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

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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)

Holstein-Primakoff transformation

Introduction of H-P transformation along z-axis¹:

¹T. Holstein and H. Primakoff. "Field Dependence of the Intrinsic Domain Magnetization of a Ferromagnet". *Phys. Rev.* 58 (1940): 1098–1113. ²Jürgen König and Fred Hucht. "Newton series expansion of bosonic operator functions". *SciPost Physics* 10, no. 1 (2021). Domain and the series are series and the series are series and the series and the series are seri

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Operators b_i^{\dagger} and b_i either create or annihilate magnons at ith site. $P(n_i)$ assures the ladder operators have a bounded spectrum². For brevity I will use $P(n_i)b_i = \tilde{b}_i$.

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Bosonic Hamiltonian

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$$\mathcal{H}_{\alpha,\lambda} = \sum_{i}^{N} -\alpha [\lambda n_{i} n_{i+1} - \frac{1}{2} (n_{i} + n_{i+1}) + \frac{1}{4}] + \frac{1}{2} (\tilde{b}_{i}^{\dagger} \tilde{b}_{i+1}^{\dagger} + \tilde{b}_{i} \tilde{b}_{i+1})$$
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$$\lambda \text{ controls the strength of magnon-magnon interactions. Original Hamiltonian obtained for } \lambda = 1.$$

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In $d \ge 2$ 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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This Hamiltonian is exactly diagonisable using Bogoliubov transformation. However, the results are completely different in 1D.

Spin correlations and spin dynamical structure factors

Focus on mostly two observables to better understand the system.

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$$S^{aa}(I) = \frac{1}{N} \sum_{i} \langle 0 | S_{i}^{a} S_{i+I}^{a} | 0 \rangle,$$

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

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

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

Gap in the $S^{xx}(k,\omega)$ spectral function

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



Figure: $S^{xx}(k,\omega)$ for various values of λ . 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 gapless³.

³Jean-Sébastien Caux et al. "Tracking the Effects of Interactions on Spinons in Gapless Heisenberg Chains". *Physical Review Letters*⊐106,@no. 21 (2011). Mikołaj Walicki, University of Warsaw Closing the gap in the XXZ chain via magnon interactions A known result (cf. eg. textbook by A. Auerbach) states that spectral function $S^{xx}(k,\omega)$ is gapless at k if:

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Connection between gap and spin correlation

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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 $\frac{1}{N}S^{xx}$ can be mapped against α, λ :

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

Tracking the phase transition

Convergence of $\frac{1}{N}S^{xx}$ can be mapped against α, λ :



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 $\alpha \leq 1$.

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

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Next steps

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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

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

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- Magnon-magnon interactions are essential for the closing of the energy gap.
- The crucial part of the Hamiltonian is balance between magnon-magnon interactions and magnon cost.

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Krzysztof Wohlfeld

University of Warsaw Jasper van Wezel University of Amsterdam





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Krzysztof Wohlfeld

University of Warsaw Jasper van Wezel University of Amsterdam **Takami Tohyama** Tokyo University of Science







(b) (4) (3) (4)

The end



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Jordan-Wigner transformation

J-W transformation inconvenient, as it involves so called "Jordan strings" $^{\!\!\!4}$:

$$n_{j} = S^{z} + \frac{1}{2}$$

$$a_{j} = e^{-i\pi \sum_{k=1}^{j-1} n_{k}} S_{j}^{-}$$

$$a_{j}^{\dagger} = e^{+i\pi \sum_{k=1}^{j-1} n_{k}} S_{j}^{+}$$
(10)

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

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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:

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

 $\alpha = 1$



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