# <span id="page-0-0"></span>Closing the gap in the XXZ chain via magnon interactions

Mikołaj Walicki, University of Warsaw

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### The model

An antiferromagnetic chain of particles of spin  $\frac{1}{2}$  with XXZ Hamiltonian and periodic boundary conditions:

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$$
H_{\alpha} = \sum_{i=1}^{N-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \alpha S_i^z S_{i+1}^z) + S_N^x S_1^x + S_N^y S_1^y + \alpha S_N^z S_1^z.
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Want to understand the difference between 1D and higher dimensions.

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### Lattice rotation

We rotate the spin operators on every other site (analogously to AF Ising):

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\tilde{S}_{2j+1}^{z} = -S_{2j+1}^{z}, \n\tilde{S}_{2j+1}^{-} = S_{2j+1}^{+}, \n\tilde{S}_{2j+1}^{+} = S_{2j+1}^{-}.
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#### <span id="page-6-0"></span>Lattice rotation

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$$
\n(2)

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This yields:

$$
H_{\alpha}^{rot} = \sum -\alpha \tilde{S}_{i}^{z} \tilde{S}_{i+1}^{z} + \frac{1}{2} (\tilde{S}_{i}^{+} \tilde{S}_{i+1}^{+} + \tilde{S}_{i}^{-} \tilde{S}_{i+1}^{-})
$$
(3)

# <span id="page-7-0"></span>Holstein-Primakoff transformation

Introduction of H-P transformation along z-axis<sup>1</sup>:

<sup>1</sup>T. Holstein and H. Primakoff. "Field Dependence of the Intrinsic Domain Magnetization of a Ferromagnet". Phys. Rev. 58 (1940): 1098–1113.  $^2$ Jürgen König and Fred Hucht. "Newton series expansion of bosonic operator functions". SciPost Physics 10, no. 1 (2021[\).](#page-6-0)  $\Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box$ Mikołaj Walicki, University of Warsaw [Closing the gap in the XXZ chain via magnon interactions](#page-0-0)

### <span id="page-8-0"></span>Holstein-Primakoff transformation

Introduction of H-P transformation along z-axis<sup>1</sup>:

$$
\tilde{S}_{i}^{z} = n_{i} - \frac{1}{2} = b_{i}^{\dagger} b_{i} - \frac{1}{2},
$$
\n
$$
\tilde{S}_{i}^{+} = b_{i}^{\dagger} P(n_{i}) = \tilde{S}_{i}^{x} + i \tilde{S}_{i}^{y},
$$
\n
$$
\tilde{S}_{i}^{-} = P(n_{i}) b_{i} = \tilde{S}_{i}^{x} - i \tilde{S}_{i}^{y},
$$
\n
$$
P(n_{i}) = \sqrt{1 - n_{i}} = 1 - n_{i}.
$$
\n(4)

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### Holstein-Primakoff transformation

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Operators  $b_i^{\dagger}$  $\mu_i^{\dagger}$  and  $b_i$  either create or annihilate magnons at i<sup>th</sup> site.  $P(n_i)$  assures the ladder operators have a bounded spectrum<sup>2</sup>. For brevity I will use  $P(n_i)b_i = \tilde{b}_i$ .

<sup>1</sup>T. Holstein and H. Primakoff. "Field Dependence of the Intrinsic Domain Magnetization of a Ferromagnet". Phys. Rev. 58 (1940): 1098–1113.  $^2$ Jürgen König and Fred Hucht. "Newton series expansion of bosonic operator functions". SciPost Physics 10, no. 1 (2021[\).](#page-8-0)  $\Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box \rightarrow \Box$ Mikołaj Walicki, University of Warsaw [Closing the gap in the XXZ chain via magnon interactions](#page-0-0)

## Bosonic Hamiltonian

Bosonic Hamiltonian:

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### Bosonic Hamiltonian

Bosonic Hamiltonian:

$$
\mathcal{H}_{\alpha,\lambda} = \sum_{i}^{N} -\alpha [\lambda n_i n_{i+1} - \frac{1}{2} (n_i + n_{i+1}) + \frac{1}{4}] + \frac{1}{2} (\tilde{b}_i^{\dagger} \tilde{b}_{i+1}^{\dagger} + \tilde{b}_i \tilde{b}_{i+1})
$$
\n(5)

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$$
\n
$$
\lambda \text{ controls the strength of magnon-magnon interactions. Original Hamiltonian obtained for } \lambda = 1.
$$
\n(5)

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In  $d \geq 2$  a good description of low lying excitations is obtained with linear spin waves approximation:

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$$
H_{LSW} = \sum_{i}^{N} \frac{1}{2}(n_i + n_{i+1}) - \frac{1}{4} + \frac{1}{2}(b_i^{\dagger}b_{i+1}^{\dagger} + b_i b_{i+1}).
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 (6)

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This Hamiltonian is exactly diagonisable using Bogoliubov transformation.

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This Hamiltonian is exactly diagonisable using Bogoliubov transformation. However, the results are completely different in 1D.

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Spin correlations and spin dynamical structure factors

Focus on mostly two observables to better understand the system.

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Focus on mostly two observables to better understand the system. Spin correlations in real and momentum space:

$$
S^{aa}(I) = \frac{1}{N} \sum_{i} \langle 0 | S_i^a S_{i+1}^a | 0 \rangle ,
$$
  
\n
$$
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<span id="page-19-0"></span>Spin correlations and spin dynamical structure factors

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$$
S^{aa}(k) = \langle 0 | S_{-k}^a S_k^a | 0 \rangle .
$$
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Spin dynamical structure factor (also known as a spectral function):

$$
S^{aa}(k,\omega) = -\lim_{\delta \to 0^+} \frac{1}{\pi} \operatorname{Im} \langle 0 | S^a_{-k} \frac{1}{E_0 + \omega + i\delta - H} S^a_k | 0 \rangle. \tag{8}
$$

In this equations  $a \in \{x, z\}$ .

# <span id="page-20-0"></span>Gap in the  $S^{xx}(k,\omega)$  spectral function

 $S^{xx}(k,\omega)$ 



Figure:  $S^{xx}(k,\omega)$  for various values of  $\lambda$ . The gap opens when magnon interactions are turned off.

The gap at  $k = \pi$  for  $\lambda = 1$  is a finite size effect, in the limit  $N\longrightarrow\infty$  the spectrum is gapless<sup>3</sup>.

 $^3$ Jean-Sébastien Caux et al. "Tracking the Effects of Interactions on Spinons in Gapless Heisenberg Chains". Physical Review Lett[ers](#page-19-0) [10](#page-21-0)[6](#page-19-0)[, n](#page-20-0)[o.](#page-21-0) [2](#page-0-0)[1 \(](#page-42-0)[201](#page-0-0)[1\)](#page-42-0)[.](#page-0-0)  $299$ Mikołaj Walicki, University of Warsaw [Closing the gap in the XXZ chain via magnon interactions](#page-0-0)

<span id="page-21-0"></span>A known result (cf. eg. textbook by A. Auerbach) states that spectral function  $S^{\times\!\times}(k,\omega)$  is gapless at  $k$  if:

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## Connection between gap and spin correlation

A known result (cf. eg. textbook by A. Auerbach) states that spectral function  $S^{\times\!\times}(k,\omega)$  is gapless at  $k$  if:

$$
\lim_{N \longrightarrow \infty} \frac{1}{N} S^{xx}(k) \neq 0. \tag{9}
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$$
\lim_{N \to \infty} \frac{1}{N} S^{xx}(k) \neq 0. \tag{9}
$$

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This gives another tool for tracking the gap, easier to do then observing the spectral functions.

