Quasiparticles in Spin Chains

Interaction – Thermodynamics – Observability

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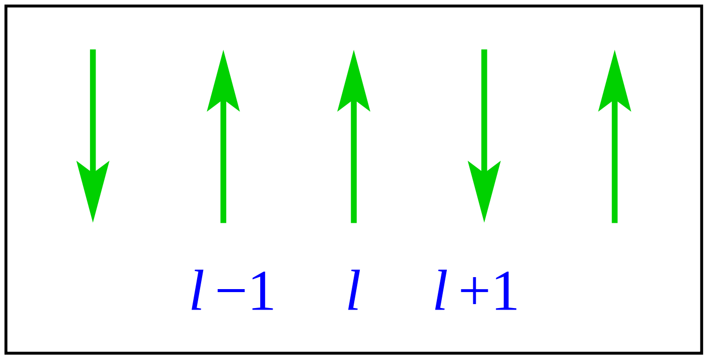
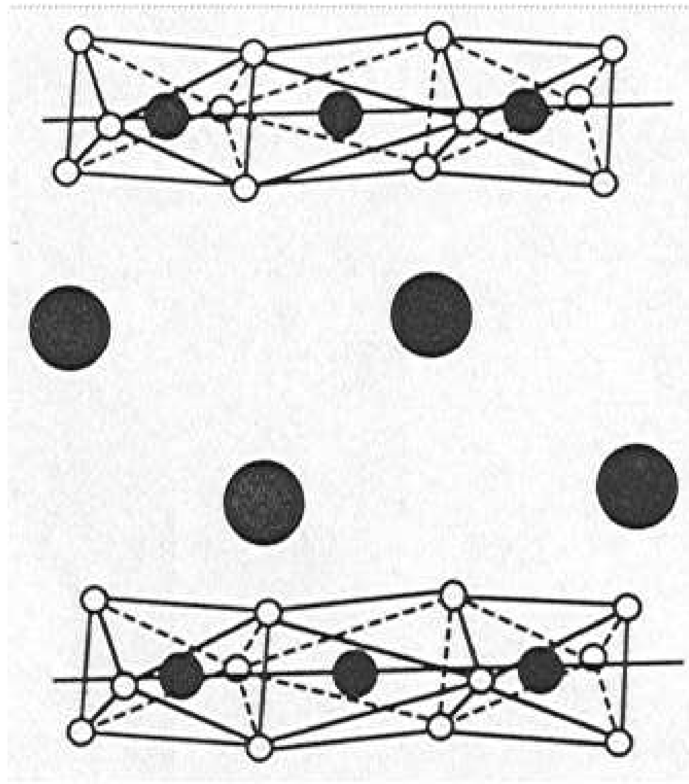
Quantum Spin Chain

- magnetic compound
- magnetic ions
- exchange coupling
- charge-spin separation
- collective spin modes
- quasiparticle composition
- quasiparticle interaction
- thermodynamics, dynamics





$CsCoCl_3$

Model Hamiltonians

XXZ model: $H = \sum_{\ell=1}^{N} \left[J_\perp \left(S_\ell^x S_{\ell+1}^x + S_\ell^y S_{\ell+1}^y \right) + J_\| S_\ell^z S_{\ell+1}^z \right]$

XX : $H = J \sum_{\ell=1}^{N} [S_\ell^x S_{\ell+1}^x + S_\ell^y S_{\ell+1}^y]$

XXX : $H = J \sum_{\ell=1}^{N} \mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1}$

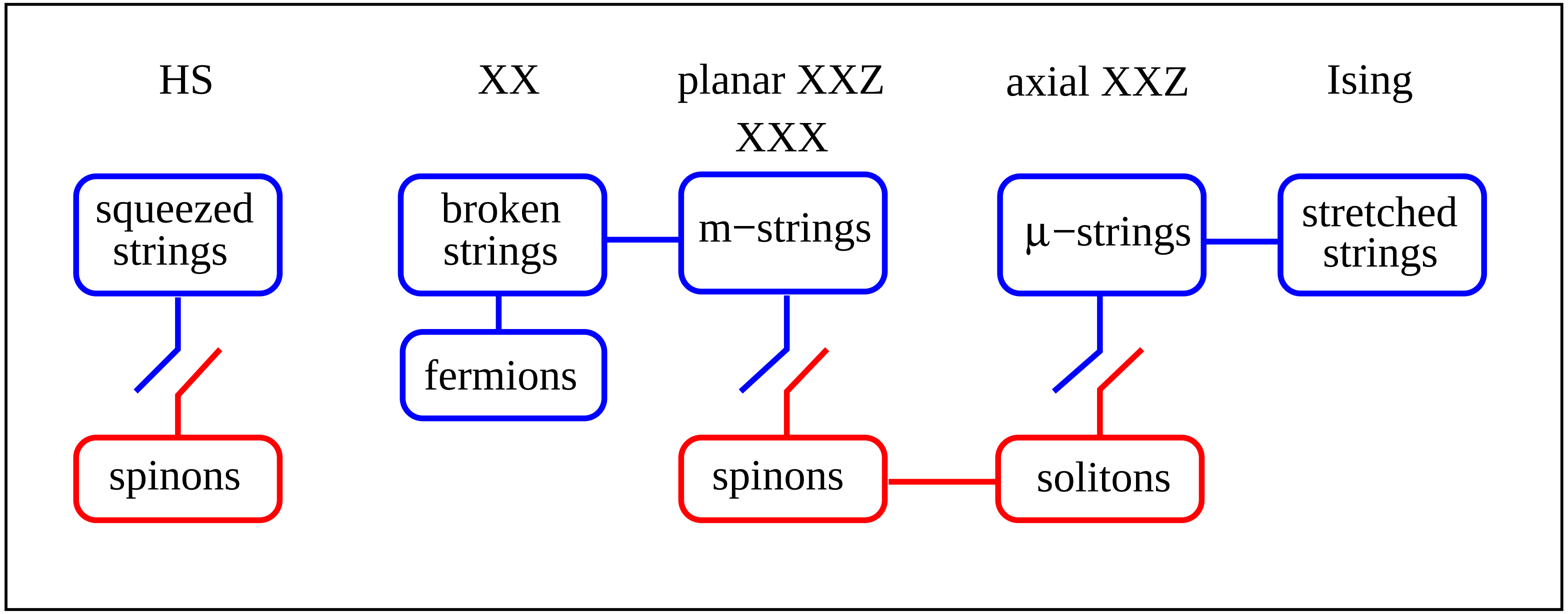
Ising : $H = J \sum_{\ell=1}^{N} S_\ell^z S_{\ell+1}^z$

- symmetries
- conservation laws, integrability
- exact analysis
- interacting quasiparticles
- pseudovacuum, physical vacuum

Haldane-Shastry model:

$$H = \sum_{\ell<\ell'} J_{\ell\ell'} \, \mathbf{S}_\ell \cdot \mathbf{S}_{\ell'}, \qquad J_{\ell\ell'} = J \left[\frac{N}{\pi} \sin \frac{\pi(\ell-\ell')}{N} \right]^{-2}$$

Zoo of Quasiparticles



- dispersion
- spin
- scattering, binding
- exclusion statistics
- selection rules

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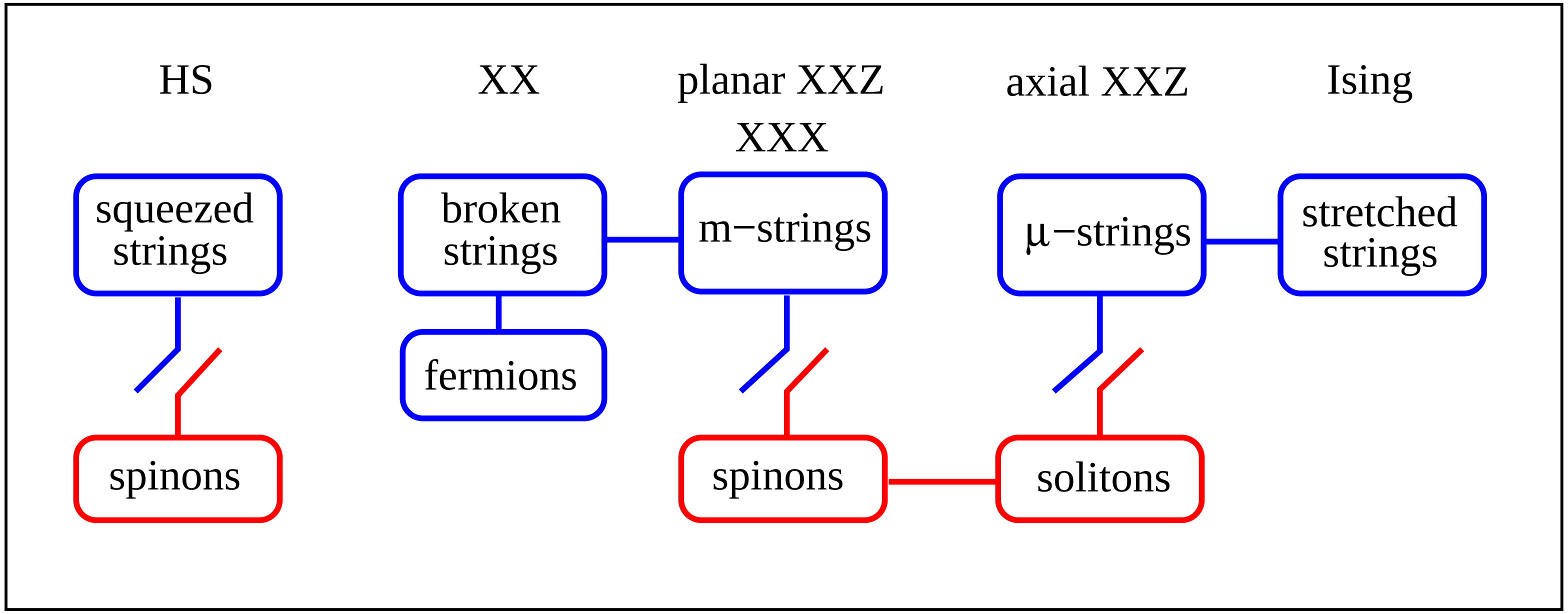

