Correlations after quantum quenches in the XXZ spin chain: Failure of the Generalized Gibbs Ensemble

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Thermalization in isolated classical systems

Isolated classical system: N degrees of freedom, energy E, volume V

$$\longrightarrow \quad \textit{microcanonical ensemble}$$

Phase space Γ : $\quad (q_1, \ldots, q_N, p_1, \ldots, p_N)$
Dynamics: Hamiltonian H

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

Fundamental postulate of statistical physics

The probability density in equilibrium is

$$\rho(q,p) = \begin{cases} \text{const.} & (q,p) \in \Gamma(N,E,V) \\ 0 & \text{otherwise} \end{cases}$$

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Boltzmann ergodic hypothesis

Boltzmann (1871): *ergodic hypothesis*

For an observable $A(q,p)$

time average: $$\bar{A} = \lim_{T\to\infty} \int_0^T dt A(q(t),p(t))$$

mc average: $$\langle A \rangle_{\text{mc}} = \frac{1}{\text{vol}(\Gamma(N,E,V))} \int_{\Gamma(N,E,V)} d^N q d^N p A(q,p)$$

Ergodicity:

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justifies use of microcanonical ensemble.

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Quantum systems differ fundamentally from classical ones:

if thermalization occurs, it must have a fundamentally different explanation as time evolution is linear!

$$|\psi(t=0)\rangle = \sum_\alpha C_\alpha |\psi_\alpha\rangle \qquad C_\alpha : \text{overlaps}$$

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

Time evolution

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

Observables

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

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Microcanonical setting: start with narrow energy distribution

$$\begin{aligned}\langle E\rangle &= \sum_\alpha |C_\alpha|^2 E_\alpha \\ \Delta E &= \sqrt{\sum_\alpha |C_\alpha|^2 \left(E_\alpha - \langle E\rangle\right)^2} \ll \langle E\rangle\end{aligned}$$

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Stationary state: for large t

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$$\langle A \rangle_{\mathrm{mc}} = \frac{1}{N(\langle E \rangle, \Delta E)} \sum_{\alpha : E_\alpha \in I} A_{\alpha\alpha} \qquad I = [\langle E \rangle - \Delta E, \langle E \rangle + \Delta E]$$

Deutsch (1991): "quantum ergodicity"

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Eigenstate thermalization hypothesis, ETH (Srednicki, 1994)

$$A_{\alpha\alpha} = \langle A \rangle_{\mathrm{mc}}(E_\alpha) \qquad \forall \alpha$$

Supposed to hold for large systems (thermodynamic limit – TDL)

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Thermalization in closed quantum systems

1. ETH is time independent: every eigenstate of Hamiltonian is already thermal. It is masked by quantum coherence, but revealed by dephasing effect of time evolution.
2. **Quantum ergodic theorem (Neumann)**: *for a typical finite family of commuting observables, every initial wave function from a microcanonical shell evolves so that for most times the averages of the given observables is close to their microcanonical value.*
   Rigol & Srednicki, 2012:
   Neumann's main technical assumption is equivalent to the Eigenstate Thermalization Hypothesis
3. What observables?
   1. local
   2. few-body

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Integrable systems violate ergodicity

Fermi-Pasta-Ulam (1953; Los Alamos technical report 1955)

$$m\ddot{x}_j = k(x_{j+1} + x_{j-1} - 2x_j)\,[1 + \alpha(x_{j+1} - x_{j-1})] \qquad j = 1, \ldots, N$$

Exciting a vibration mode: thermalization expected.
Found instead: complicated quasi-periodic behaviour!
Reason: system is integrable! (discretized version of KdV)
Integrability: action-angle variables exist

$$[Q_i, Q_j] = 0 \qquad H \in \{Q_i\}_{i=1,\ldots,N}$$

The quantities are conserved: motion along tori in phase space $\longrightarrow$
Lissajous orbits with frequencies $\omega_1, \ldots, \omega_N$
$\rightarrow$ may be ergodic on the tori
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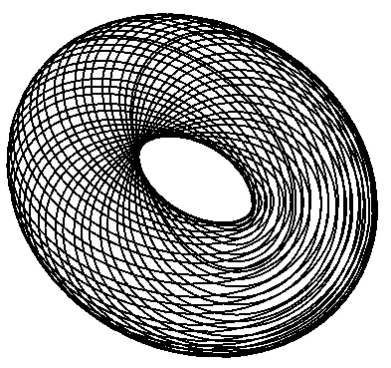

Generalized Eigenstate Thermalization Hypothesis

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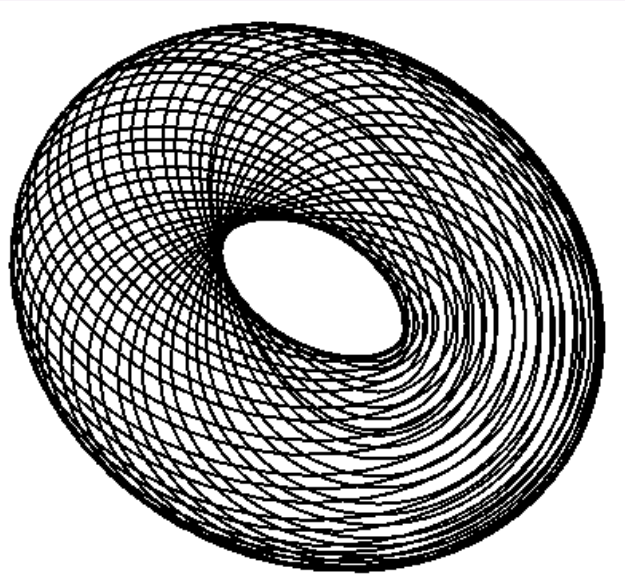

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Generalized Eigenstate Thermalization Hypothesis (GETH)

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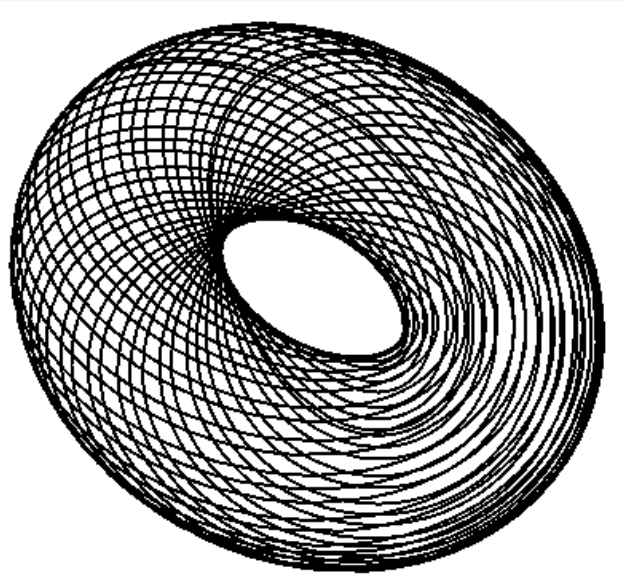

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Gibbs and generalized Gibbs ensembles

Nonintegrable system: steady state is thermal

DE is equivalent to a Gibbs ensemble for relevant observables

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Determining the temperature: $\mathrm{Tr}\ \rho_{\mathrm{GE}} H = \langle \psi(0) | H | \psi(0) \rangle \quad \rightarrow \quad \beta$

Generalized Gibbs Ensemble (GGE)

natural assumption: in integrable systems quantum ergodicity holds on common eigensubspaces of Q_i

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

Generalized temperatures/chemical potentials

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

GE/GGE: follow from conditional maximum entropy principle

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natural assumption: in integrable systems quantum ergodicity holds on common eigensubspaces of Q_i

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

Generalized temperatures/chemical potentials

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

GE/GGE: follow from conditional maximum entropy principle

Gibbs and generalized Gibbs ensembles

Nonintegrable system: steady state is thermal
DE is equivalent to a Gibbs ensemble for relevant observables

$$\begin{aligned} \mathrm{Tr}\ \rho_{\mathrm{DE}} A &= \mathrm{Tr}\ \rho_{\mathrm{GE}} A \\ \rho_{\mathrm{GE}} &= \frac{1}{Z} e^{-\beta H} \qquad Z = \mathrm{Tr}\ e^{-\beta H} \end{aligned}$$

