Quantum Heat Conduction – Local Equilibrium

Eulenhof-Seminar

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Experimental setup to meassure classical heat conduction (Deutsches Museum München)

... *local equilibrium hypothesis* i.e. on the possibility of defining a temperature for a **macroscopically small** but **microscopically large** volume ...

Lepri et al. *Thermal conduction in classical low-dimensional lattices*
Phys. Rep. **377** 1-80 (2003)

Introduction

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

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

Goal: $\rightarrow$ find a microscopical foundation (formula for κ)

Historical Attemps:

- Debye: kinetic gas theory for phonons $\kappa \propto cvl$
- Peierls-Boltzmann equation (phonon scattering, Umklapp process)
- linear response, Kubo-formulas (questionable foundation)
- Kubo-formulas in Liouville space?

Quantum Thermodynamical Approach to Heat Conduction

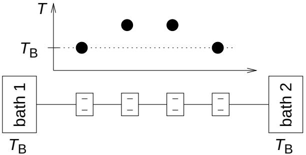
Conditions for non-equilibrium linear thermodynamics:

- system reaches a local equilibrium state
- system decays **exponentially** to this state

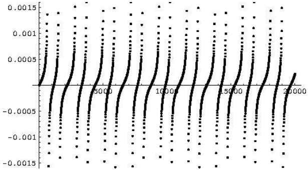
Exponential Decay?

- static κ_{s} (conductivity in a local equilibrium state)
- dynamic κ_{d} (conductivity of the decay of an exitation in the system)

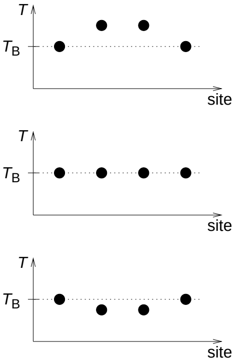
Material property *heat conductivity*: $\kappa_{\mathrm{s}} = \kappa_{\mathrm{d}}$

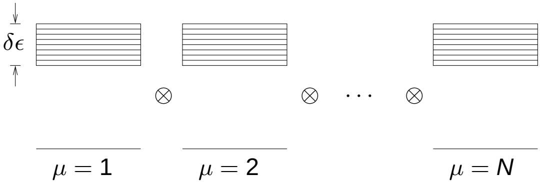


Fouriers' Law $\Rightarrow$ $\kappa = -\dfrac{J}{\Delta T}$



Remember Lepri: "**macroscopically small** but **microscopically large**"





Initial state: only one exitation inside the system

$$\hat{H} = \left(\begin{array}{ccc|ccc} \ddots & & 0 & & & \\ & i\delta\epsilon/n & & & \hat{I} & \\ 0 & & \ddots & & & \\ \hline & & & \ddots & & 0 \\ & \hat{I} & & & j\delta\epsilon/n & \\ & & & 0 & & \ddots \end{array}\right) \begin{array}{l} \left.\vphantom{\begin{array}{c}a\\a\\a\end{array}}\right\} |\psi^{\mathrm{l}}\rangle \\ \left.\vphantom{\begin{array}{c}a\\a\\a\end{array}}\right\} |\psi^{\mathrm{r}}\rangle \end{array}$$

Time dependent perturbation $\rightarrow$ von Neumann expansion

$$|\psi(\tau)\rangle \approx \left(\hat{1} - \frac{\mathrm{i}}{\hbar}\,\hat{U}_1(\tau) - \frac{1}{\hbar^2}\,\hat{U}_2(\tau) + \cdots\right)|\psi(0)\rangle$$

$$\text{with} \quad \hat{U}_1(\tau) = \int_0^{\tau} \mathrm{d}\tau' \hat{I}(\tau')\,, \quad \hat{U}_2(\tau) = \int_0^{\tau} \mathrm{d}\tau' \hat{I}(\tau') \int_0^{\tau'} \mathrm{d}\tau'' \hat{I}(\tau'')\,.$$

Occupation probability for the respective subspaces:

