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

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# E

## Density operator for Néel-to-XXZ

Analogous to what we did in Section 7.2.1, we would like to construct a statistical density operator in terms of transfer matrices that describes the equilibrium of local observables after the Néel-to-XXZ quench. For this purpose, one must manually restrict the sums in Eq. (7.3) to Bethe states that are parity invariant and have zero magnetization, since only these states have nonzero overlaps with the Néel initial state. As already explained, these restrictions are mild and one is still left with a huge number of states out of which the density operator should select precisely the ensemble that describes the postquench equilibrium.

The Bethe state eigenvalues of the transfer matrix for the spin-1/2 XXZ model are given in Eq. (2.70). For convenience, here we use a definition of the transfer matrix that differs by an unimportant overall factor. The eigenvalues on a Bethe state  $|\lambda\rangle$  of  $M$  down spins are  $\tau(\mu, \lambda) = \tau_+(\mu, \lambda) + \tau_-(\mu, \lambda)$ , with

$$\tau_{\pm}(\mu, \lambda) = \left[ \sin\left(\mu \pm \frac{i\eta}{2}\right) \right]^N \prod_{j=1}^M \frac{\sin(\mu - \lambda_j \mp i\eta)}{\sin(\mu - \lambda_j)}. \quad (\text{E.1})$$

In analogy to Eq. (7.5), one can define a quantity  $\Theta_{\text{Néel}}$  in terms of  $\tau_+$  that, up to an irrelevant overall factor, reproduces the thermodynamically dominant part of the Néel-to-XXZ overlaps [Eqs (5.20)] when the cutoff  $w$  is sent to infinity,

$$\Theta_{\text{Néel}}(w, \tilde{\lambda}) = \prod_{m=1}^w \frac{\tau_+\left(\frac{i\eta}{2}(1+2m), \tilde{\lambda}\right)}{\tau_+\left(\frac{i\eta}{2}(1+2m) + \frac{\pi}{2}, \tilde{\lambda}\right) \tau_+(i\eta m, \tilde{\lambda}) \tau_+\left(i\eta m + \frac{\pi}{2}, \tilde{\lambda}\right)} \quad (\text{E.2a})$$

$$\sim \prod_{j=1}^{M/2} \frac{\tan(\lambda_j + \frac{i\eta}{2}) \tan(\lambda_j - \frac{i\eta}{2})}{16 \sin^2(\lambda_j) \cos^2(\lambda_j)} + O\left(\frac{1}{\eta w}\right). \quad (\text{E.2b})$$

The eigenvalues of the density operator in Eq. (7.3) must then effectively be given by  $\varrho_{\text{Néel}}(\tilde{\lambda}) = \langle \tilde{\lambda} | \hat{\varrho}_{\text{Néel}} | \tilde{\lambda} \rangle = \lim_{w \rightarrow \infty} \lim_{\text{th}} |\Theta_{\text{Néel}}(w, \tilde{\lambda})|$ . By ‘effectively’ we mean that in the thermodynamic limit this is the dominant contribution to the sums in Eq. (7.3).

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It is important to note that one is required to impose the absolute value, because unlike the Lieb-Liniger case  $\Theta_{\text{Néel}}(w, \tilde{\lambda})$  is not positive for all parity-invariant Bethe states. In particular, states with strings centered at zero could lead to negative values. For example, consider a subset of four rapidities of the Bethe state that form a rectangle of two 2-strings in the plane of rapidities:  $\{\alpha + i\eta, \alpha - i\eta, -\alpha - i\eta, -\alpha + i\eta\} \subset \tilde{\lambda}$  with  $\alpha > 0$  and for simplicity no string deviations. Their contributing factor to  $\tau_+(iy, \tilde{\lambda})$  is given by

$$\tau_+(iy, \tilde{\lambda}) \sim \left| \frac{\sinh^2(y - \eta) - \sin^2(\alpha + i\eta)}{\sinh^2(y) - \sin^2(\alpha + i\eta)} \right|^2 > 0, \quad (\text{E.3a})$$

for all  $y > 0$ . Replacing them by a ‘diamond’ of a single 2-string and two 1-strings ( $\{\alpha, -\alpha, i\eta, -i\eta\}$ ) leads to a factor

$$\tau_+(iy, \tilde{\lambda}) \sim \frac{\sinh^2(y - \eta) - \sinh^2(\eta)}{\sinh^2(y) - \sinh^2(\eta)} \frac{\sinh^2(y - \eta) + \sin^2(\alpha)}{\sinh^2(y) + \sin^2(\alpha)}, \quad (\text{E.3b})$$

which is positive when  $0 < y < \eta$  or  $y > 2\eta$  and negative if  $\eta < y < 2\eta$ .

