Heat Transport in Small Quantum Systems

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Outline

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Heat Transport

Local Equilibrium

Heat Conduction Experiment
(Deutsches Museum München)

- no global temperature
- local temperature
- temperature gradient
- constant heat current

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Jean Baptiste Joseph Fourier
(1768 - 1830)

Fourier's Law

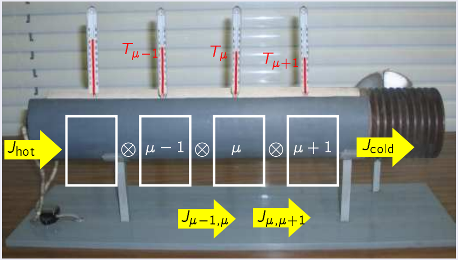
linear connection between temperature gradient ∇T and heat current $\boldsymbol{J}$

$$\boldsymbol{J} = -\kappa \nabla T$$

➜ heat conductivity κ

Heat Conductivity

Discrete Version Fourier's Law



$$J_{\mu,\mu+1} = -\kappa(T_{\mu+1} - T_\mu) = \kappa\,\Delta T_{\mu,\mu+1}$$

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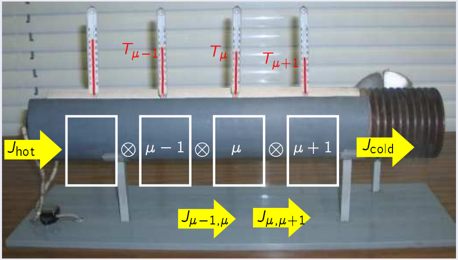

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Conditions for Local Equilibrium

$$J_{\text{hot}} = J_{\mu-1,\mu} = J_{\mu,\mu+1} = J_{\text{cold}} = J$$

for κ to be a material constant

$$\Delta T_{\mu-1,\mu} = \Delta T_{\mu,\mu+1} = \Delta T$$

except some differences at the contacts

Heat Conductivity

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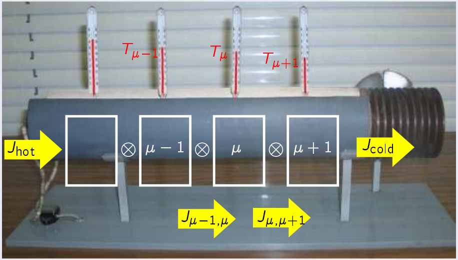

$$J_{\mu,\mu+1} = -\kappa(T_{\mu+1} - T_{\mu})$$
$$= \kappa\,\Delta T_{\mu,\mu+1}$$

Definition of the Heat Conductivity

$$\kappa = \frac{J}{\Delta T}$$

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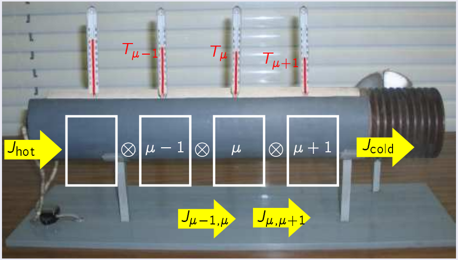

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Normal and Ballistic Transport

$\Delta T \neq 0 \quad \Rightarrow \quad$ finite κ

➜ normal transport

$\Delta T = 0 \quad \Rightarrow \quad \kappa \to \infty$

➜ ballistic transport

Microscopic Foundation

➜ Derivation of a microscopic theory for the heat conductivity κ

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Peter J. W. Debye (1884-1966)

particle current:

- mean velocity $\overline{v}$
- mean free path $\overline{l}$

$\kappa \propto c\,\overline{v}\,\overline{l}$

(c heat capacity)

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quasi-particle current:

- Boltzmann equation
- Umklapp process

$$\kappa \propto T^3$$

$$\kappa \propto \frac{1}{T} \quad \text{to} \quad \frac{1}{T^2}$$

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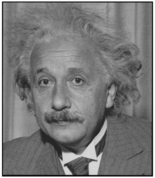
Ryogo Kubo (1920-1995)

- linear response theory (for electrical transport)
- Kubo formula ➜ current current autocorrelation
- ad hoc transferred from electrical to heat transport

Connection between Diffusion and Relaxation



Albert Einstein

(1879-1955)

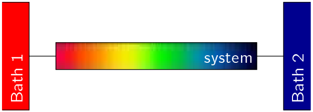
Marian Ritter von Smolan Smoluchowski

(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).

