Thermodynamic behavior from Schroedingers dynamics in incompletely observed quantum systems

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Contents

Background and projection techniques

Quantum dynamics:

- the Schrödinger equation
  $i\hbar|\dot{\psi}(t)\rangle = \hat{H}|\psi(t)\rangle$
  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:

- Observables: $A(t) \rightarrow A_{eq}$
- 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 technique, time convolutionless (TCL)

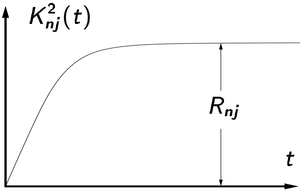
linear superoperators: $\mathcal{L}$, $\mathcal{P}$ $\qquad \hat{H} = \hat{H}_0 + \lambda \hat{V}$ $\qquad$ interaction picture $\Rightarrow$

dynamics: $\quad \frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathcal{L}(t)\hat{\rho}(t) = \mathrm{i}\lambda[\hat{V}(t), \hat{\rho}]$ $\qquad$ projection: $\quad \mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho}$

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

$\Rightarrow$ big mathematical machinery $\Rightarrow \quad \dot{B}_n = \sum_{\alpha,j} \lambda^\alpha K_{nj}^\alpha(t) B_j$

$K_{nj}^2(t)$: Integral over correlation function $C_{nj}^2 = \mathrm{Tr}\left\{\mathcal{L}(t)\hat{B}_n \mathcal{L}(0)\hat{B}_j\right\}$
If you strike it lucky $K_{nj}^\alpha(t) \approx 0$ except for $K_{nj}^2(t)$ and $K_{nj}^2(t)$ looks like this:

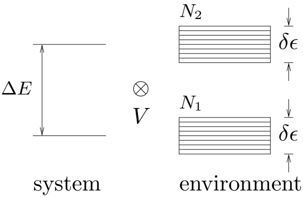


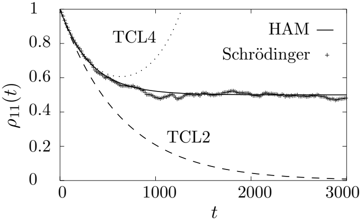
$$\dot{B}_n \approx \sum_j R_{nj} B_j$$

$R_{nj} = R_{jn} \Rightarrow$: the observables exhibit exponentially equilibrating dynamcis

Application of projection technique

Equilibration through finite environments





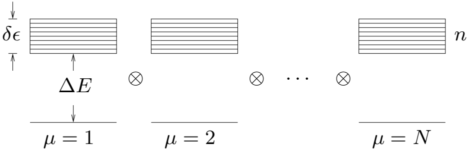
$$H_0 : \text{see sketch}, \quad \hat{V} = \lambda \sum_{n_1, n_2} C(n_1, n_2)\, |1^S\rangle\langle 0^S| \otimes |n_1^E\rangle\langle n_2^E| + \text{h.c.}$$

$C(n_1, n_2)$ normalized, random, complex Gaussian numbers

$$\mathcal{P}_1 : \hat{B}_{ij} := |i^S\rangle\langle j^S| \otimes \hat{\rho}_E(T \approx 0) \qquad \mathcal{P}_2 : \hat{B}_{ija} := |i^S\rangle\langle j^S| \otimes \frac{\hat{\Pi}_a}{\sqrt{N_a}}, \quad \hat{\Pi}_a := \sum_{n_a} |n_a^E\rangle\langle n_a^E|$$

- In both cases the correlations decay much fast on the timescale of relaxation
- $\mathcal{P}_2$(HAM) allows for an “Boltzmannian equilibrium state”, $\mathcal{P}_1$(TCL) does not!

Transport in "modular quantum systems"



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

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

- 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 "Fourier" 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"

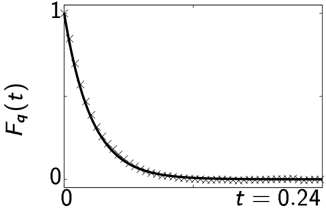
$$\dot{P}_\mu = \kappa(P_{\mu-1} + P_{\mu+1} - 2P_\mu) \quad \text{"discrete diffusion equation"}$$

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

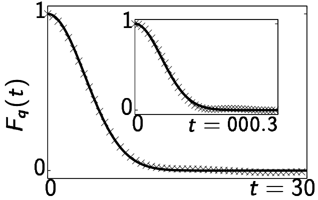
Results of the projection onto modes:

Dynamcis of modes $F_q(t)$:

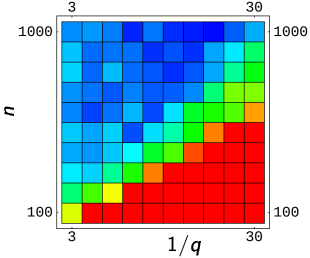
intermediate wavelength



long/short wavelength

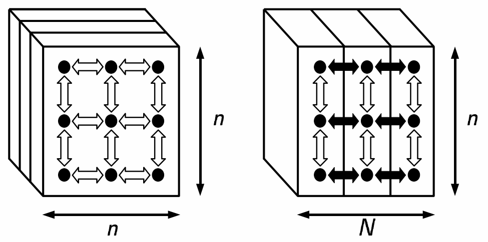


Deviation from diffusion:



- diffusive transport occurs only on an intermediate (nano-) lengthscale
- the relevant dynamics are well described by TCL to 2. order

3d-Anderson models: projection onto modes

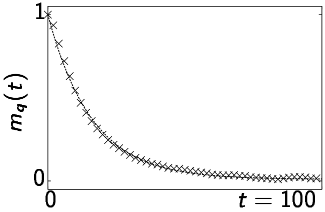


$$\hat{H} = \sum_{\mathbf{r}} \epsilon(\mathbf{r})\, \hat{a}^\dagger(\mathbf{r})\, \hat{a}(\mathbf{r}) + \sum_{NN} \hat{a}^\dagger(\mathbf{r})\, \hat{a}(\mathbf{r}')$$

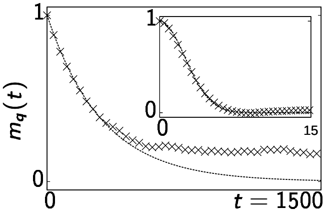
$\epsilon(\mathbf{r})$: Gaussian random numbers $\Rightarrow$

$$\hat{H} = \sum_{\mu=0}^{N-1} \hat{h}_0(\mu) + \sum_{\mu=0}^{N-1} \hat{v}(\mu, \mu+1)$$

intermediate wavelength



long/short wavelength

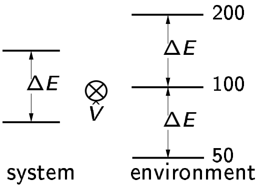


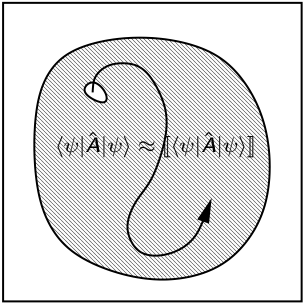
The diffusive wavelength regime appears to be rather small.

Hilbertspace Average Method (HAM) and equilibrium states

If correlation functions do not decay, projection methods can hardly be expected to converge

Extreme narrow-band model





Hilbertspace average (HA): Average of some function of $|\psi\rangle$ over states that are uniformly distributed on the hypersphere

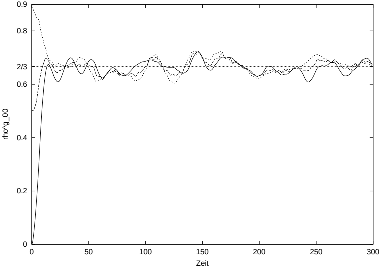
HA: $[\![\langle\psi|\hat{A}|\psi\rangle]\!] = \mathrm{Tr}\{\hat{A}\}/N$ spectral variance: $\Delta^2(A) = \mathrm{Tr}\{\hat{A}^2\}/N - (\mathrm{Tr}\{\hat{A}\}/N)^2$

Hilbertspace variance: $[\![\langle\psi|\hat{A}|\psi\rangle^2]\!] - [\![\langle\psi|\hat{A}|\psi\rangle]\!]^2 = \Delta^2(A)/(N+1)$

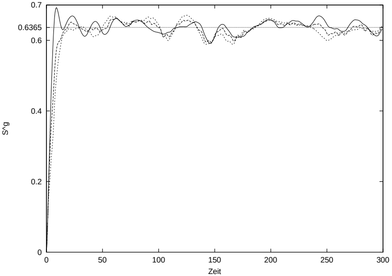
The HA equals the Boltzmannian equilibrium value $\Rightarrow$
Equilibrium values are the most frequent ones

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

The end

- Relaxation to Boltzmannian equilibrium is “typical” for some observables, even in closed quantum systems (no time or ensemble averaging needed).
- In some cases this relaxation may be described by truncating a projection expansion. The convergence crucially depnds on the choice of the projector

For further reference visit out homepage or simply ask me.

Thank you for your attention!