Quantum Thermodynamics

Global and Local Equilibrium Aspects of Small Quantum Systems

M. Michel[1] J. Gemmer[2] G. Mahler[1]

[1]Institute of Theoretical Physics I
University of Stuttgart

[2]Department of Physics
University of Osnabrück

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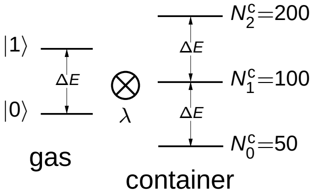
Outline

Outline

Introduction

Closed System under Schrödinger Dynamics



Hamiltonian

$$\hat{H} = \hat{H}^{g} + \hat{H}^{c} + \lambda \hat{H}^{int}$$

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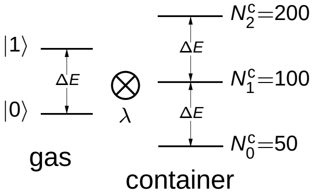

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Initial Pure Product State

- environment in the central level

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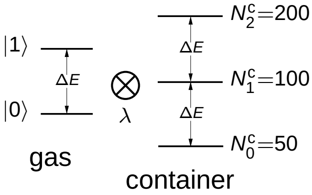

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Initial Pure Product State

- environment in the central level
- arbitrary initial state for the system $|\psi(0)\rangle \propto a|0\rangle + b|1\rangle$

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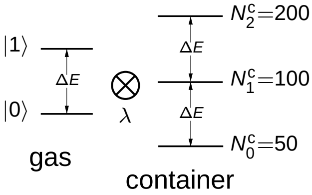

Schrödinger Dynamics

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$$

Hamiltonian

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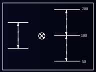
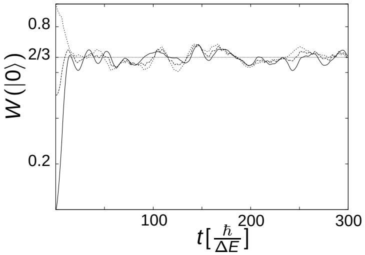
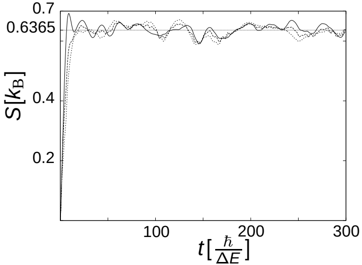


Ground state probability



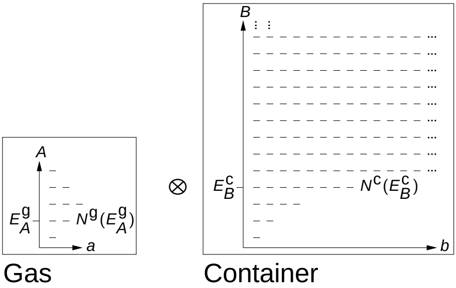
Von Neumann entropy of the gas system (2-level system)



- Borowski, Gemmer, Mahler, *Relaxation to Equilibrium under Pure Schrödinger Dynamics*, EPJB **35** (2003)
- For an intuitive example see www.physik.uni-osnabrueck.de/gemmer/ (Java-Applet by M. Exler)

Outline

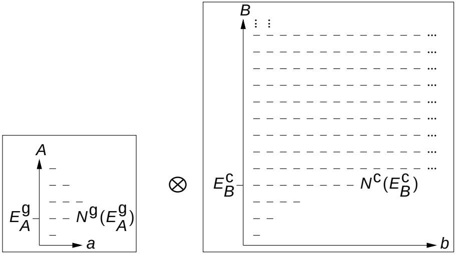
Theories of Quantum Thermodynamics
Two Partite Systems



Hamiltonian

- $\hat{H} = \hat{H}^g + \hat{H}^c + \hat{I}$
- Weak coupling:
  $\sqrt{\langle \hat{I}^2 \rangle} \ll \langle \hat{H}^g \rangle, \langle \hat{H}^c \rangle$

Theories of Quantum Thermodynamics
Two Partite Systems



Gas Container

Hamiltonian

- $\hat{H} = \hat{H}^g + \hat{H}^c + \hat{I}$
- Weak coupling: $\sqrt{\langle \hat{I}^2 \rangle} \ll \langle \hat{H}^g \rangle, \langle \hat{H}^c \rangle$

