Edge states and magnetization profiles of open spin-1 chains and open spin ladders

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Haldane gap
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

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

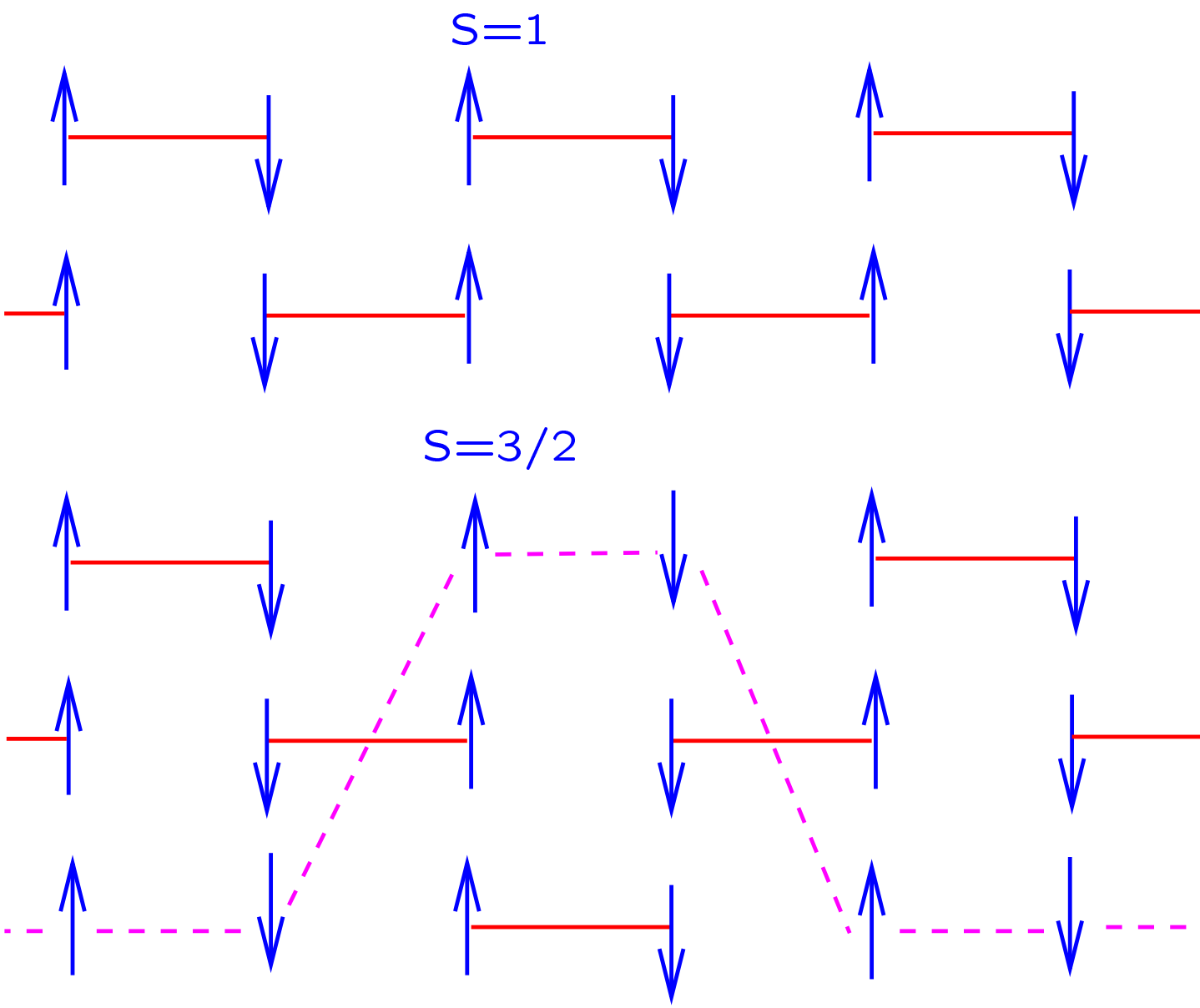
$$\vec{S}_n \sim \vec{n} \times \partial_\tau \vec{n}(na) + (-)^n S \vec{n}(na)$$

