Spontaneous dimerization and exotic critical lines in spin-1 chain

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Scope

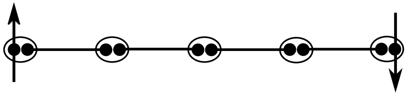
- Introduction
- Spin-1 $J_1 - J_2$ chain with three-site interaction
  - Phase diagram
  - Ising transition
  - Excitation spectrum with DMRG
    - Transverse-field Ising model
  - WZW $SU(2)_2$ critical line. End point
  - Solitons
- Spin-1 $J_1 - J_2$ chain with biquadratic interaction
  - Same phase diagram
- Spin-3/2 $J_1 - J_2$ chain with three-site interaction
  - Use conformal towers to locate the phase transition
- Summary

Introduction

Heisenberg Hamiltonian:

$$H = J_1 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

- Spin-1/2 chain is critical
- Spin-1 chain:
  - finite bulk gap
  - topologically non-trivial ground state
  - spin-1/2 edge states

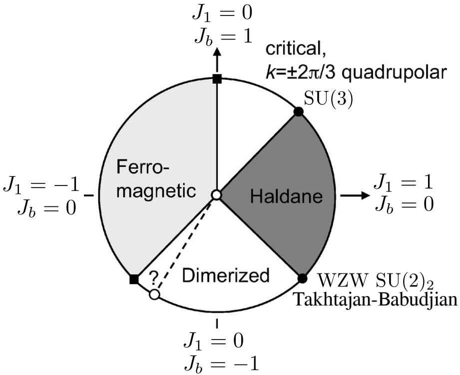


- Haldane, Phys. Lett. A **93**, 464 '83
- Affleck, Kennedy, Lieb, Tasaki, PRL **59**, 799 '87
- Kennedy J. Phys: Cond. Mat **2**, 5737 '90

Introduction

Add biquadratic interaction:

$$H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_b (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$$



Critical spin-1 chains:

- WZW $SU(2)_2$
- SU(3)

- Affleck, Nucl.Phys.B **265**, 409 '86
- Fáth, Sólyom, PRB **44**,11836 '91
- Schollwöck, Jolicœur, Garel, PRB **53**, 3304 '96
- Läuchli, Schmid, Trebst, PRB **74**, 144426 '06

The model

Hamiltonian:

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1}) + \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \text{H.c.} \right]$$

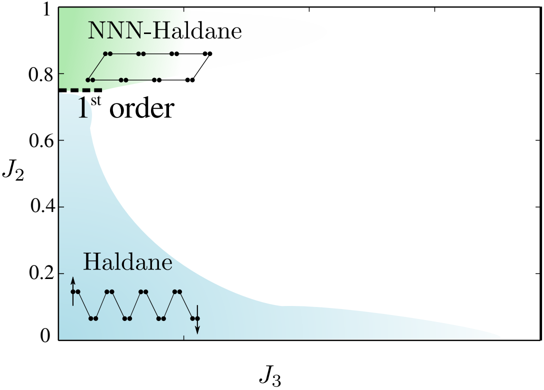
Three-site term:

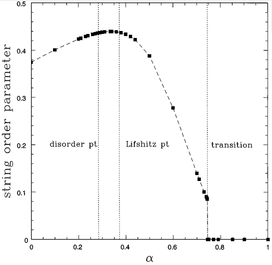
- Appears in next-to-leading order in the strong coupling expansion of the two-band Hubbard model
- Induces spontaneous dimerization
- Reduces to next-nearest-neighbor interaction for spin-1/2

Motivation

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1})$$

$$+ \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \text{H.c.} \right]$$



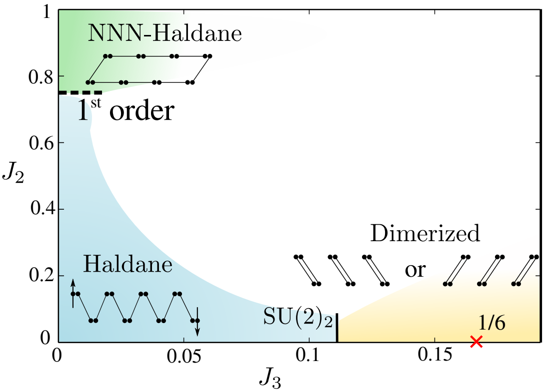


1st order transition between two topologically different phases

- Kolezhuk, Roth, Scholwöck, PRL **77**, 5142 ’96
- Kolezhuk, Scholwöck, PRB **65**, 100401 ’01

Motivation

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1}) + \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \mathrm{H.c.} \right]$$



Generalization of the Majumdar-Ghosh model: fully dimerized state is an exact ground state at $J_3/J_1 = 1/6$