System State

Reduced density operator:

$$\hat{\rho}^g = \mathrm{Tr}_c \{ |\psi\rangle\langle\psi| \}$$

Theory of Quantum Thermodynamics

Important Quantities: Entropy and Purity (Entanglement Measure)

Von Neumann Entropy:

$$S(\hat{\rho}^{\mathrm{g}}) = -k_{\mathrm{B}} \mathrm{Tr}\left\{\hat{\rho}^{\mathrm{g}} \ln \hat{\rho}^{\mathrm{g}}\right\}$$

Purity:

$$P(\hat{\rho}^{\mathrm{g}}) = \mathrm{Tr}\{(\hat{\rho}^{\mathrm{g}})^2\}$$

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Extreme Values

- min. entropy: $S = 0$ (pure state)
- max. entropy: $S = \ln N$ (totally mixed state)

Purity:

$P(\hat{\rho}^{\mathrm{g}}) = \mathrm{Tr}\{(\hat{\rho}^{\mathrm{g}})^2\}$

Extreme Values

- max. purity: $P = 1$ (pure state)
- min. purity: $P = 1/N$ (totally mixed state)

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Important Quantities: Entropy and Purity (Entanglement Measure)

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Properties

- in the limit of extreme values entropy and purity map on each other
- quantities are defined for all possible density operators $\hat{\rho}^{\mathrm{g}}$

➜ purity/entropy are functions over the Hilbert Space

Theory of Quantum Thermodynamics

Structure of Hilbert Space for bipartite systems

Parametrization of Hilbert Space

$|\psi\rangle = \sum_i (\eta_i + \mathrm{i}\xi_i)|i\rangle$

Hilbert Space

Theory of Quantum Thermodynamics

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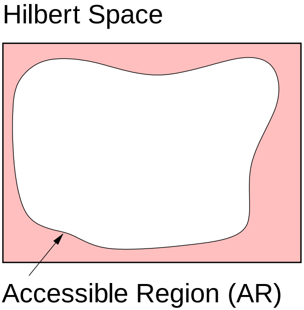
Accessible Region (AR)

- canonical contact: full system energy conservation



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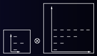

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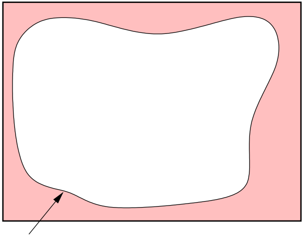
- canonical contact: full system energy conservation
- microcanonical contact: + energy conservation in each subsystem



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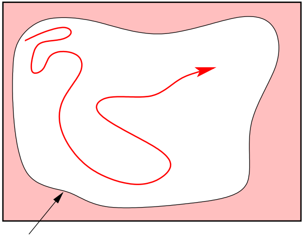
Hilbert Space Velocity

$$v = \sqrt{\langle\psi|\hat{H}^2|\psi\rangle - (\langle\psi|\hat{H}|\psi\rangle)^2} = \text{const.}$$

Hilbert Space



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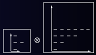

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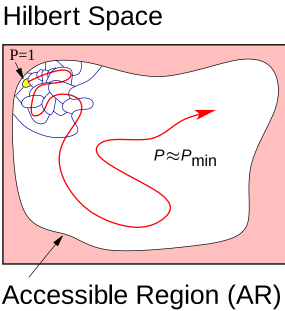

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Tools for the Investigation of the Hilbert Space

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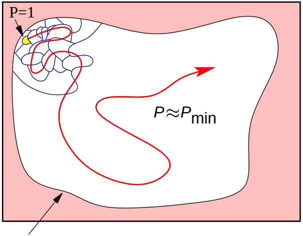

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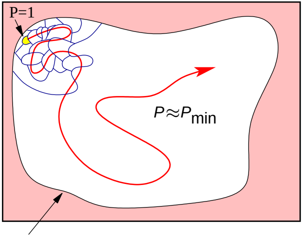

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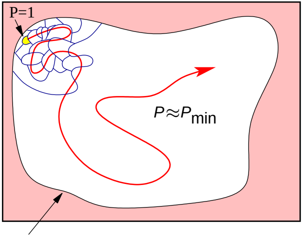

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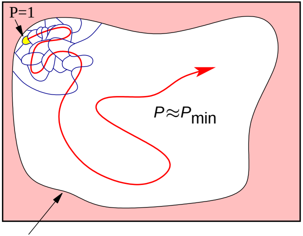

