Transport and equilibration within finite quantum systems

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Contents

Background of equilibration in quantum sytems

Do (finite) quantum systems approach equilibrium?

- The Schrödinger equation features no fixpoint
- The entropy $S(\hat{\rho}) := -k\mathrm{Tr}\left\{\hat{\rho}\ln\hat{\rho}\right\}$ is conserved under time evolution

$\Rightarrow$ Most concepts in quantum mechanics feature the concept of a "thermostat"

The standard approach

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

Consider the reduced density operator : $\hat{\rho}_S := \mathrm{Tr}_E\left\{\hat{\rho}\right\}$. For any nonzero interaction $\hat{V}$ $\frac{\mathrm{d}}{\mathrm{d}t}S(\hat{\rho}_S)$

How does one get an autonomous equation of motion for $\hat{\rho}_S$?

Projection operator techniques:

Linear Superoperators $$\frac{d\hat{\rho}}{dt} = \mathcal{L}(t)\hat{\rho}(t) \qquad \mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho} \tag{1}$$

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

$$\frac{d}{dt} = \mathcal{P}\hat{\rho} = \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{P}\hat{\rho}(t')dt' + O(\mathcal{L}^3) \tag{2}$$

Typical dynamics and choice of projection operator

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

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

Evolution non-local in time:

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \int_0^t \mathcal{R}(t-t')\hat{\rho}_S(t')\mathrm{d}t'$$

$\mathcal{R}(t-t') \approx \mathcal{R} \times \mathrm{Tr}_E\{\hat{B}(t-t')\hat{B}^\dagger(0)\hat{\rho}_E(T)\} + c.c.$ "bath correlation functions"

If decay of bath correlations short compared to relaxation dynamics of the considered system $\Rightarrow$ "Markovian" $\Rightarrow$

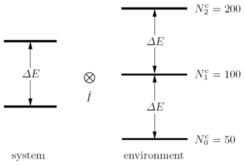
$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \gamma\mathcal{R}\hat{\rho}_S(t) \qquad \gamma = \int_0^\infty \mathrm{Tr}_E\{\hat{B}(\tau)\hat{B}^\dagger(0)\hat{\rho}_E(T)\} + c.c. d\tau$$

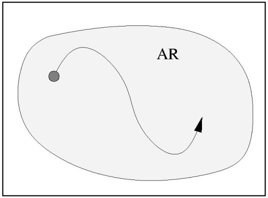
Quantum master equations

$$\frac{\mathrm{d}\rho_{ii}}{\mathrm{d}t} = \sum_j R_{ij}\rho_{jj} - \sum_l R_{li}\rho_{ii}$$ "thermalization" $$\frac{\mathrm{d}\rho_{ij}}{\mathrm{d}t} = r_{ij}\rho_{ij}$$ "decoherence"

Finite environments

extreme narrow-band design model

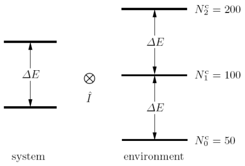




What if the environmental correlations do not decay? $\hat{\rho}_S(t \to "\infty") = ?$

- 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 expected state $\hat{\rho}_e$: $d = \mathrm{Tr}_E \left\{(\hat{\rho}_S - \hat{\rho}_e)^2\right\}$
- Compute the average of $d(|\psi\rangle)$ over all $|\psi\rangle$ that are accessible under given dynamical constraints: $[\![d(|\psi\rangle)]\!]_{AR}$

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



What to use for $\hat{\rho}_e$?
Check maximum local entropy states that are consistent with given invariants.