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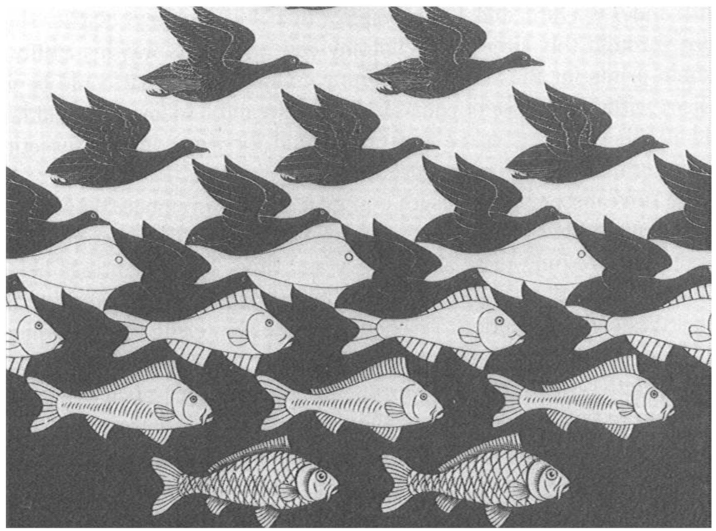


XX Model: Jordan-Wigner Fermions

Hamiltonian: $H = J \sum_n [S_n^x S_{n+1}^x + S_n^y S_{n+1}^y] = J \sum_{\{p_i\}} \cos p_i \, c_{p_i}^\dagger c_{p_i} .$

Jordan-Wigner transform: $S_n^z = c_n^\dagger c_n - \frac{1}{2}, \quad S_n^+ = S_n^x + i S_n^y = c_n^\dagger \exp\left(i\pi \sum_{j<n} c_j^\dagger c_j \right) .$

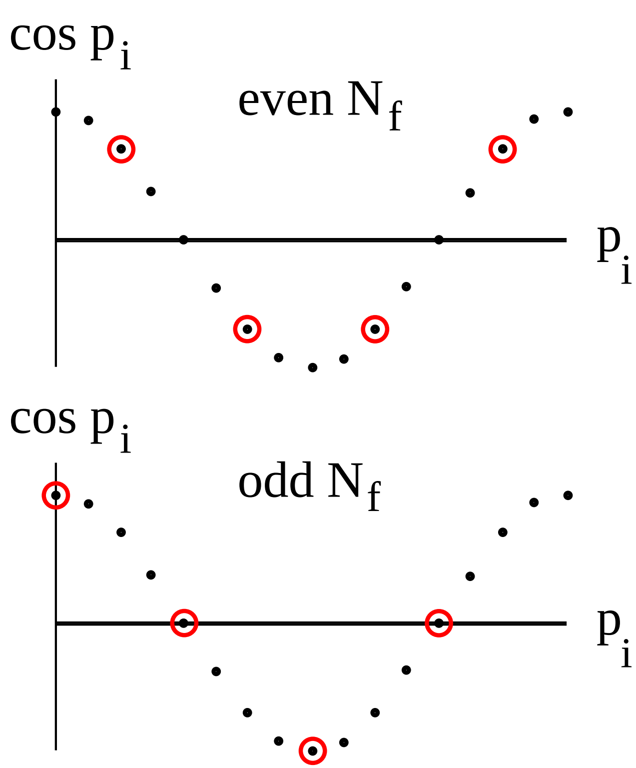
Fourier transform: $c_p = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ipn} c_n .$

Magnetization: $M_z = \frac{N}{2} - N_f .$

Fermion momenta: $p_i = \frac{\pi}{N} \bar{m}_i ,$

$$\bar{m}_i \in \begin{cases} \{1,3,\ldots,2N-1\} & (N_f \text{ even}) \\ \{0,2,\ldots,2N-2\} & (N_f \text{ odd}) \end{cases}$$

Wave number: $k = \frac{\pi}{N} \sum_{i=1}^{N_f} p_i \mod(2\pi)$



XX Model: Fermions Versus Spinons I

N_f	$\bar{m}_i$ (0 2 4 6)	M_z	k	E
0	○ ○ ○ ○	+2	0	0.000
1	○ ● ○ ○	+1	1	0.000
	○ ○ ● ○		2	−1.000
	○ ○ ○ ●		3	0.000
	● ○ ○ ○		0	1.000
2	○ ● ● ○	0	0	−1.414
	○ ● ○ ●		1	0.000
	● ● ○ ○		2	0.000
	○ ○ ● ●		2	0.000
	● ○ ● ○		3	0.000
	● ○ ○ ●		0	1.414
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	● ● ● ○		3	0.000
	● ● ○ ●		0	1.000
4	● ● ● ●	−2	0	0.000

Magnetization.

- from fermions:
  $$M_z = \frac{N}{2} - N_f;$$
- from spinons:
  $$M_z = \frac{1}{2}(N_+ - N_-),$$
  $$N_s = N_+ + N_-.$$

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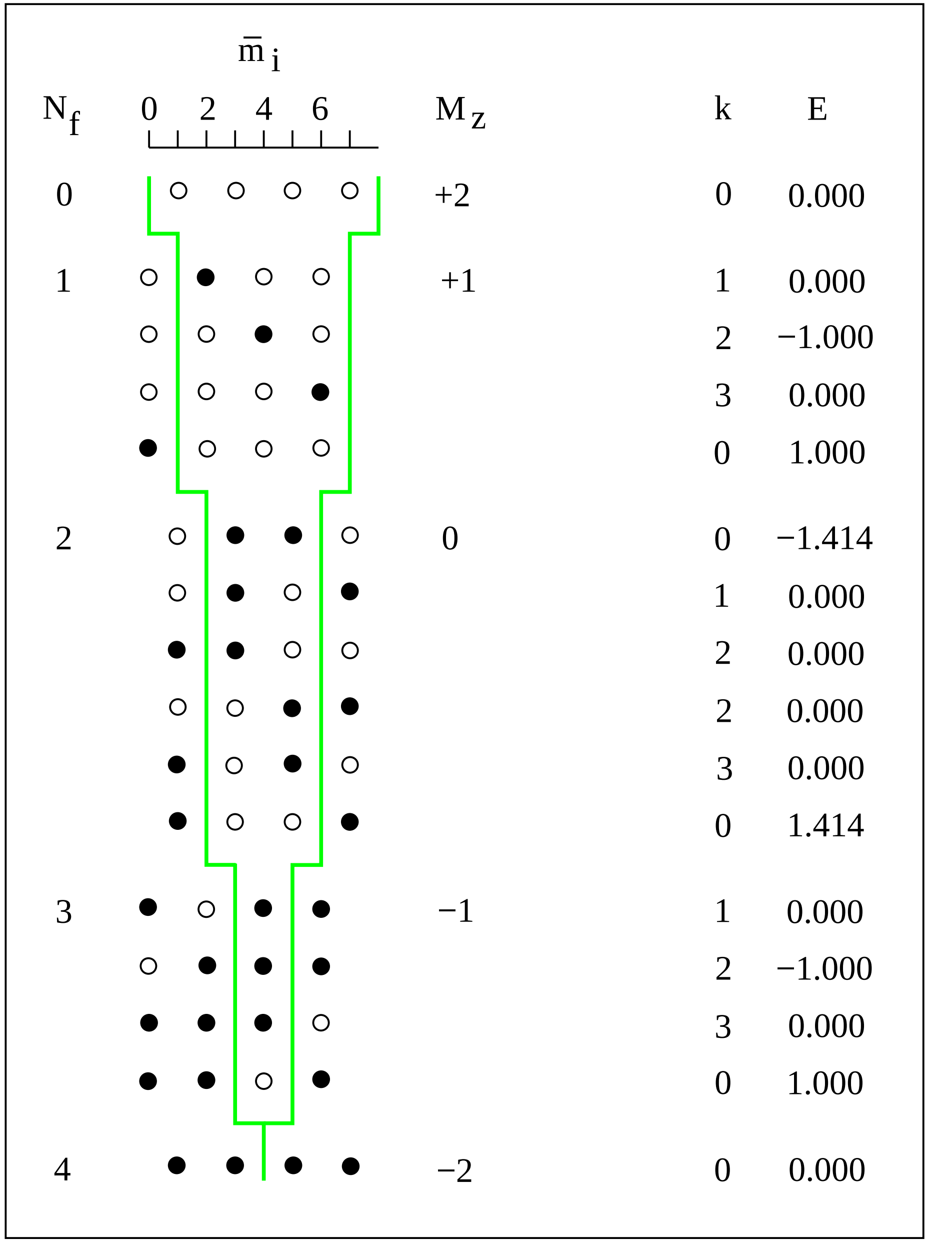