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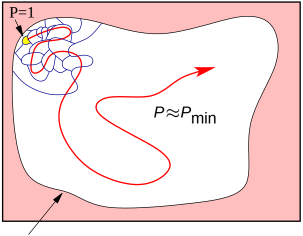
Hilbert Space Average of the Purity

$$[\![P]\!] = \frac{\int_{\mathrm{AR}} P(\{\eta_i, \xi_i\}) \prod_i \mathrm{d}\eta_i \mathrm{d}\xi_i}{\int_{\mathrm{AR}} \prod_i \mathrm{d}\eta_i \mathrm{d}\xi_i}$$

Hilbert Space



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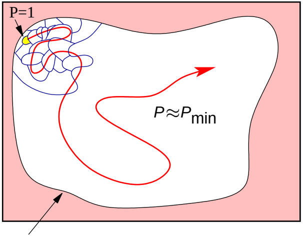
Hilbert Space Variance of the Purity

$$\Delta^2_{\mathrm{H}}(P) = [\![P^2]\!] - [\![P]\!]^2$$

Hilbert Space



Accessible Region (AR)

Theory of Quantum Thermodynamics

Quantum Thermodynamical Equilibrium: Microcanonical Conditions

Side Conditions (AR)

- overall energy conservation
- no energy exchange between gas and container

Gemmer, Michel, Mahler, *Quantum Thermodynamics*, LNP657 Springer (2004)

Theory of Quantum Thermodynamics

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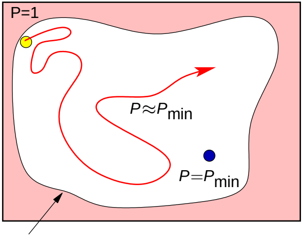

Accessible Region (AR)

Investigation of AR

- $[\![P]\!] \approx P_{min}$
- purity of almost all states within AR is very close to min. purity
- system will reach max. entropy

Gemmer, Michel, Mahler, *Quantum Thermodynamics*, LNP657 Springer (2004)

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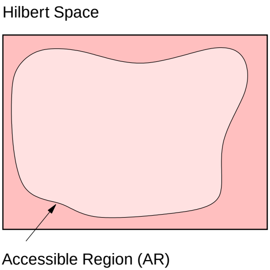
Quantum Thermodynamical Equilibrium: Energy Exchange Conditions

Side Conditions (AR)

only overall energy conservation



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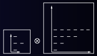


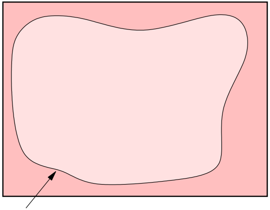
Side Conditions (AR)

only overall energy conservation

Problem

$[\![P]\!] \not\approx P_{\text{min}}$

Hilbert Space



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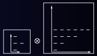

Side Conditions (AR)

only overall energy conservation

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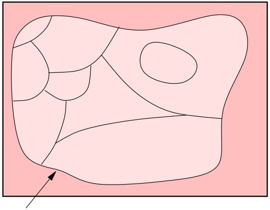
$[\![P]\!] \not\approx P_{\min}$

Regions in AR

AR consists of regions with the same energy distribution for the gas system

Hilbert Space



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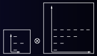

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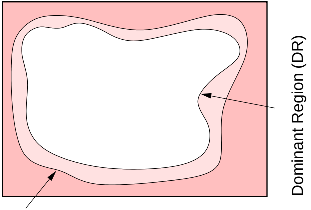
Dominant Region (DR)

- Region of all states featuring the same energy distribution for the gas system W^{dom}
- DR is exponentially larger than all other regions



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Theory of Quantum Thermodynamics

Quantum Thermodynamical Equilibrium: Energy Exchange Conditions

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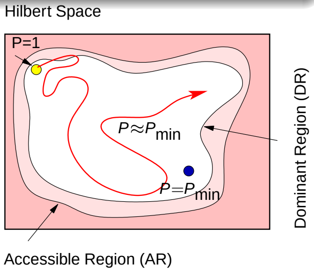
Hilbert Space Topology

in DR all consideration can be done like in case of microcanonical conditions



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Theory of Quantum Thermodynamics

Quantum Thermodynamical Equilibrium: Canonical Conditions

Dominant Distribution W^{dom}

$$W^{\text{dom}}(E_A^{\text{g}}) \propto N^{\text{g}}(E_A^{\text{g}}) N^{\text{c}}(E - E_A^{\text{g}})$$

