Thermalization and pseudolocality in extended quantum systems

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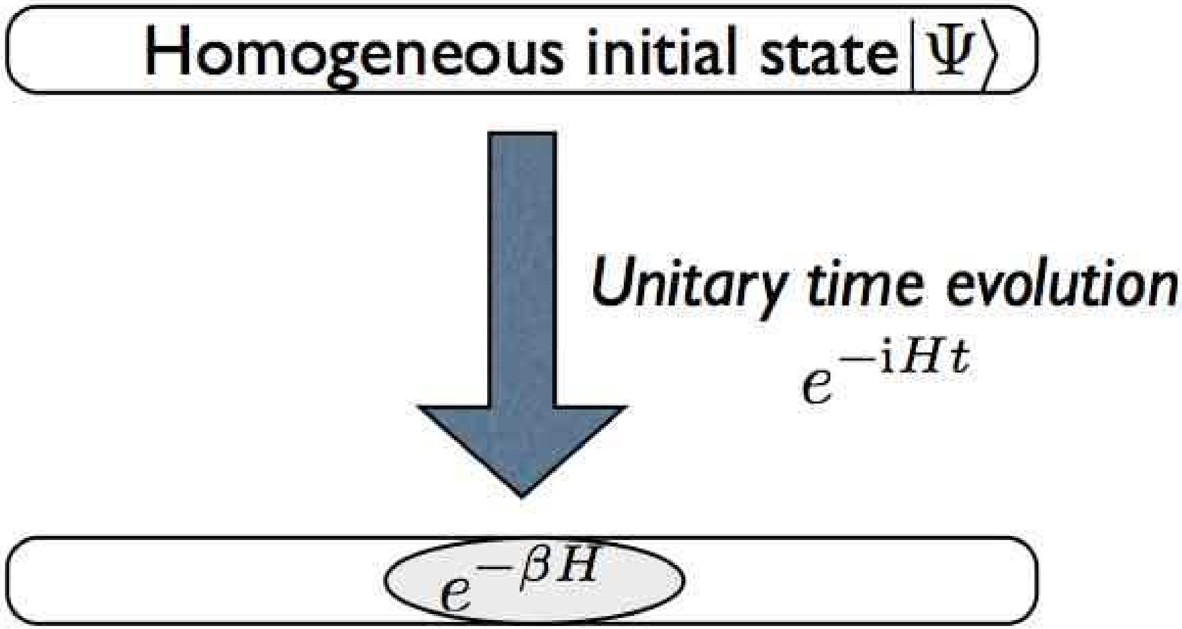


Locally thermal state?

Thermalization in extended systems

Consider a hypercubic lattice Λ of dimension $\mathtt{D}$ and linear size L, and on each site a finite-dimensional space $\mathbb{C}^N$.

Let $|\Psi\rangle$ be some normalized state vector, and $\Psi(A) := \langle\Psi|A|\Psi\rangle$ for observables A.
Let H be some evolution Hamiltonian, and $\tau_t(A) := e^{\mathrm{i}Ht}Ae^{-\mathrm{i}Ht}$.

The thermal state at inverse temperature β is

$$\omega_\beta^{\mathrm{th}}(A) := \frac{\mathrm{Tr}(e^{-\beta H}A)}{\mathrm{Tr}(e^{-\beta H})}$$

Consider all of the above in an appropriate **thermodynamic limit** $L \to \infty$.

If the large-time limit $\lim_{t\to\infty}\Psi(\tau_t(A))$ exist (equilibration),
in what situations does it equal $\omega_\beta^{\mathrm{th}}(A)$ (thermalization)?

[Quench protocols: Iglói, Rieger 2000; Altman, Auerbach 2002; Sengupta, Powell, Sachdev 2004; Calabrese, Cardy 2006] [Reviews on thermalization: Polkovnikov, Sengupta, Silva, Vengalattore 2011; Yukalov 2011; Gogolin, Eisert 2015; Eisert, Friesdorf, Gogolin 2015].

Eigenstate thermalization hypothesis

"In Hamiltonian eigenstates $|\Psi\rangle$ of a thermodynamic system, with $H|\Psi\rangle = E|\Psi\rangle$, the average $\langle\Psi|A|\Psi\rangle$ is only a function of the local observable A and the energy E. Further, it is a thermal average."

