Closed quantum systems out of equilibrium

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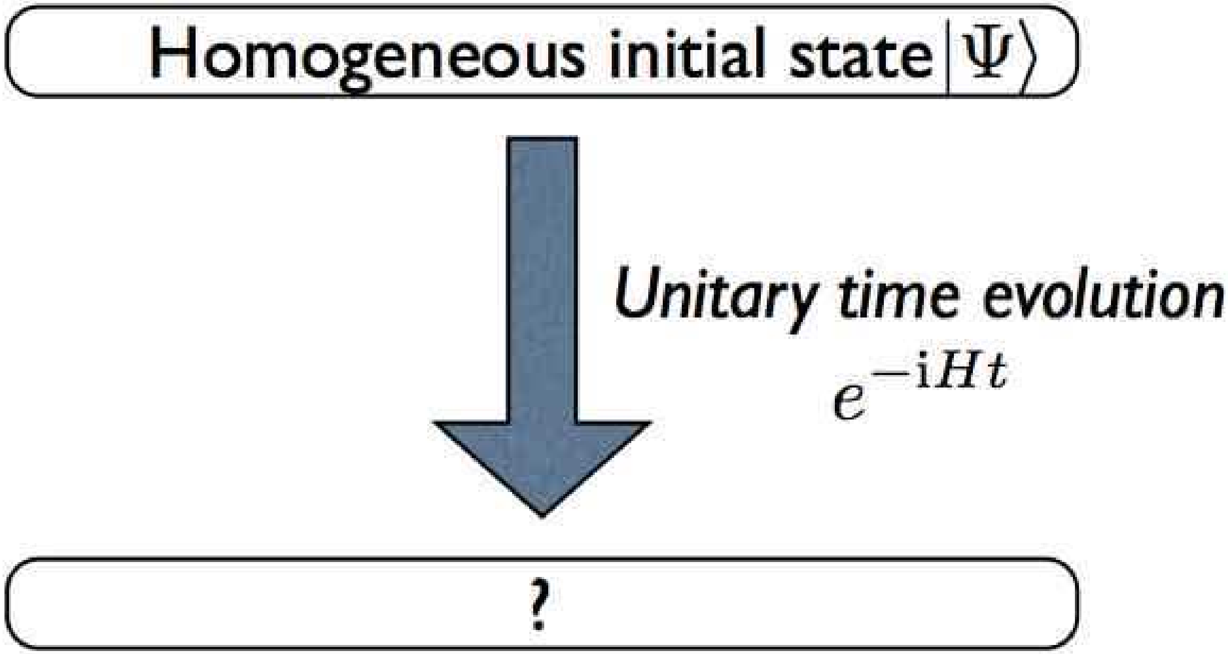
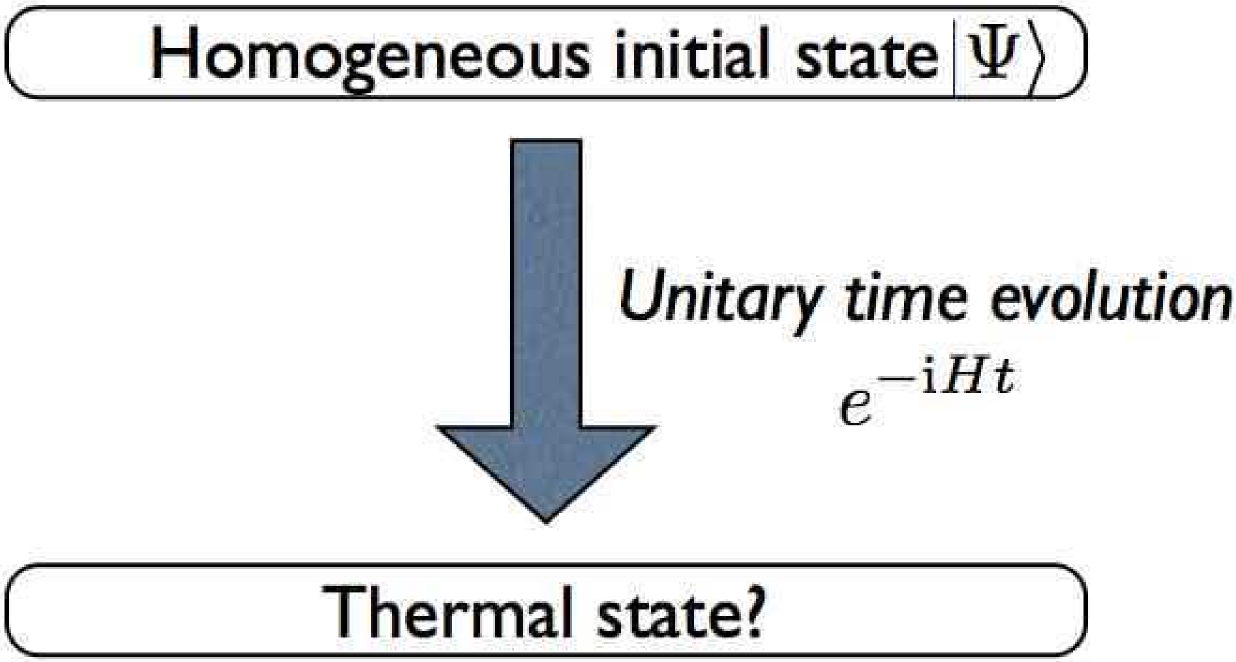
I. Some interesting questions from non-equilibrium physics...