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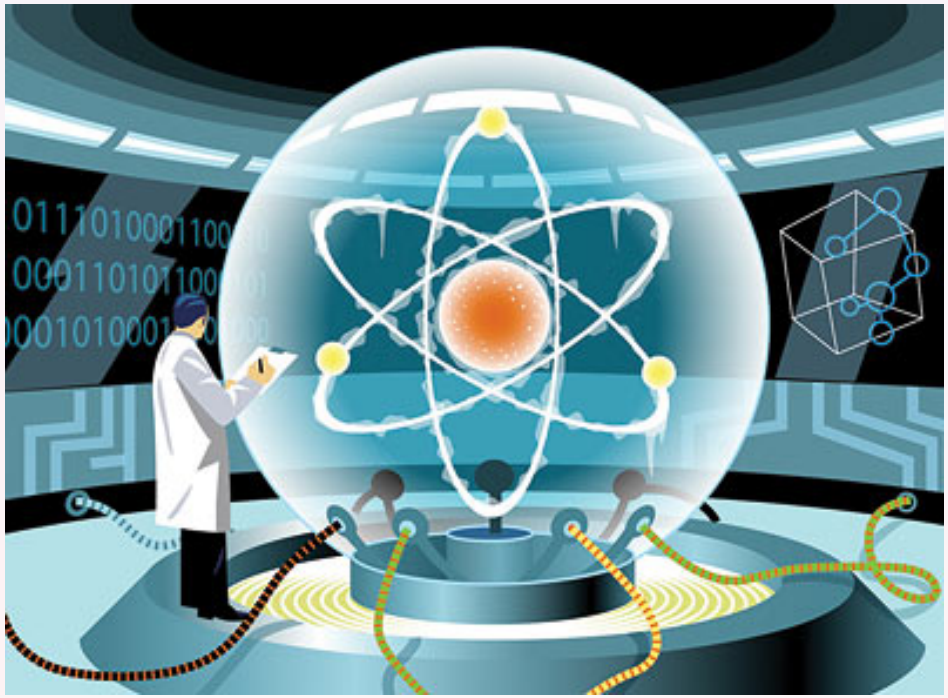
Closed quantum systems in reality

Can be realized with cold atoms...



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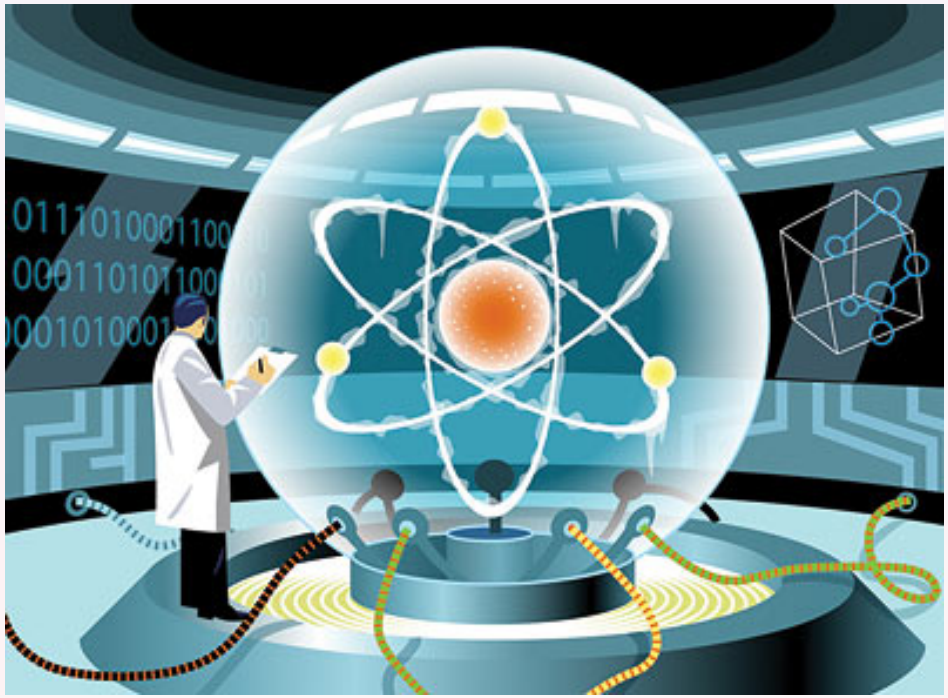

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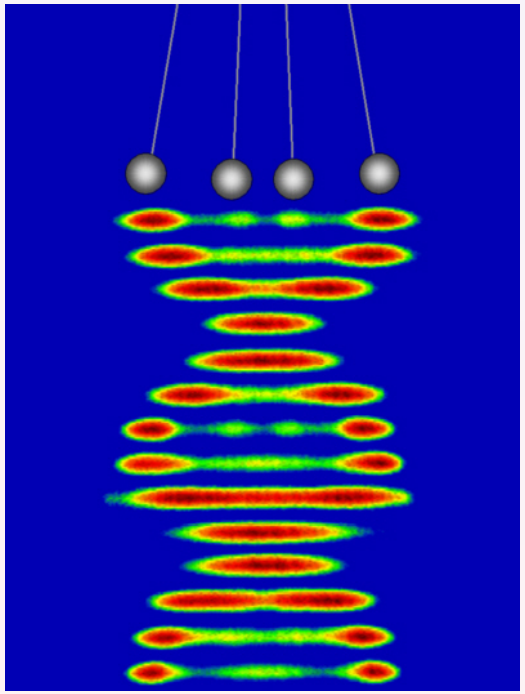

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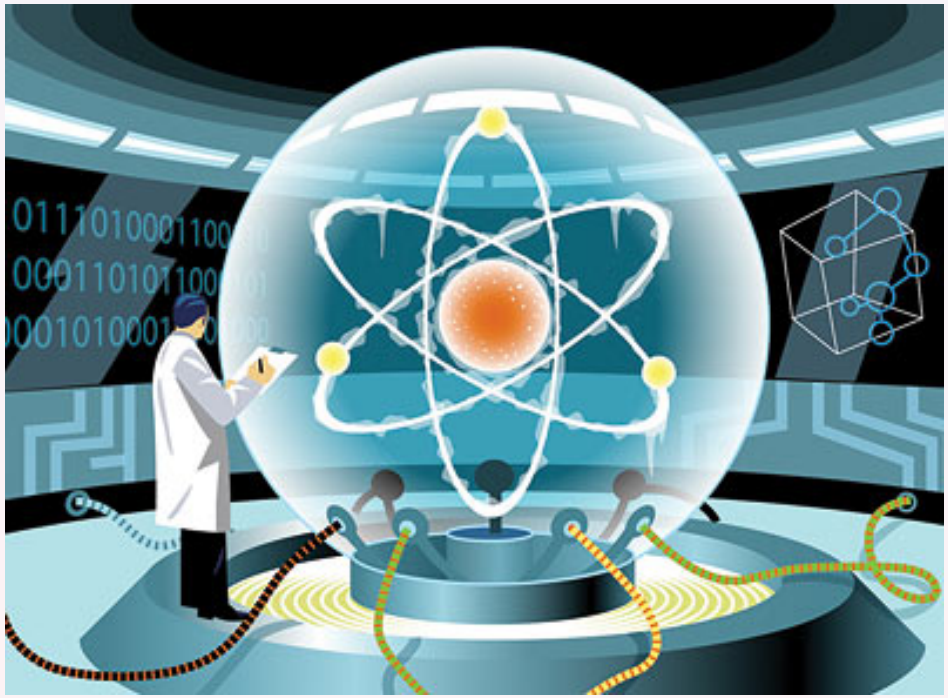

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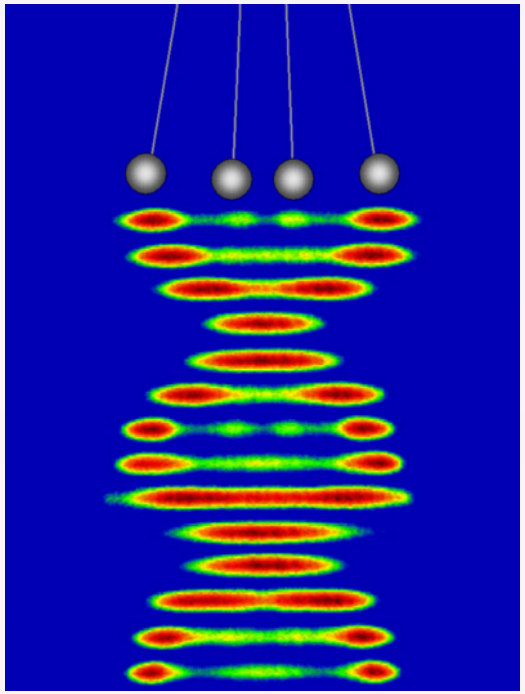

T. Kinoshita, T. Wenger and D.S. Weiss:
A quantum Newton's cradle, Nature 440 (2006) 900-903.

Outline

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The Heisenberg XXZ spin chain

A paradigmatic integrable model: chain of 1/2 spins

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

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

- $\Delta>1$: gapped phase, $\Delta\to\infty$: quantum Ising chain
- $-1<\Delta<1$: gapless phase (Luttinger liquid)

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

$$\begin{aligned}
|\lambda_1,\ldots,\lambda_N\rangle &= B(\lambda_1)\ldots B(\lambda_M)|\Omega\rangle \\
|\Omega\rangle &= |\ldots\uparrow\uparrow\uparrow\ldots\rangle \qquad \text{pseudovacuum} \\
\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,\ldots,\lambda_N\rangle &= \sum_{i=1}^{n} q_n(\lambda_i)|\lambda_1,\ldots,\lambda_N\rangle
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The conserved charges Q_n are local $\to$ additivity!