To make the transition from eigenvalues of the density operator to an actual operator, as we did for the Lieb-Liniger quench, two steps must be taken. First, one must make sense of an operator that has an absolute value as eigenvalues. Second, one must argue that instead of  $\tau_+$  one can use the full eigenvalues of the transfer matrix. We will now show that both steps encounter substantial problems.

To solve the first problem, one could try to write the density matrix as

$$\hat{\rho}_{\text{Néel}} = \lim_{w \rightarrow \infty} \lim_{\text{th}} \sum_{\tilde{\lambda}} \frac{|\tilde{\lambda}\rangle\langle\tilde{\lambda}|}{|\Theta_{\text{Néel}}(w, \tilde{\lambda})|} (\Theta_{\text{Néel}}(w, \tilde{\lambda}))^2 \quad (\text{E.4})$$

and replace  $\Theta_{\text{Néel}}(w, \tilde{\lambda})$  under the square by its corresponding operator when it is inserted in Eq. (7.3). However, the result still contains a projector onto Bethe states, which makes this solution unsatisfactory. As a projector onto the Bethe states we know what the density matrix is; up to an overall factor it should reproduce the overlaps. What we are ultimately looking for is a formulation of the density matrix in terms of local spin operators, independent of the Bethe basis.

Another approach to get rid of the absolute values is to restrict the sums in Eq. (7.3) to states for which  $\Theta_{\text{Néel}}(w, \tilde{\lambda}) \geq 0$ , as if they are representative states of a larger group of states. The other states can be accounted for via an entropic weight, which ends up in the Yang-Yang entropy. This is exactly what we did in Chapters 4 and 5 in the derivation of the GTBA equation(s) and why we demanded smooth observables and overlaps. This time the representative-state approach would be valid if  $\Theta_{\text{Néel}}(w, \tilde{\lambda})$  is a smooth function, i.e. if small changes in the configuration of rapidities would alter the value of  $\Theta_{\text{Néel}}(w, \tilde{\lambda})$  only

subleading in system size. We have just seen however that by replacing two 2-strings by a diamond of rapidities, the sign of  $\Theta_{\text{Néel}}(w, \tilde{\lambda})$  could flip. The function is not smooth and getting rid of the absolute value by means of representative states is not allowed.

In fact, this problem is a direct consequence of the fact that the transfer matrix as an operator is nonsmooth [see Eq. (3.13)]. This is the first time that we encounter a nonsmooth operator and in the next section we will illustrate this property by considering the transfer matrix in the Néel-to-XXZ quench.

Even if making sense of the absolute value is possible, there remains the problem of replacing  $\tau_+(\mu, \lambda)$  by  $\tau_+(\mu, \lambda) + \tau_-(\mu, \lambda)$ , in order to interpret it as an operator. As was shown in Section 7, for the BEC-to-LL quench this is possible since the saddle point of the term with only  $\tau_+$  elements is dominant in the thermodynamic limit. Now however there also appear  $\tau_+$  factors in the denominator [see Eqs (E.2)]. It can be shown that these cannot effectively be replaced by the full eigenvalues of the transfer matrix. We conclude that the method we used for the Lieb-Liniger quench to write the statistical density matrix in terms of the transfer matrix, is not applicable to the Néel-to-XXZ quench.

## E.1 A nonsmooth operator: the transfer matrix

In this section we use the QA approach to compute the expectation value of the transfer matrix  $\hat{\tau}(iy)$ , for  $y > 0$ , at late times after the Néel-to-XXZ quench. As we will see, this serves as a first instructive example of a nonsmooth operator and a breakdown of the QA approach due to this nonsmoothness.

Since it is a highly nonlocal operator, its eigenvalues generally diverge exponentially with system size. Instead of the expectation value of  $\hat{\tau}(iy)$ , we therefore would like to compute the quantity  $F_{\psi_0}^{\hat{\tau}}(y, t) = \lim_{t \rightarrow \infty} \frac{1}{N} \log \langle \psi_0(t) | \hat{\tau}(iy) | \psi_0(t) \rangle$  in the limit  $t \rightarrow \infty$ . The initial state  $|\psi_0(0)\rangle$  is the usual zero-momentum Néel state that we studied in Chapter 5. As the transfer matrix commutes with the Hamiltonian, it is a conserved quantity. The formalism of the algebraic Bethe Ansatz gives the transfer matrix in terms of Lax operators [see Eqs (2.68)], which can be used to compute it on the initial state. At finite size one obtains

