Thermodynamic behavior from Schroedingers dynamics in incompletely observed quantum systems

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Contents

The background, environment induced relaxation

Background and general question:

Quantum dynamics:

- the Schrödinger equation $i\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle$ features no (attractive) fixpoint
- "Hilbertspace trajectories" move with constant velocity: $\langle\dot{\psi}|\dot{\psi}\rangle$ =const.
- Entropy cannot change: $\dot{S} = 0, \; S = -k\mathrm{Tr}\{\hat{\rho}\ln\hat{\rho}\}$

Thermodynamics:

- $A(t) \rightarrow A_{eq}$
- A_{eq} are in accord with "maximum entropy principle", "a priory postulate of equal probabilities", "ergodicity", etc. $\Rightarrow \dot{S} \geq 0$
- typical dynamcis: $\dot{A}_n = \sum_m R_{nm} A_m$ where A_n^{eq} is an attractive fixpoint

How can the two pictures come together? Incomplete observation + some complexity !

Methods and concepts: projection techniques, Hilbertspace average method (HAM), entanglement, etc.

Projection operator technique (Nakajima-Zwanzig)

linear superoperators: $\mathcal{L}$, $\mathcal{P}$

dynamics: $$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathcal{L}(t)\hat{\rho}(t)$$ projection: $$\mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho}$$

$\Rightarrow$ big mathematical machinery $\Rightarrow$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\hat{\rho} = \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{P}\hat{\rho}(t')\mathrm{d}t' + O(\mathcal{L}^3)$$ **"Born approximation"**

for initial states with $\mathcal{P}\hat{\rho}(0) = \hat{\rho}(0)$

Typical quantum dynamics and standard choice of projection operator

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{V} \qquad \hat{V} = \sum_n \hat{A}_n^\dagger \hat{B}_n + \hat{A}_n \hat{B}_n^\dagger \qquad \mathcal{L}\hat{\rho} = \mathrm{i}[\hat{V}(t), \hat{\rho}(t)]$$

$$\hat{\rho}_S := \mathrm{Tr}_E\{\hat{\rho}\} \qquad \mathcal{P}\hat{\rho} := \hat{\rho}_S \otimes \hat{\rho}_E(T) \Rightarrow$$ "RWA", etc. $\Rightarrow$

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \int_0^t \mathcal{K}(t-t')\hat{\rho}_S(t')\mathrm{d}t'$$ **"time convoluted dynamics"**

$$\mathcal{K}(t-t') \propto \mathrm{Tr}\{\hat{B}(t)\hat{B}^\dagger(t')\hat{\rho}_E(T)\} + \text{c.c.}$$ "bath correlation functions"

If decay of bath correlations fast (broad and dense frequency spectrum of the bath) compared to the resulting relaxation dynamics of the considered system (weak interaction) $\Rightarrow$ **"Markov approximation"** $\Rightarrow$

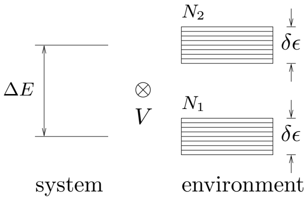
$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) \approx \int_0^t \mathcal{K}(t-t')\mathrm{d}t'\hat{\rho}_S(t) \approx: \mathcal{R}\hat{\rho}_S(t)$$

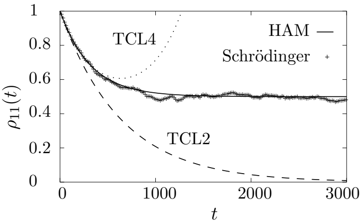
Quantum master equation with attractive Gibbsian fixpoint

Does the applicability of the Markov approximation imply the applicability of the Born approximation ?

Broad band finite environments and dynamics

Does the applicability of the Markov approximation imply the applicability of the Born approximation ?





$$\hat{V} = \lambda \sum_{n_1, n_2} C(n_1, n_2)\, \hat{\sigma}^{+} |n_1\rangle\langle n_2| + \text{h.c.}$$

No! Even if correlations decay fast enough to justify the neglect of the convolution, higher orders may not converge!

Alternative projection approach with generalized projector :

$$\mathcal{P}\hat{\rho} = \sum_n B_n \hat{B}_n \quad \text{with} \quad B_n = \mathrm{Tr}\left\{\hat{B}_n^+ \hat{\rho}\right\} \quad \text{and} \quad \mathrm{Tr}\left\{\hat{B}_n^+ \hat{B}_m\right\} = \delta_{nm}$$

