Generalizing von Neumann's approach to thermalization

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[v. Neumann, Z. Phys. 57, 30 (1929);

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"Summit" of equilibrium Statistical Mechanics (Feynman)

$$\boxed{\rho_{can} = Z^{-1}\, e^{-\beta H_S}}$$

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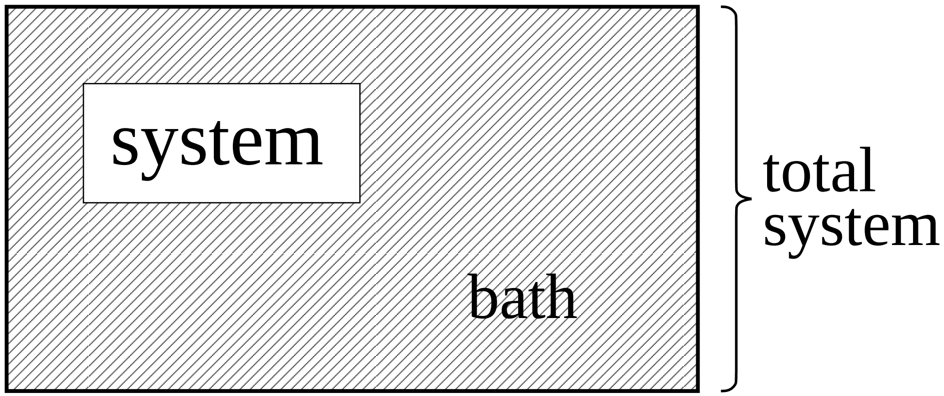
Should follow from microcanonical formalism for isolated systems



General framework

- **Model:** Isolated system (macroscopic, finite, bath(s) incorporated)

  Hamiltonian H, eigenvalues E_n, eigenvectors $|n\rangle$

  System states $\rho(t)$ (mixed or pure)

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- **Evolution:** standard QM, no further approximation/postulate/hypothesis:

  $$\rho(t) = \mathcal{U}_t\, \rho(0)\, \mathcal{U}_t^\dagger \;, \quad \mathcal{U}_t := \exp\{-iHt/\hbar\} \quad \Rightarrow$$

  $$\boxed{\mathrm{Tr}\{\boldsymbol{\rho(t)A}\} = \sum_{\boldsymbol{m,n}} \boldsymbol{e^{-i[E_m - E_n]t/\hbar}\, \langle m|\rho(0)|n\rangle\, \langle n|A|m\rangle}}$$

  Theorem: Any $\rho(t)$ returns arbitrarily "near" to $\rho(0)$!

Microcanonical setup

- Focus on $E_n \in [E, E + \Delta E]$ (**energy window**)

  Without loss of generality: $n = 1, ..., D$

  For systems with f degrees of freedom: $\boxed{\boldsymbol{D \approx 10^{\mathcal{O}(f)}}}$ e.g. $f \approx 10^{23}$

  Defs.: $P := \sum_{n=1}^{D} |n\rangle\langle n|$ projector onto **energy shell** $\mathcal{H}$

  $\rho_{mic} := P/D$ (**microcanonical ensemble**)

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  $\Rightarrow \rho(t) = P\rho(t)P$ for all $t \Rightarrow \mathrm{Tr}\{\rho(t)A\} = \mathrm{Tr}\{\rho(t)PAP\}$

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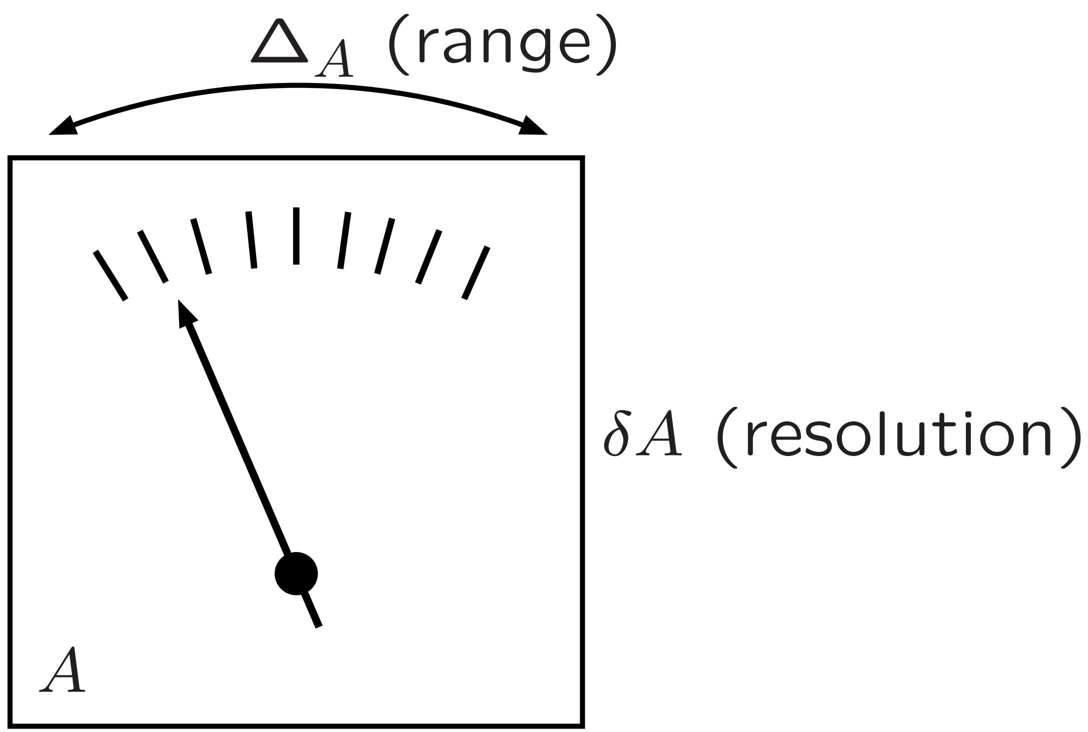
- Task: Show for arbitrary $\rho(0) : \mathcal{H} \to \mathcal{H}$ that $\mathrm{Tr}\{\rho(t)A\} \to \mathrm{Tr}\{\rho_{mic}A\}$