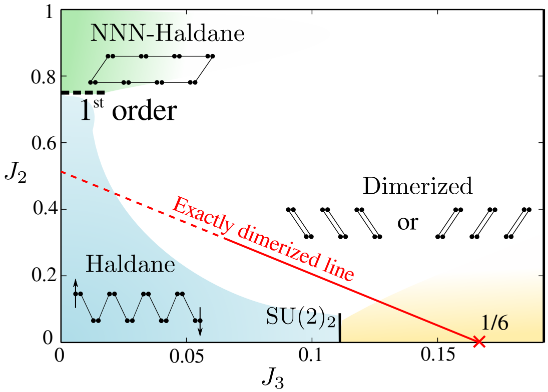
Continuous WZW $SU(2)_{k=2}$ transition at $J_3/J_1 = 0.111$

- Michaud, Vernay, Manmana, Mila, PRL **108**, 127202 '12

Motivation

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1})$$
$$+ \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \mathrm{H.c.} \right]$$

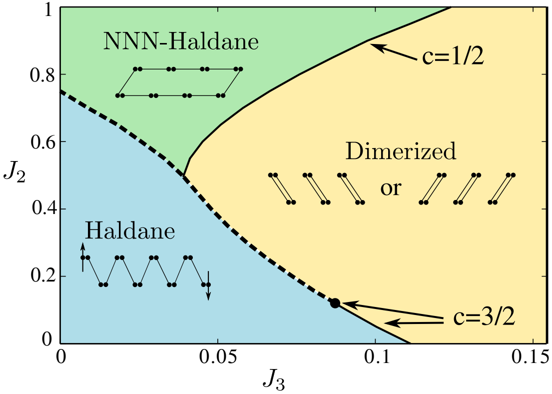
There is a line in $J_2 - J_3$ parameter space, at which the fully dimerized state is exact eigenstate



First order phase transition has to appear between the Haldane and dimerized phases

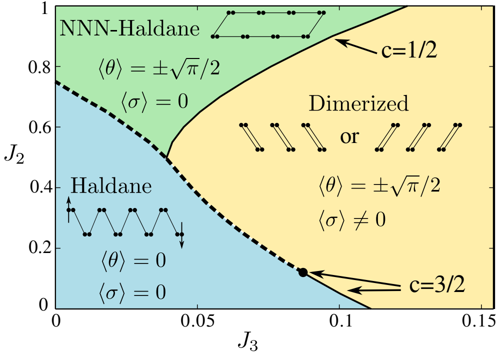
- Michaud, Vernay, Manmana, Mila, PRL **108**, 127202 '12
- Wang, Furuya, Nakamura, Komakura, PRB **88**, 224419'13

Phase diagram



- The transition between the Haldane and dimerized phases is **continuous WZW SU(2)$_2$** below and including at the end point
- The transition between the NNN-Haldane phase and the dimerized phase is in the **Ising universality class**
- Topological transition between the Haldane and NNN-Haldane phases is **always first order**

Phase diagram. Field theory



Effective Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{\text{WZW}} + \lambda_1(\text{tr}g)^2 + \lambda_2 \vec{J}_R \cdot \vec{J}_L$$

- $\lambda_2 < 0$ Continuous $\text{SU}(2)_2$
- $\lambda_2 = 0$ End point
- $\lambda_2 > 0$ First order

Free boson and Ising fields:

$$\text{tr}g \propto \sigma \sin\sqrt{\pi}\theta$$

$$(\text{tr}g)^2 \propto \epsilon - C_1 \cos\sqrt{4\pi}\theta$$

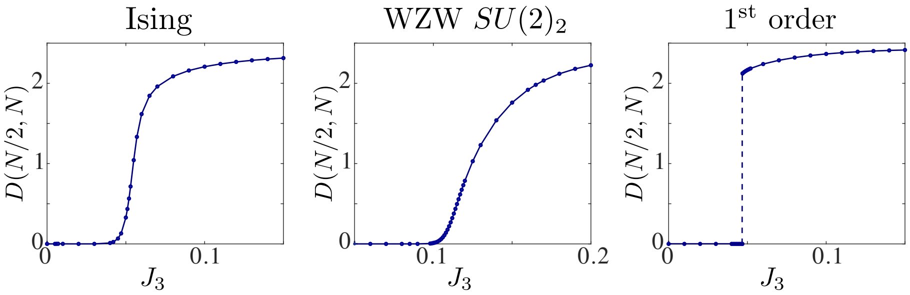
$$\vec{J}_L \cdot \vec{J}_R \propto \epsilon \cos\sqrt{4\pi}\theta + C_2 \partial_x\phi_L\partial_x\phi_R$$

Second order transition between the Haldane and dimerized phases occurs **simultaneously in Ising and boson sectors**. Far from the WZW critical end point the Ising and boson critical lines could split

Dimerization

Local dimerization:

$$D(j,N) = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle - \langle \mathbf{S}_{j-1} \cdot \mathbf{S}_j \rangle|$$



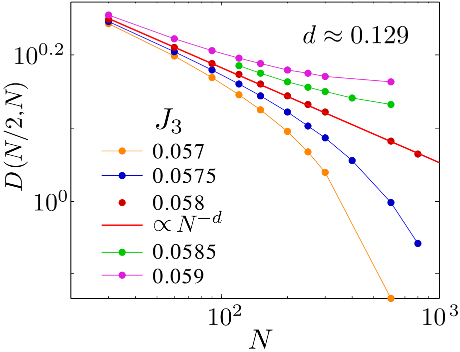
Ising transition. Dimerization

- Local dimerization: $D(j, N) = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle - \langle \mathbf{S}_{j-1} \cdot \mathbf{S}_j \rangle|$

