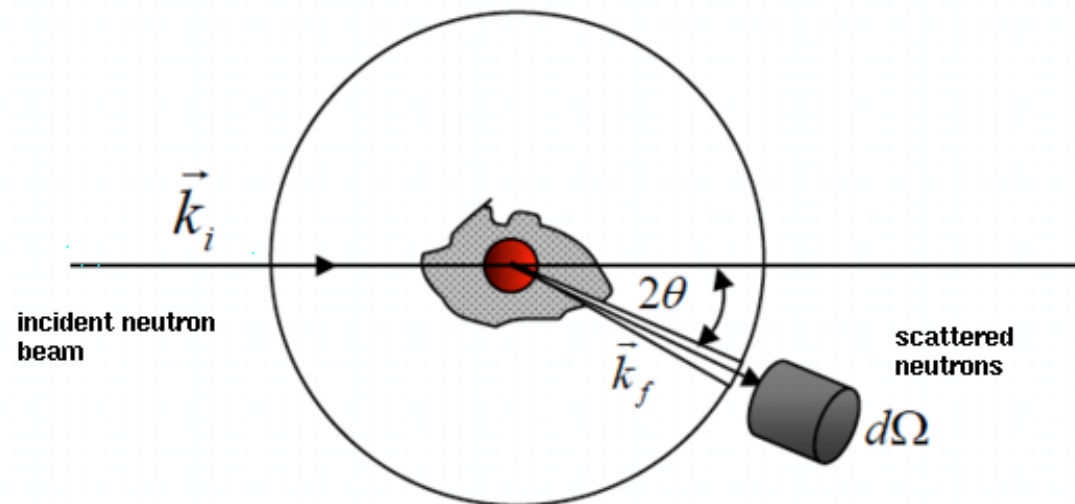


use integrability to determine
dynamical
correlation functions

Which ones?

Scattering Experiments

Scattering Experiments (neutrons, light, electrons) measure **imaginary parts of retarded 2-point functions of local operators**



Inelastic neutron scattering experiments measure

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S(\underbrace{\omega, q}_{\text{energy/mtm transferred to sample}}, T) \propto \int_0^\infty dt e^{i\omega t} \sum_j e^{-iqja_0} \frac{\text{tr} (e^{-H/T} [S_{j+n}^a(t), S_n^a])}{\text{tr} e^{-H/T}}.$$

energy/mtm transferred to sample

What we want to calculate: Spin-S Heisenberg Chain

$$H = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \quad \mathbf{S}_n^2 = S(S+1)$$

$$\mathbf{S}_j \approx S(-1)^{ja_0} \mathbf{n}(x) + \mathbf{M}(x)$$

$$\mathbf{M}(x) = \frac{1}{vg} \mathbf{n}(x) \times \frac{\partial \mathbf{n}(x)}{\partial t}$$

large integer S , low energies

$O(3)$ nonlinear
sigma model

$$\mathcal{L} = \frac{v}{2g} \partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n}$$

Constraint: $\mathbf{n} \cdot \mathbf{n} = 1$

$$v = JSa_0, \\ g = 2/S$$

Susceptibility
around $k = \pi/a_0$:

$$\chi(\omega, k = \frac{\pi}{a_0} + q) \propto -i \int dt dx e^{i\omega t - iqx} \langle [n^a(t, x), n^a(0, 0)] \rangle_T$$

around $k=0$:

$$\chi(\omega, q) \propto -i \int dt dx e^{i\omega t - iqx} \langle [M^a(t, x), M^a(0, 0)] \rangle_T$$

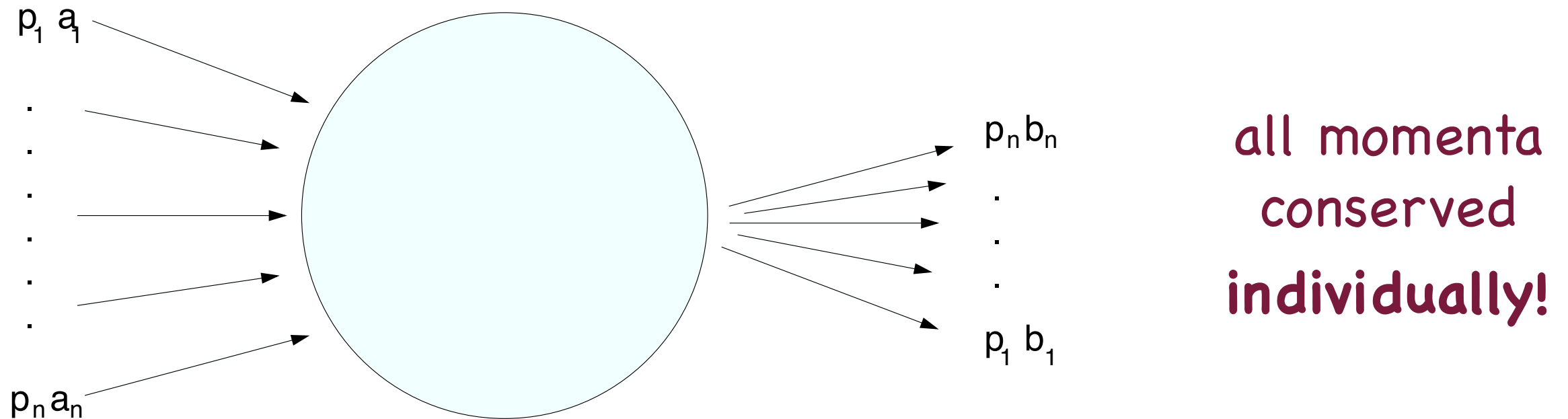
$$|qa_0| \ll \pi$$

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Integrable QFTs

Elementary excitations scatter **purely elastically**



Basis States:

$$|n\rangle = |p_1, \dots, p_n\rangle_{a_1 \dots a_n}$$

Total Momentum:

$$P_n = \sum_{j=1}^n p_j$$

Total Energy:

$$E_n = \sum_{j=1}^n \varepsilon(p_j) \geq n\Delta$$

Remarks:

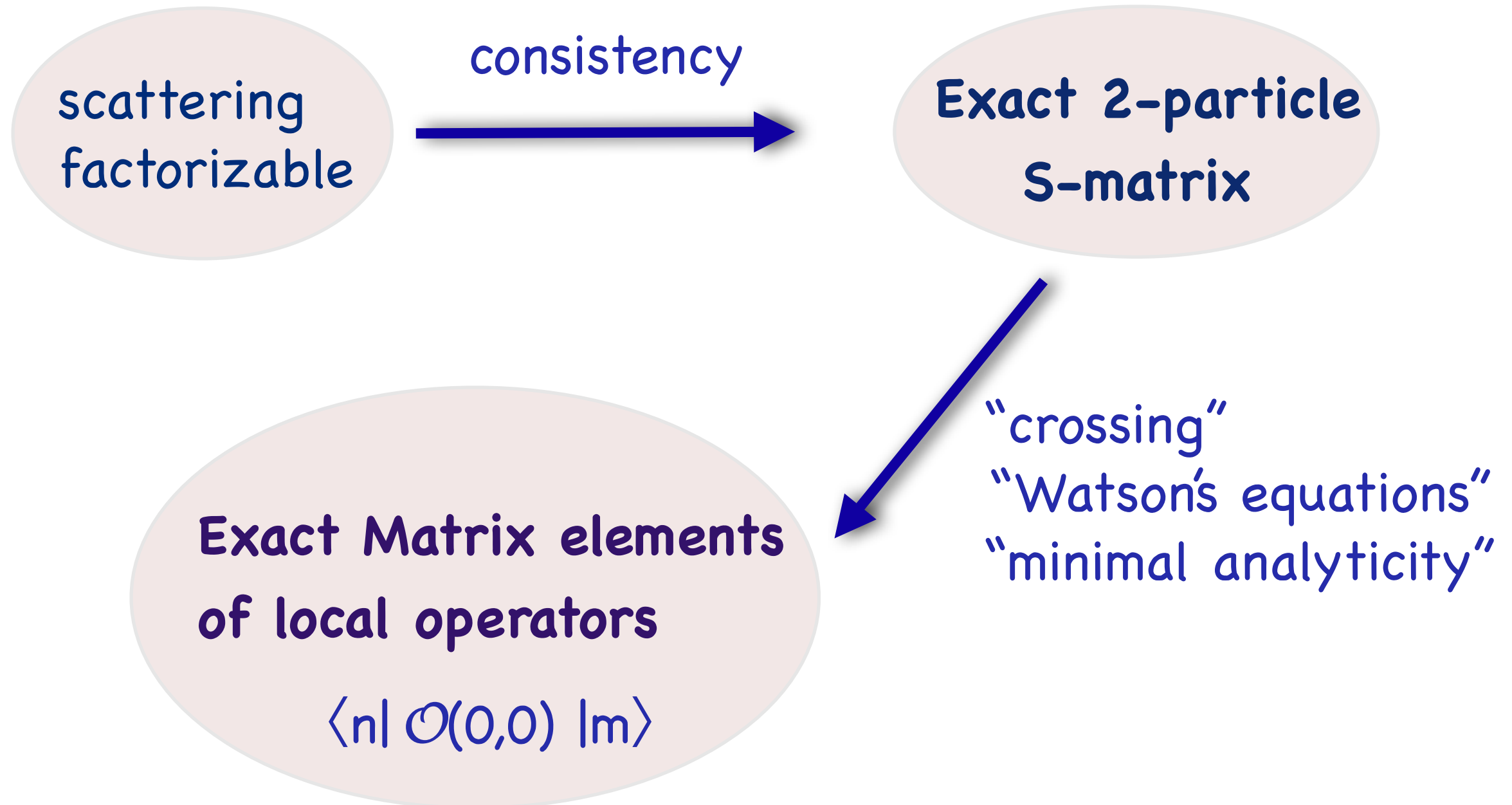
1. Elementary excitations usually very complicated in terms of the fields defining the theory (solitons rather than modes of field)
2. Elementary excitations are **neither bosons nor fermions**:
generalized commutation relations (Faddeev-Zamolodchikov algebra)

$$Z_a^\dagger(p)Z_b^\dagger(q) = S_{ab}^{cd}(p, q)Z_c^\dagger(q)Z_d^\dagger(p)$$

interpolates between fermions ($|p-q|$ small) and bosons ($|p-q|$ large)

"Form Factor Bootstrap Approach"

(Karowski/Weisz '78, Smirnov '93, Lukyanov '95, Delfino/Mussardo '95, Balog/Niedermaier '97, Babujian/Karowski '99...)



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T=0 Dynamical Structure Factor

$$S(\omega, k = \frac{\pi}{a_0} + q) \propto \int dt dx e^{i\omega t - iqx} \langle 0 | n^a(t, x) n^a(0, 0) | 0 \rangle$$

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$$\sum_m |m\rangle \langle m|$$

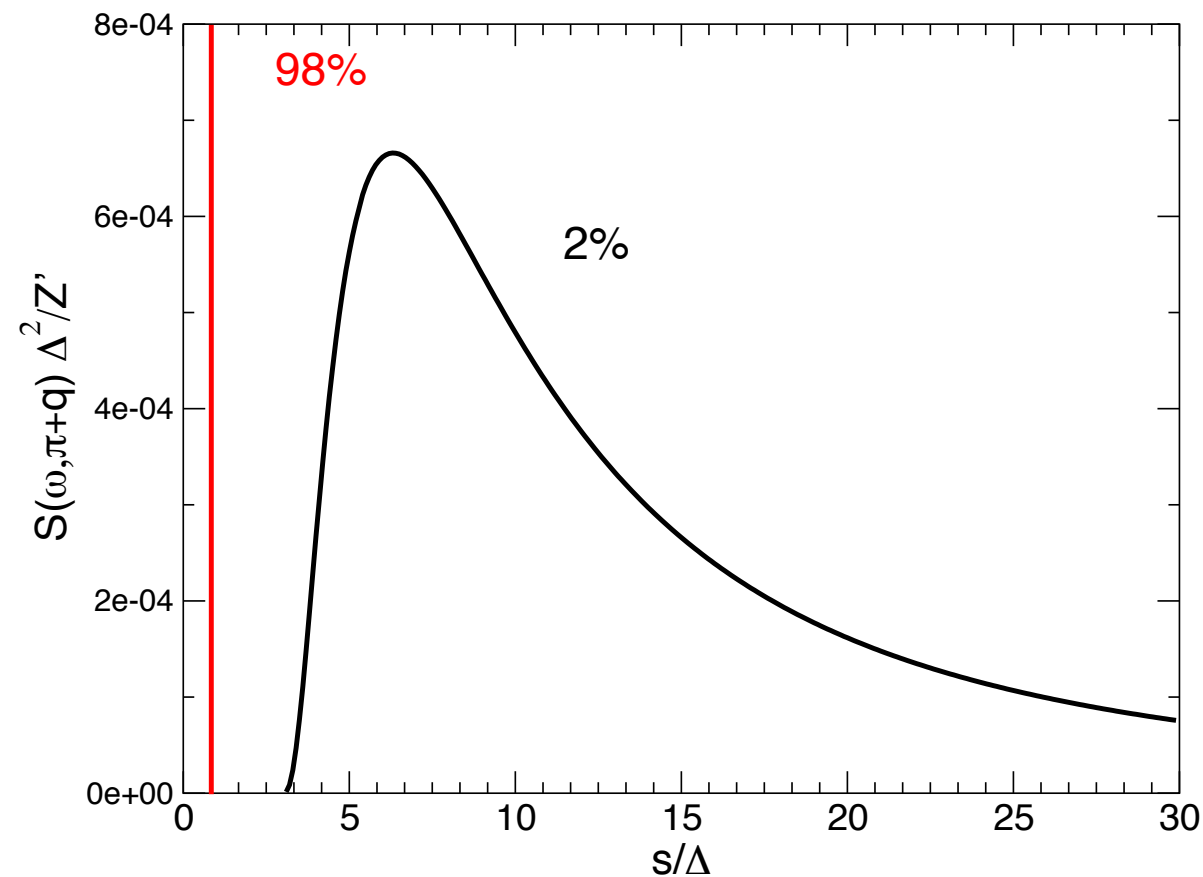

T=0 Dynamical Structure Factor

$$S(\omega, k = \frac{\pi}{a_0} + q) \propto \int dt dx e^{i\omega t - iqx} \langle 0 | n^a(t, x) n^a(0, 0) | 0 \rangle$$
$$\propto (2\pi)^2 \sum_m \left| \langle 0 | n^a(0, 0) | m \rangle \right|^2 \delta(q - P_m) \delta(\omega - E_m)$$

for $\omega < n\Delta$ at most $n-1$ part. states contribute \Rightarrow exact results.

