The quench action approach to out-of-equilibrium quantum integrable models
Wouters, B.M.

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Spin content of the Néel state

In this section we compute the expectation value of the number of infinite rapidities in the Néel state. We use that for zero-magnetization states the average number of rapidities at infinity is related to the average total spin, where spin refers to the global $SU(2)$ symmetry.

D.1 Global spin operators

It is well known that the spin-1/2 XXX Hamiltonian ($\Delta = 1$) exhibits a global $SU(2)$ symmetry. Let us consider the global $SU(2)$ operators (here and in the following we choose $N$ even, such that zero magnetization states are always possible)

$$S^\alpha = \sum_{j=1}^{N} s_j^\alpha, \quad \text{for} \quad \alpha = x, y, z, +, - .$$

The operators $s_j^\alpha = \sigma_j^\alpha / 2$ represent the local spin degrees of freedom and act locally as $SU(2)$ operators. They have the usual commutation relations

$$[s_j^\alpha, s_k^\beta] = i \delta_{jk} \epsilon_{\alpha\beta\gamma} s_k^\gamma \quad \text{for} \quad \alpha, \beta, \gamma \in \{x, y, z\}$$

where $\epsilon_{\alpha\beta\gamma}$ is the total anti-symmetric epsilon tensor. Using the definitions $s_j^\pm = s_j^x \pm i s_j^y$ these commutation relations transform into $[s_j^x, s_k^\pm] = \pm \delta_{jk} s_k^\pm$ and $[s_j^y, s_k^-] = 2 \delta_{jk} s_k^x$. Similar relations hold for the global operators,

$$[S^x, S^\pm] = \pm S^\pm \quad \text{and} \quad [S^+, S^-] = 2S^z .$$

The total spin operator

$$S^2 \equiv \vec{S}^2 = \sum_{\alpha=x,y,z} S^\alpha S^\alpha = \frac{1}{2} \left( S^+ S^- + S^- S^+ \right) + (S^z)^2 = S^+ S^- - S^z + (S^z)^2$$

(D.4)
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is a central element of $SU(2)$, i.e., $[S^2, S^\alpha] = 0$ for all $\alpha = x, y, z, +, -$.

The Hilbert space of the XXX chain is given by an $N$-fold tensor product of local spin-1/2 $SU(2)$ representation spaces. Due to the global $SU(2)$ symmetry, we can choose simultaneous eigenstates of $S^z$ and $S^2$ with eigenvalues $s^z$ and $s(s+1)$, respectively, as an orthonormal basis of the Hilbert space. The eigenstates are denoted by $|s, s^z, a\rangle$, where the integer values $s$, $s^z$, and $a$ are restricted by $0 \leq s \leq N/2$, $-s \leq s^z \leq s$, and $1 \leq a \leq A_N(s)$. Here, $A_N(s)$ is the number of $(2s+1)$-multiplets in the $N$-fold tensor product of $SU(2)$ spin-1/2 representations,

$$A_N(s) = \left( \frac{N}{2} - s \right) - \left( \frac{N}{2} - s - 1 \right).$$  

(D.5)

The Bethe states, which are constructed as eigenstates of the operator $S^z$, form multiplets of the global $SU(2)$ symmetry. A highest-weight state $|s, s, a\rangle$ is a Bethe state with $N/2 - s$ finite rapidities and zero rapidities at infinity. Other states of the multiplet, with $s^z < s$, are constructed by repeatedly applying $(s-s^z)$ times the total spin-lowering operator $S^-$ to the highest-weight state. This operator can be interpreted as the creation of a magnon with zero momentum, corresponding to a rapidity at infinity, see Eq. (2.55). Infinite rapidities decouple from the Bethe equations and the newly obtained state remains an eigenstate of the Hamiltonian. A generic state $|s, s^z, a\rangle$ can therefore be seen as a Bethe state with $N/2 - s$ finite rapidities, supplemented by $s - s^z$ infinite rapidities.

Let us define the operator $\hat{N}_\infty$, counting the number of infinite rapidities, i.e., $\hat{N}_\infty|s, s^z, a\rangle = (s - s^z)|s, s^z, a\rangle$. Note that $\hat{N}_\infty$ is a conserved quantity. We are interested in the expectation value of the number of infinite rapidities on the Néel state. For a generic zero-magnetization state $|\psi\rangle$ we easily find

$$\langle \psi | \hat{N}_\infty | \psi \rangle = \sum_{s=0}^{N/2} \sum_{a=1}^{A_N(s)} |\langle \psi |s, 0, a\rangle|^2 = \sum_{s=0}^{N/2} s C_s,$$

where $C_s$ can be interpreted as a measure of how much overlap the state $|\psi\rangle$ has with the total spin-$s$ sector.

