Nonequilibrium quantum physics: Exact steps

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How to DO theoretical physics?

Ludvig D. Faddeev vs. Phillip W. Anderson

according to: L.D. Faddeev, ‘After-dinner speech’, Rome, 2010

- ‘Top-down approach’
  *Principles, symmetries, conservation laws ⇒ models ⇒ phenomenology*

- ‘Bottom-up’ approach
  *Phenomenology, effects ⇒ models, simulations ⇒ principles, symmetries, conservation laws*
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Nonequilibrium quantum physics: Experiments!

Time evolution

Newton’s cradle with the ultracold bose-atom gas ($^{87}$Rb atoms) (Konishita, Wegner and Weiss, Nature 440, 900 (2006))
Relaxation and thermalization — Generalized Gibbs Ensemble

\[ |\Psi(t)\rangle\langle\Psi(t)| \rightarrow Z^{-1} \exp \left( -\sum_j \beta_j F_j \right), \quad F_2 \equiv H \]
\[ |\Psi(t)\rangle\langle\Psi(t)| \rightarrow Z^{-1} \exp \left( - \sum_j \beta_j F_j \right), \quad F_2 \equiv H \]

Observation of prethermalization and Generalized Gibbs ensemble


Gring et al. Science 337, 1318 (2012)
Precise experimental measurement of correlation functions

![Graphs illustrating the comparison of experimental and theoretical 4-, 6-, and 10-point correlation functions.](image)

As mentioned above, the key to this surprising result lies in the particular quench protocol that was employed.

This state was observed in a system that is very well described by an integrable model, experimentally.

Robinson bound limiting the spreading of information to a finite group velocity, as originally introduced for lattice spin models.

The GGE describes well away from the diagonal (cf. Fig. 9). The limits observed here extend these ideas to continuous experimental 4-, 6-, and 10-point correlation functions. Observation of a generalized Gibbs ensemble (GGE). (a) Two-point, 4-point, and 10-point correlation functions. (b) 6-point and 10-point correlation functions.
Expansion dynamics

FIG. 1. Experimental tools for the simulation of open quantum systems with ions. a, The coherent component is realized by collective $(U_X, U_Y, U^2, U^2_Y)$ and single-qubit operations $(U_{Z_i})$ on a string of $^{40}\text{Ca}^+$ ions which consists of the environment qubit (ion 0) and the system qubits (ions 1 through n). b, The dissipative mechanism on the ancilla qubit is realized in the two steps shown on the Zeeman-split $^{40}\text{Ca}^+$ levels by (1) a coherent transfer of the population from $|0\rangle$ to $|S'\rangle$ and (2) an optical pumping to $|1\rangle$ after a transfer to the $4^2P_{1/2}$ state by a circularly-polarised laser at 397 nm.
Open quantum system’s approach:
Canonical markovian master equation for the many-body density matrix:

The Lindblad (L-GKS) equation:

\[
\frac{d\rho}{dt} = \hat{L}\rho := -i[H, \rho] + \sum_\mu \left(2L_\mu \rho L_\mu^\dagger - \{L_\mu^\dagger L_\mu, \rho\}\right).
\]
Boundary-driven steady state paradigm

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\]

- **Bulk**: Fully coherent, local interactions, e.g. \(H = \sum_{x=1}^{n-1} h_{x,x+1}.
- **Boundaries**: Fully incoherent, ultra-local dissipation, jump operators \(L_{\mu}\) supported near boundaries \(x = 1\) or \(x = n\).
Markovian model on a $2^L$ dimensional probability state vector $\rho(t)$:

$$\frac{d}{dt}\rho = M\rho$$

Analog Classical problem: Asymmetric simple exclusion process

A paradigm of a non-equilibrium system

The asymmetric exclusion model with open boundaries

RESERVOIR

$1$ $2$ $3$ $4$ $5$ $L$

RESERVOIR

$\alpha$ $\gamma$ $\beta$ $\delta$
Analog Classical problem: Asymmetric simple exclusion process

Markovian model on a $2^L$ dimensional probability state vector $p(t)$:

$$\frac{d}{dt}p = Mp$$

Nonequilibrium steady state (NESS): a fixed point probability state vector $\bar{p}_\infty$

$$Mp_\infty = 0$$
Analog Classical problem: Asymmetric simple exclusion process

Markovian model on a $2^L$ dimensional probability state vector $\underline{p}(t)$:

$$\frac{d}{dt} \underline{p} = M\underline{p}$$

Nonequilibrium steady state (NESS): a fixed point probability state vector $\underline{p}_\infty$

$$M\underline{p}_\infty = 0$$

Applications: driven diffusive systems, traffic flow, hopping conductivity in solid electrolytes, Motion of RNA templates, Brownian motors, etc.