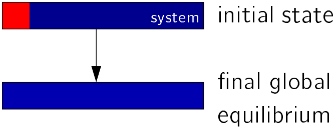
Bath Scenario



stationary local equilibrium state

➜ heat conductivity

Decay Scenario



➜ relaxation constant

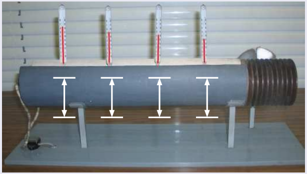
Outline

A Quantum Heat Conduction Model

Local Hamiltonian, Zeeman splitting

$$\hat{H}_{\text{loc}} = \sum_{\mu=1}^{N} \hat{\sigma}_z(\mu)$$

Model System



A Quantum Heat Conduction Model

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Interaction

Heisenberg interaction:

$$\hat{H}_{\text{H}} = \sum_{\mu=1}^{N-1} \hat{\boldsymbol{\sigma}}(\mu) \cdot \hat{\boldsymbol{\sigma}}(\mu+1)$$

Förster interaction:

$$\hat{H}_{\text{F}} = \sum_{\mu=1}^{N-1} \left[\hat{\sigma}_x(\mu)\hat{\sigma}_x(\mu+1) + \hat{\sigma}_y(\mu)\hat{\sigma}_y(\mu+1)\right]$$

Random interaction:

$$\hat{H}_{\text{R}} = \sum_{\mu=1}^{N-1} \sum_{i,j=1}^{3} p_{ij}\hat{\sigma}_i(\mu)\hat{\sigma}_j(\mu+1)$$

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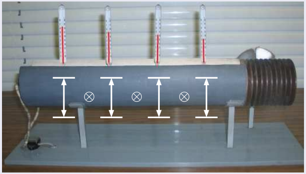

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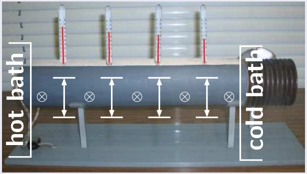

Environment

approximation of large environmental systems by a Quantum Master Equation (Open system approach)

Modelling of Environments

Liouville space

- from pure states to mixed states

Modelling of Environments

Liouville-von-Neumann Equation

$$\frac{d\psi}{dt} = i\hat{H}\psi \rightarrow \frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}]$$

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LvN Equation (Open System)

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}] + \mathcal{L}\hat{\rho}$$

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- adding phenomenological damping terms: dissipator

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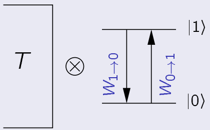
Dissipator for a single spin (Lindblad Form)



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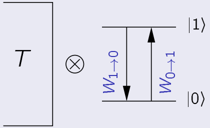

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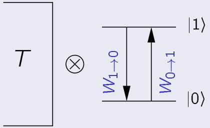

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$$\mathcal{L}\hat{\rho} = W_{1\rightarrow 0}\left(\hat{\sigma}_-\hat{\rho}\hat{\sigma}_+ - \frac{1}{2}\left\{\hat{\rho}, \hat{\sigma}_+\hat{\sigma}_-\right\}_+\right) + W_{0\rightarrow 1}\left(\hat{\sigma}_+\hat{\rho}\hat{\sigma}_- - \frac{1}{2}\left\{\hat{\rho}, \hat{\sigma}_-\hat{\sigma}_+\right\}_+\right)$$

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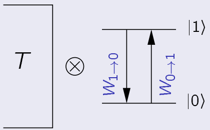

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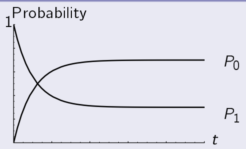

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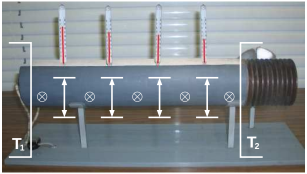
Properties of the Stationary State



Gemmer, Michel, Mahler, LNP657 (2004)

LvN Equation: Stationary State

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stationary state: $\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathcal{L}\hat{\rho}_0 = 0$