Homogeneous initial state $|\Psi\rangle$
Unitary time evolution
$e^{-\mathrm{i}Ht}$
?


Homogeneous initial state $|\Psi\rangle$
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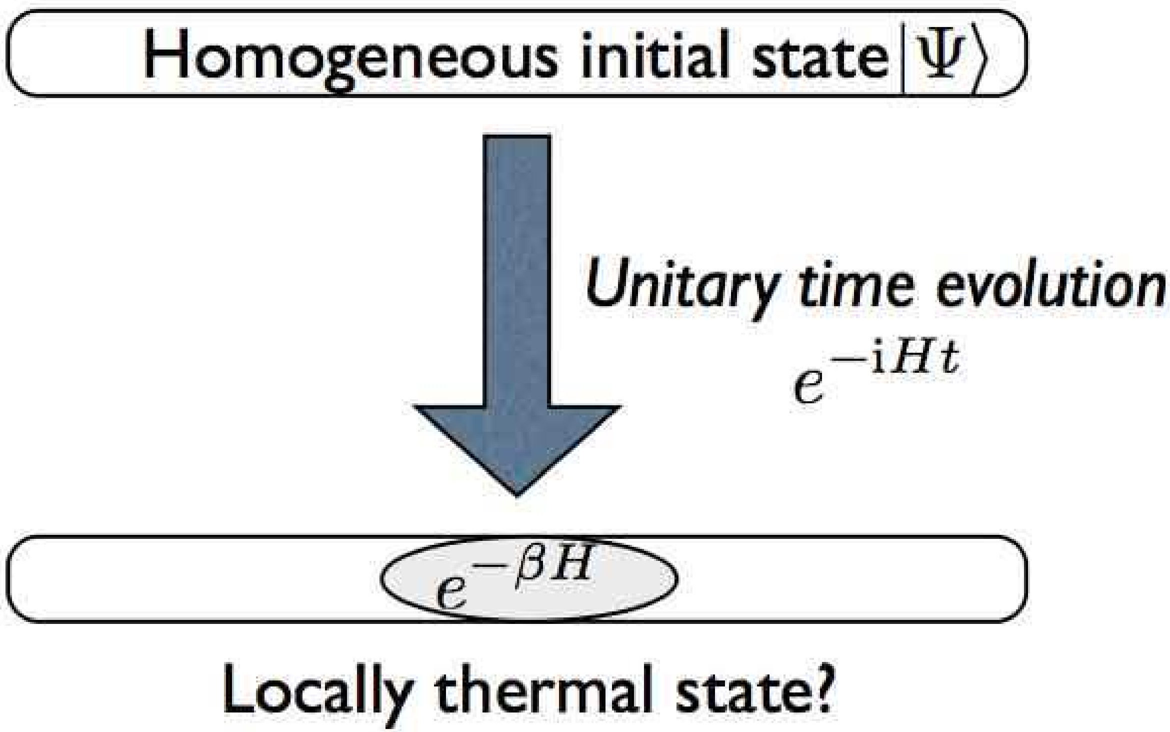
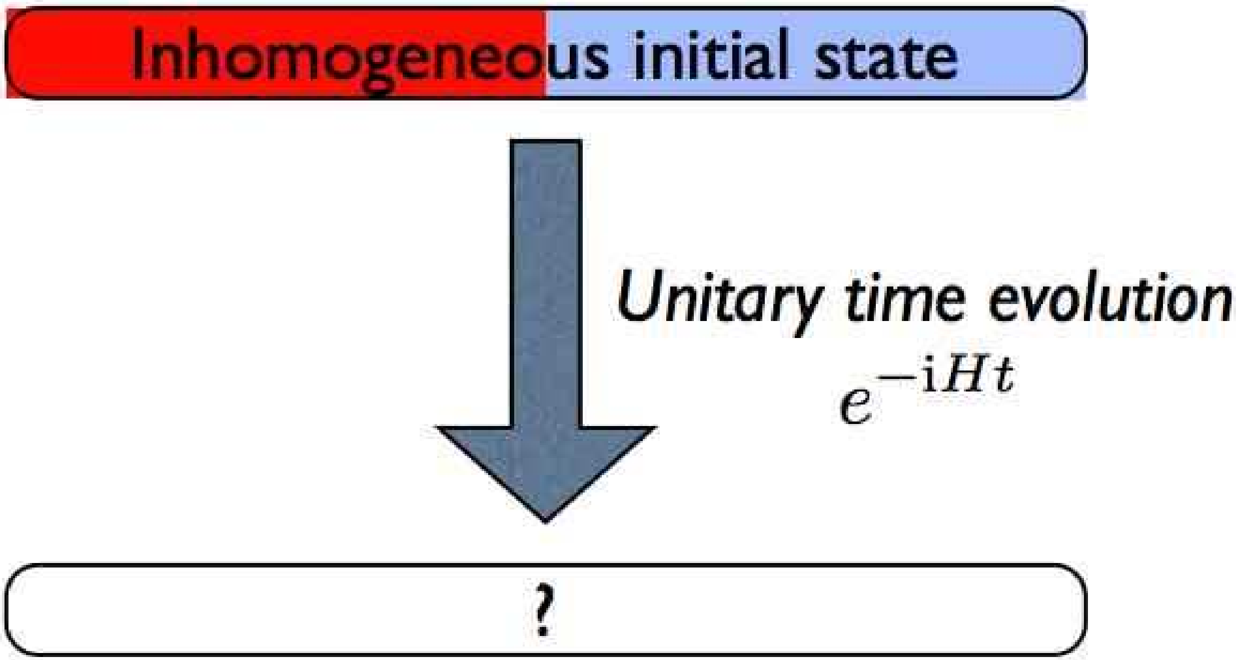
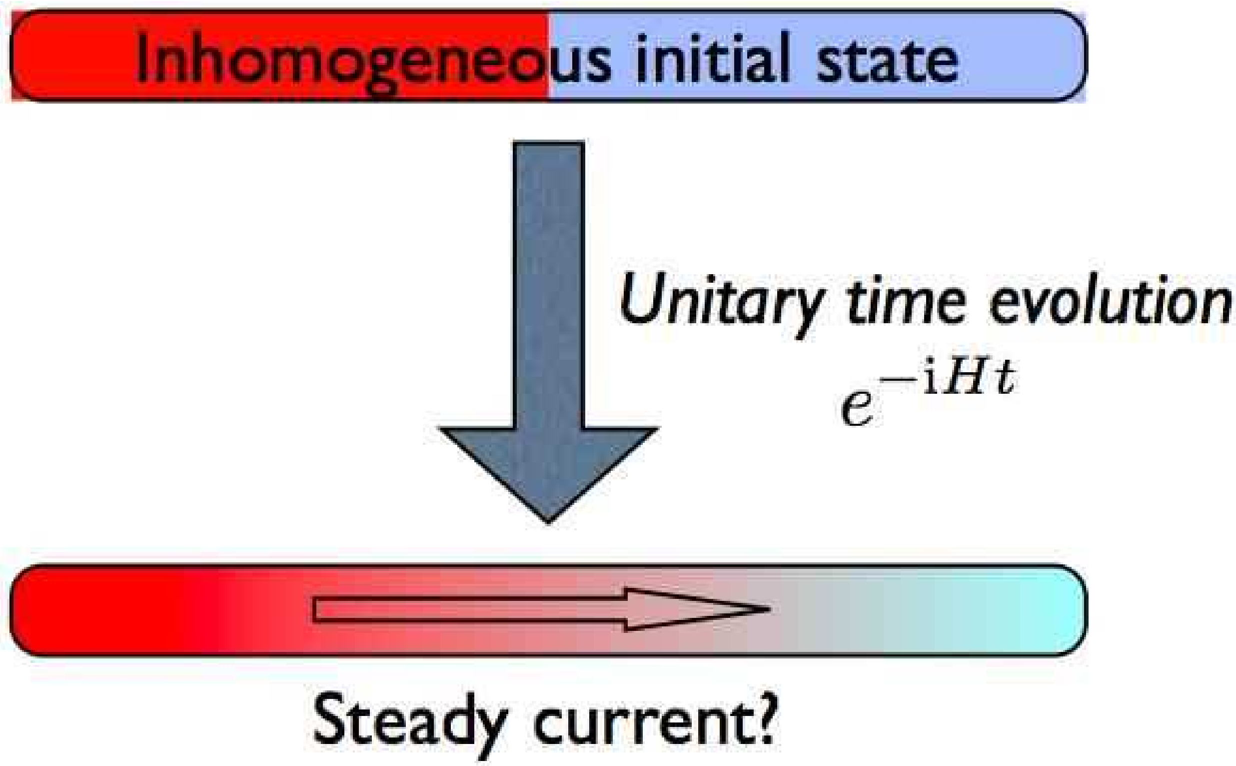
Thermal state?


