

# Thermodynamic behavior from Schroedingers dynamics in incompletely observed quantum systems

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## 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:  
 $\langle\dot{\psi}|\dot{\psi}\rangle = \text{const.}$
- Entropy cannot change:  
 $\dot{S} = 0, S = -k\text{Tr}\{\hat{\rho} \ln \hat{\rho}\}$

#### Thermodynamics:

- $A(t) \rightarrow A_{eq}$
- $A_{eq}$  are in accord with “maximum entropy principle”, “a priori postulate of equal probabilities”, “ergodicity”, etc.  $\Rightarrow \dot{S} \geq 0$
- typical dynamics:  $\dot{A}_n = \sum_m R_{nm} A_m$   
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:  $\frac{d\hat{\rho}}{dt} = \mathcal{L}(t)\hat{\rho}(t)$       projection:  $\mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho}$

$\Rightarrow$  big mathematical machinery  $\Rightarrow$

$$\frac{d}{dt}\mathcal{P}\hat{\rho} = \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{P}\hat{\rho}(t')dt' + O(\mathcal{L}^3) \quad \text{“Born approximation”}$$

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

Typical quantum dynamics and standard choice of projection operator

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

$$\hat{\rho}_S := \text{Tr}_E \{ \hat{\rho} \} \quad \mathcal{P}\hat{\rho} := \hat{\rho}_S \otimes \hat{\rho}_E(T) \Rightarrow \text{“RWA”, etc.} \Rightarrow$$

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

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

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

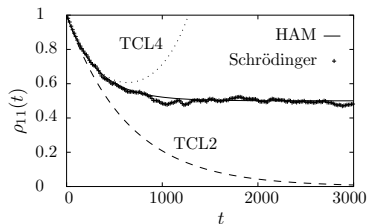
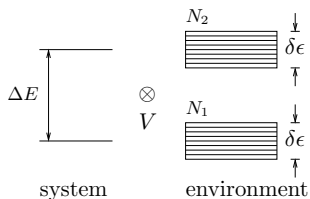
$$\frac{d}{dt} \hat{\rho}_S(t) \approx \int_0^t \mathcal{K}(t-t') dt' \hat{\rho}_S(t) \approx: \mathcal{R} \hat{\rho}_S(t)$$

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

Alternative projection approach with generalized projector :

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

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

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

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

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

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

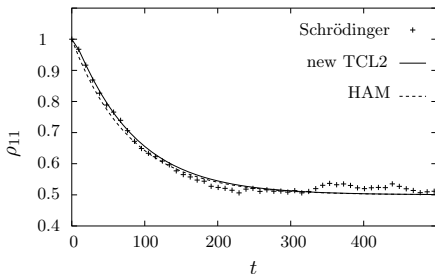
concrete projectors: (standard:  $\hat{B}_{ij} := |i\rangle\langle j| \otimes \hat{\rho}_E(T)$ ) alternative:

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

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

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

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

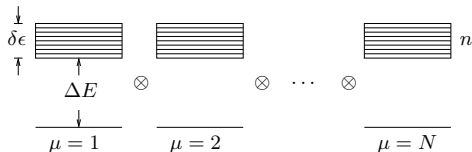


- This scheme produces reasonable results, i.e., higher orders are negligible
- Rates are in accord with Fermi's Golden Rule



## Diffusion in closed finite quantum systems

### “Finite modular quantum system”



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

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

- 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

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

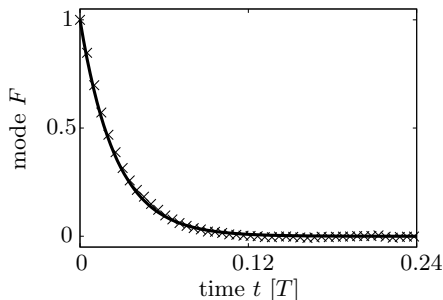
## Compare with “random walk dynamics”

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

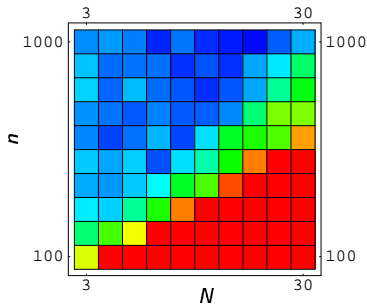
$$W_q = \sum_{\mu} \cos\left(\frac{2\pi q}{N}\mu\right) P_{\mu} \Rightarrow \dot{W}_q = 2\left(\cos\left(\frac{2\pi q}{N}\right) - 1\right) \kappa W_q$$

## Results of the projection technique:

Dynamics 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*

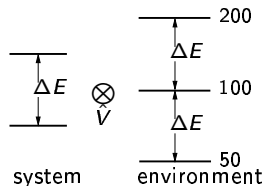
- Technically the above method only applies to states with  $\mathcal{P}\hat{\rho}(0) = \hat{\rho}(0)$
- An analysis based on the Hilbert space average method (HAM) produces the same dynamics.
- The dynamics as resulting from HAM are meant to be valid for the largest part of all pure initial states,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

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

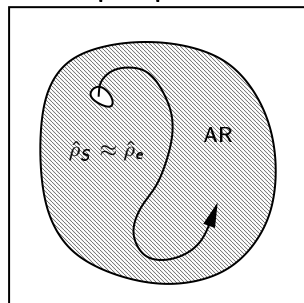
## Hilbert space Average Method (HAM) and equilibrium states

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

**Extreme narrow-band design model**



### Hilbert space portrait



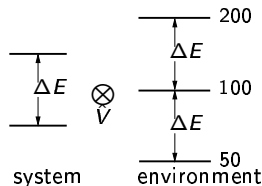
**Hilbert space average method:**

- 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  $\hat{\rho}_e$  :  

$$d^2 = \text{Tr} \{ (\hat{\rho}_S - \hat{\rho}_e)^2 \}$$
- Compute the average of  $d(|\psi\rangle)$  over all  $|\psi\rangle$  that are accessible under given dynamical constraints:  $\llbracket d(|\psi\rangle) \rrbracket_{AR}$  (AR: accessible region)

If  $\llbracket d(|\psi\rangle) \rrbracket_{AR}$  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

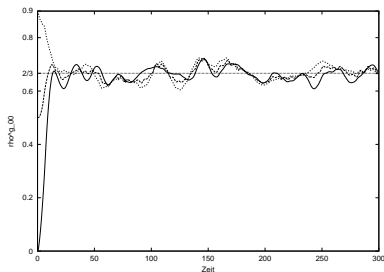
- diagonal within the energy eigenbasis of the system  $S$
- in accord with the idea of “equal a priori probabilities” under given constraints

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

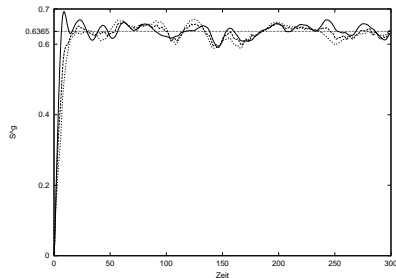
( $N_E$ : “overall size of the environment”)

## 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 equilibration.
- 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!