LORENZO CAMPOS VENUTI (USC)

ERGODICITY, EIGENSTATE THERMALIZATION, AND THE FOUNDATION OF CLASSICAL AND QUANTUM STAT-MECH

Lorenzo Campos Venuti
Lawrence Liu

arXiv:1904.02336

IARPA
BE THE FUTURE

AFRL
AIR FORCE RESEARCH LABORATORY

DOLOMITES
JULY 2019

USC Dornsife
Dana and David Dornsife
College of Letters, Arts and Sciences

GENERAL QUESTION

Question: How do we build equilibrium statistical mechanics starting from the microscopic laws?

Classical laws (Newton)

Quantum laws

What is ergodicity here?

One possibility is Boltzmann's ergodic hypothesis (to be proved in actual models)

One possibility is ETH [Deutsch91, Srednicki94, Berry77, Rigol-Dunjko-Olshanii08] (to be proved in actual models)

Large math literature: Shnirelman74, Zeldtich87, Sunada97, Rudnik&Sarnak94, Hassell08…

SETTING THE STAGE: (QUASI-) ISOLATED Q SYSTEM

$$H = \sum_n E_n \Pi_n$$

Eigendecomposition (finite dim)

Energy constrained to $V \subset \sigma(H)$

Energy shell

e.g. $V = \{E_n | \overline{E} \leq E_n \leq \overline{E} + |\Delta\}$

$$\Pi_V = \sum_{E_n \in V} \Pi_n$$

Projector

$$\mathcal{H}_V = \mathrm{Ran}(\Pi_V)$$

Energy shell's Hilbert space

$$N_V = \mathrm{Tr}(\Pi_V) = \dim(\mathcal{H}_V)$$

Dimension

$$\mathcal{S}_V$$

Set of quantum states supported in H_V

$$\langle A \rangle_V = \mathrm{Tr}(A\rho_V),$$

Statistical average

Ideally:

$$\left(\rho_V = \frac{\Pi_V}{N_V}\right)$$

Microcanonical state

More generally $\boldsymbol{\rho}_V$ invariant $\Rightarrow$ $\rho_V = \sum_{E_n \in V} f_n \Pi_n$

EIGENSTATE THERMALIZATION HYPOTHESIS (ETH)

ETH:

$$\Pi_n A \Pi_m \simeq \langle A \rangle_V \Pi_n \delta_{n,m} \qquad E_n, E_m \in V$$

$$\Pi_n A \Pi_n \simeq \langle A \rangle_V \Pi_n$$ **ETH-D (Diagonal)**

For non-degenerate levels:

$$\langle E_n | A | E_m \rangle \simeq \langle A \rangle_V \delta_{n,m}$$

Implications:

$$\left(\overline{f} := \lim_{T \to \infty} \frac{1}{T} \int_0^T dt\, f(t) \right)$$

$\rho_0 \in \mathcal{S}_V$

$$\overline{\mathrm{Tr}[A(t)\rho_0]} = \mathrm{Tr}\left(\sum_n \Pi_n A \Pi_n \rho_0 \right) \simeq \langle A \rangle_V \mathrm{Tr}(\rho_0) = \langle A \rangle_V$$

ETH

Proposition 0 If observable *A* satisfies ETH-D then *A* thermalizes (for all initial states)

Definition 1 Observable *A* thermalizes if $\overline{\mathrm{Tr}[A(t)\rho_0]} = \langle A \rangle_V \quad \forall \rho_0 \in \mathcal{S}_V$

ETH-D → thermalization

What about ← **?**

Abanin, E. Altman, I. Bloch, and M. Serbyn arXiv:1804.11065

Ergodicity, Entanglement and Many-Body Localization:

et al., 2016). While all known examples of thermalizing systems obey ETH, at present it is not clear if ETH is a necessary condition for thermalization.

What about ergodicity?

Often taken as synonym for thermalization:

[1] We note that in the context of quantum many-body systems the term ergodicity is defined somewhat differently compared to classical mechanics. Our use of this term is synonymous with thermalization, as discussed in Section II.A.

