Supplementary Material: Complete Generalized Gibbs Ensembles in an Interacting Theory

We begin by recalling some of the fundamental equations of the Bethe Ansatz solution of the XXZ chain, together with few results obtained in [21, 32] which are used in the bulk of our paper.

Thermodynamic limit of Bethe equations

In the thermodynamic limit, the Bethe equations for the XXZ chain read [28, 35, 36]

$$\rho_{n,t}(\lambda) \;=\; a_n(\lambda) - \sum_{m=1}^{\infty} (a_{nm} * \rho_m)(\lambda), \qquad \text{(S1)}$$

for $n \geq 1$, where $\rho_{n,t}(\lambda) = \rho_n(\lambda) + \rho_{n,h}(\lambda)$ and $\rho_n, \rho_{n,h}$ are respectively the particle and hole densities of n-strings. The convolution is defined by $(f * g)(\lambda) = \int_{-\pi/2}^{\pi/2} \mathrm{d}\mu\, f(\lambda-\mu)\, g(\mu)$. The kernels are

$$a_{nm}(\lambda) = (1-\delta_{nm}) a_{|n-m|}(\lambda) + 2a_{|n-m|+2}(\lambda) + \dots + 2a_{n+m-2}(\lambda) + a_{n+m}(\lambda), \qquad \text{(S2)}$$

with a_n defined in (6) in the main part of the manuscript. A convenient rewriting is in the decoupled form [36]

$$\rho_n(1+\eta_n) = s * (\eta_{n-1}\rho_{n-1} + \eta_{n+1}\rho_{n+1}), \qquad \text{(S3)}$$

for $n \geq 1$, where $\eta_n \equiv \rho_{n,h}/\rho_n$. The λ-dependence is left implicit and we use the conventions $\eta_0(\lambda) = 1$ and $\rho_0(\lambda) = \delta(\lambda)$. The kernel in (S3) reads

$$s(\lambda) = \frac{1}{2\pi} \sum_{k\in\mathbb{Z}} \frac{e^{-2ik\lambda}}{\cosh(k\eta)} \,. \qquad \text{(S4)}$$

The set $\boldsymbol{\rho} = \{\rho_n\}_{n=1}^{\infty}$ represents an ensemble of states with Yang-Yang entropy

$$S_{YY}[\boldsymbol{\rho}] = N \sum_{n=1}^{\infty} \int_{-\pi/2}^{\pi/2} \mathrm{d}\lambda \left[\rho_{n,t}(\lambda) \ln \rho_{n,t}(\lambda) - \rho_n(\lambda) \ln \rho_n(\lambda) - \rho_{n,h}(\lambda) \ln \rho_{n,h}(\lambda)\right] . \qquad \text{(S5)}$$

An important point to bear in mind is that the Bethe equations (S3) relate the set of densities $\boldsymbol{\rho}$ to the set of hole densities $\boldsymbol{\rho}_h$. Knowing one of these two sets is thus sufficient to completely determine a given state. This point is crucial to understand the effects of constraints coming from ultra-local and quasi-local charges, as is explained below.

GTBA for the GGE

The generalized TBA for the GGE based on local charges proceeds as a standard TBA, but now with the effect of additional charges beyond the Hamiltonian being taken into account by additional parameters β_n (chemical potentials) in the GGE density matrix. By applying the standard maximal entropy reasoning using these constraints results in the GTBA equations [21, 32]

$$\ln(\eta_n) = -\delta_{n,1}(s*d) + s*[\ln(1+\eta_{n-1}) + \ln(1+\eta_{n+1})] \,, \qquad \text{(S6)}$$

for $n \geq 1$, where $\eta_0(\lambda) = 0$ and $s(\lambda)$ is defined in (S4). The driving term originating from ultra-local charges is remarkably only present in the first integral equation and is specified by the chemical potentials β_m, $m \geq 2$,

$$d(\lambda) = \sum_{k\in\mathbb{Z}} e^{-2ik\lambda} \sum_{m=2}^{\infty} \beta_m \sinh^{m-1}(\eta)(ik)^{m-2} \,. \qquad \text{(S7)}$$

As shown in [21, 32], the ultra-local charges associated to the spin-1/2 transfer matrix completely fix the density of holes of 1-strings to $\rho_{1,h}^{\Psi_0}$, but leave all higher hole density functions $\boldsymbol{\rho}_{n,h}$, with $n \geq 2$, undetermined. As explained in detail in [32], the GTBA system of (S6) and (S3) for the GGE can then be solved (using the constraint $\rho_{1,h} = \rho_{1,h}^{\Psi_0}$ to eliminate the unknown driving term in (S6)).