Projected subdynamcis in a “time-convolutionless” expansion (TCL2):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\hat{\rho} \approx \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathrm{d}t'\mathcal{P}\hat{\rho}(t) \Rightarrow \mathrm{Tr}\left\{\hat{B}_n^+ \dots\right\} \Rightarrow \dot{B}_n = \sum_j K_{nj}(t) B_j$$

$$K_{nj}(t) := \int_0^t C_{nj}(t,t')\mathrm{d}t' \quad C_{nj}(t,t') = -\mathrm{Tr}\left\{[\hat{B}_n, \hat{V}(t)][\hat{B}_j, \hat{V}(t')]\right\}$$

if $C_{nj}(t,t')$ decay fast with $|t-t'|$ getting larger

$$\dot{B}_n \approx \sum_j R_{nj} B_j$$

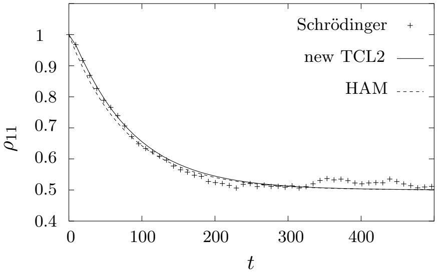
concrete projectors: (standard: $\hat{B}_{ij} := |i\rangle\langle j| \otimes \hat{\rho}_E(T)$) alternative:

$$\hat{B}_{ija} := |i\rangle\langle j| \otimes \frac{\hat{\Pi}_a}{\sqrt{N_a}}, \quad \hat{\Pi}_a := \sum_{n_a} |n_a\rangle\langle n_a| \quad \mathcal{P}\hat{\rho} = \sum_{ija} B_{ija}\hat{B}_{ija} = \sum_a \hat{\rho}_S^a \otimes \frac{\hat{\Pi}_a}{N_a}$$

$\mathcal{P}$ projects onto strongly correlated states. $\Rightarrow$ TCL2, fast decaying correaltions

$$\Rightarrow \quad \frac{d}{dt}\hat{\rho}_S^a = \sum_b \mathcal{L}_{ab}\hat{\rho}_S^b$$

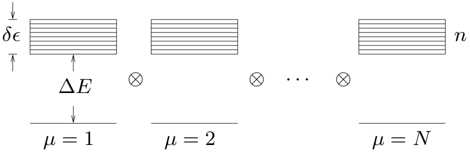
$$\hat{\rho}_S = \sum_a \hat{\rho}_S^a$$



- This scheme produces reasonable results, i.e., higher orders are negligible
- Rates are in accord with Fermi's Golden Rule

Diffusion in closed finite quantum systems

"Finite modular quantum system"



$$\hat{H} = \sum_{\mu=1}^{N} \hat{h}_\mu + \hat{v}_\mu$$

$$\hat{h}_\mu = \sum_i h_i \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu,i} \,, \quad h_i := \Delta E + i \frac{\delta\epsilon}{n}, \quad \hat{v}_\mu = \sum_{ij} c_{ij} \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu+1,j} + \text{h.c.}$$

- This may be viewed as a model for: a particle moving on lattice sites, energy exchange between molecules, etc.
- The model features: no particle-particle interaction, nearest neighbor random interband hoppings, no disorder, a finite amount of sites

How can the dynamics of the $\langle \hat{h}_\mu(t) \rangle$ be determined and understood?

Some standard tools in transport theory:

- Kubo formula: derivation based on external force acting on a carrier, not spatial gradient of the carrier density, difficult to interpret for finite systems
- (Quantum) Boltzmann equation: quasiparticles? Stosszahlansatz? (assumption of molecular chaos?)

Alternative method: Projection onto hydrodynamical modes

$$\hat{F}_q = \sqrt{\frac{2}{N}} \sum_{\mu} \cos(\frac{2\pi q}{N}\mu)\hat{h}_\mu \quad \Rightarrow \text{TCL2} \Rightarrow \quad \dot{F}_q = 2(\cos(\frac{2\pi q}{N}) - 1)K(t)F_q$$

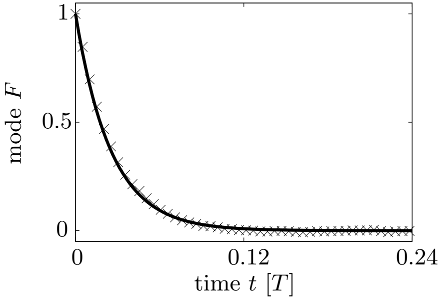
Compare with "random walk dynamics"

$$\dot{P}_\mu = \kappa(P_{\mu-1} + P_{\mu+1} - 2P_\mu) \quad \text{"discrete diffusion equation"}$$

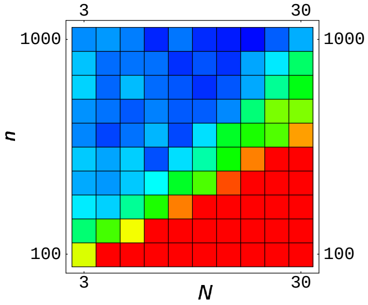
$$W_q = \sum_{\mu} \cos(\frac{2\pi q}{N}\mu)P_\mu \quad \Rightarrow \quad \dot{W}_q = 2(\cos(\frac{2\pi q}{N}) - 1)\kappa W_q$$

Results of the projection technique:

Dynamcis of a mode $F_q(t)$:



Deviation from diffusion



There may be diffusive behavior in ordered, finite "one-particle" quantum systems!

