Edge states and magnetization profiles of open spin ladders

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Haldane gap (Haldane, 1983)

antiferromagnetic spin-S Chain

$$H = J \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

$S \to \infty \Rightarrow$ O(3) Non-linear σ-model + topological term

$$\mathcal{S} = \int dx d\tau \left[(\partial_\tau \vec{n})^2 + (\partial_x \vec{n})^2 \right] + i\frac{S}{2} \int dx d\tau \vec{n} \cdot (\partial_\tau \vec{n} \times \partial_x \vec{n})$$

$$\vec{S}_n \sim \vec{n} \times \partial_\tau \vec{n}(na) + (-)^n S \vec{n}(na)$$

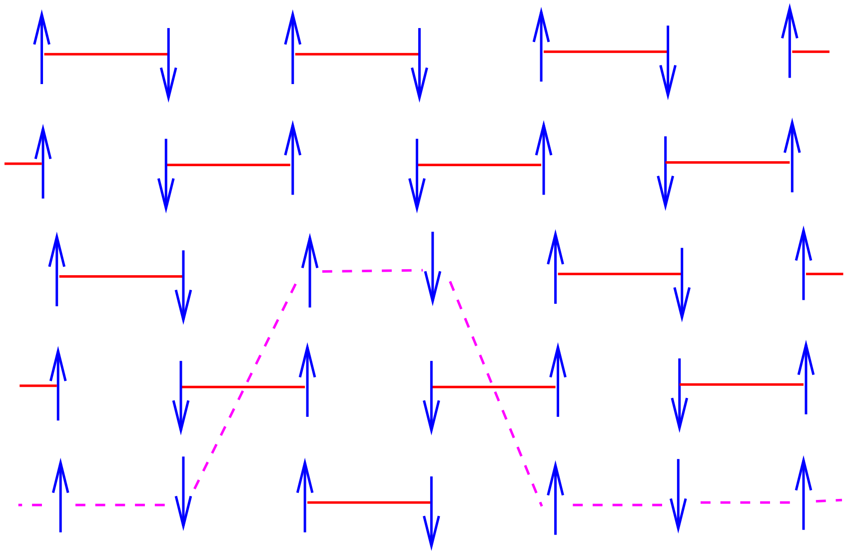
•$S \in \mathbb{N} \Rightarrow$ no effect of topological term $\Rightarrow$ spin gap

•$S \in \mathbb{N} + 1/2 \Rightarrow$ topological term prevents the formation of a gap.

The Valence Bond Solid (VBS)picture

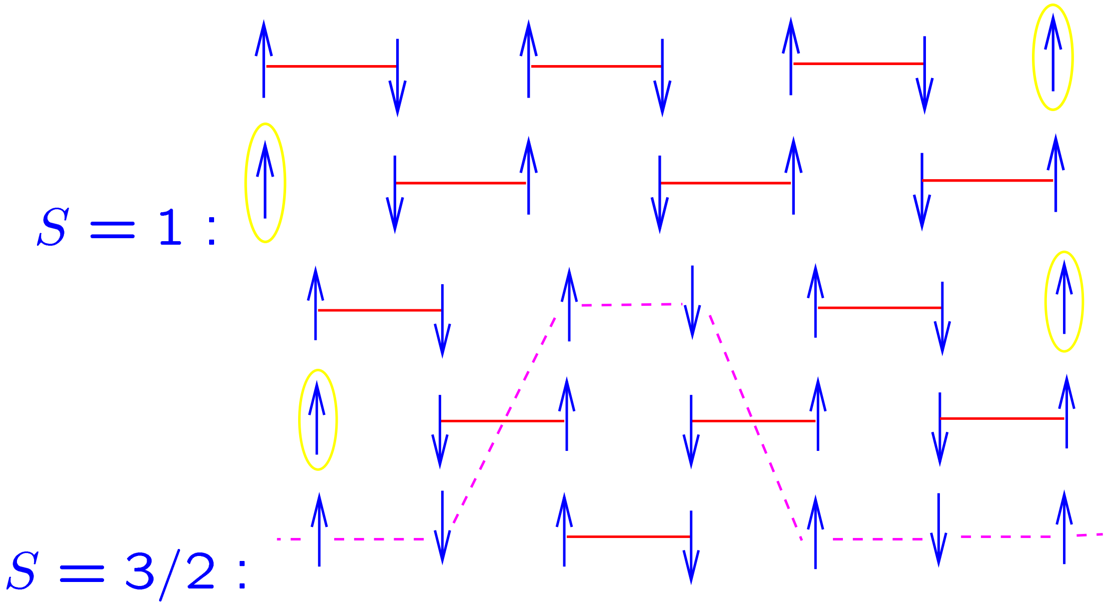
Affleck, Kennedy, Lieb, Tasaki (1987) spin S $\rightarrow$ 2S spins 1/2

