Quenching the XXZ spin chain: quench action approach versus generalized Gibbs ensemble

Gábor Takács

Department of Theoretical Physics
Budapest University of Technology and Economics
MTA-BME "Momentum" Statistical Field Theory Research Group

B. Pozsgay, M. Mestyán, M. A. Werner, M. Kormos, G. Zaránd and G. Takács, Phys. Rev. Lett. 113 (2014) 117203, arXiv: 1405.2843 .

M. Mestyán, B. Pozsgay, G. Takács and M. A. Werner, J. Stat. Mech. 1504 (2015) P04001, arXiv: 1412.4787 .

Workshop "Beyond integrability: the mathematics and physics of integrability and its breaking in low-dimensional strongly correlated quantum phenomena"

Montreal, July 13-17, 2015

Outline

Closed q-systems and eigenstate thermalization hypothesis

Time evolution

$$|\psi(t)\rangle = \sum_\alpha C_\alpha e^{-\frac{i}{\hbar}E_\alpha t}|\psi_\alpha\rangle \qquad C_\alpha = \langle\psi(0)|\psi_\alpha\rangle \ : \ \text{overlaps}$$

$$H|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$$

Observables

$$\langle A(t)\rangle = \langle\psi(t)|A|\psi(t)\rangle = \sum_\alpha C_\alpha^* C_\beta e^{-\frac{i}{\hbar}(E_\alpha - E_\beta)t}\langle\psi_\alpha|A|\psi_\beta\rangle$$

Stationary state: diagonal ensemble

$$\bar{A} = \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\,\langle A(t)\rangle = \mathrm{Tr}\,\rho_{\mathrm{DE}}A \qquad \rho_{\mathrm{DE}} = \sum_\alpha |C_\alpha|^2|\psi_\alpha\rangle\langle\psi_\alpha|$$

"Quantum ergodicity" (Deutsch, 1991); ETH (Srednicki, 1994)

$$\langle\psi_\alpha|A|\psi_\alpha\rangle = \langle A\rangle\,(E_\alpha) \qquad \text{in TDL}$$

$\Rightarrow$ DE can be replaced with microcanonical/canonical (Gibbs) ens.
– in the thermodynamic limit
– for suitable (local/few-body) observables

GETH and GGE

Integrable system: higher conserved charges

$$[Q_i, Q_j] = 0 \qquad H \in \{Q_i\}$$

Generalized Gibbs Ensemble ($\sim$ grand canonical ensemble) (Rigol, Dunjko, Yurovsky & Olshanii, 2007)

$$\rho_{\text{GGE}} = \frac{1}{Z} e^{-\sum_i \beta_i Q_i} \qquad Z = \text{Tr } e^{-\sum_i \beta_i Q_i}$$

$$\text{Tr } \rho_{\text{GGE}} Q_i = \langle \psi(0) | Q_i | \psi(0) \rangle \quad \rightarrow \quad \{\beta_i\}_{i=1,\dots,N}$$

GGE: follows from conditional maximum entropy principle.

Generalized Eigenstate Thermalization Hypothesis (GETH)

$$\langle \psi_\alpha | A | \psi_\alpha \rangle = \langle A \rangle (\{Q_i\}_\alpha) \qquad \text{in TDL}$$

ETH holds on Q-shells, i.e. subspaces determined by fixing the Q_i.

The Heisenberg XXZ spin chain

A paradigmatic integrable model: chain of 1/2 spins

$$\dots\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\dots \quad \longrightarrow \quad \mathcal{H} = \bigotimes_L \mathbb{C}^2$$

$$H_{XXZ} = \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z\right) \qquad \text{PBC: } \sigma_{L+1}^k \equiv \sigma_1^k$$

Here: $\Delta > 1$: gapped phase, $\Delta \to \infty$: Ising limit

The chain is integrable and can be diagonalized by Bethe Ansatz:

$$|\lambda_1, \dots, \lambda_M\rangle \quad : \quad \text{state with M spin waves with rapidities } \lambda_i$$

$$\left(\frac{\sin(\lambda_j + i\eta/2)}{\sin(\lambda_j - i\eta/2)}\right)^L = \prod_{k\neq j}^{M} \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k - i\eta)} \qquad \Delta = \cosh\eta$$