T=0 DSF for O(3) nonlinear sigma model at $q \approx \pi$

(Balog and Niedermaier '97, Affleck and Horton '99, Essler '00)



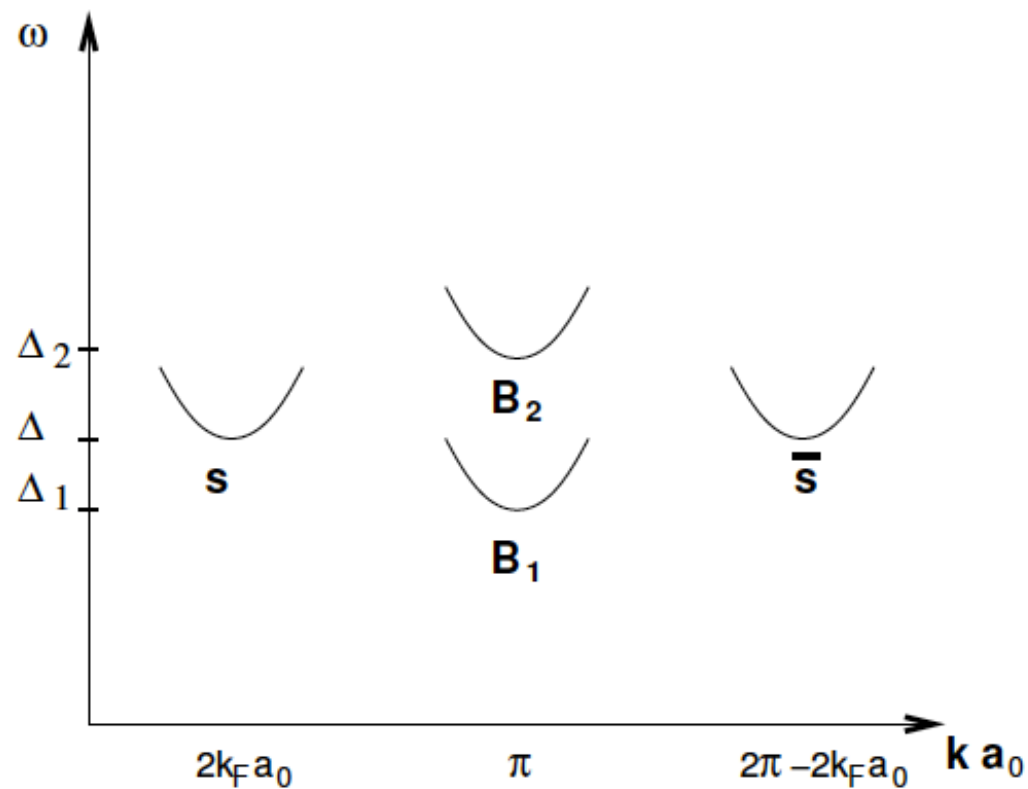
→ **very little** spectral weight above the magnon peak.

sine-Gordon model & field-induced gap systems

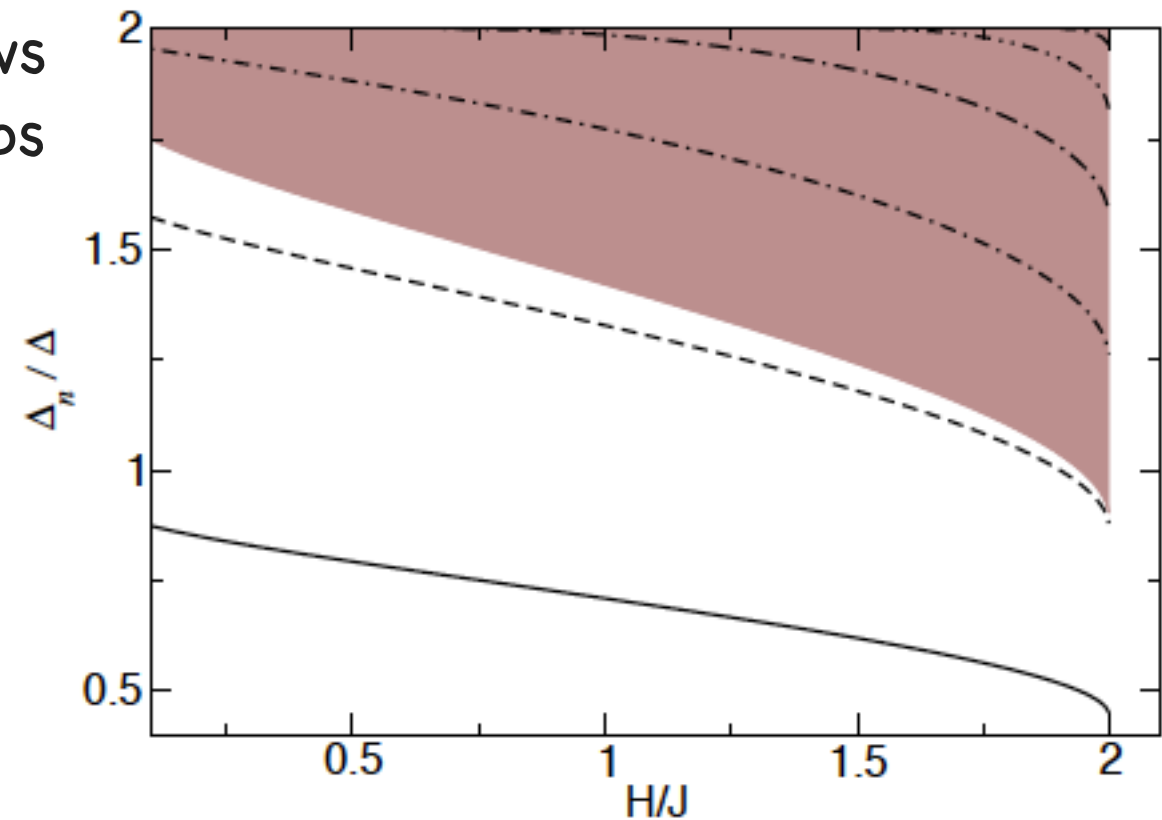
$$\mathcal{H} = \sum_j JS_j \cdot S_{j+1} - HS_j^z - h(-1)^j S_j^x .$$

where $h = \text{const } H$

elementary excitations: soliton, antisoliton and several(H) breathers

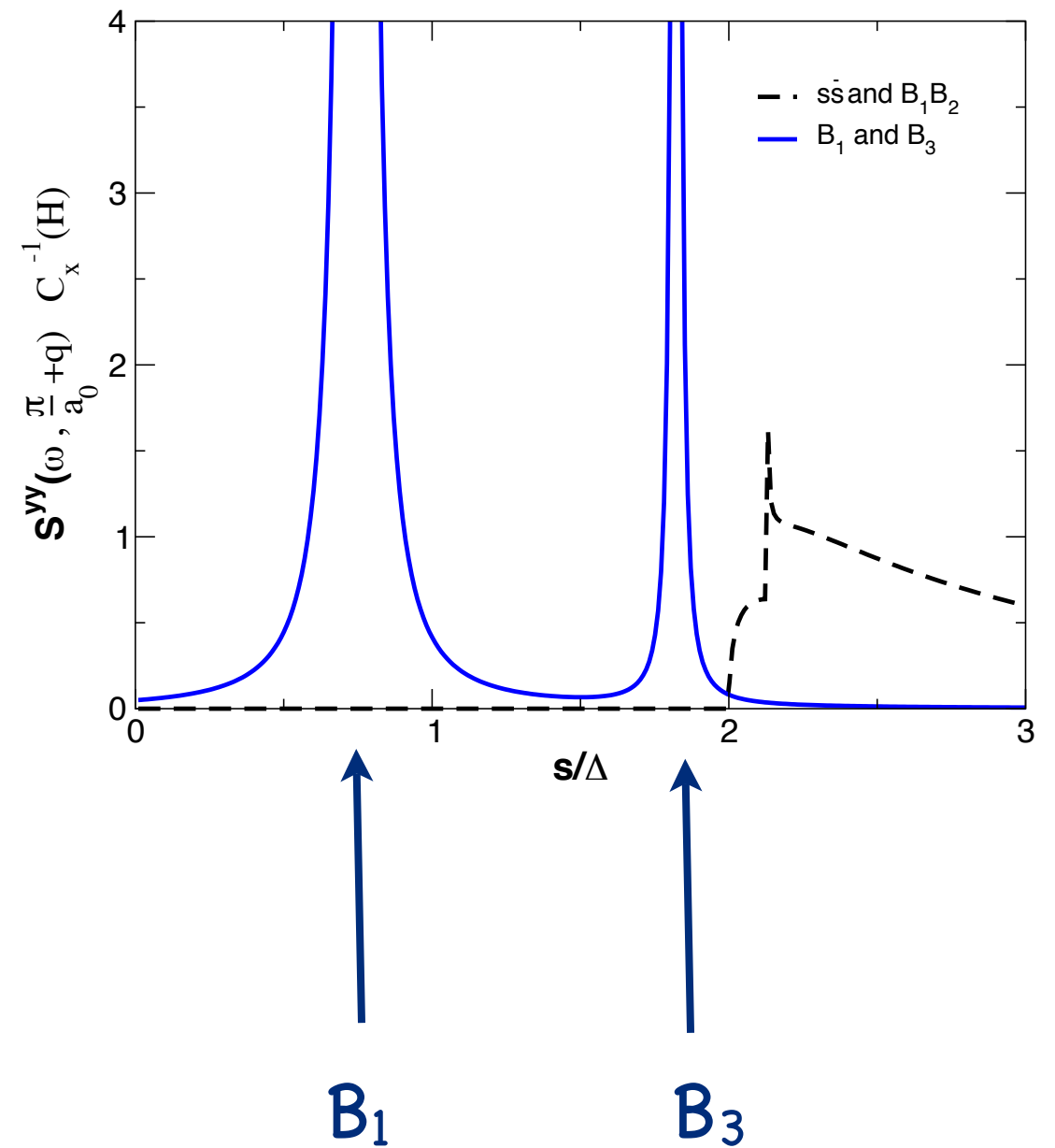
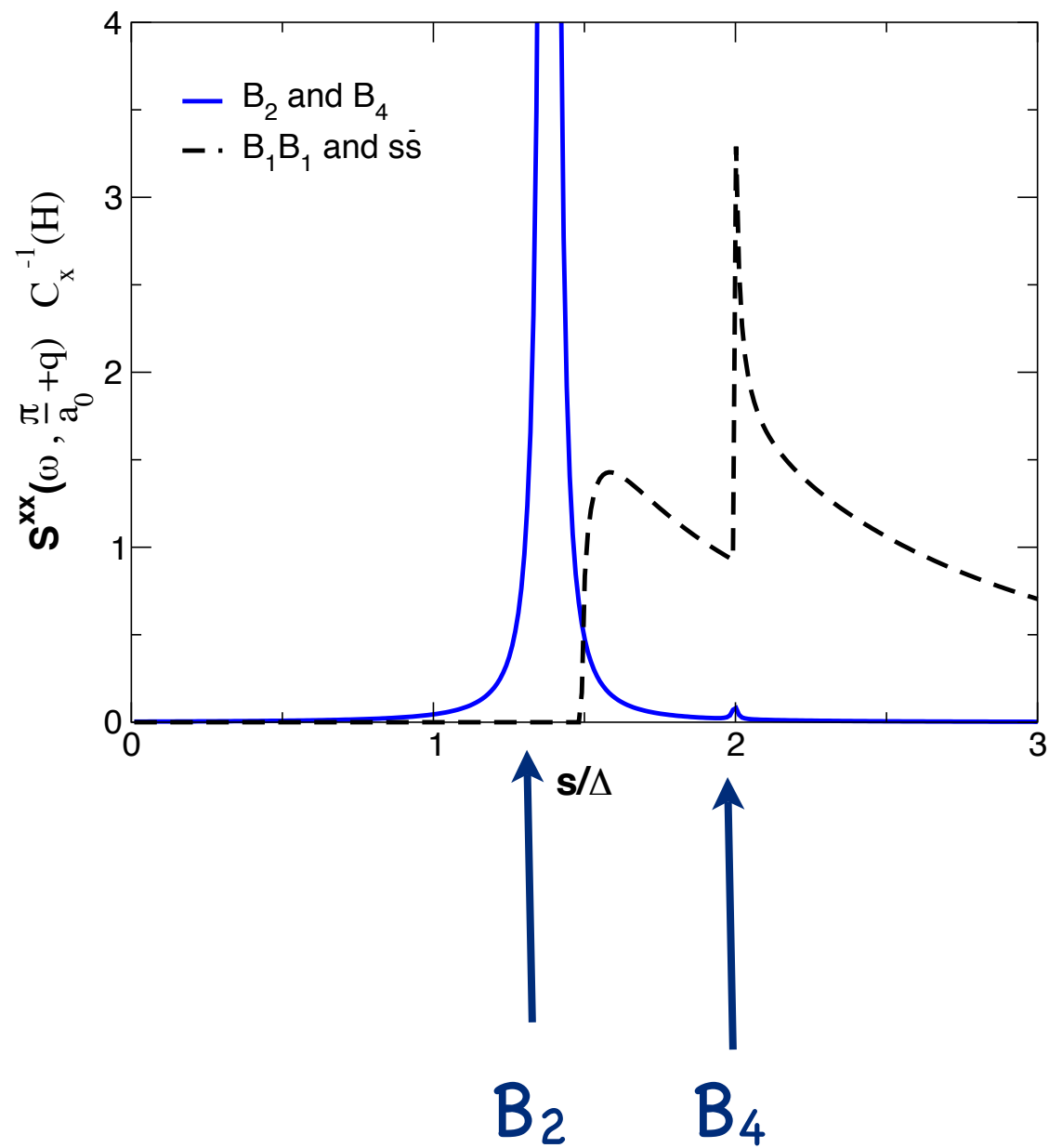


breather vs
soliton gaps



Calculated Dynamical Structure Factor Components

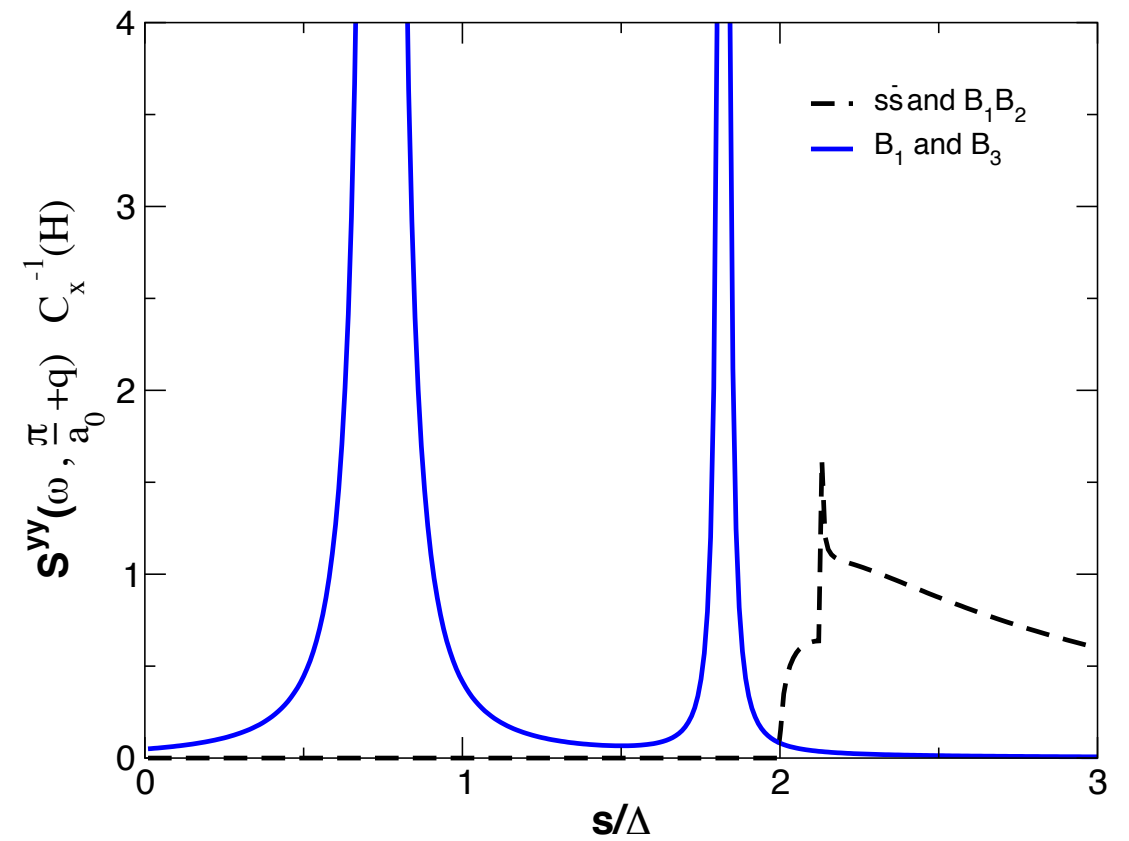
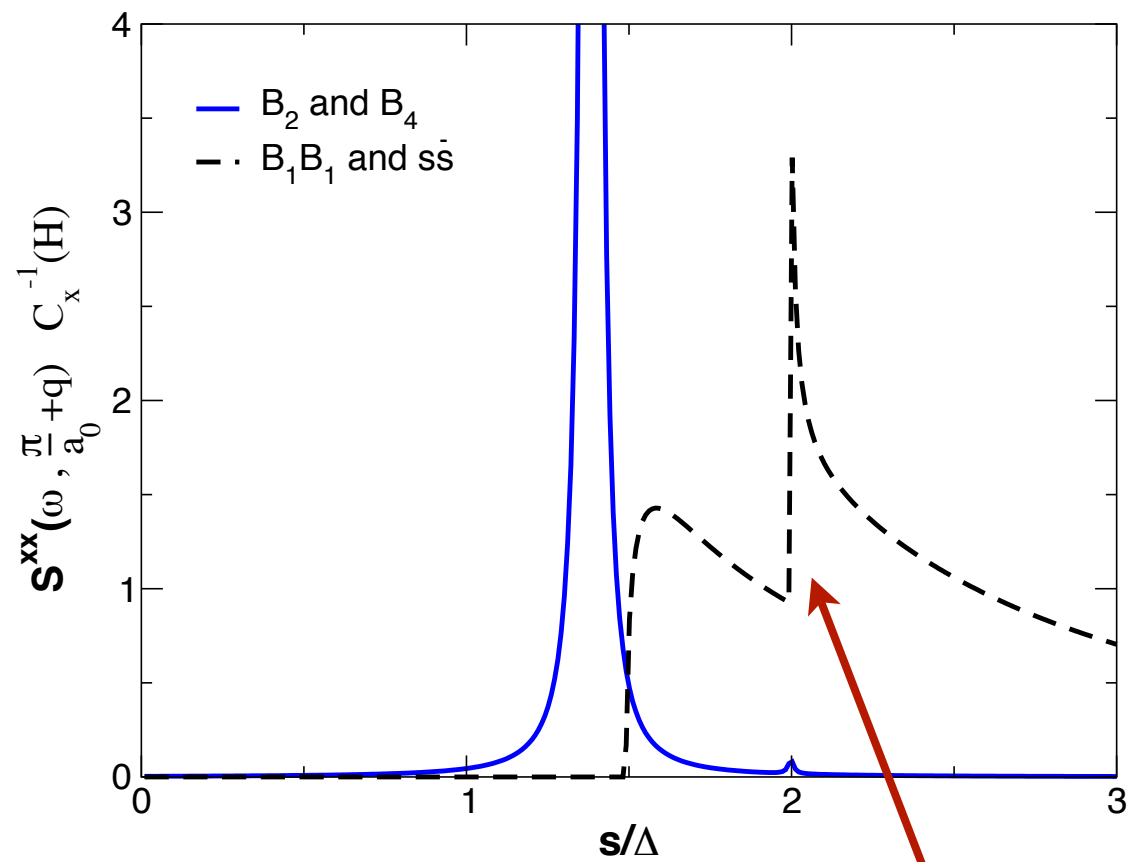
Essler et al '97, '03