$S = 1$:

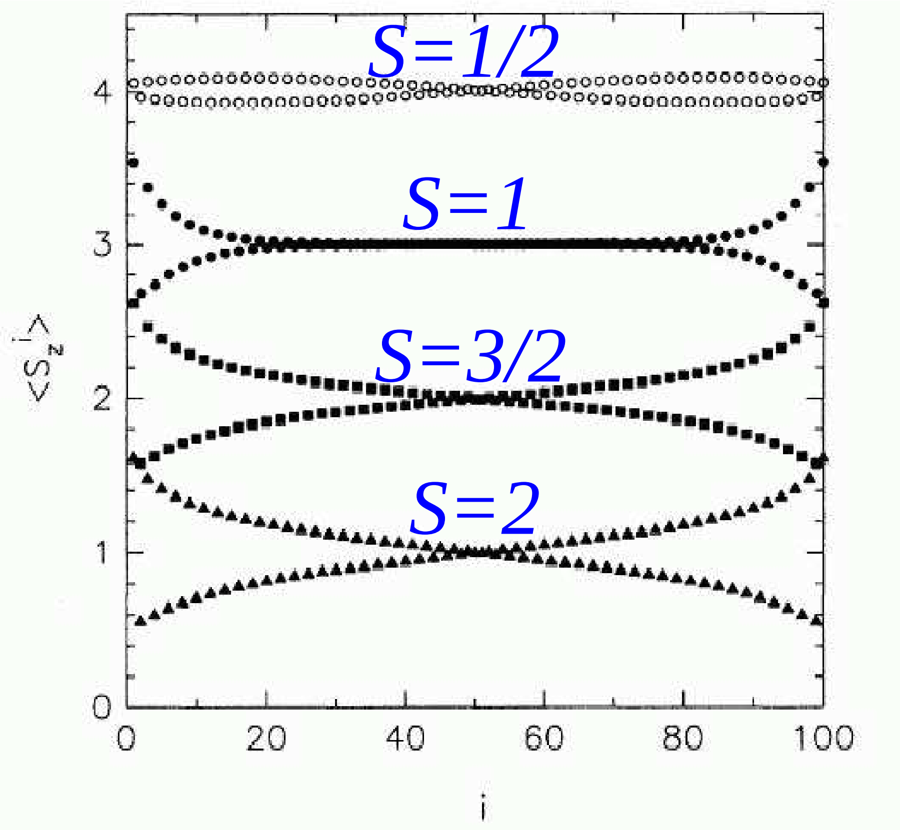


$S = 3/2$

Finite chains : presence of edge states

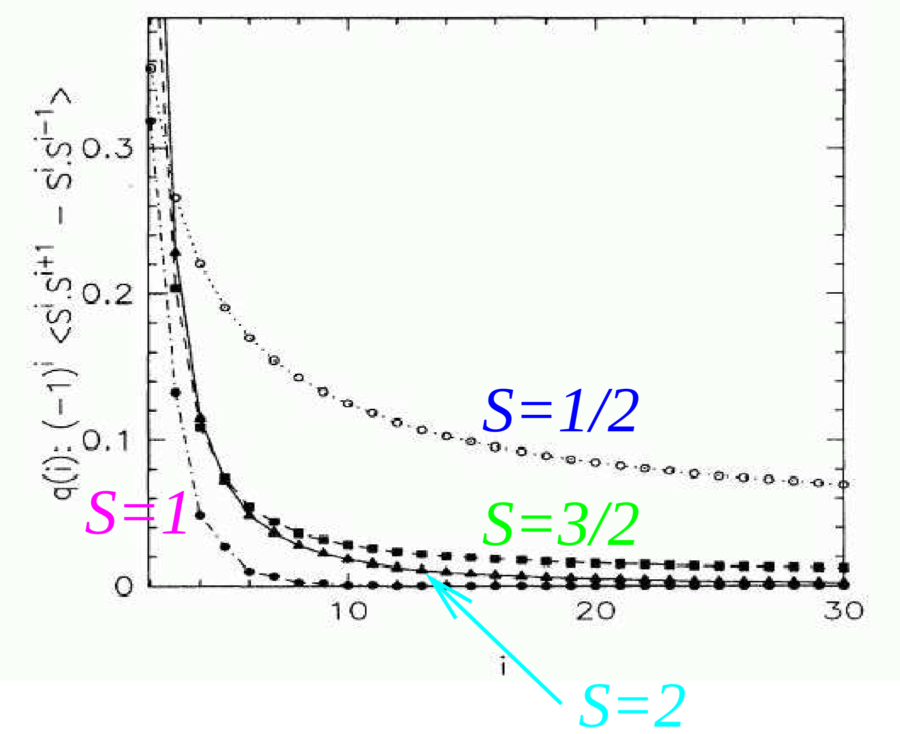


Staggered magnetization induced by edge states



From S. Qin, T. K. Ng, Z. B. Su Phys. Rev. B **52** 12844 (1995)

Staggered dimerization induced by boundary



From S. Qin, T. K. Ng, Z. B. Su Phys. Rev. B **52** 12844 (1995) spin 1/2 N leg ladder

$$H = J \sum_{\substack{i \\ p=1,\dots,N}} \vec{S}_{i,p} \cdot \vec{S}_{i+1,p} + J_\perp \sum_{\substack{i \\ p=1,\dots,N-1}} S_{i,p} \cdot S_{i,p+1}$$

$J_\perp/J \to -\infty \Rightarrow$ spin $\frac{N}{2}$ chain
$J_\perp/J \to +\infty \Rightarrow$

- $N \in 2\mathbb{N} \Rightarrow$ singlets chain $\Rightarrow$ spin gap.

- $N \in 2\mathbb{N} + 1 \Rightarrow$ spin 1/2 chain $\Rightarrow$ no spin gap.

Analogy between ladders and spin-S chains

Questions

1. spin-S chain $\Leftrightarrow$ spin ladder $\Rightarrow$ edge states in the open ladder ?

