Fourier's Law from Quantum Mechanics

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

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November 24th, 2005

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Nearly 200 years later no one doubts the empirical standing of Fourier's law [...] No one has yet managed to derive Fourier's law from truely fundamental principles.
Mark Buchanan, Nature Physics (Nov. 2005)

Outline

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Fourier's Law

Jean Baptiste Joseph Fourier
(1768 - 1830)

Local Equilibrium

Heat Conduction Experiment
(Deutsches Museum München)

- local temperature (no global temperature)
- constant heat current

Fourier's Law

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Fourier's Law

linear connection between gradient $\boldsymbol{\nabla} T$ and heat current $\boldsymbol{j}$

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

heat conductivity κ

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Prize of Paris Institute of Mathematics

... the manner in which the author arrives at these equations is not exempt of difficulties ... (*prize committee*)

Microscopic Foundation I

➜ Microscopic formula for the heat conductivity

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Peter J. W. Debye (1884-1966)

- particle current in solids with mean velocity $\overline{v}$ (e.g. electrons)
- heat current $\boldsymbol{j} \propto \eta \overline{v} c \Delta T$ (η particle density; c heat capacity)
- heat transport in conductors; what is about insulators?

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Sir Rudolph E. Peierls (1907 - 1995)

- phonons treated as classical particles
- formulation of a Boltzmann equation
- microscopic foundation on classical ideas
- quantized normal modes are treated as being well localized in both position and momentum space

Microscopic Foundation II

Ryogo Kubo (1920-1995)

- linear response theory
- for electrical transport: $\hat{H} = \hat{H}_0 + \hat{H}'$
- ad hoc transfered from electrical to heat transport
- heat current as response to a "thermal potential"?
- thermal Kubo formula

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Kubo Formula for heat conductivity

$$\kappa(\omega) = \int_0^\infty \mathrm{d}t e^{-\mathrm{i}\omega t} \int_0^\beta \mathrm{d}\lambda \mathrm{Tr}\{\hat{\rho}_0 \hat{j}(0) \hat{j}(t + \mathrm{i}\lambda)\}$$

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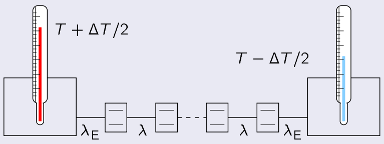
Critical Statement (Kubo et al. *Statistical Physics II* (Springer, 1991))

"It is generally accepted, however, that such formulas exist and are of the same form as those for responses to mechanical disturbances."

Microscopic Foundation III

An open system approach



Liouville von Neumann equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \mathcal{L}(T_1)\hat{\rho} + \mathcal{L}(T_2)\hat{\rho}$$

Microscopic Foundation III

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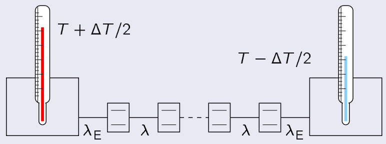

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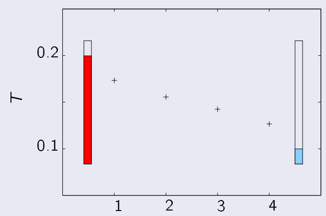
Full Numerical Solution



Microscopic Foundation III

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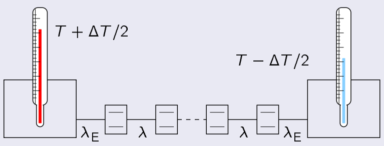

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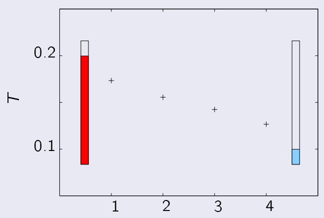
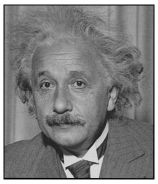


Perturbation Theory

- perturbation in Liouville space
- unperturbed system $T_1 = T_2 = T$
- perturbation ΔT
- current $\propto$ temperature difference
- formula for κ: Kubo formula in Liouville space

Connection between Diffusion and Relaxation



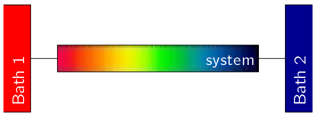
Albert Einstein
(1879-1955)

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).