To find this “spin content” of a generic state, define the function $f_N$ as the Fourier transform of the coefficient $C_s$,

$$f_N(x) = \sum_{s=0}^{N/2} C_s e^{2s(s+1)x/N}.$$  

(D.7)

The inverse transformation exists and yields

$$\frac{2}{i\pi N} \int_{0}^{i\pi N/2} \text{d}x \ f_N(x) e^{-2i(t+1)x/N} = \ldots.$$
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\[ \ldots = \sum_{s=0}^{N/2} C_s \left( \frac{2}{i \pi N} \int_0^{i \pi/2} dx \, e^{2is(s+1)-t(t+1)\frac{x}{N}} \right) = C_t, \]  

where we used that \([s(s + 1) - t(t + 1)] = 0\) if and only if \(s = t\) for nonnegative integers \(s\) and \(t\). The coefficient \(C_s\) is thus determined by the function \(f_N\), which can be expressed by its Taylor series around \(x = 0\),

\[ f_N(x) = \sum_{n=0}^{\infty} \frac{1}{n!} f_N^{(n)}(0)x^n = \sum_{n=0}^{N/2} \frac{1}{n!} \sum_{s=0}^{N/2} C_s s^n(s+1)^n \left( \frac{2x}{N} \right)^n \]

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\[ = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \frac{2x}{N} \right)^n \langle \psi | (S^+ S^-)^n | \psi \rangle. \]

For the last equality, we used Eq. (D.4), the zero-magnetization property and the following expression for the expectation value of the total-spin operator

\[ \langle \psi | (S^2)^n | \psi \rangle = \sum_{s=0}^{N/2} s^n(s+1)^n \sum_{a=1}^{A_N(s)} |\langle \psi | s, 0, a \rangle|^2 = \sum_{s=0}^{N/2} s^n(s+1)^n C_s. \]

It is convenient to bring the operators \(S^+\) and \(S^-\) of the product \((S^+ S^-)^n\) in an appropriate order,

\[ \langle \psi | (S^+ S^-)^n | \psi \rangle = \sum_{m=0}^{n} c_m^{(n)} \langle \psi | (S^+)^m (S^-)^m | \psi \rangle. \]

As shown in D.3, the coefficients \(c_m^{(n)}\) are Legendre-Stirling numbers and given by

\[ c_0^{(0)} = 1, \quad c_m^{(n)} = \sum_{r=1}^{m} \frac{(-1)^{r+m}(2r+1) r^n(r+1)^n}{(m+r+1)!(m-r)!} \]

for \(n \geq 1\). Furthermore, the expectation values of the operator \((S^+ S^-)^m\) on an arbitrary zero-magnetization state cannot be evaluated in general. However, let us focus on a special class of states that can be expressed in the local spin basis as a single product of local spin lowering operators acting on the fully-polarized state (e.g. the Néel state),

\[ |\psi\rangle = |\{n_j\}_{j=1}^{N/2} \rangle = \prod_{j=1}^{N/2} s_{n_j}^{-}\uparrow^{\otimes N}. \]

The integers \(\{n_j\}_{j=1}^{N/2}\) with \(1 \leq n_1 < \ldots < n_{N/2} \leq N\) label the positions of the downspins. One easily finds

\[ \langle \psi | (S^+)^m (S^-)^m | \psi \rangle = \langle \{n_j\}_{j=1}^{N/2} | (S^+)^m (S^-)^m | \{n_j\}_{j=1}^{N/2} \rangle = (m!)^2 \binom{N/2}{m}. \]
Plugging Eqs (D.12) and (D.14) into Eq. (D.9), we eventually obtain

$$f_N(x) = c_0^{(0)} + \sum_{n=1}^{\infty} \sum_{m=1}^{n} \frac{(m!)^2}{n!} \left( \frac{N/2}{m} \right) \sum_{r=1}^{m} \frac{(-1)^{r+m}(2r+1)r^n(r+1)^n}{(m+r+1)!(m-r)!} \left( \frac{2x}{N} \right)^n$$

$$= 1 + \sum_{m=1}^{N/2} \sum_{r=1}^{m} \frac{(m!)^2}{(m+r+1)!(m-r)!} \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{2r(r+1)x}{N} \right)^n$$