GTBA for the Quench Action

In the case of the QA treatment, the GTBA equations take the form

$$\ln(\eta_n) = d_n + s * \left[\ln(1+\eta_{n-1}) + \ln(1+\eta_{n+1})\right] \,, \qquad \text{(S8)}$$

where $n \geq 1$. The driving terms are given by the exact overlaps of Bethe states with the initial state. In the specific case of the Néel quench, these are given by

$$d_n(\lambda) = \sum_{k\in\mathbb{Z}} e^{-2ik\lambda} \frac{\tanh(k\eta)}{k} \left[(-1)^n - (-1)^k\right] = (-1)^n \ln\left[\frac{\vartheta_4^2(\lambda)}{\vartheta_1^2(\lambda)}\right] + \ln\left[\frac{\vartheta_2^2(\lambda)}{\vartheta_3^2(\lambda)}\right] \,, \qquad \text{(S9)}$$

where ϑ_j, $j = 1, \dots, 4$, are Jacobi's ϑ-functions with nome $e^{-2\eta}$.

Note the difference between this GTBA and the one associated to the ultra-local GGE: from the exact QA treatment one obtains GTBA equations with driving terms at all string lengths n, as a result yielding a different set of the steady state densities.

Relating quasi-local charges and hole densities

In the main text in (23) we provided the expectation values of the quasi-local charges on Bethe eigenstates in the limit of large system size. Strictly in the thermodynamic limit one obtains

$$\lim_{\mathrm{th}} \frac{1}{N} \langle \boldsymbol{\lambda} | \widehat{X}_s(\mu) | \boldsymbol{\lambda} \rangle = \lim_{\mathrm{th}} \frac{1}{N} \sum_{k=1}^{M} \frac{2\sinh(2s\eta)}{\cosh(2(z_k - i\mu)) - \cosh(2s\eta)} \tag{S10}$$

$$= -2\pi \sum_{n=1}^{\infty} \int_{-\pi/2}^{\pi/2} d\lambda\, \rho_n(\lambda) \sum_{j=1}^{\min(n,2s)} a_{|n-2s|-1+2j}(\lambda+\mu), \tag{S11}$$

with a_n defined in (6). In the last equality we accounted for $z_k = -i\lambda_k$, used the string hypothesis and the fact that the expectation values can be written as

$$\langle \boldsymbol{\lambda} | \widehat{X}_s(\mu) | \boldsymbol{\lambda} \rangle = -i\,\partial_\mu \ln\left(\prod_{k=1}^{M} \frac{\sin(\lambda_k + \mu + is\eta)}{\sin(\lambda_k + \mu - is\eta)} \right) + o(N). \tag{S12}$$

Using conventions for the Fourier transform

$$\hat{f}(k) = \int_{-\pi/2}^{\pi/2} \mathrm{d}\lambda\, e^{2ik\lambda} f(\lambda)\,, \quad k \in \mathbb{Z}\,, \tag{S13}$$

$$f(\lambda) = \frac{1}{\pi} \sum_{k\in\mathbb{Z}} e^{-2ik\lambda} \hat{f}(k)\,, \quad \lambda \in [-\tfrac{\pi}{2}, \tfrac{\pi}{2})\,, \tag{S14}$$

one can map Eq. (S11) to Fourier space,

$$\lim_{\mathrm{th}} \frac{1}{N} \langle \boldsymbol{\lambda} | \widehat{X}_s(\mu) | \boldsymbol{\lambda} \rangle \tag{S15}$$

$$= -2 \sum_{k\in\mathbb{Z}} e^{-i2k\mu} \sum_{n=1}^{\infty} \hat{\rho}_n(k) \sum_{j=1}^{\min(n,2s)} e^{-|k|\eta(|n-2s|-1+2j)},$$

using that $\hat{a}_n(k) = e^{-|k|\eta n}$. By performing the sum over j and using that $|n-2s| + 2\min(n,2s) = n + 2s$, one finds

$$\lim_{\mathrm{th}} \frac{1}{N} \langle \boldsymbol{\lambda} | \widehat{X}_s(\mu) | \boldsymbol{\lambda} \rangle \tag{S16}$$

$$= \sum_{k\in\mathbb{Z}} \frac{e^{-i2k\mu}}{\sinh(|k|\eta)} \sum_{n=1}^{\infty} \hat{\rho}_n(k) \left(e^{-|k|\eta(n+2s)} - e^{-|k|\eta|n-2s|} \right).$$

Using the thermodynamic Bethe equations (cf. (S3)) in Fourier space,

$$\hat{\rho}_{n,t}(k) = \frac{1}{2\cosh(k\eta)} \left(\hat{\rho}_{n-1,h}(k) + \hat{\rho}_{n+1,h}(k) \right), \tag{S17}$$

where $\hat{\rho}_{0,h}(k) = 1$, one can observe a cancellation of all terms with an exception of an expression given solely in terms $\rho_{2s,h}$:

$$\lim_{\mathrm{th}} \frac{1}{N} \langle \boldsymbol{\lambda} | \widehat{X}_s(\mu) | \boldsymbol{\lambda} \rangle = \sum_{k\in\mathbb{Z}} \frac{e^{-i2k\mu}}{\cosh(k\eta)} \left(\hat{\rho}_{2s,h}(k) - e^{-2s|k|\eta} \right). \tag{S18}$$

The quasi-local conservation laws make the left-hand side of Eq. (S18) equal to the generating function of the charges on the initial state as stated previously in (25), leading to

$$\hat{\Omega}_s^{\Psi_0}(k) \frac{\cosh(k\eta)}{\pi} = \hat{\rho}_{2s,h}(k) - e^{-2s|k|\eta}. \tag{S19}$$

Taking the inverse Fourier transform produces the main result of our Letter, namely the identification given by (24).

