The careful application of projection methods to transport and relaxation

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Projection techniques

standard open system approach (Nakajima-Zwanzig))

linear superoperators: $\mathcal{L}$, $\mathcal{P}$

dynamics: $\frac{d\hat{\rho}}{dt} = \mathcal{L}(t)\hat{\rho}(t)$ projection: $\mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho}$

$\Rightarrow$ big mathematical machinery (Nakajima-Zwanzig formalism) $\Rightarrow$

$$\frac{d}{dt}\mathcal{P}\hat{\rho}(t) = \int_0^t \mathcal{P}\mathcal{L}(t)\mathcal{L}(t')\mathcal{P}\hat{\rho}(t')dt' + O(\mathcal{L}^3) + \mathcal{I}(\hat{\rho}(0))$$ **"Born approximation"**

for initial states with $\mathcal{P}\hat{\rho}(0) = \hat{\rho}(0)$ one finds $\mathcal{I}(\hat{\rho}(0)) = 0$

Typical quantum dynamics and standard choice of projection operator

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{V} \qquad \hat{V} = \sum_n \hat{A}_n^\dagger \hat{B}_n + \hat{A}_n \hat{B}_n^\dagger \qquad \mathcal{L}\hat{\rho} = \mathrm{i}[\hat{V}(t), \hat{\rho}(t)]$$

$$\hat{\rho}_S := \mathrm{Tr}_E\{\hat{\rho}\} \qquad \mathcal{P}\hat{\rho} := \hat{\rho}_S \otimes \hat{\rho}_E(T) \Rightarrow$$ "RWA", etc. $\Rightarrow$

$$\Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) = \int_0^t \mathcal{K}(t-t')\hat{\rho}_S(t')\mathrm{d}t' \quad \textbf{autonomous dynamics of the system}$$

$$\mathcal{K}(t-t') \propto \mathrm{Tr}\{\hat{B}(t)\hat{B}^\dagger(t')\hat{\rho}_E(T)\} + \text{c.c.} \quad \text{“bath correlation functions”}$$

try the **“Markov approximation”** $\Rightarrow$ “Redfield equation”

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_S(t) \approx \int_0^t \mathcal{K}(t-t')\mathrm{d}t'\hat{\rho}_S(t) \approx: \mathcal{R}\hat{\rho}_S(t)$$

Compute relaxation dynamcis from Redfield equation. If relaxation dynamcis result as slow compared to decay of bath correlation functions $\Rightarrow$ believe Markov approximation!

Does the applicability of the Markov approximation imply the applicability of the Born approximation ?

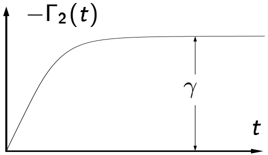
generalized projections (time-convolutionless)

quantity of interest: $A(t) := \mathrm{Tr}\{\hat{A}\hat{\rho}(t)\}$ $\Rightarrow$ pertinent projection $\Rightarrow$

$$\mathcal{P}\hat{\rho} = \hat{1} + \mathrm{Tr}\{\hat{A}\hat{\rho}\}\hat{A} \quad \text{with} \quad \mathrm{Tr}\{\hat{A}^2\} = 1, \quad \mathrm{Tr}\{\hat{A}\} = 0 \quad \Rightarrow \mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho}$$

requirements, standard situation:
“weak perturbation” $\hat{H} = \hat{H}_0 + \lambda\hat{V}$, "slow observable" $[\hat{H}_0, \hat{A}] = 0$,
initial state: $\mathcal{P}\hat{\rho}(0) = \hat{\rho}(0)$ $\Rightarrow$ "TCL machinery" yields $\Rightarrow$

$$\dot{A} = (\lambda^2\Gamma_2(t) + \lambda^4\Gamma_4(t) + \cdots)A \quad \Gamma_2(t) = \int_0^t \mathrm{Tr}\left\{[\hat{A}, \hat{V}_I(t')][\hat{A}, \hat{V}(0)]\right\} \mathrm{d}t'$$



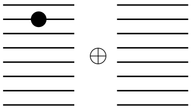
τ_C: correlation time τ_R: relaxation time

$$t > \tau_C \Rightarrow \qquad \dot{A} = -\frac{1}{\tau_R}A \qquad \tau_R := \frac{1}{\lambda^2\gamma}$$

$\tau_R \gg \tau_C \Rightarrow$ *Truncate at second order?*

importance of higher order terms

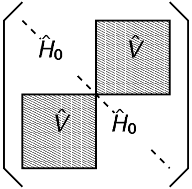
"two-site hopping model"



$$\hat{H}_0 = \sum_{i,\mu} \epsilon_i \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu,i}$$