The parameter-region in which diffusive behavior occurs and the transport coefficient may be determined without diagonalization.

Some observables relax to equilibrium in an exponential, diffusive manner

Generality with respect to initial states?

Which are the observables that do relax? And towards what? $\Rightarrow$

Connection between projection methods and Hilbert space averaging

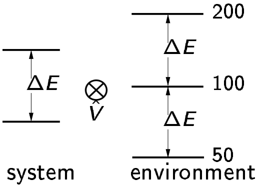
- Technically the above method only applies to states with $\mathcal{P}\hat{\rho}(0) = \hat{\rho}(0)$
- An analysis based on the Hilbert space average method (HAM) produces the same dynamics.
- The dynamcis as resulting from HAM are meant to be valid for the largest part of of all pure initial states, regardeless of whether they are entagled, correlated, etc.

$\Rightarrow$ *Most likely the above dynamcis apply even if* $\mathcal{P}\hat{\rho}(0) \neq \hat{\rho}(0)$

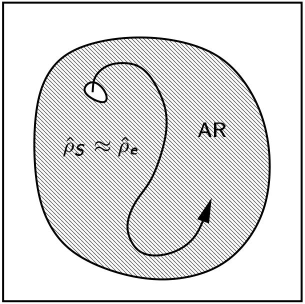
Hilbert space Average Method (HAM) and equilibrium states

What if environmental correlations do not decay?, $\hat{\rho}_S(t \to \text{“}\infty\text{”}) = ?$

Extreme narrow-band design model



Hilbert space portrait

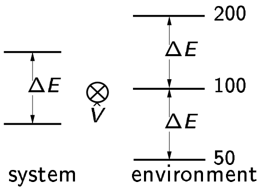


Hilbert space average method:

- Consider the reduced density operator as a function of the pure state of the full system: $\hat{\rho}_S = \hat{\rho}_S(|\psi\rangle)$
- Consider the distance d of $\hat{\rho}_S(|\psi\rangle)$ from some trial state $\hat{\rho}_e$: $d^2 = \mathrm{Tr}\left\{(\hat{\rho}_S - \hat{\rho}_e)^2\right\}$
- Compute the average of $d(|\psi\rangle)$ over all $|\psi\rangle$ that are accessible under given dynamical constraints: $[\![d(|\psi\rangle)]\!]_{AR}$ (AR: accessible region)

If $[\![d(|\psi\rangle)]\!]_{AR}$ is small, almost any pure state from the accessible region yields a reduced state closed to the trial state $\hat{\rho}_S(|\psi\rangle) \approx \hat{\rho}_e$

What trial states $\hat{\rho}_e$ are reasonable to check?



Check $\hat{\rho}_e$ which are

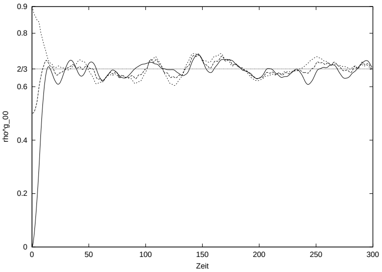
- diagonal within the energy eigenbasis of the system S
- in accord with the idea of "equal a priori probabilities" under given constraints

Using some mathematics, it can be shown that for those trial states $\hat{\rho}_e$ the average distance $[\![d]\!]_{AR}$ scales like $1/\sqrt{N_E}$

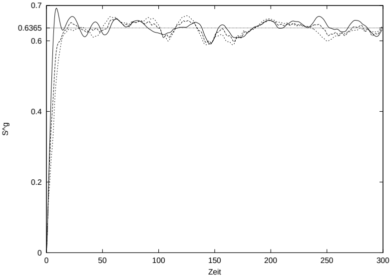
(N_E: "overall size of the environment")

Schrödinger evolutions for “weakly, randomly coupled” models

ground state occupation probability:



local entropy:



- Even though the system is not ergodic, dynamical evolutions mirror the “topology” and lead to local equlibration.
- The equilibration proceeds through increasing entanglement

Conclusion and outlook

- The relaxation of some observables towards a Boltzmann-type equilibrium is no contradiction to Schroedingers dynamcis and appears as being typical
- Projection techniques may help to analyze transport behavior in more complex systems such as "interacting" systems (Heisenberg models, Hubbard models) and/or disordered systems (Anderson systems)

Some literature concerning the addressed topics may be found on our homepage. This work has strongly been supported by M. Michel, H.-P. Breuer, R. Steinigeweg and many others.

Thank you for your attention!