Simulating the Quench-Action Method in finite integrable models

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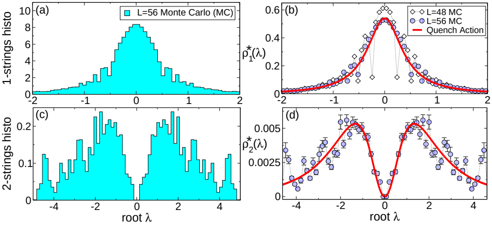
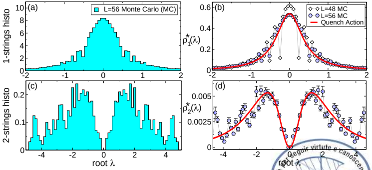
Cortona-GGI, May 18, 2016



Outline

[**V. A and P. Calabrese**, J. Stat. Mech.]

- Motivation: **Out-of-equilibrium** behavior of **isolated** quantum **many-body** systems.
- Quantum **quenches** in **integrable** 1D models.
- The **Quench Action** method.
- **Bethe ansatz** & **Monte Carlo** ⇒ numerical Quench Action.
- Hilbert space **truncation**.
- Benchmark in spin-1/2 **Heisenberg** chain.
- Quench Action **root distributions**.



Quantum quenches in **isolated** many-body systems

Quantum quench protocol

- Initial state $|\Psi_0\rangle \Rightarrow$ **unitary** evolution under a many-body Hamiltonian $\mathcal{H}$

$\{|\psi_\alpha\rangle\}$ eigenstates of $\mathcal{H}$ $\quad |\Psi_0\rangle = \sum_\alpha c_\alpha |\psi_\alpha\rangle \quad |\Psi(t)\rangle = \sum_\alpha e^{iE_\alpha t} c_\alpha |\psi_\alpha\rangle$

$c_\alpha \equiv \langle \Psi_0 | \psi_\alpha \rangle$

- For a generic observable $\widehat{\mathcal{O}}$:

$$\langle \Psi(t)|\widehat{\mathcal{O}}|\Psi(t)\rangle = \sum_{\alpha,\beta} e^{i(E_\alpha - E_\beta)t} c_\alpha^* c_\beta \widehat{\mathcal{O}}_{\alpha\beta}$$

- **Long time** $\Rightarrow$ **diagonal ensenble**.

$$\overline{\langle \Psi(t)|\widehat{\mathcal{O}}|\Psi(t)\rangle} = \langle \hat{\mathcal{O}} \rangle_{DE} = \sum_\alpha |\langle \Psi_0 | \psi_\alpha \rangle|^2 \widehat{\mathcal{O}}_{\alpha\alpha}$$

- **Main physics question**: What is the out-of-equilibrium **"phase diagram"** for **isolated** systems?

Non-thermal behavior in **integrable** 1D systems

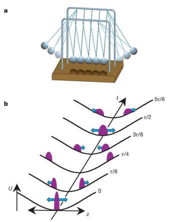
- Do isolated systems **thermalize**?

$$\rho^{Gibbs} \equiv \sum_\alpha e^{-\beta E_\alpha} |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

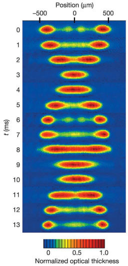
- $1D$ Bose gas $\Rightarrow$ **integrability** $\Rightarrow$ no thermalization.

$$\langle\hat{\mathcal{O}}\rangle_{DE} \neq \langle\hat{\mathcal{O}}\rangle_{Gibbs}$$

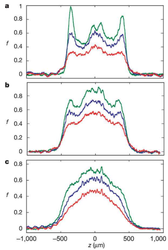
Experimental setup



Boson densities



Momentum distribution function



Quantum Newton's cradle [Kinoshita et al., Nature 440, 900 (2006)]

The Generalized Gibbs Ensemble (GGE)

- **Integrability** $\Rightarrow$ **Local** (quasi-local) conserved quantities $\mathcal{I}_j$.

$$[\mathcal{H}, \mathcal{I}_j] = 0,\ \forall j \quad \text{and} \quad [\mathcal{I}_j, \mathcal{I}_k] = 0,\ \forall j, k \qquad \mathcal{I}_2 \equiv \mathcal{H}$$