➜ $\hat{\rho}_0$ contains: temperature profile, heat currents

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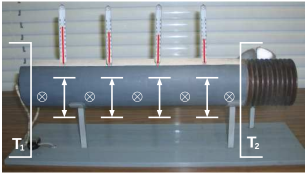

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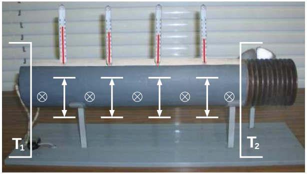

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local energy used as a measure for the local temperature:

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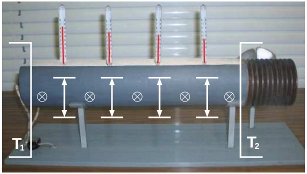

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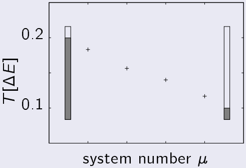
Heat Current

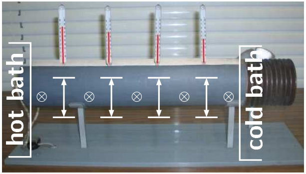
according to the current operator $\hat{J}$:

$$J = \mathrm{Tr}\{\hat{J}\hat{\rho}_0\}$$

Local Temperature Profile

Heisenberg Interaction





Michel et al. EPJB 34, 325 (2003)

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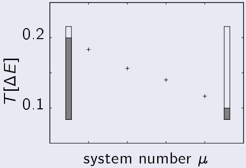
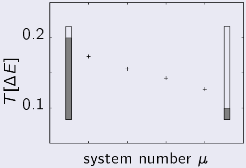
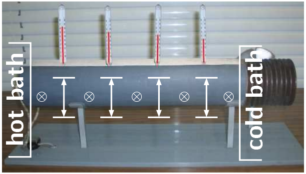


Random Interaction





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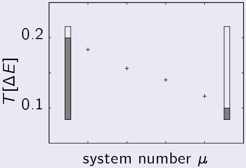

normal transport

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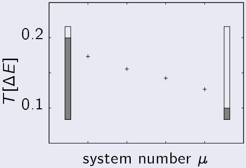

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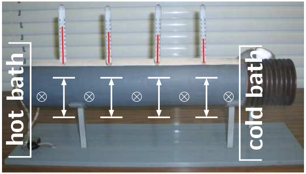

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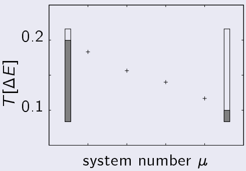

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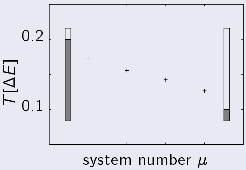

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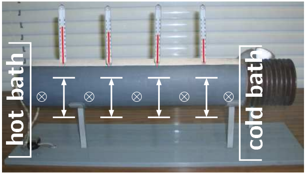

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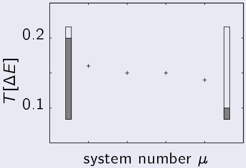
Förster Interaction (XY)



ballistic transport

Fourier's Law: Normal Behavior

Discrete Fourier's Law

linear connection between current and local temperature difference

$$J(\mu,\mu+1) = \kappa\,\Delta T(\mu,\mu+1)$$

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Procedure

- mean temperature
  $T = (T_1 + T_2)/2$
- temperature difference
  $\Delta T = (T_1 - T_2)$

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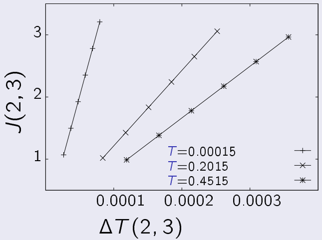
Numerical Data



J in $10^{-7}\Delta E$ (ΔE local energy splitting)

T in ΔE

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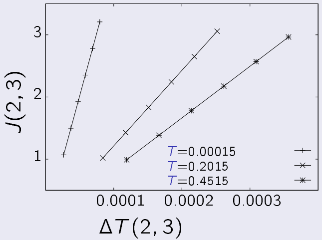