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

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

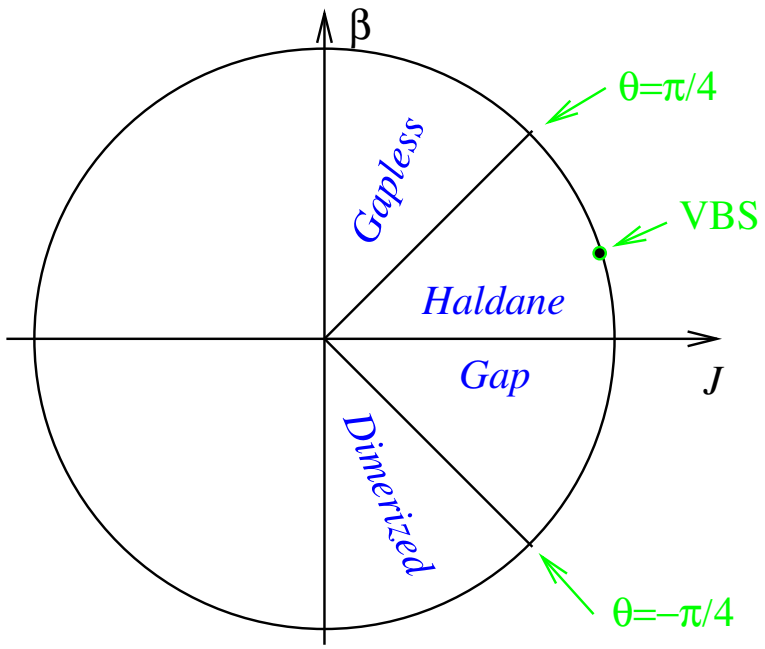
The Valence Bond Solid (VBS)

spin S $\rightarrow$ 2S spins 1/2



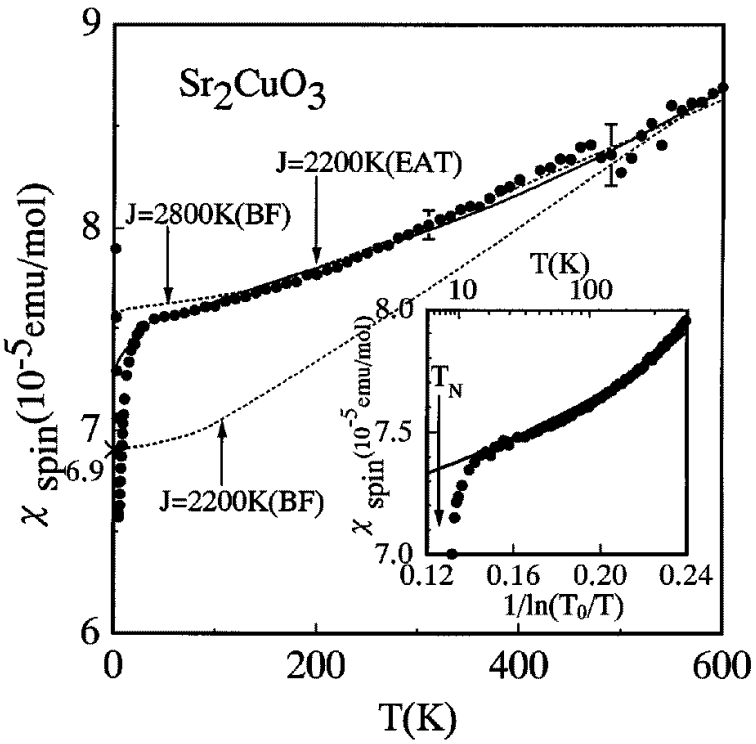
$S = 1$: Numerical Approach

$$H = J \sum_n \left[\vec{S}_n \cdot \vec{S}_{n+1} + \tan\theta (\vec{S}_n \cdot \vec{S}_{n+1})^2 \right]$$