Let $A_0, A_1$ be a pair of matrices, and $\langle L|, |R\rangle$ a pair of left and right ‘vacua’.

MPA: \[ p_{s_1,s_2,\ldots,s_L} = \langle L| A_{s_1} A_{s_2} \cdots A_{s_L} |R\rangle, \quad s_j \in \{0, 1\} \]
Let $A_0, A_1$ be a pair of matrices, and $\langle L \mid, \mid R \rangle$ a pair of left and right ‘vacua’.

\[
\text{MPA : } p_{s_1,s_2,...,s_L} = \langle L \mid A_{s_1} A_{s_2} \cdots A_{s_L} \mid R \rangle, \quad s_j \in \{0, 1\}
\]

Asking such MPA $p$ to solve the Markov fixed point condition $Mp = 0$ results in a single algebraic relation in the bulk

\[
A_1 A_0 - q A_0 A_1 = (1 - q)(A_0 + A_1)
\]

with two boundary conditions

\[
\langle L \mid (\alpha A_0 - \gamma A_1) = \langle L \mid, \quad (\beta A_1 - \delta A_0)\mid R \rangle = \mid R \rangle
\]
Matrix Product Ansatz (MPA)

Let $A_0, A_1$ be a pair of matrices, and $\langle L |, | R \rangle$ a pair of left and right ‘vacua’.

\[
\text{MPA : } \quad \rho_{s_1,s_2,\ldots,s_L} = \langle L | A_{s_1} A_{s_2} \cdots A_{s_L} | R \rangle, \quad s_j \in \{0, 1\}
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\langle L | (\alpha A_0 - \gamma A_1) = \langle L |, \quad (\beta A_1 - \delta A_0) | R \rangle = | R \rangle
\]

This algebraic structure is enough to yield all physical observables in NESS!
Rich non-equilibrium phase diagram of TASEP (q=0)
Deterministic classical interacting system driven by stochastic boundaries

E^γ, δ, E^α, β ...


Exact solution for NESS exist in terms of a specific matrix product ansatz!
Quantum noninteracting problem: phase transition in a driven XY spin chain


\[ H = \sum_j^n \left( \frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right) \]

\[ L_1 = \frac{1}{2} \sqrt{\Gamma_1} \sigma_1^- \quad L_3 = \frac{1}{2} \sqrt{\Gamma_1} \sigma_n^- \]

\[ L_2 = \frac{1}{2} \sqrt{\Gamma_2} \sigma_1^+ \quad L_4 = \frac{1}{2} \sqrt{\Gamma_2} \sigma_n^+ \]

\[ C(j, k) = \langle \sigma_j^z \sigma_k^z \rangle - \langle \sigma_j^z \rangle \langle \sigma_k^z \rangle \]
Steady state Lindblad equation $\hat{L}\rho_\infty = 0$:

$$i[H, \rho_\infty] = \sum_\mu \left( 2L_\mu \rho_\infty L_\mu^\dagger - \{L_\mu^\dagger L_\mu, \rho_\infty\} \right)$$

The XXZ Hamiltonian:

$$H = \sum_{x=1}^{n-1} (2\sigma_x^+ \sigma_{x+1}^- + 2\sigma_x^- \sigma_{x+1}^+ + \Delta \sigma_x^z \sigma_{x+1}^z)$$

and in&out (source& sink) Lindblad jump operators:

$$L_1 = \sqrt{\varepsilon} \sigma_1^+, \quad L_2 = \sqrt{\varepsilon} \sigma_n^-.$$
Again, nonequilibrium phase transition in the steady state!