(delta-function breather peaks have been broadened by hand to show the spectral weight)

Calculated Dynamical Structure Factor Components

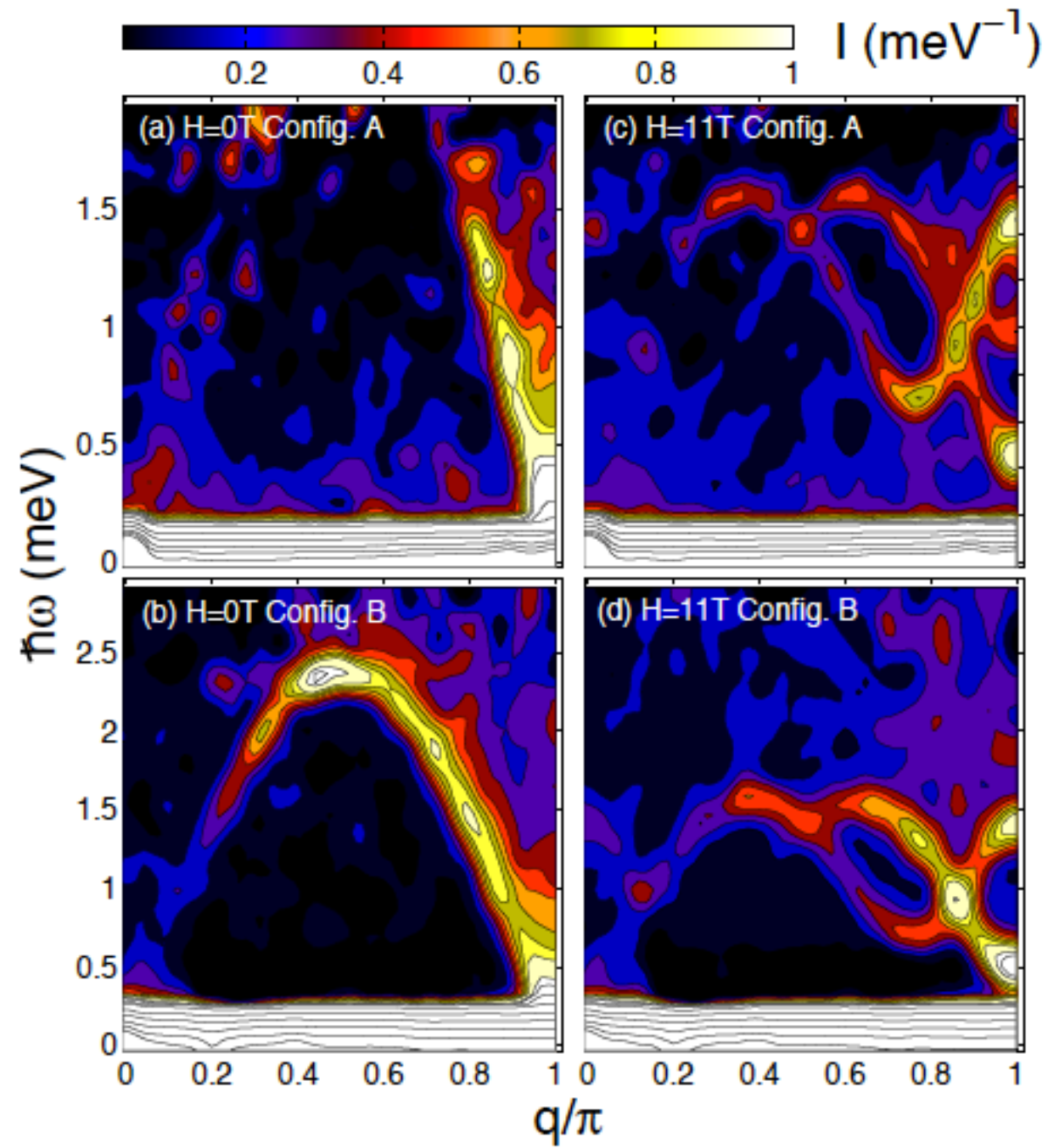
Essler et al '97, '03



threshold singularity on top of a scattering continuum.

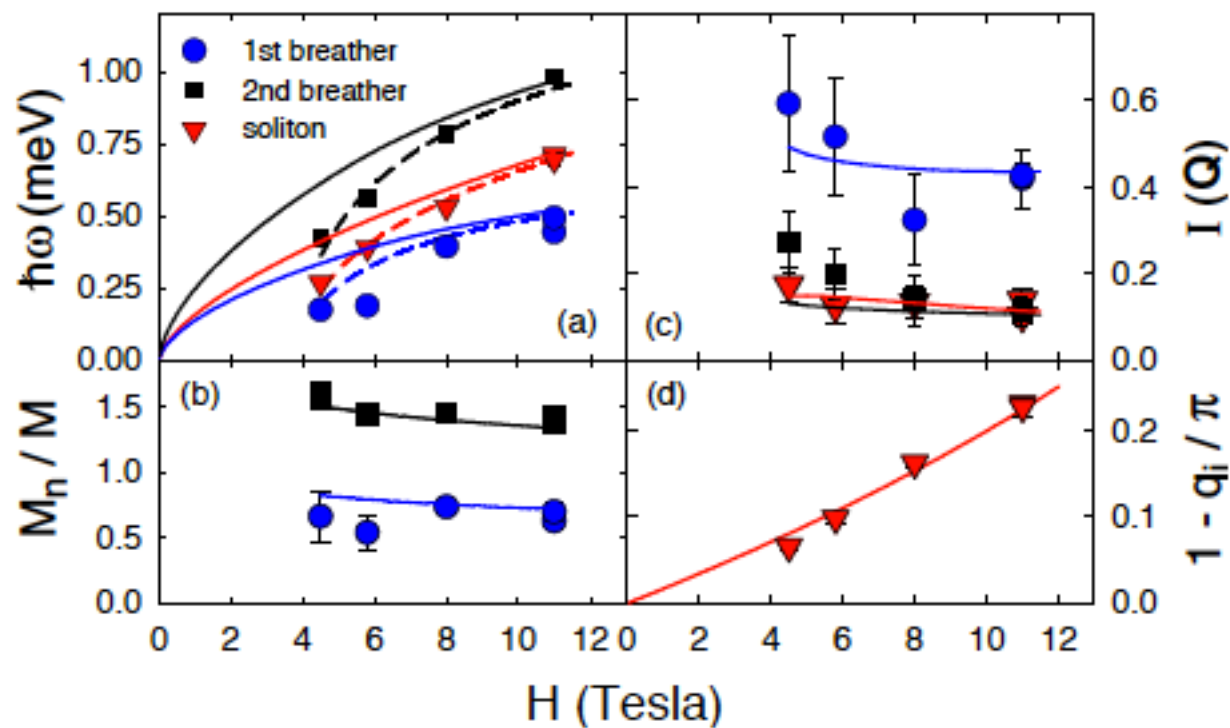
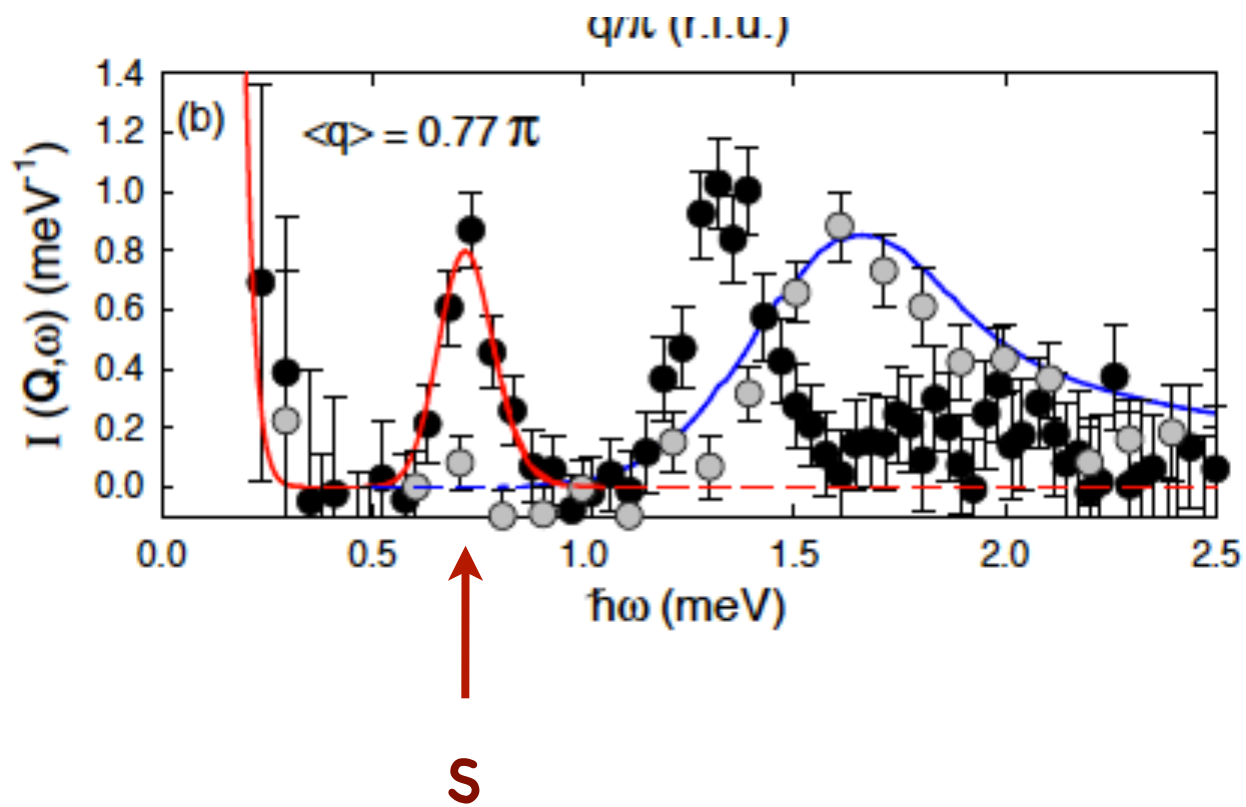
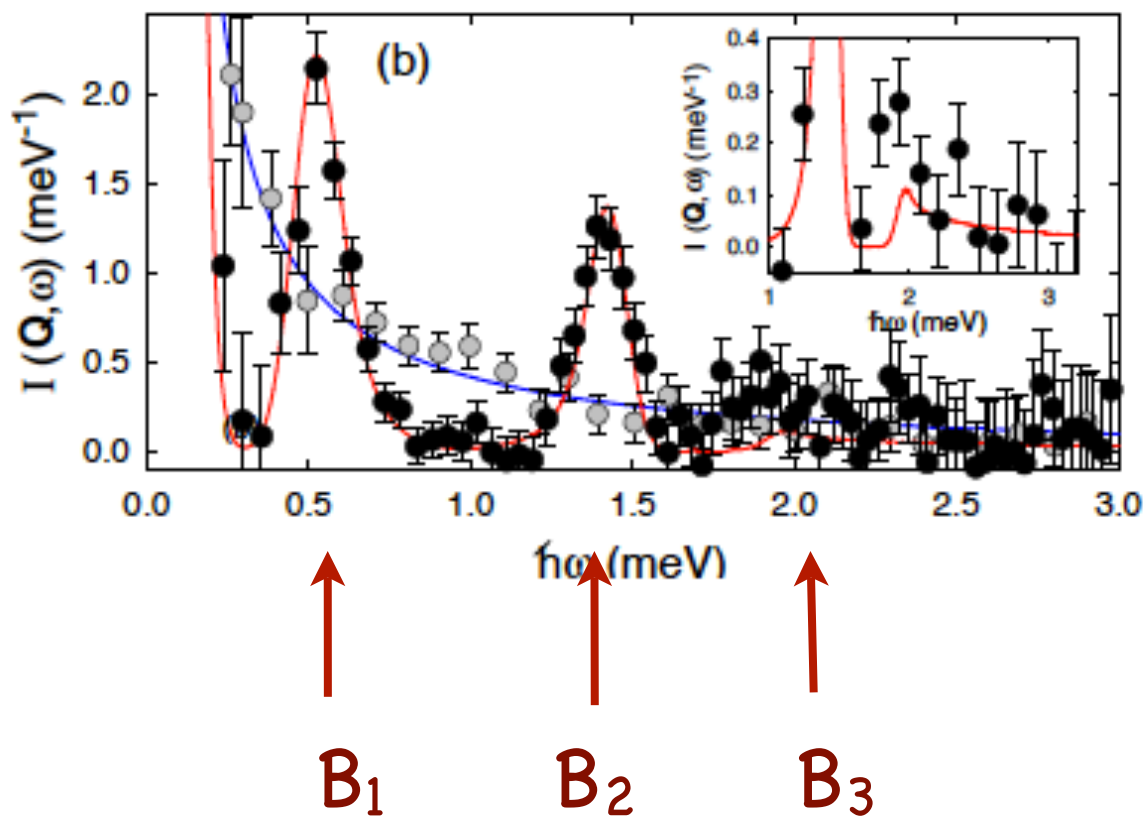
Measured DSF for CDC

Kenzelmann et al '04



Measured DSF for CDC

Kenzelmann et al '04



All of this was for $T=0$ - how about $T>0$?

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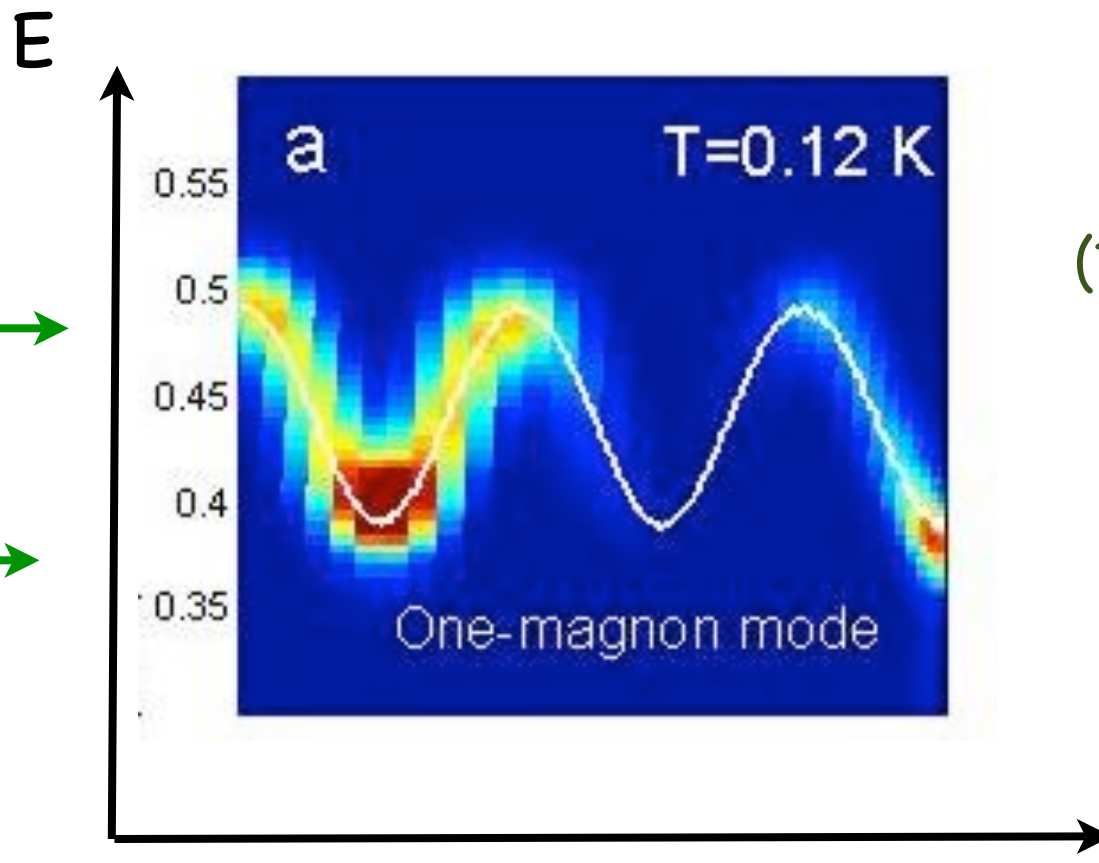
T>0 INS Studies of Gapped Quantum Spin Chains

- A. Integer Spin Heisenberg Chains (Xu et al '00, '07, Kenzelmann et al '01)
- B. 2-Leg Heisenberg Spin-1/2 Ladders (Zheludev et al '08, Rugg et al '10)
- C. Dimerized Heisenberg Spin-1/2 Chains (Xu et al '00, Tennant et al '09)