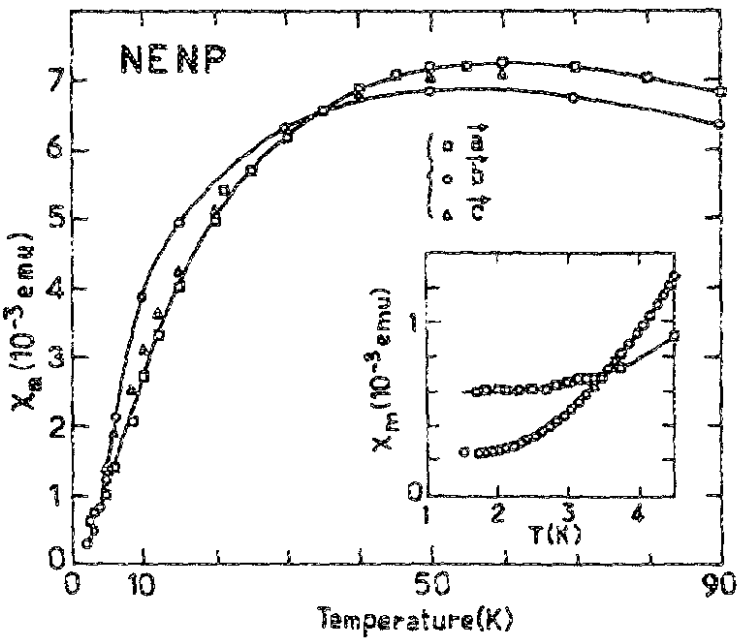
$$\begin{cases} \theta = \frac{\pi}{4} & \text{critical point} SU(3)_1 \text{ Uimin-Lai-Sutherland} \\ \theta = -\frac{\pi}{4} & \text{critical point} SU(2)_2 \text{ Takhtajan-Babujian} \end{cases}$$

Magnetic susceptibility of Sr_2CuO_3
$\simeq$ spin-1/2 chain



from N. Motoyama *et coll.*
Phys. Rev. Lett. **76** 3212 (1996)

Magnetic susceptibility of
$Ni(C_2H_8N_2)_2NO_2(ClO_4)$
$\simeq$ spin-1 chain



from J. P. Renard *et coll.*
J. Appl. Phys. **63** 3538 (1988)