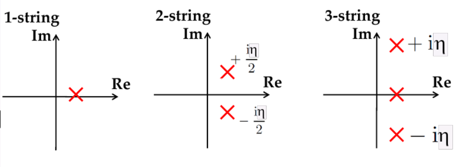
$$Q_n|\lambda_1, \dots, \lambda_M\rangle = \sum_{i=1}^{M} q_n(\lambda_i)|\lambda_1, \dots, \lambda_M\rangle$$

Conserved charges Q_n are local $\to$ additivity of eigenvalues!

Thermodynamics from string hypothesis

In TDL ($L \to \infty$)

n-string configurations



$$\lambda_j = \lambda + \frac{i\eta}{2}(n+1-2j) + O(1/L)$$

$$j = 1, \ldots, n$$

Number of n-strings centered in an interval $[\lambda, \lambda + d\lambda]$: $L\rho_n(\lambda)d\lambda$

Number of n-string holes in an interval $[\lambda, \lambda + d\lambda]$: $L\rho_n^h(\lambda)d\lambda$

Thermodynamic limit of BA: Bethe-Takahashi equations

$$\begin{aligned}
\rho_n(\lambda) + \rho_n^h(\lambda) &= a_n(\lambda) - \sum_{m=1}^{\infty} \int_{-\pi/2}^{\pi/2} d\lambda' \, T_{nm}(\lambda - \lambda')\rho_m(\lambda') \\
a_n(\lambda) &= \frac{1}{\pi} \frac{\sinh n\eta}{\cosh n\eta - \cos 2\lambda} \\
T_{nm}(\lambda) &= a_{|n-m|}(\lambda) + 2a_{|n-m|+2}(\lambda) + \cdots + a_{n+m}(\lambda)
\end{aligned}$$

Selection of initial states: the quantum quench paradigm

Quantum quench

$$H(g_0) \underset{t=0}{\longrightarrow} H(g)$$

$$\text{ground state} \longrightarrow \text{time evolution} \underset{\text{large } t}{\longrightarrow} \text{steady state}$$

Role of locality (cf. Caux & Mossel, 1012.3587)

- Start from ground state of *local* Hamiltonian, evolution by a different *local* Hamiltonian
- Relevant observables: *local* operators
  $\Rightarrow$ expect *local* charges to play a role

Example starting states for XXZ quenches:

- Neel: $|\uparrow\downarrow\uparrow\downarrow\ldots\uparrow\downarrow\rangle$ – ground state at $\Delta = \infty$
- Dimer (ground state of Majumdar-Ghosh Hamiltonian):

$$\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right)\otimes\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right)\otimes\cdots\otimes\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right)$$

GGE in XXZ spin chain

Previously: GGE for theories equivalent to free quasi-particles.
Pozsgay (2013): truncated GGE for XXZ chain
(genuinely interacting system!)

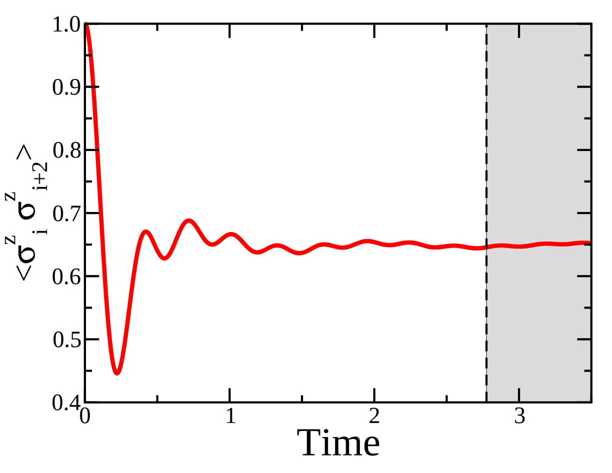
- use the quantum transfer matrix (QTM) method (Klümper)
- keep first few (up to 6) even charges
  $Q_2(= H)$, Q_4, Q_6, Q_8, Q_{10}, Q_{12}
- to predict short-range spin-spin correlators: use formulas available in QTM formalism
  (Boos, Göhmann, Klümper, Suzuki)
- converges fast in truncation level (improved by extrapolation)