- Include extra charges in Gibbs $\Rightarrow$ **Generalized Gibbs Ensemble** (GGE).
[Jaynes, 1957;Rigol,2008]

$$\rho^{GGE} = \frac{1}{Z} \exp\left(\sum_j \beta_j \mathcal{I}_j\right)$$

The Quench-Action Method (idea)

- **Thermodynamics** with the initial state **overlaps**:

[Caux & Essler, 2013]

$$|\langle\Psi_0|\Psi_i\rangle| \equiv e^{\mathcal{E}_i}$$

$\mathcal{E}_i$ Quench-Action **driving term**

- **Typical** overlap decay $\Rightarrow$ $\mathcal{E}$ is **extensive**.

$$|\langle\Psi_0|\Psi_i\rangle| \propto e^{-\alpha L}$$

- Rewrite the diagonal ensemble average

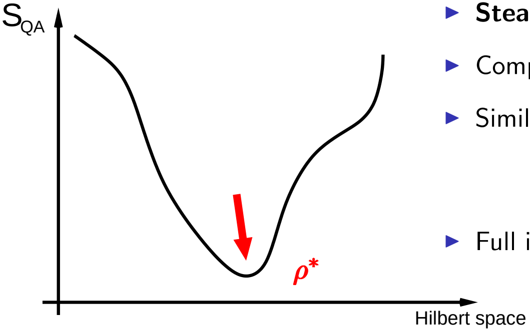
$$\mathrm{Tr}(\rho_{DE}\mathcal{O}) = \sum_\rho e^{\mathcal{E}[\rho]+S[\rho]}\langle\rho|\mathcal{O}|\rho\rangle$$

- Sum over **macrostates** ρ, with associated **entropy** $S[\rho]$.

The Q-A saddle point

- **Extensivity** of $\mathcal{E}, S \Rightarrow$ large systems $\Rightarrow$ **saddle point**.
- Minimization of **Q-A functional**:

$$S_{QA}[\rho] \equiv \mathcal{E} + S$$



- **Steady-state** physics encoded in ρ^*
- Competition between $\mathcal{E}$ and **S**.
- Similar to standard statistical physics

$$\mathcal{H} \Leftrightarrow \mathcal{E}$$

- Full information on initial state.

Numerical Quench Action for the spin-1/2 *XXX* chain

- Spin-1/2 isotropic Heisenberg (*XXX*) chain.

$$\mathcal{H}_{XXX} = \sum_{i=1}^{L} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + S_i^z S_{i+1}^z)$$

- **Bethe ansatz** + **Monte Carlo** $\Rightarrow$ Numerical Quench-Action.

- Quench from the **Néel** state.

$$|N\rangle \equiv \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle^{\otimes L/2} + |\downarrow\uparrow\rangle^{\otimes L/2})$$

Bethe ansatz for the spin-1/2 XXX chain

- Bethe-Gaudin-Takahashi (BGT) equations for string centers:

$$L\vartheta_n(x_{n;\gamma}) = 2\pi J_{n;\gamma} + \sum_{(m,\beta)\neq(n,\gamma)} \Theta_{m,n}(x_{n;\gamma} - x_{m;\beta})$$

$x_{n;\gamma}$ rapidities
$J_{n;\gamma} \in \frac{1}{2}\mathbb{Z}$, B-T quantum numbers

- Roots $\{x_{n;\gamma}\} \Rightarrow XXX$ chain eigenstates $|\{x_{n;\gamma}\}\rangle$.

$$\{J_{n;\gamma}\} \longrightarrow \{x_{n;\gamma}\} \longrightarrow |\{x_{n;\gamma}\}\rangle$$

Numerical Q-A: the overlaps

- Néel **overlaps** with **arbitrary** Bethe eigenstate:

$$\frac{\langle N|\{x_j\}_{j=1}^m, n_\infty\rangle}{|||\{x_j\}_{j=1}^m, n_\infty\rangle||} = \frac{\sqrt{2}N_\infty!}{\sqrt{(2N_\infty)!}}\left[\prod_{j=1}^m \frac{\sqrt{x_j^2+1}}{4x_j}\right]\sqrt{\frac{\det_m(G^+)}{\det_m(G^-)}}$$