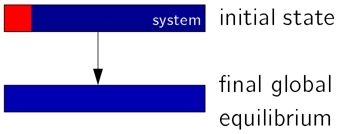
Bath Scenario



stationary local equilibrium state

➜ heat conductivity

Decay Scenario

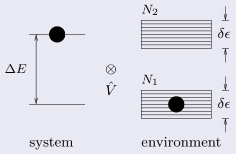


➜ relaxation constant

Outline

Model System

Spin coupled to finite environments



System parameters:

λ	coupling strength (=0.0005)
$\delta\epsilon$	band width (=0.5)
$N1$, $N2$	number of levels (=500)
ΔE	local splitting (=10)

Model System

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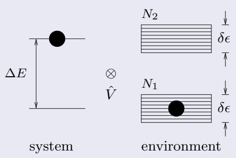

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System dynamics

Hamiltonian

$$\hat{H} = \hat{H}_{\text{sys}} + \hat{H}_{\text{env}} + \lambda\hat{V}$$

Schrödinger dynamics

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

Reduced density operator

$$\hat{\rho} = \mathrm{Tr}_{\mathrm{E}}\left\{|\psi(t)\rangle\langle\psi(t)|\right\}$$

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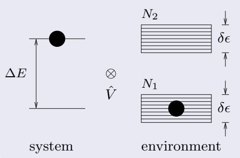

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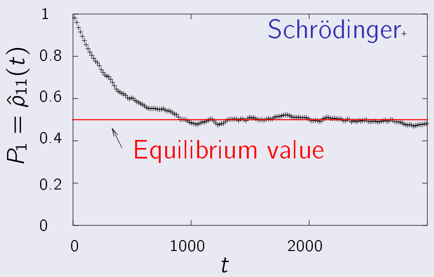
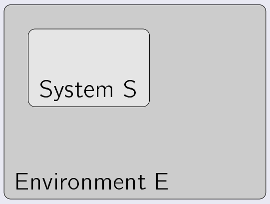
Dynamical Investigation



Reduced Description

Closed System: System and Environment



Schrödinger pure state dynamics $|\psi\rangle$ or $\hat{\rho} = |\psi\rangle\langle\psi|$ according to Liouville von Neumann Equation

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

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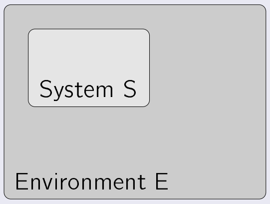

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Reduced dynamics for the system S

$$\hat{\rho}_{\mathrm{S}} = \mathrm{Tr}_{\mathrm{E}}\left\{\hat{\rho}\right\} \quad \rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}_{\mathrm{E}}\left\{\hat{\rho}\right\} = \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_{\mathrm{S}} = \mathrm{Tr}_{\mathrm{E}}\left\{\mathcal{L}\hat{\rho}\right\} \quad \rightarrow \quad \text{no closed equation}$$

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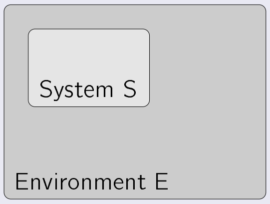

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Approaches to a closed equation

- Projection Operator Techniques: Nakajima-Zwanzig (NZ), Time Convolutionless (TCL)
- Hilbert Space Average Method (HAM)

Quantum Master Equation

Projection operator to relevant (irrelevant) part of the system

Super operator: $\mathcal{P}\hat{\rho} =$ relevant part $\quad \mathcal{Q}\hat{\rho} = \hat{\rho} - \mathcal{P}\hat{\rho} =$ irrelevant part

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Time local exact master equation (TCL)

Application of the projector on the Liouville von Neumann equation

$$\frac{\partial}{\partial t}\mathcal{P}\hat{\rho}(t) = \underbrace{\mathcal{K}(t)}_{\text{TCL generator}} \mathcal{P}\hat{\rho}(t) \quad \rightarrow \text{TCL master equation}$$

- formal exact equation for relevant part of the system
- expansion of $\mathcal{K}$ in the coupling strength
- very challenging in higher than second order

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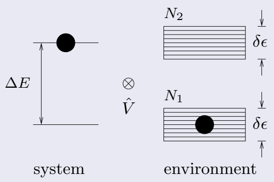
Quantum Master Equation (TCL2)