Theory of Quantum Thermodynamics

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Note for Canonical Contact

Dominant distribution W^{dom} is not necessarily the Boltzmann distribution $W_A^{\mathrm{dom}} \propto \exp(-\beta E_A^{\mathrm{g}})$

Theory of Quantum Thermodynamics

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Special Container

Exponential increase of the degeneracy in the container system: $N^{\mathrm{c}}(E_B^{\mathrm{c}}) \propto \exp(\alpha E_B^{\mathrm{c}})$

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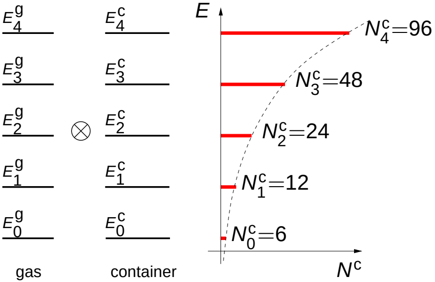

Theory of Quantum Thermodynamics

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States in DR

→ Boltzmann distribution

→ Canonical Contact Conditions

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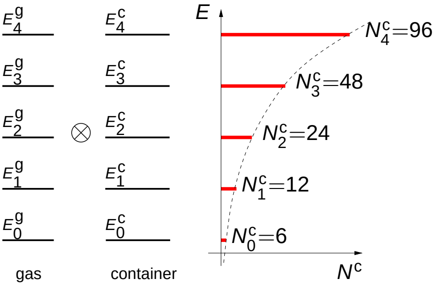

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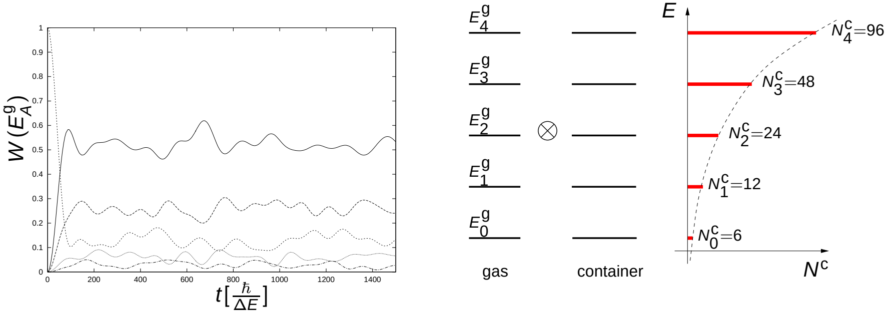
Boltzmann Distribution in a 5-Level-System



Modular Systems

It is very likely that a container system built up of a great amount of identical systems (same spectrum) has an exponential increase of degeneracy with energy.

Borowski, Gemmer, Mahler, EPJB **35** (2003)

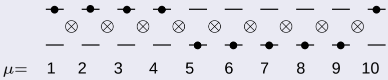
Outline

Signatures of Thermodynamical Behavior

Spin Chains: Local Properties

Heisenberg Spin Chain

$$\hat{H} = \frac{1}{2}\sum_{\mu=1}^{N} \hat{\sigma}_z(\mu) + \lambda \sum_{\mu=1}^{N-1} \vec{\sigma}(\mu)\cdot\vec{\sigma}(\mu+1)$$



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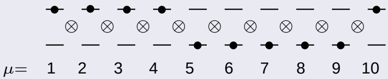

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Reduced Density Operator

$$\hat{\rho}_\nu(t) = \mathrm{Tr}_{\mu\neq\nu}\{|\psi(t)\rangle\langle\psi(t)|\}$$

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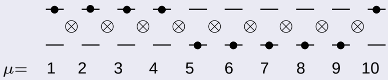

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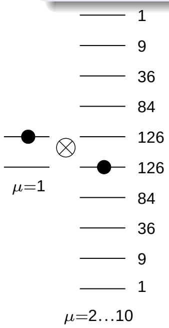


Reduced Density Operator

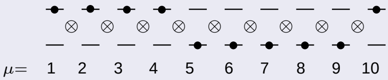
$$\hat{\rho}_\nu(t) = \mathrm{Tr}_{\mu\neq\nu}\{|\psi(t)\rangle\langle\psi(t)|\}$$

Signatures of Thermodynamical Behavior

Spin Chains: Local Properties

Heisenberg Spin Chain

$$\hat{H} = \frac{1}{2}\sum_{\mu=1}^{N} \hat{\sigma}_z(\mu) + \lambda \sum_{\mu=1}^{N-1} \vec{\sigma}(\mu)\cdot\vec{\sigma}(\mu+1)$$