Homogeneous initial state $|\Psi\rangle$
Unitary time evolution
$e^{-\mathrm{i}Ht}$
$e^{-\beta H}$
Locally thermal state?


Inhomogeneous initial state
Unitary time evolution
e^{-iHt}
?



Inhomogeneous initial state
Unitary time evolution
$e^{-\mathrm{i}Ht}$
Steady current?

Setup – quasi-local $C^\star$ algebras

Consider hypercubic lattice $\mathbb{Z}^{\mathtt{D}}$, on each site a copy of $\mathbb{C}^N$. Space of local observables $\mathcal{O}$ is completed to $C^\star$-algebra $\mathcal{A}$. Natural translation isomorphism $A \mapsto \iota_x(A) = A(x)$. With $h \in \mathcal{O}$ a local observable, homogeneous Hamiltonian of density h has formal expression

$$H = \sum_{x \in \mathbb{Z}^{\mathtt{D}}} h(x).$$

With $\mathtt{B}(n)$ "ball" of radius n centered at origin, partial sums are $H^{(n)} = \sum_{x \in \mathtt{B}(n)} h(x)$, and $\tau_t^H(A) = \lim_{n\to\infty} e^{\mathrm{i}H^{(n)}t} A e^{-\mathrm{i}H^{(n)}t}$ ($A \in \mathcal{O}$), which extends continuously to $\mathcal{A}$. A (β, H)-KMS state ω satisfy $\omega(AB) = \omega(\tau^H_{-\mathrm{i}\beta}(B)A)$. An example is given by the infinite-volume limit (for $A \in \mathcal{O}$, extended to $\mathcal{A}$ by continuity)

$$\omega_\beta^H(A) = \lim_{n\to\infty} \frac{\mathrm{Tr}_{\mathcal{H}^{(n)}}\left(\exp\left[-\beta H^{(n)}\right] A\right)}{\mathrm{Tr}\left(\exp\left[-\beta H^{(n)}\right]\right)}$$

[Araki 1969; ... For textbooks see: Bratteli, Robinson 1997]

Thermalization in extended systems

If the large-time limit $\lim_{t\to\infty} \Psi(\tau_t^H(A))$ exists (relaxation),
in what situations does it equal $\omega(A)$ for some (β, H)-KMS state ω (thermalization)?

[Some recent rigorous results: Reimann, Kastner 2012; Riera, Gogolin, Eisert 2012; Müller, Adlam, Masanes, Wiebe 2015. Reviews: Polkovnikov, Sengupta, Silva, Vengalattore 2011; Yukalov 2011; Gogolin, Eisert 2015; Eisert, Friesdorf, Gogolin 2015; BD 2017].

Eigenstate thermalization hypothesis (simplified version)

Denote $|\Psi_n\rangle : n = 1, 2, 3, \ldots$ a sequence of $H^{(n)}$-eigenstates in balls $\mathtt{B}(n)$. Assume that the following limit exists and equal $\lim_{n\to\infty} \langle \Psi_n | h | \Psi_n \rangle = e$, where h is the density of H.

In what situation does the large-volume limit give $\lim_{n\to\infty} \langle \Psi_n | A | \Psi_n \rangle = \omega(A)$

for some (β, H)-KMS state ω?

That is:

"In Hamiltonian eigenstates $|\Psi\rangle$ of a thermodynamic system, with $H|\Psi\rangle = E|\Psi\rangle$,

the average $\langle \Psi | A | \Psi \rangle$ is a thermal average."

[Jensen, Shankar 1985; Deutsch 1991; Srednicki 1994; Rigol, Dunjko, Olshanii 2008]

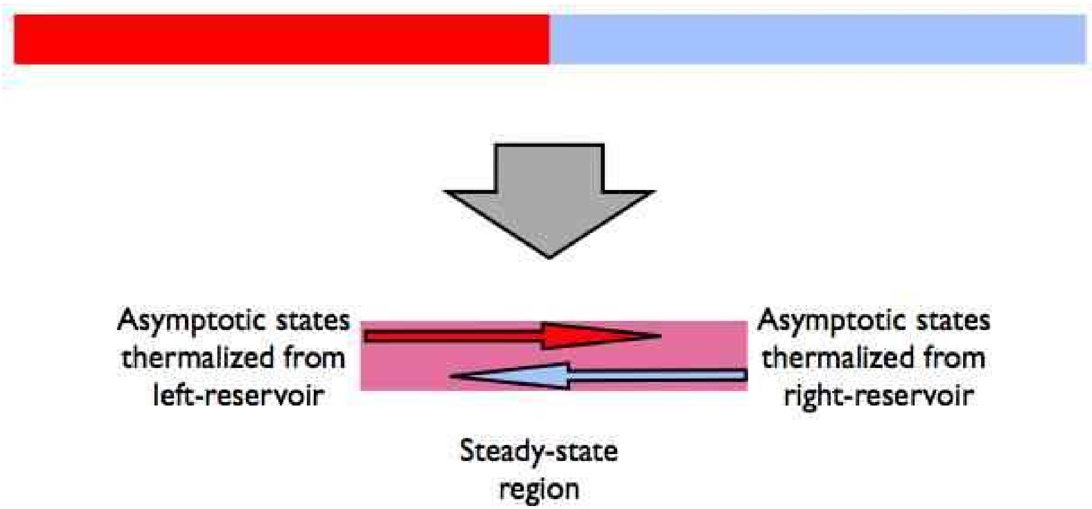
Or perhaps more generally:

"Any suitable H-stationary state ω is a (β, H)-KMS state."

