Quantum spin dynamics of the axial XXZ spin chain in the longitudinal field

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Ref. W. Yang, J. D. Wu, S. L. Xu, Zhe Wang, and C. Wu, submitted.

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Outline

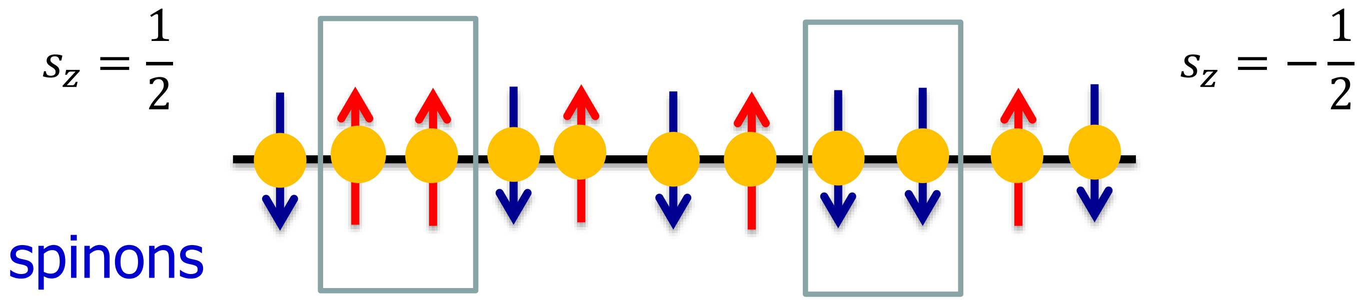
- Introduction to spin-1/2 spin chain – doped Mott insulators.
- Spin dynamics – why Bethe ansatz.
- Methodology – procedure of calculation.
- Dynamic spin structure factors – low, intermediate and high energy regimes.

Strong correlation physics in 1D systems

- Often exactly solvable (Bethe Ansatz): the Heisenberg model, Hubbard model, etc.

- Low energy effective theory -- Luttinger liquid.

- Fractionalized excitations – holon and spinon, spin-charge separations, power-law correlations.



- However, quantum dynamics remains a challenging problem.

Spin-1/2 XXZ model

$$H_{XXZ} = J\sum_{n=1}^{N}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z) - H\sum_{n=1}^{N} S_n^z$$

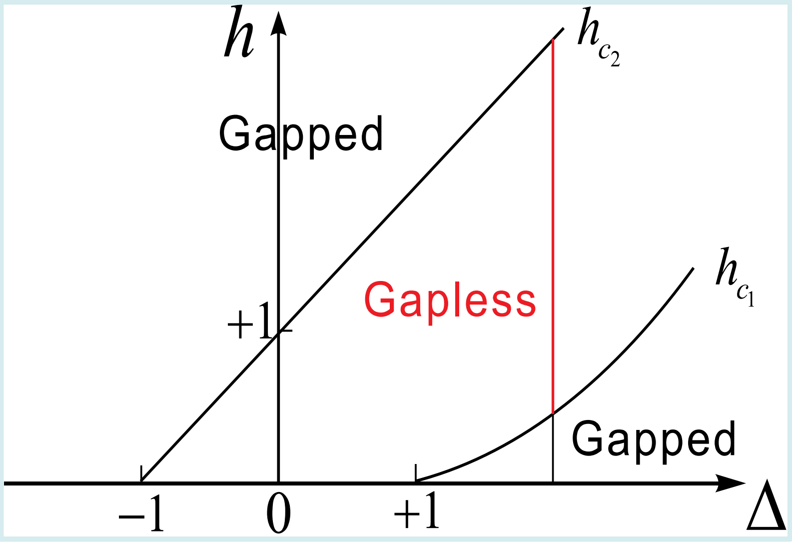
Δ: anistropy due to spin-orbit coupling, h: magnetic field.

- $\Delta \leq 1$: Power-law correlation, gapless.

  $\Delta = 1$ (Heisenberg): $\langle \vec{S}(0)\vec{S}(x)\rangle \sim (-)^x (ln x)^{1/2}/x$.

- $\Delta > 1$ (axial): commensurate Neel long-range order at H=0, spin gapped.

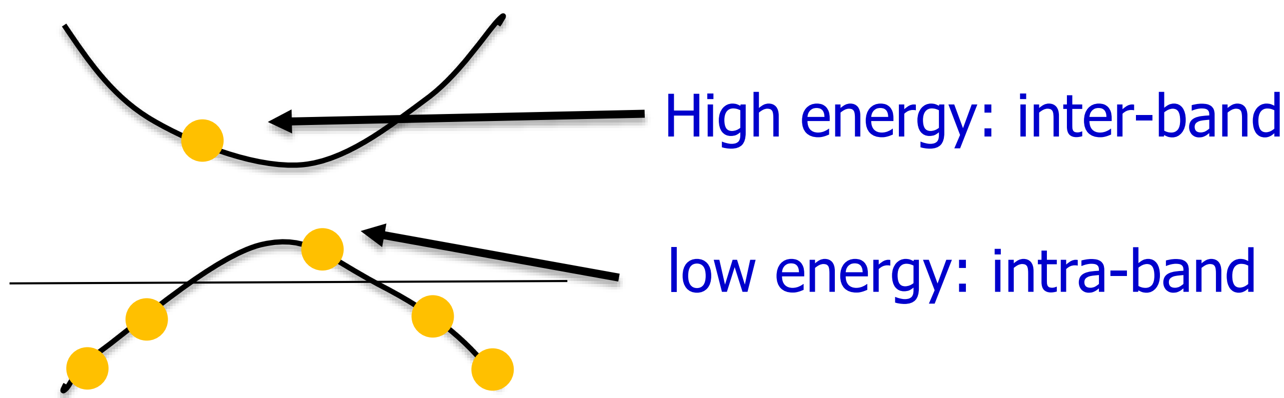
Field-induced incommensurability
→ gapless above $h_c(\Delta)$.



Relation to doped Mott insulator $\Delta > 1$

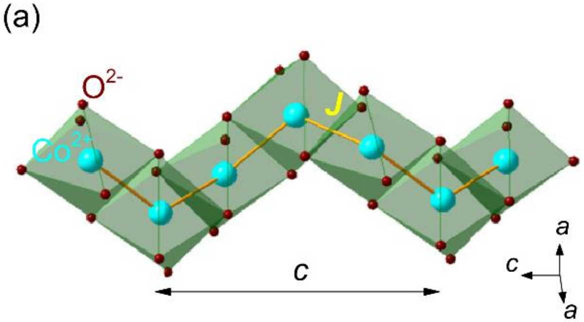
- Spin-↑→ vacuum, spin-↓→ hard-core boson.