2. Magnetization/dimerization profile ?

Generalized spin ladder

$$
\begin{aligned}
H &= J_{\|} \sum_{\substack{i=1,\infty \\ p=1,2}} \mathbf{S}_{i,p} \cdot \mathbf{S}_{i+1,p} + \sum_{i=1,\infty} J_{\perp} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} \\
&+ J'_{\perp} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i+1,2} + J''_{\perp} \mathbf{S}_{i,2} \cdot \mathbf{S}_{i+1,1}
\end{aligned}
$$

spin-1/2 chain:

Bosonization

$$H = u \int \frac{dx}{2\pi} \left[(\pi \Pi)^2 + (\partial_x \phi)^2 \right]$$

$$[\phi(x), \Pi(x')] = i\delta(x - x'),\ \theta(x) = \pi \int^x \Pi(x') dx'$$

$$S^\alpha(x) = (J_+^\alpha + J_-^\alpha)(x) + (-)^{x/a} n^\alpha(x)$$

$$J_r^+ = \frac{e^{i\sqrt{2}(r\theta - \phi)}}{2\pi\alpha} J_r^z = \frac{1}{2\pi\sqrt{2}} \partial_x (r\theta - \phi)$$

$$n_x = \frac{\cos\sqrt{2}\theta}{\pi\alpha}\ n_y = \frac{\sin\sqrt{2}\theta}{\pi\alpha} n_z = \frac{\sin\sqrt{2}\phi}{\pi\alpha}$$