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Excitations and string hypothesis

$$S^z = \frac{L}{2} - M$$

Ground state: unique solution with $M = L/2$ and all λ_i real

$$|0\rangle = B(\lambda_1)\dots B(\lambda_{L/2})|\Omega\rangle \qquad \lambda_i \in \mathbb{R}$$

Excitations: can be holes in the Dirac sea, or

n-string configurations

$$\begin{aligned} \lambda_j &= \lambda + \frac{i\eta}{2}(n+1-2j) \\ &\quad + O(1/L) \\ &\quad j = 1, \dots, n \end{aligned}$$

String hypothesis

Thermodynamics can be described by string degrees of freedom

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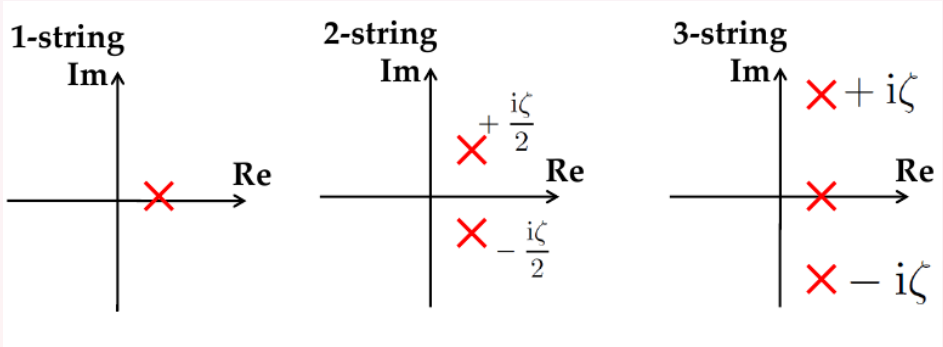

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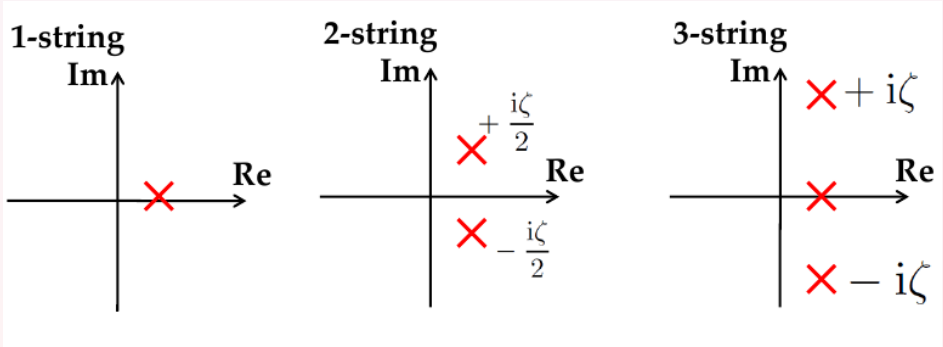

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Thermodynamic limit of Bethe Ansatz

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

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\begin{aligned}
\rho_n(\lambda) + \rho_n^h(\lambda) &= a_n(\lambda) - \sum_{m=1}^{\infty} (T_{nm} * \rho_m)(\lambda) \\
a_n(\lambda) &= \frac{1}{\pi} \frac{\sinh n\eta}{\cosh n\eta - \cos 2\lambda} \\
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Selection of initial states: the quantum quench paradigm

Quantum quench

$$H(g_0) \xrightarrow[t=0]{} H(g)$$

$$\text{ground state} \longrightarrow \text{time evolution} \xrightarrow[\text{large } t]{} \text{steady state}$$

Role of locality in our considerations

- Start from ground state of *local* Hamiltonian
- Evolved by a *local* Hamiltonian
- Relevant observables: *local* operators
- 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 $\Delta = \infty$
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$$\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right)\otimes\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right)\otimes\cdots\otimes\left(\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right)$$

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Truncated GGE

Previously: GGE only for theories equivalent to free particles.

Pozsgay (2013): truncated GGE for XXZ chain

– the first GGE realization in a genuinely interacting model

Idea:

- use the quantum transfer method (QTM) to solve the chain
- keep first few (up to 6) even charges
  $Q_2(= H)$, Q_4, Q_6, Q_8, Q_{10}, Q_{12}
- use QTM formula to predict correlators

Observations:

- converges fast in truncation level (improved by extrapolation)
- truncated GGE is "the GGE" as a matter of principle

Fagotti & Essler (2013): construct full/untruncated GGE

Fagotti, Collura, Essler & Calabrese (2013):

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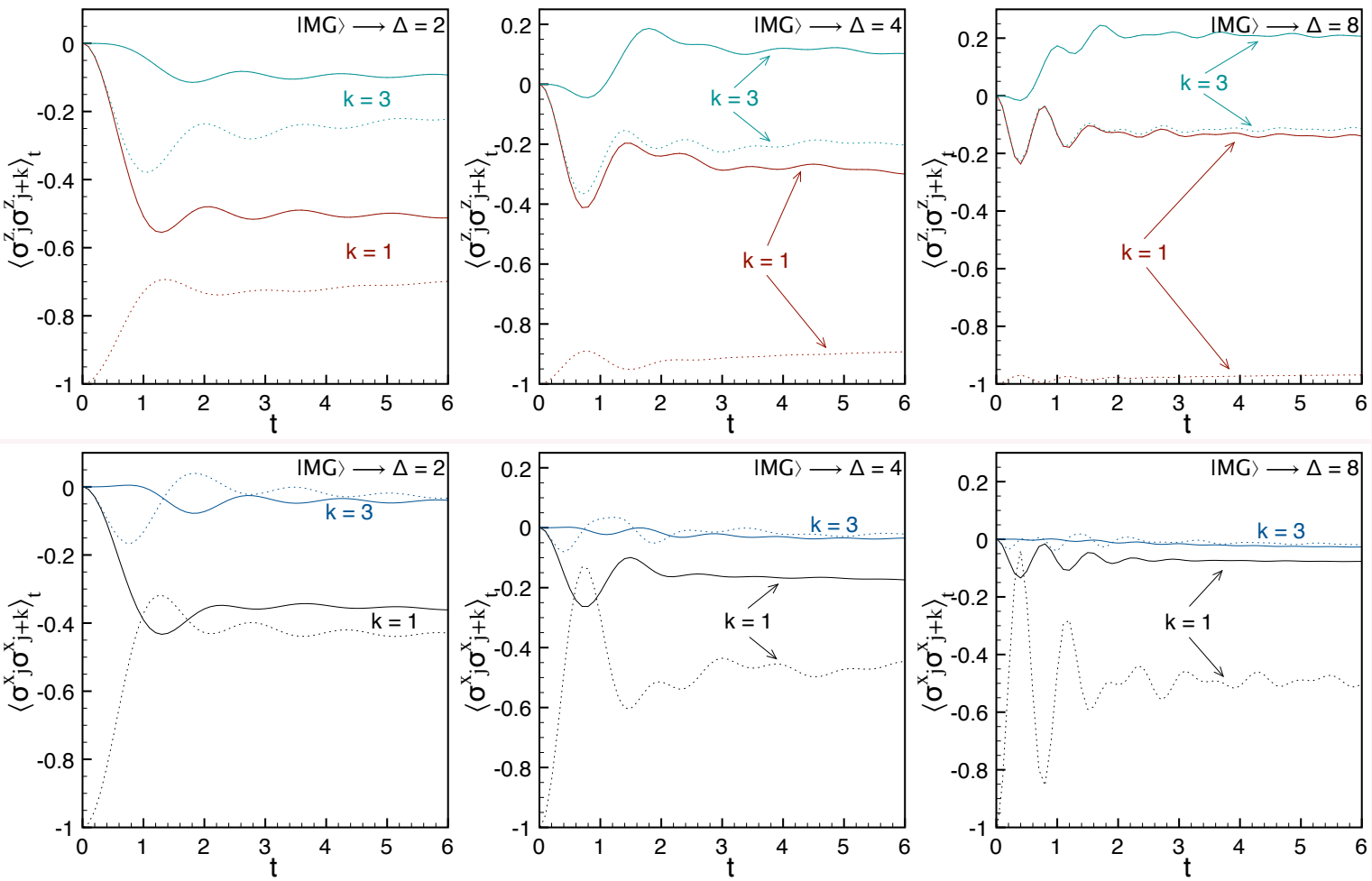

