Droplet Excitations in the Spin-1/2 XXZ Chain

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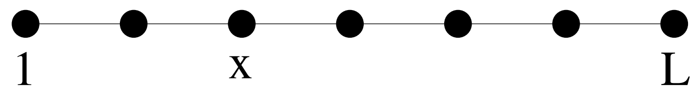
(in preparation)



One-dimensional chain $[1, L] \subset \mathbb{Z}$

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:

$$[S^1, S^2] = iS^3 \quad \text{and cyclic permutations.}$$

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

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

$$\begin{aligned} h_{x,x+1} &= \frac{1}{4} - \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1} \\ &= \frac{1}{4} - S_x^1 \, S_{x+1}^1 - S_x^2 \, S_{x+1}^2 - S_x^3 \, S_{x+1}^3 \end{aligned}$$

Raising and lowering operators: $S^{\pm} = S^1 \pm iS^2$
$S^+ \left|\downarrow\right\rangle = \left|\uparrow\right\rangle$, $S^+ \left|\uparrow\right\rangle = 0$, $S^- \left|\uparrow\right\rangle = \left|\downarrow\right\rangle$, $S^- \left|\downarrow\right\rangle = 0$

Nearest neighbor interaction is

$$h_{x,x+1} = \frac{1}{4} - S_x^3 S_{x+1}^3 - \frac{1}{2}\left(S_x^+ \, S_{x+1}^- + S_x^- \, S_{x+1}^+\right) .$$

The XXZ Kink Hamiltonian

The XXZ model breaks symmetry.

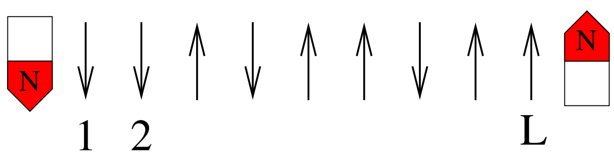
Choose $\Delta > 1$,

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

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

$$h^{\mathrm{k}}_{x,x+1} = h_{x,x+1} + \frac{\alpha}{2}\left(S_x^3 - S_{x+1}^3\right) \quad \text{where} \quad \alpha = \frac{1-q^2}{1+q^2}\,.$$



Special features of the XXZ Kink Hamiltonian:

- Quantum group symmetry $\mathrm{SU}_q(2)$.
- 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 $SU_q(2)$ on $\mathcal{H}$

The quantum group $SU_q(2)$ is a deformation of SU(2).
Representation determined by three matrices.
The total "magnetization" matrix:

$$S^3_{[1,L]} = \sum_{x=1}^{L} S^3_x \,,$$

and the q-deformed total raising and lowering operators

$$S^+_{[1,L]} := \sum_{x=1}^{L} S^+_x \, q^{-2S^3_{[x+1,L]}} \,,$$

$$S^-_{[1,L]} := \sum_{x=1}^{L} q^{2S^3_{[1,x-1]}} \, S^-_x \,,$$

where $S^3_{[a,b]} := \sum_{x=a}^{b} S^3_x$.