Steady states and the partitioning protocol

Let $\Psi = \Psi_l \otimes \Psi_r$ be the tensor product of two states, one acting on the left subalgebra $\mathcal{A}_l = \mathcal{A}_{(-\infty,0)\times\mathbb{Z}^{\mathrm{D}-1}}$, the other on the right subalgebra $\mathcal{A}_r = \mathcal{A}_{[0,\infty)\times\mathbb{Z}^{\mathrm{D}-1}}$.

If the large-time limit $\lim_{t\to\infty} \Psi(\tau_t^H(A))$ exists (relaxation),
in what situations does it generate a non-equilibrium steady state ω
($\omega \circ \tau_t^H = \omega$, and ω is not invariant under time reversal)?



[Spohn, Lebowitz 1977; Ruelle 2000; Bernard, BD 2012; Hollands, Longo 2016;Castro-Alvaredo, BD, Yoshimura 2016; Bertini, Collura, De Nardis, Fagotti 2016; Review (physics): Bernard, BD 2016]

A unifying idea

"The large time limit is a H-stationary state ω that is a (β, Q)-KMS state for some local enough Q that commutes with H."

Let Q_i be **local charges**, $Q_i = \sum_{x\in\mathbb{Z}^{\mathrm{D}}} q_i(x)$ with $q_i \in \mathcal{O}$ that are **conserved**, $[H, q_i] \in \oplus_{x\in\mathbb{Z}^{\mathrm{D}}} \mathrm{im}(\iota_x - 1)$ (that is, formally $\sum_x [H, q_i(x)] = 0$).

Then, formally, the stationary state "density operator", in **all the above cases**, has the form

$$\exp\left[-\sum_i \beta_i Q_i\right]$$

This maximizes entropy under the constraints of the average values of Q_i.

- **Thermalization.** If the only local conserved charge is H itself, then the above idea implies thermalization,

$$\exp\left[-\beta H\right]$$

- **Flows in CFT.** Take the example of CFT in dimension $\mathtt{D}$ (not a quantum lattice so outside our setup, but similar ideas apply...). Natural local conserved charges are the Hamiltonian H and the momenta $\vec{P}$. Then

$$\exp\left[-\beta H + \vec{\nu}\cdot\vec{P}\right].$$

  Stationary states are Lorentz boosts of thermal states.

  [Bernard, BD 2012; Bhaseen, BD, Lucas, Schalm 2015; Hollands, Longo 2016]

Generalized thermalization and generalized Gibbs ensembles

But what if the system is **integrable**? There are infinitely many Q_i...

The state corresponding to the formal density operator

$$\exp\left[-\sum_{i=1}^{\infty}\beta_i Q_i\right]$$

is called a **generalized Gibbs ensemble** (GGE). The process of reaching a GGE is generalized thermalization.

[Jaynes 1957; Rigol, Muramatsu, Olshanii 2006; Rigol, Dunjko, Yurovsky, Olshanii 2007; Review: Essler, Fagotti (2016)]

In fact, it was found in some examples that **quasi-local conserved charges** whose densities have **exponentially decaying tails**, must be included in the GGE expression.

[Ilievski, Medenjak, Prosen, Zadnik 2013 – 2016; Pereira, Pasquier, Sirker, Affleck 2014; Ilievski, De Nardis, Wouters, Caux, Essler, Prosen 2015]

Exponentially decaying tails? Perhaps:

$$|| \, [q_i(x), A(y)] \, || < C||A|| \, e^{-\,\mathrm{dist}(x,y)/\xi} \quad \forall A \in \mathcal{O}_{\{0\}}$$

GGEs are at the basis of a great many studies of non-equilibrium physics in closed integrable quantum systems. This includes “quantum quenches”, as well as (more recently) transport in inhomogeneous cases through the notion of generalized hydrodynamics [Castro-Alvaredo, BD, Yoshimura 2016; Bertini, Collura, De Nardis, Fagotti 2016].

GGEs form an infinite-dimensional manifold of states.

How to characterize this manifold? How is the formal sum $\sum_i \beta_i Q_i$ converging?

What conditions guarantee generalized thermalization? ...

II. A generalized thermalization theorem

Based on BD, Commun. Math. Phys. 351, 155 (2017)

Instead of looking to define and characterize (β, Q)-KMS states for appropriately quasi-local conserved charges Q, I use a different method.

Remark that, thanks to $\mathrm{d}e^{-\beta H}/\mathrm{d}\beta = -He^{-\beta H}$, we have

$$-\frac{\mathrm{d}}{\mathrm{d}\beta}\omega_\beta^H(A) = \sum_{x\in\mathbb{Z}^{\mathrm{D}}} \left[\frac{1}{2}\omega_\beta^H\big(h(x)A + Ah(x)\big) - \omega_\beta^H(h)\omega_\beta^H(A)\right]$$

This can be used to define (β, H)-KMS states for high enough temperatures (when there is unicity). This is what I generalize to charges with extended locality properties.

Clustering and integrated correlation functions

Clustering condition: at large distances, correlations between local observables decay fast enough, faster than distance$^{-\mathtt{D}}$ (recall $\mathtt{D}$ = dimension of space).