- For $|\Delta| < 1$, $\langle J \rangle \sim n^0$ (ballistic)
- For $|\Delta| > 1$, $\langle J \rangle \sim \exp(-\text{const}n)$ (insulating)
- For $|\Delta| = 1$, $\langle J \rangle \sim n^{-2}$ (anomalous)
Two-point spin-spin correlation function in NESS

\[
C \left( \frac{x}{n}, \frac{y}{n} \right) = \langle \sigma_x^z \sigma_y^z \rangle - \langle \sigma_x^z \rangle \langle \sigma_y^z \rangle
\]

for isotropic case \( \Delta = 1 \) (XXX)

\[
C(\xi_1, \xi_2) = -\frac{\pi^2}{2n} \xi_1 (1 - \xi_2) \sin(\pi \xi_1) \sin(\pi \xi_2), \text{ for } \xi_1 < \xi_2
\]
Exact solution for the steady state: Matrix product ansatz

\[ \rho_\infty = (\text{tr } R)^{-1} R, \quad R = \Omega \Omega^\dagger \]

\[ \Omega = \sum_{(s_1, \ldots, s_n) \in \{+, -, 0\}^n} \langle 0 | A_{s_1} A_{s_2} \cdots A_{s_n} | 0 \rangle \sigma^{s_1} \otimes \sigma^{s_2} \cdots \otimes \sigma^{s_n} = \langle 0 | \left( \begin{array}{cc} A_0 & A^+ \\ A^- & A_0 \end{array} \right)^\otimes n | 0 \rangle \]


**Exact solution for the steady state: Matrix product ansatz**

TP, PRL\textbf{106}(2011); PRL\textbf{107}(2011); Karevski, Popkov, Schütz, PRL\textbf{111}(2013)

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\[ A_0 = \sum_{k=0}^{\infty} a_k^0 |k\rangle \langle k|, \]

\[ A_+ = \sum_{k=0}^{\infty} a_k^+ |k\rangle \langle k+1|, \]

\[ A_- = \sum_{k=0}^{\infty} a_k^- |k+1\rangle \langle r|, \]
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\[
\begin{align*}
A_0 &= \sum_{k=0}^{\infty} a_k^0 |k\rangle \langle k|, \\
A_+ &= \sum_{k=0}^{\infty} a_k^+ |k\rangle \langle k+1|, \\
A_- &= \sum_{k=0}^{\infty} a_k^- |k+1\rangle \langle r|,
\end{align*}
\]

\[
\begin{align*}
a_k^0 &= \cos((s - k) \eta) & \cos \eta := \Delta, \\
a_k^+ &= \sin((k + 1) \eta) & \tan(\eta s) := \frac{\varepsilon}{2i \sin \eta} \\
a_k^- &= \cos((2s - k) \eta) & s \text{ is a q-deformed complex spin } q = e^{i \eta}
\end{align*}
\]
Local conservation laws

*Example:* Hamiltonian with local interactions

\[ H = \sum_{j} h_{j,j+1} \]
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Continuity equation — local conservation laws:

\[ \frac{d}{dt} h_{j,j+1} = i[H, h_{j,j+1}] = J_j - J_{j+1} \equiv -\nabla \cdot J, \quad J_j := i[h_{j-1,j}, h_{j,j+1}] \]

\( J_j \equiv \) energy current density
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\( J_j \equiv \) energy current density

In general: \( F \) some general extensive quantity, \( F = \sum_j f_j, f_j \) local around site \( j \).

From \([H, F] = 0 \) we have

\[ \frac{d}{dt} f_j = i[H, f_j] = g_j - g_{j+1} \]

\( g_j \equiv \) corresponding density of current of \( F \).
Near equilibrium transport and conservation laws

Green-Kubo formula:

$$\kappa(\omega) = \lim_{t \to \infty} \lim_{n \to \infty} \frac{\beta}{n} \int_0^t dt' e^{i\omega t} \langle J(t')J(0) \rangle_\beta$$

Divergence of d.c. conductivity defines the Drude weight $D$,

$$\kappa(\omega) = 2\pi D \delta(\omega) + \kappa_{\text{reg}}(\omega)$$

which again can be expressed in terms of a linear response formula

$$D = \lim_{t \to \infty} \lim_{n \to \infty} \frac{\beta}{2tn} \int_0^t dt' \langle J(t')J(0) \rangle_\beta$$
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\]

For integrable systems, Zotos et al. (1997) proposed to apply Mazur (1969) / Suzuki (1971) bound to estimate Drude weight in terms of conserved quantities \(F_j\), \([H, F_j] = 0\):

\[
D \geq \lim_{n \to \infty} \frac{\beta}{2n} \sum_j \frac{\langle JF_j \rangle^2}{\langle F_j^2 \rangle \beta}
\]

where operators \(F_j\) may be chosen mutually orthogonal \(\langle F_jF_k \rangle = 0, j \neq k\).
Conclusion: Integrable systems are ballistic conductors at any temperature, unless ...
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... unless all conserved quantities $F_j$ orthogonal to current operator $J$, $\langle JF_j \rangle = 0$, which may happen due to discrete symmetries.
‘Square root’ NESS $\rho_\infty \propto \Omega(s)\Omega^\dagger(s)$, $s = s(\varepsilon)$, generates non-Hermitian commuting family

$$[\Omega(s), \Omega(s')] = 0, \quad \forall s, s' \in \mathbb{C}$$
Nonequilibrium integrability

