Aspects of Non-Equilibrium Quantum Thermodynamics

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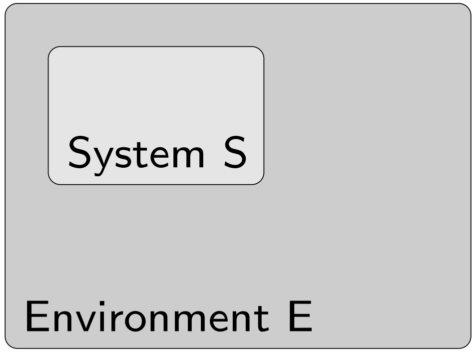
1 Introduction

Schrödinger Dynamics:



Closed system (system+environment) Schrödinger dynamics:

$$\text{pure state} \quad |\psi\rangle \quad \text{or} \quad \hat{\rho} = |\psi\rangle\langle\psi|$$

Liouville von Neumann Equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = -\mathrm{i}[\hat{H}, \hat{\rho}] = \hat{\mathcal{L}}\hat{\rho}$$

Reduced dynamics for the system S:

$$\hat{\rho}_{\mathrm{S}} = \mathrm{Tr}_{\mathrm{E}}\left\{\hat{\rho}\right\} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}_{\mathrm{E}}\left\{\hat{\rho}\right\} = \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}} = \mathrm{Tr}_{\mathrm{E}}\left\{\hat{\mathcal{L}}\hat{\rho}\right\}$$

not a closed equation for S

Nakajima-Zwanzig Projection Operator Technique

Projection operator to relevant (irrelevant) part of the system:

$$\hat{\mathcal{P}}\hat{\rho} = \mathsf{Tr}_{\mathsf{E}}\left\{\hat{\rho}\right\} \otimes \hat{\rho}_{\mathsf{E}} = \hat{\rho}_{\mathsf{S}} \otimes \hat{\rho}_{\mathsf{E}} \qquad \hat{\mathcal{Q}}\hat{\rho} = \hat{\rho} - \hat{\mathcal{P}}\hat{\rho}$$

Nakajima-Zwanzig equation (factorizing initial conditions $\hat{\rho}(0) = \hat{\rho}_{\mathsf{S}}(0) \otimes \hat{\rho}_{\mathsf{E}}$):

$$\frac{\mathsf{d}}{\mathsf{d}t}\hat{\mathcal{P}}\hat{\rho}(t) = \int_0^t \mathsf{d}s\hat{\mathcal{K}}(t,s)\hat{\mathcal{P}}\hat{\rho}(s)$$

- exact equation for relevant part of the system
- non-local in time (future time evolution depends on the history)
- integro-differential equation

Born-, Redfield-, Markov- and rotating wave approximation

➜ quantum master equation (Linblad form): $\frac{\mathsf{d}}{\mathsf{d}t}\hat{\rho}_{\mathsf{S}} = -\mathsf{i}[\hat{H}_{\mathsf{S}}, \hat{\rho}_{\mathsf{S}}] + \hat{\mathcal{D}}\hat{\rho}_{\mathsf{S}}$

Time Convolutionless (TCL) Technique

- TCL uses the same projection operator as Nakajima-Zwanzig.
- slightly different derivation
- exact, time-local, inhomogenious linear differential equation
- here factorizing initial conditions

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathcal{P}}\hat{\rho}(t) = \hat{\mathcal{K}}(t)\hat{\mathcal{P}}\hat{\rho}(t) + \hat{\mathcal{I}}(t)\hat{\rho}(0)$$

To find a solution of this equation it is common to expand the TCL generator $\hat{\mathcal{K}}$.

Hilbert Space Average Method

Dyson expansion of the complete time evolution (time dependent perturbation theory)

$$|\psi(t+\Delta t)\rangle = \hat{D}|\psi(t)\rangle\,, \qquad \hat{\rho}_{\mathsf{S}}(t+\Delta t) = \mathsf{Tr}_{\mathsf{E}}\left\{\hat{D}|\psi(t)\rangle\langle\psi(t)|\hat{D}^\dagger\right\}$$

Hilbert Space Average ($\hat{D}$ in 2. order)

