Local Equilibrium Aspects of Small Quantum Systems: Kubo Formula in Liouville Space (DY 13.14)

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Berlin, March 4th 2005

Contents

- Introduction to Quantum Heat Conduction
- Perturbation Theory in Liouville Space
- Quantum Thermodynamical Approach to Heat Conduction

Introduction


Experimental setup: heat conduction
(Deutsches Museum München)

Local behavior is accomplished by *phenomenological Fourier's Law:*

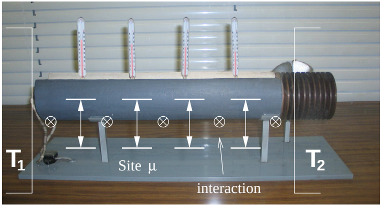
$$J = -\kappa \nabla T$$

Goal: find a microscopical foundation (formula for κ)

Different Approaches:

- Debye phonon gas $\kappa \propto cvl$ (c heat capacity, v mean velocity, l mean path)
- Peierls-Boltzmann equation (phonon scattering, Umklapp process)
- Linear response, Kubo-formulas (questionable foundation)
- Perturbation theory in Liouville space (static approach)
- Quantum thermodynamical approach (dynamic approach)

Quantum Heat Conduction Model



Hamiltonian:

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

Bath ➜ Lindblad Formalism

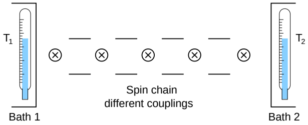
Liouville von Neumann Equation for the open system:

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

Super Operator

- A super operator acts on operators of the Hilbert space
- Density operators $|\hat{\rho})$ are states in the Liouville space

Perturbation Theory: Unperturbed System



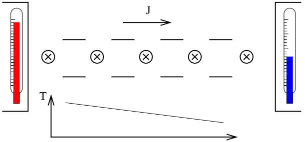
Liouville von Neumann Eq.: $T_1 = T_2 = T$

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

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

- Solution of the unperturbed system: $\hat{\mathcal{L}}_0|\hat{\rho}_j) = l_j|\hat{\rho}_j)$
- non-orthogonal eigenstates $|\hat{\rho}_j)$
- 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

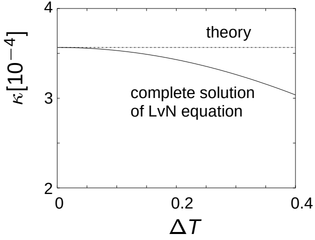
$J\ ,\Delta T(\mu, \mu+1) \propto \Delta T$

$$\rightarrow \kappa = \frac{J}{\Delta T(\mu, \mu+1)}$$

independent of the perturbation ΔT

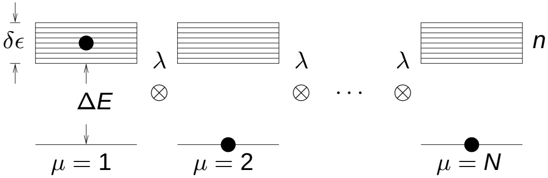
Michel, Gemmer, Mahler, EPJB **42**, 555 (2004).

Conductivity



Quantum Thermodynamical Approach to Heat Conduction

so far: local equilibrium state
now: investigation of the decay to 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
- closed master equation for the probability $P(\mu)$ finding an exitation in the μth subsystem (see also DY 13.17)

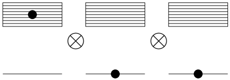
Rate Eq.:

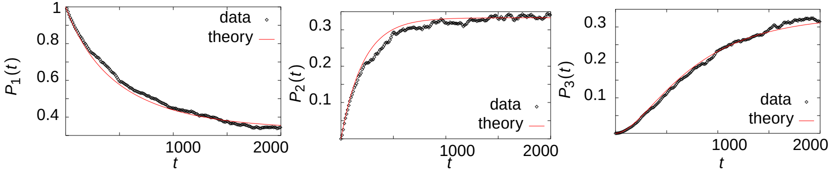
$$\frac{\mathrm{d}P_1}{\mathrm{d}t} = -\frac{1}{\tau}(P_1 - P_2)$$

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

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

$$\frac{1}{\tau} = \frac{2\pi\lambda^2 n}{\delta\epsilon}$$





Conductivity: $J \propto \frac{\mathrm{d}P}{\mathrm{d}t}$ and $\Delta T \propto P(\mu) - P(\mu+1)$

$$\Rightarrow \kappa = \frac{1}{\tau} = \frac{2\pi\lambda^2 n}{\delta\epsilon}$$

Summary

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

Outlook

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

Thanks to

- the department of physics in Osnabrück, especially J. Gemmer, J. Schnack and H.-J. Schmidt
- the group members in Stuttgart M. Hartmann, M. Henrich, H. Schmidt, M. Stollsteimer and F. Tonner
- Financial support by the Deutsche Forschungsgesellschaft is gratefully aknowledged