T=0: spin singlet ground state & gapped triplet of coherent "magnon" excitations

" δ -function" arising from single particle

Gap



CuNitrate

(D.A. Tennant et al '09)

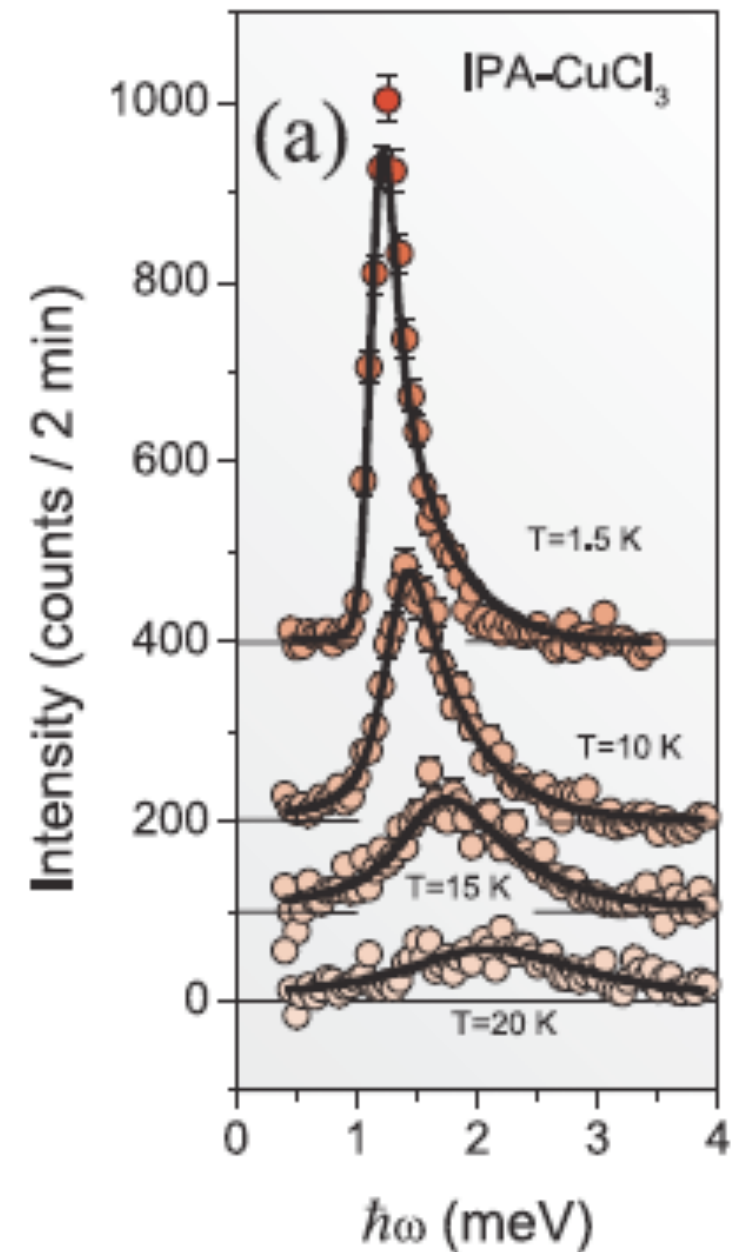
Linewidth and "T-dependent gap"

(A. Zheludev et al '08)

2-leg spin-1/2 ladder

(A) Line broadens with increasing T.

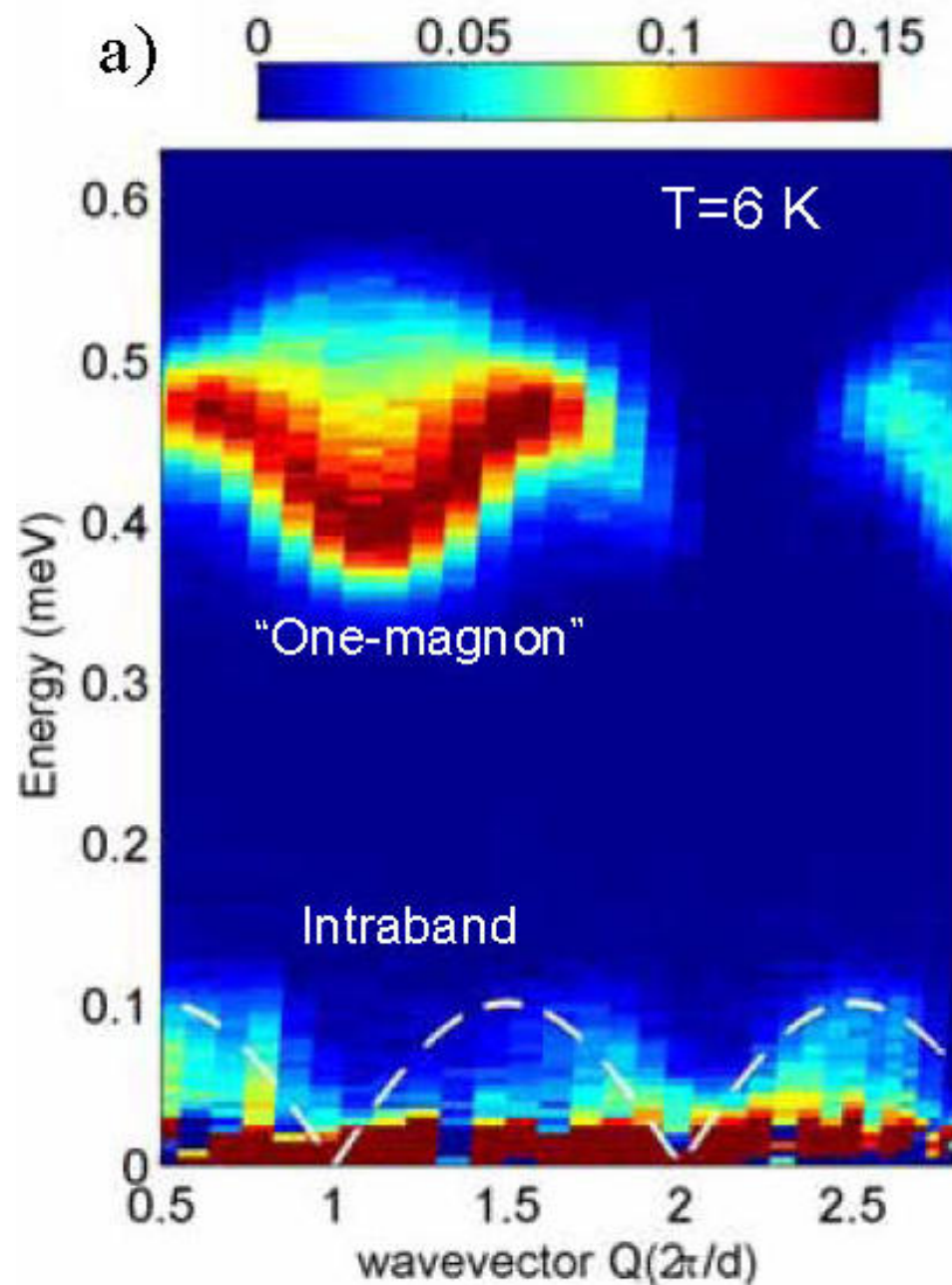
(B) Maximum shifts in energy: "T-dependent gap".



Thermally Activated Scattering

CuNitrate

$$H = \sum_j JS_{2j} \cdot S_{2j+1} + J'S_{2j+1} \cdot S_{2j+2}, \quad J' \ll J.$$



(D.A. Tennant et al '09, '12)

← asymmetric broadening
of magnon line

Thermally activated
scattering
← magnon already present in
state of thermal equilibrium
changes its spin

Why $T > 0$ dynamics is a difficult problem

Dynamical Structure
Factor

$$S(\omega, q) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \sum_l e^{-ikl} \langle S_{j+l}^a(t) S_j^a \rangle$$

$T=0:$

$$S(\omega, q) = 2\pi \sum_{\text{states } k} |\langle 0 | S_j^a | k \rangle|^2 \delta(\omega - E_k + E_0) \delta(q - P_k)$$

Only need ground state and 1 magnon excitation

$T > 0:$

$$S(\omega, q) = \frac{2\pi}{\text{tr}(e^{-\beta H})} \sum_{\text{states } n, k} e^{-\beta E_n} |\langle n | S_j^a | k \rangle|^2 \delta(\omega - E_k + E_n) \delta(q - P_k + P_n)$$

Have to deal with a **finite density** of magnons !

Lineshape of weakly interacting gapped fermions

- Single-particle spectral function of non-interacting fermions at $T > 0$

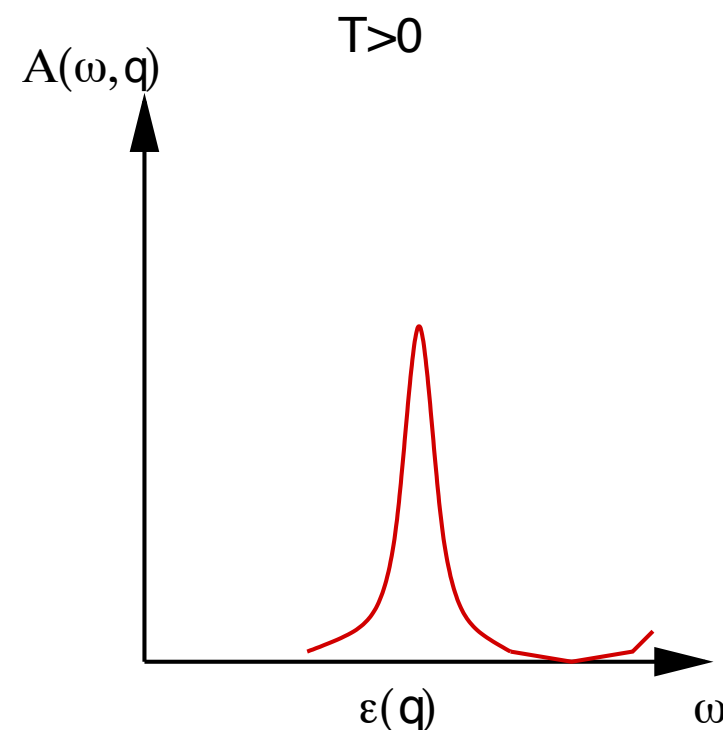
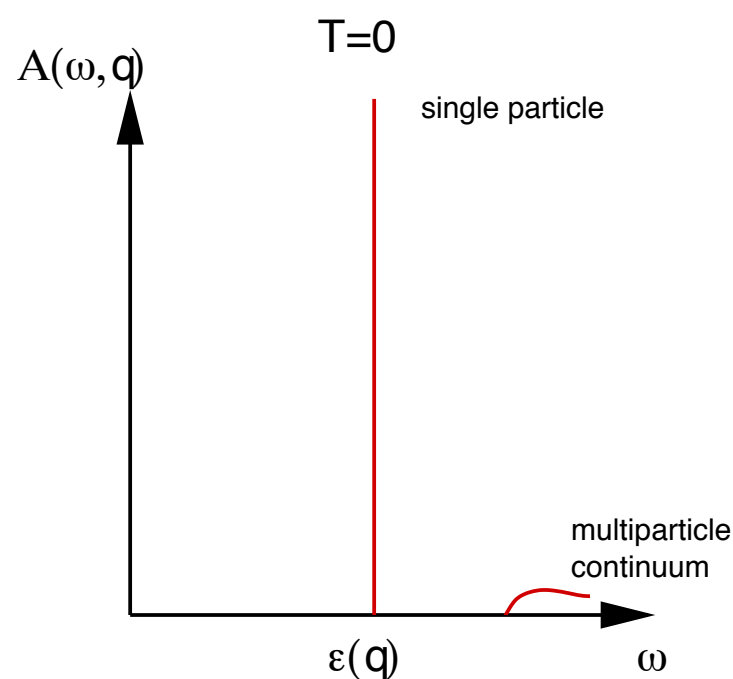
$$A(\omega, q) = -\frac{1}{\pi} \text{Im} G_{\text{ret}}(\omega > 0, q) \propto \delta(\omega - \epsilon(q))$$

→ **T-independent**. Need interactions to get non-trivial lineshape.

- Dynamical Response of weakly interacting, massive particles

$$A(\omega, q) \propto \text{Im} \frac{1}{\omega + i0 - \epsilon(q) + \Sigma(\omega, q, T)}$$

$\Sigma(\omega, q, T)$ calculable in (Matsubara) PT for **low T**.



Line-broadening gives fingerprint of interactions between particles.

Semiclassical Approach

(Sachdev, Damle '98)

(Rapp&Zarand '06,'09)

Consider gapped 1D quantum magnet with coherent single-particle excitation at $T=0$, dispersion $\varepsilon(q)$, gap $\Delta = \varepsilon(Q)$
(e.g. Haldane-gap chains, 2-leg ladder, transverse-field Ising model)

$$\text{DSF} \quad S(\omega, q, T=0) \sim A(q) \delta(\omega - \varepsilon(q)) + \text{multi-particle}$$

For "low T " the delta-function broadens in a **universal Lorentzian way** (at $q \approx Q$) as

$$S(\omega, q, T > 0) \sim A(q) \tau^{-1}(T) [(\omega - \varepsilon(q))^2 + \tau^{-2}(T)]^{-1} + \text{multi-particle}$$

widely used to analyze neutron data

Questions: Regime of applicability? How to go beyond?

Dynamical Correlations at $T > 0$

(LeClair et al '96
LeClair/Mussardo '99
Konik '03)

Basis of Hamiltonian eigenstates: $H |r\rangle = E_r |r\rangle$

$$\chi(\omega, q) = \frac{1}{\text{tr}(e^{-\beta H})} \sum_{r,s} |\langle r | S^a(0,0) | s \rangle|^2 \frac{e^{-\beta E_r} - e^{-\beta E_s}}{\omega + i\delta - E_s + E_r} 2\pi \delta(q + P_r - P_s)$$

Magnon Gap $\Rightarrow E_r \approx r\Delta$

Dynamical Correlations at $T > 0$

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Magnon Gap $\Rightarrow E_r \approx r\Delta$



Must be regularized!

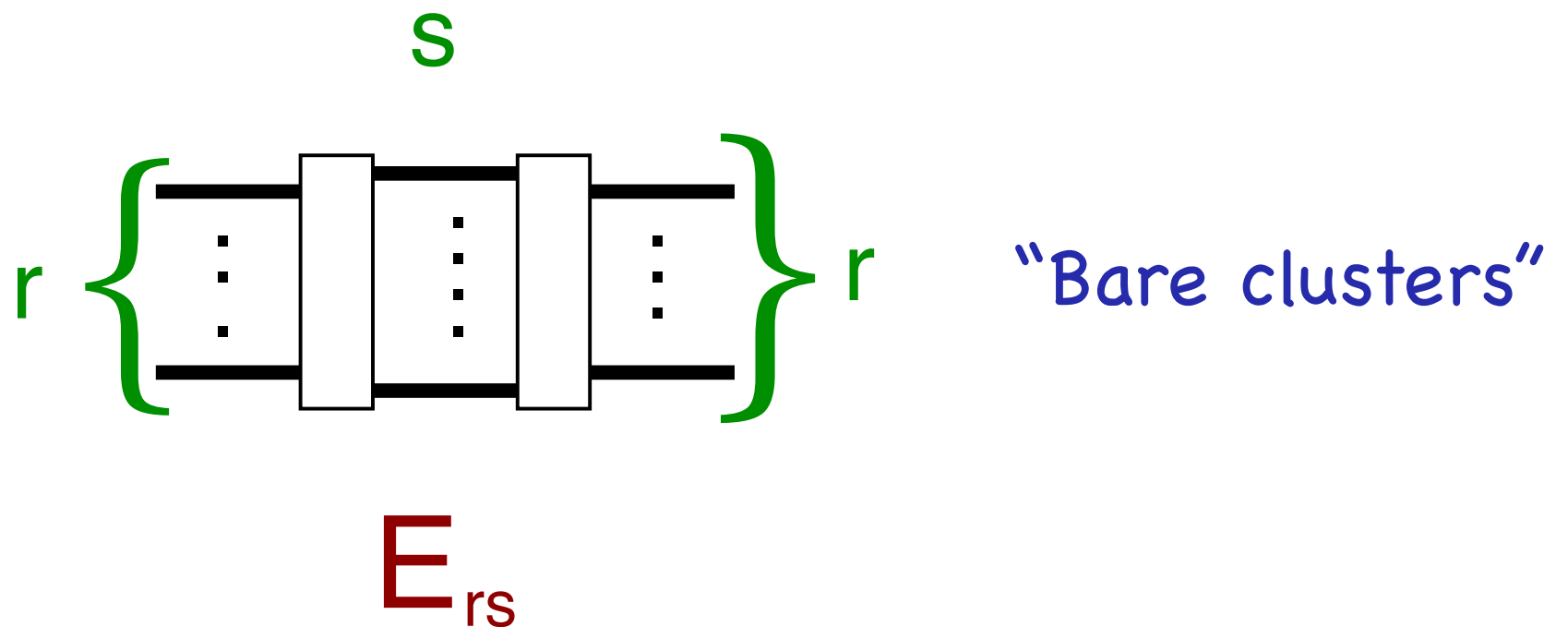
- (1) Finite Volume Regularization (Essler&Konik '08, Pozsgay& Takacs '08)
- (2) Infinite Volume Regularization (Essler& Konik '09)