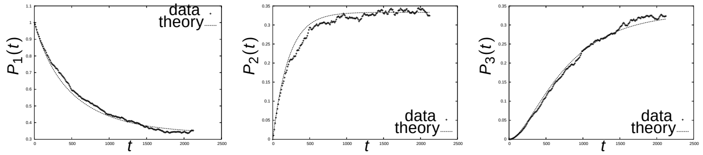
$$\begin{aligned}
W^{\mathrm{l}}(\tau) = \langle\psi^{\mathrm{l}}(\tau)|\psi^{\mathrm{l}}(\tau)\rangle =& \langle\psi^{\mathrm{l}}|\psi^{\mathrm{l}}\rangle - \frac{\mathrm{i}}{\hbar}\langle\psi^{\mathrm{r}}|\hat{U}_1|\psi^{\mathrm{l}}\rangle + \frac{\mathrm{i}}{\hbar}\langle\psi^{\mathrm{l}}|\hat{U}_1|\psi^{\mathrm{r}}\rangle \\
&+ \frac{1}{\hbar^2}\langle\psi^{\mathrm{r}}|\hat{U}_1^2|\psi^{\mathrm{r}}\rangle - \frac{1}{\hbar^2}\langle\psi^{\mathrm{l}}|\hat{U}_1^2|\psi^{\mathrm{l}}\rangle \\
W^{\mathrm{r}}(\tau) = \langle\psi^{\mathrm{r}}(\tau)|\psi^{\mathrm{r}}(\tau)\rangle =& \langle\psi^{\mathrm{r}}|\psi^{\mathrm{r}}\rangle - \frac{\mathrm{i}}{\hbar}\langle\psi^{\mathrm{l}}|\hat{U}_1|\psi^{\mathrm{r}}\rangle + \frac{\mathrm{i}}{\hbar}\langle\psi^{\mathrm{r}}|\hat{U}_1|\psi^{\mathrm{l}}\rangle \\
&+ \frac{1}{\hbar^2}\langle\psi^{\mathrm{l}}|\hat{U}_1^2|\psi^{\mathrm{l}}\rangle - \frac{1}{\hbar^2}\langle\psi^{\mathrm{r}}|\hat{U}_1^2|\psi^{\mathrm{r}}\rangle\,.
\end{aligned}$$

Expectation values $\Rightarrow$ by Hilbert space averages

Rate Equations:

$$\frac{\mathrm{d}W^{\mathrm{l}}}{\mathrm{d}t} = C(W^{\mathrm{r}} - W^{\mathrm{l}}) \qquad C = \frac{2\pi\lambda_0^2 n}{\delta\epsilon} = \frac{1}{\tau}$$

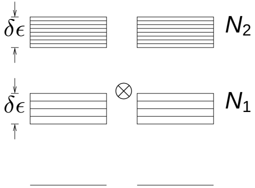
$$\frac{\mathrm{d}W^{\mathrm{r}}}{\mathrm{d}t} = C(W^{\mathrm{l}} - W^{\mathrm{r}}) \qquad \lambda_0^2 = \frac{1}{2n^2}\mathrm{Tr}\{\hat{I}^2\}$$



Conductivity: $J \propto \frac{\mathrm{d}W^{\mathrm{l}}}{\mathrm{d}t}$ and $\Delta T \propto (W^{\mathrm{r}} - W^{\mathrm{l}})$

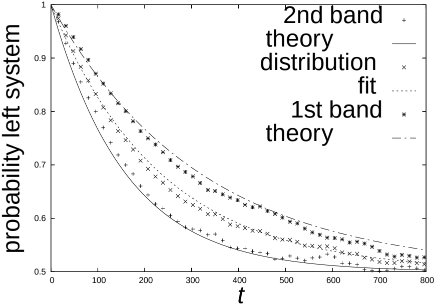
$$\Rightarrow \kappa = \frac{2\pi\lambda_0^2 n}{\delta\epsilon}$$

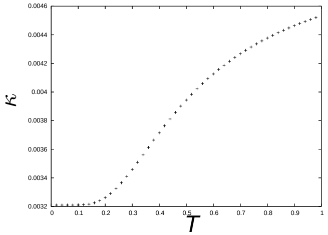
Temperature Dependence



Two decay times (dependent on the initial state):

$$\tau_1 = \frac{\delta\epsilon}{2\pi\lambda^2 N_1}\ , \quad \tau_2 = \frac{\delta\epsilon}{2\pi\lambda^2 N_2}$$





$$\frac{1}{\tau} = C = \kappa$$