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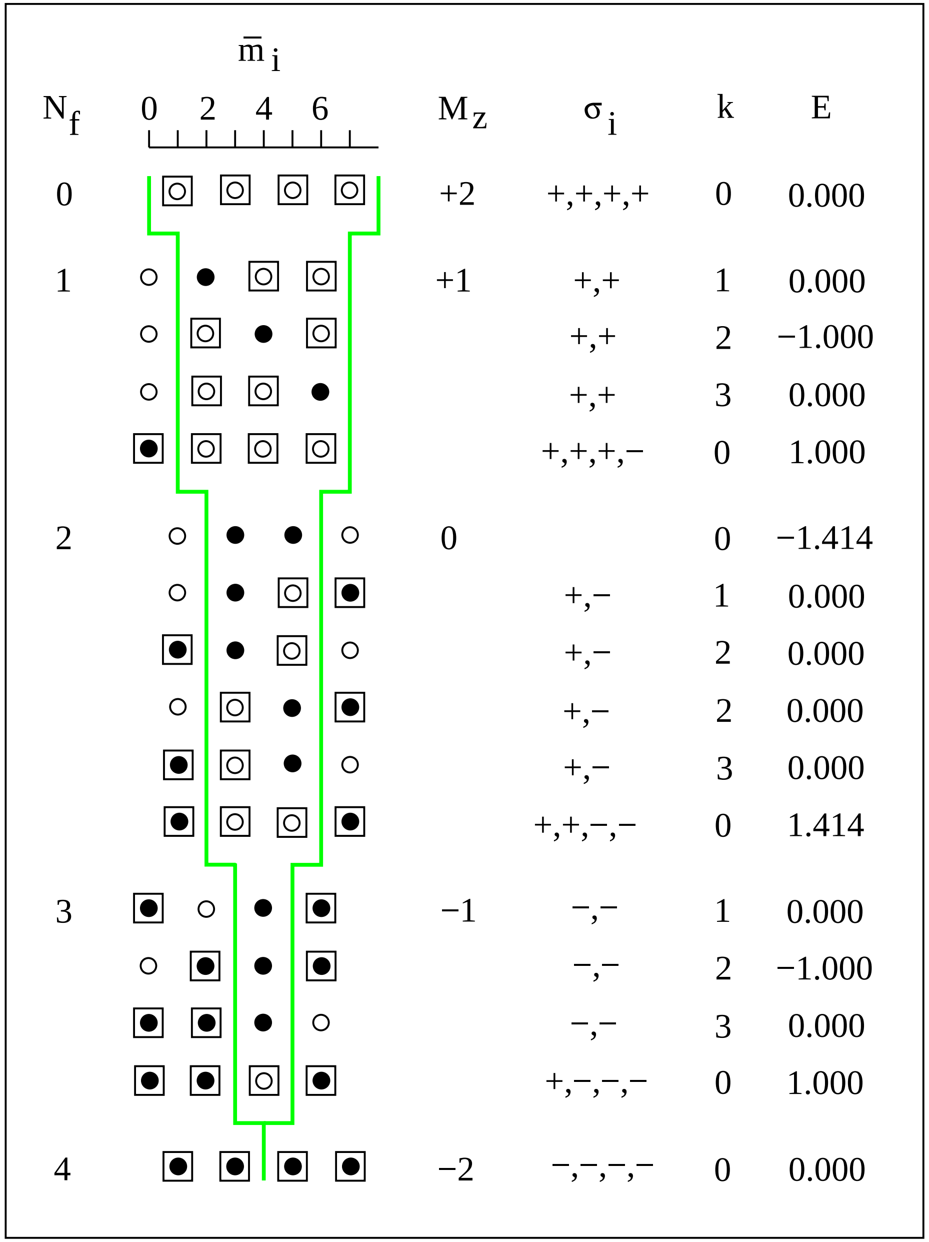

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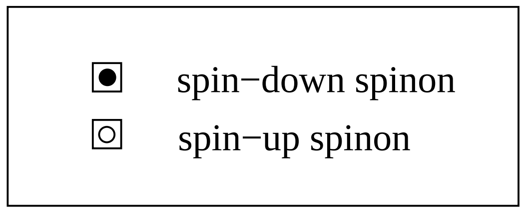
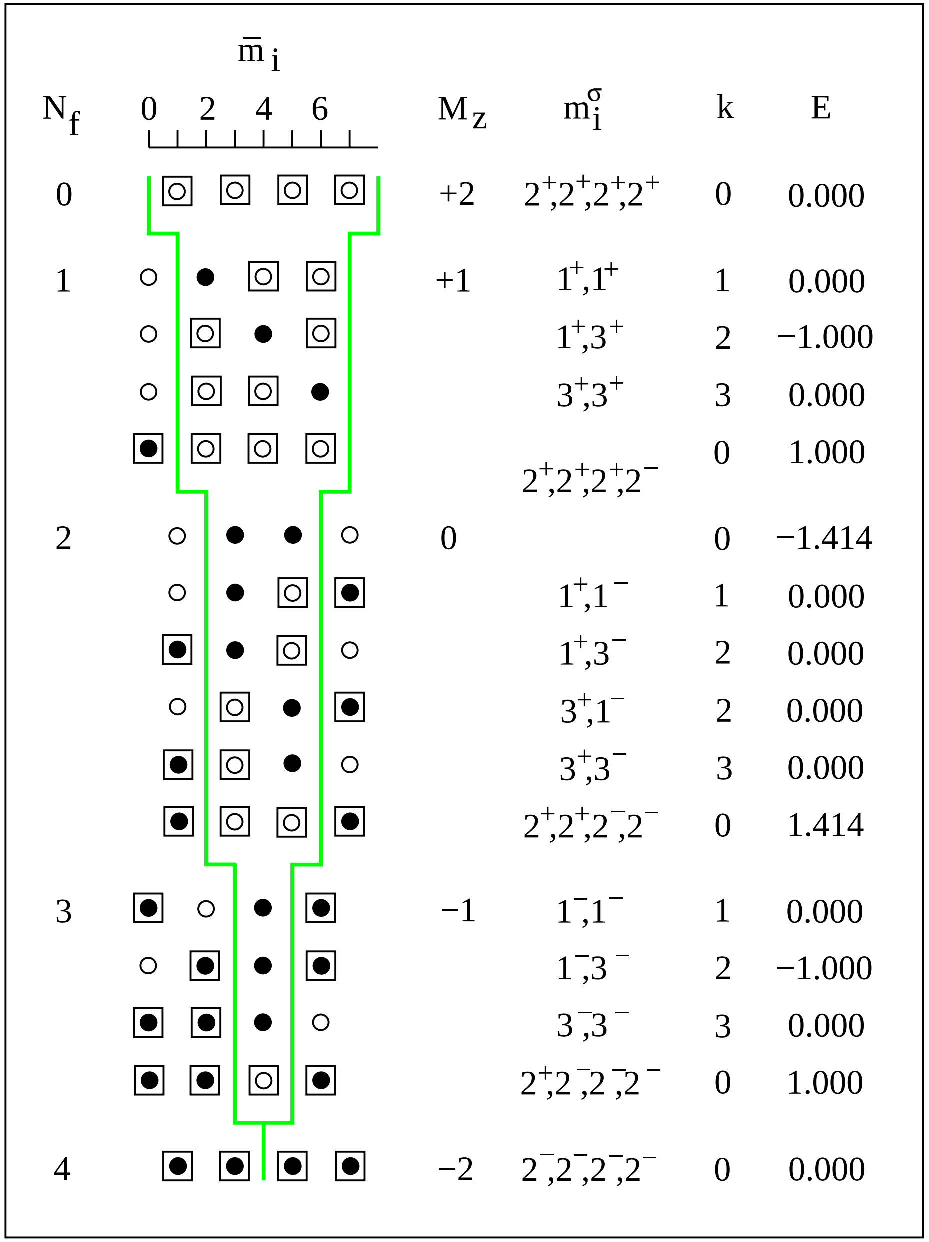
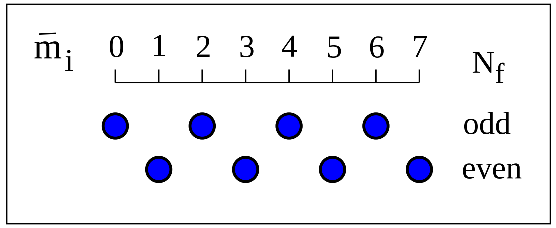


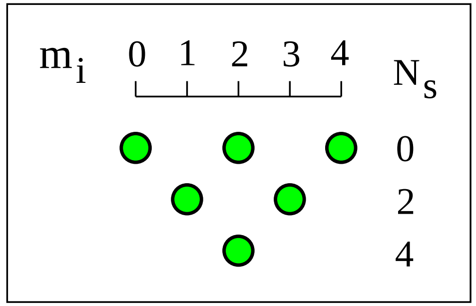
XX Model: Fermions Versus Spinons II



Fermion momenta: $p_i = (\pi/N)\bar{m}_i$



Spinon orbital momenta: $\kappa_i = (\pi/N)m_i$



Wave number:

$$k = \frac{\pi}{N}\sum_{i=1}^{N_f} p_i \mod(2\pi)$$

$$k = \left(\frac{\pi}{N}\sum_{\sigma=\pm}\sum_{j_\sigma=1}^{N_\sigma} m_{j_\sigma}^{\sigma} - \frac{N\pi}{2}\right) \mod(2\pi)$$