Dynamical Correlations at $T > 0$

$$\chi(\omega, q) = \frac{1}{\text{tr}(e^{-\beta H})} \sum_{r,s} |\langle r | S^a(0,0) | s \rangle|^2 \frac{e^{-\beta E_r} - e^{-\beta E_s}}{\omega + i\delta - E_s + E_r} 2\pi \delta(q + P_r - P_s)$$

$$\equiv \frac{1}{\text{tr}(e^{-\beta H})} \sum_{r,s} \mathcal{E}_{r,s}(\omega, q) + \mathcal{F}_{r,s}(\omega, q).$$

Formally we have: $\mathcal{E}_{r,s}(\omega, q) = \mathcal{O}(e^{-r\beta\Delta})$



Dynamical Correlations at $T > 0$

$$\begin{aligned} \chi(\omega, q) &= \frac{1}{\text{tr}(e^{-\beta H})} \sum_{r,s} |\langle r | S^a(0,0) | s \rangle|^2 \frac{e^{-\beta E_r} - e^{-\beta E_s}}{\omega + i\delta - E_s + E_r} 2\pi \delta(q + P_r - P_s) \\ &\equiv \frac{1}{\text{tr}(e^{-\beta H})} \sum_{r,s} \mathcal{E}_{r,s}(\omega, q) + \mathcal{F}_{r,s}(\omega, q). \end{aligned}$$

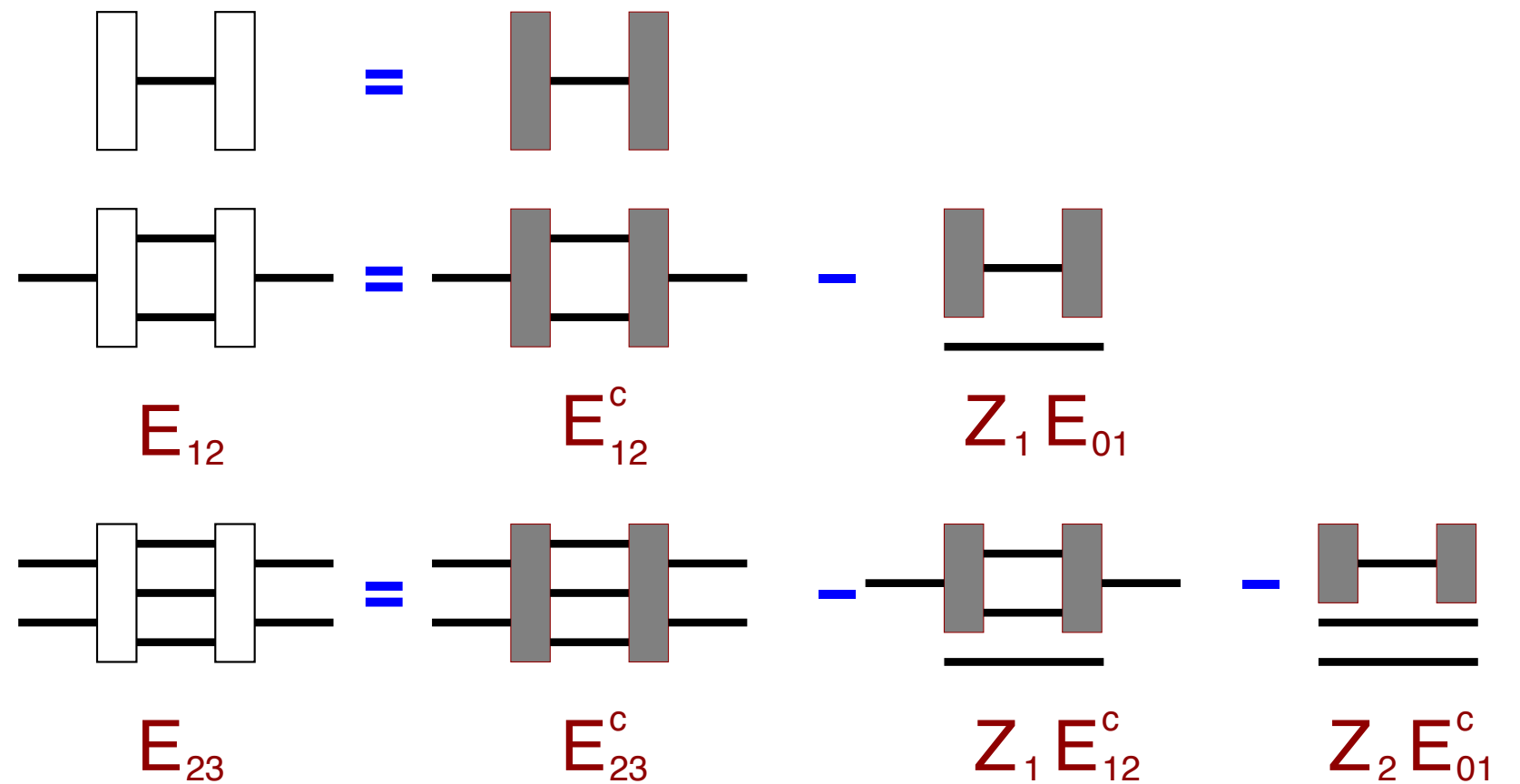
Formally we have: $\mathcal{F}_{r,s}(\omega, q) = \mathcal{O}(e^{-s\beta\Delta})$

Partition Function:

$$\text{tr}(e^{-\beta H}) = \sum_m e^{-\beta E_l} \langle l | l \rangle \equiv 1 + \sum_{n=1}^{\infty} Z_n, \quad Z_n = \mathcal{O}(e^{-n\beta\Delta}). \quad r \left\{ \begin{array}{c} \text{---} \\ \vdots \\ \text{---} \\ Z_r \end{array} \right.$$

Low-Temperature Expansion

Define "linked clusters":



$$\chi \varepsilon(\omega, q) = \frac{1}{\text{tr}(e^{-\beta H})} \sum_{r,s} \left\{ \begin{array}{c} s \\ \vdots \\ \vdots \\ \vdots \end{array} \right\}_r$$

$$= \sum_{r,s} \left\{ \begin{array}{c} s \\ \vdots \\ \vdots \\ \vdots \end{array} \right\}_r \underbrace{E_{rs}^c}_{O(\exp(-r\beta\Delta))}$$

low-T expansion for $\chi(\omega, q)$:

$$\chi(\omega, q) = \underbrace{C_0}_{\mathcal{O}(1)} + \underbrace{C_1}_{\mathcal{O}(e^{-\beta\Delta})} + \underbrace{C_2}_{\mathcal{O}(e^{-2\beta\Delta})} + \dots \quad (\text{LTE})$$

Problem: subleading (in $\exp(-\beta\Delta)$) terms in $\chi(\omega, q)$ more and more divergent when $\omega^2 \rightarrow \varepsilon^2(q)$

Solution:

(1) define $\Sigma(\omega, q)$ through

$$\chi(\omega, q) = \frac{C_0(\omega, q)}{1 - C_0(\omega, q)\Sigma(\omega, q, T)} .$$

(2) Match expansion $\chi(\omega, q) \approx C_0(\omega, q) + C_0^2(\omega, q)\Sigma(\omega, q, T) + \dots$

to LTE $\Rightarrow \Sigma(\omega, q, T)$

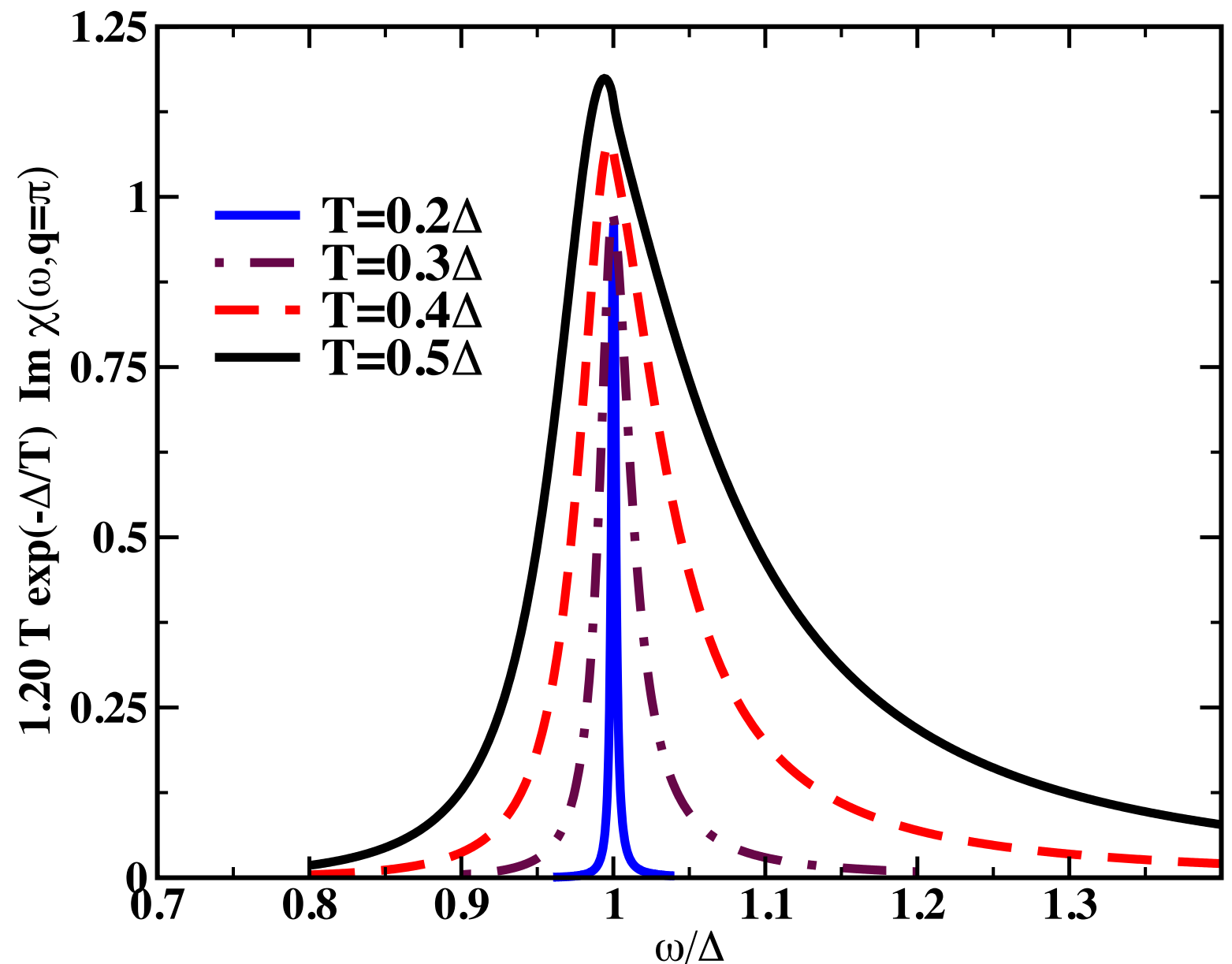
Results for $T > 0$ Lineshape in $O(3)$ nl Σ m

DSF at $q = \pi/a_0$ for integer spin- S Heisenberg chain at low energies

- width $\propto T \exp(-\beta\Delta)$
- height $\propto T^{-1} \exp(\beta\Delta)$
- lineshape **Lorentzian** for $T \ll \Delta$, $\omega \approx \Delta \Rightarrow$ agrees w. semiclassical approx.

(Damle/Sachdev '98)

- lineshape **asymmetric** for any T and $\omega \neq \Delta$
- asymmetry increases w. T

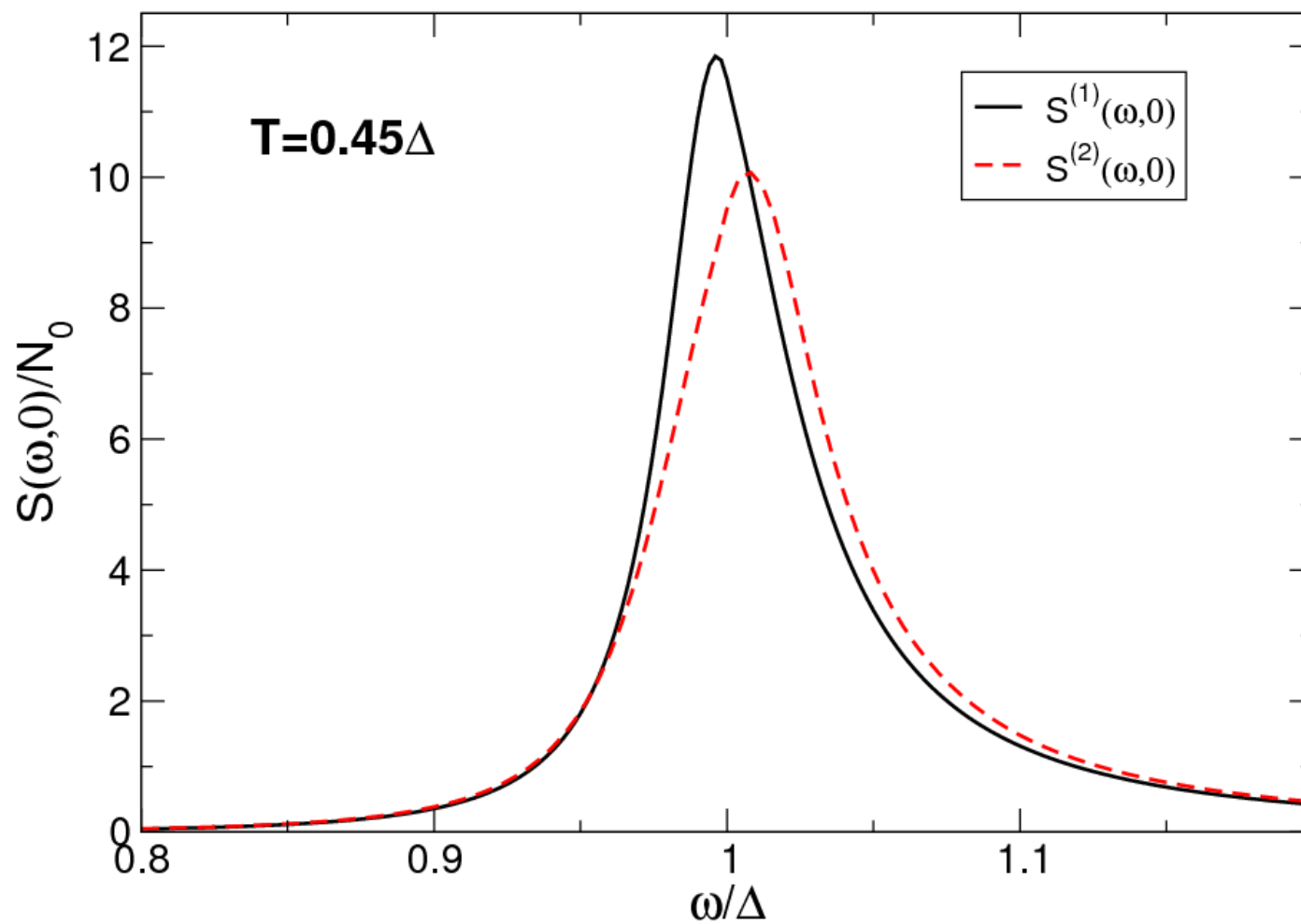


Damle/Sachdev result recovered at rather low $T < 0.1\Delta$

Higher Orders in Low-T Expansion

$$H_{\text{TFIM}} = J \sum_n S_n^z S_{n+1}^z - h \sum_n S_n^x, \quad 1 \gg \frac{h}{J} - 1 > 0$$

$$S^{zz}(\omega, q=0, T)$$



Maximum moves in energy

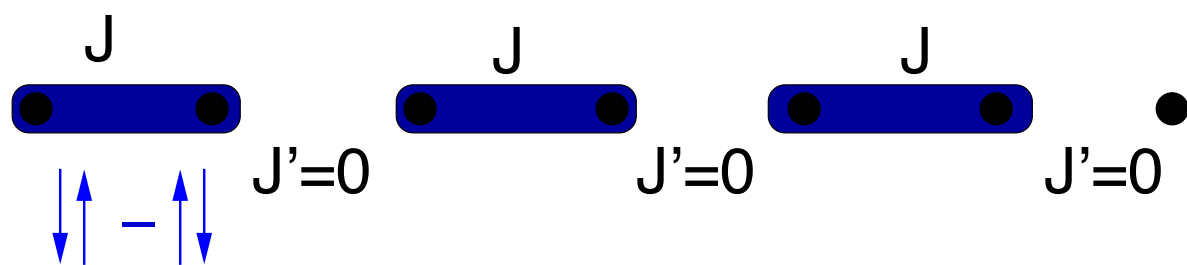
“T-dependent gap”