$$\begin{aligned} \langle \uparrow \downarrow \uparrow \dots | \hat{\tau}(\mu) | \uparrow \downarrow \uparrow \dots \rangle &= \langle \downarrow \uparrow \downarrow \dots | \hat{\tau}(\mu) | \downarrow \uparrow \downarrow \dots \rangle \\ &= 2 \left[ \sin \left( \mu + \frac{i\eta}{2} \right) \sin \left( \mu - \frac{i\eta}{2} \right) \right]^{N/2}, \end{aligned} \quad (\text{E.5})$$

$$\langle \uparrow \downarrow \uparrow \dots | \hat{\tau}(\mu) | \downarrow \uparrow \downarrow \dots \rangle = \langle \downarrow \uparrow \downarrow \dots | \hat{\tau}(\mu) | \uparrow \downarrow \uparrow \dots \rangle = \sinh^N(\eta), \quad (\text{E.6})$$

implying that on the zero-momentum initial state

$$F_{\text{Néel}}^{\hat{\tau}}(y, 0) = \begin{cases} \log[\sinh(\eta)], & 0 < y < y_\star, \\ \frac{1}{2} \log \left[ \sinh \left( y + \frac{\eta}{2} \right) \sinh \left( y - \frac{\eta}{2} \right) \right], & y > y_\star. \end{cases} \quad (\text{E.7a})$$

At  $y$ -value

$$y_\star = \sinh^{-1} \left( \sinh(\eta/2) \sqrt{1 + 4 \cosh^2(\eta/2)} \right) \quad (\text{E.7b})$$

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the expectation value has a cusp.

Let us now turn to late times and apply the QA approach to the transfer matrix. Unlike local observables, the eigenvalues of the transfer matrix contain a factor that is exponentially in system size. This factor deforms the usual saddle point of the Néel-to-XXZ quench [see Section 5.5], because the GTBA equations receive an extra driving term. For the  $\tau_+$  part of the transfer matrix the GTBA equations are of the same form as Eqs (5.27), but with different driving terms  $g_n(\lambda) = g_{0,n}(\lambda) + g_{\tau_+,n}(\lambda)$ . The terms  $g_{0,n}$  are the original driving terms given in Eqs (5.25), whereas the terms coming from  $\tau_+$  are given by

$$g_{\tau_+,n}(\lambda) = -\log \left[ \frac{\sinh^2 \left( y - \frac{\eta}{2}(n+1) \right) + \sin^2(\lambda)}{\sinh^2 \left( y + \frac{\eta}{2}(n-1) \right) + \sin^2(\lambda)} \right], \quad (\text{E.8})$$

which can be derived from Eq. (E.1) using the string hypothesis.

The partially decoupled GTBA equations [see Section 5.4.2] get driving terms  $\tilde{d}_n(\lambda) = \tilde{d}_{0,n}(\lambda) + \tilde{d}_{\tau_+,n}(\lambda)$ . The new part of the driving terms can be expressed in terms of the function  $f_\beta(\lambda) = \log(\sin^2(\lambda) + \sinh^2(\beta))$  and we use that  $a_n * f_\beta(\lambda) = f_{n\eta/2+|\beta|}(\lambda) - n\eta$ . For  $0 < 2y \leq \eta$ ,

$$\tilde{d}_{\tau_+,1} = f_y - f_{\eta-y}, \quad (\text{E.9a})$$

$$\tilde{d}_{\tau_+,n} = 0, \quad n > 1, \quad (\text{E.9b})$$

and for  $\eta < 2y$ ,

$$\tilde{d}_{\tau_+,n} = 0, \quad n \leq \lfloor 2y/\eta \rfloor - 2, \quad (\text{E.9c})$$

$$\tilde{d}_{\tau_+,n} = f_{y-\frac{\eta}{2}(n+3)} - f_{y-\frac{\eta}{2}(n+1)}, \quad \lfloor 2y/\eta \rfloor - 2 < n \leq \lfloor 2y/\eta \rfloor - 1, \quad (\text{E.9d})$$

$$\tilde{d}_{\tau_+,n} = f_{y-\frac{\eta}{2}(n-1)} - f_{y-\frac{\eta}{2}(n+1)}, \quad \lfloor 2y/\eta \rfloor - 1 < n \leq \lfloor 2y/\eta \rfloor, \quad (\text{E.9e})$$

$$\tilde{d}_{\tau_+,n} = 0, \quad \lfloor 2y/\eta \rfloor < n, \quad (\text{E.9f})$$

where  $\lambda$  dependence was suppressed. Note that the driving terms have a divergence at  $\lambda = 0$  for special values of  $y$ . For  $y = 0$  there is a divergence in  $\tilde{d}_{\tau_+,1}$ , leading to  $\eta_1(\lambda = 0) = 0$ . For  $y = m\eta/2$ , where  $m \geq 2$  is an integer, there is a divergence in  $\tilde{d}_{\tau_+,m-1}$  leading to  $\eta_{m-1}(\lambda = 0) = +\infty$ .