Neel order	←→	CDW
spin gap	←→	charge gap of hard core bosons
magnetization	←→	doping
incommensurability	←→	quantum melting of CDW



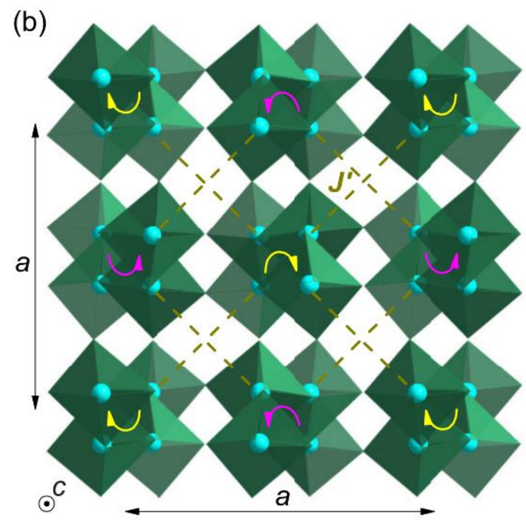
Experimental systems

Co^{2+} spin-1/2



Screw chain consisting of $\mathrm{CoO_6}$ octahedra running along the crystalline c-axis

$SrCo_2V_2O_8$



$$H = J\sum_{n=1}^{N}\left\{S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta(S_n^z S_{n+1}^z - \frac{1}{4})\right\} - g\mu_B h\sum_{n=1}^{N} S_n^z$$

- ESR experiment: THZ light along the c-axis. $S^{-+}(q,\omega)$ and $S^{+-}(q,\omega)$ detected for $q = 0, \pm\frac{\pi}{2}, \pi$.

Wang, Zhe, M. Schmidt, A. K. Bera, A. T. M. N. Islam, B. Lake, A. Loidl, and J. Deisenhofer, *PRB* 91, no. 14 140404 (2015).

Why Bethe Ansatz?

Question to address : spin dynamics over the low, intermediate and high frequency regimes.

- **Exact diagonalization:** very small size.
- **TEBD:** difficult to handle gapless systems.
- **QMC**: difficult to handle real frequency.
- **Perturbative method:** lacking small parameter.
- **Luttinger liquid:** only applies at low energy; difficult to manipulate transverse response

Dynamic spin structure factor

- Real-time spin correlation:

$$\langle G|S_i^a(t)S_j^{\bar{a}}(t')|G\rangle \qquad \text{a=+,-,z; } S_i^{\pm} = S_i^x \pm iS_i^y$$

- Fourier transform – (q, ω):

$$S^{a\bar{a}}(q,\omega) = 2\pi \sum_{\mu} \left|\langle G|S_q^a|\mu\rangle\right|^2 \delta(\omega - E_\mu + E_{GS})$$

propto differential cross sections in inelastic neutron, ESR

$$S^{zz}(q,\omega),\ S^{+-}(q,\omega),\ S^{-+}(q,\omega)$$

longitudinal transverse

Dominant excitatoins

- Bethe ansatz approach:

$$S^{\alpha\overline{\alpha}}(q,\omega) = 2\pi \sum_{\mu} |\langle GS|S_q^{\alpha}|\mu\rangle|^2 \delta(\omega - E_\mu + E_{GS})$$

- Dominant excitations:

S^{-+}: scattering states (real momenta) – psinon pairs ($1\psi\psi$, $2\psi\psi$)

S^{+-} { scattering states: psinon-antipsinon pair ($1\psi\psi^*$, $2\psi\psi^*$)
bound (string) states: 2, 3-strings ($1\chi^{(2)}$R, $1\chi^{(3)}$R)

S^{zz} { scattering states (real momenta) -- psinon anti-psinons ($1\psi\psi^*$, $2\psi\psi^*$)
bound states: 2-string states ($1\chi^{(2)}$R)

- Dominance of selected excitations checked ←→ exact sum rules.

Sum rules

- Integrated intensity: $c_a = \pm 1, 0$, for $a = \pm, z$.

$$R_{a\bar{a}} = \frac{1}{N}\sum_q \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} S^{a,\bar{a}}(q,\omega) = \frac{1}{4} + \frac{m}{2}c_a$$

- Transverse first frequency moment (FFM).

$$W_\perp(q) = \frac{1}{2}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\omega\left(S^{+-}(q,\omega) + S^{-+}(q,\omega)\right) = \alpha_\perp + \beta_\perp \cos q$$

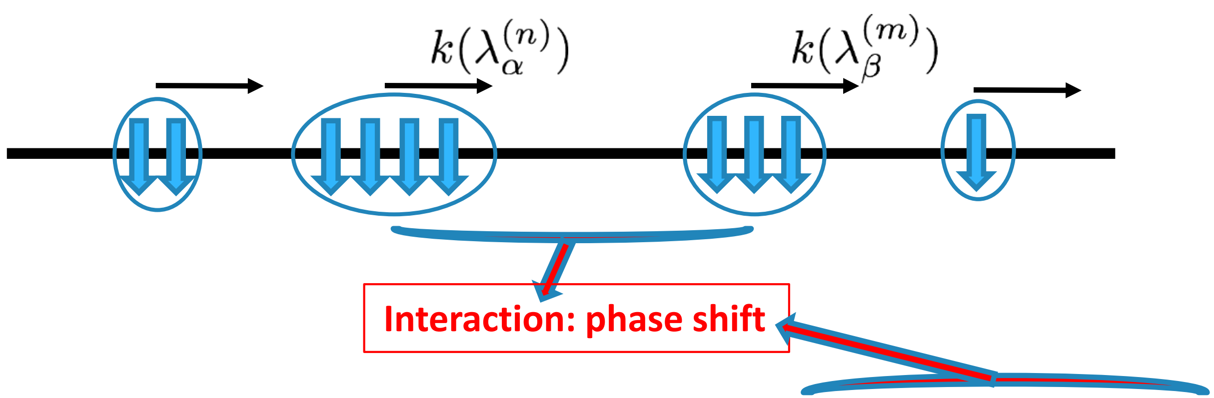
$$\alpha_\perp = -e_0 - \Delta\frac{\partial e_0}{\partial_\Delta} + mh \qquad \beta_\perp = (2-\Delta^2)\frac{\partial e_0}{\partial_\Delta} + \Delta e_0$$

- Longitudinal first frequency moment (FFM).

$$W_\parallel(q) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\omega S^{zz}(q,\omega) = (1-\cos q)\alpha_\parallel \qquad \alpha_2 = -e_0 + \Delta\frac{\partial}{\partial_\Delta}e_0$$

Bethe-Gaudin-Takahashi (BGT) equations

- Reference state: all spins up. Spin-down particles act as particles.
- String states: multi-particle bound states with complex rapidities.