Non-Integrable Models

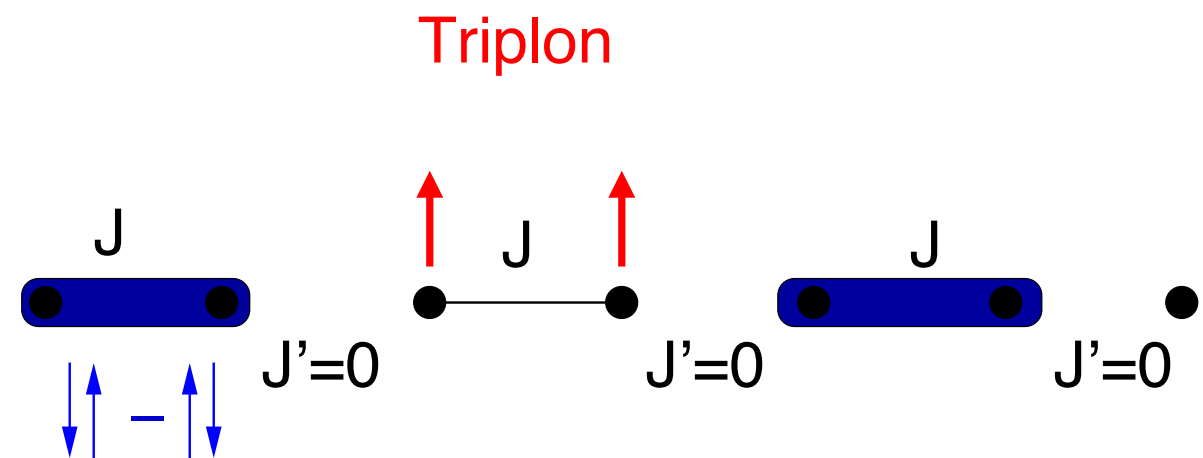
e.g. Alternating spin- $\frac{1}{2}$ Heisenberg Chain:

$$H = \sum_j JS_{2j} \cdot S_{2j+1} + J'S_{2j+1} \cdot S_{2j+2}, \quad J' \ll J.$$

$J'=0$ limit: uncoupled dimers



Ground State



"Triplon" $S=1$ Excitation

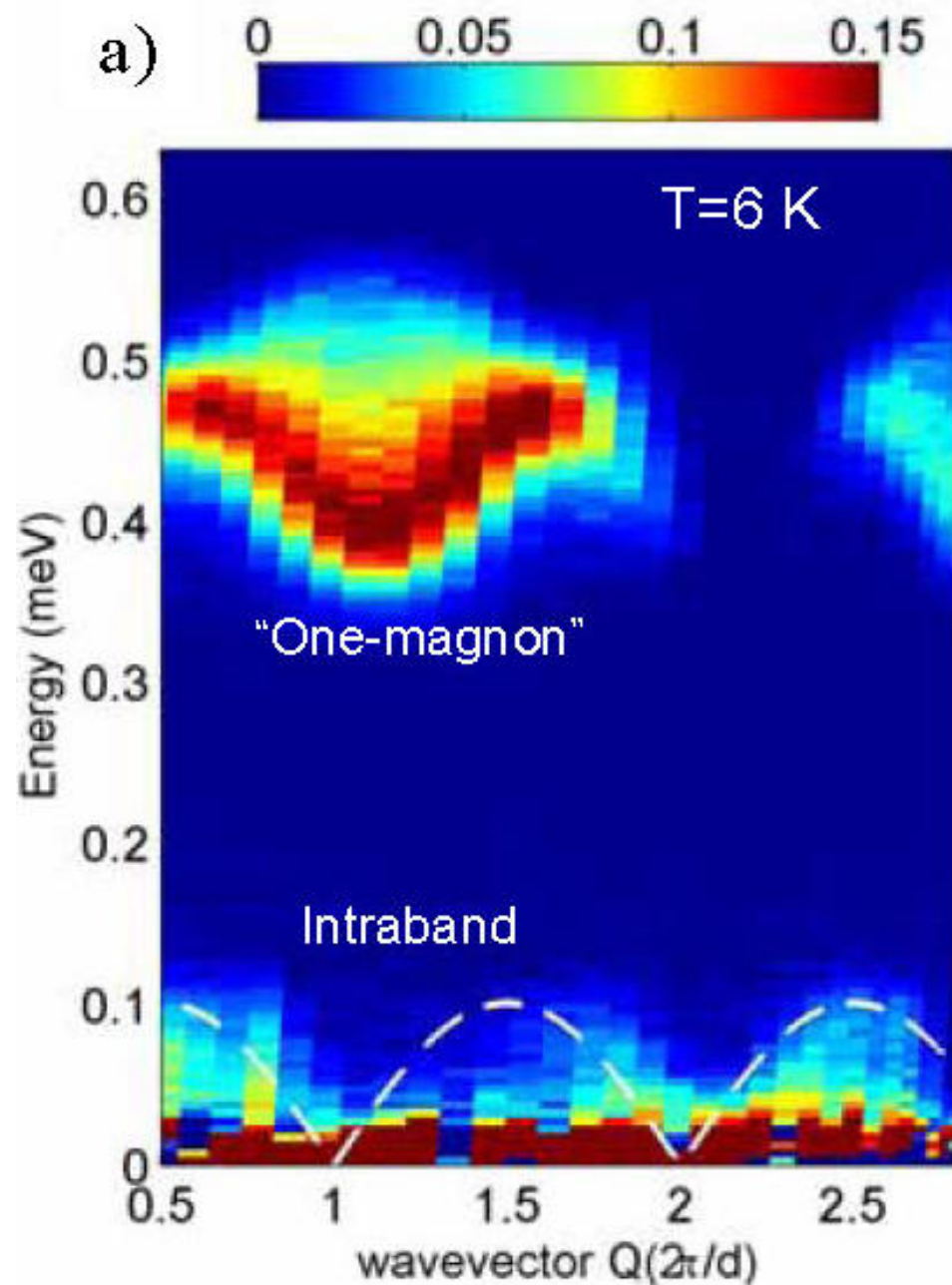
combine low- T expansion with Perturbation Theory in J'

Alternating spin-1/2 Heisenberg Chain CuNitrate

(D.A. Tennant et al '09)

$$H = \sum_j JS_{2j} \cdot S_{2j+1} + J'S_{2j+1} \cdot S_{2j+2}, \quad J' \ll J.$$

$$J' \approx 0.23J$$



← asymmetric broadening of magnon line

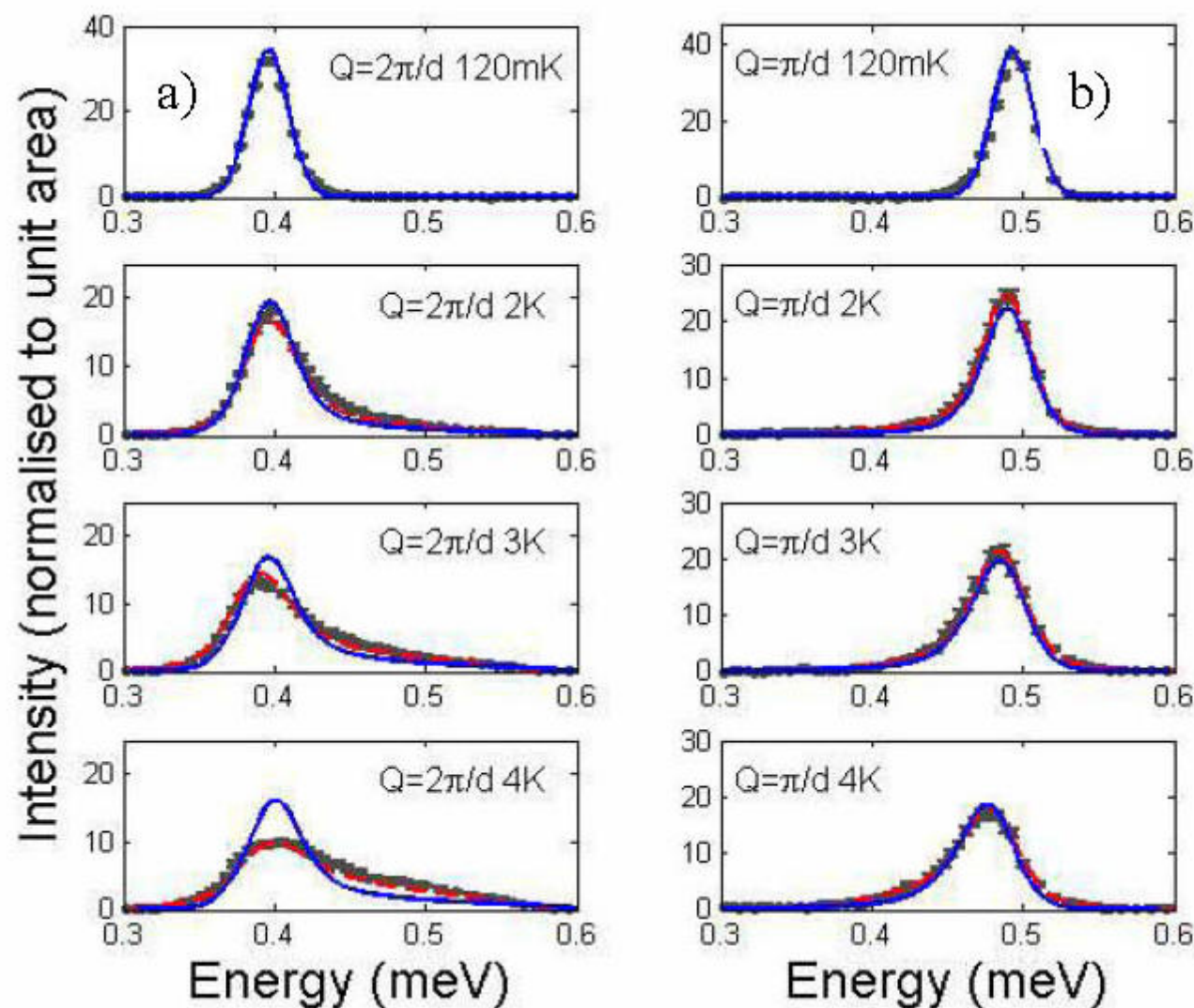
Thermally activated scattering
← magnon already present in state of thermal equilibrium changes its spin

Experiments on CuNitrate

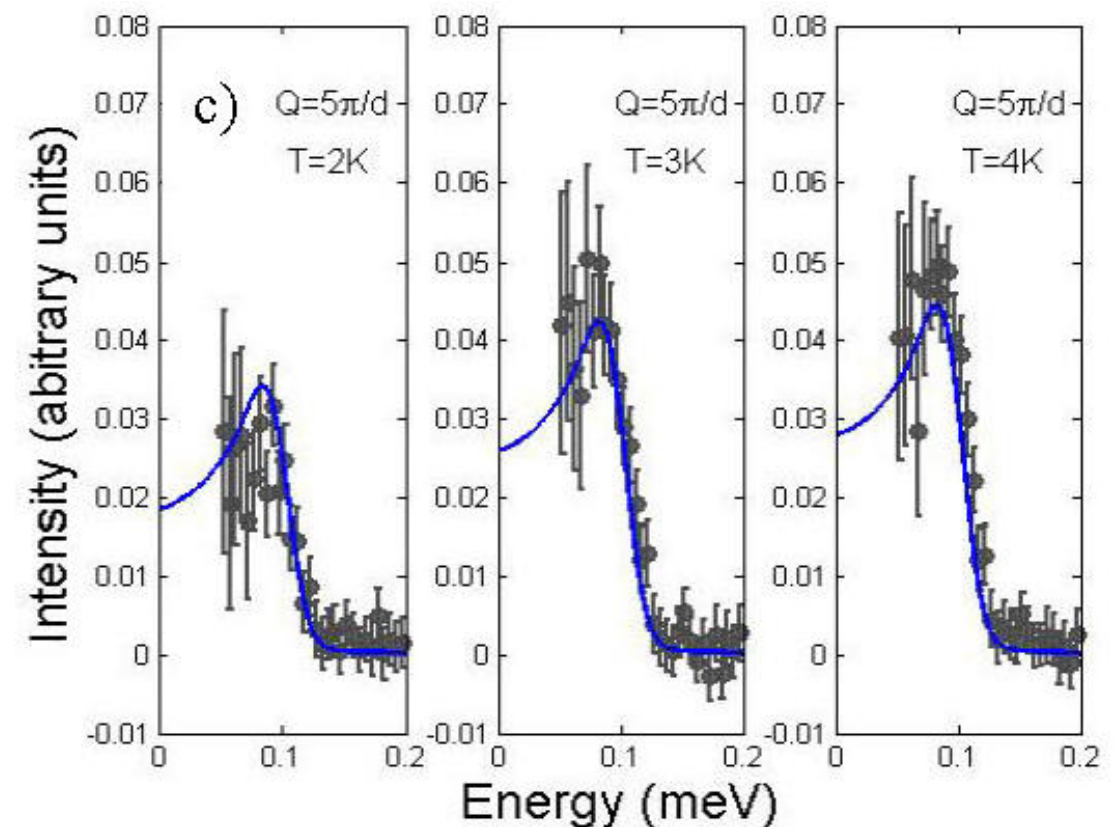
(D.A. Tennant et al)

Constant Q scans: $S(\omega, Q, T)$ for fixed Q and T

“Triplon” Broadening



low-energy $T > 0$ Resonance



Summary

- Many gapped quantum spin chains reduce to integrable QFTs at low energies.
- There is an efficient method to calculate $T=0$ dynamical response functions in these QFTs.
- Low- T expansion for finite temperature dynamics.
- Low- T expansion applicable to certain non-integrable spin chains.
- Methods developed for $T>0$ dynamics allow analysis of non-equilibrium problems.

Outline

1. Why low-D Quantum Spin Systems are interesting.
2. Some Gapped Quantum Spin Chains and their Quantum Field Theory Limits.
3. Integrable QFTs.
4. $T=0$ Dynamical Response Functions in integrable QFTs.
5. $T>0$ Dynamical Response Functions (in integrable QFTs).
6. Nonequilibrium Dynamics.

Quantum systems out of equilibrium

Idea:

- A. Consider a quantum many-particle system with Hamiltonian H
- B. Prepare the system in a state $|\psi\rangle$ that is **not** an eigenstate.
- C. Time evolution $|\psi(t)\rangle = \exp(-iHt) |\psi\rangle$
- D. Study time evolution of local observables $\langle\psi(t)|O(x)|\psi(t)\rangle$ in the **thermodynamic limit**.