Exclusion Statistics of Spinons

- $N_S = N_+ + N_-$
- $M_z = \frac{1}{2}(N_+ - N_-)$

$M_z \backslash N_S$	0	2	4	6	
3	–	–	–	1	1
2	–	–	5	1	6
1	–	6	8	1	15
0	1	9	9	1	20
-1	–	6	8	1	15
-2	–	–	5	1	6
-3	–	–	–	1	1
	1	21	35	7	64

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$7/2$	–	–	–	1	1
$5/2$	–	–	6	1	7
$3/2$	–	10	10	1	21
$1/2$	4	18	12	1	35
$-1/2$	4	18	12	1	35
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$-5/2$	–	–	6	1	7
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	8	56	56	8	128

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Multiplicity expression [Haldane 1991]:

- $W(N_+, N_-) = \prod_{\sigma=\pm} \begin{pmatrix} d_\sigma + N_\sigma - 1 \\ N_\sigma \end{pmatrix}$
- $d_\sigma = A_\sigma - \sum_{\sigma'} g_{\sigma\sigma'}(N_{\sigma'} - \delta_{\sigma\sigma'})$
- $A_\sigma = \frac{1}{2}(N+1)$
- $g_{\sigma\sigma'} = \frac{1}{2}$
- $\sum_{N_+,N_-} W(N_+, N_-) = 2^N.$

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Bethe Ansatz for Spinons

Spinon quantum numbers: $\frac{N_s}{2} \leq m_1^\sigma \leq m_2^\sigma \leq \cdots \leq m_{N_\sigma}^\sigma \leq N - \frac{N_s}{2}, \quad \sigma = \pm.$

Energy of XX eigenstate: $E\big(\{m_{j_+}^+\}, \{m_{j_-}^-\}\big) = E_0(M_z) + \sum_{\sigma=\pm} \sum_{j_\sigma=1}^{N_\sigma} \sin k_{j_\sigma}^\sigma.$

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Bethe ansatz equations: $Nk_i^\sigma = \pi m_i^\sigma + \sum_{\sigma'=\pm} \sum_{j=1}^{N_{\sigma'}} \theta_{XX}(k_i^\sigma - k_j^{\sigma'}),$

Dynamical spinon interaction: $\theta_{XX}(k_i^\sigma - k_j^{\sigma'}) = \pi \, \mathrm{sgn}(k_i^\sigma - k_j^{\sigma'})\delta_{\sigma\sigma'}.$

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Spinon momenta: $k_{j_\sigma}^\sigma = \frac{\pi}{N}\big(m_{j_\sigma}^\sigma - N_\sigma - 1 + 2j_\sigma\big), \quad j_\sigma = 1,\ldots,N_\sigma, \quad \sigma = \pm.$

Range: $\frac{\pi}{N}\left(\frac{1}{2}N_s - N_\sigma + 1\right) \leq k_1^\sigma < k_2^\sigma < \cdots < k_{N_\sigma}^\sigma \leq \frac{\pi}{N}\left(N - \frac{1}{2}N_s + N_\sigma - 1\right).$

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Statistical spinon interaction: $\Delta d_\sigma = -\sum_{\sigma'=\pm} g_{\sigma\sigma'} \Delta N_{\sigma'}, \quad g_{\sigma\sigma'} = \dfrac{1}{2}.$

Thermodynamics of Spinons I

Gibbs free energy per site: $g = u - Ts - hm_z$

- $u = \frac{1}{2\pi}\sum_\sigma \int_{k^\sigma_{\rm min}}^{k^\sigma_{\rm max}} dk\,\rho_\sigma(k)\sin k - \frac{1}{\pi}\cos(\pi m_z)$
- $s = -\frac{k_B}{2\pi}\sum_\sigma \int_{k^\sigma_{\rm min}}^{k^\sigma_{\rm max}} dk\left[\rho_\sigma(k)\ln\rho_\sigma(k) + \Big(1-\rho_\sigma(k)\Big)\ln\Big(1-\rho_\sigma(k)\Big)\right]$
- $m_z = \frac{1}{2}\sum_\sigma \sigma n_\sigma = \frac{1}{4\pi}\sum_\sigma \int_{k^\sigma_{\rm min}}^{k^\sigma_{\rm max}} dk\,\sigma\rho_\sigma(k)$

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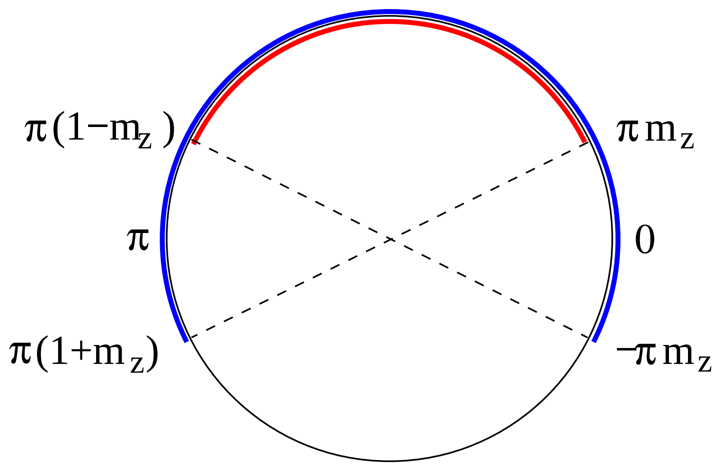
where $k^\sigma_{\min} = -\sigma\pi m_z, \quad k^\sigma_{\max} = \pi(1+\sigma m_z)$



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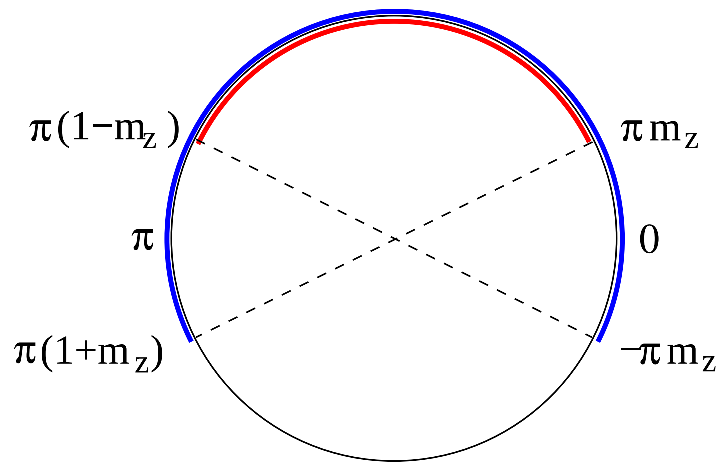

$$\Rightarrow g = -\frac{1}{\pi}\cos(\pi m_z) + \frac{1}{2\pi}\sum_\sigma \int_{-\sigma\pi m_z}^{\pi(1+\sigma m_z)} dk\Big\{\rho_\sigma(k)\sin k$$
$$+k_BT\left[\rho_\sigma(k)\ln\rho_\sigma(k) + \Big(1-\rho_\sigma(k)\Big)\ln\Big(1-\rho_\sigma(k)\Big)\right] - \frac{h}{2}\sigma\rho_\sigma(k)\Big\}$$

Thermodynamics of Spinons II

Extension of domains: $\rho_+(k) + \rho_-(k-\pi) = 1$

$$g = \frac{1}{4\pi}\sum_\sigma \int_{-\pi}^{+\pi} dk \Big\{ \rho_\sigma(k)\sin k + k_B T \Big[\rho_\sigma(k)\ln\rho_\sigma(k) + \Big(1-\rho_\sigma(k)\Big)\ln\Big(1-\rho_\sigma(k)\Big)\Big] - h\sigma\rho_\sigma(k)\Big\}.$$

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Spinon densities from $\delta g = 0$: $\rho_\sigma(k) = \Big[e^{\beta(\sin k - h\sigma)} + 1\Big]^{-1}$

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Gibbs free energy per site: $\beta g(T,h) = -\frac{1}{2\pi}\int_{-\pi}^{+\pi} dk \ln\left(2\cosh\left(\frac{\beta}{2}(\sin k - h)\right)\right)$