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

Denote $|\Psi_L\rangle : L = 1, 2, 3, \ldots$ a sequence of H-eigenstates in quantum lattices of linear sizes L. Assume that $\lim_{L\to\infty}\langle\Psi_L|h|\Psi_L\rangle = e$ where h is density of H. Then:

$$\lim_{L\to\infty}\langle\Psi_L|A|\Psi_L\rangle = f(A, e)$$

where $f(A, e)$ depends smoothly on e. Further,

$$f(A, e) = \omega^{\mathrm{th}}_{\beta(e)}(A).$$

"$\Rightarrow$ Stationary states must be thermal (thermalization)."

Generalized thermalization and generalized Gibbs ensembles

Clearly the above only works if the H-dynamics "does not possess local conserved charges other than H itself". If there exists many conserved charges $H_1(= H),\ H_2,\ H_3,\ldots$:

- With infinitely-many H_i one considers **generalized Gibbs ensembles**, formally [Jaynes 1957; Rigol, Muramatsu, Olshanii 2006; Rigol, Dunjko, Yurovsky, Olshanii 2007]

$$\omega^{\mathrm{GGE}}(A) = \lim_{L\to\infty} \frac{\mathrm{Tr}\left(e^{-\sum_i \beta_i H_i} A\right)}{\mathrm{Tr}\left(e^{-\sum_i \beta_i H_i}\right)}$$

- A natural generalization of the ETH is [cf. Caux, Essler 2013]

$$\lim_{L\to\infty} \langle \Psi_L | A | \Psi_L \rangle = \omega^{\mathrm{GGE}}(A)$$

  where β_i's are smooth functions of the quantities $\lim_{L\to\infty} \langle \Psi_L | h_i | \Psi_L \rangle$

- If stationary state is ω^{GGE}, the process is **generalized thermalization.** [Cazalilla 2006; Calabrese, Cardy 2007; Cramer, Dawson, Eisert, Osborne 2008; Barthel, Schollwöck 2008; ...]

In fact, it was found in some examples that **quasi-local conserved charges** [Ilievski, Medenjak, Prosen, Zadnik 2013 – 2016; Pereira, Pasquier, Sirker, Affleck 2014], whose densities have **exponentially decaying tails**, must be used in the GGE expression.

[...; Ilievski, De Nardis, Wouters, Caux, Essler, Prosen 2015]

Many questions remain...

- Meaning and definition of generalized Gibbs ensembles. What is the meaning of

$$\lim_{L\to\infty} \frac{\mathrm{Tr}\left(e^{-\sum_i \beta_i H_i} A\right)}{\mathrm{Tr}\left(e^{-\sum_i \beta_i H_i}\right)}?$$

  Convergence of $\sum_i \beta_i H_i$? Is $\sum_i \beta_i H_i$ still quasi-local, or can it be any non-local conserved charge? How to fundamentally characterize the GGE "density matrices"? Is generalized thermalization meaningful?

- Conditions for thermalization / generalized thermalization. What conditions guarantee thermalization or generalized thermalization?

  [For recent rigorous results: Reimann, Kastner 2012; Riera, Gogolin, Eisert 2012; Müller, Adlam, Masanes, Wiebe 2015; Gluza, Krumnow, Friesdorf, Gogolin, Eisert 2016]

The $C^\star$-algebra structure

[Araki 1969; ...; Kliesch, Gogolin, Kastoryano, Riera, Eisert 2014. Textbooks: Bratteli, Robinson 1997]

- Space of local observables $\mathcal{O}$ may be completed under operator norm $||\cdot||$ to a $C^\star$-algebra $\mathcal{A}$. There is a natural translation $\star$-isomorphism $A \mapsto A(x),\ x \in \Lambda$.

- A state ω is a continuous linear functional on $\mathcal{A}$ normalized to $\omega(\mathbf{1}) = 1$. We assume translation invariance.

- With $h \in \mathcal{O}$ a local observable, a local Hamiltonian has the formal expression $H = \sum_{x\in\Lambda} h(x)$. Denoting $\mathtt{B}(n)$ the "ball" of radius n centered at the origin, we may define $H^{(n)} = \sum_{x\in\mathtt{B}(n)} h(x)$, the partial sums of the formal expression.

- One can show that $\lim_{n\to\infty} e^{\mathrm{i}H^{(n)}t} A e^{-\mathrm{i}H^{(n)}t}$ and $\lim_{n\to\infty} \frac{\mathrm{Tr}(e^{-\beta H^{(n)}} A)}{\mathrm{Tr}(e^{-\beta H^{(n)}})}$ exist for any local $A \in \mathcal{O}$, and define, respectively, a strongly continuous one-parameter unitary group, and a translation-invariant state, on $\mathcal{A}$.