Quantum systems out of equilibrium

Idea:

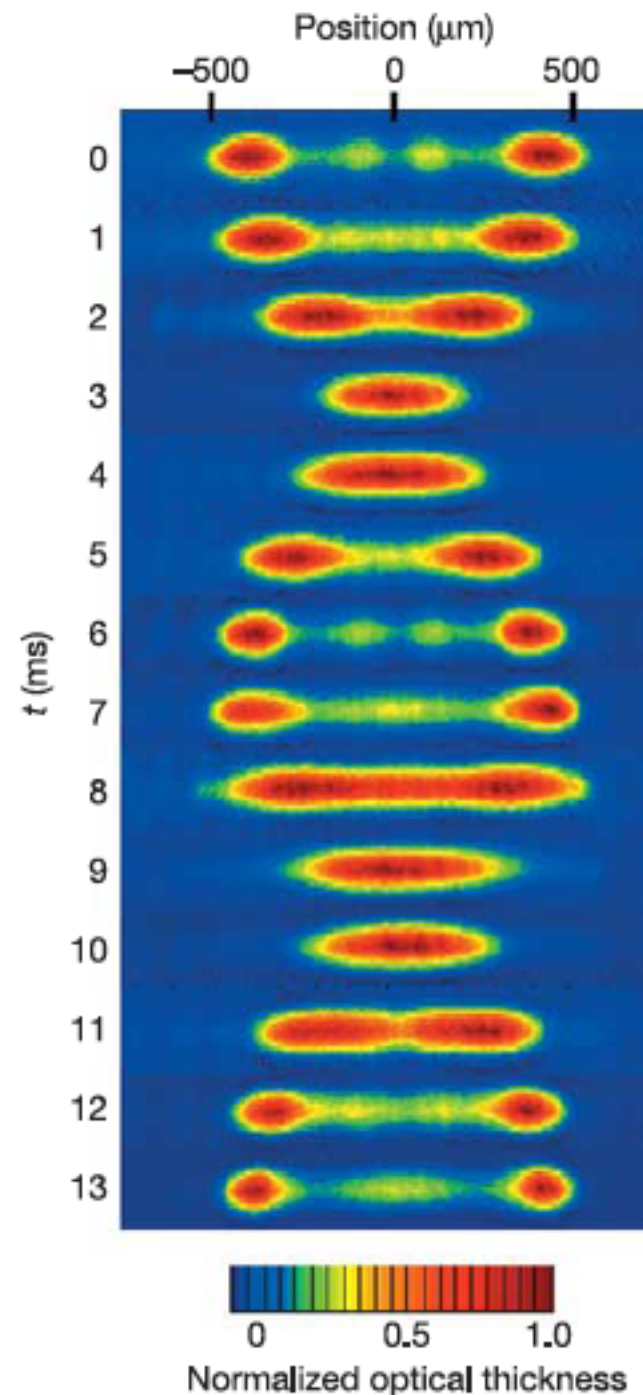
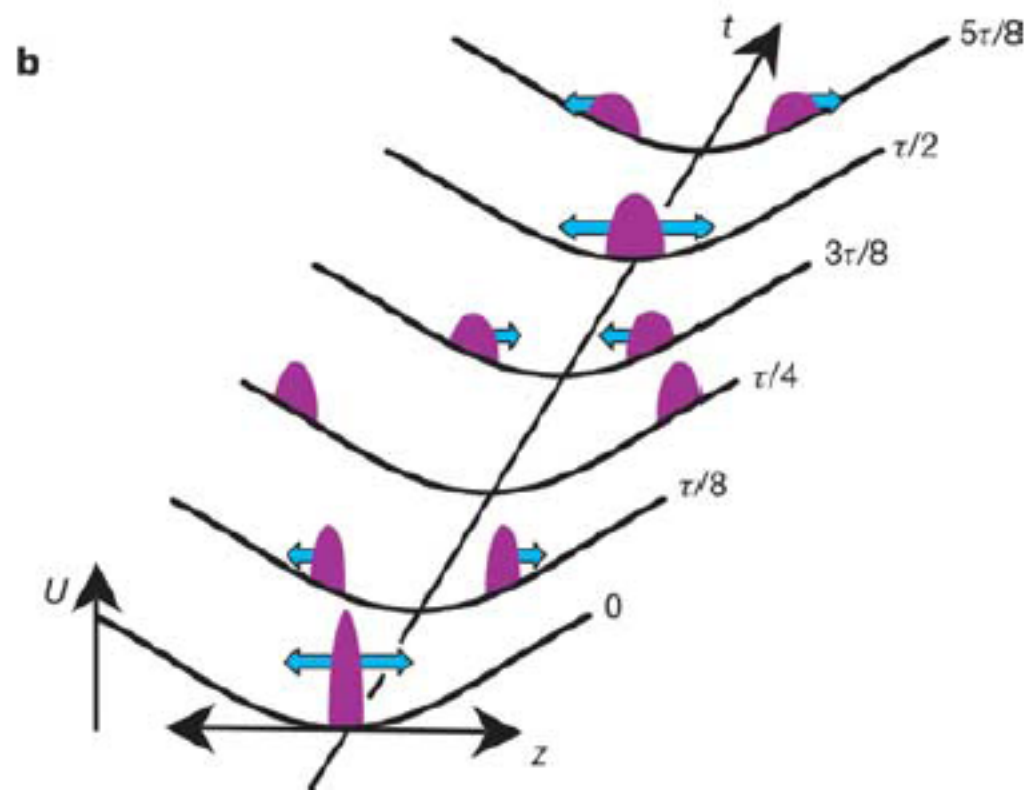
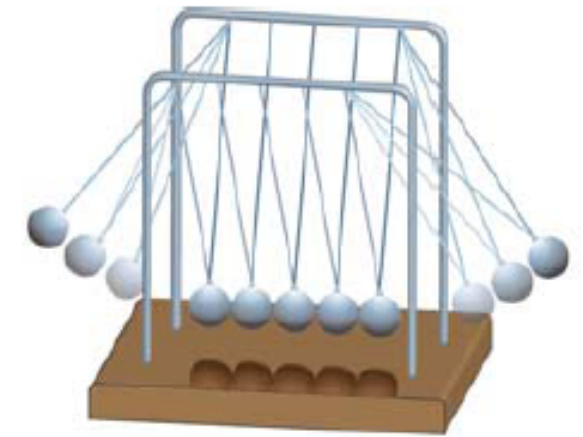
- A. Consider a quantum many-particle system with Hamiltonian H
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- D. Study time evolution of local observables $\langle\psi(t)|O(x)|\psi(t)\rangle$
in the **thermodynamic limit**.

$|\psi(t)\rangle$ has a **finite density** of elementary excitations of the new
Hamiltonian $H \rightarrow$ **like $T>0$**

Experiments: "Quantum Newton's Cradle"

T. Kinoshita, T. Wenger and D.S. Weiss, Nature 440, 900 (2006)

40–250 ^{87}Rb atoms in a 1D optical trap



Essentially unitary
time evolution.

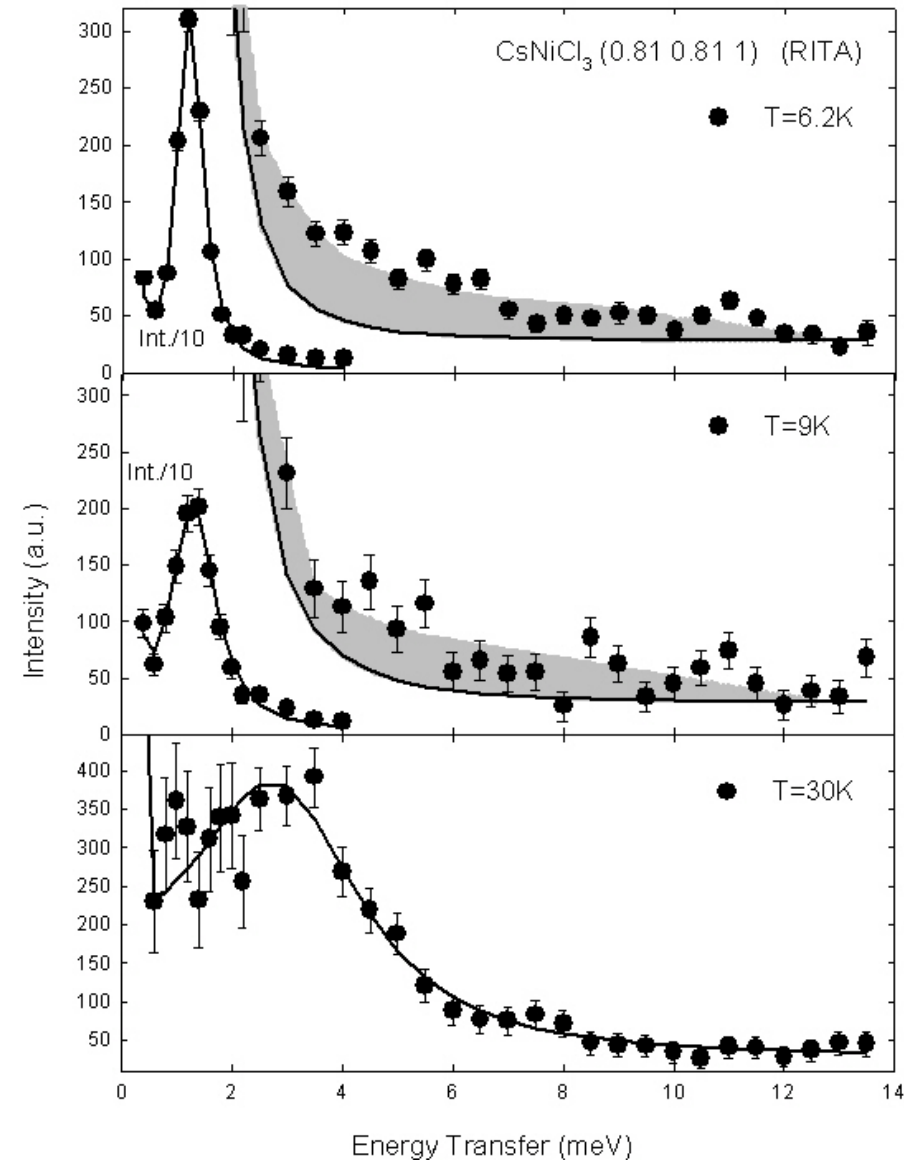
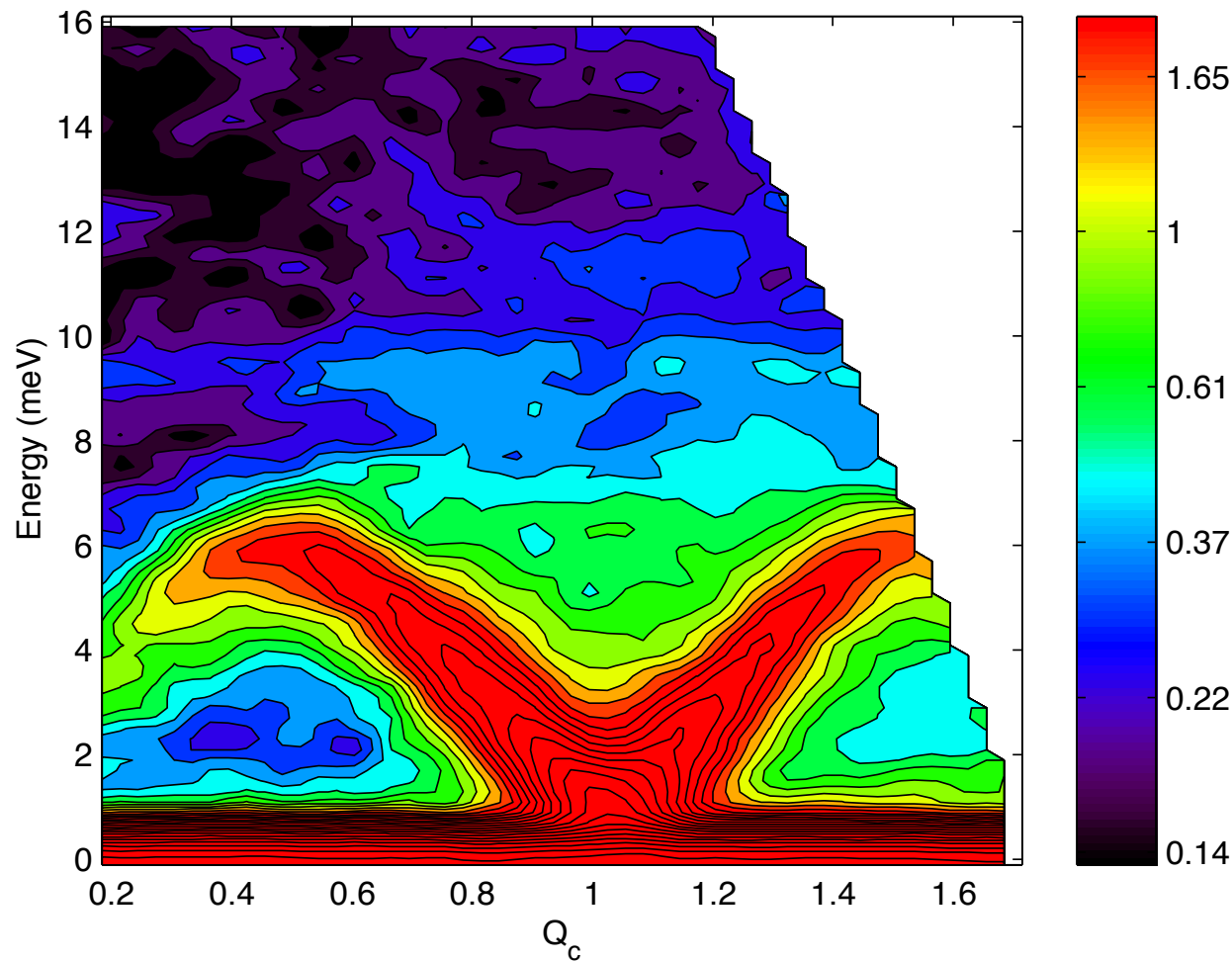
A different talk !



T>0 Dynamical Structure Factor of CsNiCl₃

(M. Kenzelmann et al '01)

(spin-1 Heisenberg chain)



T=0 delta-function → asymmetric continuum at T>0

Dynamical Structure Factor

Continuum limit of lattice spin operators:

$$\mathbf{S}_j \approx S(-1)^{j a_0} \mathbf{n}(x) + \mathbf{M}(x), \quad \mathbf{M}(x) = \frac{1}{v g} \mathbf{n}(x) \times \frac{\partial \mathbf{n}(x)}{\partial t}.$$

Dynamical structure factor around $q = \pi$:

$$S(\omega, k = \frac{\pi}{a_0} + q) \propto \int dt dx e^{i\omega t - i q x} e^{i q (R_j - R_l)} \langle n^a(t, x) n^a(0, 0) \rangle$$

Dynamical structure factor around $q = 0$:

$$S(\omega, q) \propto \int dt dx e^{i\omega t - i q x} e^{i q (R_j - R_l)} \langle M^a(t, x) M^a(0, 0) \rangle$$

Restrictions: formally $S \gg 1$, $\omega \ll J$ ($\Leftrightarrow |q a_0| \ll \pi$).

Non-Integrable Models

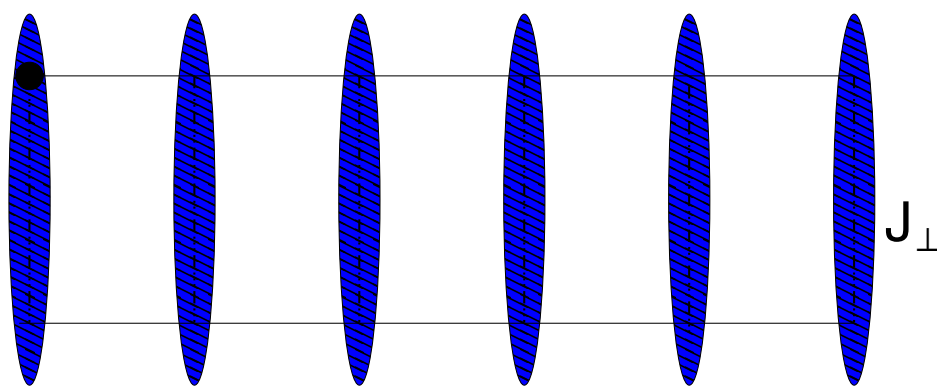
A. Alternating spin- $\frac{1}{2}$ Heisenberg Chain:

$$H = \sum_j JS_{2j} \cdot S_{2j+1} + J'S_{2j+1} \cdot S_{2j+2}, \quad J' \ll J.$$

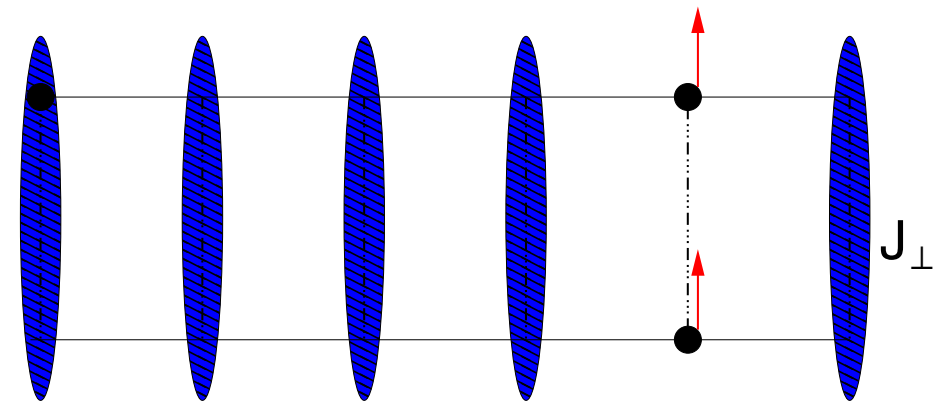
B. 2-leg spin- $\frac{1}{2}$ Heisenberg ladder:

$$H = J_{\parallel} \sum_{a=1,2} \sum_j S_{a,j} \cdot S_{a,j+1} + J_{\perp} \sum_j S_{1,j} \cdot S_{2,j}, \quad J_{\parallel} \ll J_{\perp}.$$

$J_{\parallel}=0$: uncoupled dimers (for A. along chain)