ETH-INTERLUDE

Theorem Let (M, g^t, μ) be a dynamical system. M measure space, g^t flow, μ g^t-invariant measure (normalized). The following are equivalent:

1. For any (almost) invariant set $X \subseteq M$, either $\mu(X)=0$ or $\mu(X)=1$.

   aka metric indecomposability

2. For any two functions $f,g \in L^\infty(M,\mu)$

$$\overline{\langle f(t) g \rangle_\mu} = \langle f \rangle_\mu \langle g \rangle_\mu$$

3. For any $f \in L^1(M,\mu)$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T dt f(g^t(x_0)) = \langle f \rangle_\mu$$

   for almost any initial point x_0

QUANTUM DYNAMICAL SYSTEMS

Definition Observable A is shell-ergodic if $\overline{\langle A(t)A\rangle_V} = \left(\langle A\rangle_V\right)^2$

(characterization 2.)

✓

Proposition 1 Observable A is shell-ergodic if and only if $\overline{A(t)}\Pi_V = \langle A\rangle_V \Pi_V$

(characterization 3.)

✓

Proposition 2 Observable A thermalizes if and only if is shell-ergodic

✓

Proposition 3 Observable A is shell-ergodic if and only if it satisfies ETH-D

ETH-D ⟺ ergodicity ⟺ thermalization

METRIC INDECOMPOSABILITY

What about characterization 1.? **Heisenberg evolution:** $\mathcal{E}_t^* : \ \mathcal{E}_t^*(A) = e^{itH} A e^{-itH}$

Shell-ergodicity for all observables *A* $\overline{A(t)}\Pi_V = \langle A \rangle_V \Pi_V$

$$\mathcal{T}(X) := \overline{\mathcal{E}_t^*}(\Pi_V X \Pi_V) = \Pi_V \langle X \rangle_V$$

$$\mathcal{T} = |\Pi_V\rangle\rangle\langle\langle\rho_V|$$ **Moreover**

$$\mathcal{T} = \mathcal{T}^* \ \Rightarrow \ \rho_V = \frac{\Pi_V}{N_V} =: \rho_{MC}$$

However: NOT possible unless H_V is one-dimensional!

Thermalization only for *some* observables

BETTER DEFINITIONS

Definition 1′ Observable *A* thermalizes with precision **ε** if

$$\left| \overline{\mathrm{Tr}\,(A(t)\rho_0)} - \langle A \rangle_V \right| \leq \epsilon \, \|A\|$$

Definition 2′a Observable *A* is shell-ergodic with precision **ε** if

$$\left| \overline{\langle A(t) A \rangle_V} - (\langle A \rangle_V)^2 \right| \leq \epsilon^2 \|A\|^2$$

Definition 2′b Observable *A* is strong shell-ergodic with precision **ε** if

$$\left\| \left(\overline{A(t)} - \langle A \rangle_V \right) \Pi_V \right\| \leq \epsilon \, \|A\|$$

Definition 3′ Observable *A* satisfies ETH-D to precision **ε** if

$$\| \, \Pi_n A \Pi_n - \langle A \rangle_V \Pi_n \, \| \leq \epsilon \|A\|$$ **for all** $E_n \in V$

Non degeneracy $\longrightarrow$ $\left| \langle n | A | n \rangle - \langle A \rangle_V \right| \leq \epsilon \|A\|$

REMARK: WHAT ABOUT THE STEADY STATE?

