Projection operator techniques and Hilbert space averaging: alternative approaches to transport and relaxation

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Contents

Equilibration of quantum sytems through environments, projection methods

The standard approach

Do closed (finite) quantum systems approach equilibrium?

The Schroedinger equation features no attractive fixpoint.

$\Rightarrow$ Most approaches to relaxation in quantum mechanics feature the concept of an environment acting as a "thermostat", open quantum systems:

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{V} \qquad \hat{V} = \sum_n \hat{A}_n^\dagger \hat{B}_n + \hat{A}_n \hat{B}_n^\dagger$$

Consider the reduced density operator : $\hat{\rho}_S := \mathrm{Tr}_E \{\hat{\rho}\}$.

Can one get one get an autonomous equation of motion for $\hat{\rho}_S$ *and if so, how ?*

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 $\Rightarrow$

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

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

Typical quantum dynamics and **standard choice of projection operator**

$$\mathcal{L}\hat{\rho} = \mathrm{i}[\hat{V}(t), \hat{\rho}(t)] \qquad \mathcal{P}\hat{\rho} := \hat{\rho}_S \otimes \hat{\rho}_E(T) \Rightarrow$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = -\int_0^t \mathrm{Tr}_E\left\{[\hat{V}(t), [\hat{V}(t'), \hat{\rho}_S(t') \otimes \hat{\rho}_E(T)]]\right\}\mathrm{d}t' \quad \Rightarrow \quad \text{“RWA”} \Rightarrow$$

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \int_0^t \mathcal{K}(t-t')\hat{\rho}_S(t')\mathrm{d}t' \quad \text{“time convoluted evolution”}$$

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

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

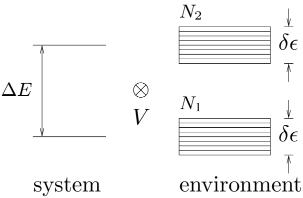
$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) \approx \int_0^t \mathcal{K}(t-t')\mathrm{d}t'\,\hat{\rho}_S(t) \approx: \mathcal{R}\hat{\rho}_S(t)$$

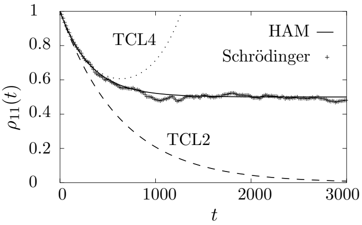
Quantum master equation with attractive Gibbsian fixpoint

Does the neglibility of the convolution justify the above truncation ?

Broad band finite environments and dynamics

Does the neglibility of the convolution justify the above truncation?





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

Although correlations decay fast enough to justify the neglection of the convolution, higher orders may not converge!

Alternative projection approach with generalized projector :

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

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

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

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

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

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

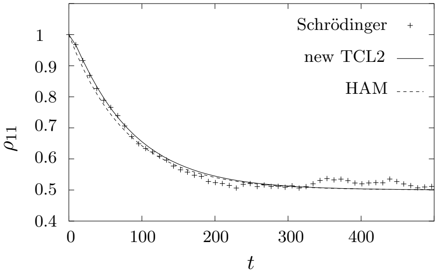
concrete projectors: (standard: $\hat{B}_{ij} := |i\rangle\langle j| \otimes \hat{\rho}_E(T)$) alternative:

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

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

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

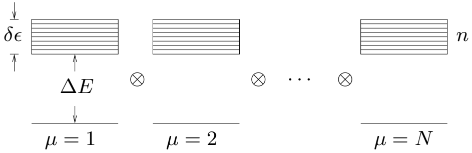
$$\hat{\rho}_S = \sum_a \hat{\rho}_S^a$$



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

Analysis of transport through projection method

"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 gradient driven transport be determined and understood? $\langle \hat{h}_\mu(t) \rangle = ?$

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?)