Ground State



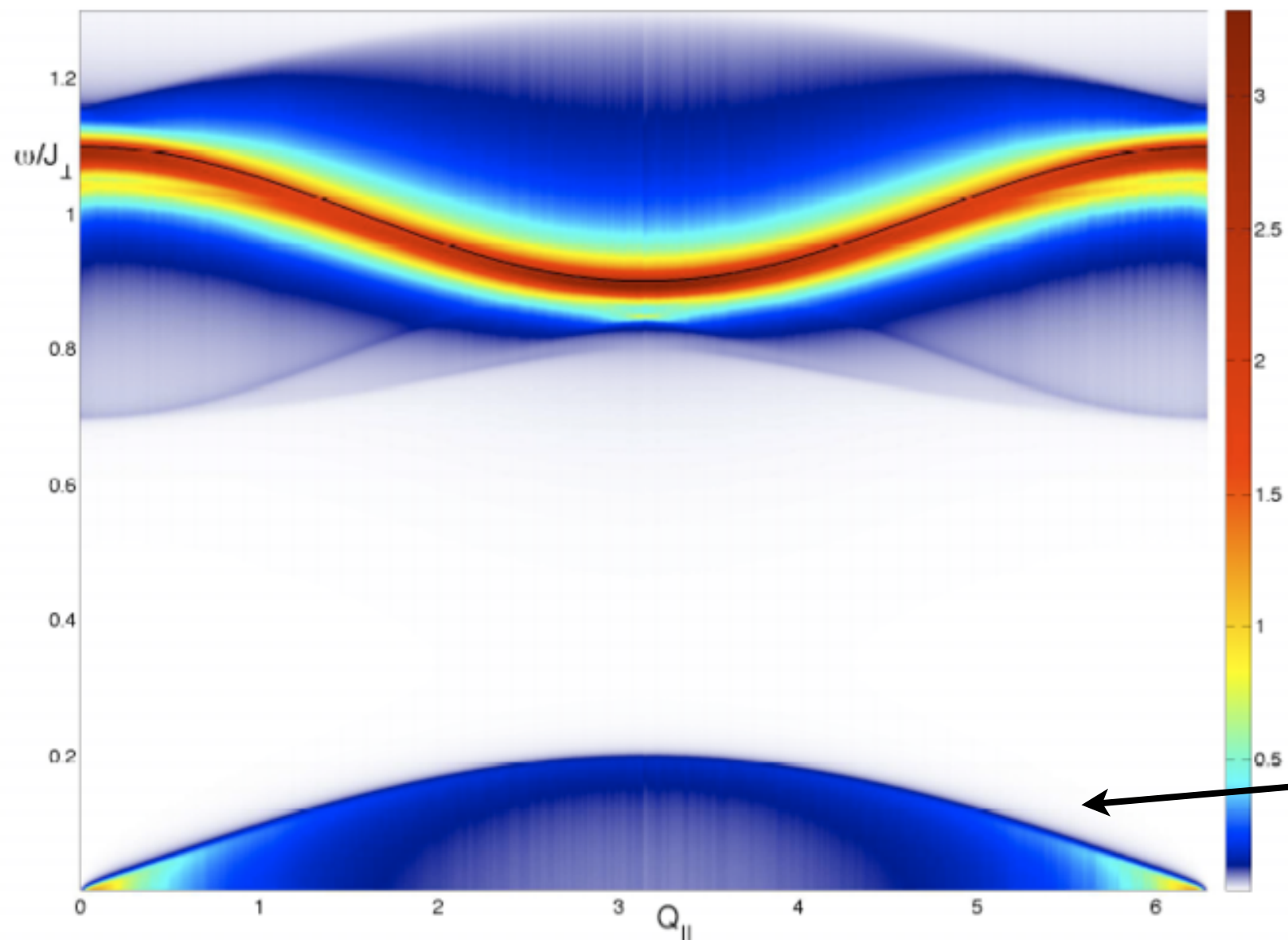
"Triplon" $S=1$ Excitation

Low-T expansion works.

For $J_{\parallel} \ll J_{\perp}$ can still use $J_{\parallel}=0$ quantum numbers (in PT)

→ combine low-T expansion with PT in J_{\parallel}

Low-T DSF for 2-leg ladder: $J_{\parallel}=0.1 J_{\perp}$, $T=0.5 J_{\perp}$, $Q_{\perp} = \pi/2$



Asymmetry in ω
depends on Q

T>0 "Resonance"



Low-T Expansion Method

Input: Energies E_n and matrix elements $\langle r|S^a(0,0)|s\rangle$

Output: Dynamical susceptibility at low T ($e^{-\beta\Delta}\ll 1$)

Can apply it to:

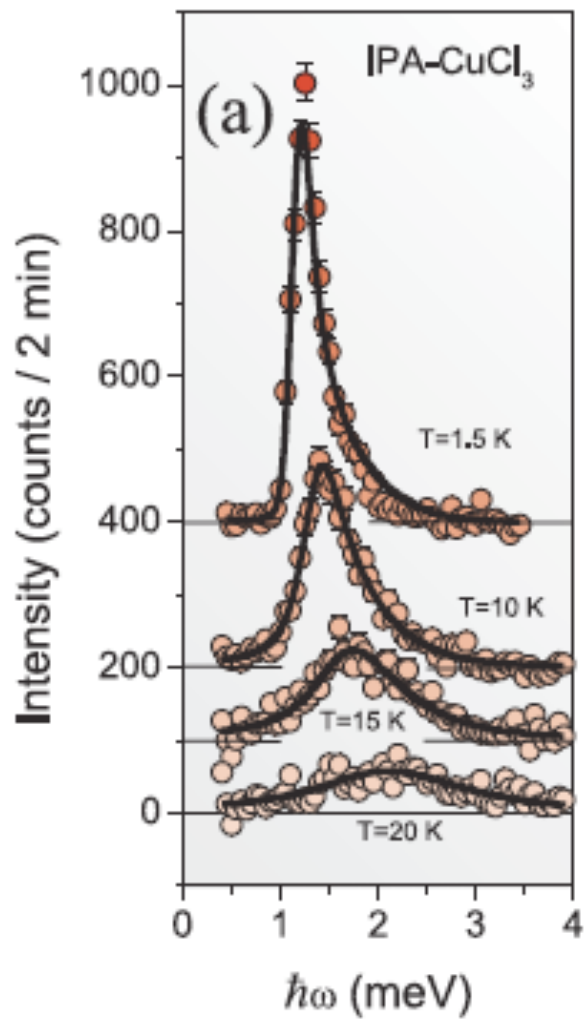
A. Integrable Models (know matrix elements exactly)
 $\Rightarrow \Sigma(\omega, q, T)$ in terms of (simple) integrals

B. Models where we know the eigenstates to a good approximation

Linewidth and "T-dependent gap"

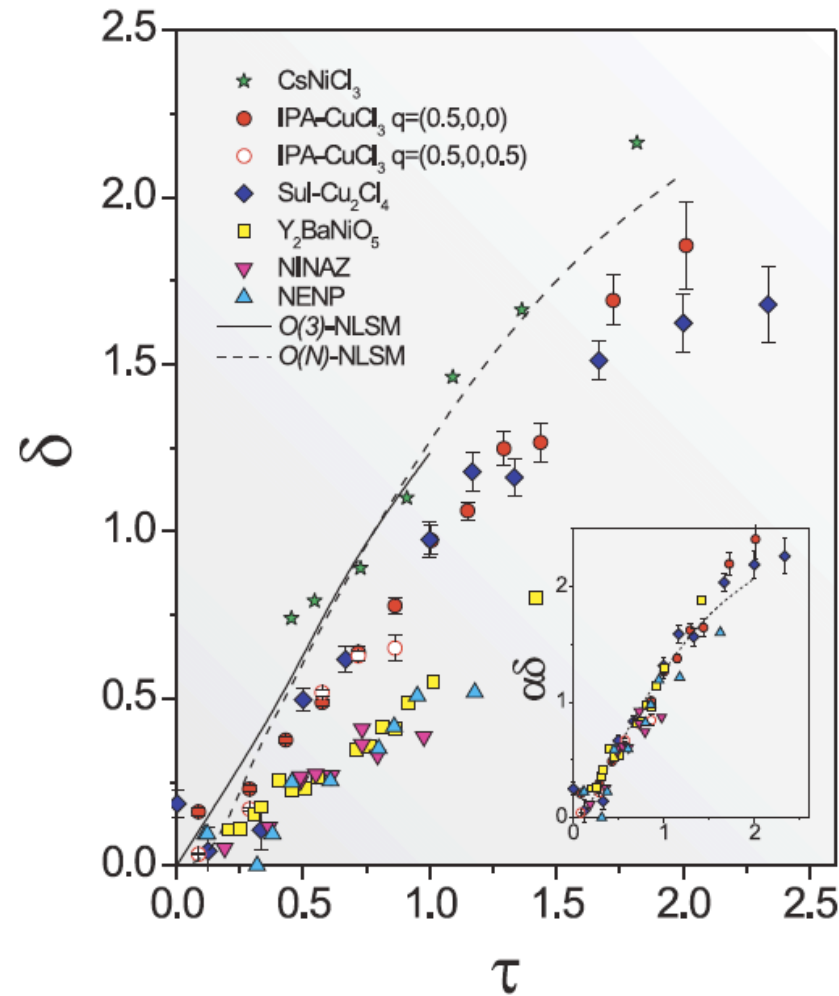
(A. Zheludev et al '08)

T=0 Gap $\Delta \ll$ Magnon Bandwidth

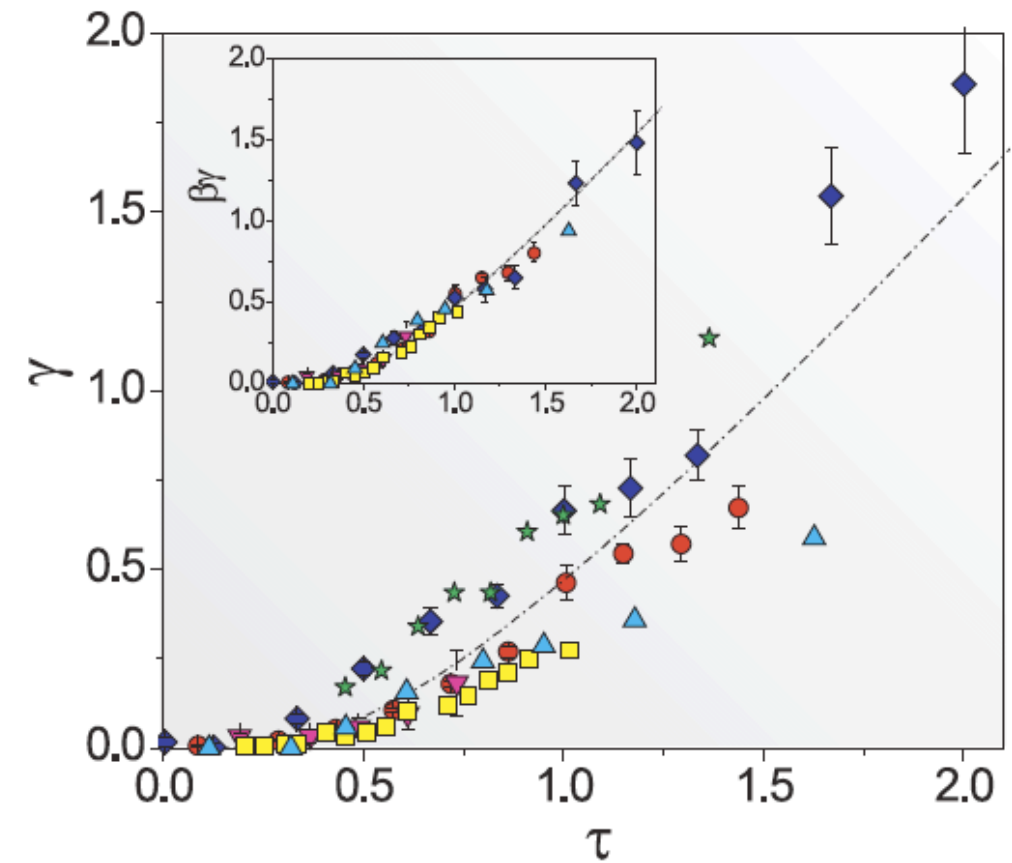


2-leg spin-1/2 ladder

"Gap" $\delta^2 = (\Delta^2(T)/\Delta^2) - 1$



Halfwidth ($\tau = T/\Delta$)



"quasi-universal" behaviour

Form Factor Bootstrap Approach

(Karowski/Weisz '78, Smirnov '93, Lukyanov '95, Delfino/Mussardo '95, Balog/Niedermaier '97, Babujian/Karowski '99...)

Exact
S-matrix



Matrix elements
of local operators

$$\langle n | \mathcal{O}(0,0) | m \rangle$$

Sigma Model is integrable



Can construct exact eigenstates labelled by n particle momenta

Basis States:

$$|n\rangle = |p_1, \dots, p_n\rangle_{a_1 \dots a_n}$$

Total Momentum:

$$P_n = \sum_{j=1}^n p_j$$

Total Energy:

$$E_n = \sum_{j=1}^n \varepsilon(p_j) \geq n\Delta$$

Form Factor Bootstrap Approach

(Karowski/Weisz '78, Smirnov '93, Lukyanov '95, Delfino/Mussardo '95, Babujian/Karowski '99...)

integrability



Matrix elements of local operators

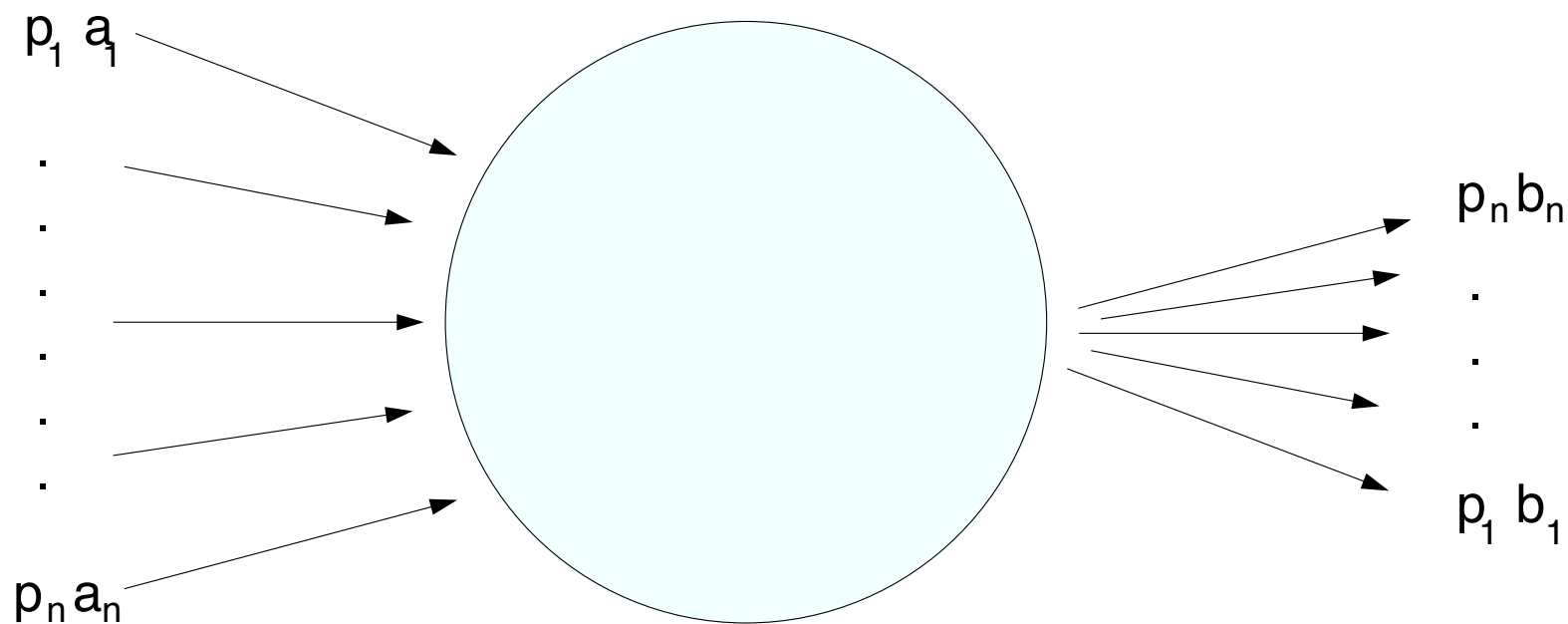
$$\langle n | \mathcal{O}(0,0) | m \rangle$$

Idea: Use Lehmann representation to calculate response functions

2-Point Functions in Integrable QFTs

e.g. $O(3)$ nonlinear sigma model $\mathcal{L} = \frac{v}{2g} \partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n} \cdot \mathbf{n} \cdot \mathbf{n} = 1$

Purely elastic scattering \Rightarrow Hamiltonian eigenbasis of scattering states



Basis States:

$$|n\rangle = |p_1, \dots, p_n\rangle_{a_1 \dots a_n}$$

Total Momentum:

$$P_n = \sum_{j=1}^n p_j$$

Total Energy:

$$E_n = \sum_{j=1}^n \varepsilon(p_j) \geq n\Delta$$

Idea: Use Lehmann representation to calculate response functions

Field Theory Limit of Integer-S Heisenberg Chain

(Haldane '83
Affleck '89)

$$H = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \quad \mathbf{S}_n^2 = S(S+1)$$



large integer S , low energies

$$\mathbf{S}_j \approx S(-1)^{ja_0} \mathbf{n}(x) + \frac{1}{vg} \mathbf{n}(x) \times \frac{\partial \mathbf{n}(x)}{\partial t}$$

$O(3)$ nonlinear
sigma model

$$\mathcal{L} = \frac{v}{2g} \partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n}$$

Constraint: $\mathbf{n} \cdot \mathbf{n} = 1$

$$v = JSa_0, \\ g = 2/S$$

Dynamical Structure Factor
around $q=\pi$:

$$S(\omega, k = \frac{\pi}{a_0} + q) \propto \int dt dx e^{i\omega t - iqx} \langle 0 | n^a(t, x) n^a(0, 0) | 0 \rangle$$