Range and resolution of A

$A \hat{=}$ measurement device with **range $\boldsymbol{\Delta_A}$** (finite number of eigenvalues)

Expectation values $\mathrm{Tr}\{\rho(t)A\}$ can only be determined with some finite accuracy **$\boldsymbol{\delta A}$ (resolution limit)**

Assumption: **$\boldsymbol{\delta A/\Delta_A}$ "reasonable", say $\boldsymbol{> 10^{-20}}$**



Technical conditions: generic H

1. **Non-degeneracy condition:** $E_m \neq E_n$ unless $m = n$

2. **Non-resonance condition:**

   $E_m - E_n \neq E_j - E_k$ unless $m = j$ and $n = k$ (or $m = n$ and $j = k$)

- "quantum ergodicity" and "quantum mixing" (?)
- Originally due to von Neumann, by now commonly accepted
- Weaker conditions still ok

Key point of von Neumann's approach

Consider unitary trafo U between eigenvectors of H and A

Key assumption: the actual U is "typical" among all possible $U : \mathcal{H} \to \mathcal{H}$

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- Common lore of random matrix theory.
- No randomness in the real system.

Main result [PRL 115, 010403 (2015)]

Consider: $$B(T) := \left\{ t \in [0,T] \ : \ |\,\mathrm{Tr}\{\rho(t)A\} - \mathrm{Tr}\{\rho_{mic}A\}\,| \geq \delta A \right\}$$

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Theorem: For any $\epsilon > 0$ there exists a T_{min} so that for all $T \geq T_{min}$

$$\mu_U\left(\frac{|B(T)|}{T} \geq \epsilon\right) \leq 6\,\exp\left\{-\frac{\epsilon\,D}{(6\pi)^3}\left(\frac{\delta A}{\Delta_A}\right)^2 + 2\ln D\right\}$$

independently of $\rho(0)$

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Recall: $D \approx 10^{\mathcal{O}(f)}$, $f \approx 10^{23}$, $\delta A/\Delta_A > 10^{-20}$ $\Rightarrow$ choose e.g. $\epsilon = D^{-1/2}$

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- **Inital relaxation included in** $B(T)$
- **Recurrences of Tr**$\{\rho(t)A\}$ **included in** $B(T)$
- **Same backward in time**
- **Already quite small** f **will do !**

Conceptual implications

Recall: pure states $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ included $\Rightarrow$

$|\psi(t)\rangle$ **"imitates"** $\boldsymbol{\rho_{mic}}$ **practically perfectly** (for "most" t and U)

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Von Neumann entropies: $S[|\psi(t)\rangle] = 0$, $S[\rho_{mic}] = k_B \ln D$ (maximal)

$\Rightarrow$ **Role of entropy overestimated ?**

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- Already contained in v. Neumann, Z. Phys. 57, 30 (1929)
- Closely related to "typicality phenomena":

Goldstein, Lebowitz, Tumulka, Zanghì, PRL 96, 050403 (2006)

Popescu, Short, Winter, Nat. Phys. 2, 754 (2006)

Sugita, Nonlinear Phenom. Complex Syst. 10, 192 (2007)

Sugiura, Shimizu, PRL 108, 240401 (2012)

Related Works

von Neumann, Z. Phys. 57, 30 (1929),
[English translation by **Tumulka**, Eur. Phys. J. H 35, 201 (2010)],
approximating all relevant observables ("macro-observers") by commuting operators with very high-dimensional common eigenspaces.

