Reservoir coupling approach to transport in quantum systems

Jochen Gemmer

University of Osnabrück,

RWTH Aachen, Dec. 03. 2008
1 Introduction
- The "why" and the "how"
- Modelling reservoirs ⇒ Quantum Master Equations (QME)
- Stochastic unravelling: a way to solve the QME

2 Concrete set ups and results
- The Heisenberg chain
- "One particle modular quantum system"
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:
\[ \hat{H} = \hat{H}_S + \sum_n \epsilon_n \hat{a}_n^+ \hat{a}_n + \hat{V}, \quad \frac{d}{dt} \hat{\rho} = i[\hat{H}, \hat{\rho}] \]

"Project" onto \( \hat{\rho}_S(t) \otimes \hat{\rho}_B(\beta) \) and truncate the, e.g., Nakajima-Zwanzig equation at leading order
\[ \frac{d}{dt} \hat{\rho}_S^D(t) = \int_0^\infty G'(t, t') \hat{\rho}_S^D(t') \]

Redfield approximation (QME):
\[ \frac{d}{dt} \hat{\rho}_S(t) = i[\hat{H}_S, \hat{\rho}_S(t)] + \mathcal{G} \hat{\rho}_S(t) \]

\( \mathcal{G} \): superoperator, linearly 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):
\[ \frac{d}{dt} \hat{\rho}_S(t) = i[\hat{H}_S, \hat{\rho}_S(t)] + \mathcal{L} \hat{\rho}_S \]
\[ \mathcal{L} \hat{\rho}_S = \sum_k \alpha_k \left( \hat{E}_k \hat{\rho}_S \hat{E}_k^\dagger - \frac{1}{2} \left[ \hat{E}_k^\dagger \hat{E}_k, \hat{\rho}_S \right]_+ \right) \]

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):

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

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

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

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

If the dimension of the PDDE is $n$, then the dimension of the QME is $n^2$
The Heisenberg chain set up

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

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

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

local coupling to two bosonic baths

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

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

$$\hat{E}_L,R^{+,\pm} = \hat{\sigma}_+^{(L,R)} + \eta(T_L,R)\hat{\sigma}^{(L,R)}_- \quad \alpha_L,R^{+,\pm} = \alpha^{+,\pm}(T_L,R)$$

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

"One particle modular quantum system"

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 chain length.

*Heisenberg chain only appears to be diffusive*
Dependence of current and gradient in the Heisenberg chain on the bath coupling strength $\lambda$ and the chain length. The bulk conductivity of any finite chain depends on the bath coupling strength.
Results on different anisotropies (particle-particle interactions) $\Delta$

The gradients for all $\Delta$ 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

\[ \delta \varepsilon \]

\[ \Delta E \]

\[ \mu = 0 \quad \mu = 1 \quad \mu = N-1 \]

probability for the excitation to be at site \( \mu \): \( P_\mu = \langle \hat{P}_\mu \rangle \)

long (short) wavelength:

intermediate wavelength:

density wave: \( F_k = \sum_\mu \cos(k_\mu)P_\mu \)
diffusive: \( F_k \propto e^{-Dk^2t} \)
ballistic: e.g. \( F_k \propto e^{-Dk^2t^2} \)
diffusion condition: \( \frac{4\pi^2 n \lambda k}{\delta \varepsilon} \gg 1 \)
diffusion coefficient: \( D = \frac{2\pi n \lambda^2}{\delta \varepsilon} \)
the “one particle modular quantum system” with baths

Lindblad operators and rates:
\[ \hat{E}^L = (\sum_n |n, L\rangle \langle 0|, \alpha^L = l \]
\[ \hat{E}_k^R = |0\rangle \langle n, R|, \alpha_k^R = r \]

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

dependence of transport coefficient on the bath coupling strength

local currents and probabilities
The “take home message”:

Carefully designed 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.

Many thanks to M. Michel, R. Steinigeweg, H. Wichterich, M. Ogiewa, .... and the audience!