Two-leg ladder: Bosonization

$$
\begin{aligned}
H &= H_1 + H_2 (\text{Free}) \\
&+ (J_\perp - J'_\perp - J''_\perp) \int dx \vec{n}_1(x) \cdot \vec{n}_2(x) (\text{relevant}) \\
&+ (J_\perp + J'_\perp + J''_\perp) \int dx (\vec{J}_{1+} + \vec{J}_{1-})(x) \cdot (\vec{J}_{2+} + \vec{J}_{2-})(x) (\text{Marginal})
\end{aligned}
$$

relevant term:

$$
\int dx \left[\cos 2\theta^{(-)} + \frac{1}{2} \cos 2\phi^{(-)} - \frac{1}{2} \cos \phi^{(+)} \right]
$$

where $\phi^{(\pm)} = (\phi_1 \pm \phi_2)/\sqrt{2}$, $\theta^{(\pm)} = (\theta_1 \pm \theta_2)/\sqrt{2}$

Fermionization (Nersesyan, Shelton, Tsvelik 1996)

$$\xi_{r,1} = \frac{\cos(\theta^{(+)} - r\phi^{(+)})}{\sqrt{2\pi\alpha}} \xi_{r,2} = \frac{\sin(\theta^{(+)} - r\phi^{(+)})}{\sqrt{2\pi\alpha}}$$

$$\xi_{r,3} = \frac{\cos(\theta^{(-)} - r\phi^{(-)})}{\sqrt{2\pi\alpha}} \xi_{r,0} = \frac{\sin(\theta^{(-)} - r\phi^{(-)})}{\sqrt{2\pi\alpha}}$$

Fermionized Hamiltonian

$$H = -\frac{iv}{2} \sum_{\substack{\alpha=0 \\ r=\pm}}^{3} \int dx r \xi_r^\alpha \partial_x \xi_r^\alpha + im \int dx \left[\sum_{\alpha=1}^{3} \xi_+^\alpha \xi_-^\alpha - 3\xi_+^0 \xi_-^0 \right]$$

$m = -\frac{J_\perp - J'_\perp - J''_\perp}{2\pi}$; $J_r^{1,a}(x) + J_r^{2,a}(x) = \frac{i}{2}\epsilon_{abc}\xi_r^b \xi_r^c.$

semi-infinite spin-1/2 chain: Bosonization

(Eggert, Affleck 1992) Condition:

$$\vec{n}(0,t) = 0 \Rightarrow \phi(0,t) = 0$$

Chiral components:

$$\Phi_r(x,t) = \frac{1}{2}(\phi(x,t) - r\theta(x,t)) = \Phi_r(x - rvt)$$

$$\Rightarrow \Phi_+(0,t) = -\Phi_-(0,t)$$

$$\Rightarrow \Phi_+(x,t) = \Phi_+(0,t-x/v) = -\Phi_-(0,t-x/v) = -\Phi_-(-x,t)$$

$$\Rightarrow \phi(x,t) = \Phi_+(x,t) - \Phi_+(-x,t)$$

$$\Delta(x = na) = (-)^n \vec{S}_n \cdot \vec{S}_{n+1} \sim \cos\sqrt{2}\phi$$

$$\Rightarrow \langle\Delta(x)\rangle \sim \frac{1}{x^{1/2}} \Rightarrow \langle\vec{S}(x)\rangle = \vec{0}$$

Ladder with open boundary conditions

$$\phi_1(0) = \phi_2(0) = 0$$

Change of variables:

$$\phi^{(\pm)} = \frac{1}{\sqrt{2}}(\phi_1 \pm \phi_2)$$

$$\Rightarrow \phi^{(r)}(0) = 0$$

Fermionization: $\Rightarrow \xi_+^\alpha(0) = \xi_-^\alpha(0) \Rightarrow$ Preserves the non-interacting character.