Definition. Let ω be a state. We say that ω is *sizably clustering* if there exist $\nu, a > 0$ and $p > \mathtt{D}$ such that for every $\ell > 0$ and every $A, B \in \mathcal{O}$ of sizes $|A|, |B| < \ell$, we have

$$\Big|\omega(AB) - \omega(A)\omega(B)\Big| \leq \nu\ell^a \, ||A|| \, ||B|| \, \mathrm{dist}(A,B)^{-p}.$$

(With some more general function $\nu(\ell)$ in place of $\nu\ell^a$ the state is simply *clustering*.)

This guarantees finiteness of integrated correlation functions (clustering is sufficient):

$$\langle\langle A, B\rangle\rangle_\omega := \sum_{x\in\mathbb{Z}^{\mathtt{D}}} \left[\frac{1}{2}\omega\big(A^\star(x)B + BA^\star(x)\big) - \omega(A^\star)\omega(B)\right]$$

The Hilbert space of correlation functions

The sesquilinear form $\langle\langle\cdot,\cdot\rangle\rangle$ is non-negative on $\mathcal{O}$. It has a null space $\widehat{\mathcal{N}}_\omega$ that contains $\mathrm{im}(\iota_x - 1)$. Taking the quotient $\widehat{\mathcal{L}}_\omega = \mathcal{O}/\widehat{\mathcal{N}}_\omega$ we obtain a non-degenerate inner product. We can thus extends $\widehat{\mathcal{L}}_\omega$ to a Hilbert space $\widehat{\mathcal{H}}_\omega$ (similar to GNS construction).

High-temperature Gibbs states

Time-evolved high-temperature Gibbs states are uniformly sizably clustering.

Let $\omega_\beta^{H_0}$ and τ_t^H be associated to possibly **different local Hamiltonians**.

Theorem. There exists $\beta_* > 0$ [Kliesch, Gogolin, Kastoryano, Riera, Eisert 2014] (with $\beta_* = \infty$ in one dimension $\mathtt{D} = 1$ [Araki 1969]) such that the sizably clustering property holds uniformly for $\omega_\beta^{H_0} \circ \tau_t^H$ in every compact subset of $\{|\beta| < \beta_*, t \in \mathbb{R}\}$.

[Araki 1969; Lieb, Robinson 1972; Bravyi, Hastings, Verstraete 2006; Kliesch, Gogolin, Kastoryano, Riera, Eisert 2014; BD 2016]

Pseudolocality

[Prosen 1998, 1999, 2011; BD 2017]

A pseudolocal charge (conserved or not) is the limit of a sequence of observables Q_n, supported on balls $\mathtt{B}(n)$ centered at the origin and of growing radius n, with in particular the condition that their second cumulants diverge at most like the volume.

Three conditions (assume without loss of generality $\omega(Q_n) = 0$) :

I. *Volume growth.* There exists $\gamma > 0$ such that $\omega(\{Q_n^\star, Q_n\}) \leq \gamma n^{\mathtt{D}}$ for all $n > 0$.

II. *Limit action.* For every $A \in \mathcal{O}$, $\widehat{Q}_\omega(A) := \lim_{n\to\infty} \frac{1}{2}\omega(\{Q_n^\star, A\})$ exists in $\mathbb{C}$.

III. *Bulk homogeneity.* There exists $0 < k < 1$ such that for every $A \in \mathcal{O}$,

$$\lim_{n\to\infty} \max_{x,y\in\mathtt{B}(kn)} |\omega(\{Q_n^\star, A(x)\}) - \omega(\{Q_n^\star, A(y)\})| = 0.$$

The limit action $\widehat{Q}_\omega$ is referred to as a **pseudolocal charge** with respect to ω. We denote the linear space of pseudolocal charges with respect to ω as $\widehat{\mathcal{Q}}_\omega$.

A subset of pseudolocal charges is that of **local charges**, obtained from **sequences of partial sums**,

$$n \mapsto Q_n = \sum_{x \in \mathrm{B}(n)} A(x)$$

for any $A \in \mathcal{O}$. The associated limit action is the correlation function,

$$\widehat{Q}_\omega(B) = \sum_{x \in \mathbb{Z}^{\mathrm{D}}} \left(\frac{1}{2} \omega(\{A(x), B\}) - \omega(A)\omega(B) \right) = \langle\langle A, B \rangle\rangle_\omega$$

Theorem. [BD 2017] Let ω be a clustering state on $\mathcal{O}$. There exists a bijection $\widehat{\mathfrak{D}} : \widehat{\mathcal{Q}}_\omega \to \widehat{\mathcal{H}}_\omega$ such that, for every $Q_\omega \in \mathcal{Q}_\omega$ and every $A \in \mathcal{O}$,

$$Q_\omega(A) = \langle\langle \widehat{\mathfrak{D}}(Q_\omega), A \rangle\rangle_\omega.$$

In particular, $\widehat{Q}_\omega$ can be extended to a continuous linear functional on $\widehat{\mathcal{H}}_\omega$.