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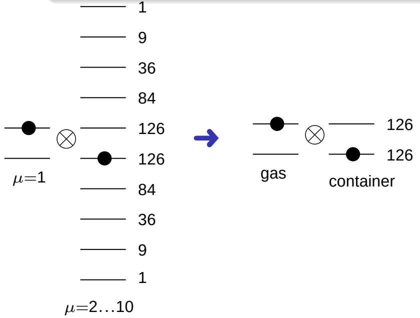

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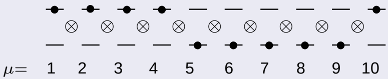

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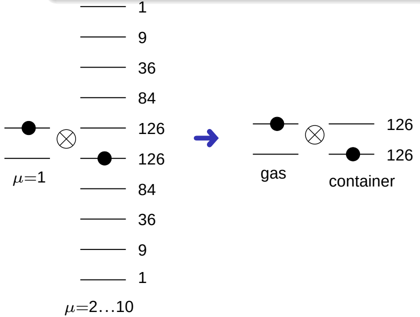

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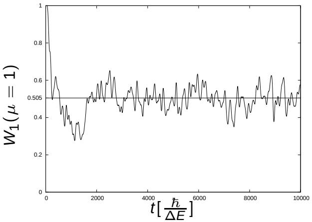
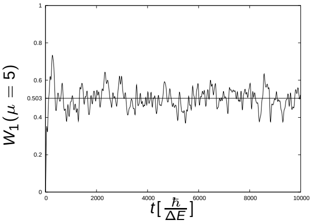
Theoretical Expectation

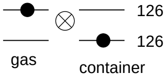
- ➜ system $\mu = 1$ enters the totally mixed state
- ➜ $W_0(1) \propto N_1^c$, $W_1(1) \propto N_0^c$

Signatures of Thermodynamical Behavior

Spin Chain Result







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Outline

Introduction

Non-Equilibrium Quantum Thermodynamics

Systems Near Equilibrium

- the route from non-equilibrium initial states to a global equilibrium state

Introduction

Non-Equilibrium Quantum Thermodynamics

Systems Near Equilibrium

- the route from non-equilibrium initial states to a global equilibrium state
- local equilibrium states ➜ heat conduction

Heat Conduction

Heat Conduction Experiment
(Deutsches Museum München)

- no global equilibrium state (linear temperature gradient)
- locally the system is in equilibrium (const. local temperature)

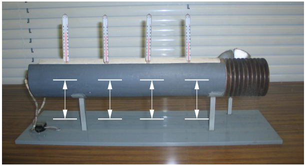
Outline

A Quantum Heat Conduction Model

Minimal Quantum Model

Local Hamiltonian

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



A Quantum Heat Conduction Model

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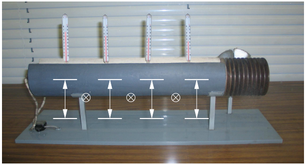
Interaction

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

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

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



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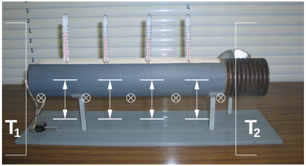
Next Neighbor Interaction

- Heisenberg Interaction
- XY Interaction (Förster)
- Random Interaction

→ weak coupling



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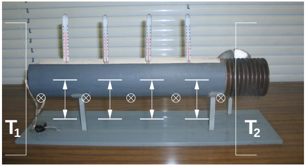

Environmental Systems

- too many levels for a complete Schrödinger investigation
- approximation of environmental systems by Lindblad Formalism (from Quantum Optics)

A Quantum Heat Conduction Model

Open System Approach: Lindblad Formalism

Liouville-Von-Neumann Equation

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = -\mathrm{i}[\hat{H}, \hat{\rho}]$$

A Quantum Heat Conduction Model

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LvN Equation (Open System)

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- phenomenological operator
- computation not in n dimensional Hilbert space but in n^2 dimensional Liouville space