- Finite-size scaling of the middle-chain dimerization in log-log scale

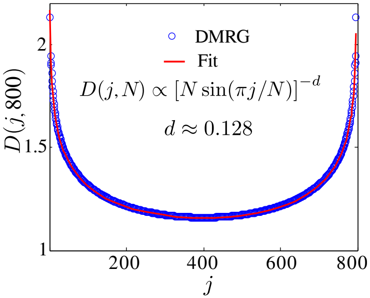
- The **separatrix** is associated with the phase transition

- The **slope** corresponds to the critical exponent



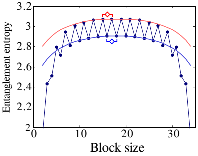
Ising transition. Dimerization

- Local dimerization: $D(j,N) = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle - \langle \mathbf{S}_{j-1} \cdot \mathbf{S}_j \rangle|$
- Open boundary favors dimerization
- In the transverse-field Ising chain it is equivalent to the applied **boundary magnetic field**
- At the critical point the magnetization decays away from the edges as $\sigma(x) \propto [N \sin(\pi j/N)]^{-1/8}$



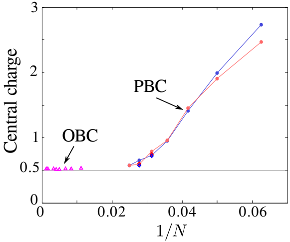
- In spin-1 chain the dimerization decays away from the boundaries in the same way and with the same **critical exponent**

Ising transition. Central charge



Entanglement entropy in **periodic** system:

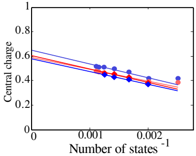
$$S_N(n) = \frac{c}{3}\ln\left[\frac{N}{\pi}\sin\left(\frac{\pi n}{N}\right)\right] + s_1$$



Mid-chain central charge:

$$c_k = \frac{3[S_N(\frac{N}{2}-(k+2)) - S_N(\frac{N}{2}-k)]}{\ln[\cos(\frac{(k+2)\pi}{N})/\cos(\frac{k\pi}{N})]}$$

with $k = 0, 1$



Entanglement entropy in **open** system:

$$S_N(n) = \frac{c}{6}\ln\left[\frac{2N}{\pi}\sin\left(\frac{\pi n}{N}\right)\right] + s_1 + \log g$$

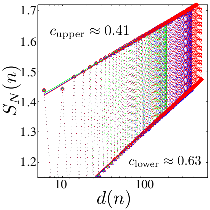
Conformal distance:

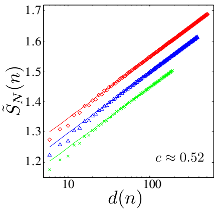
$$d(n) = \frac{2N}{\pi}\sin\left(\frac{\pi n}{N}\right)$$

Reduced entanglement entropy:

$$\tilde{S}_N(n) = \frac{c}{6}\ln d(n) + \zeta\langle \mathbf{S}_n \cdot \mathbf{S}_{n+1}\rangle$$

$$+ s_1 + \log g$$





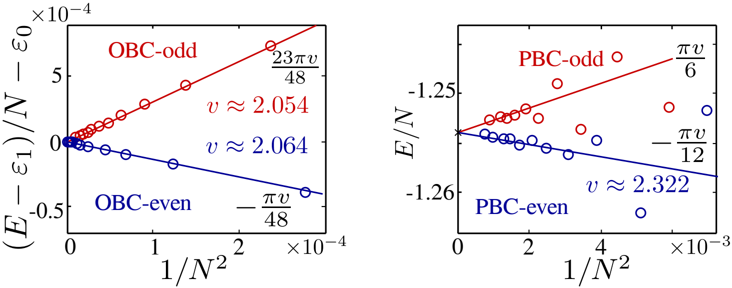
- Calabrese, Cardy, J.Phys.A **42**, 504005'09
- Capponi, Lecheminant, Moliner, PRB **88**, 0.75132'13

Universality class from the energy spectrum:

1. Ground-state energy

2. Excitation spectrum

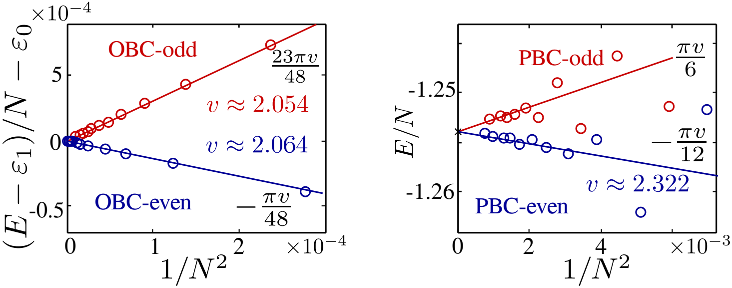
Finite-size scaling of the ground-state energy



$$E_{\text{OBC}} = \varepsilon_0 N + \varepsilon_1 + \frac{\pi v}{N}\left[-\frac{c}{24} + x\right]$$

