Droplet Excitations in the Spin-1/2 XXZ Chain
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(in preparation)

One-dimensional chain \([1, L] \subseteq \mathbb{Z}\)

Single-site spin Hilbert space: \(\mathcal{H}_x \cong \mathbb{C}^2\), o.n. basis \(\{|\uparrow\rangle, |\downarrow\rangle\}\)

Spin matrices:

\[
S^1 = \begin{bmatrix} 0 & 1/2 \\ 1/2 & 0 \end{bmatrix}, \quad S^2 = \begin{bmatrix} 0 & -i/2 \\ i/2 & 0 \end{bmatrix}, \quad S^3 = \begin{bmatrix} 1/2 & 0 \\ 0 & -1/2 \end{bmatrix}.
\]

Defines spin-1/2 representation of SU(2) at each site \(x\):

\([S^1, S^2] = iS^3\) and cyclic permutations.
Hilbert space for chain $\mathcal{H} = \bigotimes_{x=1}^{L} \mathcal{H}_x$.
O.n. basis, all Ising–$\{\uparrow, \downarrow\}$ configurations for $[1, L]$.

Isotropic Heisenberg Hamiltonian

$$H = \sum_{x=1}^{L-1} h_{x,x+1},$$

$$h_{x,x+1} = \frac{1}{4} - S_x \cdot S_{x+1}$$

$$= \frac{1}{4} - S^1_x S^1_{x+1} - S^2_x S^2_{x+1} - S^3_x S^3_{x+1}$$

Raising and lowering operators: $S^\pm = S^1 \pm i S^2$
$S^+ |\downarrow\rangle = |\uparrow\rangle$, $S^+ |\uparrow\rangle = 0$, $S^- |\uparrow\rangle = |\downarrow\rangle$, $S^- |\downarrow\rangle = 0$

Nearest neighbor interaction is

$$h_{x,x+1} = \frac{1}{4} - S^3_x S^3_{x+1} - \frac{1}{2} (S^+_x S^-_{x+1} + S^-_x S^+_x).$$
The XXZ Kink Hamiltonian

The XXZ model breaks symmetry.

Choose $\Delta > 1$,

$$ h_{x,x+1} = \frac{1}{4} - S_{x}^{3} S_{x+1}^{3} - \frac{1}{2\Delta} (S_{x}^{+} S_{x+1}^{-} + S_{x}^{-} S_{x+1}^{+}) $$

Nice parametrization: $\Delta = (q + q^{-1})/2$ for $q \in [0, 1]$.

$q = 0$ Ising model, $q = 1$ isotropic Heisenberg

Kink Hamiltonian adds special boundary fields

$$ h_{x,x+1}^{k} = h_{x,x+1} + \frac{\alpha}{2} (S_{x}^{3} - S_{x+1}^{3}) \quad \text{where} \quad \alpha = \frac{1 - q^2}{1 + q^2}. $$
Special features of the XXZ Kink Hamiltonian:

- Quantum group symmetry $SU_q(2)$.
- Exact (and simple) formula for groundstates of $H^k$.
- Groundstates are “frustration free”: they minimize every n.n. interaction separately.
- Finite volume groundstates are restrictions of approximately half of all the infinite volume groundstates. (Other half are ”antikinks”.)
- The Kink Hamiltonian is equivalent by a similarity transformation to the Markov generator for the ASEP on $[1, L]$.
- $H^k$ is Bethe ansatz solvable.
- Exact formula known for the spectral gap $\gamma = 1 - \Delta^{-1}$. 
Representation of $\text{SU}_q(2)$ on $\mathcal{H}$

The quantum group $\text{SU}_q(2)$ is a deformation of $\text{SU}(2)$. Representation determined by three matrices.

The total ”magnetization” matrix:

$$S_{[1,L]}^3 = \sum_{x=1}^{L} S_x^3 ,$$

and the $q$-deformed total raising and lowering operators

$$S_{[1,L]}^+ := \sum_{x=1}^{L} S_x^+ q^{-2S_{[x+1,L]}^3} ,$$

$$S_{[1,L]}^- := \sum_{x=1}^{L} q^{2S_{[1,x-1]}^3} S_x^- ,$$

where $S_{[a,b]}^3 := \sum_{x=a}^{b} S_x^3$. 