Using the Symmetry

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

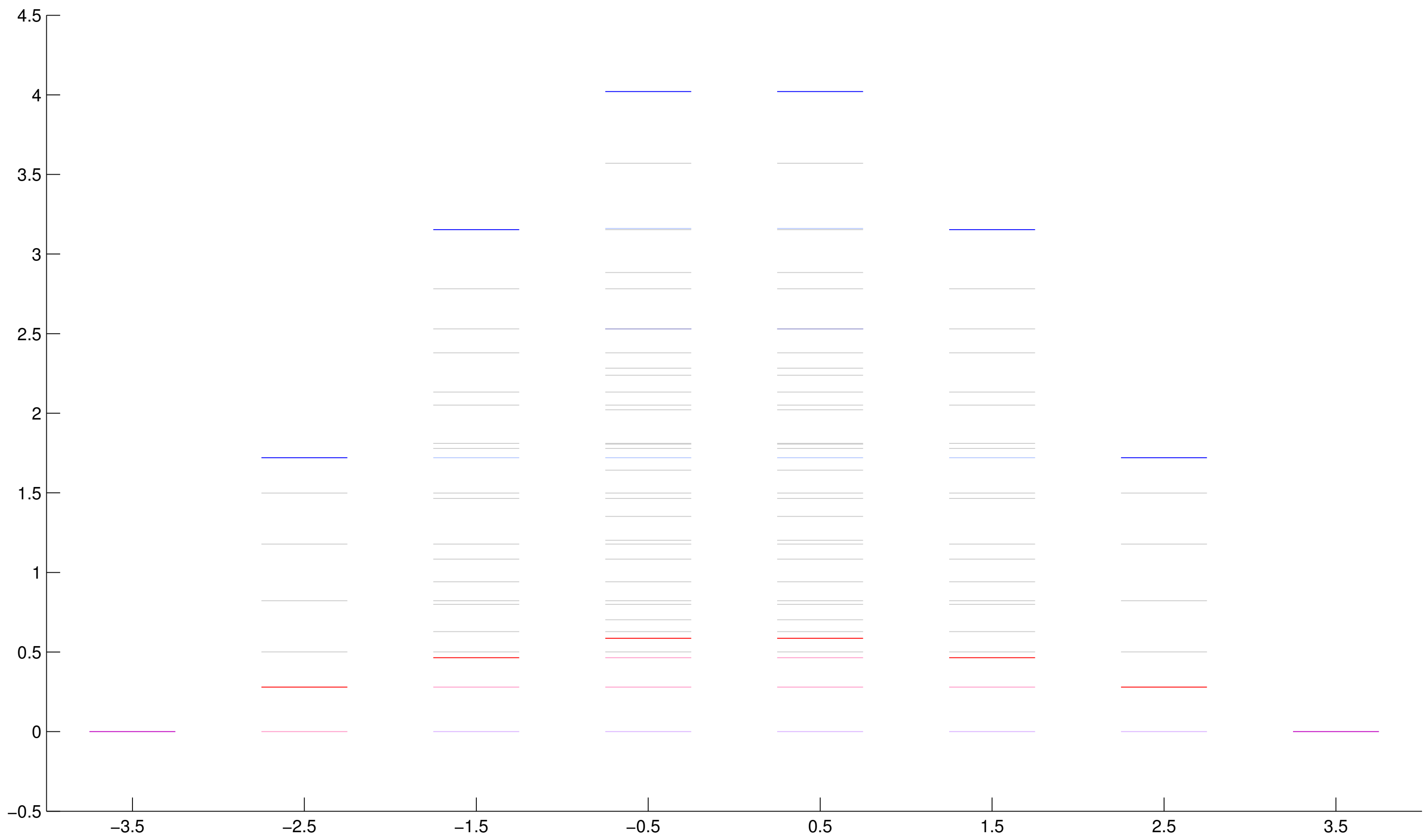
The spin lowering matrix maps $S^-_{[1,L]} : \mathcal{H}(n) \to \mathcal{H}(n+1)$.
Define $\mathcal{H}^{\mathrm{hw}}(0) = \mathcal{H}(0)$, and for $n = 1, \dots, \lfloor L/2 \rfloor$, define $\mathcal{H}^{\mathrm{hw}}(n)$ such that

$$\mathcal{H}(n) \;=\; \mathcal{H}^{\mathrm{hw}}(n) \oplus S^-_{[1,L]}\mathcal{H}(n-1)\,.$$

Then $\mathcal{H}^{\mathrm{hw}}(n)$ is the set of "highest weight vectors" for the representation of $\mathrm{SU}_q(2)$.

The highest weight subspaces are also invariant subspaces for H^{k}.

Numerical Diagonalization for $L = 7$ and $\Delta = 1.25$



Abscissa: $S^3_{[1,L]}$-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

$$E_L(n) \;=\; \min \mathrm{spec} \left(H^{\mathrm{k}} \restriction \mathcal{H}^{\mathrm{hw}}(n) \right) .$$

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

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

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_x^3 is $-1/2$ if there is a particle at site x and $+1/2$ otherwise;
- $S_x^+ : \mathcal{H}(n) \to \mathcal{H}(n-1)$ removes the particle at site x if one is present, and otherwise annihilates the vector;
- $S_x^- : \mathcal{H}(n) \to \mathcal{H}(n+1)$ places a particle at site x if one is not present, and otherwise annihilates the vector.

There is a densely defined, positive semidefinite operator

$$H_{\mathbb{Z}} = \sum_{x \in \mathbb{Z}} h_{x,x+1} = \sum_{x \in \mathbb{Z}} h^{\mathrm{k}}_{x,x+1} ,$$

defined in terms of the $S^{3,\pm}_x$ 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 $\mathrm{SU}_q(2)$ on $\mathcal{H}_{\mathbb{Z}}$.