Localized eigenstates

For $m > 0$, $\exists$ localized solutions in triplet sector:

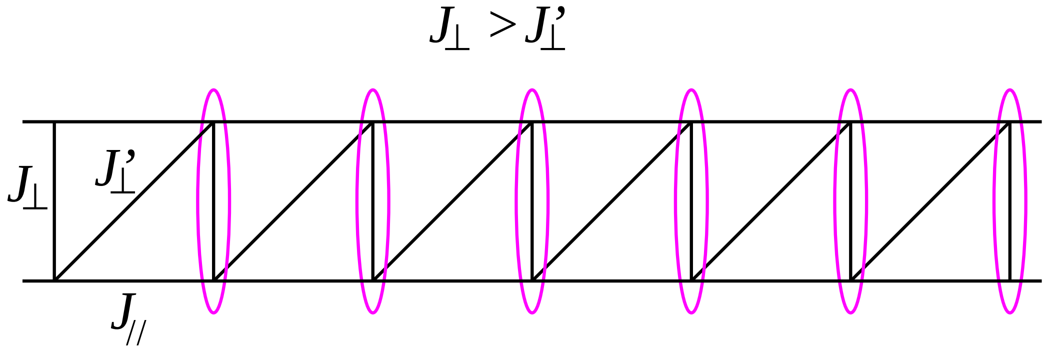
$$\xi_r^\alpha = \sqrt{\frac{m}{v}} e^{-mx/v} \eta^\alpha + \ldots$$

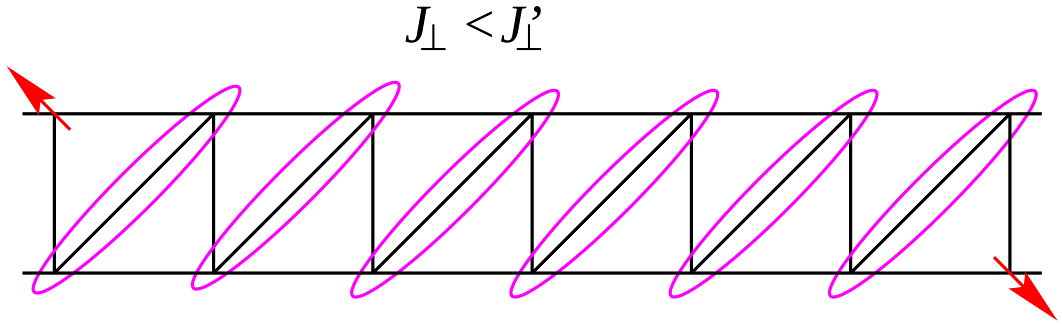
$\Rightarrow M^\alpha = \int dx S^\alpha(x) = \frac{i}{2}\epsilon_{\alpha\beta\gamma}\eta^\beta\eta^\gamma + \ldots$
$\Rightarrow$ $\exists$ spin 1/2 edge state at chain end in:

- Haldane gap phase of spin-1 chain ($|\theta| < \frac{\pi}{4}$))
- 2-leg ladder for $J_\perp < J'_\perp + J''_\perp$

No edge states if $m < 0$

Simple interpretation for $J''_\perp = 0$.





$\Rightarrow$ Two different types of hidden order.