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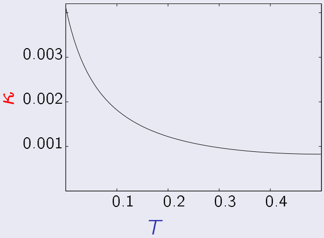
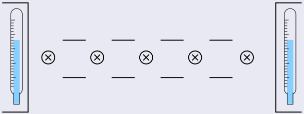
Conductivity



Perturbation Theory

Unperturbed System: $T_1 = T_2 = T$



Michel et al. EPJB 42, 555 (2004)

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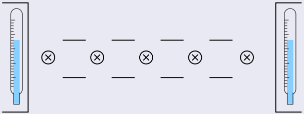

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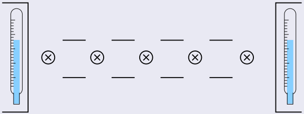

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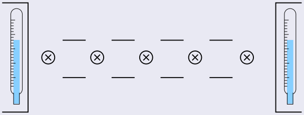

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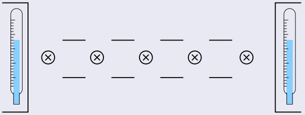

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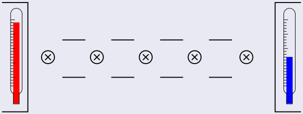

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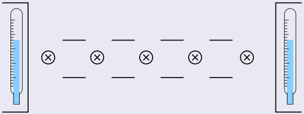

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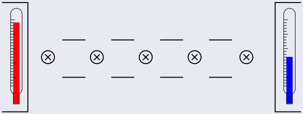

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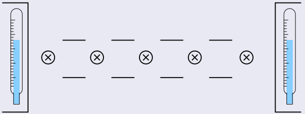

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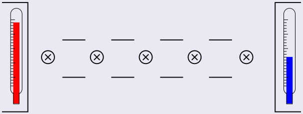

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stationary local equilibrium state

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Results of the Perturbation Theory

Stationary State

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Local Equilibrium State

- $\hat{\rho}_0$ contains neither a temperature profile nor any currents

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the current through the system is linear in the external perturbation

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Global Fourier's Law

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

➜ independent of ΔT

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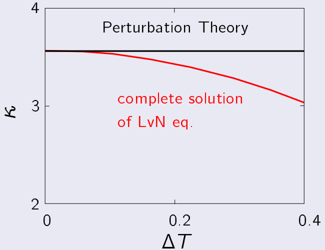
Discussion of the Perturbation Theory

Conductivity



➜ complete solution shows a weak ΔT dependence

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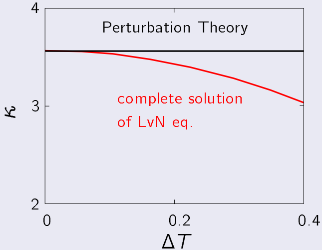


➜ complete solution shows a weak ΔT dependence

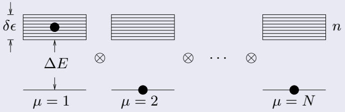
Why this talk doesn't end here?

- shortcoming 1: it isn't possible to observe large systems at the moment
- shortcoming 2: the systems heat conductivity depends on the environmental coupling strength in a nontrivial way

Outline

The Hamiltonian Model

Hamiltonian: Design Model



$$\hat{H} = \sum_{\mu=1}^{N} \hat{H}_{\text{loc}}(\mu) + \lambda \sum_{\mu=1}^{N-1} \hat{V}(\mu, \mu + 1)$$

$\hat{H}_{\text{loc}}$	local Hamiltonian
$\hat{V}$	random interaction
λ	coupling strength

further reading: Michel, Mahler, Gemmer, PRL 95, 180602 (2005)
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The Hamiltonian Model

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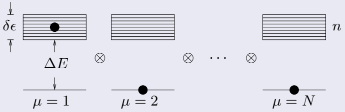

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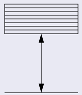
- Energy in a subunit ➜ $\Delta E \cdot$excitation probability P_μ



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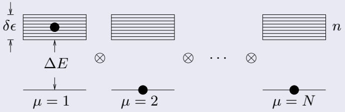

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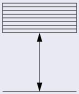

Subunit μ

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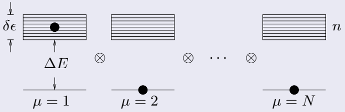