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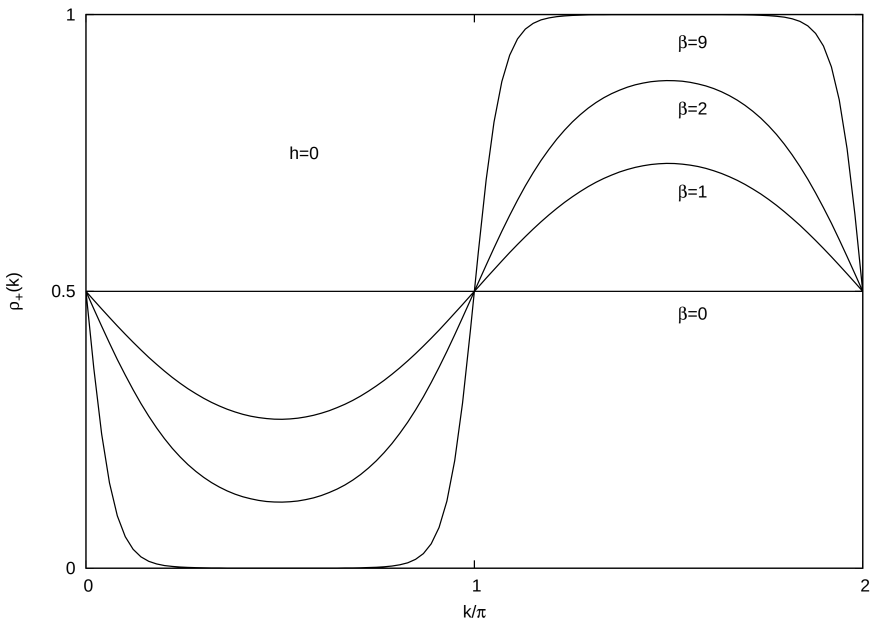
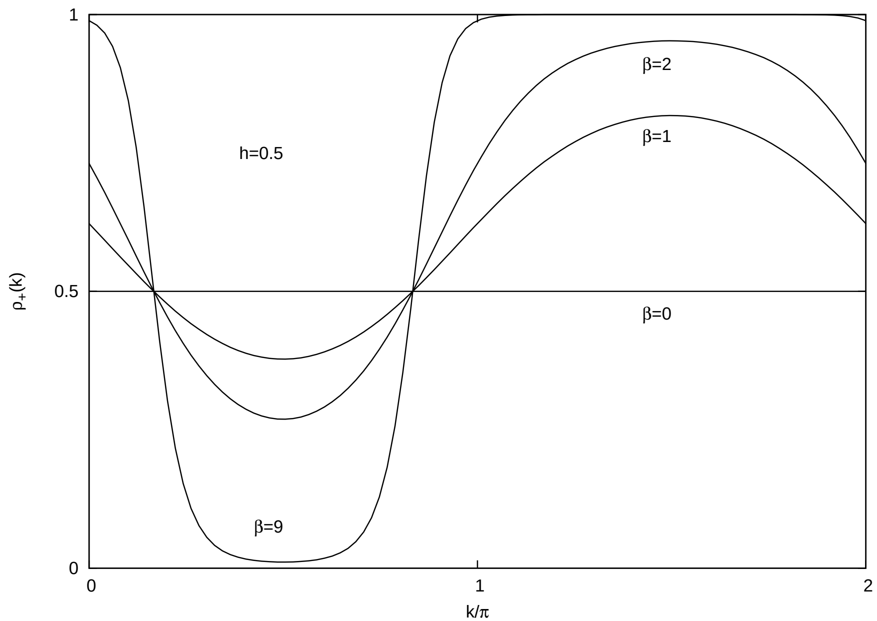
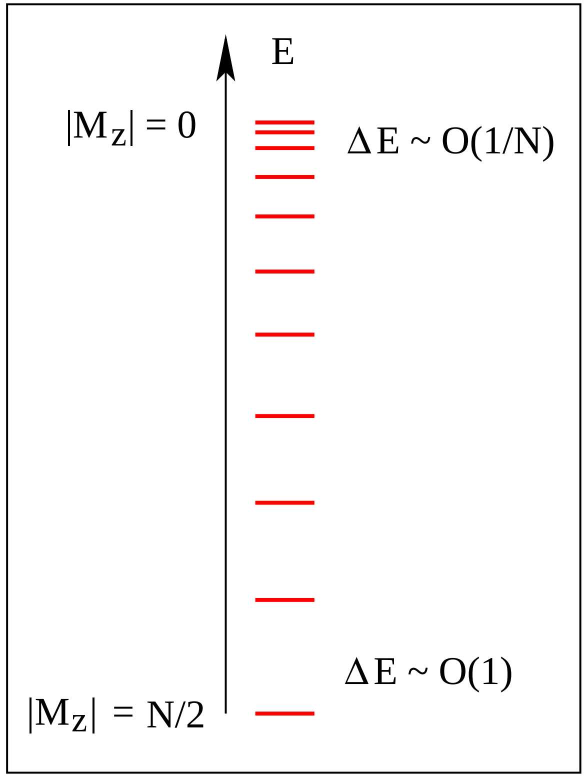




Spinon Spin Interaction

Spinon orbital filled to capacity $(N_s = N)$.

- non-uniform level splitting,
- $n_s = \dfrac{N_s}{N}, \quad m_z = \dfrac{M_z}{N}, \quad \epsilon = \dfrac{E}{N},$
- $\epsilon = \dfrac{1}{\pi}\cos(\pi m_z), \quad -\dfrac{1}{2} \le m_z \le +\dfrac{1}{2},$



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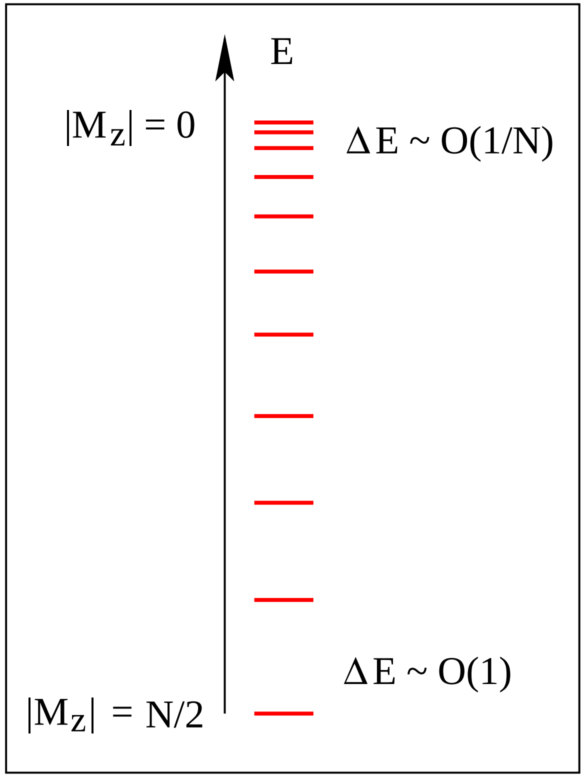


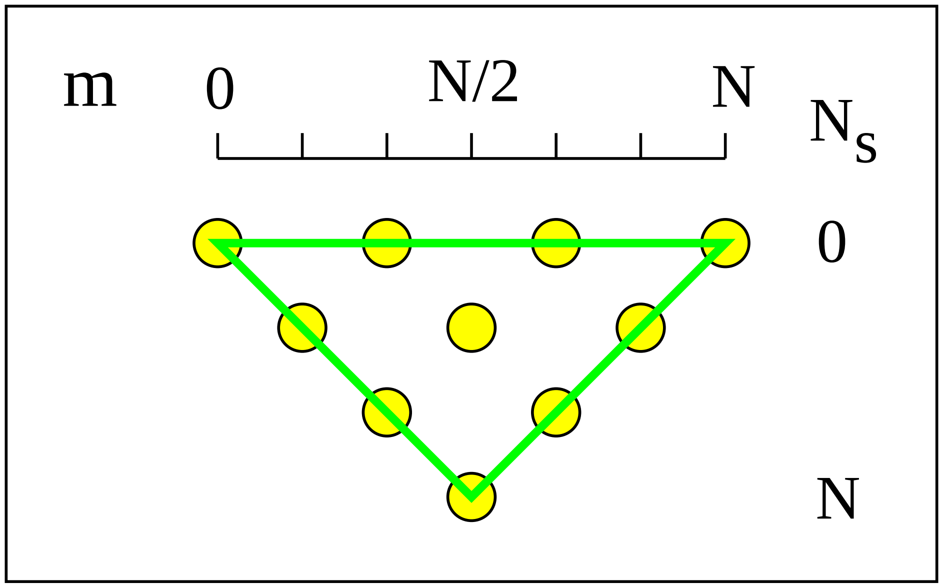
Spinon spin interaction:

- $\mathcal{H}_e = -J_e \sum_{i<j} [\sigma_i \sigma_j - 1], \quad \sigma_i = \pm 1, \quad J_e = \dfrac{2}{\pi N},$
- $\epsilon_e = \dfrac{1}{\pi}\left(1 - 4m_z^2\right), \quad -\dfrac{1}{2} \le m_z \le +\dfrac{1}{2}.$

Hund's Rule

Partially filled spinon orbital $(0 < N_s \leq N)$.

- filling: $0 \leq n_s \leq 1$,
- magnetization: $|m_z| \leq \frac{n_s}{2}$,
- orbital momentum: $\kappa = \frac{\pi m}{N}, \quad \frac{\pi n_s}{2} \leq \kappa \leq \pi - \frac{\pi n_s}{2}$,
- energy: $\epsilon = \frac{1}{\pi}\cos(\pi m_z)\left[2\sin\left(\frac{\pi}{2}n_s\right)\sin\kappa - 1\right]$.