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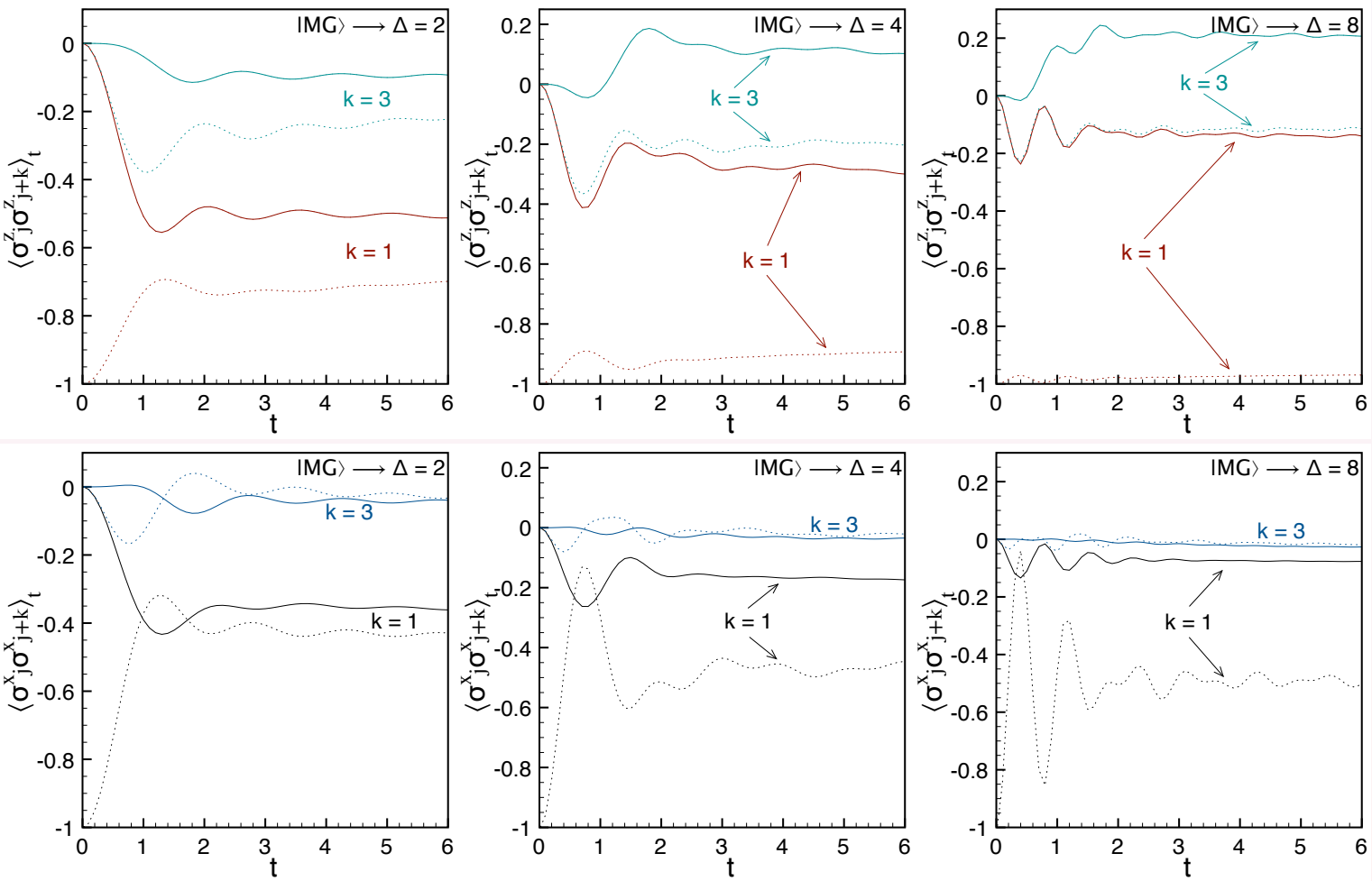