Just two weeks later:
Fagotti & Essler (2013): construct full/untruncated GGE for XXZ

Fagotti, Collura, Essler & Calabrese (2013):
compare GGE to tDMRG $\quad \rightarrow \quad$ mainly seemed to work, but:

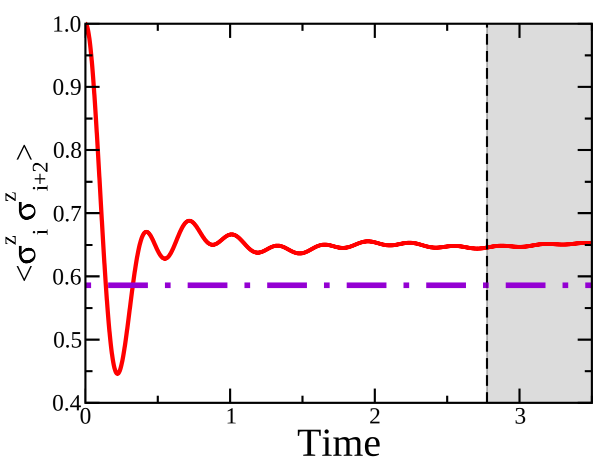
- translational invariance not restored for dimer initial state;
- relaxation for dimer?

Numerics from iTEBD (Werner & Zaránd)