Magnetization profiles

1D Massive Majorana Fermions $\Leftrightarrow$ 2D non-critical Ising model

$\Rightarrow$ mapping to 4 non-critical 2D Ising models

$$
\begin{aligned}
n_1^x + n_2^x &= \mu_1 \sigma_2 \sigma_3 \mu_0 \\
n_1^y + n_2^y &= \sigma_1 \mu_2 \sigma_3 \mu_0 \\
n_1^z + n_2^z &= \sigma_1 \sigma_2 \mu_3 \mu_0
\end{aligned}
$$

$$
\begin{cases}
m > 0 & : \langle \mu_0 \rangle \neq 0, \langle \sigma_i \rangle \neq 0 (i = 1, 2, 3) \\
m < 0 & : \langle \sigma_0 \rangle \neq 0, \langle \mu_i \rangle \neq 0 (i = 1, 2, 3)
\end{cases}
$$

massive Majorana Fermions $\Leftrightarrow$ 2D noncritical Ising model

Boundary condition for fermions $\rightarrow$ B. C.'s for Ising spins ?

(Ghoshal, Zamolodchikov 1994) $\Rightarrow$

If $m = (T_c - T)$:

$\bullet \xi_+(0) = \xi_-(0)$: Free B. C.'s on order parameter σ at $x = 0$

$\bullet \xi_+(0) = -\xi_-(0)$: Fixed B. C.'s on order parameter σ at $x = 0$

$\Rightarrow$ Calculate the magnetization of a non-critical Ising model of a half-plane with free/fixed B. C.'s of the origin

(R. Z. Bariev, 1980)

Non-critical 2D Ising model on a half-plane

$\diamond\langle\sigma\rangle_{\text{free}}(x, T > T_c) = 0$

$\diamond\langle\sigma\rangle_{\substack{\text{free}\\ \text{fixed}}}(x, T) = \langle\mu\rangle_{\substack{\text{fixed}\\ \text{free}}}(x, 2T_c - T)$ duality

$\diamond\langle\sigma\rangle_{\text{fixed}}(x, T < T_c) = \langle\sigma(x = \infty, T < T_c)\rangle G(x/\xi)$

$\diamond\langle\sigma\rangle_{\text{fixed}}(x, T > T_c) = \langle\mu(x = \infty, T > T_c)\rangle e^{-x/\xi} G(x/\xi)$

$\diamond\langle\sigma\rangle_{\text{free}}(x, T > T_c) = \langle\sigma(x = \infty, T < T_c)\rangle H(x/\xi)$

$$u \to 0 \begin{cases} G(u) \sim u^{-1/8} \\ H(u) \sim u^{3/8} \end{cases} \quad u \to \infty \begin{cases} G(u) \sim 1 + \dfrac{e^{-2u}}{16\sqrt{\pi}u^{3/2}} \\ H(u) \sim 1 - \dfrac{e^{-2u}}{2\sqrt{\pi}u^{1/2}} \end{cases}$$

Magnetization profile of the ladder with $J_\perp < J'_\perp + J''_\perp$

$T < T_c$ for i=1,2,3 $T > T_c$ for $i = 0$

$$\begin{aligned}\langle n_1^a + n_2^a\rangle(x) &= \langle\mu_1\rangle_{\text{free}}\langle\sigma_2\rangle_{\text{free}}\langle\sigma_3\rangle_{\text{free}}\langle\mu_0\rangle_{\text{free}} \\ &= m^{1/2}e^{-mx/v}G(\frac{mx}{v})H(\frac{mx}{v})H(\frac{mx}{v})G(3\frac{mx}{v})\end{aligned}$$

•$mx/v \to 0 \Rightarrow \langle n_1^a + n_2^a\rangle(x) \sim mx^{1/2} \to \Rightarrow$ 2 decoupled chains.
•$mx/v \to \infty \Rightarrow \langle n_1^a + n_2^a\rangle(x) \sim e^{-mx/v} \to$ No power law prefactor
$\neq$ bosons with mass: $n^a(x) \sim K_0(mx)$.

