Microscopic origin of macroscopic thermalization time

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Bounding Transport and Chaos

Nordita, August 22, 2018

Motivation

Non-equilibrium statistical mechanics from quantum mechanics

timescales of thermalization:
-short (local) timescales (governed by local couplings)
-macroscopic timescales (grow polynomially with L)
-exponentially long scales (Heisenberg,...)

- macroscopic timescales of thermalization from underlying microscopic physics
  - $\langle A(t)A(0)\rangle$
- macroscopic timescales of thermalization from underlying quantum mechanics
  - $\langle \Psi|A(t)|\Psi\rangle$

Thermalization: classical vs quantum mechanical

- assuming classical transport (diffusion)
  - $\langle\Psi|A(t)|\Psi\rangle = \sum_n C_n e^{-\Gamma_n t}, \quad \Gamma_n = Dn^2/L^2$

  even classically the space of all possible $A(t) \equiv \langle\Psi|A(t)|\Psi\rangle$ is not very well understood. E.g. can time-averaged A can be parametrically longer than the diffusion time Γ_1^{-1},

$$\frac{1}{\max_{t>0} A(t)} \int_0^\infty A(t)dt \gg \Gamma_1^{-1} \qquad ?$$

- quantum mechanically

  how to define the spectrum Γ_n and longest thermalization timescale Γ_1^{-1} a priori is not clear

This talk: outline

- quantum-mechanical definition of Γ_1^{-1}
- uniform (for all Ψ) bound on time dynamics of $\langle\Psi|A(t)|\Psi\rangle$

$$\text{“}\left|\frac{1}{T}\int_0^T dt\langle\Psi|A(t)|\Psi\rangle\right|\text{”} \leq x(1/T)$$

- presence of quantum states that thermalize parametrically longer than Γ_1^{-1}
- presence of new macroscopic timescales besides Γ_1^{-1}

New technical ingredient – deviation function

- connection between time evolution and linear algebra of $\hat{A}$

$$\int_{-\infty}^{\infty} dt \frac{\sin(t/T)}{\pi t} \langle \Psi | A(t) | \Psi \rangle = \langle \Psi | \begin{bmatrix} * & \diagdown & & & 0 \\ \diagdown & * & & & \\ & & \dots & & \swarrow \\ & & & * & \diagdown \\ 0 & & \underset{2/T}{\nearrow} & \diagdown & * \end{bmatrix} | \Psi \rangle$$

- deviation function, arXiv:1702.07722

$$x(\Delta E) = \lambda_{\max} \left(\begin{bmatrix} 0 & & 0 \\ & \underbrace{[\dots]}_{2\Delta E}\}2\Delta E & \\ 0 & & 0 \end{bmatrix} \right)$$

Uniform bound on averaged time evolution

- Heuristic argument: after time t energies E_i, E_j, $|E_i - E_j|t \geq 1$ are mutually de-phased

  $$\langle \Psi | A(t) | \Psi \rangle = \sum_{ij} C_i^* C_j A_{ij} e^{-i(E_i - E_j)t} \approx \sum_k \langle \Psi_k | A(t) | \Psi_k \rangle$$

  $\cdot$ here $\Psi_k = P_k \Psi$, P_k – projector on an energy band of size $1/t$ centered at $E + k/t$

  $\cdot$ $|\langle \Psi_k | A(t) | \Psi_k \rangle| \leq x(1/t)$

  finally, we have:

  $$|\langle \Psi | A(t) | \Psi \rangle| \leq x(1/t)$$

- Conjecture: uniform bound on time-averaged dynamics

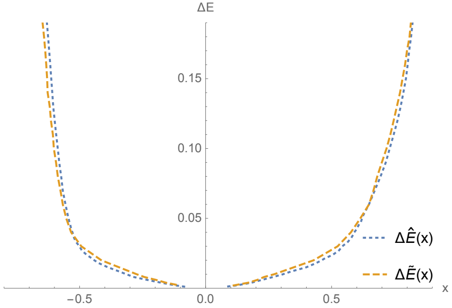
  $$\left| \int_{-\infty}^{\infty} dt \frac{\sin(t/T)}{t} \langle \Psi | A(t) | \Psi \rangle \right| \leq 3x(1/t)$$

Uniform bound on averaged time evolution

- numerical check for chaotic spin-chain

  $\cdot\ \Delta\tilde{E}(x)$ inverse function to maximal eigenvalue $x = \lambda_{\max}$ of a "narrow strip" matrix of width $1/T = \Delta E$

  $\cdot\ \Delta\hat{E}(x)$ inverse function to deviation function $x(\Delta E)$ (maximal eigenvalue of small "square" matrix)



Uniform bound on averaged time evolution

- numerics confirms validity of the uniform bound for chaotic and integrable models, arxiv:1806.04187

$$\left| \int_{-\infty}^{\infty} dt \frac{\sin(t/T)}{t} \langle \Psi | A(t) | \Psi \rangle \right| \leq 3x(1/t)$$

- the bound holds for $t \geq t^*$
- there are states Ψ which approximately saturate the bound

additional numerics shows:

- time t^* is the macroscopic thermalization (diffusion) time

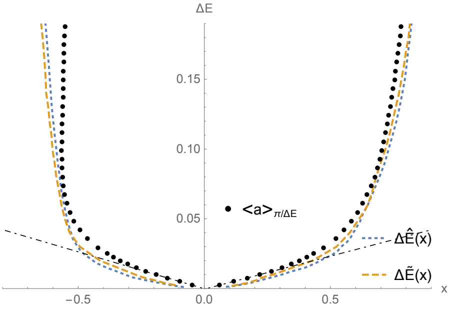
- macroscopic diffusive states approximately saturate the bound

Time-dynamics of quasi-classical diffusive states

- states Ψ with macroscopic spatial inhomogeneities
  $\langle\Psi|A(t)|\Psi\rangle \approx e^{-t/\tau}$

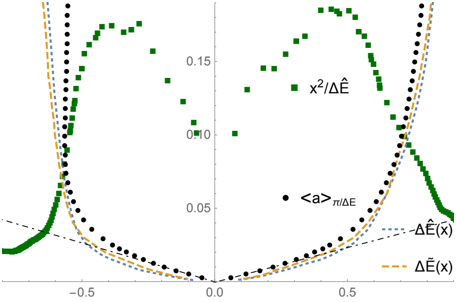
$$\langle a\rangle_T \equiv \int_{-\infty}^{\infty} dt \frac{\sin(t/T)}{t}\langle\Psi|A(t)|\Psi\rangle$$

$$\langle a\rangle_T = \begin{cases} \sim 1, & T \ll \tau \\ \tau/T, & T \gtrsim \tau \end{cases}$$



Non-perturbative definition of Thouless time

- macroscopic thermalization time Γ_1^{-1} is associated with the maximum of $x^2/\Delta\hat{E}(x) \sim \Gamma_1^{-1}$



- for a quantum diffusive system Thouless (diffusion) time is the longest thermalization time for all initial states Ψ with a macroscopic initial amplitude $\langle\Psi|A(0)|\Psi\rangle \sim 1$

Recap

- deviation function of an observable A, arXiv:1702.07722

$$x(\Delta E) = \lambda_{\max}\left(\begin{bmatrix} 0 & & 0 \\ & \underbrace{[\dots]}_{2\Delta E}\}2\Delta E & \\ 0 & & 0 \end{bmatrix}\right)$$

- non-perturbative definition of thermalization time, arxiv:1806.04187

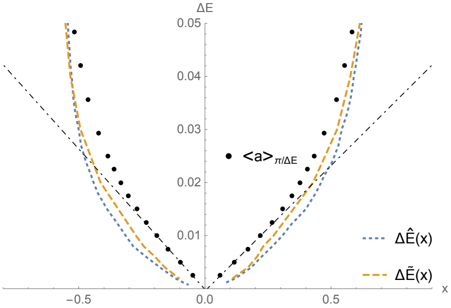
$$\max_x \frac{x^2}{\Delta E(x)} \sim \Gamma_1^{-1}$$

- uniform bound on time-averaged dynamics

$$\left|\int_{-\infty}^{\infty} dt \frac{\sin(t/T)}{t} \langle\Psi|A(t)|\Psi\rangle\right| \leq 3\,x\left(\frac{1}{t}\right)$$

Difference between classical and quantum thermalization

- Γ_1^{-1} is the longest thermalization time for all configurations/states Ψ with a macroscopic initial amplitude $\langle\Psi|A(0)|\Psi\rangle \sim 1$
- at quantum level there are states Ψ with size-suppressed amplitudes that thermalize parametrically slower than Thouless time Γ_1^{-1} (in fact arbitrarily slowly)



$$\Delta E(x) \leq x^2/f^2(0)$$

Outstanding questions

- is spectrum Γ_n a useful notation quantum-mechanically?
  - $\langle\Psi|A(t)|\Psi\rangle = \sum_n C_n e^{-\Gamma_n t}$

  - exponential decay of $\langle\Psi|A(t)|\Psi\rangle$ is not natural at quantum level

  - presence of "non-classical" states with non-intuitive dynamics (e.g. arbitrary long thermalization time)

  - relation to 2pt function $\langle A(t)A(0)\rangle$

- evidence of new timescale(s) beyond Γ_1^{-1}

Thermalization – conventional picture

Diffusive system thermalizes at the scale of Thouless (diffusive) time $\tau \sim L^2$ necessary for the slowest diffusive modes to propagate across the system. After time $t \sim \tau$ the system is fully ergodic.

There are no other (longer) timescales, except those exponential in system size – we debunk that.

ETH "reduces" to RMT?

For small $\omega \leq \Delta E_{RM}$, $f(\omega)$ is constant and r_{nm} is GOE

$$\langle E_n|A|E_m\rangle = A^{\rm eth}\delta_{nm} + e^{-S/2} f(\omega) r_{nm}$$

D'Alessio, Kafri, Polkovnikov, Rigol'15

- Gaussian distribution of r_{nn} and r_{nm}
  Beugeling, Moessner, Haque'14, ...
- ratio $\langle r_{nn}^2\rangle = 2\langle r_{nm}^2\rangle$
  AD, Liu'17, Mondaini, Rigol'17

Expectation: ETH reduces to RMT at Thouless energy $|\omega| \leq E_{\rm Th} \equiv D/L^2$.