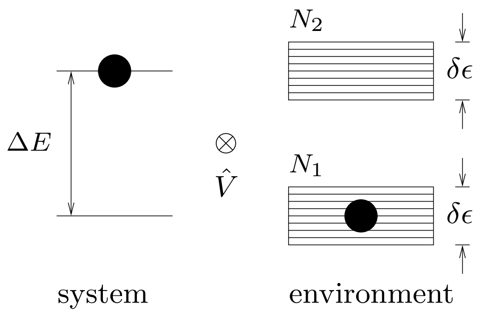
$$\hat{\rho}_{\mathsf{S}}(t+\Delta t) \approx [\![\mathsf{Tr}_{\mathsf{E}}\left\{\hat{D}|\psi(t)\rangle\langle\psi(t)|\hat{D}^\dagger\right\}]\!]$$

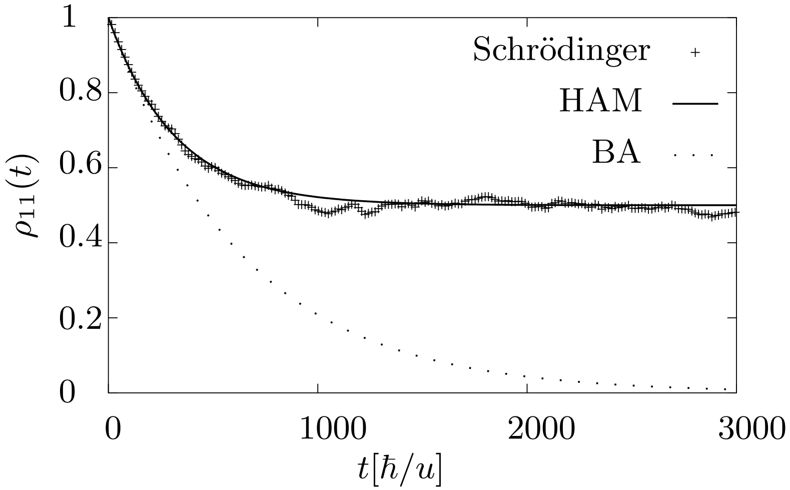
Result:

- rate equation for $\hat{\rho}_{\mathsf{S}}$
- criteria for applicability
- not necessarily factorizing initial states

2 Relaxation Processes

Design model (finite bath system)





$N_1 = N_2 = 500$, $\lambda = 0.001$, $\delta\epsilon = 0.5$

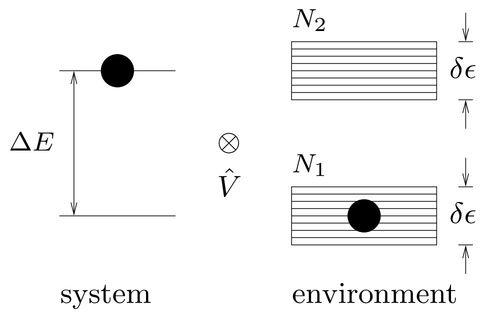
The TCL master equation:

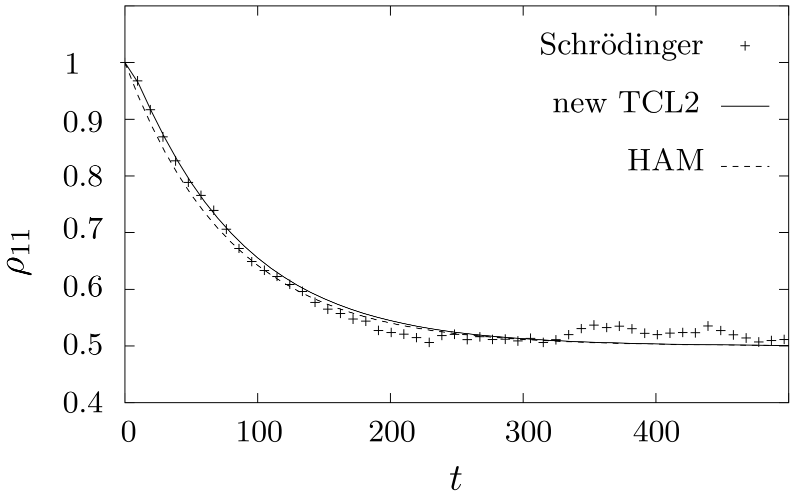
- expansion does not converge in arbitrary high order
- new projector for TCL from HAM (Breuer)