[Tsuchiya, 1998; Koslowski et al., 2012; Brockmann et al., 2014]

- Total number Z_{Neel} of non-zero overlap eigenstates:

$$Z_{Neel} = 2^{\frac{L}{2}-1} + \frac{1}{2}\binom{L/2}{L/4} + 1$$

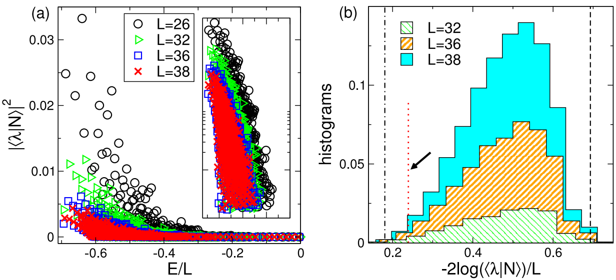
- Fictitious singularities for $x_j \to 0$ (**zero-momentum** strings).

- Vast majority of eigenstates contain zero-momentum strings.

$$\widetilde{Z}_{Neel}/Z_{Neel} \propto 1/\sqrt{L}$$

Overlap distribution function

- **All Néel** overlaps for $L \lesssim 40$ (exact **Bethe ansatz**).
- **No** zero-momentum strings. $\sim$ 200000 eigenstates

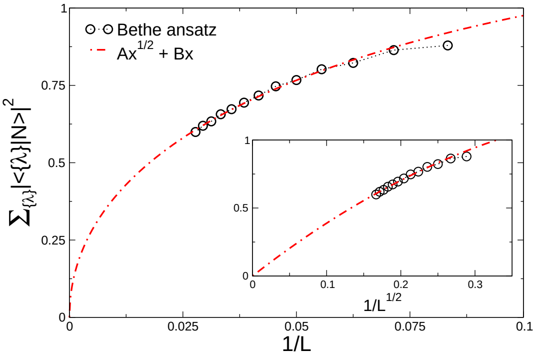


- Largest overlaps at **low energy**.
- Competition between **overlaps** and **entropy**.

Effects of zero-momentum strings (Néel)

- Trivial sum rule:

$$\langle N|N\rangle = \sum_{\lambda} |\langle\lambda|N\rangle|^2 = 1$$



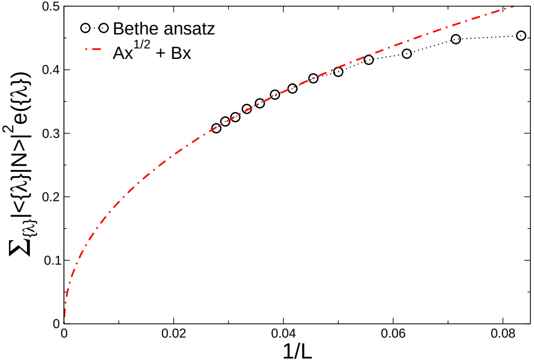
$$\frac{\tilde{Z}_{Neel}}{Z_{Neel}} \propto \frac{1}{\sqrt{L}}$$

- Violation of normalization sum rule.
- Vanishing $\propto 1/\sqrt{L}$ reflects the fraction of eigenstates kept.

Local sum rules violations

- **Energy** sum rules (no zero-momentum strings):

$$\langle N|\mathcal{H}|N\rangle/L = \sum_\lambda |\langle\lambda|N\rangle|^2 e(\lambda) = -1/2$$

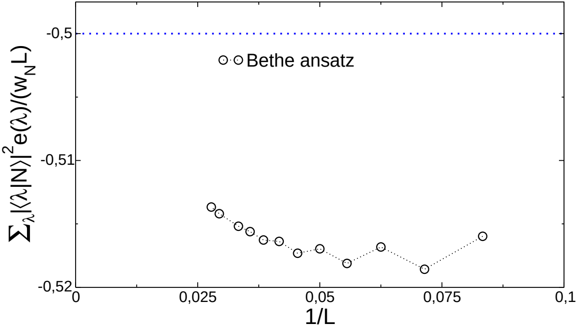


- Same vanishing behavior as the normalization

Quench-Action reweighting

- Quench-Action **reweigthing** for conserved quantities:

$$\langle \mathcal{I} \rangle = \frac{\sum_\lambda |\langle \lambda | \Psi_0 \rangle|^2 \langle \lambda | \mathcal{I} | \lambda \rangle}{w_{\Psi_0}}, \qquad w_{\Psi_0} \equiv \sum_\lambda |\langle \lambda | \Psi_0 \rangle|^2 ,$$



- Neglecting zero-momentum strings $\Rightarrow$ **scaling corrections**.