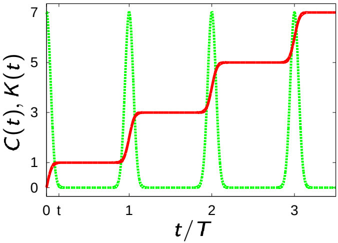
Alternative method: Projection onto hydrodynamical modes

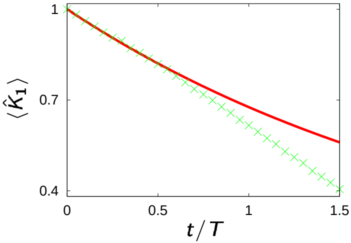
$$\hat{B}_k = \sqrt{\frac{2}{N}} \sum_{\mu} \cos(\frac{2\pi k}{N}\mu)\hat{h}_{\mu} \quad \Rightarrow \text{TCL2} \Rightarrow \quad \dot{B}_k = 2(\cos(\frac{2\pi k}{N}) - 1)K(t)B_k$$

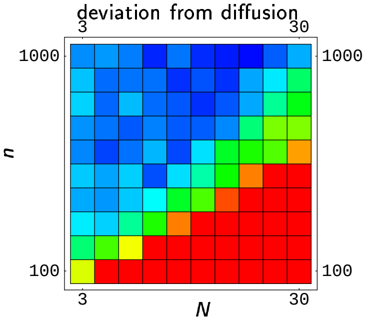
Compare with "random walk dynamics"

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

$$W_k = \sum_{\mu} \cos(\frac{2\pi k}{N}\mu)P_{\mu} \quad \Rightarrow \quad \dot{W}_k = 2(\cos(\frac{2\pi k}{N}) - 1)\kappa W_k$$







With increasing system “lenght” N the longest wavelength hydrodynamical mode undergoes a transition from diffusive to ballistic behavior!
This result, including the “phase boundary”, the diffusion constant κ, etc, may be obtained through a TCL projection analysis to second order.

Moderately sized systems (featuring adequate parameters) seem to relax to some equilibrium in a exponential, diffusive manner

Generality with respect to initial states? $\Rightarrow$

Connection between alternative projection methods and Hilbert space averaging

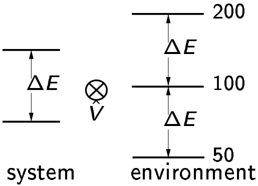
- Technically the above method only applies to states with $\mathcal{P}\hat{\rho}(0) = \hat{\rho}(0)$
- An analysis based on the Hilbert space average method (HAM) produces the same dynamics.
- The dynamcis as resulting from HAM are meant to be valid for the largest part of of all pure initial states,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

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

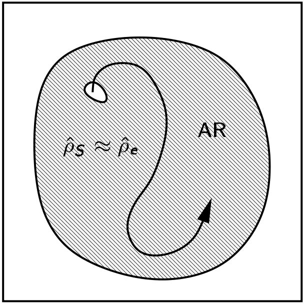
Hilbert space Average Method (HAM) and equilibrium states

What if environmental correlations do not decay?, $\hat{\rho}_S(t \rightarrow \text{``}\infty\text{''}) = ?$

Extreme narrow-band design model



Hilbert space portrait

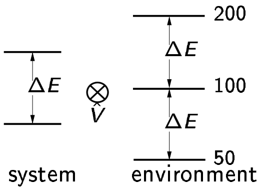


Hilbert space average method:

- 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 $\hat{\rho}_e$: $d^2 = \text{Tr}\left\{(\hat{\rho}_S - \hat{\rho}_e)^2\right\}$
- 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

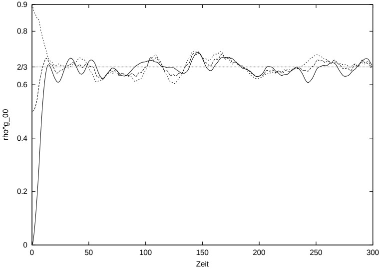
- diagonal within the energy eigenbasis of the system S
- in accord with the idea of "equal a priori probabilities" under given constraints

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

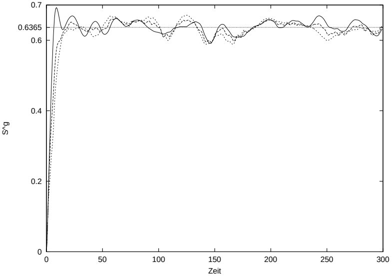
(N_E: "overall size of the environment")

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

- Diffusive transport and equilibration exist and may be analyzed in finite quantum systems
- 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)

All our literature concerning the addressed topics may be found on our homepage

Thank you for your attention!