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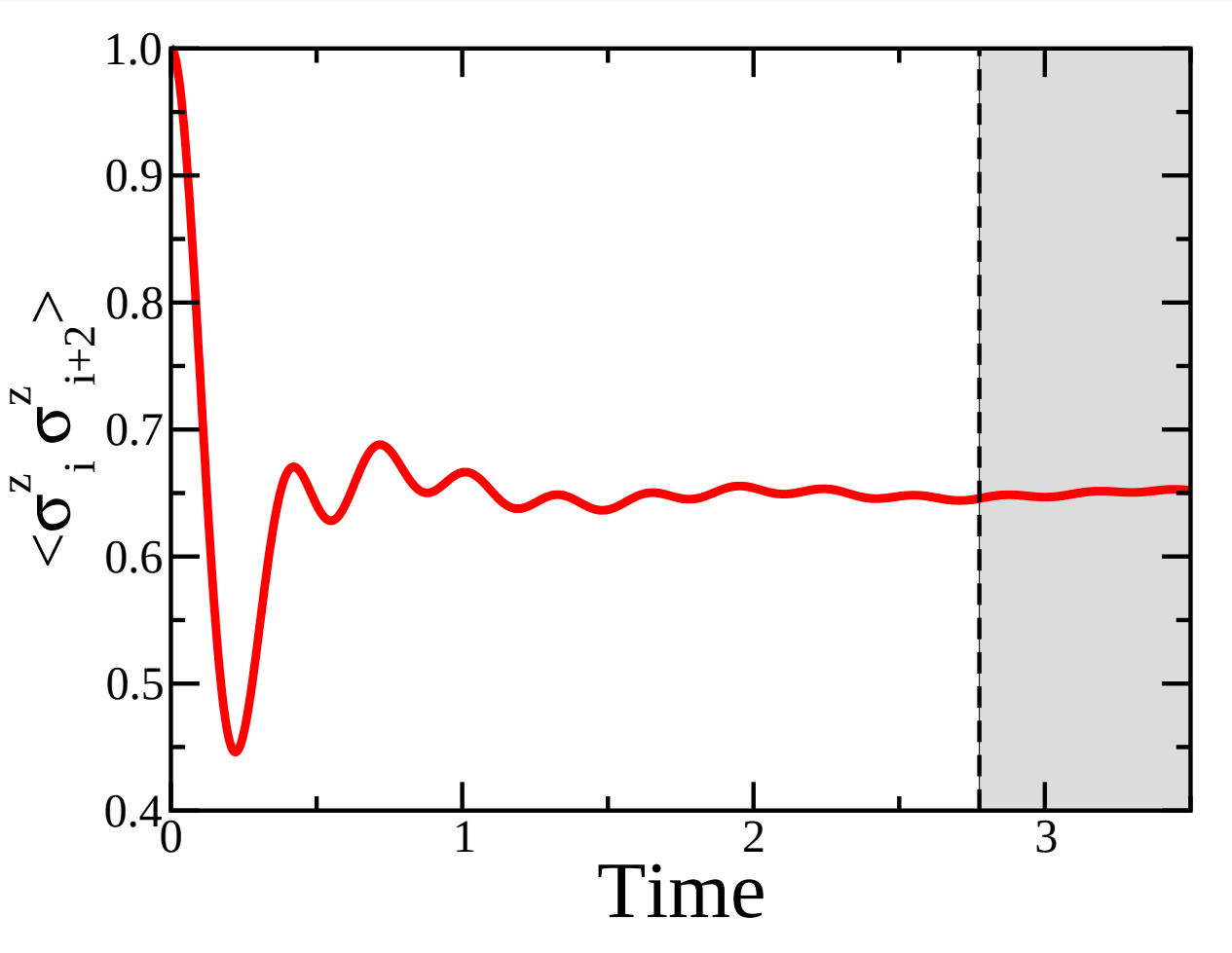
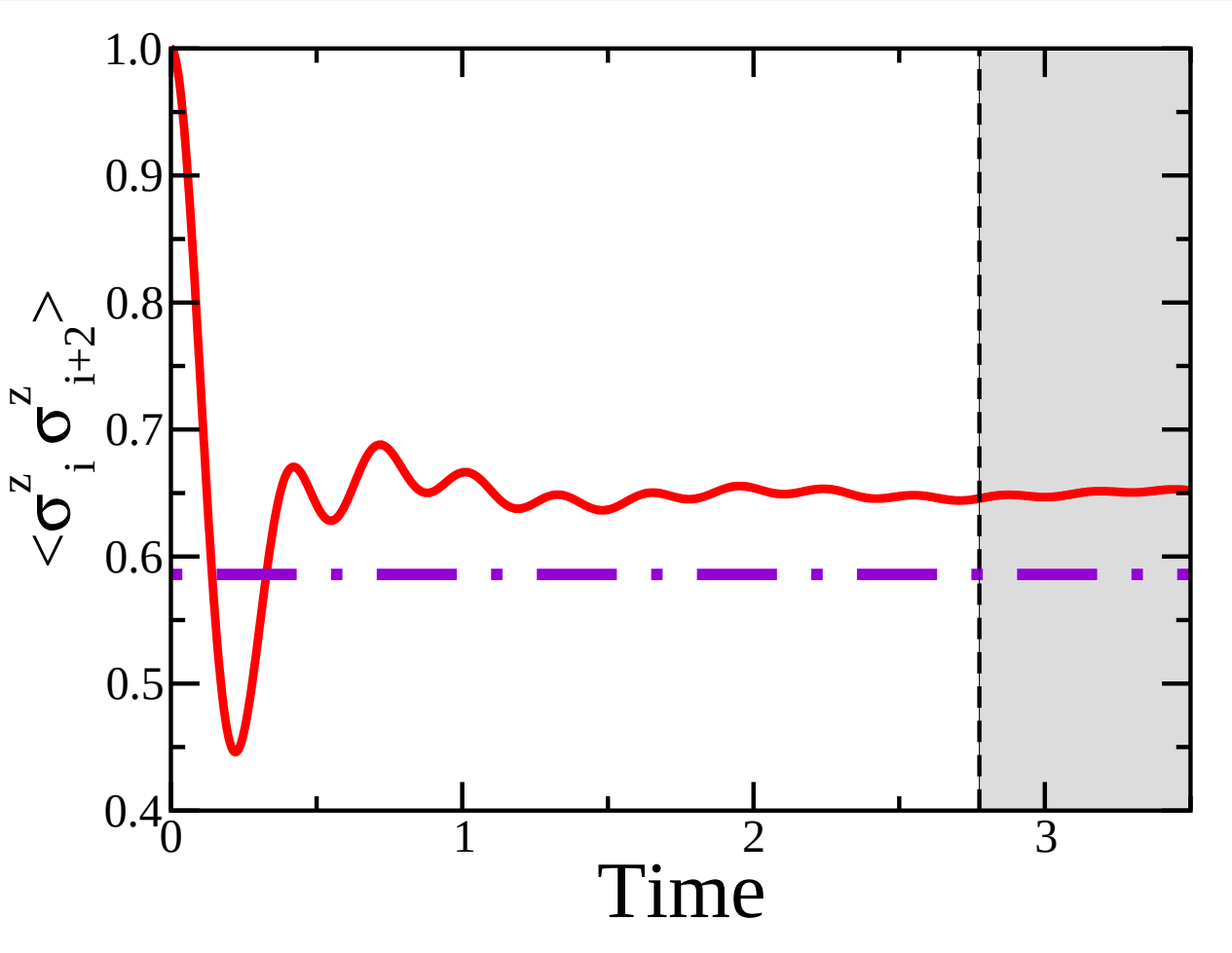


Neel $\Delta = 3$

Result of iTEBD compared to thermal



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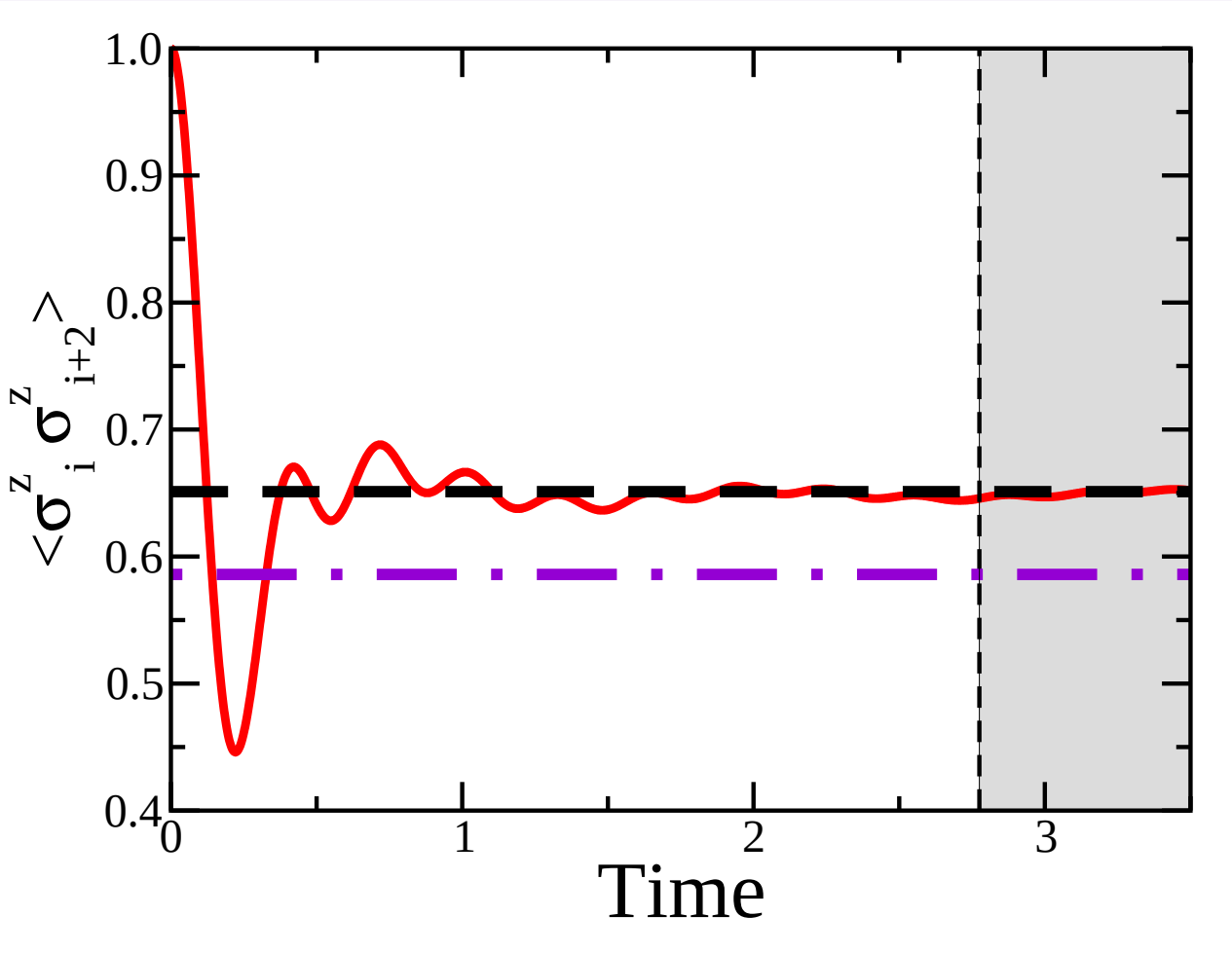