Non-interacting:
$Nk = 2\pi I$

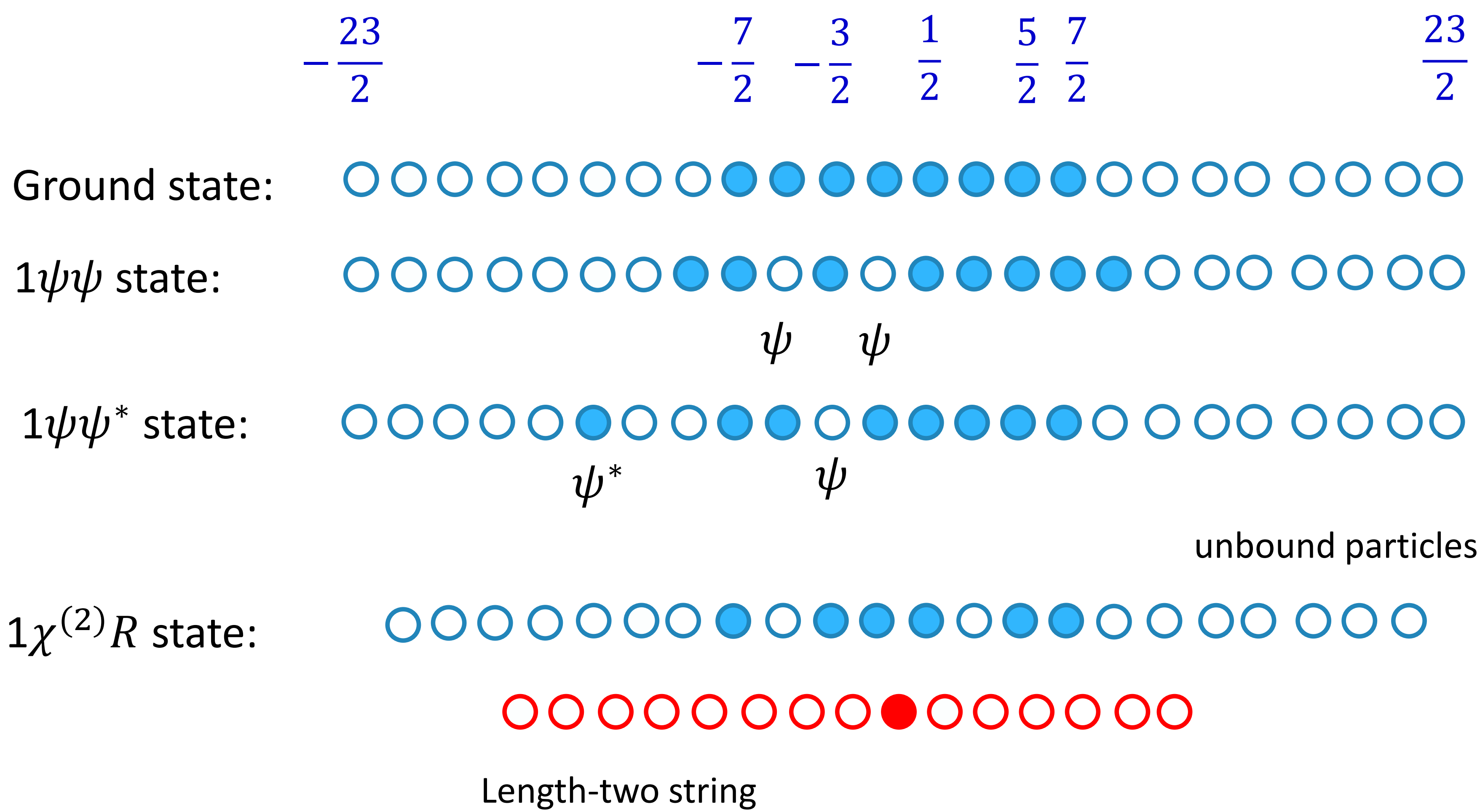
$$N\theta_n(\lambda_\alpha^{(n)}) = 2\pi I_\alpha^{(n)} + \sum_{(m,\beta)\neq(n,\alpha)} \Theta_{nm}(\lambda_\alpha^{(n)} - \lambda_\beta^{(m)})$$

$\lambda_\alpha^{(n)}$: rapidity $\quad$ $I_\alpha^{(n)}$: Bethe quantum number

Θ_{nm} : phase shift due to interaction

Bethe quantum numbers

$-\frac{M-1}{2} - S^z < I_\alpha^{(n)} < \frac{M-1}{2} + S^z$: N=32, M=8 (spin-down).



Determinant Formulas for Form Factors

$$|\langle\mu|S_q^-|\lambda\rangle|^2 = N\delta_{q,q\{\lambda\}-q\{\mu\}}|\sin(i\eta)|\frac{\Pi_{j=1}^{M+1}|\sin(\mu_j - i\eta/2)|^2}{\Pi_{j=1}^{M}|\sin(\lambda_j - i\eta/2)|^2}$$
$$\Pi_{j>k=1}^{M+1}|\sin^2(\mu_j - \mu_k) - \sin^2(i\eta)|^{-1}\Pi_{j>k=1}^{M}|\sin^2(\lambda_j - \lambda_k) - \sin^2(i\eta)|^{-1}$$
$$\frac{|\det H^-|^2}{|\det\Phi(\{\mu\})|\ |\det\Phi(\{\lambda\})|}$$

V. E. Korepin *Commun. Math. Phys.* 86, 391 (1982)
J. M. Maillet and J. Sanchez De Santos *arXiv: q-alg/9612012* (1996)
N. Kitanine, J. M. Maillet and V. Terras *Nucl. Phys. B* 554, 647 (1999)