Quasilocal charges [Ilievski, Prosen 2013], whose densities have **exponentially decaying tails**, are also pseudolocal charges.

A **clustering property** holds (similar to an asymptotic differentiation property) [BD 2017]:

$$\lim_{\mathrm{dist}(B,C)\to\infty} \widehat{Q}_\omega(BC) = \widehat{Q}_\omega(B)\omega(C) + \omega(B)\widehat{Q}_\omega(C)$$

A larger family of states: pseudolocal states

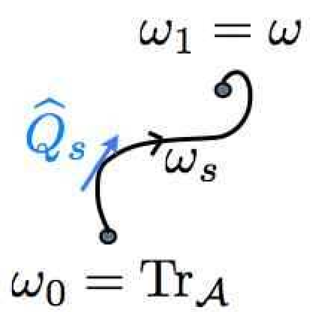
[BD 2017]

We extend the family of high-temperature Gibbs states using pseudolocal charges. Since (formally) $\mathrm{d}e^{-\beta H}/\mathrm{d}\beta = -He^{-\beta H}$, we have

$$-\frac{\mathrm{d}}{\mathrm{d}\beta}\omega_\beta^H(A) = \langle\langle h, A\rangle\rangle_{\omega_\beta^H} = \widehat{H}_{\omega_\beta^H}(A)$$

We interpret $\widehat{H}_{\omega_\beta^H}$ as a **tangent vector at the "point"** ω_β^H, and this is a **"flow equation"** along a curve that connects ω_β^H to the **infinite-temperature state** $\mathrm{Tr}_{\mathcal{A}}$ at $\beta = 0$.

A pseudolocal state is a state at the end-point of a curve connecting it to the infinite-temperature state, and whose tangent is determined by pseudolocal charges.



The integrated version is more useful in practice:

Definition. Let $\{\omega_s : s \in [0,1]\}$ be a one-parameter family of uniformly sizably clustering states, with $\omega_1 = \omega$ and $\omega_0 = \mathrm{Tr}_{\mathcal{A}}$. If there exists a one-parameter family $\{\widehat{Q}_s \in \widehat{\mathcal{Q}}_{\omega_s} : s \in [0,1]\}$ of uniformly bounded pseudolocal charges such that, for every $A \in \mathcal{O}$, the function $s \mapsto \widehat{Q}_s(A)$ is Lebesgue integrable on $[0,1]$ and

$$\omega_s(A) = \mathrm{Tr}_{\mathcal{A}}(A) + \int_0^s \mathrm{d}s' \, \widehat{Q}_{s'}(A),$$

then we say that ω is a **pseudolocal state**.

Theorem. High-temperature Gibbs states are pseudolocal states.

Theorem. If ω is a pseudolocal state and τ_t^H is a time evolution associated to a local Hamiltonian H, then $\omega \circ \tau_t^H$ is a pseudolocal state for all $t \in \mathbb{R}$.

Stationarity and conserved charges

We denote

$$[H, A] = \sum_{x \in \mathbb{Z}^{\mathrm{D}}} [h(x), A]$$

(note: the sum is finite!)

A clustering state is stationary if $\omega([H, A]) = 0$ for all $A \in \mathcal{O}$.

In a stationary state, the condition that a pseudolocal charge $\widehat{Q}_\omega$ be **conserved** is simply $\widehat{Q}_\omega([H, A]) = 0$ for all $A \in \mathcal{O}$.

(Intuitively, $\omega(Q[H, A]) = \omega([Q, H]A) = 0$.)

Generalized Gibbs ensembles

We then have a natural definition of **generalized Gibbs ensembles**:

A generalized Gibbs ensemble with respect to H is a pseudolocal state whose entire flow is stationary with respect to H.

Definition. [BD 2017] A GGE with respect to H is a pseudolocal state ω with the property that for almost all $s \in [0,1]$, we have $\omega_s([H,A]) = 0$ and $\widehat{Q}_s([H,A]) = 0$ for all $A \in \mathcal{O}$.

Intuitively and formally, the GGE "density operator" would be a product of **path-ordered exponentials** of pseudolocal conserved charges:

$$\rho^{\rm GGE} = \overleftarrow{\mathcal{P}\exp} \int_0^1 {\rm d}s\, Q(s) \cdot \overrightarrow{\mathcal{P}\exp} \int_0^1 {\rm d}s\, Q(s) \quad \text{instead of} \quad \rho^{\rm GGE} = e^{-\sum \beta_i Q_i}$$

Generalized thermalization

Under conditions of uniform clustering and existence of large-time dynamical response functions, the large-time limit of a time-evolved pseudolocal state exists and is a GGE.

Theorem. [BD 2017] Let τ_t^H be an evolution dynamics, and let ω be a pseudolocal state with flow $\{\omega_s : s \in [0,1]\}$. Suppose

(a) $\{\omega_s \circ \tau_t^H : (s,t) \in [0,1] \times [0,\infty)\}$ is uniformly sizably clustering, and

(b) for every $A, B \in \mathcal{O}$ and almost all $s \in [0,1]$, the limit $\lim_{t\to\infty} \langle\langle \tau_t^H(A), B\rangle\rangle_{\omega_s}$ exists in $\mathbb{C}$.