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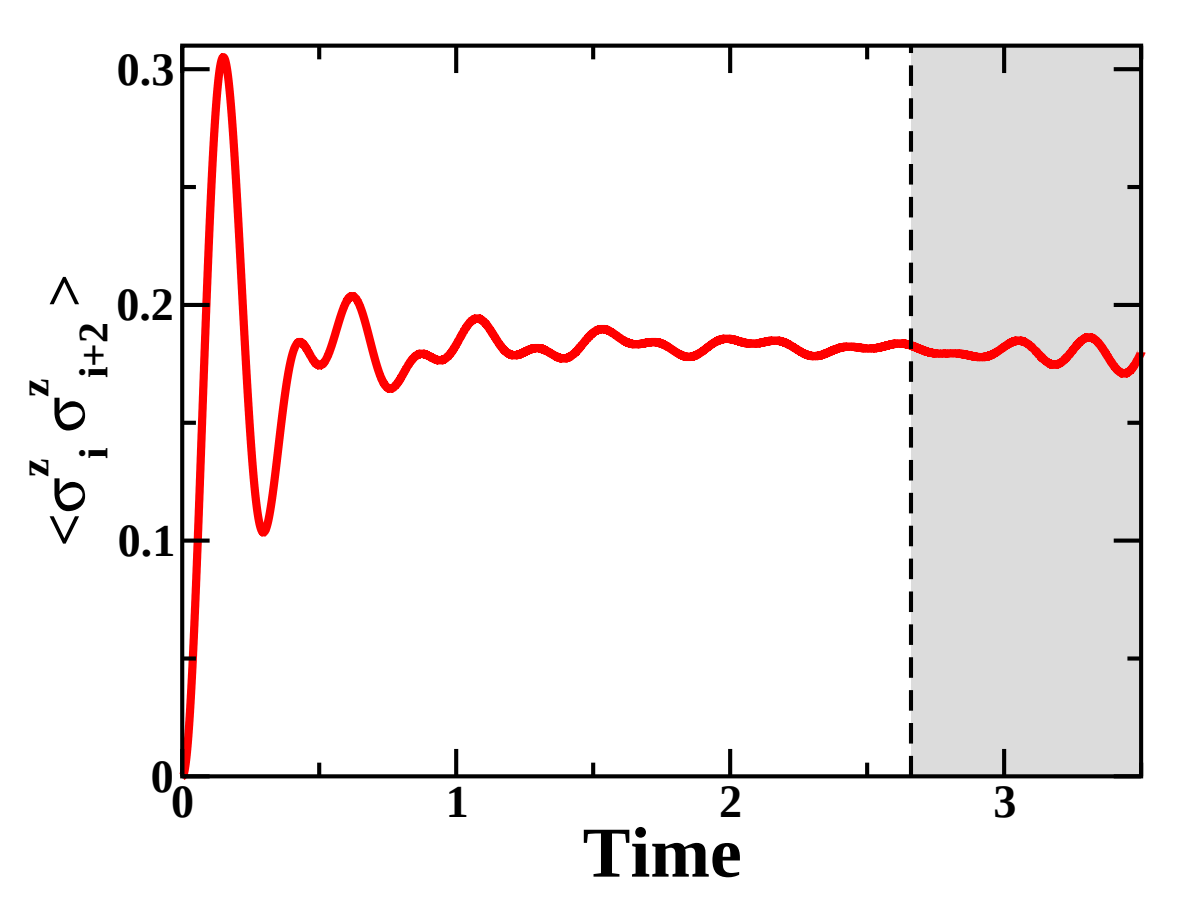

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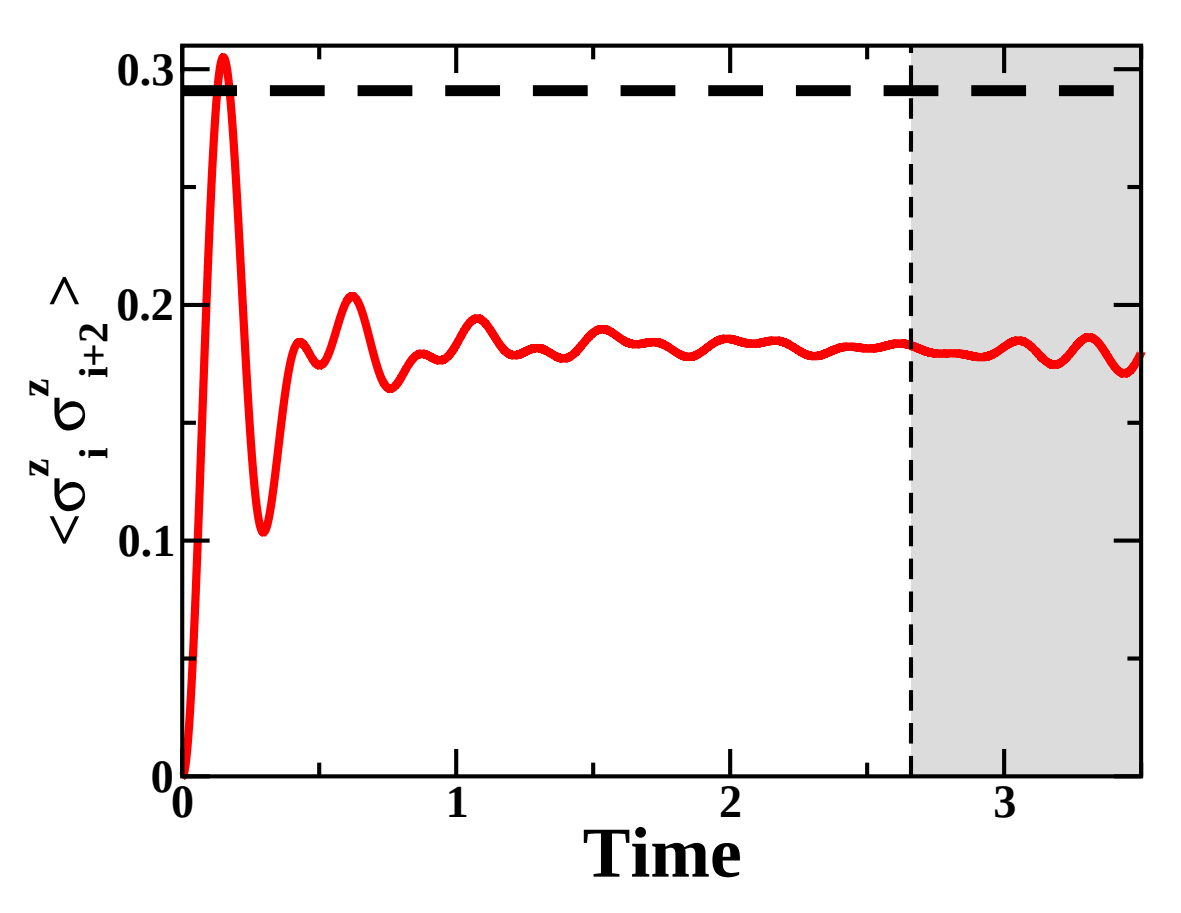

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Outline

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The quench action

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

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.
Supposing that C_α and $A_{\alpha\alpha}$ only depend on $\{\rho_n(\lambda)\}$ in the TDL:

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

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J.-S. Caux & F.H.L. Essler, 2013

The quench action

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

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Outline

Initial states and overlap

Initial states: translation invariant Neel and dimer states
($\hat{T}$ is translation by one site)

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

Only overlaps with $S^z = 0$ states built upon "Cooper pairs":

$$|\{\lambda_k\}\rangle_C = |\lambda_1, -\lambda_1, \lambda_2, -\lambda_2, \ldots, \lambda_{L/4}, -\lambda_{L/4}\rangle$$

Neel overlaps (Brockmann, De Nardis, Wouters & Caux, 2014)

$$\frac{\langle\Psi_N|\{\lambda_k\}\rangle_C}{\sqrt{{}_C\langle\{\lambda_k\}|\{\lambda_k\}\rangle_C}} = \prod_{j=1}^{L/4} \frac{\sqrt{\tan(\lambda_j + i\eta/2)\tan(\lambda_j - i\eta/2)}}{2\sin(2\lambda_j)} \times (\text{Fredholm det})$$

Dimer overlaps (Pozsgay, 2014)

$$\langle\Psi_D|\{\lambda_k\}\rangle = \langle\Psi_N|\{\lambda_k\}\rangle \prod_k \frac{1}{\sqrt{2}} \left(1 - \frac{\sin(\lambda_j - i\eta/2)}{\sin(\lambda_j + i\eta/2)} \right)$$

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Overlaps in the thermodynamic limit

Integral form for $L \to \infty$

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\begin{aligned}
-2\mathrm{Re}\ln\langle\psi(0)|\{\rho_n(\lambda)\}\rangle &= \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)
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For our translation invariant Neel and dimer states

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

The overlap TBA equations

Entropy: 1/2 of Yang-Yang expression (only paired states!)

$$s[\{\rho_n(\lambda)\}] = \frac{1}{2}\sum_{n=1}^{\infty}\int_{-\pi/2}^{\pi/2} d\lambda \left[\rho_n(\lambda)\ln\left(1+\frac{\rho_n^h(\lambda)}{\rho_n(\lambda)}\right) + \rho_n^h(\lambda)\ln\left(1+\frac{\rho_n(\lambda)}{\rho_n^h(\lambda)}\right)\right]$$

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. before us.