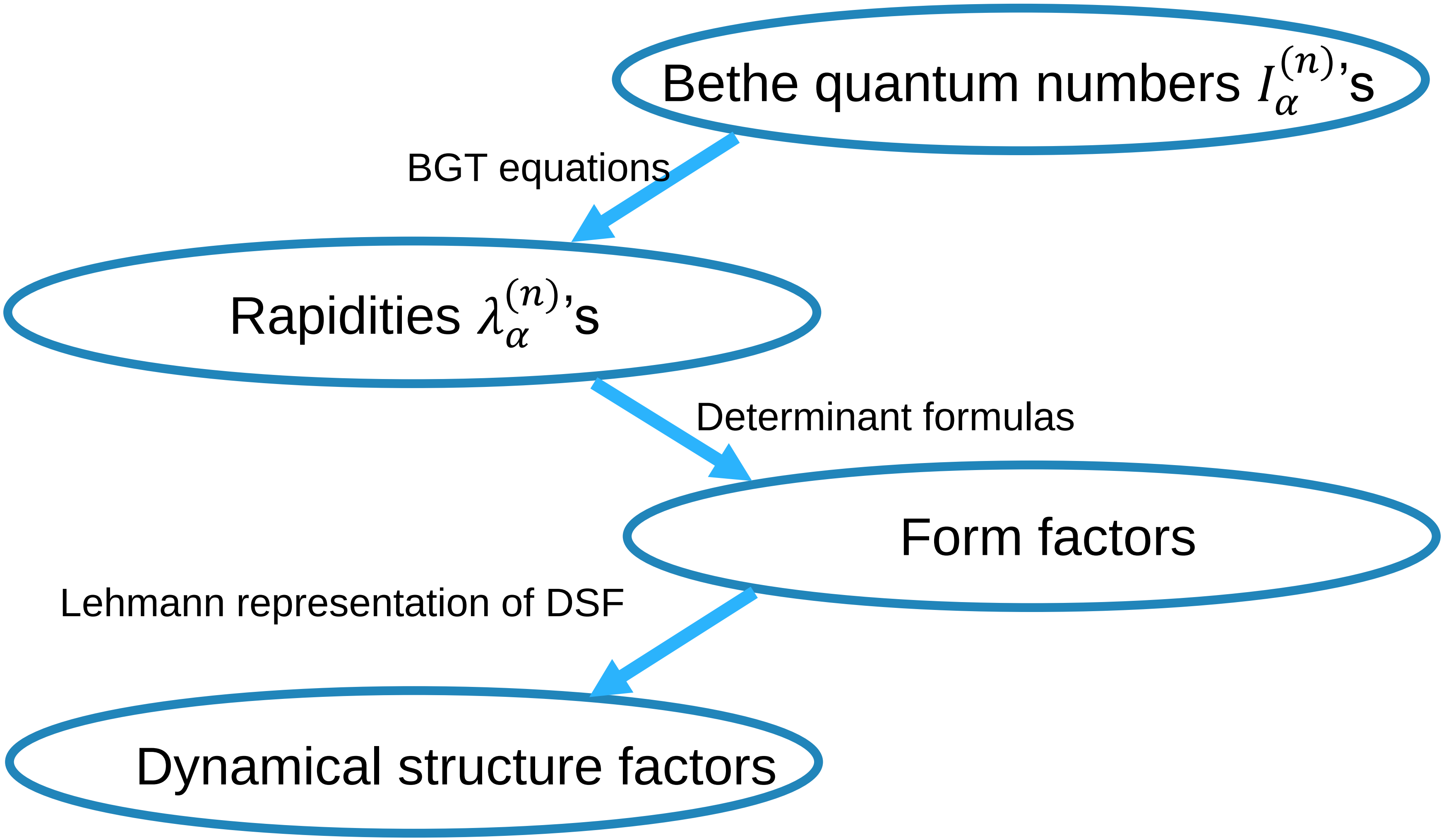
- For string states, the formulas need to be regularized.

J. Mossel, and J-S Caux *New J. Phys.,* 12.5 (2010)

- String deviations can be treated in exact manner.

R Hagemans, and J-S Caux. J. *Phys. A* 40.49 (2007)

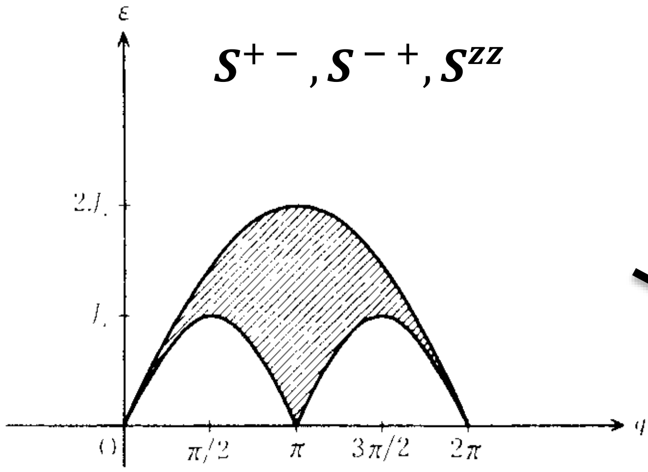
Algorithm for calculating DSF



Transverse DSF S^{+-}, S^{-+}

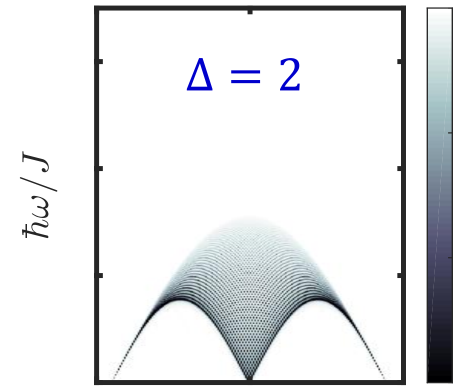
$2m = 0.1$

des Cloiseaux-Pearson (DCP) mode, h=0, $\Delta = 1$

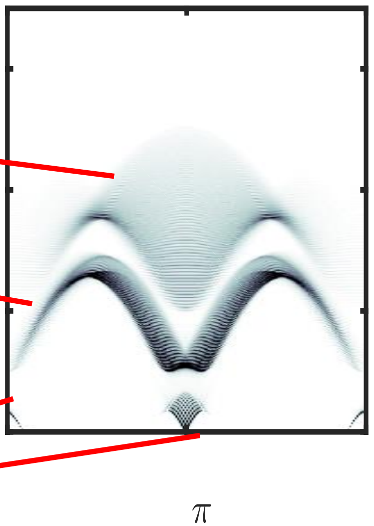


h breaks TR symm.

S^{-+}

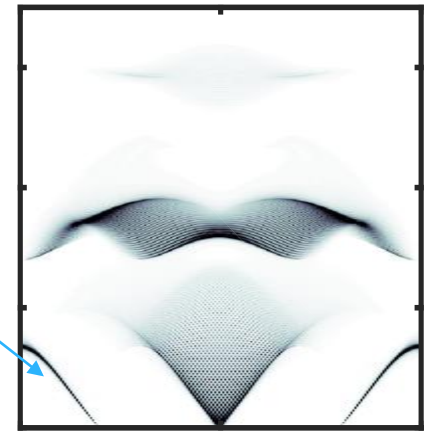


S^{+-}



Transverse DSF - S^{+-}

$2m = 0.4$

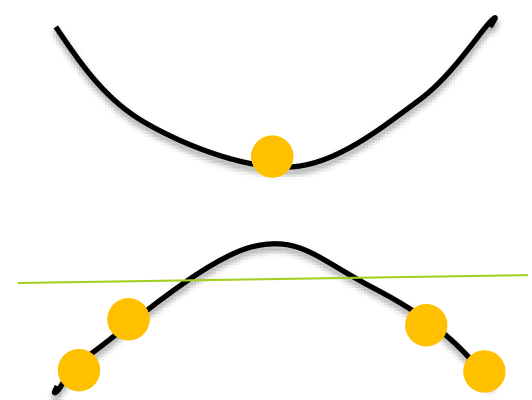


π

- Low energy: collective Larmor mode.
- Magnetic field induced incommensurability.

$$\frac{1}{i\hbar}[S^{+-}(q=0), H] = hS^{+-}(q=0) \quad \text{at } \Delta = 1$$

2 and 3-string states: excitations see the gapped Neel ordered background.