microcanonical:

$$\hat{\rho}_e := \sum_{n,A} \frac{W_A}{N_S(E_A)} |A,n\rangle\langle A,n|$$

energy exchange

$$\hat{\rho}_e \propto \sum_E W_E \sum_{A,n} N_E(E-E_A)|A,n\rangle\langle A,n|$$

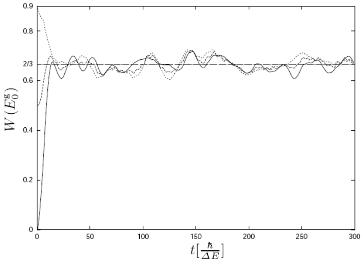
$N_{S(E)}(U)$: degree of degeneracy of the system (environment) at the energy U
$|A,n\rangle$: energy eigenstate of the system with energy E_A
W_A: probability to find the system initially at energy E_A

W_E: probability to find the system+environment initially at energy E

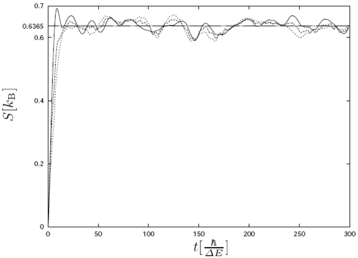
For those trial states $\hat{\rho}_e$ $[\![d]\!]$ decreases like $1/N_E$

Schrödinger evolutions for "randomly coupled" models

ground state occupation probability:



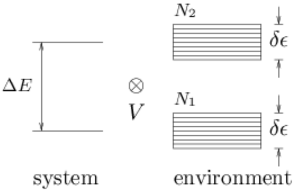
local entropy:

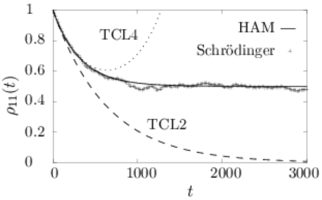


Even though the system is not ergodic, dynamical evolutions mirror the "topology"

Broad band finite environments , dynamics and HAM

Do standard methods always work if the environmental correlations do decay?





$$\hat{H}_0 = \Delta E \hat{\sigma}_z + \sum_{n_1} \frac{\delta\epsilon}{N_1} n_1 |n_1\rangle\langle n_1| + \sum_{n_2} (\Delta E + \frac{\delta\epsilon}{N_2} n_2)|n_2\rangle\langle n_2|$$

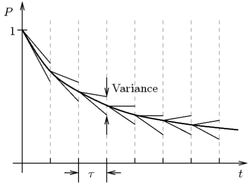
$$\hat{V} = \lambda \sum_{n_1, n_2} C(n_1, n_2)\, \hat{\sigma}^+ |n_1\rangle\langle n_2| + \text{h.c.} \qquad (3)$$

Although correlations decay fast, higher orders may not converge!

The HAM approach: $\langle \hat{P}_\xi(t+\tau)\rangle \approx [\![\langle\phi|\hat{U}^\dagger(t,\tau)\hat{P}_\xi\hat{U}(t,\tau)|\phi\rangle]\!]_{\{\langle\phi|\hat{P}_{\xi'}|\phi\rangle = \langle\hat{P}_{\xi'}(t)\rangle\}}$

$\hat{U}(t,\tau)$: propagator in the interaction picture as given by a Dyson series truncating $\hat{U}(t,\tau)$ at second order in λ yields under some conditions

$$\langle \hat{P}_\xi(t+\tau)\rangle \approx \langle \hat{P}_\xi(t)\rangle + \tau\sum_{\xi'}(R_{\xi\xi'}\langle\hat{P}_{\xi'}(t)\rangle - R_{\xi'\xi}\langle\hat{P}_\xi(t)\rangle)$$

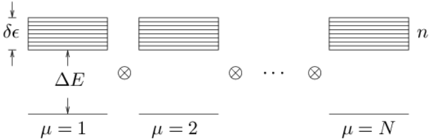


"iterative guessing" As a guess the result is valid for all initial states of the full system, including pure, mixed, correlated, entangled, etc. It leads to autonomous dynamic in the variables of interest $\langle\hat{P}_\xi(t)\rangle$:

masterequation: $$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{P}_\xi\rangle = \sum_{\xi'} R_{\xi\xi'}\langle\hat{P}_{\xi'}\rangle - R_{\xi'\xi}\langle\hat{P}_\xi\rangle$$