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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.

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

2nd idea: Hellmann-Feynman theorem

$$\begin{aligned} H_{XXZ} &= \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z \right) \\ \Rightarrow \frac{\partial E_\Psi}{\partial \Delta} &= L \langle \Psi | (\sigma_1^z \sigma_2^z - 1) | \Psi \rangle \end{aligned}$$

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3rd idea: a real stroke of genius (B. Pozsgay)

Hellmann-Feynman result analogous to QTM correlator formulas
$\longrightarrow$ 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 $\mathcal{S}[\{\rho_n^*(\lambda)\}] = 0$. GGE gives $-\infty$!)
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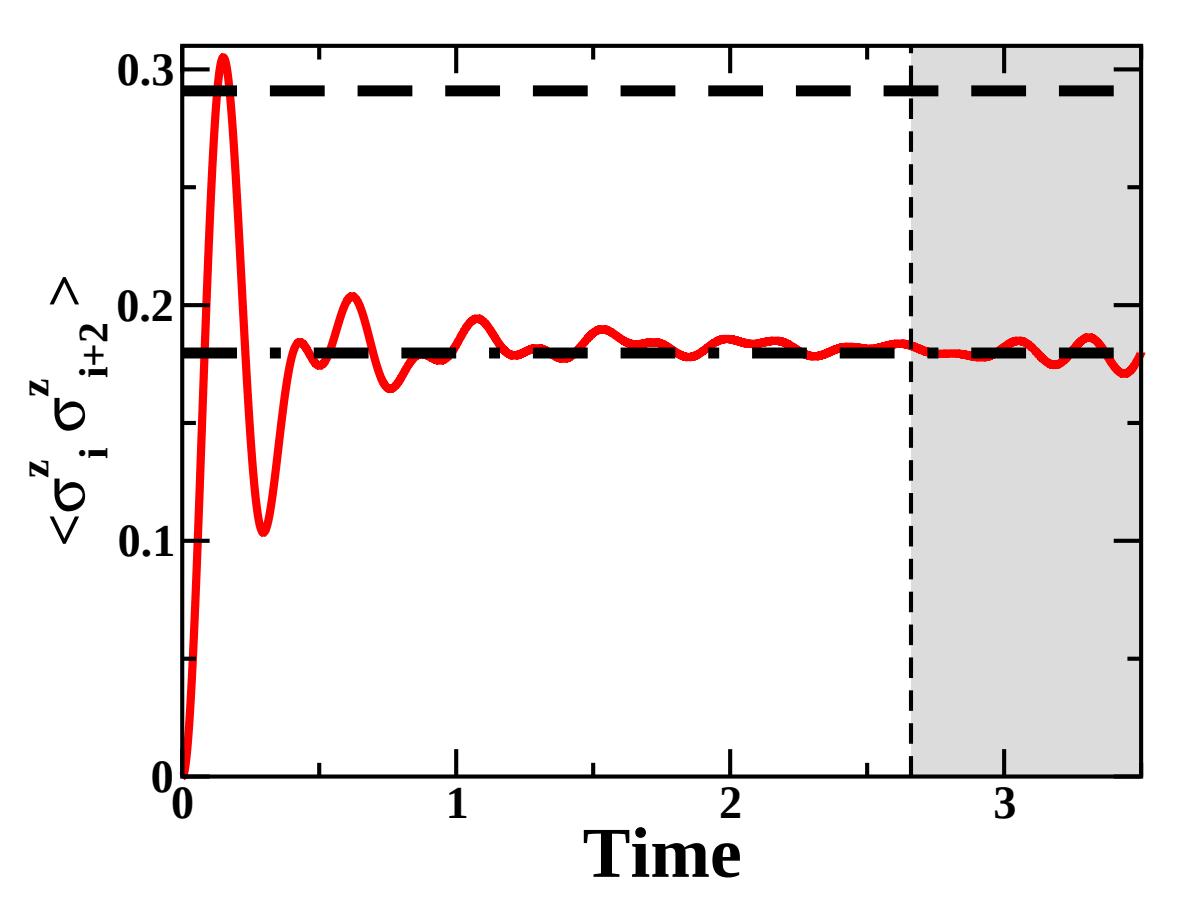
Result of iTEBD compared to GGE and oTBA

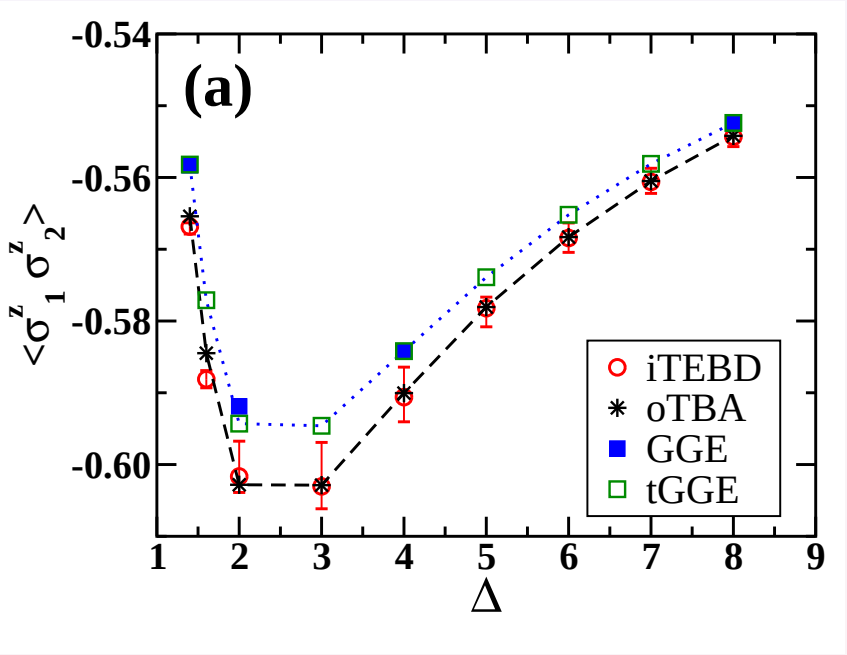


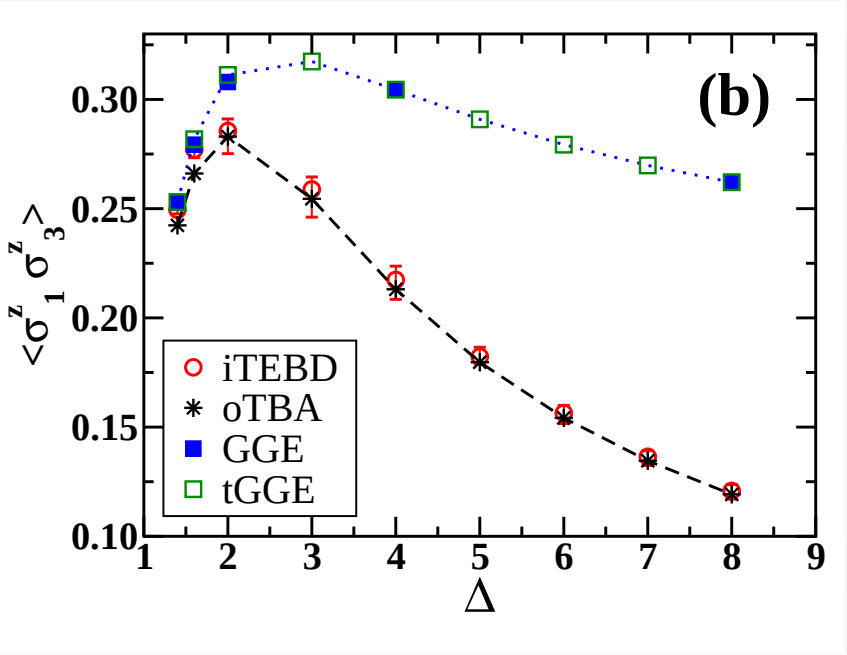
Dimer $\Delta = 3$

This is very strong evidence for breakdown of GGE

1. $n = 2$: sublattice independent (projection is immaterial)
2. Agreement with oTBA shows system has relaxed