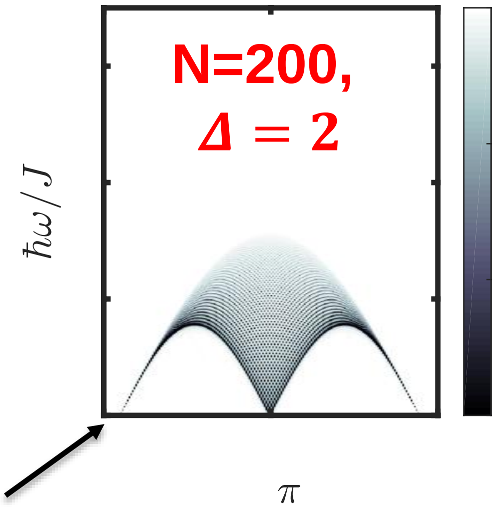
Transverse DSF - S^{-+}

- Analogy of the des Cloiseaux-Pearson mode

$2m = 0.1$

S^{-+}:

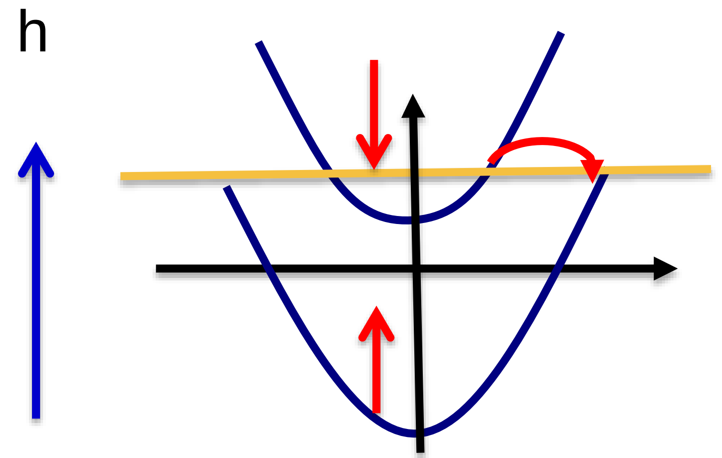
$\langle \mu | S^{+} | G \rangle$



$q = 2m\pi$

$|G\rangle \rightarrow \; |\mu\rangle: flip\; \downarrow to\; \uparrow$

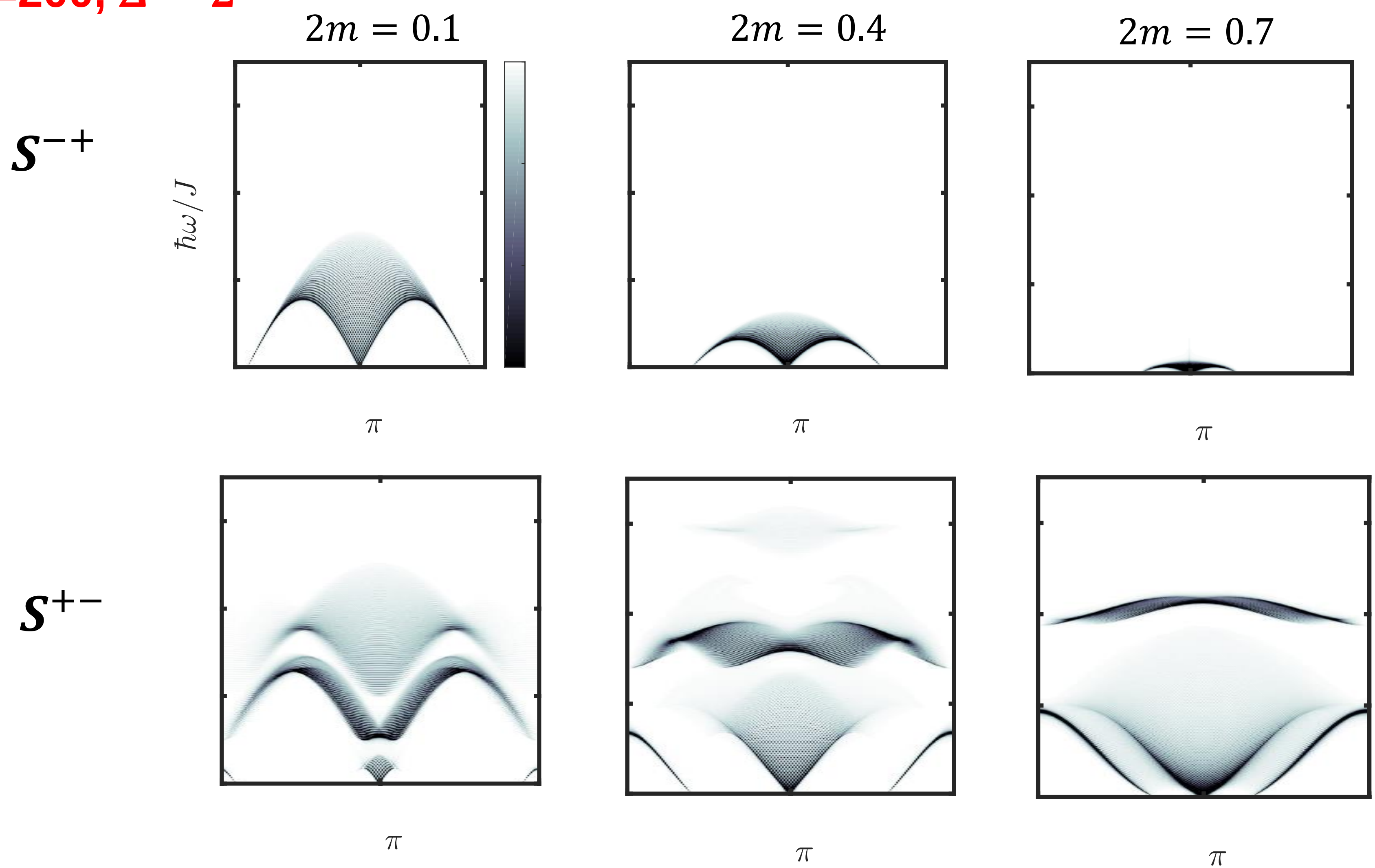
Hubbard chain at half-filling → Heisenberg



$k_{f\uparrow,\downarrow} = \pi(\frac{1}{2} \pm m)$

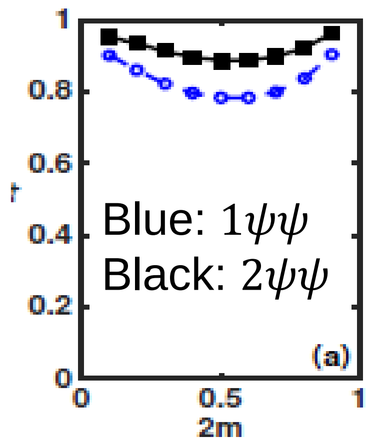
Transverse DSF – Evolution with magnetization

