Reservoir coupling approach to transport in quantum systems

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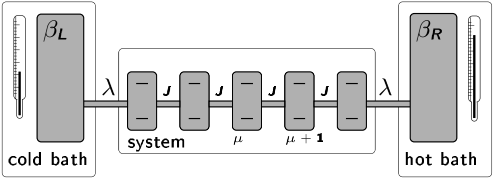
Introduction

The "why" and the "how"



Why? ⇒ To determine (bulk) transport properties of systems

Other tools:

- map onto a Boltzmann equation
- linear response (Kubo formula)
- project onto density waves
- Landauer formula ... etc.

How?

- find a pertinent equation of motion for $\hat{\rho}$ coupled to different baths
- find its stationary non-equilibrium state
- extract density gradient $\nabla n(x)$ and current $j(x)$ and compute $D = j/\nabla n$

Is the so described transport behavior due to the system or the bath contacts?
How does this transport description compare to other descriptions?

Modelling reservoirs ⇒ Quantum Master Equations (QME)

"microscopical"

model system+bath+coupling:

$$\hat{H} = \hat{H}_S + \sum_n \epsilon_n \hat{a}_n^+ \hat{a}_n + \hat{V}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = \mathrm{i}[\hat{H}, \hat{\rho}]$$

"Project" onto $\hat{\rho}_S(t) \otimes \hat{\rho}_B(\beta)$ and truncate the, e.g., Nakajima-Zwanzig equation at leading order

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S^D(t) = \int_0^\infty \mathcal{G}'(t,t')\hat{\rho}_S^D(t')$$

Redfield approximation (QME):

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \mathrm{i}[\hat{H}_S, \hat{\rho}_S(t)] + \mathcal{G}\hat{\rho}_S(t)$$

$\mathcal{G}$: superoperator, linearily maps a matrix onto another

"phenomenological"

find a linear, time local equation which evolves a density matrix into a density matrix, i.e., "Lindblad form" (QME):

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \mathrm{i}[\hat{H}_S, \hat{\rho}_S(t)] + \mathcal{L}\hat{\rho}_S$$

$$\mathcal{L}\hat{\rho}_S = \sum_k \alpha_k \left(\hat{E}_k \hat{\rho}_S \hat{E}_k^\dagger - \tfrac{1}{2}[\hat{E}_k^\dagger \hat{E}_k, \hat{\rho}_S]_+ \right)$$

Determine $\hat{E}_k, \alpha_k$ from the "result"

The problem: $\mathcal{G}$ is not necessarily of Lindblad form.

"Lindbladization" is a subtle thing, crucial features may be lost

But why Lindblad form?

Stochastic unravelling: a way to solve the QME

The solution $\hat{\rho}(t)$ of a QME in Lindblad form is equivalent to an ensemble of trajectories generated by , e.g., this piecewise deterministic differential equation (PDDE):

$$\mathrm{d}|\psi(t)\rangle = -\mathrm{i}\,\hat{G}(|\psi(t)\rangle)\,|\psi(t)\rangle\,\mathrm{d}t + \sum_k \left(\frac{\hat{E}_k|\psi(t)\rangle}{\|\hat{E}_k|\psi(t)\rangle\|} - |\psi(t)\rangle \right) \mathrm{d}n_k$$

$$\hat{G}(|\psi(t)\rangle) = \hat{H} - \frac{\mathrm{i}}{2}\sum_k \alpha_k \hat{E}_k^\dagger \hat{E}_k - \alpha_k \|\hat{E}_k|\psi(t)\rangle\|^2$$

$$\langle \mathrm{d}n_k \rangle = \|\hat{E}_k|\psi(t)\rangle\|^2\,\mathrm{d}t\,, \quad \mathrm{d}n_k\,\mathrm{d}n_l = \delta_{kl}\,\mathrm{d}n_k$$