Using the Symmetry

The eigenspaces of $S_{[1,L]}^3$ are invariant subspaces for $H^k$. Let $\mathcal{H}(n)$ be the eigenspace of $S_{[1,L]}^3$ with eigenvalue $L/2 - n$.

The spin lowering matrix maps $S_{[1,L]}^- : \mathcal{H}(n) \rightarrow \mathcal{H}(n + 1)$. Define $\mathcal{H}^{\text{hw}}(0) = \mathcal{H}(0)$, and for $n = 1, \ldots, \lfloor L/2 \rfloor$, define $\mathcal{H}^{\text{hw}}(n)$ such that

$$\mathcal{H}(n) = \mathcal{H}^{\text{hw}}(n) \oplus S_{[1,L]}^- \mathcal{H}(n - 1).$$

Then $\mathcal{H}^{\text{hw}}(n)$ is the set of “highest weight vectors” for the representation of $SU_q(2)$.

The highest weight subspaces are also invariant subspaces for $H^k$. 
Numerical Diagonalization for $L = 7$ and $\Delta = 1.25$

Abscissa: $S_{[1,L]}^3$-eigenvalues, “total magnetization” $M$

Minimum energies in hw subspace. Maximum energies. Both.
Ferromagnetic Ordering of Energy Levels

For each $n \in \{0, 1, \ldots, \lfloor L/2 \rfloor\}$ define

$$E_L(n) = \min \text{spec} \left( H^k \upharpoonright \mathcal{H}^{\text{hw}}(n) \right).$$

Note that $E_L(0) = 0$ is the ground state energy.

Previously the same authors proved (for more general spin chains)

$$E_L(0) < E_L(1) < \cdots < E_L(\lfloor L/2 \rfloor).$$

They also proved that for any $n \in \mathbb{N}$, the sequences $(E_L(n) : L \geq 2n)$ is strictly decreasing in $L$.

We can define

$$E(n) = \lim_{L \to \infty} E_L(n),$$

for each $n \in \mathbb{N}$. We know

$$E(0) \leq E(1) \leq \ldots \leq E(n) \leq \ldots$$

**Question:** Is the ordering strict?
Main result.

**Theorem** For $n \in \mathbb{N}$,

$$E(n) = \frac{(1 - q^2)(1 - q^n)}{(1 + q^2)(1 + q^n)}.$$

**Note.** For $n = 0$ this gives $E(0) = 0$, which is the ground state energy.

For $n = 1$ this gives

$$E(1) = \frac{(1 - q^2)(1 - q)}{(1 + q^2)(1 + q)} = \frac{(1 - q)^2}{1 + q^2} = 1 - \Delta^{-1} = \gamma.$$

**Also note.** This formula agrees with a calculation of Yang and Yang for a related quantity. Our method is related to theirs, but not exactly the same. Particularly, our approach is simpler.
The GNS Representation for the All-Up-Spin Groundstate

Define $\mathcal{X}_0 := \{\emptyset\}$.  
For each $n \in \mathbb{N}_+$, define  

$$\mathcal{X}_n := \{\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{Z}^n : x_1 < \cdots < x_n\}.$$  

For each $n \in \mathbb{N}$, let $\mathcal{H}_\mathbb{Z}(n) := \ell^2(\mathcal{X}_n)$, with counting measure.  
Let $\mathcal{H}_\mathbb{Z} := \bigoplus_{n \in \mathbb{N}} \mathcal{H}_\mathbb{Z}(n)$.  
There is a standard representation of SU(2) for each site $x \in \mathbb{Z}$:  

- $S^3_x$ is $-1/2$ if there is a particle at site $x$ and $+1/2$ otherwise;  
- $S^+_x : \mathcal{H}(n) \rightarrow \mathcal{H}(n - 1)$ removes the particle at site $x$ if one is present, and otherwise annihilates the vector;  
- $S^-_x : \mathcal{H}(n) \rightarrow \mathcal{H}(n + 1)$ places a particle at site $x$ if one is not present, and otherwise annihilates the vector.
There is a densely defined, positive semidefinite operator
\[ H_{\mathbb{Z}} = \sum_{x \in \mathbb{Z}} h_{x,x+1} = \sum_{x \in \mathbb{Z}} h_{x,x+1}^k, \]
defined in terms of the $S^3_{x, \pm}$ operators.
Kink boundary fields telescope to $\pm \infty$ and cancel in this representation.