spin ladder

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

$$\vec{S}_{i,p}^2 = \frac{1}{2}\left(\frac{1}{2}+1\right)$$

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

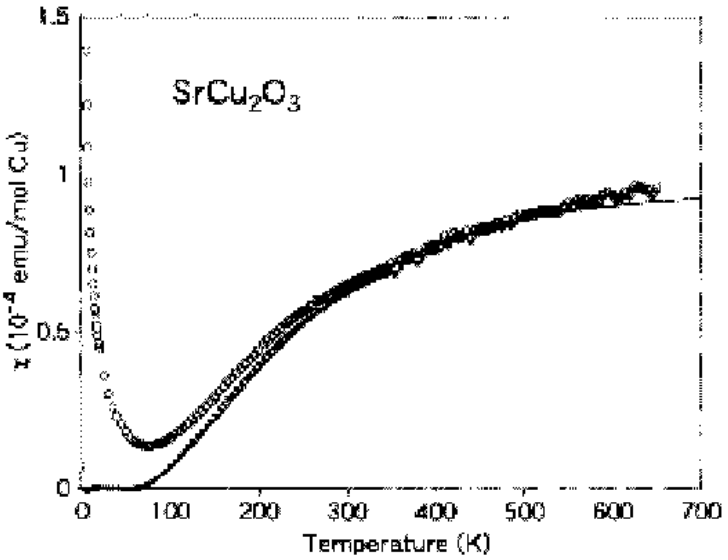
$$J_\perp/J \to +\infty \Rightarrow$$

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

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

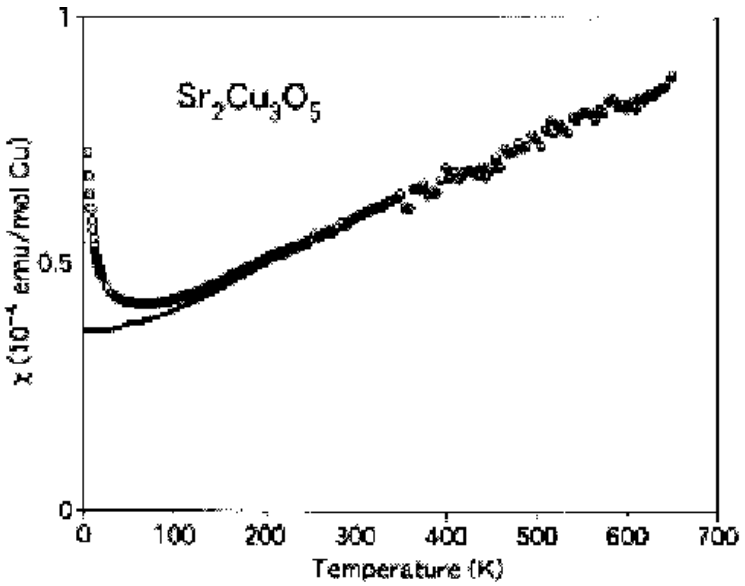
Analogy between ladders and spin-S chains

Magnetic susceptibility of $SrCu_2O_3$
$\simeq$ 2 leg spin-1/2 ladder



from M. Azuma *et coll.*
Phys. Rev. Lett. **73** 3463 (1994)

Magnetic susceptibility of $Sr_2Cu_3O_5$
$\simeq$ 3 leg spin-1/2 ladder



from M. Azuma *et coll.*
Phys. Rev. Lett. **73** 3463 (1994)

Experiments

- $KCuF_3, SrCuO_2, Sr_2CuO_3 \ldots \longrightarrow$ ions Cu^{2+} spin-1/2 chain
- YBa_2NiO_5, NENP, NINO, NDMAZ, $\ldots \longrightarrow$ ions Ni^{2+} spin-1 chain
- $CsVBr_3, CsVCl_3 \longrightarrow (V^{2+})$ spin 3/2 chain
- $MnCl_3(2, 2'$bipyridine$) \longrightarrow$ spin 2 chain
- Sr_2CuO_3, CuHpCl, $\ldots \longrightarrow$ 2 leg ladder
- $Sr_2Cu_3O_5 \longrightarrow$ 3 leg ladder
- La2Cu2O5 $\longrightarrow$ 3 leg ladder

finite length spin-S chains

topological term:

$$\frac{S}{2}\int_0^L dx \int_0^\beta d\tau \vec{n}\cdot(\partial_x\vec{n}\cdot\partial_\tau\vec{n})$$
$$= \frac{S}{2}\left[\Omega(L)-\Omega(0)+4n\pi\right]$$

$\Omega(x)$=area circumscribed on sphere S^2 by $n(x,\tau)$ for $\tau\in[0,\beta]$

$S\in\mathbb{N}$

$\frac{S}{2}\Omega(L)$ = action of a spin $\frac{S}{2}$ at $x=L$.