Using the resulting  $y$ -dependent saddle point  $\rho_{(y)}^{\text{sp}}$  one can compute  $F_{\text{Néel}}^{\hat{\tau}}(y, \infty)$  and compare it with  $F_{\text{Néel}}^{\hat{\tau}}(y, 0)$ , as is done in Fig. E.1. The saddle-point prediction has a cusp at  $y = \eta$ , coming from the divergence of the driving term  $\tilde{d}_{\tau_+,1}$ . One finds perfect agreement for  $0 < y < \eta$  and disagreement for  $y > \eta$ . The latter can be attributed to the nonsmoothness of the transfer matrix, which was illustrated earlier by showing that a diamond of rapidities can lead to negative eigenvalues. This nonsmoothness renders the quench action method inapplicable.

The exponential part of  $\tau_-$  in Eq. (E.1) can be computed likewise. As in Section. 7.2.1, the result is always smaller than the  $\tau_+$  result. The  $\tau_-$  term is thus exponentially suppressed and can be neglected in the thermodynamic limit.

Repeating the procedure for  $\hat{\tau}^2$  instead of  $\hat{\tau}$  is easy, as the extra driving terms simply get doubled:  $\tilde{d}_{\tau_+,n}^2 = 2\tilde{d}_{\tau_+,n}$ . Again, the  $\tau_-$  terms can be neglected. Since the eigenvalues of  $\hat{\tau}^2$  on Bethe states are never negative, the operator is smooth and the QA logic can be applied. On the initial state one finds

$$F_{\text{Néel}}^{\hat{\tau}^2}(y, 0) = \frac{1}{2} \log \left( \frac{1}{2} [\cosh(\eta) - \cosh(2y)]^2 + \sinh^4(\eta) + \dots \right. \quad (\text{E.10}) \\ \left. \dots + \sinh^2(\eta) \sqrt{\sinh^4(\eta) + [\cosh(\eta) - \cosh(2y)]^2} \right) - \frac{1}{2} \log(2),$$

which is compared with the late-time result in Fig. E.1. As expected, the agreement is perfect for all values  $y > 0$ . Note that there is no cusp in the saddle-point result at  $y = \eta$ . This is nontrivial, since the driving term  $\tilde{d}_{\tau_+,1}^2$  still has a divergence at  $\lambda = 0$ .

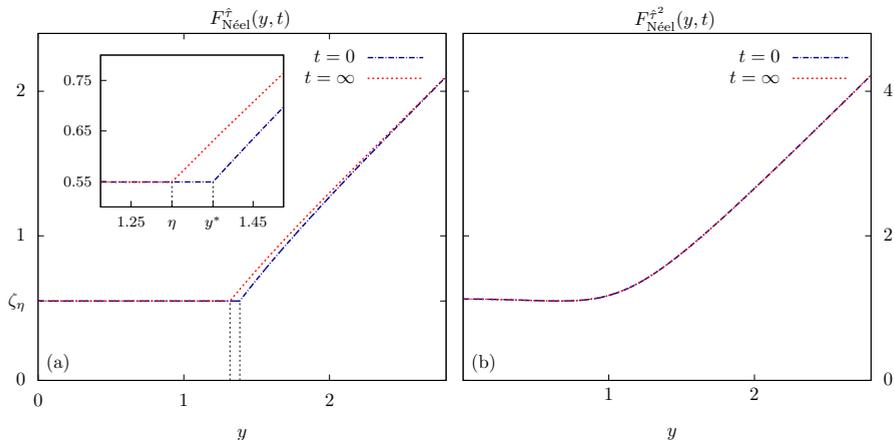


Figure E.1: (a) Comparison of  $F_{\text{Néel}}^{\hat{\tau}}(y, t)$  at  $t = 0$  from a direct computation and  $t = \infty$  from a saddle-point computation. For  $0 < y < \eta$  the saddle-point correctly predicts  $F_{\text{Néel}}^{\hat{\tau}}(y, \infty) = \zeta_\eta = \log[\sinh(\eta)]$ . For  $y > \eta$  the transfer matrix is a nonsmooth operator, rendering the QA method inapplicable and causing a discrepancy. (b) As in (a), now for  $\hat{\tau}^2$ . Since this operator is smooth for all  $y$  there is no discrepancy. All data were obtained for anisotropy  $\Delta = 2$ .