For each $n$, $\mathcal{H}_{\mathbb{Z}}(n)$ is an invariant subspace for $H_{\mathbb{Z}}$.
On this subspace, the Hamiltonian is bounded.
There is no representation of SU$_q(2)$ on $\mathcal{H}_{\mathbb{Z}}$.

**Lemma** For each $n \in \mathbb{N}$, define
\[ E_{\mathbb{Z}}(n) := \inf \text{spec} \left( H_{\mathbb{Z}} \mid \mathcal{H}_{\mathbb{Z}}(n) \right). \]
Then
\[ E(n) = E_{\mathbb{Z}}(n). \]
There is another symmetry of $H \mid \mathcal{H}_Z(n)$, shift-invariance. Let $\tau : \mathcal{X}_n \to \mathcal{X}_n$ be the map $\tau(x) = x + (1, \ldots, 1)$. Let $\mathcal{Y}_n = \{ y \in \mathcal{X}_n : 0 \leq y_1 + \cdots + y_n \leq n - 1 \}$. Then $\mathcal{Y}_n \cong \mathcal{X}_n/\tau$ in a natural way.

Define the shift operator

$$T \delta_x = \delta_{\tau(x)}.$$ 

Let $\ell(\mathcal{X}_n)$ be the set of all sequences, and let $\ell_0(\mathcal{X})$ be the set of $T$-invariant sequences. Define $\ell_0^2(\mathcal{X}_n)$ to be the subspace of $\ell_0(\mathcal{X}_n)$ with Hilbert space norm

$$\|f\|^2 = \sum_{y \in \mathcal{Y}_n} |f(y)|^2.$$
Direct Integral Decomposition

Using the usual Fourier transform from $\mathbb{Z}$ to $S^1$

$$\mathcal{H}_\mathbb{Z}(n) = \ell^2(\mathcal{X}_n) \cong \int_{S^1} \ell^2_0(\mathcal{X}_n) \frac{d\theta}{2\pi},$$

and

$$(H_\mathbb{Z} \upharpoonright \mathcal{H}_\mathbb{Z}(n)) \cong \int_{S^1} A_n(\theta) \frac{d\theta}{2\pi},$$

where $A_n(\theta)$ is the image of $H_\mathbb{Z}$ conjugated by appropriate (Bloch-type) transformations, restricted to $\ell^2_0(\mathcal{X}_n)$. 
The operator $A_n(\theta)$ is the restriction to $\ell^2_0(\mathcal{X}_n)$ of an operator $\tilde{A}_n(\theta)$ on all of $\ell(\mathcal{X}_n)$ defined through the kernel

$$K_n(x, y; \theta) = \sum_{k=0}^{n} K_n^{(k)}(x, y; \theta),$$

where

$$K_n^{(0)}(x, y; \theta) = \frac{1}{2} \delta_{y,x} - \frac{1}{2\Delta} e^{i\theta} \delta_{y,x-e_1},$$

$$K_n^{(n)}(x, y; \theta) = \frac{1}{2} \delta_{y,x} - \frac{1}{2\Delta} e^{-i\theta} \delta_{y,x+e_n},$$

and for $k = 1, \ldots, n-1$,

$$K_n^{(k)}(x, y; \theta) = \left(1 - \delta_{x_{k+1}, x_{k+1}}\right) \delta_{y,x} - \frac{1}{2\Delta} \left(e^{-i\theta} \delta_{y,x+e_k} + e^{i\theta} \delta_{y,x-e_{k+1}}\right).$$
Each $A_n(\theta)$ is a self-adjoint operator on $\ell^2_0(\mathcal{X}_n)$, and the map $\theta \mapsto A_n(\theta)$ is norm-continuous. Therefore,

$$\inf \text{spec} \left( H_Z \upharpoonright \mathcal{H}_Z(n) \right) = \min_{\theta \in S^1} \inf \text{spec} A_n(\theta).$$