### Tracking the phase transition

Convergence of  $\frac{1}{N}S^{\times \times}$  can be mapped against  $\alpha, \lambda$ :

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### <span id="page-25-0"></span>Tracking the phase transition

Convergence of  $\frac{1}{N}S^{\times \times}$  can be mapped against  $\alpha, \lambda$ :



Figure: Calculated convergence of  $\frac{1}{N}S^{xx}(k)$ . The calculations were done exactly for small systems and then confirmed with DMRG.

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## Tracking the phase transition

Convergence of  $\frac{1}{N}S^{\times \times}$  can be mapped against  $\alpha, \lambda$ :



Figure: Calculated convergence of  $\frac{1}{N}S^{xx}(k)$ . The calculations were done exactly for small systems and then confirmed with DMRG.

We see a critical line along  $\lambda = 1$  up to  $\alpha = 1$ .

### Real space spin correlations

Another observable that can be linked to the energy gap is real space correlations–the crucial distinction is power-law vs. exponential decay of correlations.

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Figure:  $S^{xx}(i)$  for range of systems with  $\alpha$  < 1.

Figure:  $S^{xx}(i)$  for range of systems with  $\alpha \geq 1$ .

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### Next steps

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#### Next steps

 $\blacktriangleright$  But what about  $S^z$ ? Initial results suggest that spin correlations in  $S^{zz}$  take over in the regions with exponential decay of  $S^{xx}$  and can even create a true long range order-neds to be verified.

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### Next steps

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- ▶ Come up with a intuitive 'cartoon' picture of the excitations.

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 $\blacktriangleright$  Linear spin waves break down in  $d = 1$ , but the magnon description is still useful.

 $\left\{ \left\vert \Theta\right\vert \right\}$  , and if  $\left\vert \Phi\right\vert$ 

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- ▶ Linear spin waves break down in  $d = 1$ , but the magnon description is still useful.
- ▶ Magnon-magnon interactions are essential for the closing of the energy gap.

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- $\blacktriangleright$  Linear spin waves break down in  $d = 1$ , but the magnon description is still useful.
- ▶ Magnon-magnon interactions are essential for the closing of the energy gap.
- $\blacktriangleright$  The crucial part of the Hamiltonian is balance between magnon-magnon interactions and magnon cost.

 $\mathcal{L}$  and  $\mathcal{L}$  is a set of  $\mathcal{L}$  in the  $\mathcal{L}$ 

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#### Jasper van Wezel University of Amsterdam





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#### Jasper van Wezel University of Amsterdam

#### Takami Tohyama Tokyo University of Science







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## The end



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# Jordan-Wigner transformation

J-W transformation inconvenient, as it involves so called "Jordan strings" <sup>4</sup>:

$$
n_j = S^z + \frac{1}{2}
$$
  
\n
$$
a_j = e^{-i\pi \sum_{k=1}^{j-1} n_k} S_j^-
$$
  
\n
$$
a_j^{\dagger} = e^{+i\pi \sum_{k=1}^{j-1} n_k} S_j^+
$$
\n(10)

These assure correct anticommutation relations between fermions at different sites, but prove hard to compute in larger systems.

<sup>4</sup>Paul Jordan and Eugen Wigner. "Über das Paulische Äquivalenzverbot". Zeitschrift für Physik 47 (1928): 631-651.

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#### <span id="page-42-0"></span>Disturbing the balance the other way

Add chemical potential (can be interpreted as magnetic field) to tip the balance between magnon interactions and magnon cost:

$$
H_{\mu} = \sum_{i}^{N} -\alpha [\lambda n_{i} n_{i+1} - \frac{1}{2} (n_{i} + n_{i+1}) + \frac{1}{4}] + \frac{1}{2} (b_{i}^{\dagger} b_{i+1}^{\dagger} + b_{i} b_{i+1}) + \mu n_{i}.
$$
\n(11)

 $\alpha = 1$ 



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