Fourier's Law from Schrödinger Dynamics
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Contents

- Introduction to Heat Conduction
- Hilbert Space Average Method (HAM)
- Quantum Thermodynamical Approach to Heat Conduction

Joseph Fourier
(1768 - 1830)

Fourier's Law (1807)

$$J_{\text{th}} = -\kappa_{\text{th}} \nabla T$$

heat conductivity κ_{th}

Heat Conduction Experiment
(Deutsches Museum München)

- local temperature gradient
- constant heat current

Microscopic Approaches:

- Peierls-Boltzmann equation
- Kubo-formula
- Open systems approach

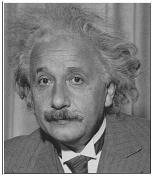
Recent Statements:

- Buchanan: "No one has yet managed to derive Fourier's Law truly from fundamental principles."

  (Nature Physics 2005)

- Bonetto, Lebowitz et al.: "Fourier's Law: a challenge to theorists"

  (World Scientific 2000)



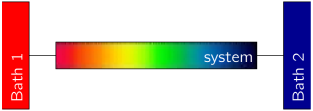
Albert Einstein
(1879-1955)

Marian Ritter von
Smolan Smoluchowski
(1872-1917)

Diffusion

The diffusion constant in a *local equilibrium steady state* (bath scenario) is equivalent to the relaxation constant from a far from equilibrium state into the global equilibrium (decay scenario).

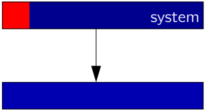
Bath Scenario



stationary local equilibrium state

➜ heat conductivity

Decay Scenario

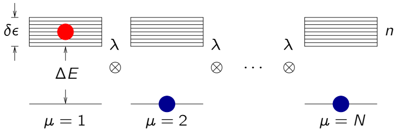


initial state

final global equilibrium

➜ relaxation constant

Quantum Thermodynamical Approach to Heat Conduction

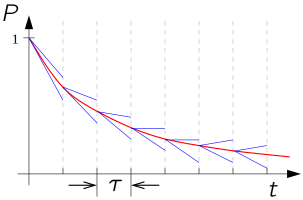


Energy in μth subunit

- excitation probability
- projector $\hat{P}_\mu$ to the band
- probability $P_\mu(t) \equiv \langle\psi(t)|\hat{P}_\mu|\psi(t)\rangle$

Dyson series: $$|\psi(\tau)\rangle \approx \left(\hat{1} - \frac{\mathrm{i}}{\hbar}\hat{U}_1(\tau) - \frac{1}{\hbar^2}\hat{U}_2(\tau)\right)|\psi(0)\rangle = \hat{D}_2(\tau)|\psi(0)\rangle$$

Probability (2nd order): $$P_\mu(\tau) \approx \langle\psi(0)|\hat{D}_2^\dagger(\tau)\hat{P}_\mu\hat{D}_2(\tau)|\psi(0)\rangle$$



Hilbert Space Average:

$$P_\mu(\tau) \approx [\![\langle\phi|\hat{D}_2^\dagger(\tau)\hat{P}_\mu\hat{D}_2(\tau)|\phi\rangle]\!]$$

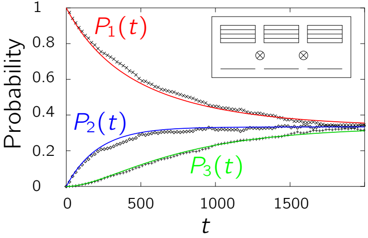
Diffusive Behavior

Rate Eq.:

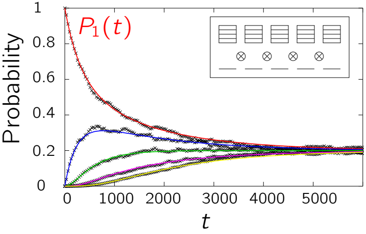
$$\frac{\mathrm{d}P_1}{\mathrm{d}t} = -\kappa(P_1 - P_2)$$

$$\frac{\mathrm{d}P_\mu}{\mathrm{d}t} = -\kappa(2P_\mu - P_{\mu-1} - P_{\mu+1}) \qquad \kappa = 2\pi\lambda^2 \frac{n}{\delta\epsilon}$$

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



($N = 3,\ n = 500,\ \delta\epsilon = 0.05,\ \lambda = 5 \cdot 10^{-5}$)