Poisson increments: $\mathrm{d}n_k \in \{0, 1\}$

If the dimension of the PDDE is n, then the dimension of the QME is n^2

Concrete set ups and results

The Heisenberg chain set up

Hamiltonian $\hat{H}$, local energies $\hat{h}^{(\mu)}$ and local energy currents $\hat{J}^{(\mu)}$

$$\hat{H}_S = \sum_\mu \frac{\Omega}{2}\,\hat{\sigma}_z^{(\mu)} + J(\hat{\sigma}_x^{(\mu)} \otimes \hat{\sigma}_x^{(\mu+1)} + \hat{\sigma}_y^{(\mu)} \otimes \hat{\sigma}_y^{(\mu+1)} + \Delta\hat{\sigma}_z^{(\mu)} \otimes \hat{\sigma}_z^{(\mu+1)})$$

$$\hat{h}^{(\mu)} = \frac{\Omega_\mu}{2}\,\hat{\sigma}_z^{(\mu)} \quad \hat{J}^{(\mu)} = \mathrm{i}J\Omega_\mu[\hat{\sigma}_+^{(\mu)}\hat{\sigma}_-^{(\mu+1)} - \hat{\sigma}_-^{(\mu)}\hat{\sigma}_+^{(\mu+1)}]$$

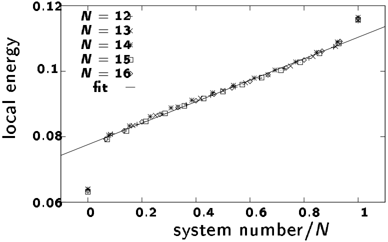
local coupling to two bosonic baths baths

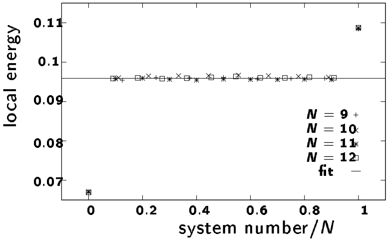
$$\hat{V} = (\hat{\sigma}_x^{(1)} \sum_n \hat{a}_{L,n}^+ + \hat{a}_{L,n}) + (\hat{\sigma}_x^{(N)} \sum_n \hat{a}_{R,n}^+ + \hat{a}_{R,n})$$

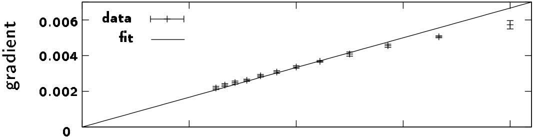
Project onto $\hat{\rho}_S(t) \otimes \hat{\rho}_B^L(\beta_L) \otimes \hat{\rho}_B^R(\beta_R)$, assume $\Omega >> J$, "minimum invasive Lindbladization" $\Rightarrow$ four Lindblad operators and rates:

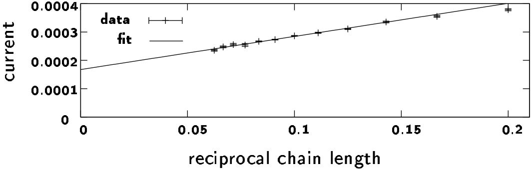
$$\hat{E}_{L,R}^{+,-} = \hat{\sigma}_{+,-}^{(L,R)} + \eta(T_{L,R})\hat{\sigma}_{-,+}^{(L,R)} \quad \alpha_{L,R}^{+,-} = \alpha^{+,-}(T_{L,R})$$

Minimum invasive means $\eta \neq 0$, for $\Omega \approx J$ it is unclear whether or not a reasonable Lindbladization exists.