- OBC N even $\leftrightarrow$ Ising with $\uparrow\uparrow$ BC $\leftrightarrow$ $x_I = 0$
- OBC N odd $\leftrightarrow$ Ising with $\uparrow\downarrow$ BC $\leftrightarrow$ $x_\epsilon = 1/2$

Finite-size scaling of the ground-state energy



$$E_{\mathrm{PBC}} = \varepsilon_0 N + \frac{2\pi v}{N}\left[-\frac{c}{12} + x_R + x_L\right]$$

- PBC N even $\leftrightarrow$ Ising with PBC $\leftrightarrow x_L = x_R = x_I = 0$
- PBC N odd $\leftrightarrow$ Ising with APBC $\leftrightarrow x_L = x_R = x_\sigma = 1/16$

Universality class from the energy spectrum:

1. Ground-state energy
2. Excitation spectrum

Excitation spectrum with DMRG/MPS

1. The excited state is the 'ground-state' of the different symmetry sector
2. Conventional DMRG: Mixed states
   - Heavy memory usage
3. MPS: Construct the lowest-energy state orthogonal to the previously constructed ones
   - Time consuming
   - Accumulation of the error

Excitation spectrum with DMRG/MPS

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2. Conventional DMRG: Mixed states
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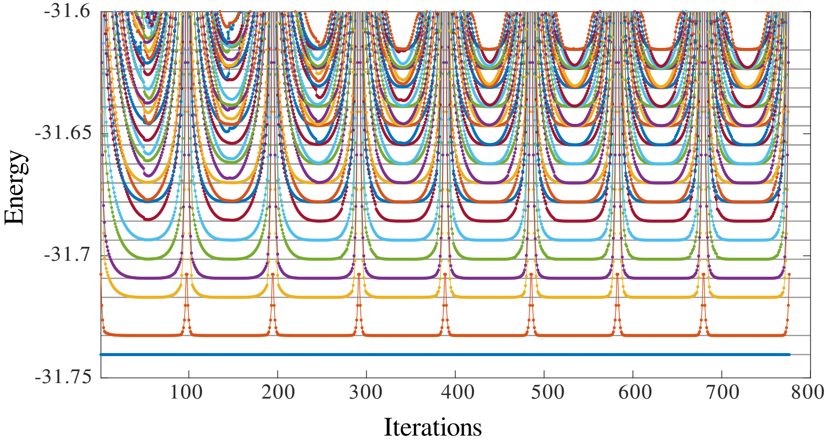
3. MPS: Construct the lowest-energy state orthogonal to the previously constructed ones
   - Time consuming
   - Accumulation of the error

However...

One can extract the excitation spectrum of the critical system **directly** from the effective Hamiltonian while searching for the ground state

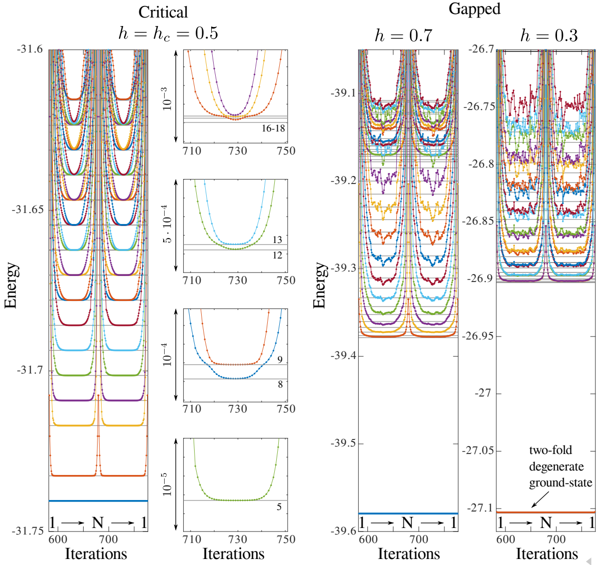
Transverse field Ising model

Transverse field Ising model. Excitation spectrum



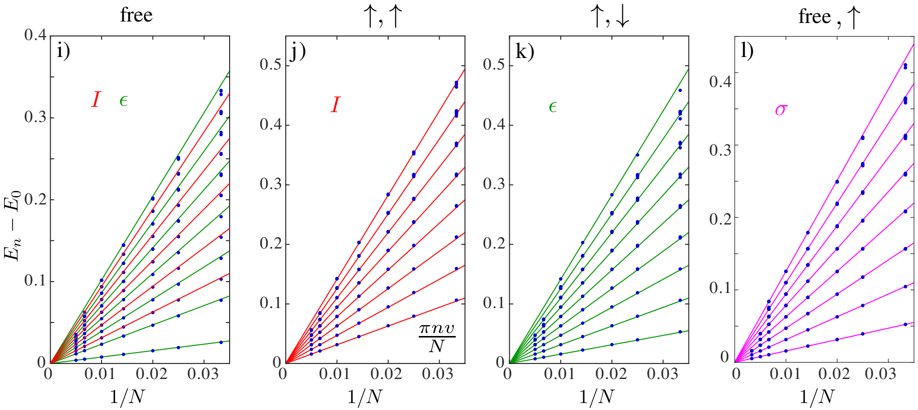
- 30 states within a single run!
- Flattening signals convergence