Dimer correlators as function of Δ





Remarks:

1. oTBA≠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, but iTEBD is less accurate

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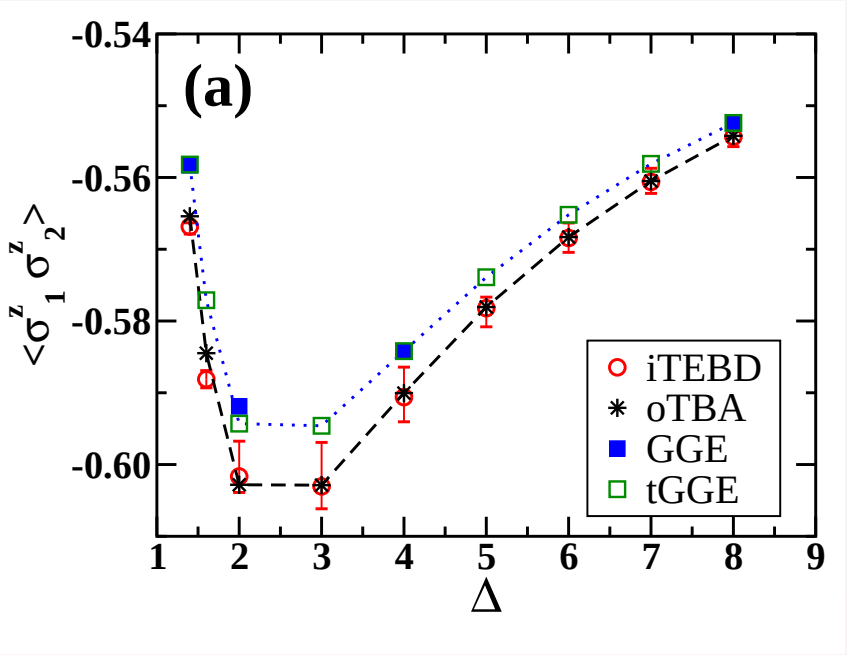

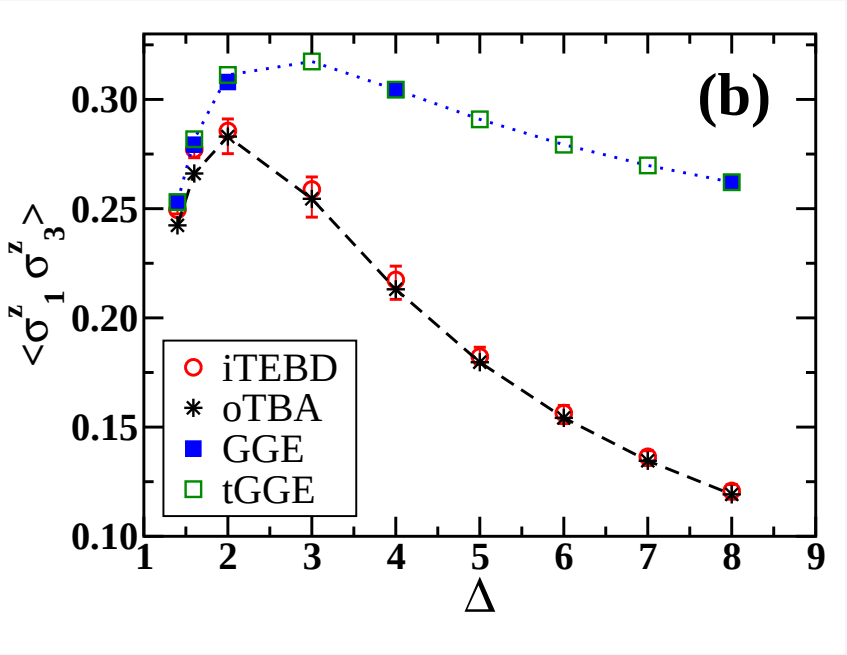

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Outline

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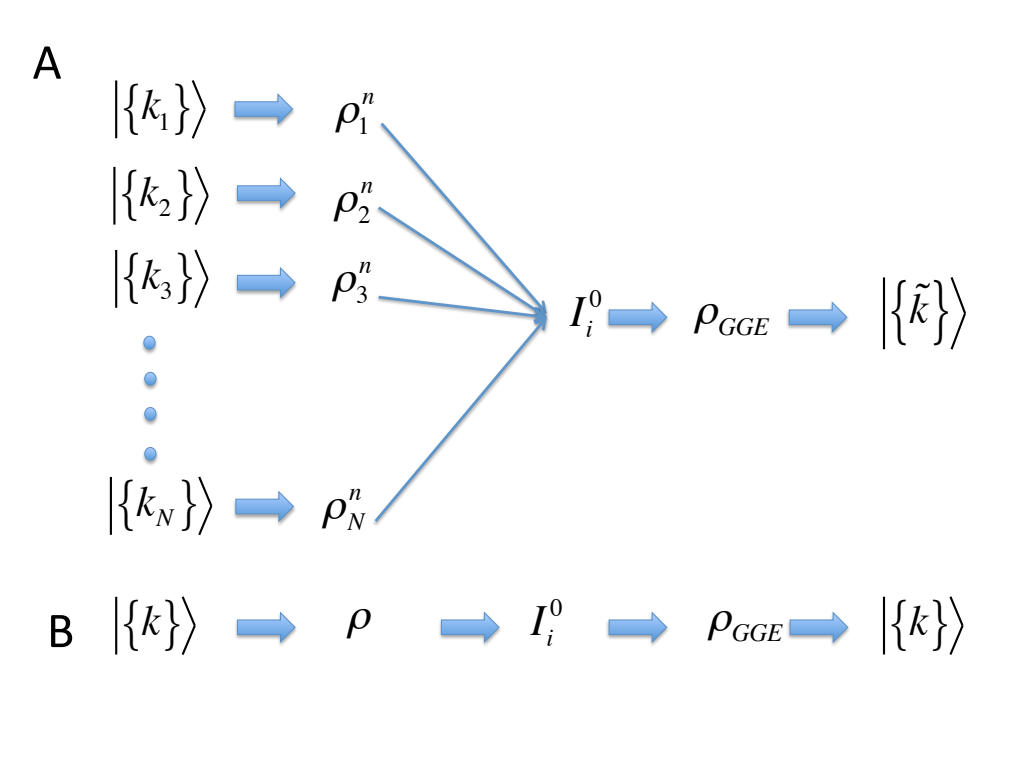
Role of bound states

XXZ spectrum: $n \geq 2$ strings are bound states of $n = 1$ magnons
in such a case the Q_i do not uniquely determine the ρ
GGE: maximum entropy with given Q_i
... but that is irrelevant ($\mathcal{S}[\{\tilde{k}\}] = -\infty$)!)



G. Goldstein and N. Andrei: Phys. Rev. A 90, 043625

Outline

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!

Indeed, this is how non-integrable systems thermalize.

However: GETH is broken!

B. Pozsgay: *Failure of the generalized eigenstate thermalization hypothesis in integrable models with multiple particle species*, J. Stat. Mech. (2014) P09026.

This also shows that GGE is broken for almost all initial states!

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Outline

Conclusions

1. The GGE description is not generally valid for genuinely interacting integrable systems.
2. Failure of GGE is caused by failure of the generalized eigenstate thermalization hypothesis. (Classical version: ergodicity on action-angle tori.)
3. Failure of GGE seems to be tied with existence of bound states.
4. The quench action correctly captures the steady state. However, it is a microscopic description!

Open issues

1. Are there more local charges? Very-very likely: NO!

2. Non-local charges?
   Known to exist for $-1 < \Delta < 1$, recently also for $\Delta > 1$!

   Must be careful (!) under what condition they can play a role:

   derivation of canonical from microcanonical ensemble assumes subsystem additivity of conserved quantities (e.g. energy)!

   Additivity is needed in TDL only: quasi-local charges?

3. Any other ideas?

The quest is open:

the ensemble describing the steady state of integrable systems is **presently unknown.**

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Pozsgai Balázs: Junior Prima Díj 2014