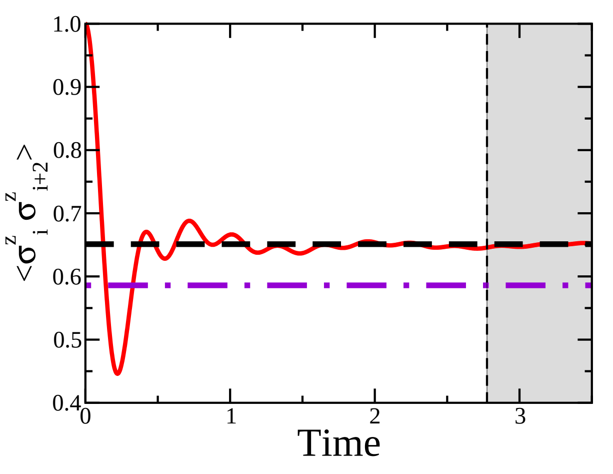
Neel $\Delta = 3$

Numerics from iTEBD compared to thermal



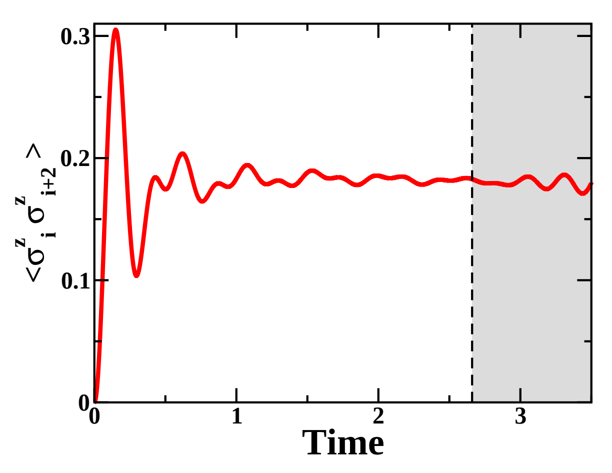
Neel $\Delta = 3$

Numerics from iTEBD compared to thermal and GGE



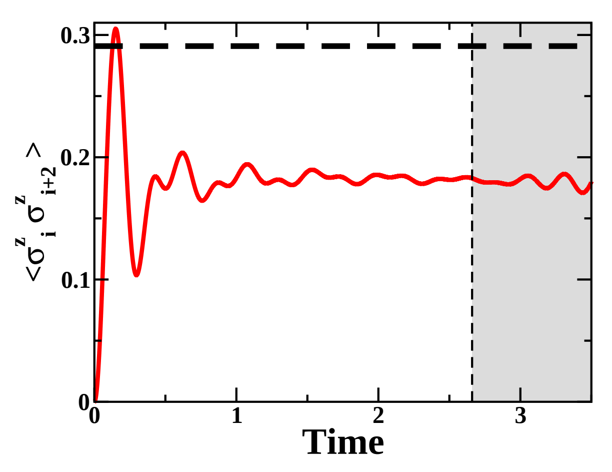
Neel $\Delta = 3$

Numerics from iTEBD



Dimer $\Delta = 3$

Numerics from iTEBD compared to GGE



Dimer $\Delta = 3$

The quench action for steady state expectation values

$$\bar{A} = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, \langle A(t)\rangle = \sum_\alpha |\langle\psi(0)|\alpha\rangle|^2 \langle\psi_\alpha|A|\psi_\alpha\rangle$$

$$\text{Replace sum: } \sum_\alpha \longrightarrow \int \prod_{n=1}^{\infty} D\rho_n(\lambda) e^{Ls[\{\rho_n(\lambda)\}]}$$

$e^{Ls[\{\rho_n(\lambda)\}]}$: number of Bethe states scaling to $\{\rho_n(\lambda)\}$ in the TDL.

In the TDL: $\langle\psi(0)|\alpha\rangle$ and $\langle\psi_\alpha|A|\psi_\alpha\rangle$ only depend on $\{\rho_n(\lambda)\}$

$$\bar{A} = \int \prod_{n=1}^{\infty} D\rho_n(\lambda) e^{-L\left(-\frac{2}{L}\mathrm{Re}\ln\langle\psi(0)|\{\rho_n(\lambda)\}\rangle - s[\{\rho_n(\lambda)\}]\right)} \langle\{\rho_n(\lambda)\}|A|\{\rho_n(\lambda)\}\rangle$$

In TDL: determined by saddle point of quench action functional

$$\begin{aligned} \mathcal{S}[\{\rho_n(\lambda)\}] &= -\frac{2}{L}\mathrm{Re}\ln\langle\psi(0)|\{\rho_n(\lambda)\}\rangle - s[\{\rho_n(\lambda)\}] \\ \bar{A} &= \langle\{\rho_n^*(\lambda)\}|A|\{\rho_n^*(\lambda)\}\rangle \end{aligned}$$

J.-S. Caux & F.H.L. Essler, 2013 (also describes time evolution)

Initial states and overlap

Initial states: translation invariant Neel and dimer states

$$|\Psi_N\rangle = \frac{1+\hat{T}}{\sqrt{2}} \bigotimes_{L/2} |\uparrow\downarrow\rangle \qquad |\Psi_D\rangle = \frac{1+\hat{T}}{\sqrt{2}} \bigotimes_{L/2} \left(\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \right)$$

Log overlap is extensive in TDL: integral form for $L \to \infty$

$$\begin{aligned} -2\mathrm{Re}\ln\langle\psi(0)|\{\rho_n(\lambda)\}\rangle &= L\sum_{n=1}^{\infty}\int_{-\pi/2}^{\pi/2} d\lambda \rho_n(\lambda) g_n^{\psi}(\lambda) \\ g_n^{\psi}(\lambda) &= \sum_{j=1}^{n} g_1^{\psi}\left(\lambda + \frac{i\eta}{2}(n+1-2j)\right) \end{aligned}$$

Neel overlaps (Brockmann, De Nardis, Wouters & Caux, 2014;
– based on Kozlowski & Pozsgay, 2012; Pozsgay, 2014)

$$g_1^N(\lambda) = -\ln\left(\frac{\tan(\lambda+i\eta/2)\tan(\lambda-i\eta/2)}{4\sin^2(2\lambda)}\right)$$

Dimer overlaps (Pozsgay, 2014)

$$g_1^D(\lambda) = -\ln\left(\frac{\sinh^4(\eta/2)\cot(\lambda)}{\sin(2\lambda+i\eta)\sin(2\lambda-i\eta)}\right)$$