Lemma For each $n \in \mathbb{N}$, define

$$E_{\mathbb{Z}}(n) := \inf \operatorname{spec} \left(H_{\mathbb{Z}} \restriction \mathcal{H}_{\mathbb{Z}}(n) \right) .$$

Then

$$E(n) = E_{\mathbb{Z}}(n) .$$

There is another symmetry of $H_{\mathbb{Z}} \restriction \mathcal{H}_{\mathbb{Z}}(n)$, shift-invariance.
Let $\tau : \mathcal{X}_n \to \mathcal{X}_n$ be the map $\tau(\boldsymbol{x}) = \boldsymbol{x} + (1, \ldots, 1)$.
Let $\mathcal{Y}_n = \{\boldsymbol{y} \in \mathcal{X}_n \,:\, 0 \le y_1 + \cdots + y_n \le n - 1\}$.
Then $\mathcal{Y}_n \cong \mathcal{X}_n/\tau$ in a natural way.

Define the shift operator

$$T\,\delta_{\boldsymbol{x}} \;=\; \delta_{\tau(\boldsymbol{x})}\,.$$

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

$$\|f\|^2 \;=\; \sum_{\boldsymbol{y} \in \mathcal{Y}_n} |f(\boldsymbol{y})|^2\,.$$

Direct Integral Decomposition

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

$$\mathcal{H}_{\mathbb{Z}}(n) = \ell^2(\mathcal{X}_n) \cong \int_{\mathbb{S}^1}^{\oplus} \ell_0^2(\mathcal{X}_n)\, \frac{d\theta}{2\pi}\,,$$

and

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

where $A_n(\theta)$ is the image of $H_{\mathbb{Z}}$ conjugated by appropriate (Bloch-type) transformations, restricted to $\ell_0^2(\mathcal{X}_n)$.

The operator $A_n(\theta)$ is the restriction to $\ell^2_0(\mathcal{X}_n)$ of an operator $\widetilde{A}_n(\theta)$ on all of $\ell(\mathcal{X}_n)$ defined through the kernel

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

where

$$\begin{aligned} K_n^{(0)}(\boldsymbol{x},\boldsymbol{y};\theta) \;&=\; \frac{1}{2}\,\delta_{\boldsymbol{y},\boldsymbol{x}} - \frac{1}{2\Delta}\,e^{i\theta}\,\delta_{\boldsymbol{y},\boldsymbol{x}-\boldsymbol{e}_1}\;, \\ K_n^{(n)}(\boldsymbol{x},\boldsymbol{y};\theta) \;&=\; \frac{1}{2}\,\delta_{\boldsymbol{y},\boldsymbol{x}} - \frac{1}{2\Delta}\,e^{-i\theta}\,\delta_{\boldsymbol{y},\boldsymbol{x}+\boldsymbol{e}_n}\;, \end{aligned}$$

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

$$\begin{aligned} K_n^{(k)}(\boldsymbol{x},\boldsymbol{y};\theta) \;&=\; \Big(1 - \delta_{x_{k+1},x_k+1}\Big)\,\delta_{\boldsymbol{y},\boldsymbol{x}} \\ &\quad - \frac{1}{2\Delta}\,\Big(e^{-i\theta}\,\delta_{\boldsymbol{y},\boldsymbol{x}+\boldsymbol{e}_k} + e^{i\theta}\,\delta_{\boldsymbol{y},\boldsymbol{x}-\boldsymbol{e}_{k+1}}\Big)\,. \end{aligned}$$

Each $A_n(\theta)$ is a self-adjoint operator on $\ell_0^2(\mathcal{X}_n)$, and the map $\theta \mapsto A_n(\theta)$ is norm-continuous. Therefore,

$$\inf \operatorname{spec} \Big(H_{\mathbb{Z}} \restriction \mathcal{H}_{\mathbb{Z}}(n) \Big) \;=\; \min_{\theta \in \mathbb{S}^1} \inf \operatorname{spec} A_n(\theta)\,.$$