Transverse field Ising model. Excitation spectrum



Works well for critical systems, but not for gapped ones

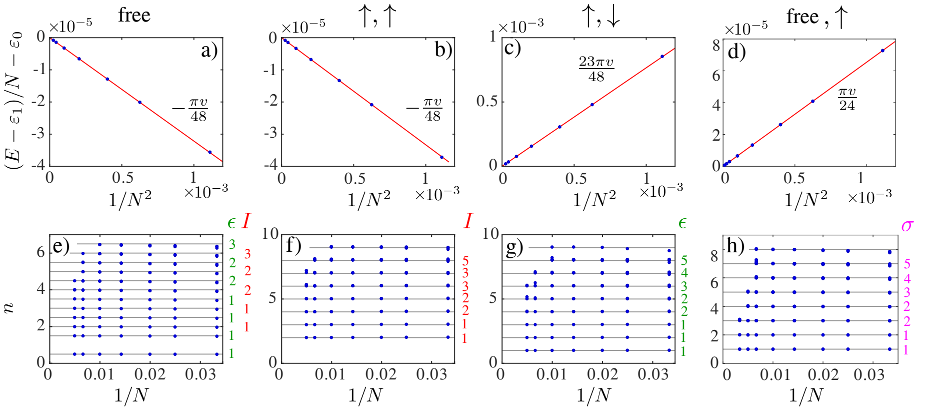
Finite-size scaling of the excitation energy



$$\chi_I(q) = q^{-1/48}\left(1 + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 3q^7 + 5q^8\right)$$

- BCFT prediction: Cardy, Nuc. Phys. B, **324** 581-596'89
- DMRG results: NC, Mila, unpublished

Transverse field Ising model. Conformal towers

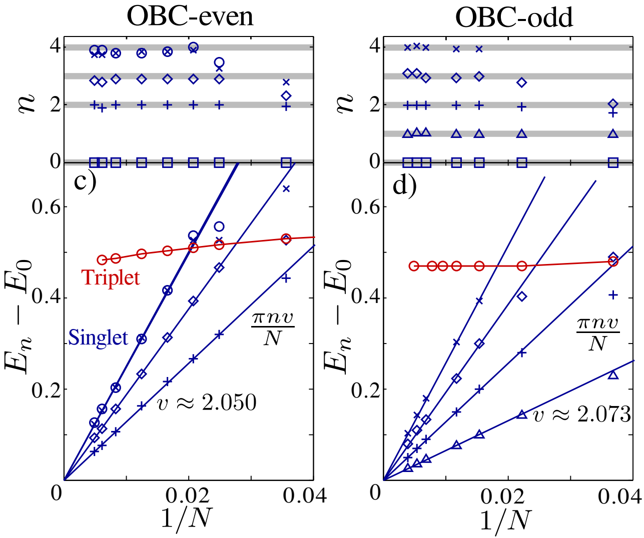


$$\chi_I(q) = q^{-1/48}\left(1 + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 3q^7 + 5q^8\right)$$

- BCFT prediction: Cardy, Nuc. Phys. B, **324** 581-596'89
- DMRG results: NC, Mila, unpublished

Ising transition in spin-1 chain

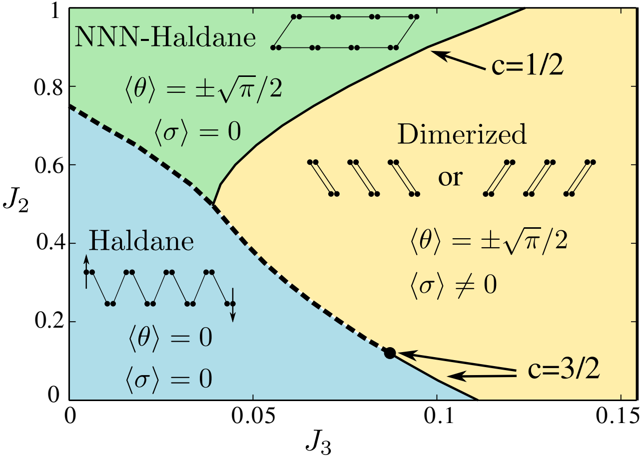
Ising conformal towers in spin-1 chain



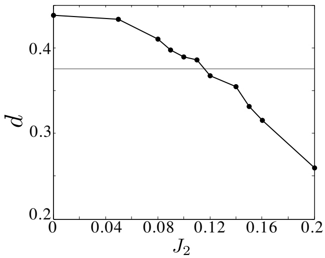
- Singlet-triplet gap is **open**
- Critical scaling of the gap in the singlet sector
- N **even**
  I conformal tower
- N **odd**
  ϵ conformal tower