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$$[\Omega(s), \Omega(s')] = 0, \quad \forall s, s' \in \mathbb{C}$$

Derivative of such non-equilibrium ’transfer matrix’ defines a quasi-local conserved quantity

$$Z = \frac{d}{ds} \Omega(s)|_{s=0}, \quad \langle Z^\dagger Z \rangle \propto n.$$
Nonequilibrium integrability

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The operator $Z$ in fact defines a conservation law $Q = i(Z - Z^\dagger)$ with a continuity equation

$$[H, Q] = 2\sigma^z_1 - 2\sigma^z_n$$
Nonequilibrium integrability

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$Q$ is in fact the first-order of NESS

$$\rho_\infty \propto \mathbb{1} + \varepsilon Q + \mathcal{O}(\varepsilon^2).$$
Corollary: Rigorous lower bound on spin Drude weight

∃ spin flip symmetry \( P = \prod_j \sigma_j^x \): \([H, P] = 0\) ter \([F_j, P] = 0\) for all local conserved quantities \( F_j \), but \( PJ = -JP \), hence \( \langle F_j J \rangle = 0 \).
∃ spin flip symmetry $P = \prod_j \sigma_j^x$: $[H, P] = 0$ and $[F_j, P] = 0$ for all local conserved quantities $F_j$, but $PJ = -JP$, hence $\langle F_j J \rangle = 0$.

However, new conservation law has odd parity, $Q = i(Z - Z^\dagger)$, $PQ = -QP$, hence allows $\langle QJ \rangle \neq 0$. 
Corollary: Rigorous lower bound on spin Drude weight

\[ \exists \text{ spin flip symmetry } P = \prod_j \sigma_j^x: [H, P] = 0 \text{ and } [F_j, P] = 0 \text{ for all local conserved quantities } F_j, \text{ but } PJ = -JP, \text{ hence } \langle F_j J \rangle = 0. \]

However, new conservation law has odd parity, \( Q = i(Z - Z^\dagger) \), \( PQ = -QP \), hence allows \( \langle QJ \rangle \neq 0 \).

Fractal Mazur bound on Drude weight

\[
\frac{D}{\beta} \geq D_Z := \frac{\sin^2(\pi l/m)}{\sin^2(\pi/m)} \left( 1 - \frac{m}{2\pi} \sin \left( \frac{2\pi}{m} \right) \right), \quad \Delta = \cos \left( \frac{\pi l}{m} \right)
\]

TP, Ilievski, PRL 111, 057203 (2013); TP, NPB 886, 1177 (2014)
Generalized Gibbs ensemble $\rho_{GGE} = \exp(\sum_{j=1}^{n-1} \beta_j F_j)$ for the steady state after a quantum quench of XXZ Hamiltonian gives incorrect results!

$$H = \sum_{x=1}^{n-1} \left( 2\sigma_x^+ \sigma_{x+1}^- + 2\sigma_x^- \sigma_{x+1}^+ + \Delta \sigma_x^z \sigma_{x+1}^z \right)$$


![Graphs showing correlation functions](image)


**FIG. 1:** Numerical simulation of the time evolution of correlation functions (a) $\langle \sigma_i^z \sigma_j^z \rangle$, (b) $\langle \sigma_i^z \sigma_j^x \rangle$, (c) $\langle \sigma_i^x \sigma_j^x \rangle$.
Resolution of the puzzle: analytical construction of new QL charges