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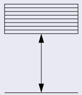

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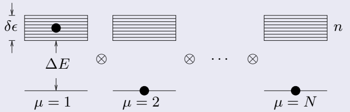
Reduced and Full Dynamics

Model System



Full Dynamics

solution of the Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \mathrm{i}\hbar\hat{H}|\psi(t)\rangle$$

exact time-dependend probability to find the μth system excited

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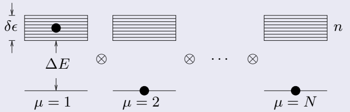

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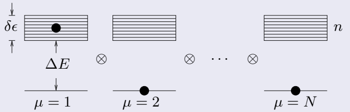

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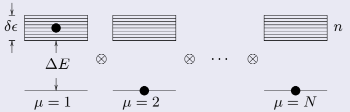

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Reduced Dynamics of Probabilities

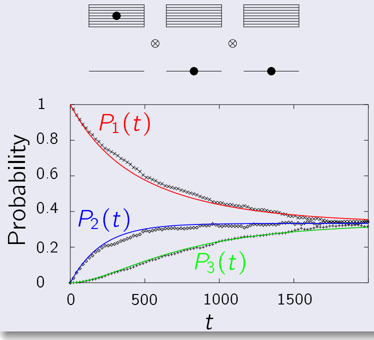
approximated dynamics: Rate Equation (derived after TCL/HAM)

$$\frac{\mathrm{d}}{\mathrm{d}t}P_1 = -\kappa\left(P_1 - P_2\right)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}P_\mu = -\kappa\left(2P_\mu - P_{\mu+1} - P_{\mu-1}\right)$$
$$\frac{\mathrm{d}}{\mathrm{d}t}P_N = -\kappa\left(P_N - P_{N-1}\right)$$

- Decay constant $\kappa = 2\pi\lambda^2\frac{n}{\delta\epsilon}$
- N differential equations

Comparison of Full and Reduced Dynamics

N=3



Model Parameter

- levels in the band $n = 500$
- band width $\delta\epsilon = 0.05$
- coupling strength $\lambda = 5 \cdot 10^{-5}$

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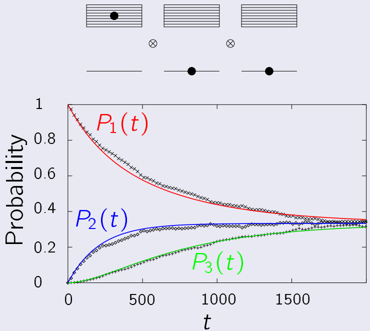

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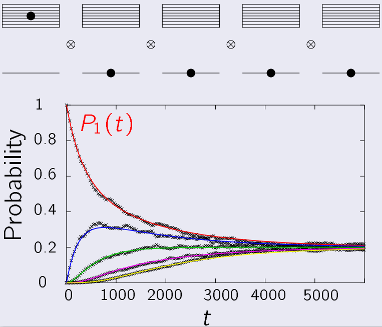

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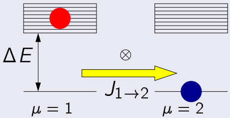
Energy Transport

HAM rate equation



rate equation
➜ exponential decay

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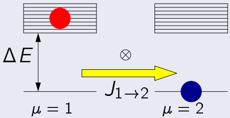

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Energy Current

defined as the change of internal energy U_μ in the two subunits

$$J_{1\to 2} = \frac{1}{2}\left(\frac{dU_2}{dt} - \frac{dU_1}{dt}\right)$$

internal energy: $U_\mu = \Delta E P_\mu$

$$J_{1\to 2} = \frac{\Delta E}{2}\left(\frac{dP_2}{dt} - \frac{dP_1}{dt}\right)$$

and with rate equation

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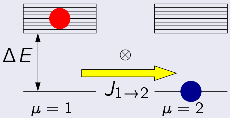

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Energy Fourier's law

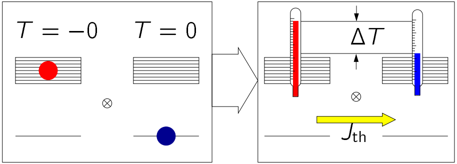
energy current $\propto$ energy gradient

$$J_{1\to 2} = -\kappa(U_2 - U_1)$$

Energy Conduction Coefficient:

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

Heat Transport



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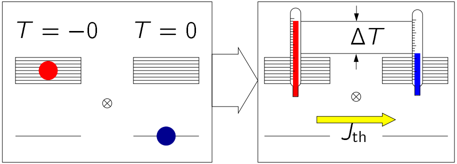
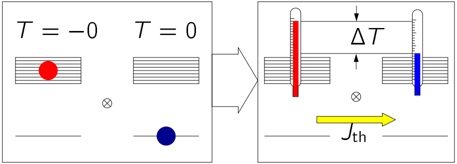


Fourier's Law

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

Heat Transport



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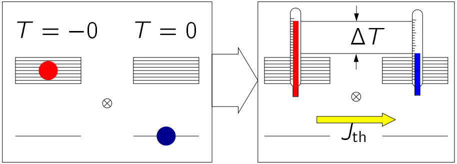
Heat conductivity

$$\kappa_{\rm th} = \kappa c$$

κ energy diffusion constant
c heat capacity of subunit

Heat Transport



Fourier's Law

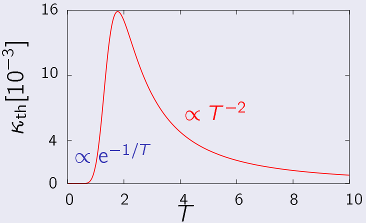
$$J_{th} = -\kappa_{th} \Delta T$$

Heat conductivity

$$\kappa_{th} = \kappa c$$

κ energy diffusion constant
c heat capacity of subunit

Heat Conductivity

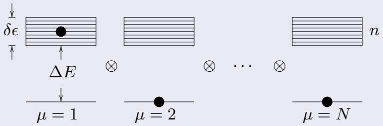


Expectation (Peierls)

- small temperatures $\propto T^3$
- high temperatures $\propto T^{-1}$-T^{-2}

Beyond the Design Model

Design Model

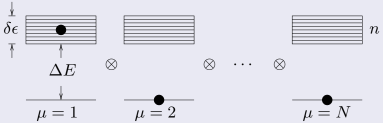


Assets

- local energy and temperature

Beyond the Design Model

Design Model

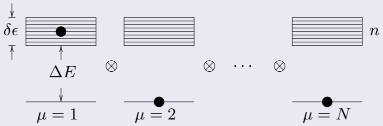


Assets

- local energy and temperature
- full solution feasible

Beyond the Design Model

Design Model



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Drawbacks

- not a real microscopic model

Beyond the Design Model

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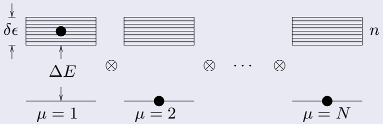

Assets

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Drawbacks

- not a real microscopic model
- large gap is not typical

Beyond the Design Model

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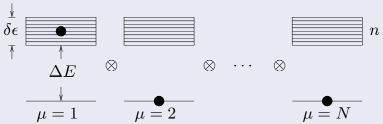

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General Requirements for a Heat Conduction Model

- organize the microscopic system as a "net-structure" of subunits
- high state density, weakly interacting subunits

Beyond the Design Model

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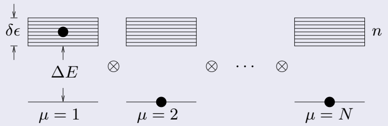

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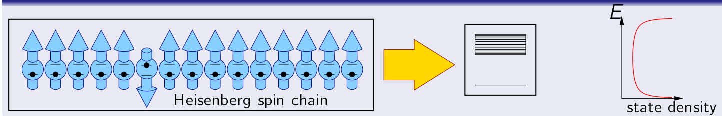
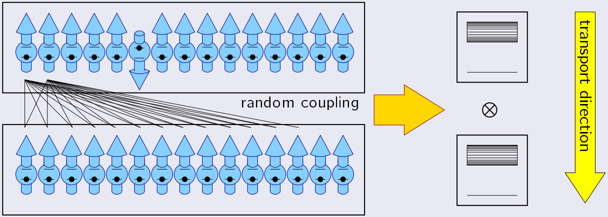
Spin Chains as Subunits