NC, Affleck, Mila, PRB **93**, 241108'16

WZW $SU(2)_2$ end point

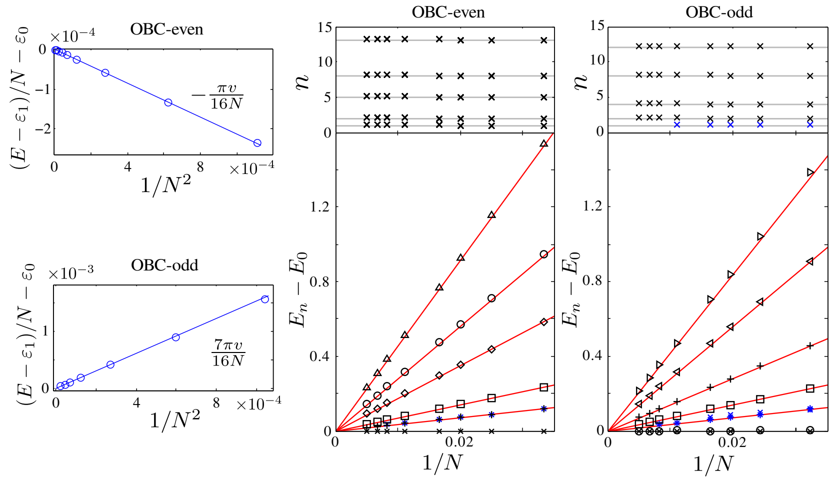


WZW $SU(2)_2$ end point



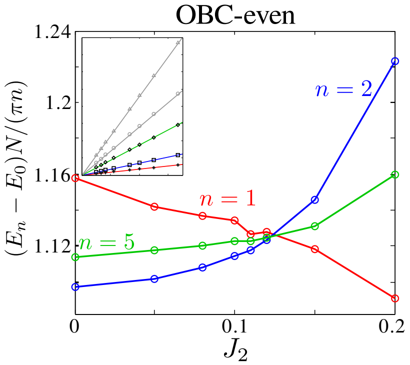
- Associate the critical point with the separatrix in the log-log plot of the finite-size scaling of the dimerization
- The slope gives an **apparent** critical exponent. It is different from the WZW $SU(2)_2$ due to logarithmic corrections
- At the end point the logarithmic corrections vanish and the critical exponent is $\mathbf{d = 3/8}$

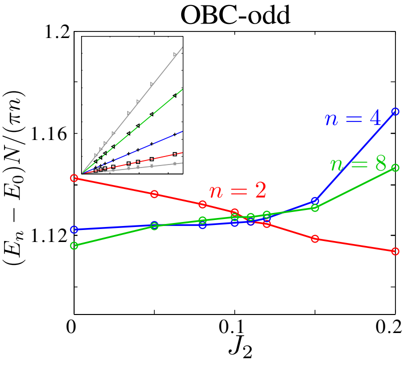
WZW SU(2)$_2$ end point



NC, Affleck, Mila, PRB **93**, 241108'16

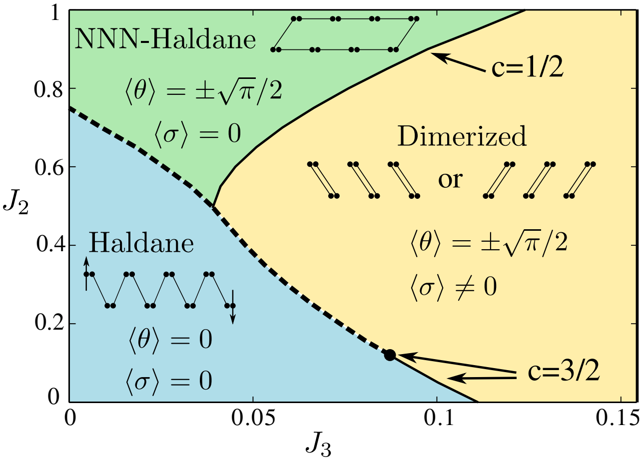
WZW $SU(2)_2$ end point



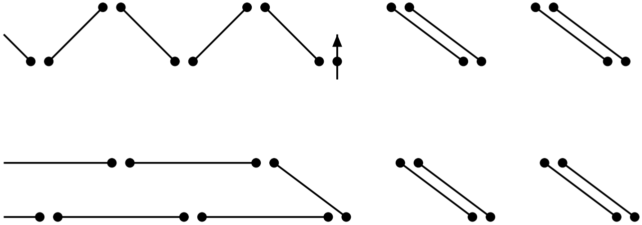


- The 'velocities' extracted from the gap between the ground state and a few lowest excited states cross at the end point
- Away from this point the lines are divergent and the conformal towers are destroyed