A Quantum Heat Conduction Model

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Bath Super Operators

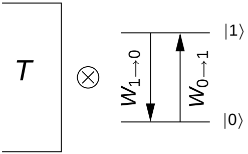
$$\begin{aligned}\hat{\mathcal{L}}^1 \hat{\rho} =& \frac{W_{1\to 0}}{2}\left(2\hat{\sigma}_-^{(1)}\hat{\rho}\hat{\sigma}_+^{(1)} - \hat{\rho}\hat{\sigma}_+^{(1)}\hat{\sigma}_-^{(1)} - \hat{\sigma}_+^{(1)}\hat{\sigma}_-^{(1)}\hat{\rho}\right) + \\ & \frac{W_{0\to 1}}{2}\left(2\hat{\sigma}_+^{(1)}\hat{\rho}\hat{\sigma}_-^{(1)} - \hat{\rho}\hat{\sigma}_-^{(1)}\hat{\sigma}_+^{(1)} - \hat{\sigma}_-^{(1)}\hat{\sigma}_+^{(1)}\hat{\rho}\right)\end{aligned}$$

A Quantum Heat Conduction Model

Example: Spin and Single Bath

LvN Equation

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



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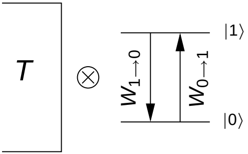

Properties

- Rates are functions of bath temperature T and bath coupling strength λ
- $W_{0\to 1} < W_{1\to 0}$

A Quantum Heat Conduction Model

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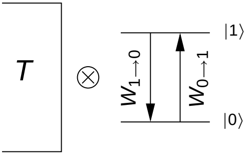
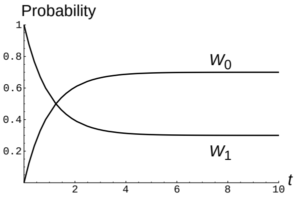
Stationary State

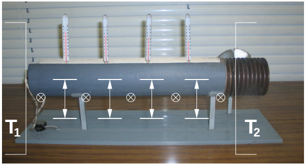
$$\hat{\rho} = \frac{1}{W_{0\to1} + W_{1\to0}} \begin{pmatrix} W_{1\to0} & 0 \\ 0 & W_{0\to1} \end{pmatrix}$$





Outline

Properties of the Stationary State
Temperature and Current



Gemmer, Michel, Mahler, LNP657 (2004)

LvN Equation: Stationary State

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

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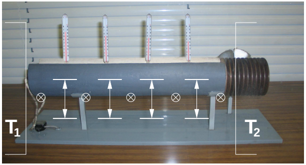

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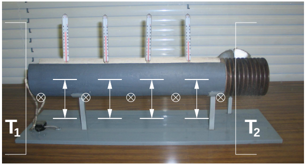

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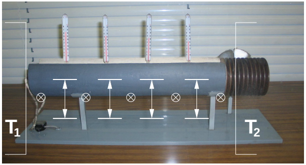

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Current Operator

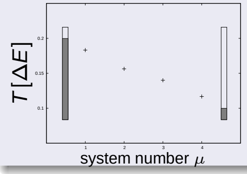
Equation of continuity for the local energy leads to the current operator:

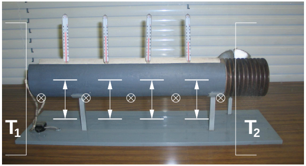
$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{H}^{\mathrm{loc}}(\mu) = \mathrm{i}\left[\hat{H},\hat{H}^{\mathrm{loc}}(\mu)\right] = \hat{J}^{(\mu-1,\mu)} - \hat{J}^{(\mu,\mu+1)}$$

Temperature and Current

Local Temperature Profile for Different Interactions

Heisenberg Interaction





Michel, Hartmann, Gemmer, Mahler EPJB **34** (2003)

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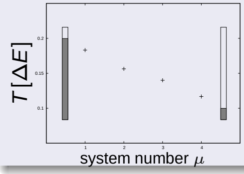
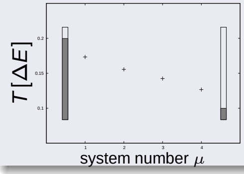
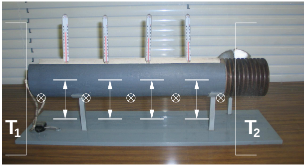


Random Interaction





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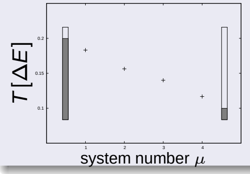

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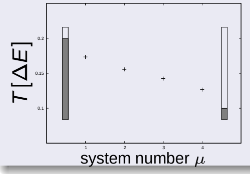

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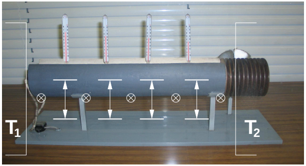