But it is easy to see that the optimal $\theta$ is 0 because for any $f \in \ell^2_0(\mathcal{X}_n)$,

$$(f, A_n(\theta)f) \geq (|f|, A_n(0)|f|).$$
**Lemma** Let $\mathbb{C}^\times = \mathbb{C} \setminus \{0\}$. Suppose that $\xi \in (\mathbb{C}^\times)^n$ satisfies

$$\xi_k + \xi_k^{-1} = 2\Delta,$$

for $k = 1, \ldots, n - 1$. Define $f_\xi \in \ell(\mathcal{X}_n)$,

$$f_\xi(x) = \prod_{k=1}^{n} \xi_k^{x_k}.$$

Then $f$ is an eigenvector of $\tilde{A}_n(0)$ with eigenvalue equal to

$$E(\xi) = \sum_{k=1}^{n} \left(1 - \frac{1}{2\Delta} \left[\xi_k + \xi_k^{-1}\right]\right).$$
Proof. Define two kernels on $\mathbb{Z}^n$ not $\mathcal{X}_n$:

$$\tilde{K}_n^1(x, y) = \sum_{k=1}^{n} \left( \delta_{y,x} - \frac{1}{2\Delta} (\delta_{y,x-e_k} + \delta_{y,x+e_k}) \right),$$

$$\tilde{K}_n^2(x, y) = \sum_{k=1}^{n-1} \delta_{y_{k+1},y_{k+1}} \left( \delta_{y,x} - \frac{1}{2\Delta} (\delta_{y,x-e_k} + \delta_{y,x+e_{k+1}}) \right).$$

Let $\tilde{K}_n = \tilde{K}_n^1 - \tilde{K}_n^2$. Then

1. for any $x, y \in \mathcal{X}_n$, $\tilde{K}_n(x, y) = K_n(x, y)$, and
2. for any $y \in \mathcal{X}_n$ and $x \in \mathbb{Z}^n \setminus \Omega_n$, $\tilde{K}_n(x, y) = 0$.

By these two properties, if $f \in \ell(\mathbb{Z}^n)$ is any eigenvector, its restriction to $\ell(\mathcal{X}_n)$ is an eigenvector of $\tilde{A}_n(0)$.

The first kernel corresponds to the discrete Laplacian for $n$ noninteracting particles. Its energy is just what was written in the lemma, $E(\xi)$. We try to find null-vectors for the second kernel.
Meeting Conditions

For each $k = 1, \ldots, n$, let $M_k$ be the operator on $\ell(\mathbb{Z}^n)$ defined through the kernel

$$\tilde{K}_{n,k}^2(x, y) = \delta_{y_{k+1}, y_{k+1}} \left( \delta_{y, x} - \frac{1}{2\Delta} \left( \delta_{y, x-e_k} + \delta_{y, x+e_{k+1}} \right) \right).$$

Their sum equals $\tilde{K}_n^2$.

Given $f_\xi(x) = \prod_{k=1}^n \xi_k^{x_k}$, let us consider the linear equation $M_k f_\xi = 0$.

This requires

$$2\Delta \tilde{f}_\xi(y) = \tilde{f}_\xi(y + e_k) + \tilde{f}_\xi(y - e_{k+1}),$$

for every $y \in \mathbb{Z}^n$ such that $y_{k+1} = y_k + 1$. But this means

$$2\Delta \xi_k \xi_{k+1} = \xi_{k+1} \xi_{k+1} + \xi_k \xi_k.$$

Dividing through by $\xi_k \xi_{k+1}$, gives precisely $\xi_k + \xi_{k+1}^{-1} = 2\Delta$. 
By the lemma, we will have an eigenvector of $\tilde{A}_n(0)$ in $\ell_0(\mathcal{X}_n)$ if we choose $\xi \in (\mathbb{C}^x)^n$ such that both

$$\xi_k + \xi_{k+1}^{-1} = 2\Delta,$$

for $k = 1, \ldots, n - 1$, and such that $\prod_{k=1}^n \xi_k = 1$.