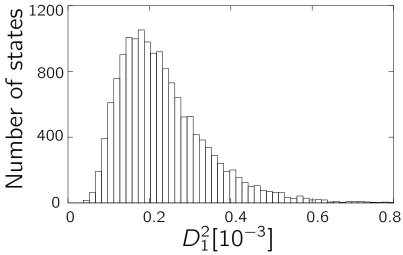
($N = 5,\ n = 500,\ \delta\epsilon = 0.05,\ \lambda = 5 \cdot 10^{-5}$)

Deviation of HAM from the Exact Solution

Quadratic deviation of the exact result from the HAM prediction

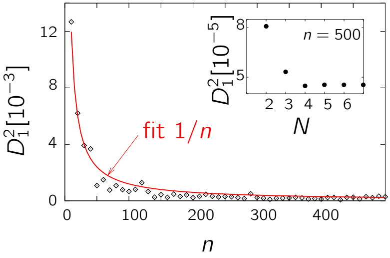
$$D_1^2 = \frac{1}{5\tau}\int_0^{5\tau}\left(P_1^{\mathrm{HAM}}(t) - P_1^{\mathrm{exact}}(t)\right)^2 \mathrm{d}t \leq 1$$

Different initial states



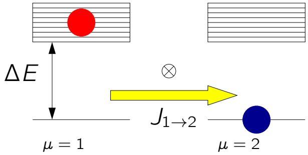
15000 equally distributed initial states ($N = 2,\ n = 500$)

Different system sizes



dependence of D_1^2 on n for $N = 3$.
Inset: dependence on N for $n = 500$.

Energy Diffusion



HAM rate equation

$$\frac{\mathrm{d}P_1}{\mathrm{d}t} = -\kappa\left(P_1 - P_2\right)$$
$$\frac{\mathrm{d}P_2}{\mathrm{d}t} = -\kappa\left(P_2 - P_1\right)$$

Relaxation Coefficient:

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

Energy current: change of internal energy $U_\mu = \Delta E P_\mu$

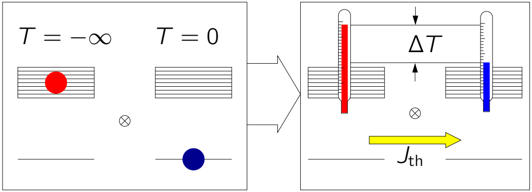
$$J_{1\to 2} = \frac{1}{2}\left(\frac{\mathrm{d}U_2}{\mathrm{d}t} - \frac{\mathrm{d}U_1}{\mathrm{d}t}\right) = \frac{\Delta E}{2}\left(\frac{\mathrm{d}P_2}{\mathrm{d}t} - \frac{\mathrm{d}P_1}{\mathrm{d}t}\right)$$

with rate equation

$$J_{1\to 2} = -\kappa\Delta E\left(P_2 - P_1\right) = -\kappa\left(U_2 - U_1\right)$$

➜ energy current $\propto$ energy gradient (energy Fourier's law)

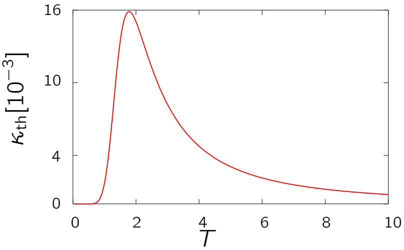
Heat Diffusion



Fourier's Law:

$$J_{\text{th}} = -\kappa_{\text{th}} \Delta T$$

heat conductivity: $\kappa_{\text{th}} = \kappa\, c$
c heat capacity of a subunit



Expectation

- small temperatures $\propto T^3$
- high temperatures between T^{-1} and T^{-2} (Peierls)

Result

- small temperatures $\propto e^{-1/T}$
- high temperatures $\propto T^{-2}$

Summary

- HAM a new method for observing the decay in small quantum systems
- energy, heat diffusion and Fourier's Law from Schrödinger dynamics
- Conclusion: Regular diffusive behavior follows from quantum mechanics and a coarse grained level of description.

Outlook

- more realistic model systems
- comparison with bath scenario

Further reading:

- Michel, Mahler, Gemmer, PRL 95, 180602 (2005)
- Michel, Gemmer, Mahler, PRE 73, 016101 (2006)
- Gemmer, Michel, Mahler, *Quantum Thermodynamics*, Springer (2004)

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