Quantum Thermodynamical Approach to Transport Phenomena

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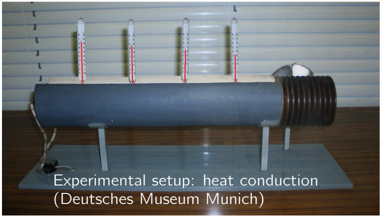
Entanglement between subsystems may be a central source of local decoherence and therefore also the reason for local thermodynamical behavior.

Gemmer, Michel, Mahler,
Quantum Thermodynamics
Springer (2004).

Introduction


Experimental setup: heat conduction
(Deutsches Museum Munich)

Local behavior is accomplished by phenomenological Fourier's Law:

$$J = -\kappa \nabla T$$

Goal: find a microscopical foundation (formula for κ)

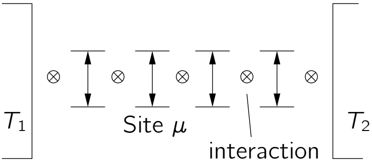
Historic Approaches:

- Peierls-Boltzmann equation (phonon scattering, Umklapp process)
- Linear response, Kubo-formula (questionable foundation)

New Approaches:

- Perturbation Theory in Liouville space (stationary approach)
- Quantum thermodynamical approach (dynamic approach)

Perturbation Theory in Liouville Space: Model System



- System:

$$\hat{H} = \sum_{\mu} \left(\hat{H}_{\text{loc}}(\mu) + \hat{H}_{\text{int}}(\mu, \mu+1) \right)$$

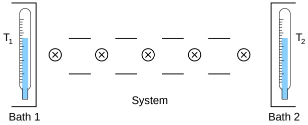
- Bath: Quantum Master Equation

Liouville von Neumann equation for the open quantum system:

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \underbrace{[\hat{H}, \hat{\rho}]}_{=\hat{\mathcal{L}}^{\text{sys}}\hat{\rho}} + \hat{\mathcal{L}}^{1}(T_1)\hat{\rho} + \hat{\mathcal{L}}^{2}(T_2)\hat{\rho} = \hat{\mathcal{L}}\,|\hat{\rho})$$

- Super operator acts on operators of the Hilbert space.
- Density operator $|\hat{\rho})$ is a state in Liouville space

Perturbation Theory: Unperturbed System



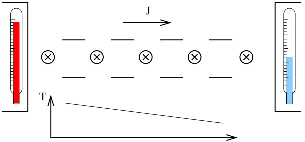
Liouville von Neumann eq.: $T_1 = T_2 = T$

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \underbrace{\left(\hat{\mathcal{L}}^{\mathrm{sys}} + \hat{\mathcal{L}}^{1}(T) + \hat{\mathcal{L}}^{2}(T)\right)}_{=\hat{\mathcal{L}}_0} \hat{\rho}$$

➜ stationary state $|\hat{\rho}_0)$ is a global equilibrium state with T

- Solution of the unperturbed system: $\hat{\mathcal{L}}_0|\hat{\rho}_j) = l_j|\hat{\rho}_j)$
- non-orthogonal eigenbasis $|\hat{\rho}_j)$
- dual basis: $|\hat{\rho}^j)$ with $\sum_j |\hat{\rho}_j)(\hat{\rho}^j| = \hat{1}$

Perturbed System



Perturbation: $\hat{\mathcal{L}}^{\text{per}} = \hat{\mathcal{L}}^1(T_1) + \hat{\mathcal{L}}^2(T_2)$

with $T_1 = T + \Delta T$ and $T_2 = T - \Delta T$

Stationary State: $\hat{\rho}_{\text{stat}} = \hat{\rho}_0 + \Delta\hat{\rho}$

$$\Delta\hat{\rho} = -\Delta T \lambda \sum_{j=1}^{n^2-1} \frac{(\hat{\rho}^j|\hat{\mathcal{L}}^{\text{per}}|\hat{\rho}_0)}{l_j} |\hat{\rho}_j)$$

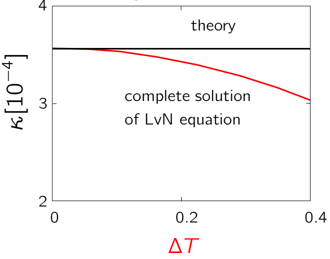
$\Delta\hat{\rho}$ ➜ Temperature current and profile
➜ J , $\delta T(\mu, \mu+1) \propto \Delta T$

➜ $\kappa = -\dfrac{J}{\delta T(\mu, \mu+1)}$ (Fourier)

independent of the perturbation ΔT

Michel, Gemmer, Mahler, EPJB 42, 555 (2004).

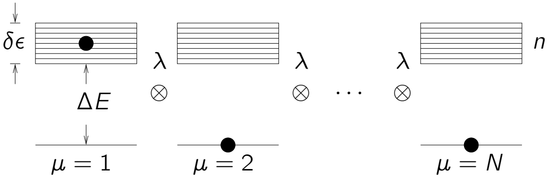
Conductivity



Quantum Thermodynamical Approach to Heat Conduction

so far: stationary local equilibrium state

now: decay to global equilibrium



Hilbert Space Average Method: Gemmer et al., *Quantum Thermodynamics* Springer (2004).

- time-dependent perturbation theory of 2nd order
- replacement of exact terms by the mean of the quantity in Hilbert space
- rate equation for the probability P_μ finding an excitation in the μth system.

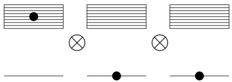
Rate eq.:

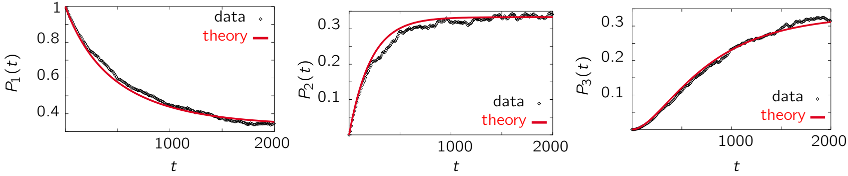
$$\frac{dP_1}{dt} = -\kappa(P_1 - P_2)$$

$$\frac{dP_\mu}{dt} = -\kappa(2P_\mu - P_{\mu-1} - P_{\mu+1})$$

$$\frac{dP_N}{dt} = -\kappa(P_N - P_{N-1})$$

$$\kappa = \frac{2\pi\lambda^2 n}{\delta\epsilon}$$





Current $\propto \frac{dP}{dt}$; Gradient $\propto P(\mu) - P(\mu+1)$ ➜ Conductivity $\kappa = \frac{2\pi\lambda^2 n}{\delta\epsilon}$

Summary

- Perturbation theory in Liouville space
- Quantum thermodynamical approach to heat conduction

Outlook

- Temperature dependence of the heat conductivity
- Comparison of the two approaches

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