$\rightarrow$ spins $\frac{S}{2}$ at chain ends

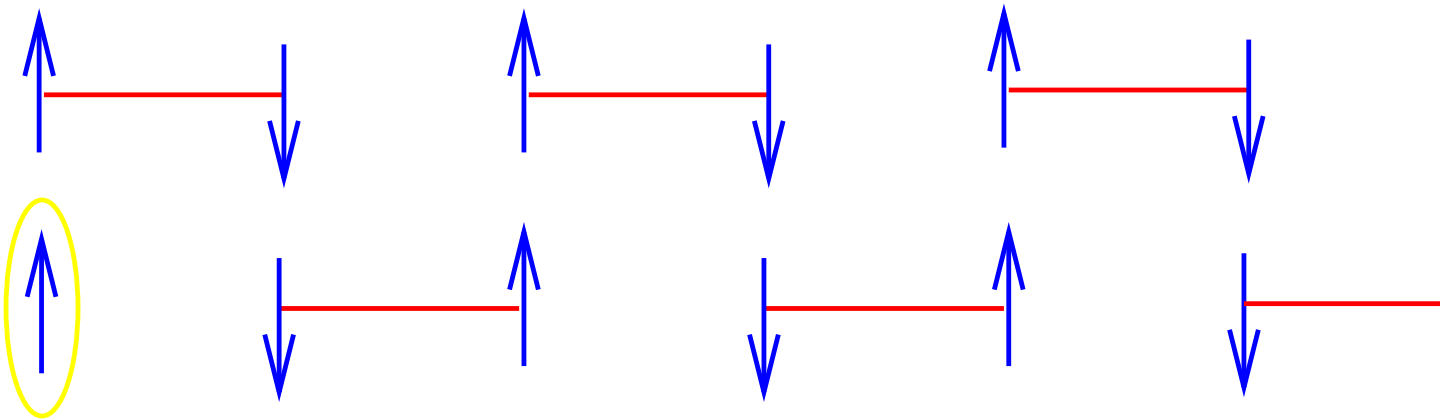
$S\in\mathbb{N}+\frac{1}{2}$

$$\frac{S}{2}\left[\Omega(L)-\Omega(0)+4n\pi\right] = \frac{1}{2}\left(S-\frac{1}{2}\right)\left[\Omega(L)-\Omega(0)+\right.$$
$$(S=1/2 chain) + \frac{1}{2}\times\frac{1}{2}\left[\Omega(L)-\Omega(0)+4n\pi\right.$$

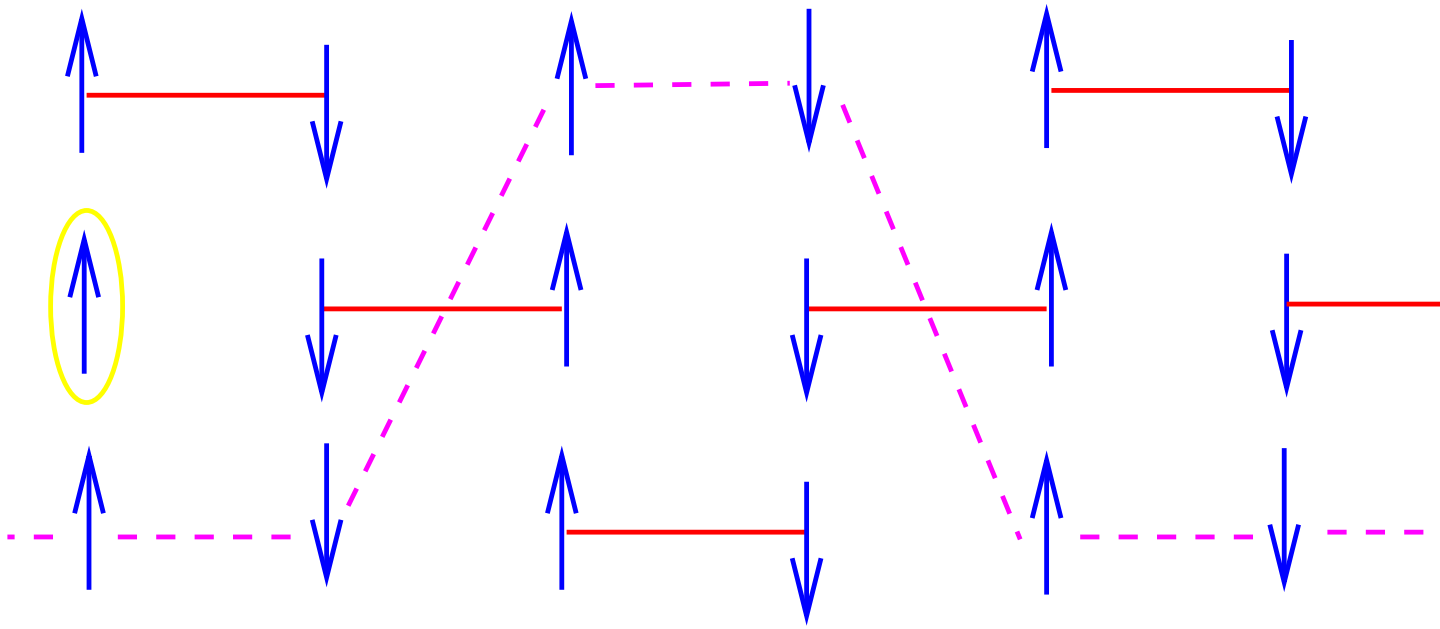
$\rightarrow \frac{(S-1/2)}{2}$ spins at chain ends