New TCL in 2. order

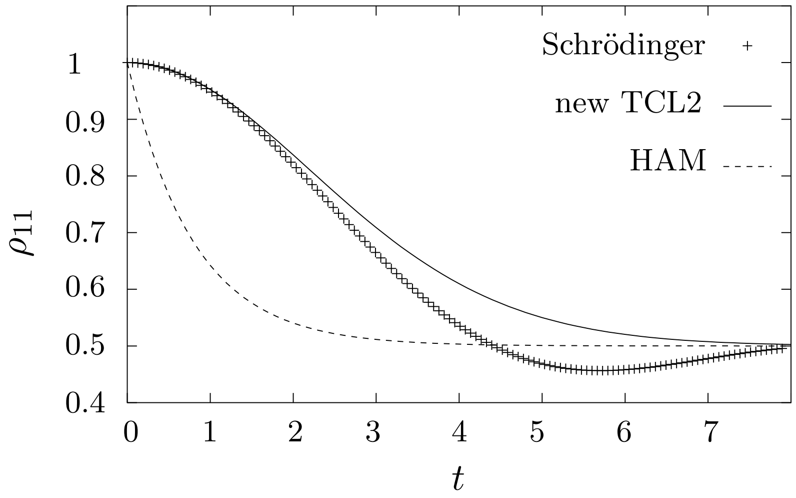
HAM Criteria 1: $C_1 = \lambda \frac{N_1}{\delta\epsilon} \geq 0.5$

HAM Criteria 2: $C_2 = \lambda^2 \frac{N_1}{\delta\epsilon^2} \ll 1$





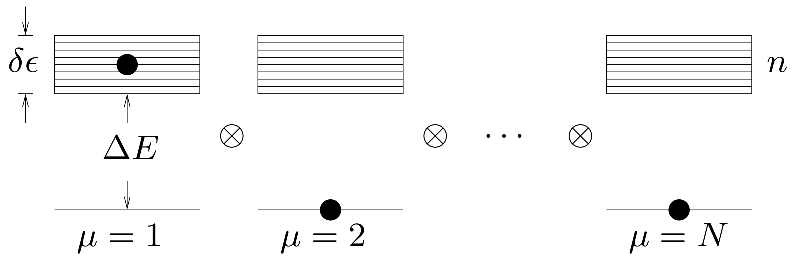
$\lambda = 0.001,\ C_1 = 1,\ C_2 = 0.002$



$\lambda = 0.01,\ C_1 = 10,\ C_2 = 0.2$

3 Application of HAM to Heat Conduction Models

Design Model: Energy Diffusion

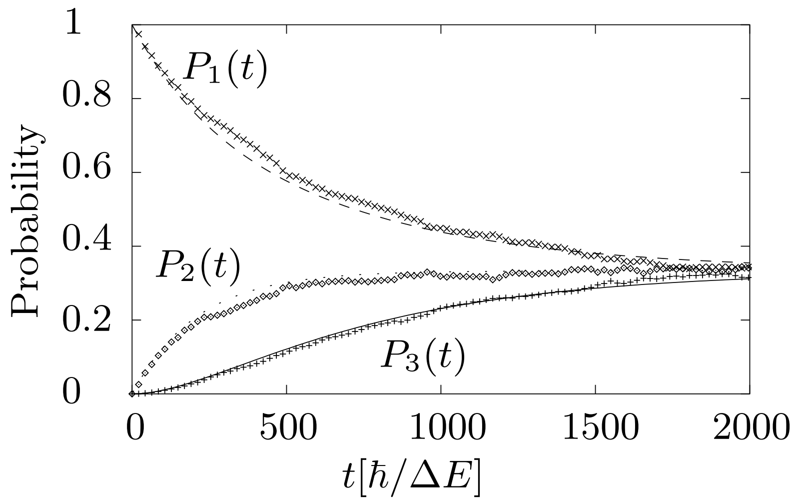


HAM-Rate Equation:

$$\frac{\mathrm{d}P_1}{\mathrm{d}t} = -\gamma(P_1 - P_2) \ ,$$

$$\frac{\mathrm{d}P_\mu}{\mathrm{d}t} = -\gamma(2P_\mu - P_{\mu-1} - P_{\mu+1}) \ ,$$