Born-, Redfield-, Markov- and rotating wave approximation

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

Comparison of QME and Schrödinger

Results



$\lambda = 0.0005$, $\delta\epsilon = 0.5$,
$N1 = N2 = N = 500$

see Breuer et al. PRE submitted (2005)

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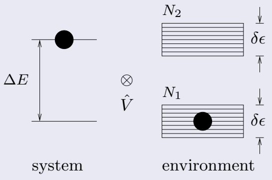

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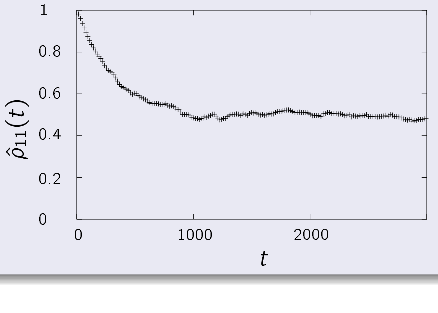

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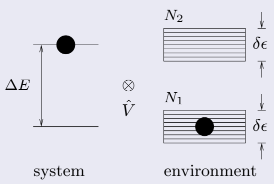

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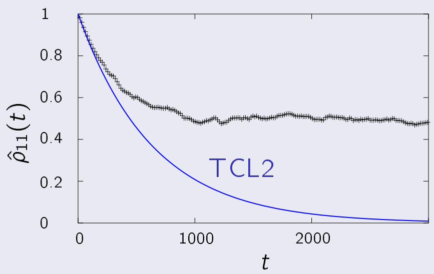

Solution of the QME in TCL2

$$\hat{\rho}_{11}(t) = \hat{\rho}_{11}(0)e^{-\gamma t}$$

with the decay rate $\gamma = \frac{2\pi\lambda^2 N}{\delta\epsilon}$

see Breuer et al. PRE submitted (2005)

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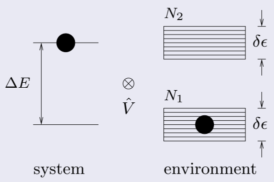

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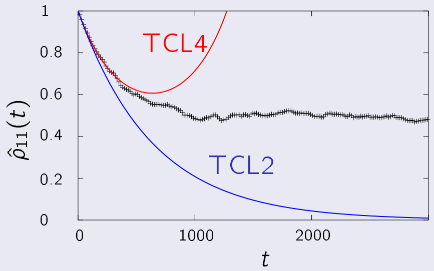

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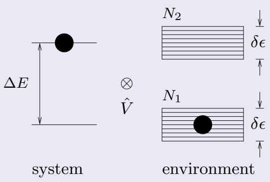
Problem

- TCL2 converges to the wrong equilibrium value
- all higher orders of the TCL expansion are divergent

Hilbert Space Average Method

Freeman Dyson
(*1923)

Dyson expansion of the Schrödinger equation



$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = -\mathrm{i}\hat{V}(t)\,|\psi(t)\rangle$$

short time step τ

$$|\psi(\tau)\rangle = \hat{D}(\tau)\,|\psi(0)\rangle$$

Dyson operator $\hat{D}(\tau) = \hat{1} + \sum_{j=1}^{\infty}\Big(-\frac{\mathrm{i}}{\hbar}\Big)^j \hat{U}_j(\tau)$

$$\hat{U}_1(\tau) = \int_0^{\tau} \mathrm{d}\tau'\,\hat{V}(\tau')\,, \quad \hat{U}_2(\tau) = \int_0^{\tau}\mathrm{d}\tau'\int_0^{\tau'}\mathrm{d}\tau''\,\hat{V}(\tau')\,\hat{V}(\tau'')$$

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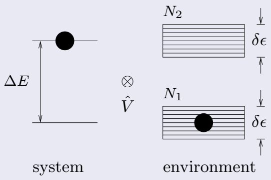

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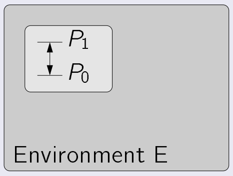
Second Order Approximation for a short time τ