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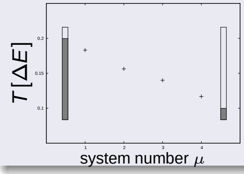

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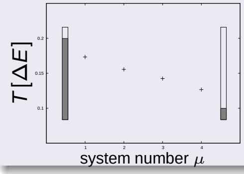

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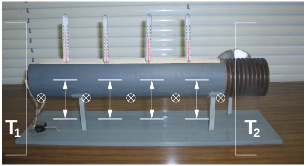

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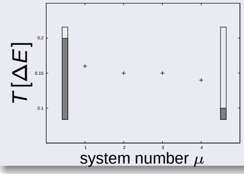
Förster Interaction (XY)



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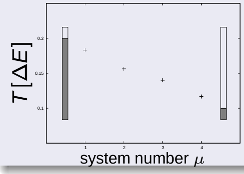

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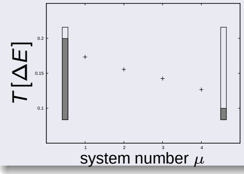

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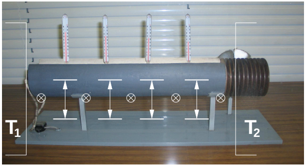

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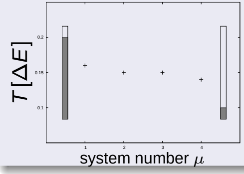

ballistic transport

Fourier's Law

Normal Heat Conduction (Heisenberg Chain)

Fourier's Law

linear connection between current and local temperature difference

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

Fourier's Law

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- fixed mean temperature $T = (T_1 + T_2)/2$
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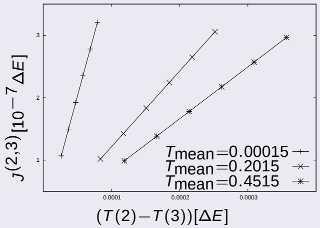
Numerical Data



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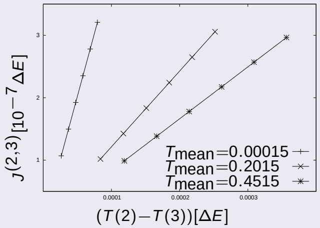
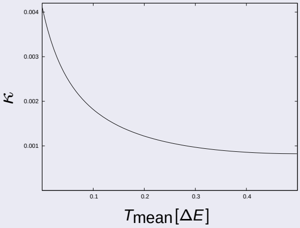


Conductivity



Outline

Kubo Formulas

Background (F. Heidrich-Meisner, TU Braunschweig, 22.6.2004)

- Theory of linear response: $\hat{H} = \hat{H}_0 + \hat{F}$
  $\hat{H}_0$ system Hamiltonian, $\hat{F}$ external perturbational potential

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- linear response of the system: current
- Ohm's Law: $\vec{J} = \sigma \vec{E}$ with σ electric conductivity

Kubo Formulas

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- Theory of linear response: $\hat{H} = \hat{H}_0 + \hat{F}$
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Problematic Derivation

What is $\hat{F}$ in the thermal case?

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Extension of Kubo Formulas for the Thermal Case

Include heat baths: Theory of Perturbation in Liouville Space

Kubo Formulas in Liouville Space

Perturbation Theory: Unperturbed System

LvN Equation

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \hat{\mathcal{L}}\hat{\rho} \quad \text{with}$$

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

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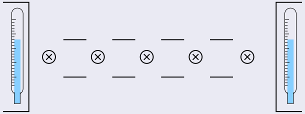

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Kubo Formulas in Liouville Space

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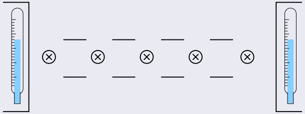

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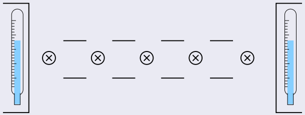

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Kubo Formulas in Liouville Space

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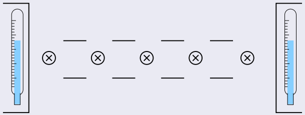

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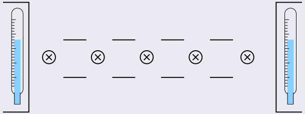

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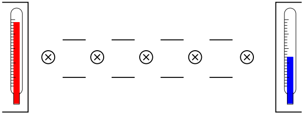
- dual basis: $|\hat{\rho}^j)$ with $\sum_j |\hat{\rho}_j)(\hat{\rho}^j| = \hat{1}$