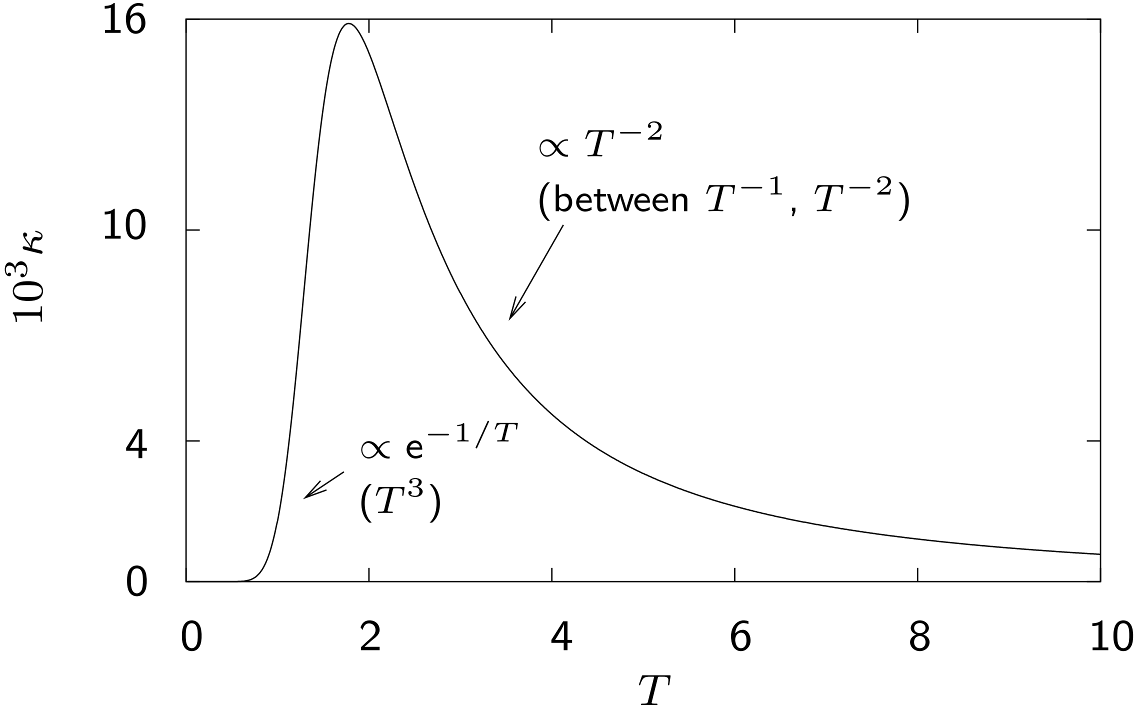
$$\frac{\mathrm{d}P_N}{\mathrm{d}t} = -\gamma(P_N - P_{N-1}) \ .$$



$N = 3$, $n = 500$, $\lambda = 0.005$, $\delta\epsilon = 0.5$

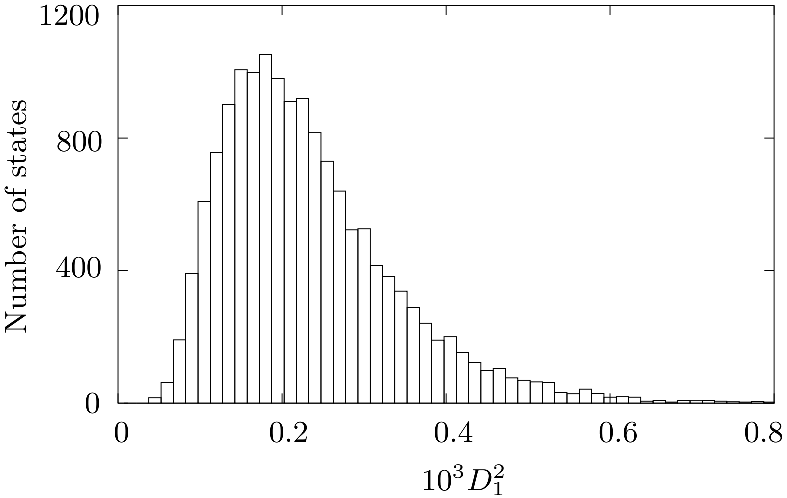
Design Model: Heat Diffusion

- quasi thermal initial state: eigenstates superposed according to Boltzmann probability
- heat conductivity $\kappa = \gamma c$ (energy diffusion constant γ, heat capacity c of single subunit)