The overlap TBA equations

Compute saddle point of quench action

$$\mathcal{S}[\{\rho_n(\lambda)\}] = -\frac{2}{L}\mathrm{Re}\ln\langle\psi(0)|\{\rho_n(\lambda)\}\rangle - s[\{\rho_n(\lambda)\}]$$

with the condition that the Bethe-Takahashi equations must hold

$$\rho_n(\lambda) + \rho_n^h(\lambda) = a_n(\lambda) - \sum_{m=1}^{\infty}(T_{nm} * \rho_m)(\lambda)$$

Result: the overlap thermodynamic Bethe Ansatz equations

$$\log\eta_n(\lambda) = g_n^{\psi}(\lambda) - \mu n + \sum_{m=1}^{\infty} T_{nm} \star \ln(1+\eta_m^{-1}) \qquad \eta_n(\lambda) = \frac{\rho_n^h(\lambda)}{\rho_n(\lambda)}$$

μ: chemical potential for S^z (external magnetic field).
Independently obtained for the Neel case by Caux et al., prior to us (J-S. Caux, lecture at NY meeting, 14-18 April 2014).

Correlations on the XXZ chain

We want observables: spin-spin correlators

$$\langle \sigma_i \sigma_{i+n} \rangle$$

But: it was only known how to get these in the QTM formalism!

1st idea: get from oTBA to QTM

14-18 April 2014: conference lecture by J-S Caux in New York: discrepancy between GGE-TBA and oTBA densities $\{\rho_n(\lambda)\}$
$\longrightarrow$ first idea killed :(

2nd idea: Hellmann-Feynman theorem

$$\begin{aligned} H_{XXZ} &= \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z \right) \\ \Rightarrow \frac{\partial E_\Psi}{\partial \Delta} &= L \langle \Psi | \sigma_i^z \sigma_{i+1}^z | \Psi \rangle \end{aligned}$$

(also $\sigma_i^x \sigma_{i+1}^x$ from $\langle H \rangle = E_\Psi$)

Correlations on the XXZ chain

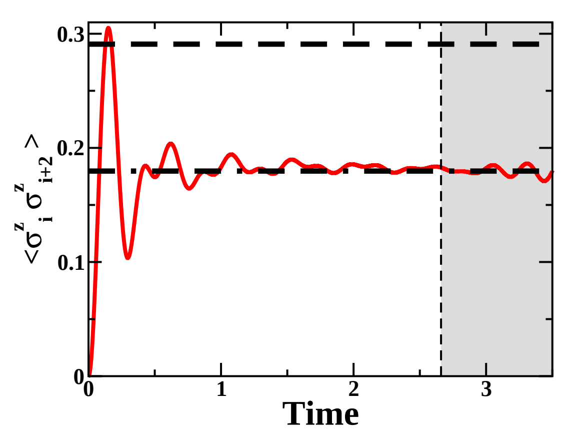
3rd idea: a surprising conjecture (B. Pozsgay)

Hellmann-Feynman result analogous to QTM correlator formulas (Boos, Göhmann, Klümper, Suzuki)
$\longrightarrow$ can be extended to a conjecture for all $\langle \sigma_i \sigma_{i+n} \rangle$
M. Mestyán and B. Pozsgay, J. Stat. Mech. (2014) P09020.

How does it work? (without formulas)

1. Solve oTBA for the η_n functions.
2. Solve Bethe-Takahashi for the ρ_n and ρ_n^h.
3. Check that $\langle Q_i \rangle$ agree with initial state (+overlap sum rule).
4. Solve auxiliary integral equations for some auxiliary functions.
5. Substitute the auxiliary functions into the place of their analogues in the QTM correlator formulas.

iTEBD compared to GGE and oTBA

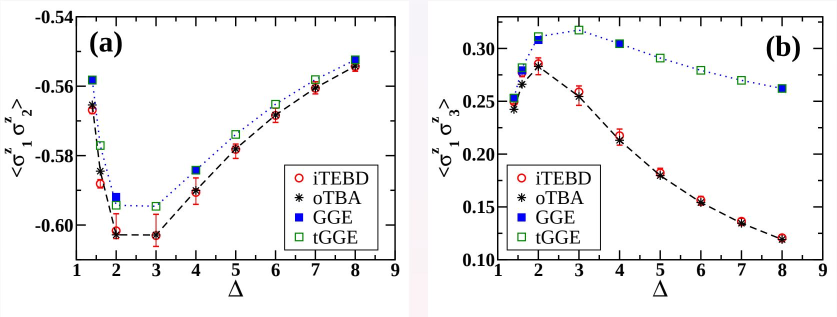


Dimer $\Delta = 3$

This is very strong evidence for breakdown of GGE

1. $n = 2$: sub-lattice independent ($\hat{T}$ projection is immaterial)
2. Agreement with oTBA (=DE in TDL) shows system has relaxed.