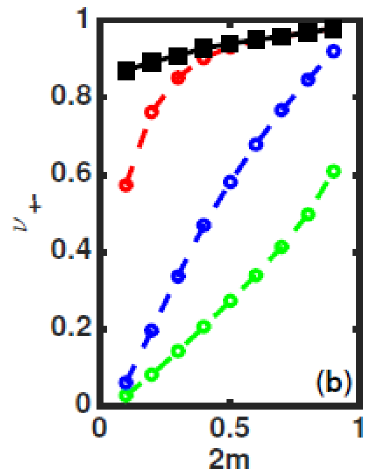
N=200, $\Delta = 2$



Comparison with sum rules – transverse DSF

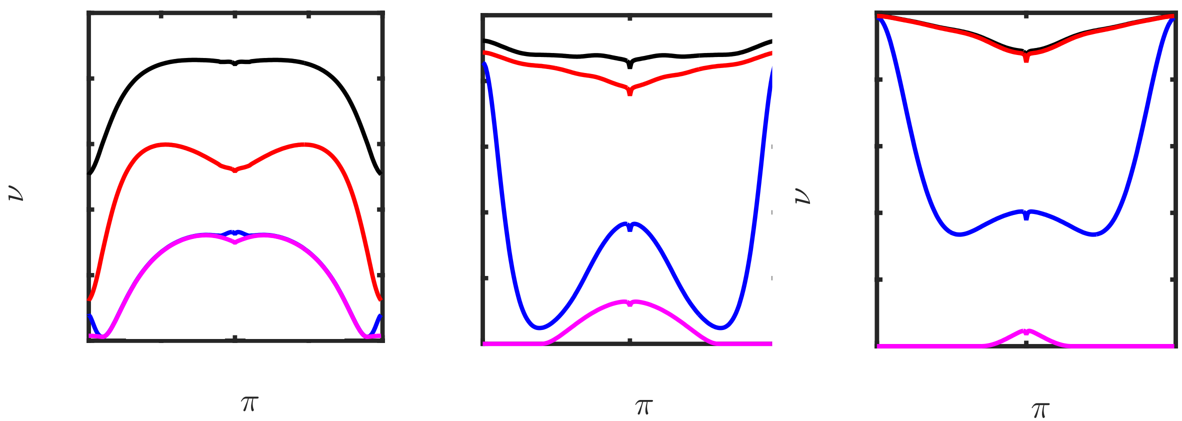
- Saturation of sum rule of integrated intensity: (a) for S^{-+}, (b) for S^{+-}.





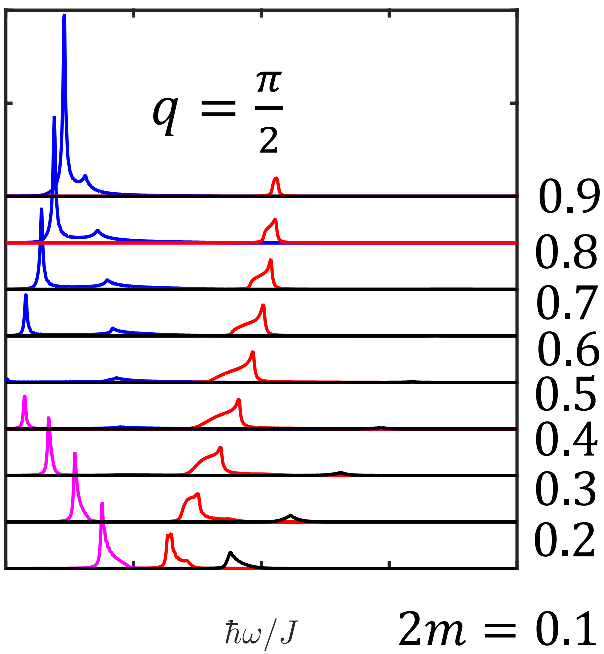
Green: $1\psi\psi^*$
Blue: $2\psi\psi^*$
Red: two-string states
Black: three-string states

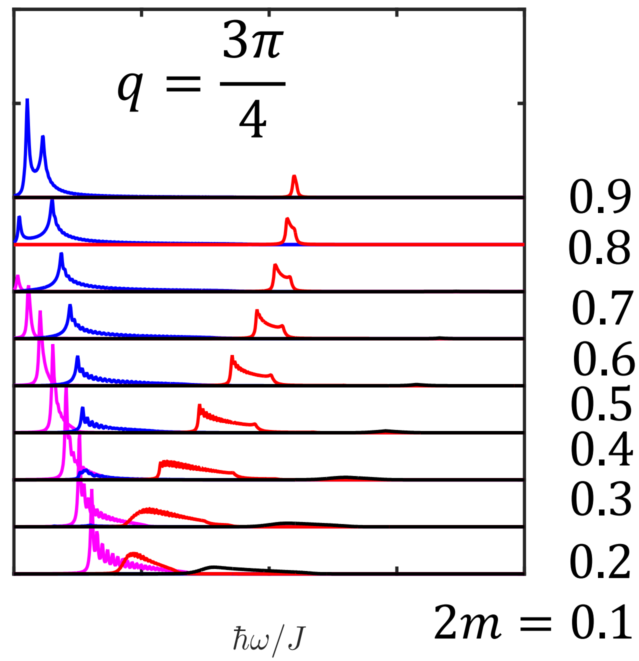
- Momentum-resolved: (a) for 2m=0.1, (b) for 2m=0.4, (c) for 2m=0.7.



Pink: S^{-+}
Blue: real states in S^{+-}
Red: two-string states in S^{+-}
Black: three-string states in S^{+-}

Evolution of DSF intensity at specific momenta

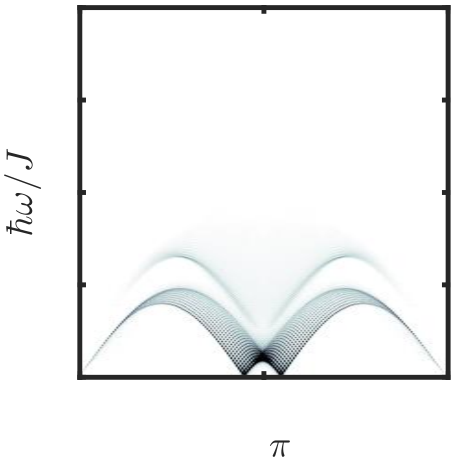




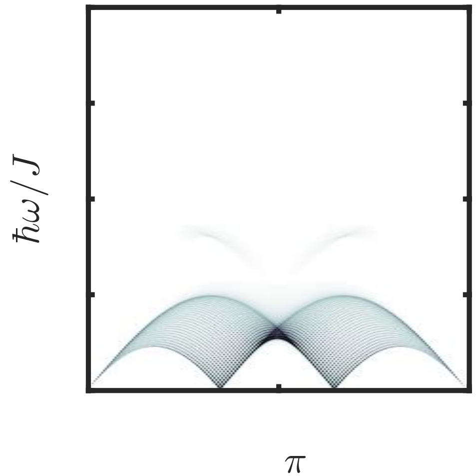
Pink: S^{-+}
Blue: real states in S^{+-}
Red: two-string states in S^{+-}
Black: three-string states in S^{+-}

String stats occupy regions of higher energies,
and the peaks are more smeared.