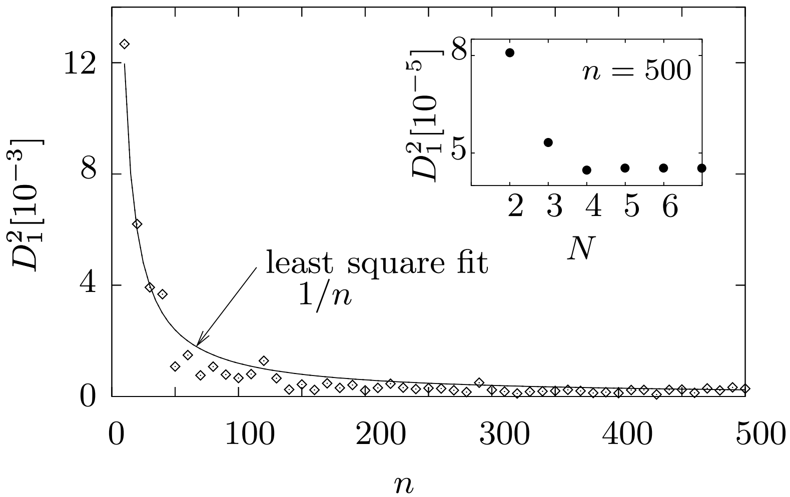


Deviations of the HAM Prediction from the Exact Dynamics

$$D_1^2 = \frac{1}{\tau}\int_0^{5\tau} (P_1^{\mathsf{HAM}}(t) - P_1^{\mathsf{exact}}(t))^2 \mathrm{d}t \quad \text{with} \quad \tau = \frac{1}{\kappa}$$



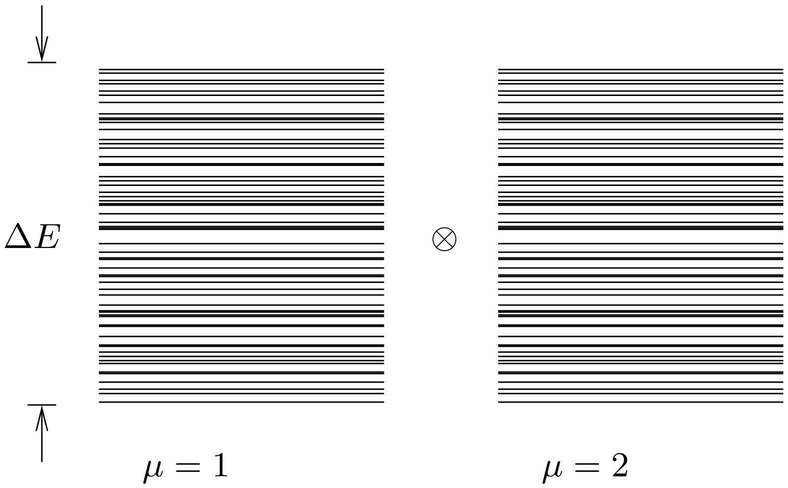
Fluctuations for random initial states

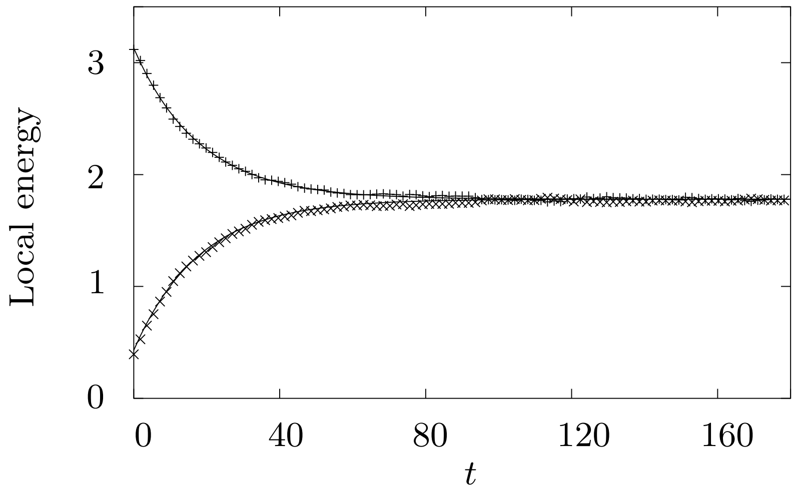


Fluctuations over n and N

The Route to More Realistic Models

- system must exhibit a topological structure in real space
- coarse-graining of the system → weakly coupled subunits
- HAM criteria?