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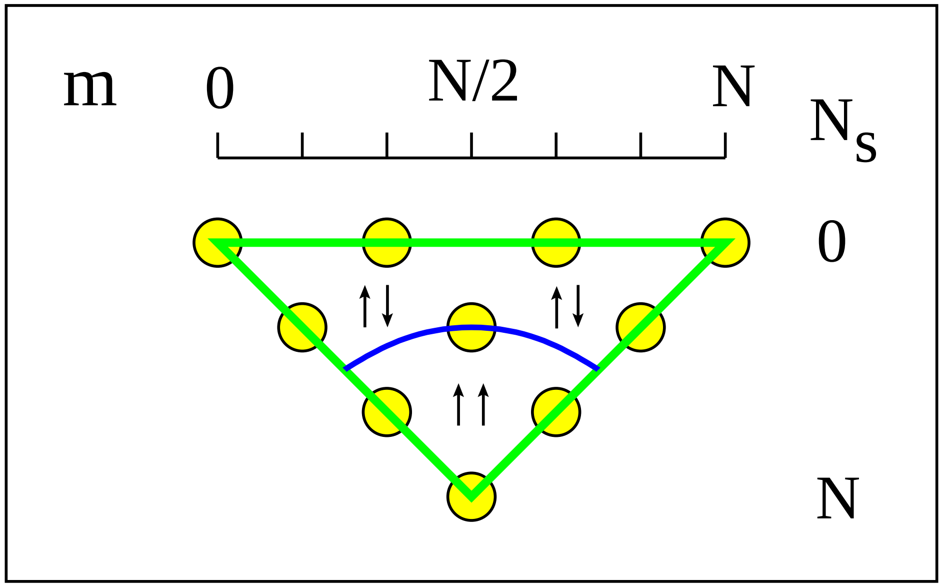
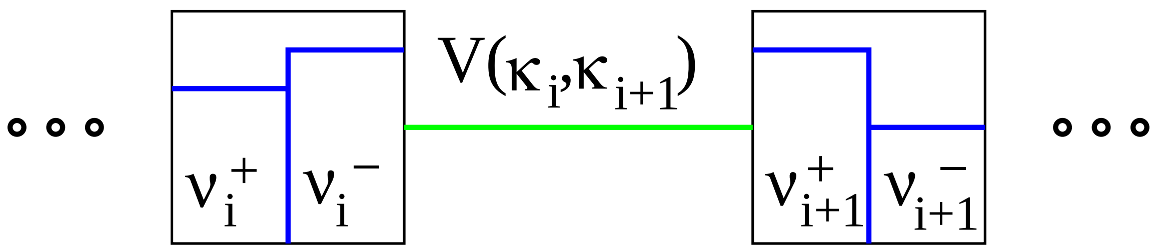
- magnetization: $|m_z| \leq \frac{n_s}{2}$,
- orbital momentum: $\kappa = \frac{\pi m}{N}, \quad \frac{\pi n_s}{2} \leq \kappa \leq \pi - \frac{\pi n_s}{2}$,
- energy: $\epsilon = \frac{1}{\pi} \cos(\pi m_z) \left[2 \sin\left(\frac{\pi}{2} n_s\right) \sin\kappa - 1 \right]$.



Interacting Spinon Orbitals

Spinons in several orbitals:

- $\nu_s \leq \kappa_1 < \kappa_2 < \cdots < \kappa_t \leq \pi - \nu_s,$
- $\nu_i \doteq \dfrac{\pi N_s^{(i)}}{2N} = \nu_i^+ + \nu_i^-, \quad \mu_i \doteq \dfrac{\pi M_z^{(i)}}{N} = \nu_i^+ - \nu_i^-, \quad i = 1, 2, \ldots, t; \quad \nu_s \doteq \sum_{i=1}^{t} \nu_i,$
- $\bar{\mu}_{i,k} \doteq \sum_{j=1}^{i} \mu_j - \sum_{j=k}^{t} \mu_j, \qquad \bar{\nu}_{i,k} \doteq \sum_{j=1}^{i} \nu_j - \sum_{j=k}^{t} \nu_j,$
- $$\pi\epsilon = \sum_{i=1}^{t-1} \cos\bar{\mu}_{i,i+1} \left\{ \cos\bar{\nu}_{i,i+1} \Big[\cos\kappa_{i+1} - \cos\kappa_i \Big] + \sin\bar{\nu}_{i,i+1} \Big[\sin\kappa_i - \sin\kappa_{i+1} \Big] \right\}$$
$$+ \cos\bar{\mu}_{t,t+1} \left\{ \cos\bar{\nu}_{t,t+1} \Big[\cos\kappa_1 - \cos\kappa_t \Big] + \sin\bar{\nu}_{t,t+1} \Big[\sin\kappa_1 + \sin\kappa_t \Big] - 1 \right\}.$$



Comparison of XX and HS Models

XX model

- $s\ell_2$ loop symmetry.

HS model

- Yangian symmetry.

Comparison of XX and HS Models

XX model

- $s\ell_2$ loop symmetry.
- Free fermions $(g = 1)$.

HS model

- Yangian symmetry.
- Free pseudomomenta $(g = 2)$

Comparison of XX and HS Models

XX model

- $s\ell_2$ loop symmetry.
- Free fermions $(g = 1)$.
- Interacting spinons $(g = 1/2)$.

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Comparison of XX and HS Models

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- $s\ell_2$ loop symmetry.
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- Spinon spin coupling present.

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Comparison of XX and HS Models

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- $s\ell_2$ loop symmetry.
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- Motif: $\boxed{\bullet}\ \circ \mid \bullet\ \boxed{\circ}\ \bullet \mid \circ\ \ \circ$

HS model

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- Motif: ⊡● ○ | ● ⊡○ ● | ○ ○
- Bethe quantum numbers: $\{m_i^\sigma\}$.
- Spinon scattering:
  $\theta_{XX}(k_i^\sigma - k_j^{\sigma'}) = \pi\,\mathrm{sgn}(k_i^\sigma - k_j^{\sigma'})\delta_{\sigma\sigma'}$.

HS model

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Comparison of XX and HS Models

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- $E - E_0 = \sum_{\sigma=\pm} \sum_{j_\sigma=1}^{N_\sigma} \sin k_{j_\sigma}^\sigma$.

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- Interacting spinons $(g = 1/2)$.
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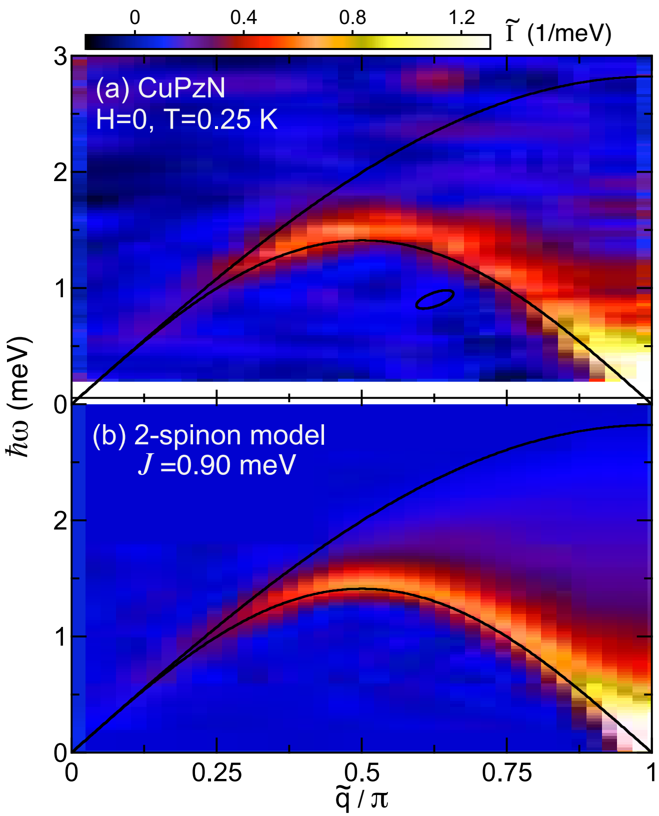
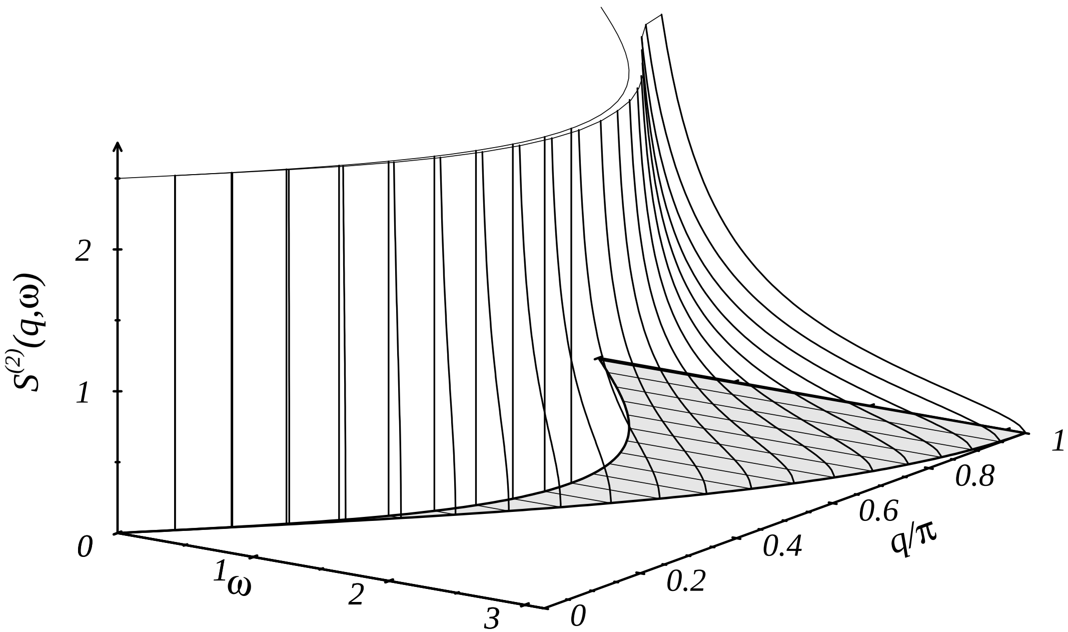
- Bethe quantum numbers: $\{m_i\}$.
- Spinon scattering:
  $\theta_{HS}(k_i - k_j) = \pi \,\mathrm{sgn}(k_i - k_j)$.
- $E - E_0 = -\frac{v_s}{\pi} \sum_{j=1}^{N_s} \kappa_j k_j, \quad \kappa_j = \frac{\pi}{N} m_j$.