The first of these is a linear fractional recurrence relation

$$\xi_{k+1} = \frac{1}{2\Delta - \xi_k}.$$

It can be easily solved just as for a linear recurrence relation. The most general solution is

$$\xi_k = \frac{z^{1/2} q^{k-1/2} + z^{-1/2} q^{-k+1/2}}{z^{1/2} q^{k+1/2} + z^{-1/2} q^{-k-1/2}}.$$
There is only one $T$-invariant solution

$$\xi_k = \zeta_{k-(n+1)/2} \quad \text{where} \quad \zeta_m = \frac{q^{m-1/2} + q^{-m+1/2}}{q^{m+1/2} + q^{-m-1/2}}.$$

For this one can easily calculate (by induction on $n$)

$$E(\xi) = \frac{(1 - q^2)(1 - q^n)}{(1 + q^2)(1 + q^n)}.$$

Also, one can see that the $\xi_k$ are strictly decreasing in $k$; therefore, the norm,

$$\|f_\xi\|^2 := \sum_{y \in \mathcal{Y}_n} |f_\xi(y)|^2,$$

is finite. So $f_\xi$ is not only in $\ell_0(\mathcal{X}_n)$. It is actually an eigenvector of $A_n(0)$ in $\ell_0^2(\mathcal{X}_n)$.
An Easy Application of PF

We want to know that \( \inf \text{spec } A_n(0) \) is equal to the eigenvalue for \( f_\xi \). We get this from the following lemma, which can be proved by appealing to the PF theorem.

**Lemma** Suppose \( \mathcal{Y} \) is a countable set, and \( A \) is a bounded, self-adjoint operator on \( \ell^2(\mathcal{Y}) \) defined through a nonnegative kernel. If there is some strictly positive \( f \in \ell^2(\mathcal{Y}) \) such that \( Af = \lambda f \), then \( \rho(A) = \lambda \).

(This is applied to \((cI - A_n(0))\) for \( c \) large enough.)
Droplet Excitations

The wavefunction is \( f_\xi(x) = \prod_{k=1}^{n} \xi^{x_k}_k \) where

\[
\xi_k = \zeta_{k-(n+1)/2} \quad \text{where} \quad \zeta_m = \frac{q^{m-1/2} + q^{-m+1/2}}{q^{m+1/2} + q^{-m-1/2}}.
\]

This is a “droplet” of downspins, exponentially bound together.

In a previous paper [CMP 2001], Naftergaele and S* studied 1d droplets in the XXZ model.

Two natural Hamiltonians suggest themselves, in addition to those already suggested.

For the finite chain \([1, L] \subset \mathbb{Z}\),

\[
H^{\text{cycl}} = H + h_{n,1}
\]

\[
H^{\text{drop}} = H + \left( \frac{1}{2} - S_1^3 \right) + \left( \frac{1}{2} - S_2^3 \right).
\]

We found the asymptotic description of all low-energy states.
Using the methods of that paper, we can also prove

**Corollary.** For each \( n \leq \lfloor L/2 \rfloor \), define

\[
E_{L}^{\text{cycl}}(n) = \min \text{spec} \left( H_{[1,L]}^{\text{cycl}} \upharpoonright \mathcal{H}_{[1,L]}(n) \right),
\]

\[
E_{L}^{\text{drop}}(n) = \min \text{spec} \left( H_{[1,L]}^{\text{drop}} \upharpoonright \mathcal{H}_{[1,L]}(n) \right).
\]

Then

\[
\lim_{L \to \infty} E_{L}^{\text{cycl}}(n) = \lim_{L \to \infty} E_{L}^{\text{drop}}(n) = \frac{(1 - q^2)(1 - q^n)}{(1 + q^2)(1 + q^n)}.
\]

For the case of cyclic b.c.’s, this rederives a result of Yang and Yang [Phys.Rev. 1966].
It also recovers the asymptotic droplet energy

\[
\lim_{n \to \infty} E(n) = \frac{1 - q^2}{1 + q^2} = \alpha.
\]