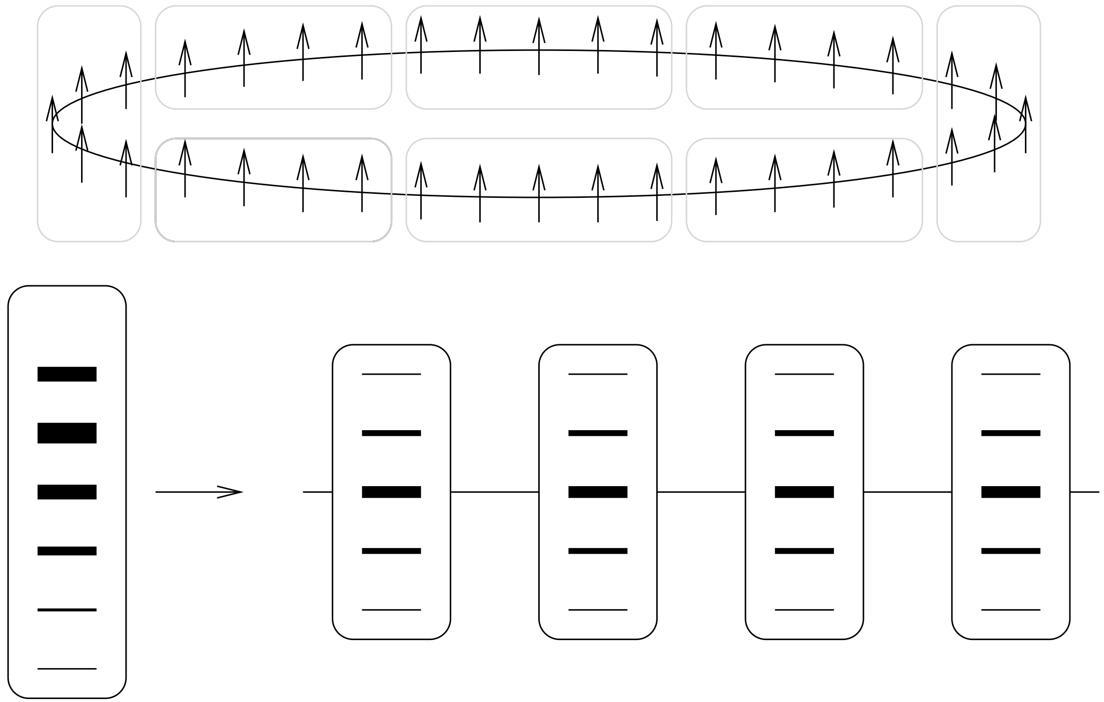




$n = 60$, $\lambda = 0.005$, $\Delta E = 7$

initial state: quasi thermal $T_1 = 40$, $T_2 = 1$

Subspace Conduction in Spin Systems (Pedro Vidal)