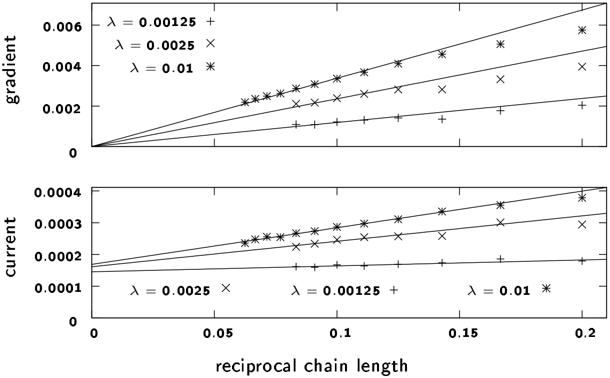


Heisenberg chain results

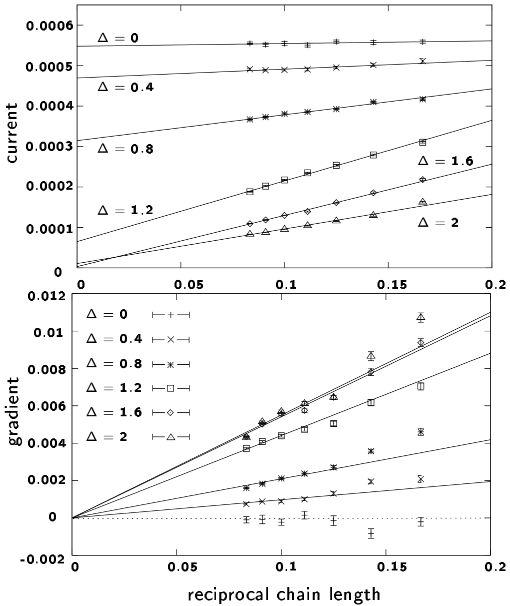
top:
local energies for up to 16 sites for $\Delta = 0$ and $\Delta = 1$.
Other parameters: $\Omega = 1$, $J = 0.01$, $\lambda = 0.01$, $\beta_L = 0.5$, $\beta_R = 0.25$

bottom:
scaling of internal gradient and current with chainlength.

Heisenberg chain only appears to be diffusive



Dependence of current and gradient in the Heisenberg chain on the bath coupling strength λ and the chain length.
The bulk conductivity of any finite chain depends on the bath coupling strength.

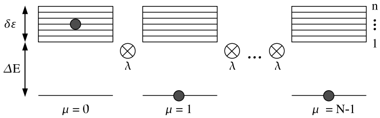


Results on different anisotropies (particle-particle interactions) Δ

The gradients for all Δ seem to vanish for infinite chains.
Only for $\Delta \approx 1.6$ the current seems to vanish for the infinite chain.

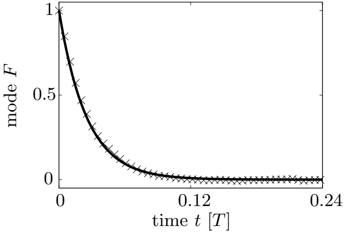
For $\Delta \approx 1.6$ there may be regular diffusive transport. If so, we expect the respective energy diffusion coefficient to be $D = 2.34 \cdot 10^{-2}$ with a computational error on the order of 5%

The "one particle modular quantum system", results on decay of density waves

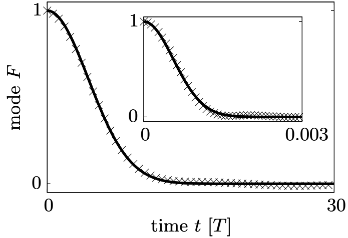


probability for the exitation to be at site μ: $P_\mu = \langle \hat{P}_\mu \rangle$

intermediate wavelength:



long (short) wavelength:



density wave: $F_k = \sum_\mu \cos(k\mu) P_\mu$

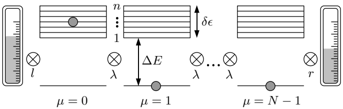
diffusive: $F_k \propto e^{-Dk^2 t}$

ballistic: e.g. $F_k \propto e^{-Dk^2 t^2}$

diffusion condition: $\frac{4\pi^2 n \lambda k}{\delta\epsilon} \gg 1$

diffusion coefficient: $D = \frac{2\pi n \lambda^2}{\delta\epsilon}$

the "one particle modular quantum system" with baths



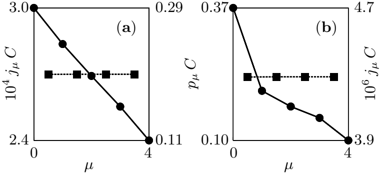
Lindblad operators and rates:

$$\hat{E}^L = (\sum_n |n, L\rangle)\langle 0|,\ \alpha^L = l$$

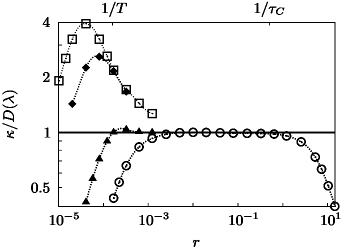
$$\hat{E}^R_k = |0\rangle\langle n, R|,\ \alpha^R_k = r$$

- diffusion coeffients from bath-scenario and denisty wave decay may be in quantitative accord
- Internal diffusion coefficent is independent of bath coupling strength over a wide range
- an adequate bath-scenario may make the diffusive-ballistic transition visible

local currents and probabilities



dependence of transport coefficient on the bath coupling strength



The "take home message":

Carefully desigend bath-coupling scenarios may help to quantitatively describe bulk transport properties of quantum systems. However, a detailed understanding of the role of the bath modelling and powerful tools to solve the resulting equations are required.

More information, literature, etc. : ask me or visit our webpage.

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.... and the audience!