New quasilocal conserved charges [E. Ilievski, M. Medenjak, TP, PRL 115, 120601 (2015)] close the gap between GGE and QA:


\[ \langle \sigma_1^z \sigma_3^z \rangle \]

\[ \left| \delta \langle \sigma_1^z \sigma_3^z \rangle \right| \]

\[ \Delta \]

\[ \Delta \]

\[ \Delta \]

\[ \Delta \]
Consider 2s + 1 dimensional spin–s auxiliary space $\mathcal{H}_a = \mathcal{V}_s$ with SU(2) generators represented as

$$s^z|m\rangle = m|m\rangle, \quad s^\pm|m\rangle = \sqrt{(s + 1 \pm m)(s \mp m)}|m \pm 1\rangle$$

and define Lax operators acting over $\mathcal{H}_p \otimes \mathcal{H}_a, \mathcal{H}_p = \mathcal{V}_1^{\otimes n}$,

$$L_{x,a}(\lambda) = \lambda \mathbb{1} + \sigma^z_{x} s^z_{a} + \sigma^+_{x} s^-_{a} + \sigma^-_{x} s^+_{a} = \lambda \mathbb{1} + \vec{\sigma}_x \cdot \vec{s}_a,$$

in turn defining a commuting set of transfer matrices

$$T_s(\lambda) = \text{tr}_a L_{0,a}(\lambda)L_{1,a}(\lambda)\cdots L_{n-1,a}(\lambda),$$

$$[T_s(\lambda), T_{s'}(\lambda')] = 0, \quad \forall s, s', \lambda, \lambda'.$$
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\]

and define Lax operators acting over \(\mathcal{H}_p \otimes \mathcal{H}_a\), \(\mathcal{H}_p = \mathcal{V}_{1/2}^\otimes\),

\[
L_{x,a}(\lambda) = \lambda \mathbb{1} + \sigma^z s^z_a + \sigma^+_x s^-_a + \sigma^-_x s^+_a = \lambda \mathbb{1} + \vec{\sigma}_x \cdot \vec{s}_a,
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\]

\[
[T_s(\lambda), T_{s'}(\lambda')] = 0, \quad \forall s, s', \lambda, \lambda'.
\]

The fundamental TM \(T_{1/2}(\lambda)\) generates all local charges as

\[
F_k = -i \partial_t^{k-1} \log T_{1/2}(\frac{1}{2} + it)|_{t=0},
\]

with \(H_{XXX} = Q_2\).
Theorem (PRL 115, 120601 (2015)):

Traceless operators $X_s(t)$, $s \in \frac{1}{2} \mathbb{Z}^+$, $t \in \mathbb{R}$, defined as

\[
X_s(t) = [\tau_s(t)]^{-n} \left\{ T_s\left( -\frac{1}{2} + it \right) T'_s\left( \frac{1}{2} + it \right) \right\},
\]

\[
\tau_s(t) = -t^2 - \left( s + \frac{1}{2} \right)^2,
\]

where $T'_s(\lambda) \equiv \partial_\lambda T_s(\lambda)$ and $\{A\} \equiv A - (\text{tr } A) \mathbb{1}/(\text{tr } \mathbb{1})$, are quasilocal for all $s$, $t$ and linearly independent from $\{F_k; k \geq 2\}$ for $s > \frac{1}{2}$. 

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Nonequilibrium quantum physics
Theorem (PRL 115, 120601 (2015)):

Traceless operators \( X_s(t) \), \( s \in \frac{1}{2} \mathbb{Z}^+ \), \( t \in \mathbb{R} \), defined as

\[
X_s(t) = [\tau_s(t)]^{-n} \{ T_s(-\frac{1}{2} + it) T'_s(\frac{1}{2} + it) \},
\]

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\tau_s(t) = -t^2 - (s + \frac{1}{2})^2,
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where \( T'_s(\lambda) \equiv \partial_\lambda T_s(\lambda) \) and \( \{ A \} \equiv A - (\text{tr} A) \mathbb{1} / (\text{tr} \mathbb{1}) \), are quasilocal for all \( s, t \) and linearly independent from \( \{ F_k; k \geq 2 \} \) for \( s > \frac{1}{2} \).

Inspiration: for \( s = 1/2 \), TM is asymptotically, \( n \to \infty \), a unitary operator

\[
T_{1/2}(\frac{1}{2} + it) \simeq \exp \left( \sum_{k=1}^\infty F_{k+1} t^k / k! \right),
\]

[Fagotti and Essler, JSTAT P07012 (2013)] hence \( X_{1/2}(t) \) is a logarithmic derivative, since \( T_s^\dagger(\lambda) \equiv T_s^T(\overline{\lambda}) = (-1)^n T_s(-\overline{\lambda}) \).
Conclusions and open problems

- Quasi-local charges exist in integrable lattice models and are as relevant for non-equilibrium physics and relaxation to equilibrium as the local ones!
- Stability of quasilocal charges and integrable nonequilibrium steady states against perturbations?
- Quantum field theories?
- Classical integrable lattice systems?
- Integrable bosonic lattices/field theories?

Acknowledgements:
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