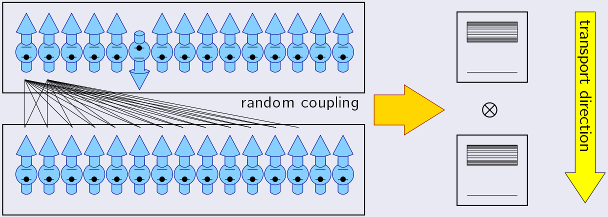
Spin Chain Model

Coupling Model

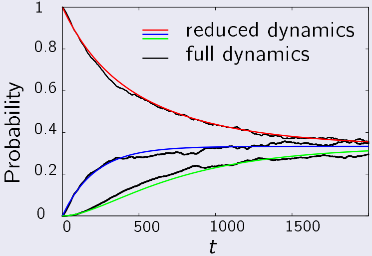


Spin Chain Model

Coupling Model



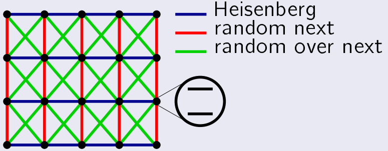
Comparison of Theory and Schrödinger Dynamics



- normal transport behavior
- heat conductivity as before
  ➜ $\kappa = 2\pi\lambda^2 \frac{n}{\delta\epsilon}$

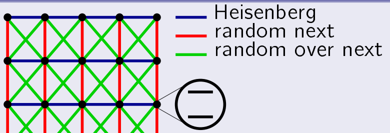
Anisotropic Model

Coupling Model

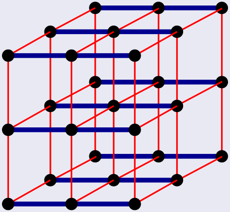


Anisotropic Model

Coupling Model

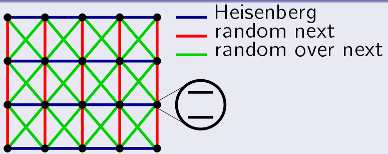


3D Model



Anisotropic Model

Coupling Model



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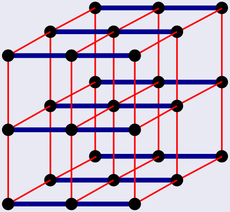
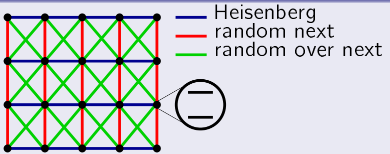


Hamiltonian

$$\hat{H} = \hat{H}_{\text{loc}} + \hat{H}_{\text{Heis}} + \hat{H}_{\text{rand1}} + \hat{H}_{\text{rand2}}$$

Anisotropic Model

Coupling Model



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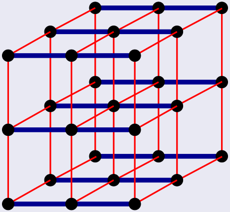

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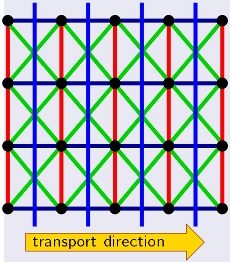
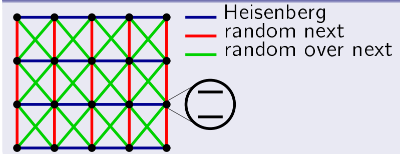
Parallel to Chains



Anisotropic Model

Coupling Model



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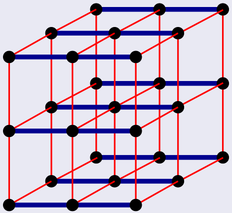

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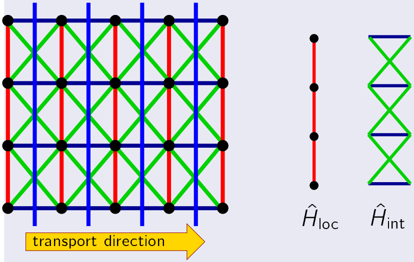

Anisotropic Model

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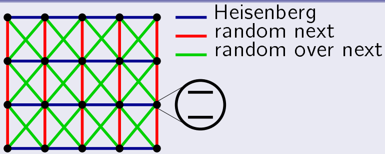