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

Approximation Scheme I

Short time evolution of probabilities



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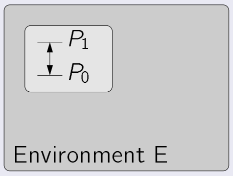

$$P_1(\tau) = \langle\psi(\tau)|\hat{P}_1|\psi(\tau)\rangle$$
$$= \langle\psi(0)|\hat{D}^\dagger(\tau)\hat{P}_1\hat{D}(\tau)|\psi(0)\rangle$$

second order approximation of Dyson operator

$$P_1(\tau) \approx \langle\psi(0)|\hat{D}_2^\dagger(\tau)\hat{P}_1\hat{D}_2(\tau)|\psi(0)\rangle$$

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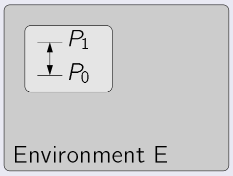


$$
\begin{aligned}
P_1(\tau) &= \langle \psi(\tau) | \hat{P}_1 | \psi(\tau) \rangle \\
&= \langle \psi(0) | \hat{D}^\dagger(\tau) \hat{P}_1 \hat{D}(\tau) | \psi(0) \rangle
\end{aligned}
$$

second order approximation of Dyson operator

$$
P_1(\tau) \approx \langle \psi(0) | \hat{D}_2^\dagger(\tau) \hat{P}_1 \hat{D}_2(\tau) | \psi(0) \rangle
$$

Hilbert Space Average

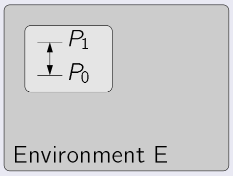
Method to guess the value of a quantity defined as a function of the full state $|\psi\rangle$ of the system

Hilbert Space

- only available information is the initial probability $P_1(0) = \langle \psi(0) | \hat{P}_1 | \psi(0) \rangle$

Approximation Scheme I

Short time evolution of probabilities



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$$= \langle \psi(0) | \hat{D}^\dagger(\tau) \hat{P}_1 \hat{D}(\tau) | \psi(0) \rangle$$

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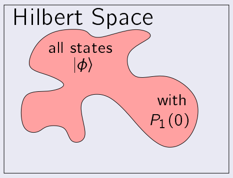
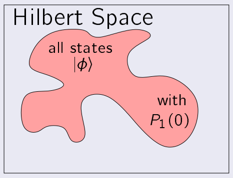


- only available information is the initial probability $P_1(0) = \langle \psi(0) | \hat{P}_1 | \psi(0) \rangle$
- take all states $|\phi\rangle$ featuring $P_1(0)$

➜ take the average over all $\langle \phi | \hat{D}_2^\dagger \hat{P}_1 \hat{D}_2 | \phi \rangle$

Approximation Scheme II

Hilbert Space Average



replace the actual expectation value

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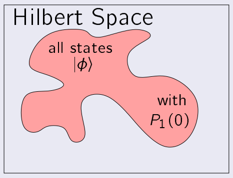
Approximation Scheme II

Hilbert Space Average



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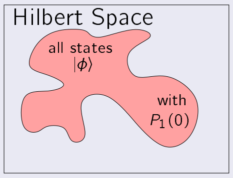

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HAM Rate equation

$$\frac{\mathrm{d}}{\mathrm{d}t} P_1(t) = \gamma\big(2P_1(t) + P_1(0)\big) \quad \text{with} \quad \gamma = \frac{2\pi\lambda^2 N}{\delta\epsilon}$$

further reading:

Gemmer, Michel EPL accepted (2005)
Gemmer, Michel, Physica E, 29, 136 (2005)
Gemmer, Michel, Mahler, *Quantum Thermodynamics*, Springer (2004)

Results of HAM

Criteria for applicability of HAM

From theory one gets criteria for the validity of HAM

$$2\lambda \frac{N}{\delta\epsilon} \geq 1\,, \quad \lambda^2 \frac{N}{\delta\epsilon^2} \ll 1$$

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Solution of the HAM rate equation

Solving the rate equation

$$P_1(t) = P_1(0)\big(0.5 + 0.5\mathrm{e}^{-2\gamma t}\big)$$

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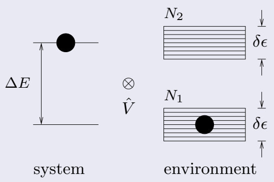
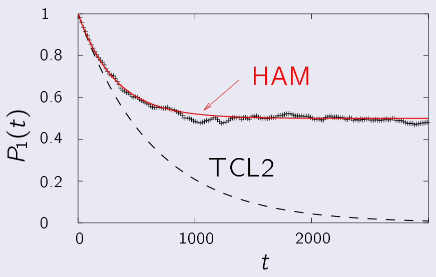