Buildup: Random Matrix Theory

- form-factor $f^2(\omega) = \sum_j r_{ij}^2 \, \delta(\omega - E_i + E_j)$

- assuming fluctuations r_{ij} are *independent* maximal eigenvalue of band random matrix is bounded by

$$x^2(\Delta E) \le 8 \int_0^{2\Delta E} d\omega \, |f(\omega)|^2, \qquad A_{\Delta E} = \begin{bmatrix} * & \diagdown & & & 0 \\ \diagdown & * & & & \\ & & \ldots & & \swarrow \\ & & & * & \diagdown \\ 0 & & \nearrow & \diagdown & * \end{bmatrix}$$

$$2\Delta E$$

arXiv:1702.07722

◇ Gaussian Random Matrix, $f^2 = \text{const}$,
$\Delta E(x) = x^2/(8f^2), \qquad x \propto \Delta E^{1/2}$

Upper bound on ΔE_{RM} from transport

Idea: to go from energy domain to time domain

$$\int dt \frac{\sin(t\Delta E)}{t\pi} \langle \Psi(t)|A|\Psi(t)\rangle = \langle \Psi(0)|A_{\Delta E}|\Psi(0)\rangle$$

$$f^2_{\mathrm{new}}(\omega) = \begin{cases} f^2(\omega) : |\omega| \leq 2\Delta E \\ 0 \qquad\quad : |\omega| > 2\Delta E \end{cases} \qquad A_{\Delta E} = \begin{bmatrix} * & \diagdown & & 0 \\ \diagdown & * & & \\ & & \dots & \swarrow \\ & & * & \diagdown \\ 0 & \nearrow\diagdown & & * \end{bmatrix}$$

$$2\Delta E$$

- for $\Delta E < \Delta E_{\mathrm{RM}}$ all elements of $A_{\Delta E}$ are random (uncorrelated) by assumption

$$\max_{\Psi} |\langle \Psi(0)|A_{\Delta E}|\Psi(0)\rangle|^2 \leq 8 \int_0^\infty d\omega\, f^2_{\mathrm{new}}(\omega) = \int_0^{2\Delta E} d\omega\, f^2(\omega)$$

Upper bound on ΔE_{RM} from transport

- form-factor $f^2(\omega)$ is a Fourier transform of two-point function

$$\max_{\Psi}\left|\int dt \frac{\sin(t\Delta E)}{t\ \pi}\langle\Psi(t)|A|\Psi(t)\rangle\right|^2 \le \int dt \frac{\sin(t\Delta E)}{t\ \pi}\langle E|A(t)A(0)|E\rangle_{\mathrm{c}}$$

this inequality holds for sufficiently small $\Delta E \le \Delta E_{\mathrm{RM}}$

- for a diffusive 1D system, $\langle E|A(t)A(0)|E\rangle_{\mathrm{c}} \sim (t_D/t)^{1/2}$, and we take Ψ to be a quasi-classical state describing slowest diffusive mode $\langle\Psi(t)|A|\Psi(t)\rangle \sim e^{-t/\tau}, \quad \tau = t_D L^2$

$$(\Delta E\tau)^2 \le \Delta E\sqrt{t_D\tau} \quad \Rightarrow \quad \Delta E_{\mathrm{RM}} \le \frac{1}{t_D L^3}$$

arxiv:1804.08626

Summary

- There is a new "Random Matrix" time-scale $\Delta E_{\mathrm{RM}}^{-1}$ which is parametrically longer than the Thouless (diffusive) time

- Off-diagonal matrix elements A_{ij} encode slow hydrodynamic modes (transport) through cross–correlations; a framework to connect ETH and dynamics?

$$\langle \Psi | A(t) | \Psi \rangle = \sum_n C_n e^{-\Gamma_n t} \qquad ?$$

- Conjecture: time-scale $\Delta E_{\mathrm{RM}}^{-1}$ is the time when the exponential decay of $\langle \Psi | A(t) | \Psi \rangle$ saturates into quantum fluctuations $\langle \Psi | A(t) | \Psi \rangle \sim e^{-S/2}$

Conclusions

- Thermalization of quantum systems is a very rich subject: approach toward equilibrium

$$\langle\Psi|A(t)|\Psi\rangle$$

"knows" about transport and much more

- We identified macroscopic timescale of thermalization starting from the underlying quantum-mechanical formulation

$$\Gamma^{-1} = \max \frac{x^2}{\Delta E(x)}$$

- Beyond Γ^{-1} there is a new "Random Matrix" time-scale $\Delta E_{\rm RM}^{-1}$ which is parametrically longer than Γ^{-1}. It might be related to the "end of exponential decay" timescale

- Quantum dynamics is richer than classical: there are special states Ψ with arbitrarily long thermalization time. But there is also a uniform bound on thermalization dynamics for all Ψ