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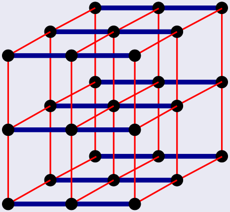

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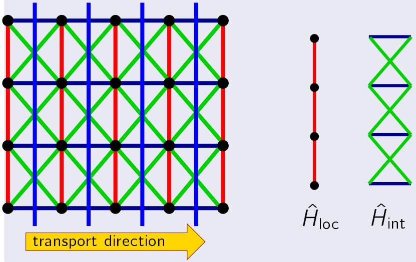
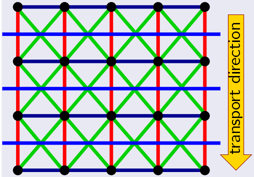
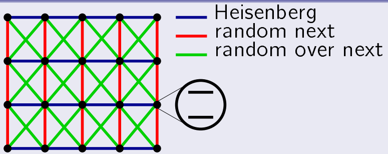


Perpendicular to Chains



Anisotropic Model

Coupling Model



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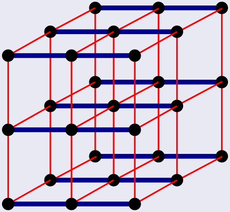

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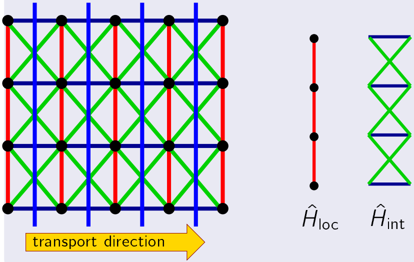
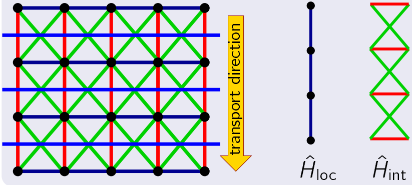
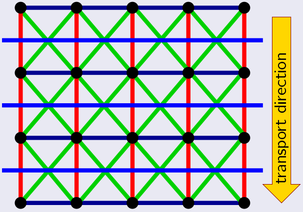


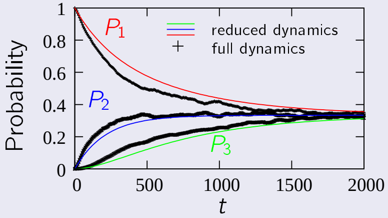
Perpendicular to Chains



Anisotropic Model

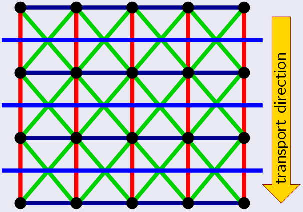
Perpendicular to Chains (Normal Transport)

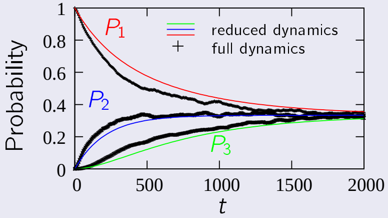




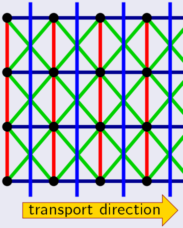
Anisotropic Model

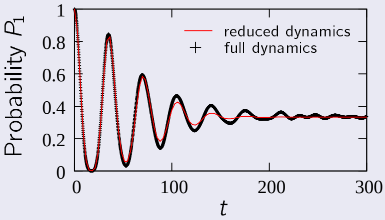
Perpendicular to Chains (Normal Transport)





Parallel to Chains (Ballistic Transport)

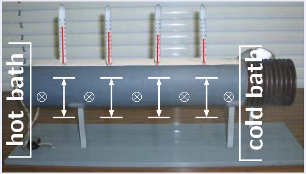




Summary

Bath Scenario

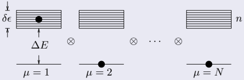
bath assisted transport of heat in small quantum systems

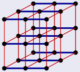


- ballistic and normal behavior
- Fourier's Law

Relaxation Scenario

investigation of decay behavior of small quantum systems





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Thanks to

- the members of the Institute of Theoretical Physics I (Stuttgart)
- special thanks to Hendrik Weimer
- Financial support by the DFG is gratefully acknowledged