$\lambda = 0.0005$, $\delta\epsilon = 0.5$, $N1 = N2 = N = 500$



Breuer TCL

a new TCL projection operator for finite environments

- convergence of the second order to the correct equilibrium state
- no divergence in higher orders

Breuer et al. PRE submitted (2005)

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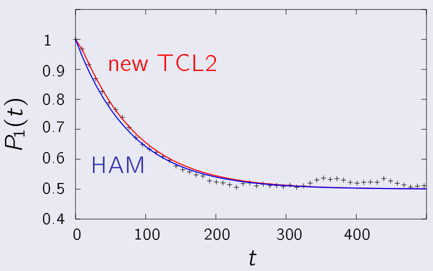

$$2\lambda \frac{N}{\delta\epsilon} = 1 \geq 1\,, \quad \lambda^2 \frac{N}{\delta\epsilon^2} = 0.002 \ll 1$$

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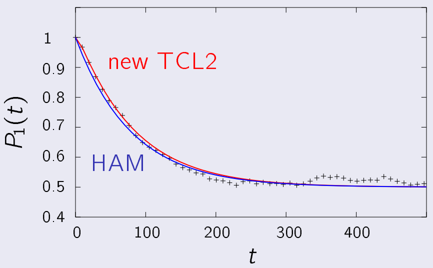
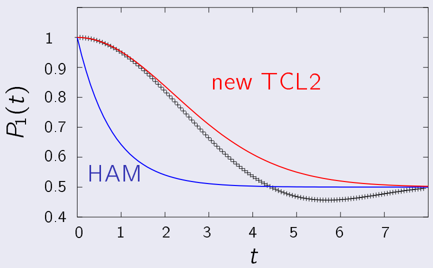


$$2\lambda \frac{N}{\delta\epsilon} = 1 \geq 1\,, \quad \lambda^2 \frac{N}{\delta\epsilon^2} = 0.002 \ll 1$$

$\lambda = 0.01$



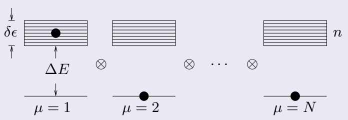
$$2\lambda \frac{N}{\delta\epsilon} = 10 \geq 1\,, \quad \lambda^2 \frac{N}{\delta\epsilon^2} = 0.2 \ll 1$$

Breuer et al. PRE submitted (2005)

Outline

The Hamiltonian Model

Hamiltonian



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

Operators

$\hat{H}_{\text{loc}}$	local Ham.
$\hat{V}$	interaction

Parameters

λ	coupling strength
$\delta\epsilon$	band width
ΔE	gap
n	number of levels

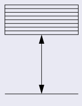
One Excitation Subspace Hamiltonian

$$\hat{H} = \left(\begin{array}{c|c|c} \begin{matrix}\ddots & & 0\\ & i\frac{\delta\epsilon}{n} & \\ 0 & & \ddots\end{matrix} & v_{12} & 0 \\ \hline v_{21} & \begin{matrix}\ddots & & 0\\ & j\frac{\delta\epsilon}{n} & \\ 0 & & \ddots\end{matrix} & v_{23} \\ \hline 0 & v_{32} & \begin{matrix}\ddots & & 0\\ & k\frac{\delta\epsilon}{n} & \\ 0 & & \ddots\end{matrix} \end{array}\right)$$

Application of HAM

Observed quantity: probability to find an excitation in subsystem μ

- Energy in a subunit ➜ excitation probability
- Projector on the excitation band of μth subunit $\hat{P}_{\mu}$
- Probability $P_{\mu}(t) \equiv \langle \psi(t) | \hat{P}_{\mu} | \psi(t) \rangle$



Subunit μ

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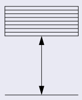

Short time evolution according to Dyson series expansion

$$P_\mu(\tau) = \langle \psi(0) | \hat{D}^\dagger(\tau) \hat{P}_\mu \hat{D}(\tau) | \psi(0) \rangle$$

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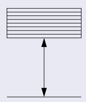

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Second order truncation of Dyson series