Transport through finite systems

the model



$$\hat{H} = \sum_{\mu=1}^{N} \hat{h}_\mu + \hat{v}_\mu \qquad (4)$$

$$\hat{h}_\mu = \sum_n \epsilon_n \hat{a}^\dagger_{\mu,n} \hat{a}_{\mu,n} \quad \hat{v}_\mu = \sum_{nm} c_{nm} \hat{a}^\dagger_{\mu,n} \hat{a}_{\mu+1,m} + h.c. \qquad (5)$$

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

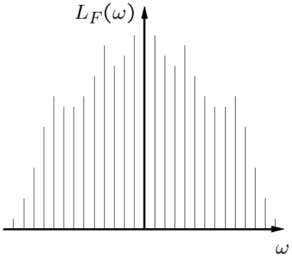
How can gradient driven transport be determined and understood? $\langle \hat{h}_\mu(t) \rangle = ?$

Kubo formula? Derived for force driven transport:

$$\hat{H} = \hat{H}_0 + \hat{U}(t) \quad E = -\nabla U$$

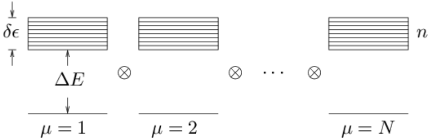
$$j(\omega) = L(\omega)E(\omega) \quad L(\omega) = \frac{1}{V}\int_0^{\infty} \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}\omega t} \int_0^{\beta} \mathrm{d}\tau\, \mathrm{Tr}\{\hat{\rho}_0 \hat{j}(0)\hat{j}(t+\mathrm{i}\tau)\}, \qquad (6)$$

Does the proportionality of force driven transport (viscosity) and gradient driven transport from Brownian motion hold in this case?



How does one extract the coefficient for gradient driven transport for a finite system, i.e., from a discrete spectrum ?

Extract transport behavior from a (linearized) Boltzmann equation?



$$\dot{f}(x,v,t) + v\nabla f(x,v,t) = \int \mathrm{d}v' R(v,v') f(x,v',t) \qquad (7)$$

- What are the (quasi-)particles?
- What are the velocities v of the (quasi-)particles ?
- What are the rates $R(v, v')$?
- Is the stosszahlansatz justified?

The HAM approach to transport:
consider local occupation numbers :$P_\mu := \sum_n \hat{a}^\dagger_{\mu,n}\hat{a}_{\mu,n}$
Compute the HA for $\langle \hat{P}_\mu(t+\tau)\rangle$ under the restriction of given $\langle \hat{P}_{\mu'}(t)\rangle$

$$\langle \hat{P}_\mu(t+\tau)\rangle \approx [\![\langle\phi|\hat{U}^\dagger(t,\tau)\hat{P}_\mu\hat{U}(t,\tau)|\phi\rangle]\!]_{\{\langle\phi|\hat{P}_{\mu'}|\phi\rangle = \langle\hat{P}_{\mu'}(t)\rangle\}}$$

Under some conditions on the model parameters this yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{P}_\mu\rangle = R(\langle\hat{P}_{\mu+1}\rangle + \langle\hat{P}_{\mu-1}\rangle - 2\langle\hat{P}_\mu\rangle) \Longleftrightarrow \tag{8}$$

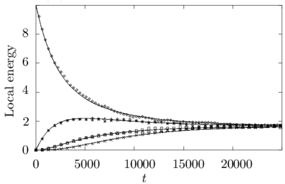
- autonomous dynamics for the variables of interest
- dynamics generate diffusive