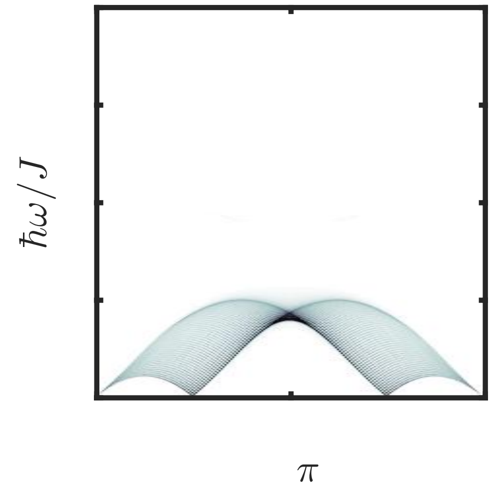
Longitudinal DSF $S^{zz}(q,\omega)$- intensity plot



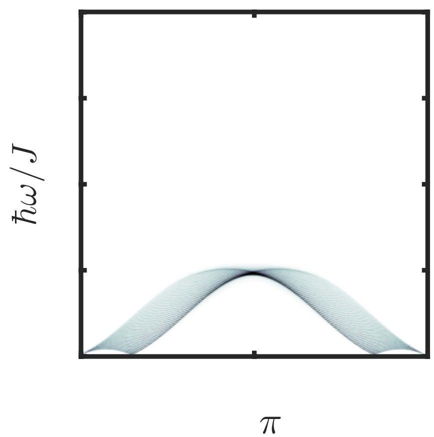
2m=0.1



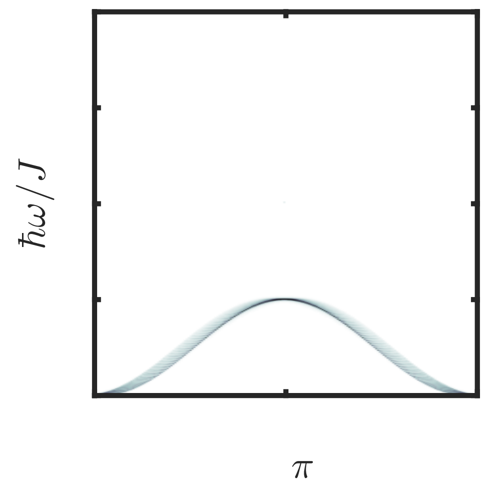
2m=0.3



2m=0.5



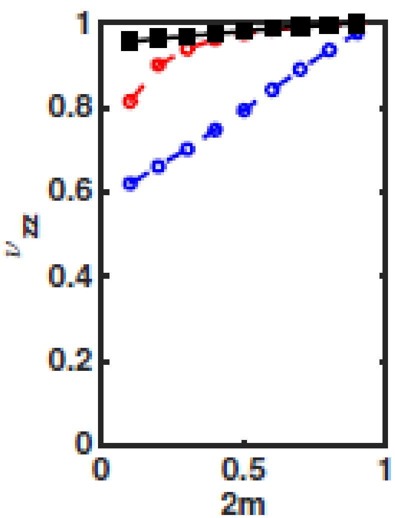
2m=0.7



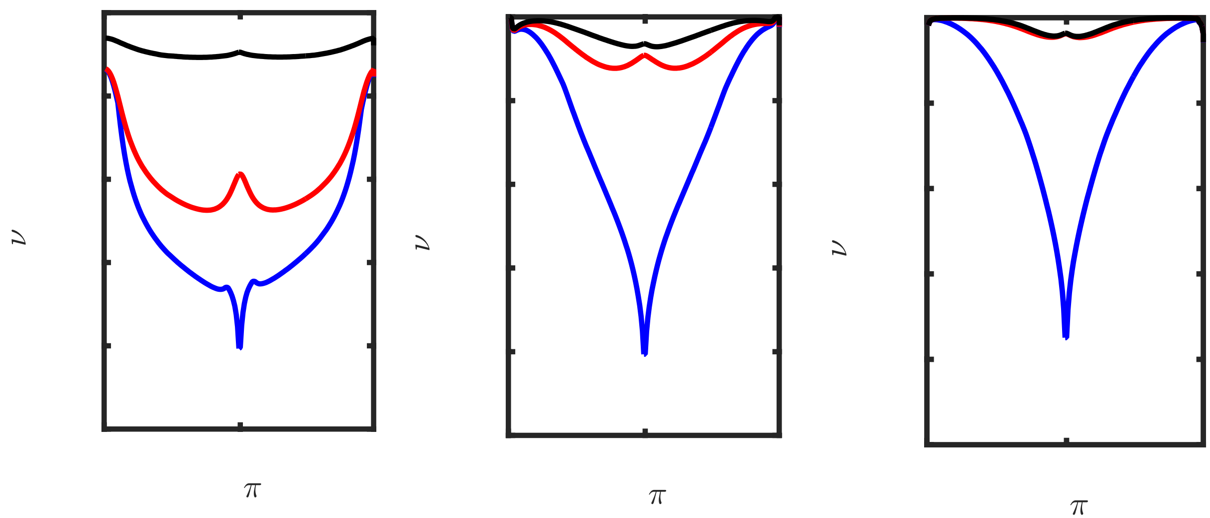
2m=0.9

Comparison with sum rules for longitudinal DSF

Saturation of momentum-integrated intensity



momentum-resolved intensity



2m=0.1

2m=0.4

2m=0.7

Blue: $1\psi\psi^*$

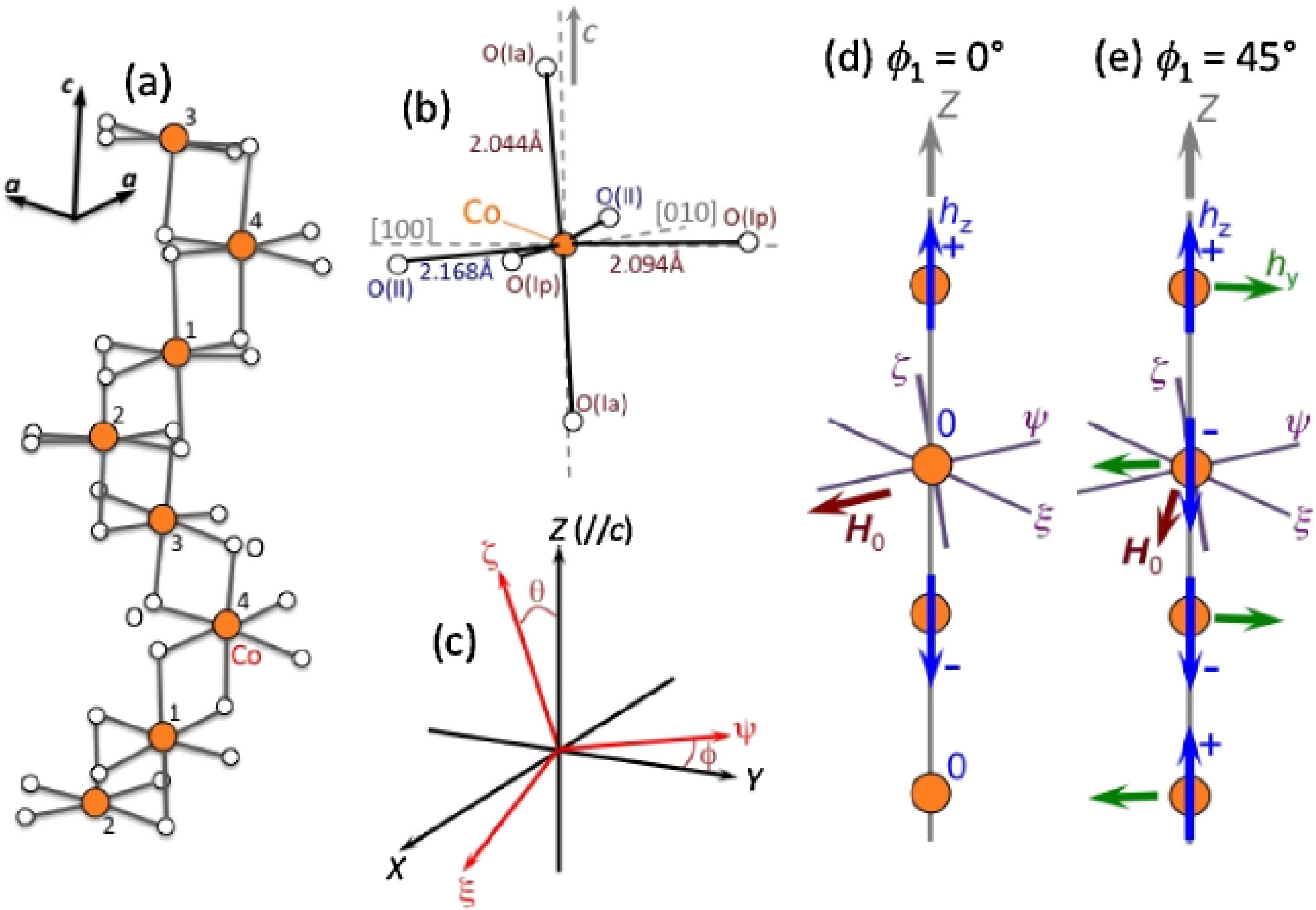
Red: $2\psi\psi^*$

Black: two-string states

Summary

- Dynamic spin structure factor S^{-+}, S^{+-} and S^{zz} for the axial XXZ model.
- Dominant excitations identified-- excellent agreement with sum rules.
- Low energy – gapless, magnetic-field-induced incommensurability

Intermediate and high energies -- gapped Neel background



(a)
c
a
a
3
4
1
2
3
4
Co
1
2
(b)
c
O(Ia)
2.044Å
Co
O(II)
[010]
O(Ip)
[100]
2.168Å
O(Ip)
2.094Å
O(II)
O(Ia)
(c)
Z (//c)
ζ
θ
ψ
ϕ
Y
X
ξ
(d) ϕ1 = 0°
Z
hz
+
ζ
0
ψ
ξ
H0
-
0
(e) ϕ1 = 45°
Z
hz
+
hy
ζ
-
ψ
ξ
H0
-
+

Derivation of determinant formulae

$$\langle \mu | S_n^a | \lambda \rangle = \frac{\langle \Psi(\{\mu_i\}) | S_j^a | \Psi(\{\lambda_j\}) \rangle}{\sqrt{\langle \Psi(\{\mu_i\}) | \Psi(\{\mu_i\}) \rangle} \cdot \sqrt{\langle \Psi(\{\lambda_j\}) | \Psi(\{\lambda_j\}) \rangle}}$$

Quantum inverse problem:

$$\sigma_i^- = \prod_{\alpha=1}^{i-1} (A+D)(\xi_\alpha) \cdot B(\xi_i) \cdot \prod_{\alpha=i+1}^{N} (A+D)(\xi_\alpha),$$