Magnetization profile of the ladder with $J_\perp - (J'_\perp + J''_\perp) > 0$

$T > T_c$ for i=1,2,3 $T < T_c$ for $i = 0$

$$
\begin{aligned}
\langle n_1^a + n_2^a \rangle (x) &= \langle \mu_1 \rangle_{\text{free}} \langle \sigma_2 \rangle_{\text{free}} \langle \sigma_3 \rangle_{\text{free}} \langle \mu_0 \rangle_{\text{free}} \\
&= 0.
\end{aligned}
$$

Dimerization profile of the ladder

Staggered dimerization operator:

$$\Delta_n = (-)^n(\vec{S}_{n,1} \cdot \vec{S}_{n+1,1} + \vec{S}_{n,2} \cdot \vec{S}_{n+1,2})$$

Continuum:

$$\Delta(x) \sim \mu_1\mu_2\mu_3\mu_0$$

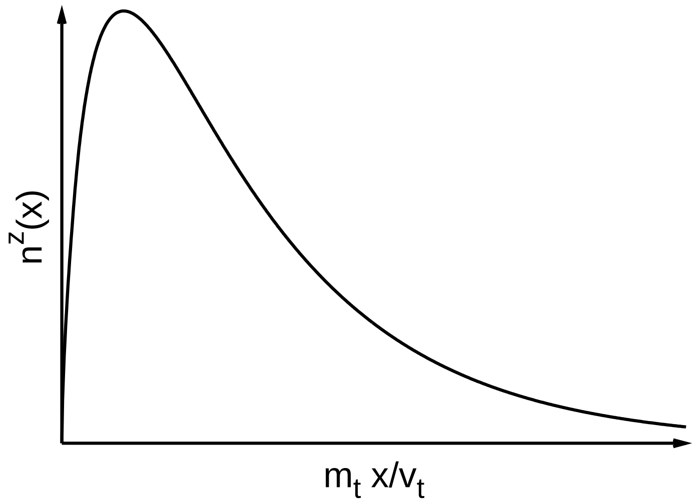
- $|m|x/v \ll 1 \Rightarrow \langle \Delta(x) \rangle \sim \frac{1}{x^{1/2}}$ 2 decoupled chains
- $|m|x/v \gg 1 \Rightarrow \langle \Delta(x) \rangle \sim m^{1/2} e^{-|m|x/v}$

Independent of sign of $J_\perp$!

Magnetization profile of the spin-1 chain

Deduced from the ladder with $J_\perp < 0$ by $\mu_0 \to 1$

$$\langle n^a(x)\rangle \sim m^{3/8} e^{-mx/v} G(\tfrac{mx}{v}) H^2(\tfrac{mx}{v})$$



$$\begin{cases} x \to 0 & \Rightarrow \langle n^a(x)\rangle \sim m x^{5/8} \\ x \to \infty & \Rightarrow \langle n^a(x)\rangle \sim m^{3/8} e^{-mx/v} \end{cases}$$

Dimerization profile of the spin-1 chain

- $mx/v \ll 1 \Rightarrow \langle \Delta(x) \rangle \sim \frac{1}{x^{3/8}}$ (Marston, Tsai 2000)

- $|m|x/v \gg 1 \Rightarrow \langle \Delta(x) \rangle \sim m^{3/8} e^{-mx/v}$

Anisotropic interactions

Ex: (a)interchain coupling $J_\perp(S^x_{i,1}S^x_{i,2}+S^y_{i,1}S^y_{i,2})+J^z_\perp S^z_{i,1}S^z_{i,2}$

(b) anisotropy in the spin 1 chain $-D(S^z_i)^2$

$\Rightarrow$ mass term:

$$i\sum_a m_a \xi^a_+ \xi^a_-$$

$m_a > 0 \forall a \Rightarrow\ \exists$ edge states.

effective g factors $2g_c^{-1} = \sqrt{m_a/m_b} + \sqrt{m_b/m_a}$.

Staggered magnetization: $n_a(x) \sim\sim e^{-m_a x/v}$

Staggered dimerization: $e^{-(m_1+m_2+m_3)x/v}$

Conclusion & perspectives

- field theory description of semi-infinite spin-1 chain and 2 leg spin-1/2 ladder
- edge states description
- calculation of dimerization profile

Generalizations ?

- n-leg ladders or spin-S chains
- explicitly dimerized spin-1/2 chain (sine-Gordon model)
- spontaneously dimerized chains