Ising vs WZW SU(2)$_2$

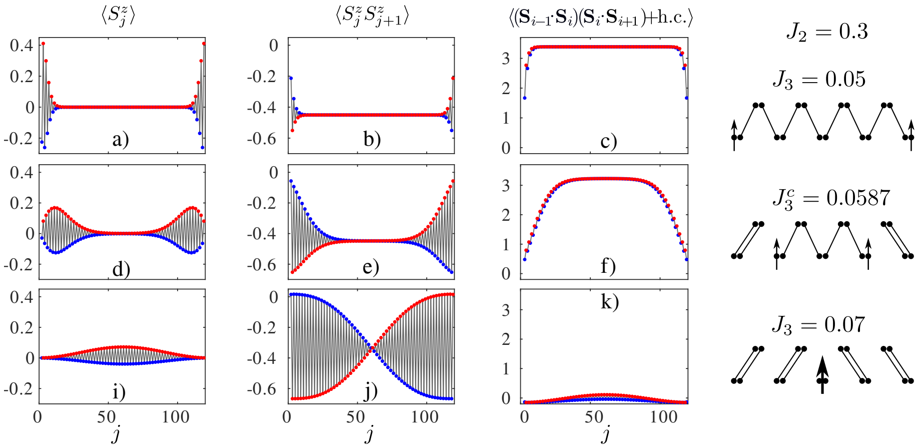


Ising vs WZW $SU(2)_2$



- The domain wall between the Haldane and dimerized phase carries spin-1/2 and corresponds to the **magnetic** WZW $SU(2)_2$ transition
- The domain wall between the NNN-Haldane phased and the dimerized phase does not carry any spin and therefore the singlet-triplet gap remains open

Solitons at the transition between the Haldane and dimerized phases

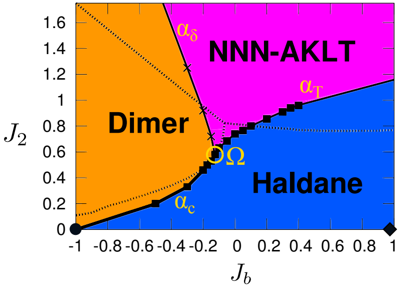


NC, Affleck, Mila, PRB **94**, 205112'16

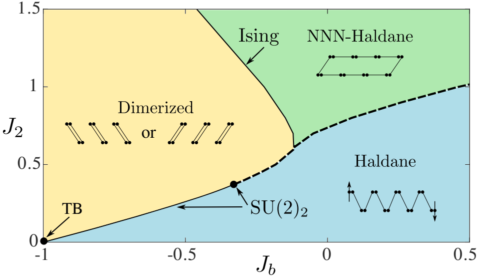
Bilinear-biquadratic model with NNN-interaction

Hamiltonian:

$$H = J_1 \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_b \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2 + J_2 \sum_i \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1}$$



Pixley, Shashi, Nevidomskyy, PRB **90**, 214426'14



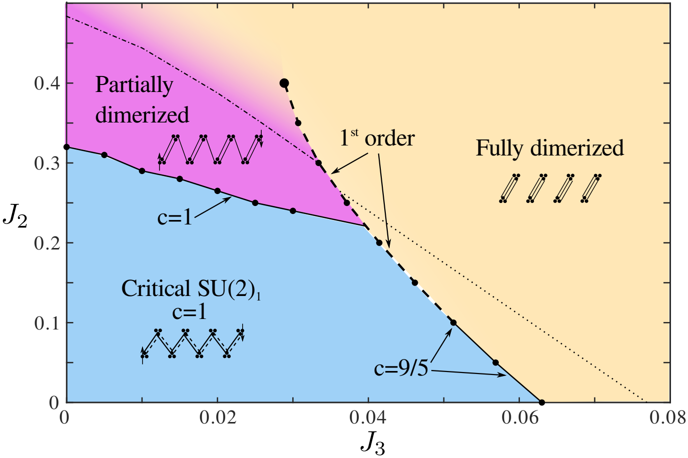
NC, Affleck, Mila, PRB **94**, 136401'16

Conclusions

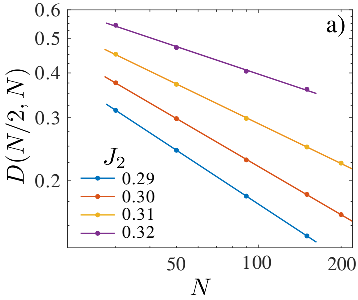
- In spin-1 chains the transition to spontaneously dimerized phase can be either continuous in the **WZW SU(2)$_2$** or in the **Ising** universality class, or **first order**
- The choice between the Ising and WZW SU(2)$_2$ transition depends on the nature of the **domain walls** between the corresponding phases
- Continuous WZW SU(2)$_2$ critical line turn into a first order phase transition at the end point due to presence of marginal operator
- Universality class can be deduced from the finite-size scaling of the energy spectrum

Spin-3/2 chain with three-site interaction

Spin-3/2 chain with three-site interactions

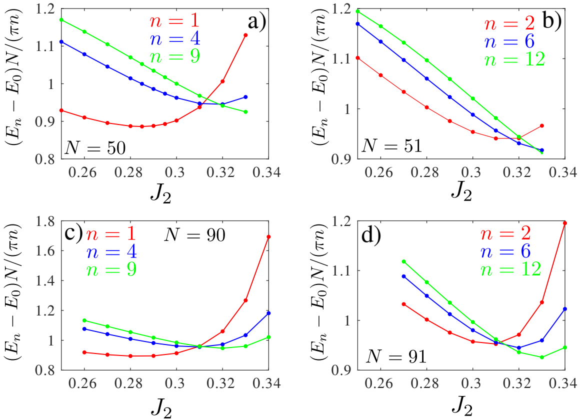


Kosterlitz-Thouless transition



- Difficult to identify the separatrix
- The location of the critical line can be **roughly** estimated from the central charge