But it is easy to see that the optimal θ is 0 because for any $f \in \ell_0^2(\mathcal{X}_n)$,

$$(f, A_n(\theta) f) \;\geq\; (|f|, A_n(0)|f|)\,.$$

One-binding Vectors for the Bethe Ansatz

Lemma Let $\mathbb{C}^\times = \mathbb{C} \setminus \{0\}$. Suppose that $\boldsymbol{\xi} \in (\mathbb{C}^\times)^n$ satisfies

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

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

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

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

$$E(\boldsymbol{\xi}) \;=\; \sum_{k=1}^{n} \left(1 - \frac{1}{2\Delta}\left[\xi_k + \xi_k^{-1}\right]\right) \,.$$

Proof. Define two kernels on $\mathbb{Z}^n$ <u>not $\mathcal{X}_n$</u> :

$$\widetilde{K}_n^1(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{k=1}^{n}\left(\delta_{\boldsymbol{y},\boldsymbol{x}} - \frac{1}{2\Delta}\left(\delta_{\boldsymbol{y},\boldsymbol{x}-\boldsymbol{e}_k} + \delta_{\boldsymbol{y},\boldsymbol{x}+\boldsymbol{e}_k}\right)\right),$$

$$\widetilde{K}_n^2(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{k=1}^{n-1}\delta_{y_{k+1},y_k+1}\left(\delta_{\boldsymbol{y},\boldsymbol{x}} - \frac{1}{2\Delta}\left(\delta_{\boldsymbol{y},\boldsymbol{x}-\boldsymbol{e}_k} + \delta_{\boldsymbol{y},\boldsymbol{x}+\boldsymbol{e}_{k+1}}\right)\right).$$

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

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

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 $\widetilde{A}_n(0)$.

The first kernel corresponds to the discrete Laplacian for n noninteracting particles. Its energy is just what was written in the lemma, $E(\boldsymbol{\xi})$. 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

$$\widetilde{K}^2_{n,k}(\boldsymbol{x}, \boldsymbol{y}) \;=\; \delta_{y_{k+1}, y_k+1} \left(\delta_{\boldsymbol{y},\boldsymbol{x}} - \frac{1}{2\Delta} \left(\delta_{\boldsymbol{y},\boldsymbol{x}-\boldsymbol{e}_k} + \delta_{\boldsymbol{y},\boldsymbol{x}+\boldsymbol{e}_{k+1}} \right) \right).$$

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

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

This requires

$$2\Delta\, \widetilde{f}_{\boldsymbol{\xi}}(\boldsymbol{y}) \;=\; \widetilde{f}_{\boldsymbol{\xi}}(\boldsymbol{y} + \boldsymbol{e}_k) + \widetilde{f}_{\boldsymbol{\xi}}(\boldsymbol{y} - \boldsymbol{e}_{k+1}),$$

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

$$2\Delta\, \xi_k^{y_k}\, \xi_{k+1}^{y_k+1} \;=\; \xi_k^{y_k+1}\, \xi_{k+1}^{y_k+1} + \xi_k^{y_k}\, \xi_{k+1}^{y_k}.$$

Dividing through by $\xi_k^{y_k}\, \xi_{k+1}^{y_k+1}$, gives precisely $\xi_k + \xi_{k+1}^{-1} = 2\Delta$.

Linear Fractional Recurrence Relation

By the lemma, we will have an eigenvector of $\widetilde{A}_n(0)$ in $\ell_0(\mathcal{X}_n)$ if we choose $\boldsymbol{\xi} \in (\mathbb{C}^x)^n$ 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)

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

Also, one can see that the ξ_k are strictly decreasing in k; therefore, the norm,

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

is finite. So $f_{\boldsymbol{\xi}}$ 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 $\inf \operatorname{spec} A_n(0)$ is equal to the eigenvalue for $f_{\boldsymbol{\xi}}$. 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 $f_{\boldsymbol{\xi}}(\boldsymbol{x}) = \prod_{k=1}^{n} \xi_k^{x_k}$ 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], Nacthergaele 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 $n \le \lfloor L/2 \rfloor$, define

$$E_L^{\text{cycl}}(n) \;=\; \min\operatorname{spec}\left(H_{[1,L]}^{\text{cycl}} \restriction \mathcal{H}_{[1,L]}(n)\right),$$
$$E_L^{\text{drop}}(n) \;=\; \min\operatorname{spec}\left(H_{[1,L]}^{\text{drop}} \restriction \mathcal{H}_{[1,L]}(n)\right).$$

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

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