Then the limit $\omega^{\rm sta} := \lim_{t\to\infty} \omega \circ \tau_t^H$ exists ($\star$-weakly) and is a GGE with respect to the evolution Hamiltonian H.

Integrability vs non-integrability?

What about thermalization in non-integrable model? We need a “definition” of non-integrability.

Consider a local Hamiltonian H. It is **completely mixing** if it does not possess conserved pseudolocal charges other than scalar multiples of itself.

Definition. [BD 2017] A local hamiltonian H is completely mixing if for every stationary clustering state ω, the condition that $\widehat{Q}_\omega$ be conserved ($\widehat{Q}_\omega([H,A]) = 0$ for all $A \in \mathcal{O}$) implies $\widehat{Q}_\omega = \lambda \widehat{H}_\omega$ for some $\lambda \in \mathbb{C}$.

A re-thermalization theorem

A pseudolocal state whose entire flow is stationary with respect to a completely mixing local Hamiltonian must be a high-temperature Gibbs state with respect to this Hamiltonian.

The inverse temperature is

$$\beta = -\int_0^1 \mathrm{d}s\, \lambda(s)$$

where $\lambda(s)$ is the proportionality constant in $\widehat{Q}_s = \lambda(s)\widehat{H}_{\omega_s}$.

This implies a **re-thermalization theorem** under the "quantum quench" $H_0 \to H$

Theorem. Suppose

(a) $\{\omega_s^{H_0} \circ \tau_t^H : (s,t) \in [0,\beta] \times [0,\infty)\}$ is uniformly sizably clustering,

(b) for every $A, B \in \mathcal{O}$ and almost all $s \in [0,\beta]$, the limit $\lim_{t\to\infty} \langle\langle \tau_t^H(A), B\rangle\rangle_{\omega_s^{H_0}}$ exists in $\mathbb{C}$, and

(c) the H is completely mixing.

Then $\omega_\beta^{\mathrm{sta}} = \lim_{t\to\infty} \omega_\beta^{H_0} \circ \tau_t^H$ is a high-temperature Gibbs state with respect to H.

Geometry and the second law of thermodynamics

The Hilbert space structure suggests an infinite-dimensional Riemannian manifold of quantum states. Is there a aelation between geometry and (non-equilibrium) thermodynamics?

Consider the distance from a pseudolocal state ω to the infinite-temperature state $\mathrm{Tr}_{\mathcal{A}}$: the minimal length over all paths connecting $\mathrm{Tr}_{\mathcal{A}}$ to ω,

$$\mathsf{Dist}(\omega) = \inf \left\{ \int_0^1 \mathrm{d}s \, ||\widehat{Q}_s|| : \begin{array}{l} s \mapsto \widehat{Q}_s \in \widehat{\mathcal{Q}}_{\omega_s} \text{ tangent to } s \mapsto \omega_s \\ \omega_0 = \mathrm{Tr}_{\mathcal{A}}, \; \omega_1 = \omega \end{array} \right\}$$

If $\omega^{\mathrm{sta}} = \lim_{t\to\infty} \omega \circ \tau_t^H$ exists in the sense of generalized thermalization theorem, then

$$\mathsf{Dist}(\omega) \geq \mathsf{Dist}(\omega^{\mathrm{sta}})$$

That is, there is a preorder on the set of pseudolocal states determined by infinite-time evolution $\Rightarrow$ second law of thermodyanmics.

A “fluctuation-dissipation” theorem

Commutators are response functions,

$$\mathrm{i}\omega([H, A])$$

while anti-commutators are correlation functions,

$$\langle\langle h, A\rangle\rangle_\omega.$$

A relation between response functions and correlation functions is a fluctuation-dissipation theorem.

There exists a continuous linear map $\mathcal{M}_\omega : \widehat{\mathcal{H}}_\omega \to \widehat{\mathcal{H}}_\omega$ such that

$$\mathrm{i}\omega([H, A]) = \langle\langle \mathcal{M}_\omega(h), A\rangle\rangle_\omega$$

for all $A \in \mathcal{O}$.

Conclusions

- Framework, directly in infinite systems, for non-equilibrium quantum dynamics and for generalized Gibbs ensembles, based on pseudolocal charges. Suggests other results, such as "If all Rényi entropies satisfy a volume law, then the state is a pseudolocal state" $\Rightarrow$ ETH...
- Are GGEs, as defined here, really some (β, Q)-KMS state for appropriate β, Q? How are they related to standard structures of integrability?
- Similar framework for IQFT? Connection with scattering states?
- Use similar framework in other non-equilibrium situations? E.g. non-homogeneous initial states, non-equilibrium steady states? Local GGEs [Castro-Alvaredo, BD, Yoshimura 2016; Bertini, Collura, De Nardis, Fagotti 2016], description in terms of the quasi-particles of Bethe ansatz?