Kubo Formulas in Liouville Space

Perturbation Theory: Perturbed System



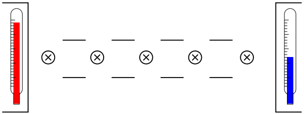
Perturbation Operator

$\hat{\mathcal{L}}^{\text{per}} = \hat{\mathcal{L}}^1(T_1) + \hat{\mathcal{L}}^2(T_2)$
with $T_1 = T + \Delta T$ and $T_2 = T - \Delta T$

Michel, Gemmer, Mahler, submitted to EPJB (2004)

Kubo Formulas in Liouville Space

Perturbation Theory: Perturbed System



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Perturbed Stationary State (local Equilibrium)

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

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Kubo Formulas in Liouville Space

Temperature Profile and Heat Current

Local Equilibrium Properties

- $\hat{\rho}_0$ contains no profile or current

Stationary State

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

Kubo Formulas in Liouville Space

Temperature Profile and Heat Current

Local Equilibrium Properties

- $\hat{\rho}_0$ contains no profile or current
- expectation values as before

Expectation Value

$$A = \mathrm{Tr}\{\hat{A}\Delta\hat{\rho}\}$$

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Temperature Profile and Heat Current

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Current

$$J^{(\mu,\mu+1)} = \mathrm{Tr}\{\hat{J}^{(\mu,\mu+1)}\Delta\hat{\rho}\}$$

Current

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

the current through the system is linear in the external perturbation

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current is independent of the concrete internal profile

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Profile

$$\Delta T^{(\mu,\mu+1)} = \mathrm{Tr}\{(\hat{H}_{\mathrm{loc}}^{(\mu)} - \hat{H}_{\mathrm{loc}}^{(\mu+1)})\Delta\hat{\rho}\}$$

Current

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the current through the system is linear in the external perturbation

Local Temperature Profile

$$\Delta T^{(\mu,\mu+1)} \propto \Delta T$$

the profile is also linear in the external perturbation

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Local Properties

material constant conductivity defined as

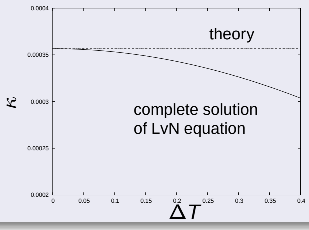
$$\kappa = -\frac{J^{(\mu,\mu+1)}}{\Delta T^{(\mu,\mu+1)}}$$

is independent of ΔT

Kubo Formulas in Liouville Space

Results

Conductivity



Kubo Formulas in Liouville Space

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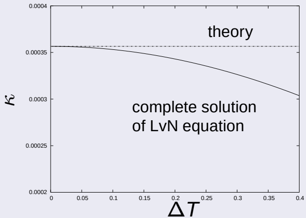

Theoretical Results

- Formula for current and temperature profile

Kubo Formulas in Liouville Space

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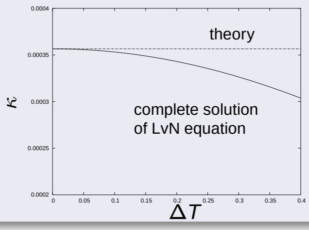

Theoretical Results

- Formula for current and temperature profile
- Formula for material property conductivity (κ)

Kubo Formulas in Liouville Space

Results

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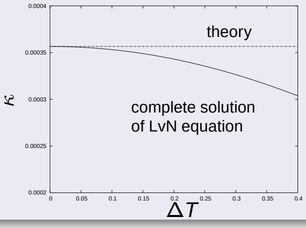
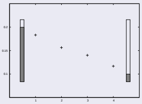


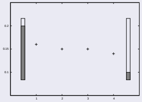
Theoretical Results

- Formula for current and temperature profile
- Formula for material property conductivity (κ)
- Numerical investigation of the above mentioned formulas is showing the correct dependence of the interaction type

Heisenberg

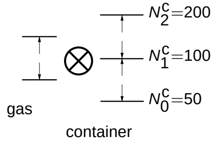


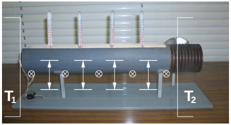
Förster



Summary

- Emergence of quantum thermodynamical equilibrium in really small quantum systems (global equilibrium).
- Non-equilibrium quantum thermodynamics: minimal heat conduction model (local equilibrium).





- Outlook: investigation of the route from non-equilibrium states into equilibrium.

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