$Cu(C_4H_4N_2)(NO_3)_2$

$S^{(2)}(q, \omega)$





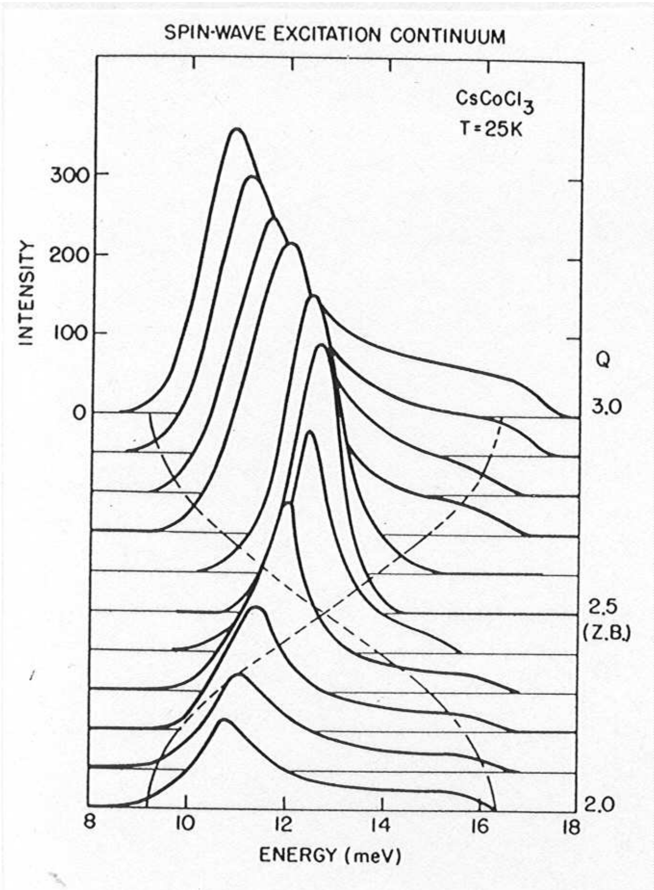
[Stone, Reich, Broholm, Lefmann, Rischel, Landee, and Turnbull 2003]

[Karbach, Müller, Bougourzi, Fledderjohann, and Mütter 1997]

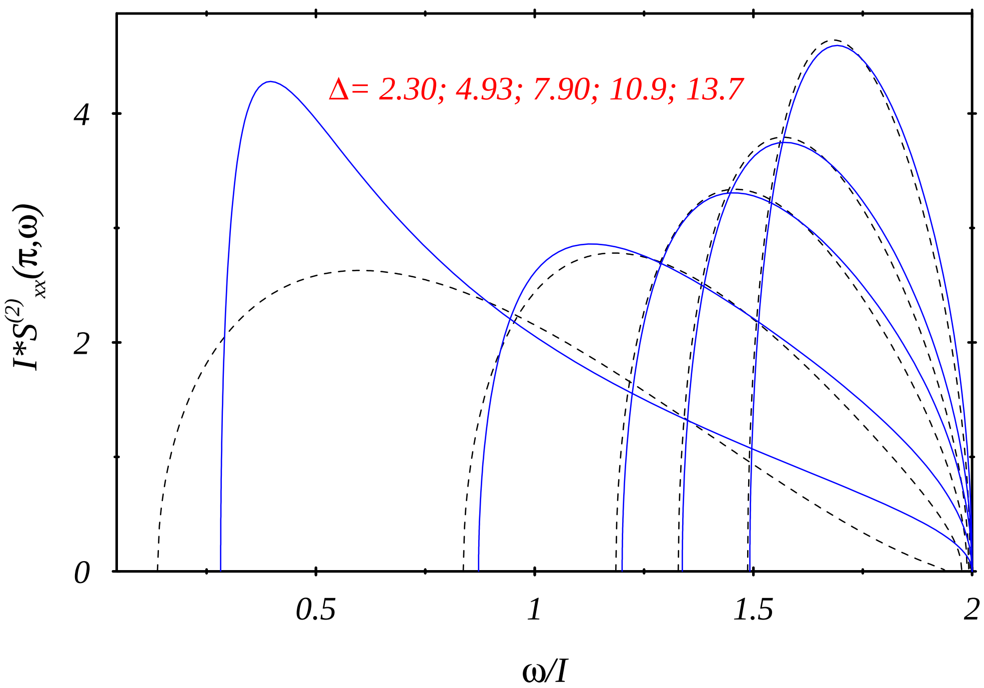
Observation of Solitons in Axial XXZ Model

$CsCoCl_3$

$S^{(2)}(\pi, \omega)$



[Yoshizawa, Hirakawa, Satija, and Shirane 1981]



[Müller and Karbach 2000]

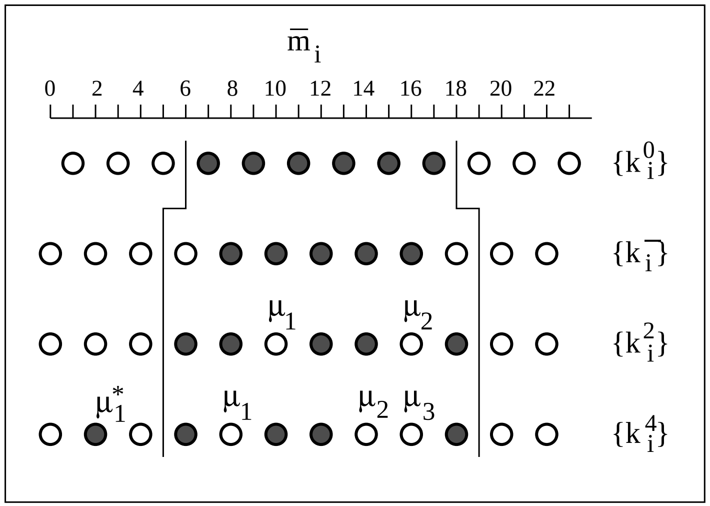
Observability of Spinons in XX Model?

- Physical realizations
- Spinon composition of XX spectrum
- Transition rate expressions
  - Free fermions
    [McCoy, Barouch, and Abraham 1971]
  - Algebraic Bethe ansatz
    [Korepin 1982, Kitanine, Maillet, and Terras 1999]
  - Product expressions for XX transition rates
    [Biegel, Karbach, Müller, and Wiele 2004]
  - Observability
    [Arikawa, Karbach, Müller, and Wiele 2006]

Transition Rates

Product expressions for $M_\lambda^\pm(q) \doteq \dfrac{|\langle\psi_0|S_q^\pm|\psi_\lambda\rangle|^2}{\|\psi_0\|^2\|\psi_\lambda\|^2}$:

$$M_\lambda^-(q) = \frac{\prod_{i<j}^{r-1} \sin^2 \frac{k_i - k_j}{2} \prod_{i<j}^{r} \sin^2 \frac{k_i^0 - k_j^0}{2}}{\prod_{j=1}^{r-1} N^2 \prod_{i=1}^{r} \sin^2 \frac{k_i^0 - k_j}{2}}.$$