A re-thermalization theorem

Clustering and susceptibilities

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 susceptibilities (clustering is sufficient):

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

Gibbs states

Time-evolved Gibbs states are analytic and uniformly sizably clustering.

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

Theorem. [BD 2015] Let

$$\beta_* := \begin{cases} \frac{1}{2||h||} \log \left[\frac{1+\sqrt{1+2/(\mathtt{D}e)}}{2}\right] & (\mathtt{D} > 1) \\ \infty & \mathtt{D} = 1. \end{cases}$$

[Kliesch, Gogolin, Kastoryano, Riera, Eisert 2014, Araki 1969]

(i) The sizably clustering property holds uniformly for $\omega_\beta^{\mathrm{th}} \circ \tau_t$ in every compact subset of $\{|\beta| < \beta_*, t \in \mathbb{R}\}$.

(ii) For every $t \in \mathbb{R}$ and $A \in \mathcal{A}$, the function $\omega_\beta^{\mathrm{th}}(\tau_t(A))$ is analytic on $|\beta| < \beta_*$.

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

Re-thermalization theorem

Let $\omega_\beta^{\rm th}$ and τ_t be associated to possibly different local Hamiltonians.

Under conditions of uniform clustering, existence of large-time dynamical susceptibilities, and the time evolution being **completely mixing**, the large-time limit of a time-evolved Gibbs state exists and is a Gibbs state.

Theorem. [BD 2015] Suppose there exists a neighborhood K of $[0,\beta]$ such that:

(a) $\{\omega_s^{\rm th}\circ\tau_t : (s,t)\in K\times[0,\infty)\}$ is uniformly sizably clustering,

(b) for every $A,B\in\mathcal{O}$ and almost all $s\in K$, the limit $\lim_{t\to\infty}\langle\langle\tau_t(A),B\rangle\rangle_{\omega_s^{\rm th}}$ exists in $\mathbb{C}$, and

(c) the τ_t dynamics is completely mixing.

Then $\omega_\beta^{\rm sta}$ is a thermal Gibbs state with respect to H.

How do we define "completely mixing"? We need **pseudolocality**.

Pseudolocality

[Prosen 1998, 1999, 2011; Ilievski, Prosen 2013; BD 2015]

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 WLOG $\omega(Q_n) = 0$ for all n):

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**,

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

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

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

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

- A **clustering property** holds (similar to an asymptotic derivation property) [BD 2015]:

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

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

- The generator $\mathfrak{L}H$ of time evolution of local observables $A \in \mathcal{O}$ is (the sum is finite)

$$\mathfrak{L}H(A) = \sum_{x\in\Lambda}[h(x), A]$$

- A clustering state ω is stationary if $\omega(\mathfrak{L}H(A)) = 0$ for all $A \in \mathcal{O}$.
- In a stationary state, the condition that a pseudolocal charge $\widehat{Q}_\omega$ be conserved is simply $\widehat{Q}_\omega(\mathfrak{L}H(A)) = 0$ for all $A \in \mathcal{O}$.

$$\widehat{Q}_\omega(\mathfrak{L}H(A)) = \lim_n \omega\big(\{Q_n, [H, A]\}\big) = -\lim_n \omega\big(\{[H, Q_n], A\}\big) = 0$$

Definition. [BD 2015] A local hamiltonian H is *completely mixing* if for every stationary clustering state ω, the condition that $\widehat{Q}_\omega$ be conserved implies $\widehat{Q}_\omega = \lambda \widehat{H}_\omega$ for some $\lambda \in \mathbb{C}$.

A larger family of states: pseudolocal states

[BD 2015]

In order to get stronger results, we extend the family of Gibbs states using pseudolocal charges. Since $\mathrm{d}e^{-\beta H}/\mathrm{d}\beta = -He^{-\beta H}$, we have

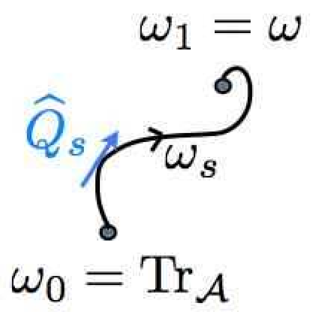
$$-\frac{\mathrm{d}}{\mathrm{d}\beta}\omega_\beta^{\mathrm{th}}(A) = \langle\langle h, A\rangle\rangle_{\omega_\beta^{\mathrm{th}}} = \widehat{H}_{\omega_\beta^{\mathrm{th}}}(A)$$

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

Generalize:

$$\frac{\mathrm{d}}{\mathrm{d}s}\omega_s(A) = \widehat{Q}_s(A), \quad \omega_0 = \mathrm{Tr}_{\mathcal{A}}$$

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.