Pauli and Fierz, Z. Phys. 106, 572 (1937),
assuming #eigenspaces $\ll D/(\ln D)^2$ (proof ok ?)

Goldstein, Lebowitz, Mastrodonato, Tumulka, Zanghì, PRE 81, 011109 (2010), assuming that one of those eigenspaces (the "equilibrium subspace") is overwhelmingly large compared to all the others.

Goldstein, Lebowitz, Tumulka, Zanghì, Eur. Phys. J. H 35, 173 (2010): Misunderstandings and rehabilitation of von Neumann's work.

Deutsch, PRA 43, 2046 (1991); **Reimann** NJoP 17, 055025 (2015):
U generated via $H = H_0 + V$ with random matrices V (banded, sparse etc.)

Eigenstate thermalization hypothesis (ETH)

Deutsch, PRA 43, 2046 (1991);

Srednicki, PRE 50, 888 (1994);

Rigol, Dunjko, Olshanii, Nature 452, 854 (2008)

Here:

ETH not required but actually fulfilled by all non-exceptional U's

Similarly to (but now for general A's):

Goldstein, Tumulka, AIP Conference Proceedings 1332, 155 (2011)

Rigol, Srednicki, PRL 108, 110601 (2012)

Disequilibrium requires fine tuning

So far: unitary trafos U between eigenvectors of H and A
$\Rightarrow$ conclusions independent of $\rho(0)$, i.e. valid for **all** $\boldsymbol{\rho(0)}$

Now: unitary trafos W between eigenvectors of $\rho(0)$ and A

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Recall: $D \approx 10^{\mathcal{O}(f)}$, $f \approx 10^{23}$, $\delta A/\Delta_A > 10^{-20}$ $\quad\Rightarrow$

- Given $\rho(t)$, most A appear equilibrated [Bocchieri & Loinger, Phys. Rev. 111, 668 (1958)]
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$\Rightarrow$ Disequilibrium requires fine tuning of $\rho(0)$ relatively to A

$\Rightarrow$ Statements about **most** $\boldsymbol{\rho(0)}$ useless for equilibration

Typical temporal relaxation (work in progress)

$\rho(0)$ kept fixed relatively to A $\Rightarrow$ $\mathrm{Tr}\{\rho(0)A\}$ arbitrary but fixed.

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$$\text{from } \text{Tr}\{\rho_{mic}A\} + F(t)\left(\text{Tr}\{\rho(0)A\} - \text{Tr}\{\rho_{mic}A\}\right)$$

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- Many common A's must be untypical ("almost conserved").
- Most of those exceptional A's still thermalize (for *any* $\rho(0)$).

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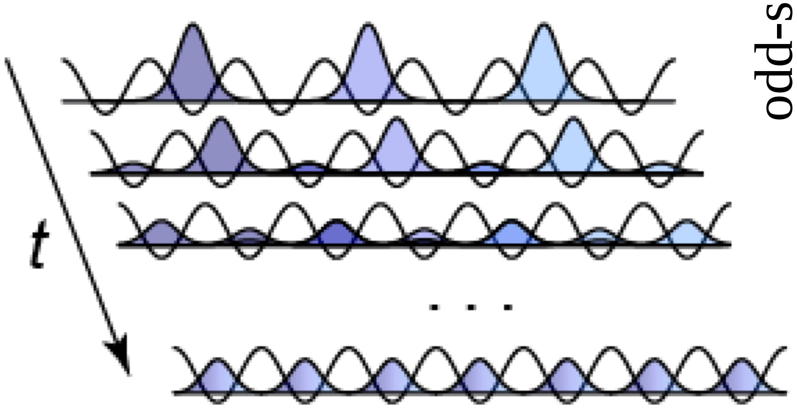
Closely related works:

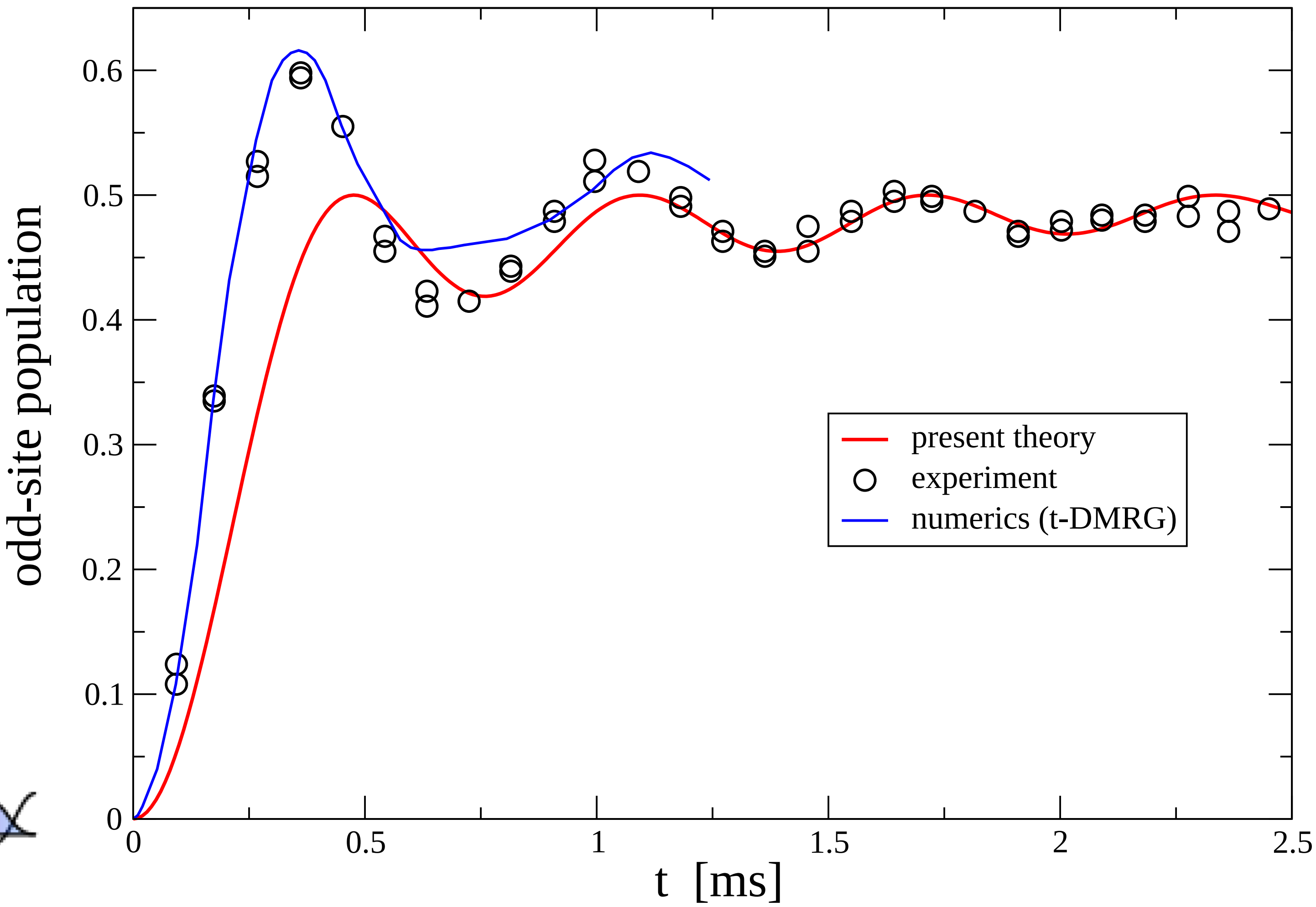
Cramer, NJoP 14, 053051 (2012)
Goldstein, Hara, Tasaki, PRL 111, 140401 (2013); NJoP 17, 045002 (2015)
Monnai, J. Phys. Soc. Jpn. 82, 044006 (2013)
Malabarba, Garcia-Pintos, Linden, Farrelly, Short, PRE 90, 012121 (2014)

Comparison with experiment

Trotzky, Chen, Flesch, McCulloch, Schollwöck, Eisert, and Bloch, *Probing the relaxation towards equilibrium in an isolated strongly correlated 1D Bose gas*, Nature Physics 8, 325 (2012)

ultracold atoms in an optical lattice





Further examples (numerical)

Thon et al., Appl. Phys. A 78, 189 (2004): Fig. 8

Bartsch and Gemmer, PRL 102, 110403 (2009): Fig. 1b

Rigol, PRL 103, 100403 (2009): Fig. 1

Rigol, PRA 80, 053607 (2009): Figs. 1, 2

Khatami et al. PRA 85, 053615 (2012): non-exponential decay

Gramsch and Rigol, PRA 86, 053615 (2012): non-exponential decay

Investigations of Loschmidt echo (fidelity, nondecay probability, ...)

...

Further example

[**Bartsch and Gemmer, PRL 102, 110403 (2009)**]

$H = H_0 + \lambda V$, $D = 6000$, $E^{(0)}_{n+1} - E^{(0)}_n = 8.33 \cdot 10^{-5}$ $(\hbar = 1)$

${}_0\langle m|V|n\rangle_0$ normally distributed, independent complex random variables

$\lambda = 2.5 \cdot 10^{-3}$ ("strong perturbation")

${}_0\langle m|A|n\rangle_0 = \delta_{mn}\, a_n$, $a_n = \pm 1$ (random)

$\rho(0) = |\psi(0)\rangle\langle\psi(0)|$ random with $\mathrm{Tr}\{\rho(0)A\} \simeq 0.2$