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{P}_\mu\rangle = j_{\mu-1} - j_\mu \quad j_\mu = -R(\langle\hat{P}_{\mu+1}\rangle - \langle\hat{P}_\mu\rangle) \tag{9}$$

numerical results for a 6-subunit-ring

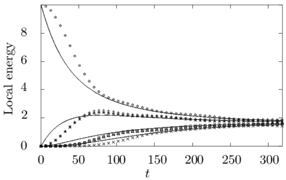
intermediate coupling

dynamics



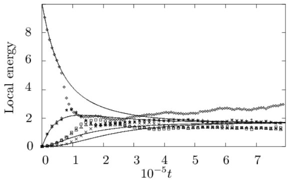
strong coupling

dynamics

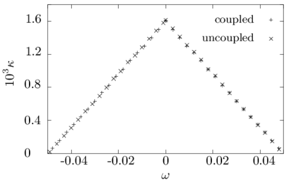


weak coupling

dynamics



kubo spectrum



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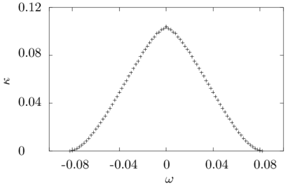
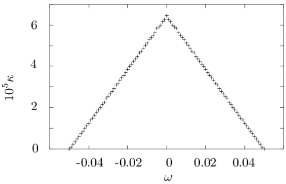
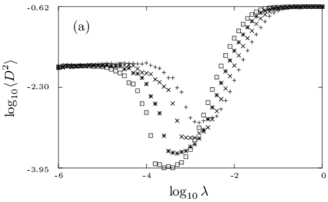


kubo spectrum

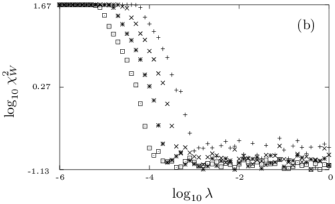


The connection to quantum chaos

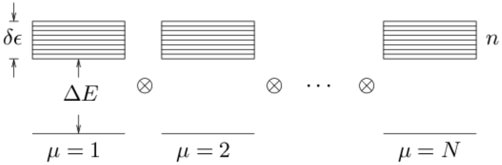
deviation from precisely diffusice behavior



deviation from Wigner-Dyson level statistics



Fourier's law



the model

$$\hat{H} = \sum_{\mu=1}^{N} \epsilon_{\boldsymbol{n}} \hat{a}^{\dagger}_{\mu,\boldsymbol{n}} \hat{a}_{\mu,\boldsymbol{n}} \tag{10}$$

$$\hat{H} = \sum_{\mu=1}^{N} \hat{h}_{\mu} + \sum_{\mu=1}^{N-1} \hat{v}_{\mu,\mu+1} \tag{11}$$

Local energy

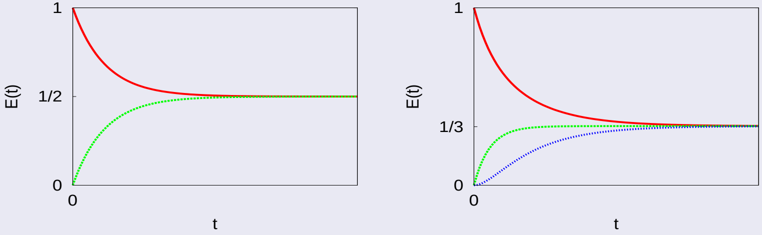
$$E_{\mu}(t) = \langle \psi(t) | \hat{h}_{\mu} | \psi(t) \rangle \tag{12}$$

Fourier's law (discrete version)

Normal transport

- Fourier's law + continuity equation

$$\begin{aligned} \dot{E}_1 &= \eta\,(E_2 - E_1) \\ \dot{E}_\mu &= \eta\left[(E_{\mu+1} - E_\mu) - (E_\mu - E_{\mu-1})\right] \\ \dot{E}_N &= \eta\,(E_{N-1} - E_N) \end{aligned} \tag{15}$$



- Measure D^2:
  - Deviation of the (numerically) exact dynamics from (15)