Formally, the "density matrix" would be a product of **path-ordered exponentials**:

$$\overleftarrow{\mathcal{P}\exp}\int_0^1 \mathrm{d}s\, Q_s \cdot \overrightarrow{\mathcal{P}\exp}\int_0^1 \mathrm{d}s\, Q_s$$

The integrated version is more useful in practice:

Definition. [BD 2015] Let $\{\omega_s : s \in [0,1]\}$ be a one-parameter family of uniformly bounded, 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. Thermal Gibbs states are pseudolocal states.

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

A stationary-state thermalization theorem
(in the spirit of ETH)

Any analytic pseudolocal state whose entire flow is stationary with respect to a completely mixing local Hamiltonian must be a thermal Gibbs state with respect to this Hamiltonian.

Here analytic means that, for any $A \in \mathcal{O}$, the function $\omega_s(A)$ is an analytic function of s in some neighborhood of $[0,1]$.

Theorem. Let H be a completely mixing local Hamiltonian, and let ω be an analytic pseudolocal state with the property that $\omega_s(\mathfrak{L}H(A)) = 0$ for all $s \in [0,1]$ and all $A \in \mathcal{O}$. Then ω is a thermal Gibbs state with respect to H. The inverse temperature is

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

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

Generalized Gibbs ensembles

More generally, 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 2015] A GGE with respect to H is a pseudolocal state ω with the property that for almost all $s \in [0,1]$, we have $\omega_s(\mathfrak{L}H(A)) = 0$ and $\widehat{Q}_s(\mathfrak{L}H(A)) = 0$ for all $A \in \mathcal{O}$.

- Formally, the GGE "density matrix" would be a product of **path-ordered exponentials** of pseudolocal **conserved charges**:

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

- This definition is mathematically accurate, and also accounts for cases where conserved charges generate **non-commuting flows** [cf. Fagotti 2014, Cardy 2015].

Generalized thermalization

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

Theorem. [BD 2015] Let τ_t be an evolution dynamics, and let ω be a pseudolocal state with flow $\{\omega_s : s \in [0,1]\}$. Suppose

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

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

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

Main structure for the proofs: Hilbert space

[BD 2015; cf Prosen 1998, 1999]

● Susceptibilities give rise to a Hilbert space structure.

Consider the positive semidefinite sesquilinear form $\langle\langle A, B\rangle\rangle_\omega$ and its null space $\widehat{\mathcal{N}}$, and Cauchy-complete the quotient space $\mathcal{O}/\widehat{\mathcal{N}}$ (similar to GNS construction). Hilbert space $\widehat{\mathcal{H}}_\omega$.

● There is a bijection between this Hilbert space and the space of pseudolocal charges.
Elements of the Hilbert space are the **densities** of pseudolocal charges.

Given $\widehat{Q}_\omega \in \widehat{\mathcal{Q}}_\omega$ there exists $A \in \widehat{\mathcal{H}}_\omega$ such that

$$\widehat{Q}_\omega(B) = \langle\langle A, B\rangle\rangle_\omega \quad \forall\ B \in \mathcal{O}.$$

The opposite also holds. Recall for local charges: $Q = \sum_{x\in\Lambda} A(x)$ for $A \in \mathcal{O}$.

● Any pseudolocal charge can be extended to a continuous linear functional on $\widehat{\mathcal{H}}_\omega$.
Any continuous linear functional on $\widehat{\mathcal{H}}_\omega$ is a pseudolocal charge.

Conclusions

- Framework, directly in infinite systems, for non-equilibrium quantum dynamics and for generalized Gibbs ensembles, based on pseudolocal charges.
- A geometric re-interpretation of quantum dynamics? Hilbert space structure $\longrightarrow$ infinite-dimensional Riemannian manifold of quantum states? Relation between geometry and (non-equilibrium) thermodynamics?
- "If all Rényi entropies satisfy a volume law, then the state is a pseudolocal state" $\Rightarrow$ ETH?
- Connection with GGE results? E.g. do quasi-local conserved charges found in [Ilievski, De Nardis, Wouters, Caux, Essler, Prosen 2015] form a basis of conserved pseudolocal charges?
- Use similar framework in other non-equilibrium situations? E.g. non-homogeneous initial states, non-equilibrium steady states? Connection with a quantum large-deviation theory?