The Quench-Action Monte Carlo approach

- **Reweighting** via **Monte Carlo** sampling of the **Hilbert space** (eigenstates).

1. Start with an eigenstate identified by roots $\{x_{n;\gamma}\}$.
2. Solve the BGT equations for a new eigenstate with no zero-momentum strings (new $\{x'_{n;\gamma}\}$).
3. Accept the new eigenstate with Metropolis probability

$$\mathbf{Min}\Big[1, \exp\Big(\mathbf{Re}(\mathcal{E}' - \mathcal{E})\Big)\Big]$$

4. Iterate steps 1-3.

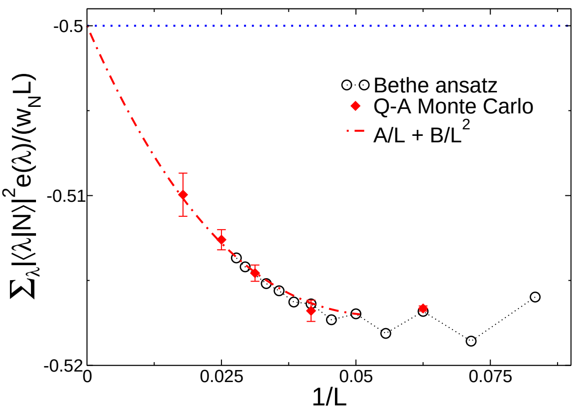
- **Quench-Action** average ⇒ **Monte Carlo** average:

$$\langle \hat{\mathcal{O}} \rangle_{QA} = \frac{1}{N_{mcs}} \sum_x \langle x | \hat{\mathcal{O}} | x \rangle$$

N_{mcs} is # eigenstates sampled

The Quench-Action Monte Carlo approach II

- Larger system sizes can be reached (**$L \sim 60$**).

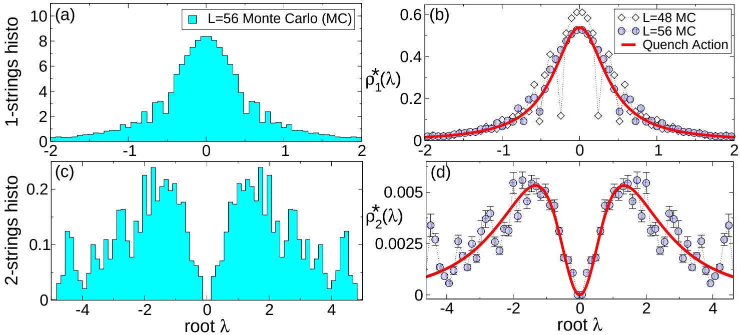


The steady-state root distributions

- In the **thermodynamic limit**:

$$\langle\mathcal{O}\rangle_{QA} = \sum_{\text{MC sampled}\{x_{\mathbf{n};\gamma}\}} \langle\{x_{\mathbf{n};\gamma}\}|\mathcal{O}|\{x_{\mathbf{n};\gamma}\}\rangle \to \sum_{\mathbf{n}} \int dx \rho^*_{\mathbf{n}}(x) \mathcal{O}_n(x)$$

$\rho_n(x)$ root distributions



- **Finite-size**: $\rho_n(x)$ approximated by histograms of BT roots.
- **Zero-momentum** strings are irrelevant.

Conclusions

- **Numerical** (Monte Carlo) implementation of **Quench Action** for **finite-size integrable** models.
- Numerical benchmarks in the **Heisenberg spin chain**.
- Steady-state **root distributions**.
- **Zero-measure** set of eigenstates contains all information about the out-of-equilibrium **steady state**.

Thanks!