The quench action approach to out-of-equilibrium quantum integrable models

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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)

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

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

$$[s_j^\alpha, s_k^\beta] = i\delta_{jk}\epsilon_{\alpha\beta\gamma}s_k^\gamma \qquad \text{for} \quad \alpha, \beta, \gamma \in \{x, y, z\} \tag{D.2}$$

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 $[s_j^z, s_k^\pm] = \pm\delta_{jk}s_k^\pm$ and $[s_j^+, s_k^-] = 2\delta_{jk}s_k^z$. Similar relations hold for the global operators,

$$[S^z, S^\pm] = \pm S^\pm \qquad \text{and} \qquad [S^+, S^-] = 2S^z \,. \tag{D.3}$$

The total spin operator

$$S^2 \equiv \vec{S}^2 = \sum_{\alpha=x,y,z} S^\alpha S^\alpha = \frac{1}{2}\left(S^+S^- + S^-S^+\right) + (S^z)^2 = S^+S^- - S^z + (S^z)^2 \tag{D.4}$$

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,

$$A_N(s) = \binom{N}{\frac{N}{2} - s} - \binom{N}{\frac{N}{2} - s - 1} . \tag{D.5}$$

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

$$\langle\psi|\hat{N}_\infty|\psi\rangle = \sum_{s=0}^{N/2} s \sum_{a=1}^{A_N(s)} |\langle\psi|s, 0, a\rangle|^2 = \sum_{s=0}^{N/2} s\, C_s , \tag{D.6}$$

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,

$$f_N(x) = \sum_{s=0}^{N/2} C_s e^{2s(s+1)x/N} . \tag{D.7}$$

The inverse transformation exists and yields

$$\frac{2}{i\pi N} \int_0^{i\pi N/2} \mathrm{d}x\, f_N(x) e^{-2t(t+1)x/N} = \dots$$

$$\ldots = \sum_{s=0}^{N/2} C_s \left(\frac{2}{i\pi N} \int_0^{i\pi N/2} \mathrm{d}x\, e^{2[s(s+1)-t(t+1)]x/N} \right) = C_t \,, \qquad \text{(D.8)}$$

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 $x = 0$,

$$\begin{aligned} f_N(x) &= \sum_{n=0}^{\infty} \frac{1}{n!} f_N^{(n)}(0) x^n = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{s=0}^{N/2} C_s s^n (s+1)^n \left(\frac{2x}{N}\right)^n \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{2x}{N}\right)^n \langle\psi| \left(S^+S^-\right)^n |\psi\rangle \,. \end{aligned} \qquad \text{(D.9)}$$

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

$$\langle\psi| \left(S^2\right)^n |\psi\rangle = \sum_{s=0}^{N/2} s^n (s+1)^n \sum_{a=1}^{A_N(s)} |\langle\psi|s,0,a\rangle|^2 = \sum_{s=0}^{N/2} s^n (s+1)^n C_s \,. \qquad \text{(D.10)}$$

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

$$\langle\psi| \left(S^+S^-\right)^n |\psi\rangle = \sum_{m=0}^{n} c_m^{(n)} \langle\psi| \left(S^+\right)^m \left(S^-\right)^m |\psi\rangle \,. \qquad \text{(D.11)}$$

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

$$c_0^{(0)} = 1, \qquad c_m^{(n)} = \sum_{r=1}^{m} \frac{(-1)^{r+m}(2r+1) r^n (r+1)^n}{(m+r+1)!(m-r)!} \qquad \text{(D.12)}$$

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),

$$|\psi\rangle = |\{n_j\}_{j=1}^{N/2}\rangle = \prod_{j=1}^{N/2} s_{n_j}^- \, |\uparrow\rangle^{\otimes N} \,. \qquad \text{(D.13)}$$

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

$$\langle\psi| \left(S^+\right)^m \left(S^-\right)^m |\psi\rangle = \langle\{n_j\}_{j=1}^{N/2}| \left(S^+\right)^m \left(S^-\right)^m |\{n_j\}_{j=1}^{N/2}\rangle = (m!)^2 \binom{N/2}{m} \,.$$

(D.14)

Plugging Eqs (D.12) and (D.14) into Eq. (D.9), we eventually obtain

$$\begin{aligned} f_N(x) & \\ &= c_0^{(0)} + \sum_{n=1}^{\infty} \sum_{m=1}^{n} \frac{(m!)^2}{n!} \binom{N/2}{m} \sum_{r=1}^{m} \frac{(-1)^{r+m}(2r+1)r^n(r+1)^n}{(m+r+1)!(m-r)!} \left(\frac{2x}{N}\right)^n \\ &= 1 + \sum_{m=1}^{N/2} \sum_{r=1}^{m} (m!)^2 \binom{N/2}{m} \frac{(-1)^{r+m}(2r+1)}{(m+r+1)!(m-r)!} \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{2r(r+1)x}{N}\right)^n \\ &= 1 + \sum_{m=1}^{N/2} \sum_{r=1}^{m} \binom{N/2}{m} \frac{(-1)^{r+m}(m!)^2(2r+1)}{(m+r+1)!(m-r)!} \left(e^{2r(r+1)x/N} - 1\right) . \qquad \text{(D.15)} \end{aligned}$$

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

$$C_s = \sum_{m=s}^{N/2} \binom{N/2}{m} \frac{(-1)^{s+m}(m!)^2(2s+1)}{(m+s+1)!(m-s)!} = \frac{(2s+1)\ (N/2)!^2}{(N/2-s)!(N/2+s+1)!} = \frac{A_N(s)}{\binom{N}{N/2}} . \qquad \text{(D.16)}$$

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,

$$C_s \sim \frac{2(2s+1)}{N} e^{-2s(s+1)/N} . \qquad \text{(D.17)}$$

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

$$\begin{aligned}
&\left\langle S^+S^- \left(S^+\right)^m \left(S^-\right)^m\right\rangle \\
&= \left\langle \left(S^+\right)^{m+1} \left(S^-\right)^{m+1}\right\rangle + (2+4+\ldots+2m)\left\langle \left(S^+\right)^m \left(S^-\right)^m\right\rangle && \text{(D.20)}\\
&= \left\langle \left(S^+\right)^{m+1} \left(S^-\right)^{m+1}\right\rangle + m(m+1)\left\langle \left(S^+\right)^m \left(S^-\right)^m\right\rangle , && \text{(D.21)}
\end{aligned}$$

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

$$c_0^{(0)} = 1 , \qquad c_m^{(n+1)} = m(m+1)c_m^{(n)} + c_{m-1}^{(n)} \qquad \text{for} \quad 0 \le m \le n+1 , \quad n \ge 0 . \tag{D.22a}$$

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

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