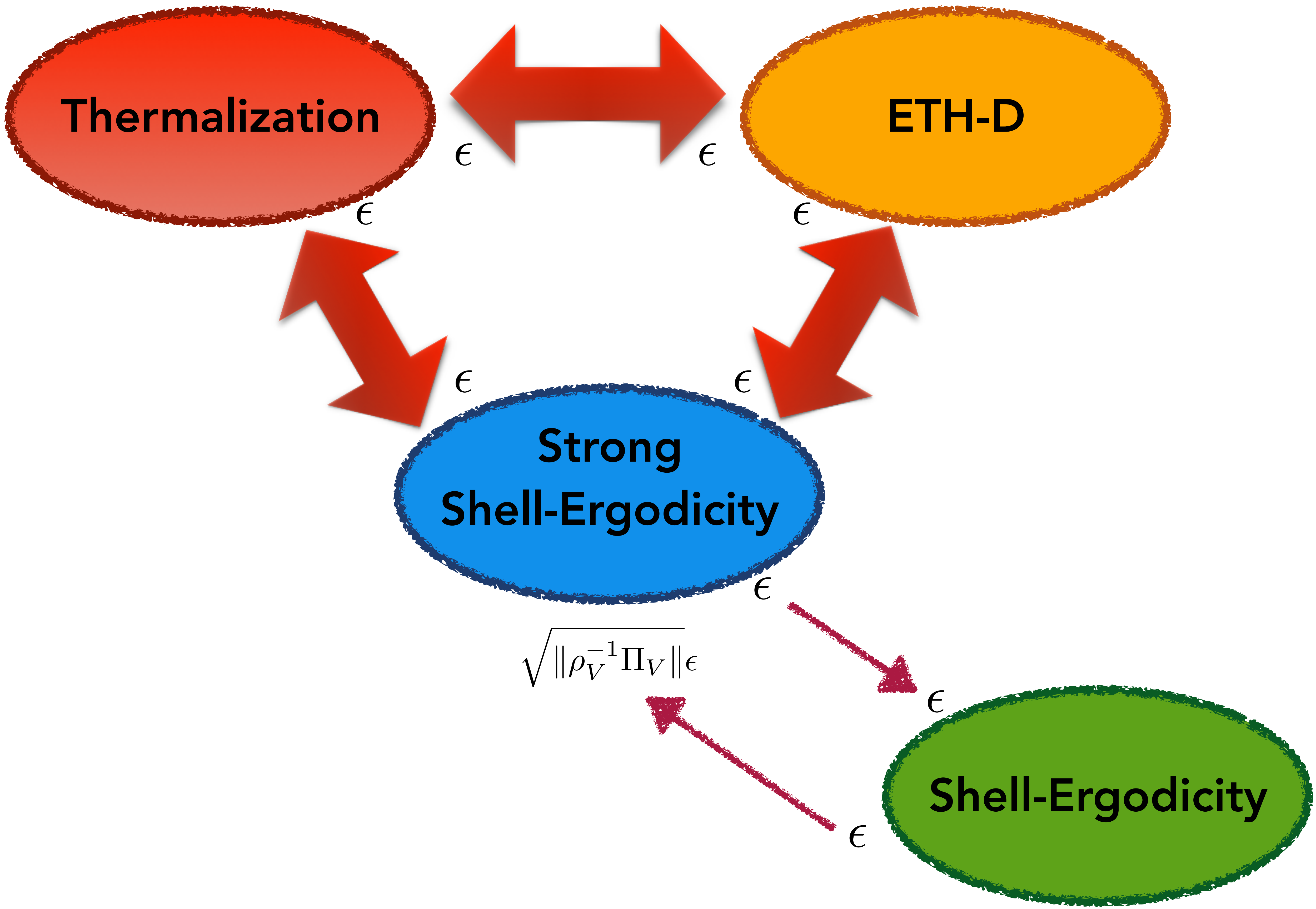
Observable *A* thermalizes with precision **ε**

$$\left| \overline{\mathrm{Tr}\left(A(t)\rho_0\right)} - \langle A \rangle_V \right| \leq \epsilon \, \|A\|$$

$$\left| \mathrm{Tr}[A \overline{\mathcal{E}_t}(\rho_0)] - \langle A \rangle_V \right| = \left| \langle A \rangle'_V - \langle A \rangle_V \right| \leq \epsilon$$

We can pick the $\boldsymbol{\rho}_V$ we prefer at the price of **ε**, e.g. $\boldsymbol{\rho}_V = \boldsymbol{\rho}_{MC}$

BETTER PROPOSITION



HOW IS CLASSICAL STAT-MECH BUILT?

Possibility a) Fix energy exactly:

$$M_E = \{(q,p) | \; H(q,p) = E\}$$

+ Metric indecomposable

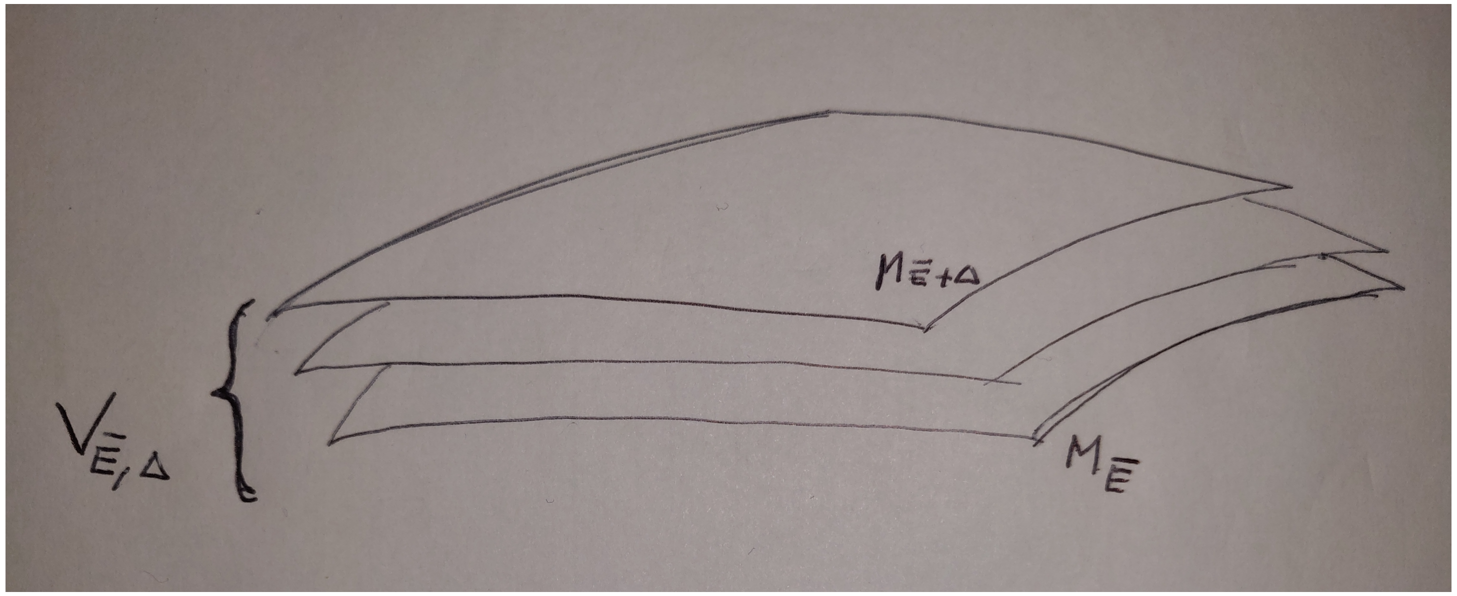
$$S(E) = k_B \ln(\omega(E))$$

$$\overline{f} = \langle f \rangle_E$$

$$\omega(E) = \int dqdp \, \delta[H(q,p) - E]$$

Possibility b) Fix energy approximately:

$$V_{\overline{E},\Delta} := \{(q,p) | \; \overline{E} \leq H(q,p) \leq \overline{E} + \Delta\}$$



STAT-MECH CONTINUED

We want uniform measure on *V*:

$$\langle f\rangle_{V_{\overline{E},\Delta}} := \frac{\int_{V_{\overline{E},\Delta}} dx\, f(x)}{\int_{V_{\overline{E},\Delta}} dx} = \frac{\int_I dE\, \omega(E)\langle f\rangle_E}{\int_I dE\, \omega(E)}.$$

Need metric indeomposable

$$\forall E \in I := [\overline{E}, \overline{E}+\Delta]$$

What we really want:

③ $$\overline{f}(x) = \langle f\rangle_{V_{\overline{E},\Delta}}$$

(for almost any *x*)

① $$\overline{f} = \langle f\rangle_E \quad \forall E \in I := [\overline{E}, \overline{E}+\Delta]$$

② $$\langle f\rangle_E = \langle f\rangle_{V_{\overline{E},\Delta}}$$

Classical ETH (ETH-C)

Obviously ① + ② $\Rightarrow$ ③

When do we have (2)? $\Delta \to 0$

$$\langle f \rangle_{V_{\overline{E},\Delta}} = \langle f \rangle_{\overline{E}} + \frac{\Delta}{2} \langle f \rangle'_{\overline{E}} + O\left(\Delta^2\right)$$

$$\Rightarrow \quad \left| \frac{\langle f \rangle_{V_{\overline{E},\Delta}} - \langle f \rangle_{\overline{E}}}{\langle f \rangle_{\overline{E}}} \right| \lesssim \frac{\Delta}{2\epsilon_f}, \qquad \epsilon_f = \langle f \rangle_{\overline{E}} / \left| \langle f \rangle'_{\overline{E}} \right|.$$

For the Hamiltonian $\epsilon_H = \overline{E}$ $\Rightarrow$ $\Delta / \overline{E} \ll 1.$

Approach a) (fix $H=E$) not possible because:

1. Time-energy uncertainty (Landau)
2. Impossible to define meaningful entropy

Approach b) :

① Hamiltonian with non-degenerate spectrum in V

② ETH-D

③ Shell-ergodicity

THANK YOU