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

second order approximation of the probability

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

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Rate Equation

Hilbert Space Average for $P_\mu(\tau)$

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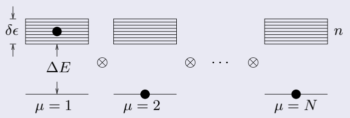
Rate equation for the probability



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

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

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

Diffusion Constant

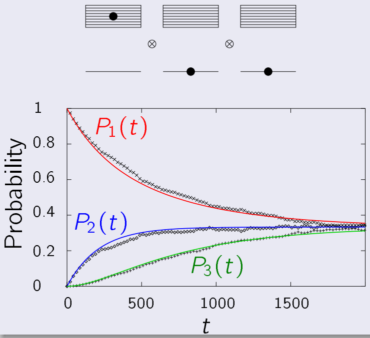
$$\kappa = \frac{2\pi\lambda^2 n}{\delta\epsilon}$$

Conditions for HAM

$$\frac{\lambda}{\delta\epsilon}n \geq \frac{1}{2}\,, \qquad \frac{\lambda^2}{\delta\epsilon^2}n \ll 1$$

Comparison to the Schrödinger Equation

N=3



Model Parameters

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

Conditions:

$\frac{\lambda}{\delta\epsilon} n = 0.5 \quad \geq \frac{1}{2}$ ✔

$\frac{\lambda^2}{\delta\epsilon^2} n = 0.5 \cdot 10^{-3} \quad \ll 1$ ✔

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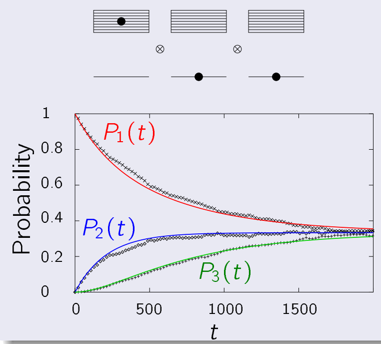
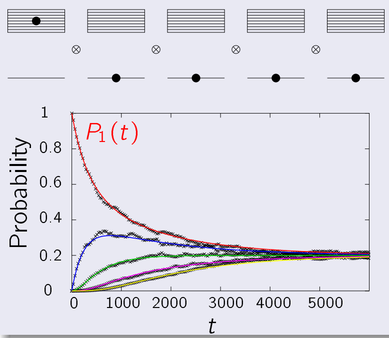


N=5



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Deviation of HAM from the Exact Solution

Deviation Measure

time-averaged quadratic deviation of the exact result from the HAM prediction

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

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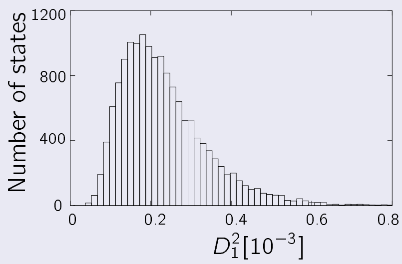
for different initial states



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

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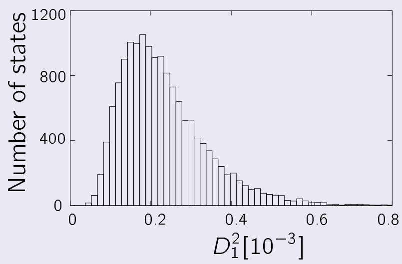
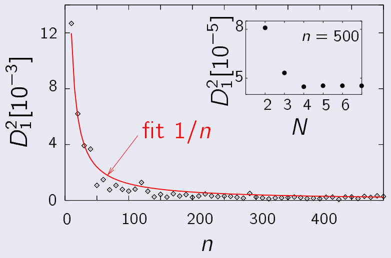


15000 equally distributed initial states ($N = 2$, $n = 500$)

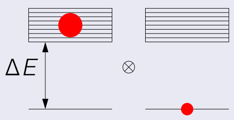
for different system sizes



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

Energy Diffusive Behavior

HAM rate equation



Respective rate equation

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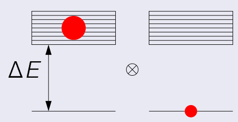