We used that $c_m^{(n)} = 0$ if $m = 0$ or $m > n$, as can be seen from Eq. (D.12). Using now the inverse Fourier transform (D.8) we can read off the coefficients $C_s$. They are given by

$$C_s = \sum_{m=s}^{N/2} \left( \frac{N/2}{m} \right) \frac{(-1)^{s+m}(m!)^2(2s+1)}{(m+s+1)!(m-s)!} = \frac{(2s+1)(N/2)!^2}{(N/2-s)!(N/2+s+1)!} = \frac{A_N(s)}{N/2}.$$  

(D.15)

The fact that $C_s$ is directly proportional to $A_N(s)$, the number of all zero-magnetization states in a fixed $s$-sector, is remarkable. It means that the average overlap squared is the same ($= (N/2)!^2/N!$) for each sector. Therefore, one cannot argue that overlaps with higher $s$, i.e., with more rapidities at infinity, $N_\infty = s$, decrease with increasing $s$. Only the number of zero-magnetization states $A_N(s)$ per $s$-sector decreases with increasing $s$ for sufficiently large $s$.

**D.2 Limit of large number of lattice sites**

The formula for $C_s$, which is a measure of how much spin $s$ is contained in a zero-magnetization state of the form (D.13) and which is directly proportional to the number $A_N(s)$ of $(2s+1)$-multiplets for a given $N$, can be further analyzed in the limit of large lattice site $N$.

In the limit $N \to \infty$ we use Stirling’s formula to manipulate Eq. (D.16). After a straightforward calculation one obtains the scaling of the coefficient $C_s$ with large $N$,

$$C_s \sim \frac{2(2s+1)}{N} e^{-2s(s+1)/N}.$$  

(D.17)

This function has a maximum at $s_0 = (\sqrt{N} - 1)/2 \sim \sqrt{N}/2$ or, to be more precise, at the integer which lies as close as possible to this generally irrational
number. Furthermore, the expectation value of the number of infinite rapidities can be computed analytically,

\[
\langle \psi | \hat{N}_\infty | \psi \rangle = \sum_{s=0}^{N/2} s C_s = \frac{1}{2} \left( \frac{2^N (N/2)!^2}{N!} - 1 \right). \tag{D.18}
\]

Using Stirling’s formula one finds that

\[
\lim_{N \to \infty} \frac{\langle \psi | \hat{N}_\infty | \psi \rangle}{\sqrt{N}} = \sqrt{\frac{\pi}{8}}. \tag{D.19}
\]

In the thermodynamic limit, the number of infinite rapidities of the steady state is negligible compared to the total number of rapidities, \(n_\infty = \lim_{N \to \infty} N_\infty / N = 0\). This serves as additional evidence for the correctness of the application of the quench action approach to the Néel-to-XXX quench.

### D.3 Legendre-Stirling numbers of the second kind

The coefficients \(c_m^{(n)}\) appear in the reordering of operators \(S^\pm\) in the product \((S^+ S^-)^n\) to get terms like \((S^+)^m (S^-)^m\), see Eq. (D.11). Since we consider this inside expectation values \(\langle \cdot \rangle\) of zero-magnetization states and since for these states

\[
\langle S^+ S^- (S^+)^m (S^-)^m \rangle = \left( (S^+)^{m+1} (S^-)^{m+1} \right) + (2 + 4 + \ldots + 2m) \langle (S^+)^m (S^-)^m \rangle \tag{D.20}
\]

we obtain the relations \((c_m^{(n)} := 0 \text{ for } m > n \text{ or } m < 0)\)

\[
c_0^{(0)} = 1, \quad c_m^{(n+1)} = m(m+1)c_m^{(n)} + c_{m-1}^{(n)} \quad \text{for} \quad 0 \leq m \leq n+1, \quad n \geq 0. \tag{D.22a}
\]

These recursion relations define the triangle of Legendre-Stirling numbers of second kind, which have an explicit representation for \(n \geq 1\),

\[
c_m^{(n)} = \sum_{r=1}^{m} \frac{(-1)^r + m(2r + 1)r^n(r + 1)^n}{(m + r + 1)!(m - r)!}. \tag{D.23}
\]