Kosterlitz-Thouless transition



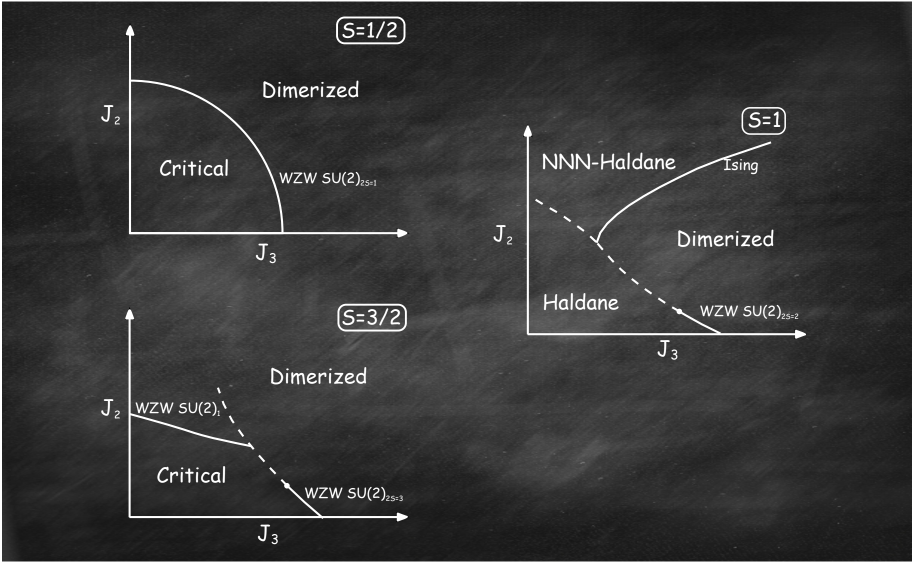
Employ the absence of the logarithmic corrections at the Kosterlitz-Thouless critical line

- More accurate way to locate the phase transition
- The finite-size effects decrease fast with system size and can be **controlled systematically**

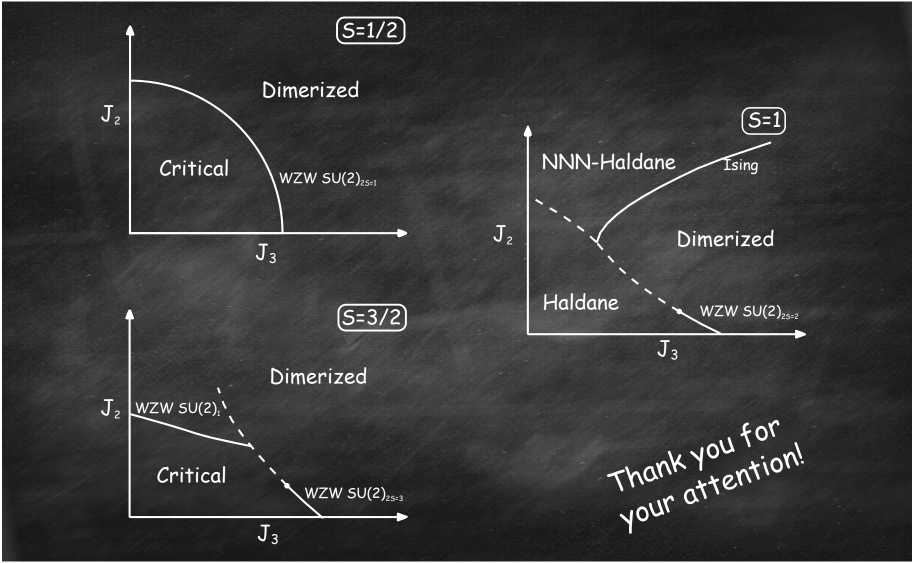
Reminder:

'Velocities' **cross** at the point where the logarithmic corrections vanish and the conformal tower is restored

Summary


S=1/2
Dimerized
J_2
Critical
WZW SU(2)$_{2S=1}$
J_3
S=3/2
Dimerized
J_2
WZW SU(2)$_1$
Critical
WZW SU(2)$_{2S=3}$
J_3
S=1
NNN-Haldane
Ising
J_2
Dimerized
Haldane
WZW SU(2)$_{2S=2}$
J_3

Summary



S=1/2
Dimerized
J_2
Critical
WZW SU(2)$_{2S=1}$
J_3
S=1
NNN-Haldane
Ising
J_2
Dimerized
Haldane
WZW SU(2)$_{2S=2}$
J_3
S=3/2
Dimerized
J_2
WZW SU(2)$_1$
Critical
WZW SU(2)$_{2S=3}$
J_3
Thank you for your attention!