Respective rate equation

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Energy Current

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

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

internal energy in this simple model: $U_\mu = \Delta E P_\mu$

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

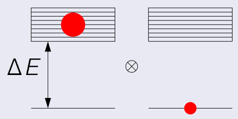
and with rate equation

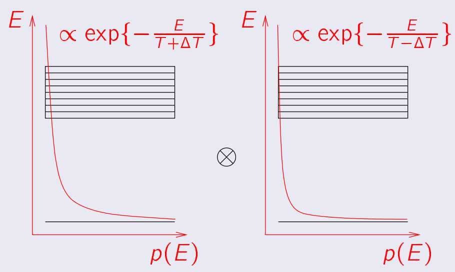
$$J_{1\to 2} = -\kappa \Delta E\left(P_1 - P_2\right)$$

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

Heat Diffusive Behavior

Quasi Thermal State





➜ not a mixed state, but a superposition of states according to the Boltzmann distribution

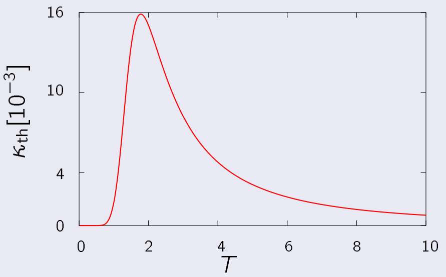
Heat Current and Conductivity

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

κ_{th}	heat conductivity
κ	energy diffusion constant
c	heat capacity of subunit

Heat Conductivity

Transport Coefficient



Expectation

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

Result

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

further reading: Michel, Mahler, Gemmer, PRL 95, 180602 (2005)
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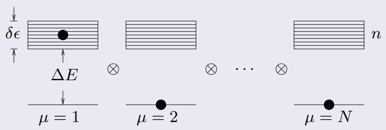
Design Model and Real Solids

Design Model



- easy definition of local energy and temperature
- such a large gap is not very typical situation

➜ HAM is not restricted to such gapped system

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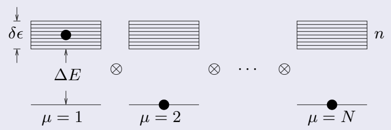

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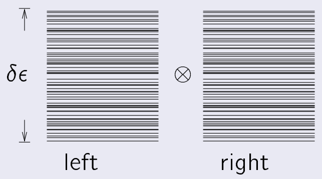
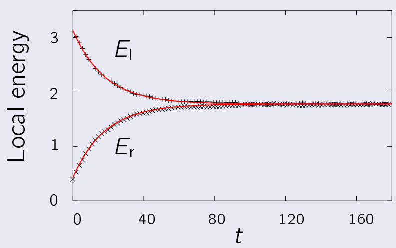
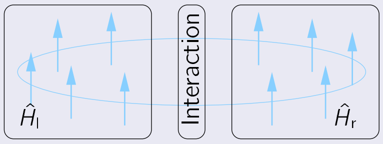
Gap free system





Spin Model

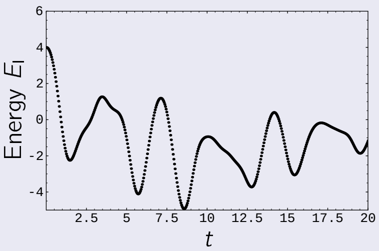
Spin ring without local field



$$\hat{H}_\mathrm{H} = \sum_\mu \vec{\sigma}(\mu)\vec{\sigma}(\mu+1)$$

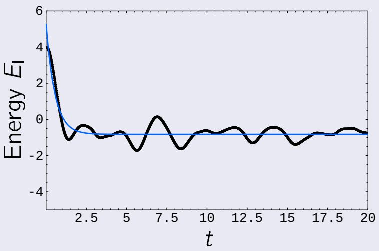
$$\hat{H}_\mathrm{R} = \sum_\mu \sum_{ij} p_{ij}\hat{\sigma}_i(\mu)\hat{\sigma}_j(\mu+1)$$

Heisenberg Ring



$$\hat{H} = \lambda \hat{H}_\mathrm{H}$$

Heisenberg and Random Ring



$$\hat{H} = \lambda \hat{H}_\mathrm{H} + 0.1\lambda \hat{H}_\mathrm{R}$$

Summary and Outlook

Summary

The new Hilbert Space Average Method is a powerful technique to describe both

- the statistical decay into the global equilibrium state within quantum mechanics
- the emergence of Fourier's Law from Schrödinger dynamics

Outlook

- more realistic models
- comparison with bath scenario

Thanks

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M. Stollsteimer, J. Teifel, F. Tonner
Financial support by the DFG is gratefully acknowledged.