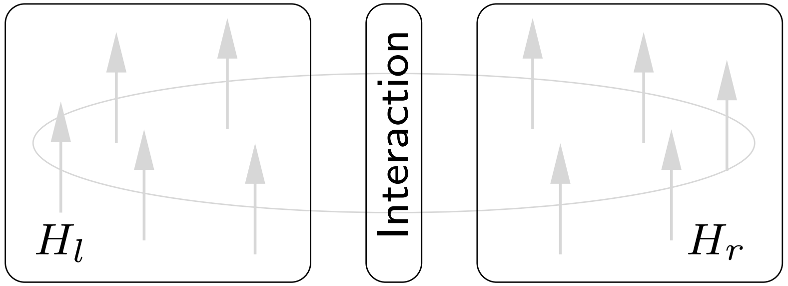


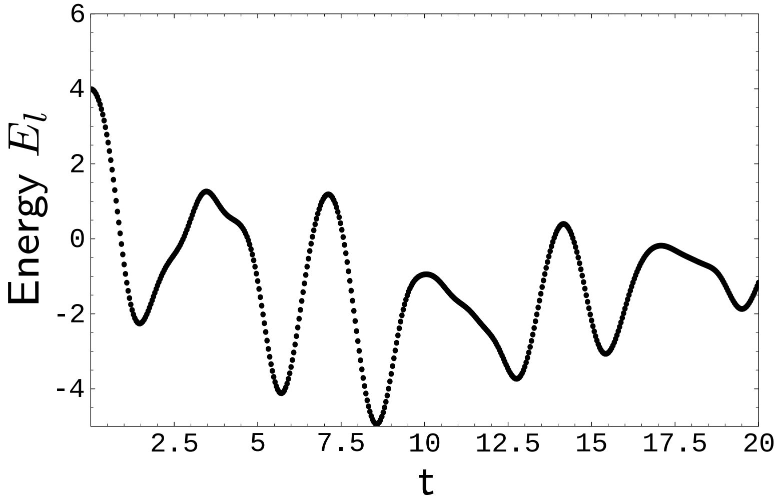
Heisenberg-Ring

- one excitation subspace
- NN coupling type
- no statistical behavior
- higher subspaces?
- ONN coupling?

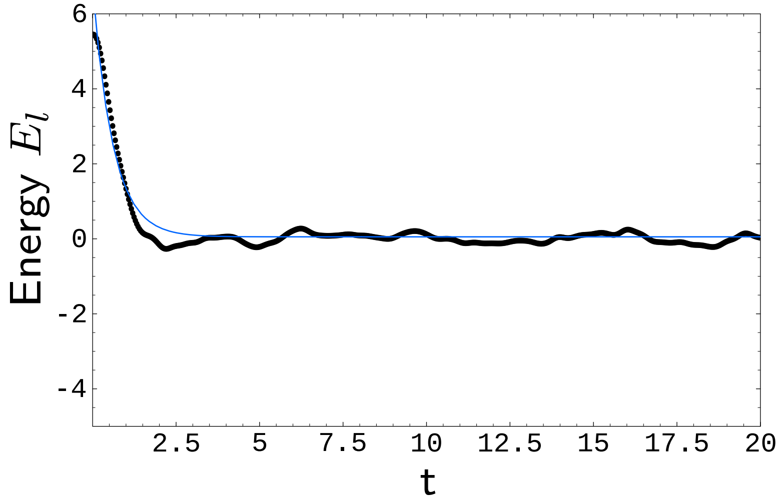
Spin-Ring: Coarse-Graining

- without local field
- Heisenberg NN interaction
- Random NN interaction, no disorder



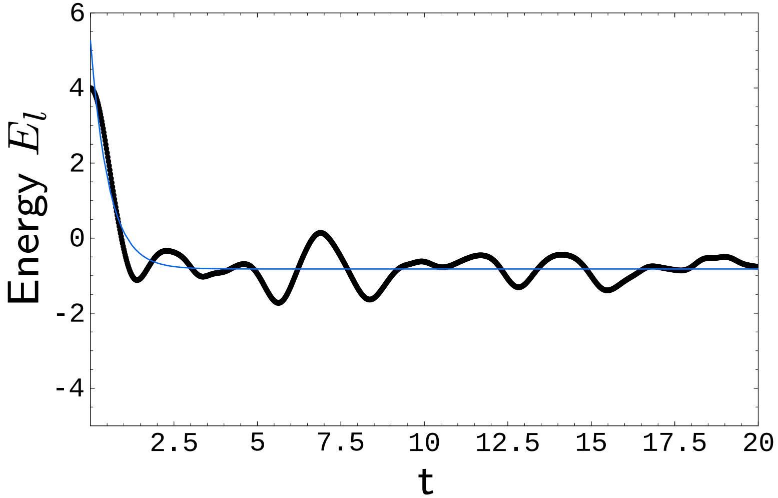


Heisenberg-Ring



Random-Ring

Spin-Ring



Heisenberg-Random-Ring

4 Conclusion

- **Relaxation via finite baths**
  - Born approximated Nakajima-Zwanzig equation fails
  - application of HAM
  - new TCL
- **Heat conduction**
  - normal heat respectively energy diffusion in design models
  - evidences for normal diffusion in realistic models
    (single band model, spin systems)
  - foundation of Kubo-formula from HAM