$$\sigma_i^+ = \prod_{\alpha=1}^{i-1} (A+D)(\xi_\alpha) \cdot C(\xi_i) \cdot \prod_{\alpha=i+1}^{N} (A+D)(\xi_\alpha),$$

$$\sigma_i^z = \prod_{\alpha=1}^{i-1} (A+D)(\xi_\alpha) \cdot (A-D)(\xi_i) \cdot \prod_{\alpha=i+1}^{N} (A+D)(\xi_\alpha)$$

F-basis:

$$\widetilde{D}_{1\ldots N}(\lambda; \xi_1, \ldots, \xi_N) \equiv F_{1\ldots N}(\xi_1, \ldots, \xi_N)\ D_{1\ldots N}(\lambda; \xi_1, \ldots, \xi_N)\ F^{-1}_{1\ldots N}(\xi_1, \ldots, \xi_N)$$

$$= \bigotimes_{i=1}^{N} \begin{pmatrix} b(\lambda, \xi_i) & 0 \\ 0 & 1 \end{pmatrix}_{[i]}.$$

$$\widetilde{B}_{1\ldots N}(\lambda) = \sum_{i=1}^{N} \sigma_i^-\ c(\lambda, \xi_i) \bigotimes_{j \neq i} \begin{pmatrix} b(\lambda, \xi_j) & 0 \\ 0 & b^{-1}(\xi_j, \xi_i) \end{pmatrix}$$

Algebraic Bethe Ansatz

Yang-Baxter Equation:

$$R_{12}(\lambda_1,\lambda_2)R_{13}(\lambda_1,\lambda_3)R_{23}(\lambda_2,\lambda_3) = R_{23}(\lambda_2,\lambda_3)R_{13}(\lambda_1,\lambda_3)R_{12}(\lambda_1,\lambda_2)$$

Monodromy matrix:

$$\mathcal{T}(\lambda) = R_{0n}(\lambda, i\frac{\eta}{2})...R_{02}(\lambda, i\frac{\eta}{2})R_{01}(\lambda, i\frac{\eta}{2}) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}_{[0]}$$

Transfer matrix and XXZ Hamiltonian:

$$T(\lambda) = \mathrm{Tr}\mathcal{T}(\lambda) \qquad H = \sin(i\eta)\frac{d}{d\lambda}\ln T(\lambda)|_{\lambda=i\eta/2} + \mathrm{const.}$$

Magnon creation operator:

$$\Psi(\lambda_1,\lambda_2,...,\lambda_r) = B(\lambda_1)B(\lambda_2)...B(\lambda_r)|\uparrow\uparrow...\uparrow\rangle$$

L. A. Takhtadzhan and L. D. Faddeev *Russ. Math. Sur.* 34,11 (1979)