Truncated GGE

For practical reasons it is useful to determine a GGE ensemble by including only a finite number $\bar{s}$ of quasi-local charges $\{\widehat{X}_s\}_{s=1}^{\bar{s}}$. Using Eq. (24) for $s = 1, \ldots, \bar{s}$ we fix the distributions of holes $\rho_{n,h} = \rho_{n,h}^{\Psi_0}$ for string of lengths $n = 1, \ldots, 2\bar{s}$. These restrictions can be in turn used as a driving term for the following GTBA equations (analogously to what has been done for the case $\bar{s} = 1/2$ in [21, 29, 32])

$$\ln(\eta_n) = s * \left[\ln(1+\eta_{n-1}) + \ln(1+\eta_{n+1}) \right] \qquad n > 2\bar{s}\,, \tag{S20}$$

with

$$\eta_n = \frac{\rho_{n,h}^{\Psi_0}}{\rho_n} \qquad n \le 2\bar{s}\,, \tag{S21}$$

where the functions ρ_n solve the Bethe equations (S3). For any $\bar{s} \ge 1/2$ we then apply an iterative procedure to find a solution for all the $\{\eta_n^{\bar{s}}\}_{n=1}^{\infty}$ and all the $\{\rho_n^{\bar{s}}\}_{n=1}^{\infty}$, ultimately leading to the results shown in figure 1.

Néel initial state

As the Néel state is a simple product state we can evaluate all scalar products in the "quantum" spaces pertaining to the physical spin-1/2 degrees of freedom. This leaves us with a staggered product of diagonal components of an auxiliary two-channel L-matrix $\mathbb{L}_s(z_1, z_2) = L_{a_1}^{(-)}(z_1, s) L_{a_2}^{(+)}(z_2, s)$, producing a transfer matrix $\mathbb{T}_s(z_1, z_2)$ operating on two copies of auxiliary spin-s spaces $\mathcal{V}_s \otimes \mathcal{V}_s$,

$$\mathbb{T}_s(z_1, z_2) = \mathbb{L}_s^{\uparrow\uparrow}(z_1, z_2) \mathbb{L}_s^{\downarrow\downarrow}(z_1, z_2). \tag{S22}$$

This is a local unit of the 'boundary partition function' $Z_s(z_1, z_2) = \lim_{\mathrm{th}} N^{-1} \mathrm{Tr}_a \mathbb{T}_s(z_1, z_2)^{N/2}$, whose large-$N$

limit on $\mathcal{D} := \{(z_\lambda^-, z_\lambda^+); \lambda \in \mathbb{R}\} \subset \mathbb{C}^2$ is dominated by a non-degenerate unit eigenvalue $\Lambda_s(z_\lambda^-, z_\lambda^+) = 1$ of $\mathbb{T}_s(z_1, z_2)|_{\mathcal{D}}$, implying

$$\Omega_s^{\text{Néel}}(\lambda) = \partial_{z_2} Z_s(z_1, z_2)|_{\mathcal{D}} = \frac{1}{2}[\partial_{z_2}\Lambda_s(z_1, z_2)]_{\mathcal{D}}. \quad \text{(S23)}$$

It also helps noticing that $\mathbb{T}_s(z_1, z_2)$ enjoys a $U(1)$-symmetry, with the leading eigenvalue always residing in the largest $(2s+1)$-dimensional subspace. Closed-form results can be readily obtained in the cases $s = \frac{1}{2}, 1$

$$\Omega_{1/2}^{\text{Néel}}(\lambda) = \frac{-\sinh(2\eta)}{1 - 2\cos(2\lambda) + \cosh(2\eta)}, \quad \text{(S24)}$$

$$\Omega_1^{\text{Néel}}(\lambda) = \frac{2\sinh(3\eta)}{3\cos(2\lambda) - \cosh(\eta) - 2\cosh(3\eta)}. \quad \text{(S25)}$$

suppressing $\Omega_s^{\text{Néel}}(\lambda)$ for higher spins $s \geq 3/2$ which become quickly cumbersome expressions. For practical implementation of the truncated GGE it however suffices to evaluate them numerically. For a class of initial states which are given in the Matrix Product State form this can be done efficiently by e.g. employing the method outlined in [20].