Valence Bond Solid point of view

$S = 1$



$S = \frac{3}{2}$



Questions

1. Field theory for the semi-infinite spin-1 chain ?

2. Magnetization/dimerization profile ?

3. Analogy of spin-S chains and spin ladder ?

spin-1/2 chain:

Bosonization

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

$$\vec{S}_n = (\vec{J}_+ + \vec{J}_-)(na) + (-)^n \vec{n}(x)$$

$$\pi \Pi(x) = \partial_x \theta$$

$$J_r^+ \sim e^{i\sqrt{2}(r\theta - \phi)}$$

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

$$n_x = \cos\sqrt{2}\theta \; n_y = \sin\sqrt{2}\theta$$

$$n_z = \sin\sqrt{2}\phi$$

Two-leg ladder: Bosonization

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

Fermionization of relevant term (Nersesyan, Shelton, Tsvelik 1996)

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

$$
m = -\frac{J_\perp}{2\pi}
$$

$$
J_r^{1,a}(x) + J_r^{2,a}(x) = \frac{i}{2} \epsilon_{abc} \xi_r^b \xi_r^c
$$

Equivalence with 4 non-critical 2D Ising models

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

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

spin-1 chain near the integrable Takhtajan-Babujian point:
(A. M. Tsvelik, 1990)

$$H = J\sum_i [\vec{S}_i \cdot \vec{S}_{i+1} - (1-\delta)(\vec{S}_i \cdot \vec{S}_{i+1})^2]$$

$\delta = 0$:

$$H = H_0 = -\frac{iv}{2}\sum_{\substack{\alpha=1\\ r=\pm}}^{3} \int dx r \xi_r^\alpha \partial_x \xi_r^\alpha$$

$\delta \neq 0$:

$$H = H_0 + im\int dx \sum_{\alpha=1}^{3} \xi_+^\alpha \xi_-^\alpha$$

$$S^a = \frac{i}{2}\sum_{r=\pm} \epsilon^{abc}\xi_r^b \xi_r^c + (-)^n n^a(x)$$

$$n^x = \mu_1\sigma_2\sigma_3 \qquad n^y = \sigma_1\mu_2\sigma_3$$

$$n^z = \sigma_1\sigma_2\mu_3$$

$$\begin{cases} \delta > 0: & \langle\sigma_i\rangle \neq 0 \text{ Haldane gap} \\ \delta < 0: & \langle\mu_i\rangle \neq 0 \text{spontaneous dimerization} \end{cases}$$

semi-infinite spin-1/2 chain:

Bosonization

(Eggert, Affleck 1992) Condition:

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

Chiral components:

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

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

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

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

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

Conséquences:

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

$$\langle \Delta(x) \rangle \sim \frac{1}{x^{1/2}}$$

Ladder with open boundary conditions

$$J_\perp \int_0^\infty dx \vec{n}_1(x) \cdot \vec{n}_2(x)$$

$$\sim \quad J_\perp \int_0^\infty dx \left[\cos\sqrt{2}(\theta_1 - \theta_2) + \frac{1}{2}\cos\sqrt{2}(\phi_1 - \phi_2) - \right.$$

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

Change of variables:

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

$$J_\perp \int_0^\infty dx \vec{n}_1(x) \cdot \vec{n}_2(x)$$

$$\sim J_\perp \int_0^\infty dx \left[\cos 2\theta_- + \frac{1}{2}\cos 2\phi_- - \frac{1}{2}\cos 2\phi_+ \right]$$

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

Fermionization

$$\xi_r^1 \sim \cos(\theta^{(+)} - r\phi^{(+)}) \quad \xi_r^3 \sim \cos(\theta^{(-)} - r\phi^{(-)})$$
$$\xi_r^2 \sim \sin(\theta^{(+)} - r\phi^{(+)}) \quad \xi_r^0 \sim \sin(\theta^{(-)} - r\phi^{(-)})$$

Boundary conditions $\phi^{(\pm)}(0) = 0$:

$$\Rightarrow \xi_+^\alpha(0) = \xi_-^\alpha(0)$$

Where:

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

Localized solutions

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

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

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

- Haldane gap phase of spin-1 chain ($|\theta| < \frac{\pi}{4}$))
- 2-leg ladder for $J_\perp < 0$

Absents if $m < 0$

Magnetization profiles

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

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

(Ghoshal, Zamolodchikov 1994) $\Rightarrow$

If $m = (T_c - T)$:

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

- $\xi_+(0) = \xi_-(0)$: Free B. C.'s on order parameter σ at $x = 0$ $(\sigma(0) = 1)$

$\Rightarrow$ 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

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

$\diamond \langle\sigma\rangle^{\text{libre}}_{\text{fixe}}(x, T) = \langle\mu\rangle^{\text{fixe}}_{\text{libre}}(x, 2T_c - T)$ duality

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

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

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

$$u \to 0 \begin{cases} G(u) \sim u^{-1/8} \\ H(u) \sim u^{3/8} \end{cases}$$

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

Magnetization profile of the ladder with $J_\perp < 0$

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

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

$mx/v \to 0 \Rightarrow \langle n_1^a + n_2^a\rangle(x) \sim mx^{1/2}$

$\to$ for $m \to 0 \Rightarrow$ 2 decoupled chains.

$mx/v \to \infty \Rightarrow \langle n_1^a + n_2^a\rangle(x) \sim e^{-mx/v}$

No power law prefactor

$\neq$ bosons with mass: $n^a(x) \sim K_0(mx) \Rightarrow$

Agreement with DMRG calculations.

Magnetization profile of the ladder with $J_\perp > 0$

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

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

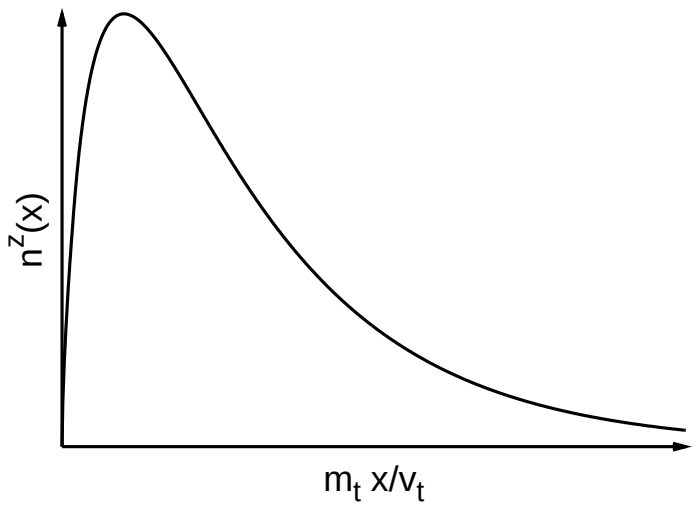
Magnetization profile of the spin-1 chain

Haldane gap phase

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

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

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



Dimerized phase

$$\langle n^a(x) \rangle = 0$$

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 $J_\perp$!

Dimerization profile of the spin-1 chain

Haldane gap phase

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

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

Dimerized phase

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

- $|m|x/v \gg 1 \Rightarrow \langle \Delta(x) \rangle \to \Delta(x = \infty)$

$\Rightarrow$ Boundary enhances dimerization !

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