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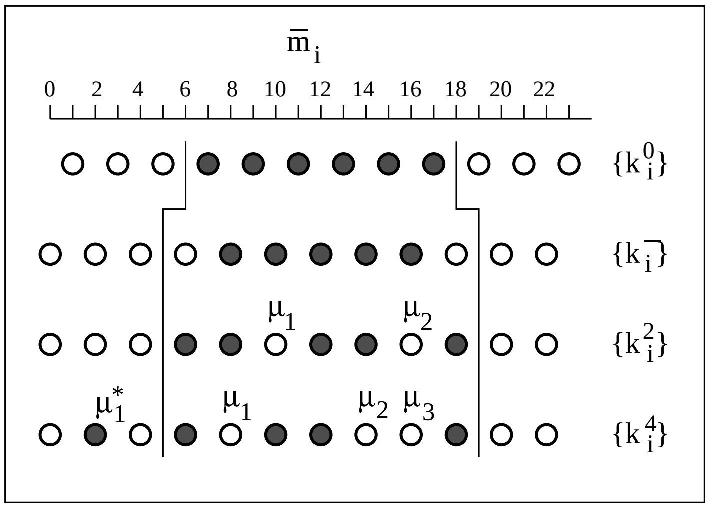
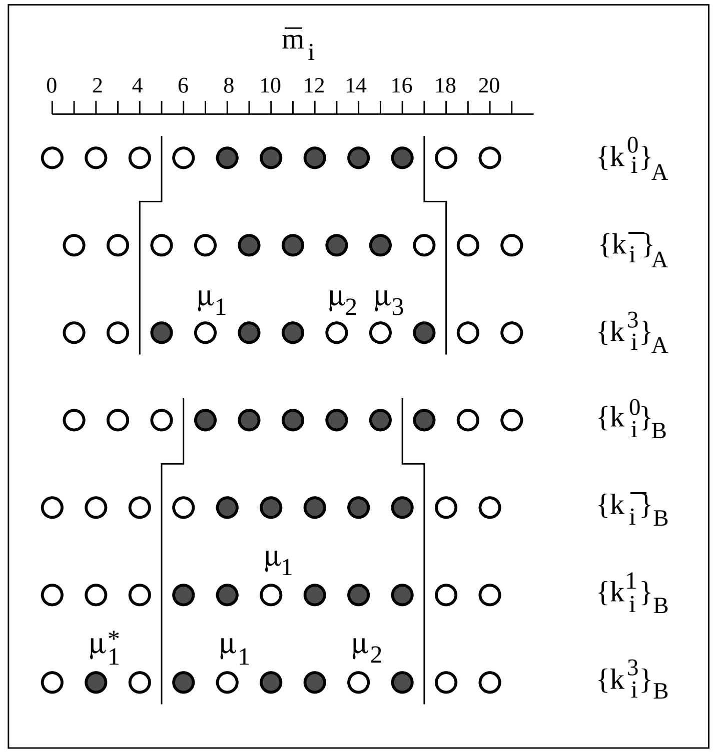
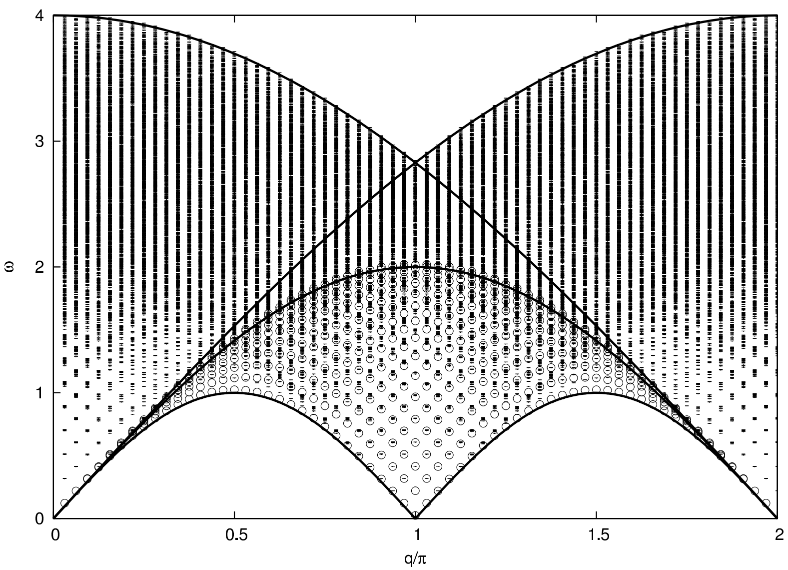
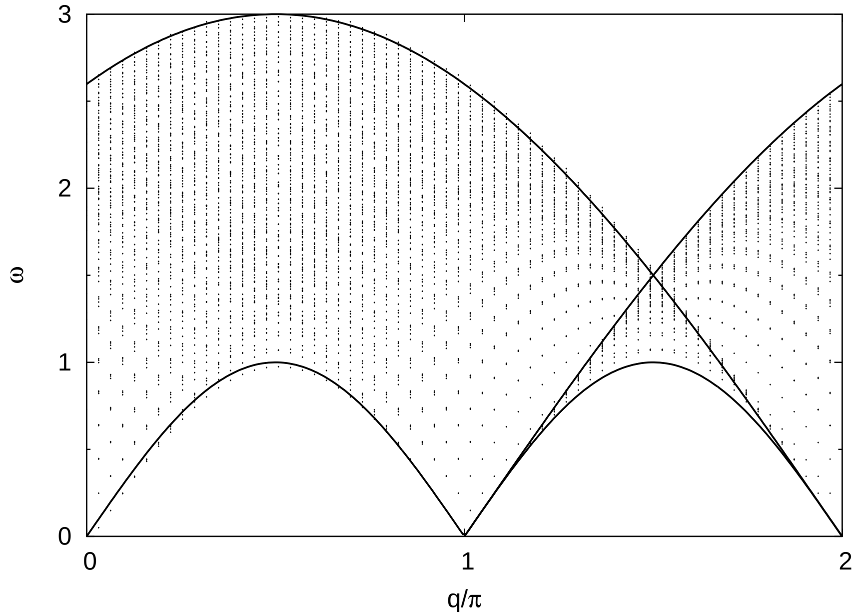




Spectrum





2-spinon spectrum:

$$\epsilon_{2L}(q) = \epsilon_{4L}(q) = |\sin q|$$

4-spinon spectrum: $\epsilon_{2U}(q) = 2\left|\sin\frac{q}{2}\right|$

$$\epsilon_{4U}(q) = 4\max\left[\left|\sin\frac{q}{4}\right|, \left|\sin\frac{q-2\pi}{4}\right|\right]$$

1-spinon spectrum:

$$\epsilon_1(q) = \epsilon_{3L}(q) = |\sin\ q|$$

3-spinon spectrum:

$$\epsilon_{3U}(q) = 3\max\left[\left|\sin\frac{q}{3}\right|, \left|\sin\frac{q-2\pi}{3}\right|\right]$$

Spectral Weight

1-spinon dynamic structure factor:

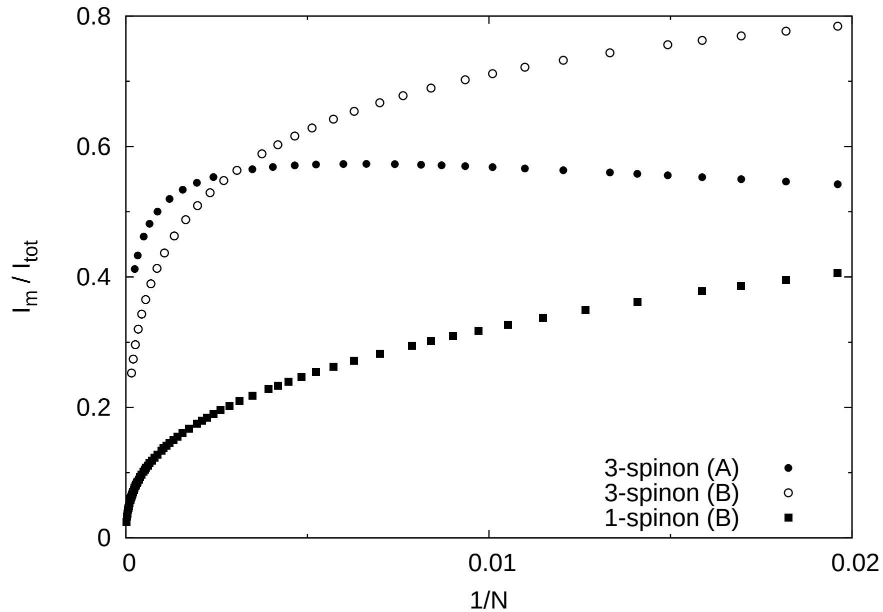
$$S_{-+}^{(1)}(q,\omega) \stackrel{a}{=} \frac{C}{4\sqrt{N}} \tan\frac{q}{2}\,\delta\left(\omega - |\sin q|\right)$$

2-spinon dynamic structure factor:

$$S_{-+}^{(2)}(q,\omega)_0 \stackrel{a}{=} \frac{2C}{\pi\sqrt{N}} \frac{\sqrt{4\sin^2(q/2)-\omega^2}}{\omega^2 - \sin^2 q}$$

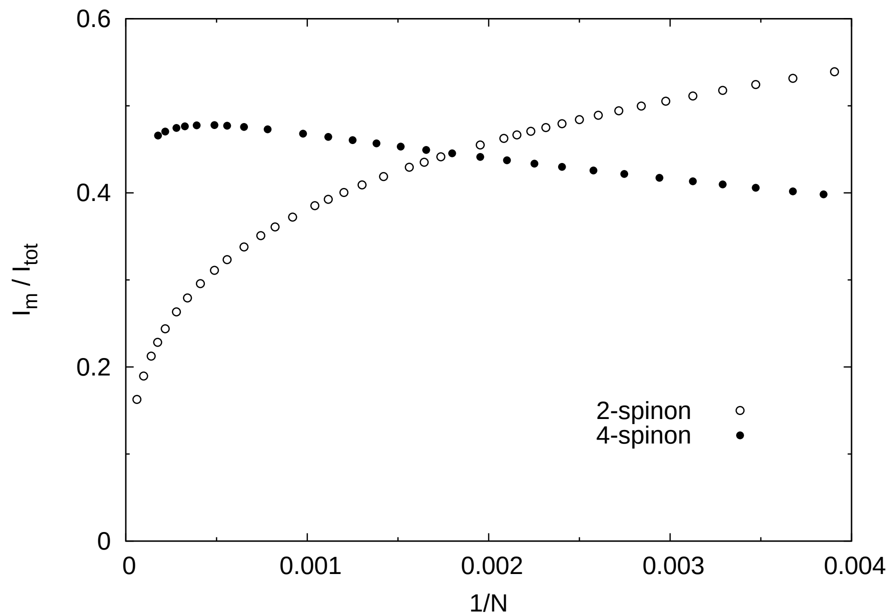
1-spinon dynamic structure factor:

$$S_{-+}^{(1)}(q,\omega) \stackrel{a}{=} \frac{C}{4\sqrt{N}} \tan\frac{q}{2}\delta\left(\omega - |\sin q|\right)$$



2-spinon dynamic structure factor:

$$S_{-+}^{(2)}(q,\omega)_0 \stackrel{a}{=} \frac{2C}{\pi\sqrt{N}} \frac{\sqrt{4\sin^2(q/2) - \omega^2}}{\omega^2 - \sin^2 q}$$



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