Dimer correlators as function of Δ



Remarks:

1. oTBA$\neq$GGE for Neel as well (observed also by Caux et al.)

... but difference is too small for iTEBD to resolve

2. xx correlators show same patterns (iTEBD is less accurate)

Role of bound states

Goldstein & Andrei, 2014:

– $n \geq 2$ strings are bound states of $n = 1$ magnons;

– due to their presence the Q_i do not fix the ρ_k uniquely, so

$$\{\langle\Psi_0|Q_i|\Psi_0\rangle\} \Rightarrow \left\{ \begin{array}{c} |\{\rho_1\}\rangle \\ |\{\rho_2\}\rangle \\ \vdots \end{array} \right\} \xrightarrow{\text{maximum entropy principle}} |\{\rho_{GGE}\}\rangle$$

... however: QA overlap sum rule (Pozsgay et al, 2014)

$$\mathcal{S}[\{\rho_n^*(\lambda)\}] = -\frac{1}{L}\log\langle\Psi_0|\Psi_0\rangle = 0$$

GGE densities violate this, but since

$$e^{-L\mathcal{S}[\{\rho_n^*(\lambda)\}]} = \text{weight of saddle point contribution}$$

$\Rightarrow \{\rho_n^{GGE}(\lambda)\}$ is irrelevant in the TDL!

Quench action principle selects the relevant densities

$$\mathcal{S}[\{\rho_{QA}\}] = 0$$

Note: QA is exactly the TDL of the diagonal ensemble!

Breakdown of GETH

However: if GETH held, any state (including GGE) on the shell

$$\Gamma(\psi(0)) = \{|\{\rho_n(\lambda)\}\rangle : \quad \langle\{\rho_n(\lambda)\}|Q_i|\{\rho_n(\lambda)\}\rangle = \langle\psi(0)|Q_i|\psi(0)\rangle\}$$

would give the same expectation value for local operators!

However: GETH is broken!

B. Pozsgay: *Failure of the generalized eigenstate thermalization hypothesis in integrable models with multiple particle species*,
J. Stat. Mech. 1409 (2014) P09026.
This also shows that GGE is broken for almost all initial states!

GGE seems to work in systems without bound states

B. Pozsgay: *Quantum quenches and Generalized Gibbs Ensemble in a Bethe Ansatz solvable lattice model of interacting bosons*,
J. Stat. Mech. 1410 (2014) P10045.

Quasi-local charges

Are there additional conserved charges?

Quasi-local charges for XXZ: previously known to exist for $-1 < \Delta < 1$

Prosen, 2011; Pereira, Pasquier, Sirker & Affleck, 2014.

New charges have recently been found for XXX!

Ilievski, Medenjak & Prosen, 1506.05049

The GGE saved (just today on arXiv)

Extending the GGE with the XXZ analogues of the new ultralocal charges agrees with the QA!

E. Ilievski, J. De Nardis, B. Wouters, J.-S. Caux, F.H.L. Essler and T. Prosen: Complete Generalized Gibbs Ensembles in interacting Theories, 1507.02993

Remark: charges completely fix densities –
no room for maximum entropy principle...

Question: do QLC always exist when there are bound states?

Conclusions

1. The standard GGE description based on only local charges is not generally valid for genuinely interacting integrable systems.
2. Underlying the failure of GGE is the failure of the GETH (generalized eigenstate thermalization hypothesis), and seems to be tied with existence of bound states.
3. The quench action correctly captures the steady state (new: can be reproduced with the GGE extended by quasi-local charges!)
4. Correlation formula in terms of TBA densities is a conjecture. Can it be proven?