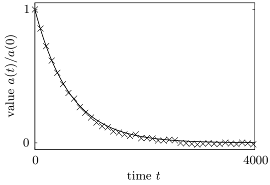
$$\hat{V} = \sum_{ij} c_{ij} \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu+1,j} + \text{h.c.}$$

$$\hat{A} \propto \sum_i \, \hat{a}^\dagger_{1,i} \hat{a}_{1,i} - \sum_j \, \hat{a}^\dagger_{2,j} \hat{a}_{2,j}$$

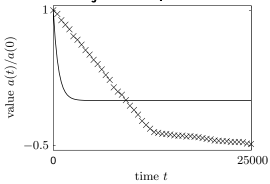


$\tau_C \approx 0.002\tau_R$ in all examples below ("Born-Markov satisfied")

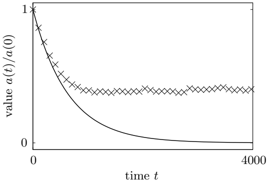
c_{ij} random



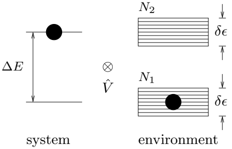
c_{ij} all equal



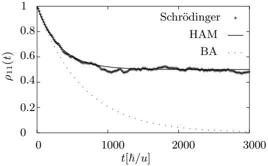
c_{ij} sparse



Statistical (exponential) decay only results for random interaction "spin-finite-environment model"



$$\hat{H}_0 = \Delta E \hat{\sigma}_z + \sum_{i,n} \epsilon_n^i |i, n\rangle\langle i, n|$$
$$\hat{V} = \hat{\sigma}^+ \sum_{nm} c_{nm} |1, n\rangle\langle 2, m| + \text{h.c.}$$
$$\hat{A}_{prod} = \hat{\sigma}_z \sum_n |1, n\rangle\langle 1, n|$$
$$\hat{A}_{corr} = \hat{\sigma}^+\hat{\sigma}^- \sum_n |1, n\rangle\langle 1, n| - \hat{\sigma}^-\hat{\sigma}^+ \sum_n |2, n\rangle\langle 2, n|$$



Truncate at second order? $\Rightarrow$

Success of second order description of relaxation depends on: i) interaction strength, ii) structure of the interaction $\hat{V}$, iii) choice of the projection operator, i.e., choice of $\hat{A}$

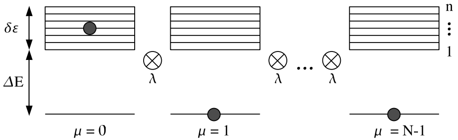
Fourth order contributions are hard to compute numerically but they are small if

$$[\hat{V}(t), [\hat{V}(t'), \hat{A}]] \propto \hat{A}$$

$\Rightarrow$ necessary (but not sufficient) is the "Van Hove structure", i.e., $\hat{V}^2$ must be essentially digonal

Transport

"one particle" modular quantum system:



$$\hat{H}_0 = \sum_{\mu=1}^{N} \hat{h}_\mu$$
$$\hat{V} = \sum_{\mu=1}^{N} \hat{v}_\mu$$

$$\hat{h}_\mu = \sum_i \epsilon_i \; \hat{a}^\dagger_{\mu,i}\hat{a}_{\mu,i}, \quad h_i := \Delta E + i\frac{\delta\epsilon}{n}, \quad \hat{v}_\mu = \sum_{ij} c_{ij} \; \hat{a}^\dagger_{\mu,i}\hat{a}_{\mu+1,j} + \text{h.c.}$$

- This may be viewed as a model for: a particle moving on lattice sites, energy exchange between molecules, etc.
- The model features: no particle-particle interaction, nearest neighbor random interband hoppings, no disorder, a finite amount of sites
- Exploiting the Bloch theorem the dynamics of this model can be directly, numerically calculated up to, e.g., $n \approx 1000$, $N \approx 30$

What are the dynamics of the particle density ?

projection onto density waves

$$\hat{A}_q = \sum_x \cos(qx)\hat{n}(x) \qquad \hat{n}(x) := \sum_i \hat{a}^\dagger_{x,i}\hat{a}_{x,i}$$

$$\Rightarrow \quad \dot{A}_q(t) = \Gamma_q(t)A_q(t)$$

Comparison with a Fourier transformed diffusion equation allows for the following classification:

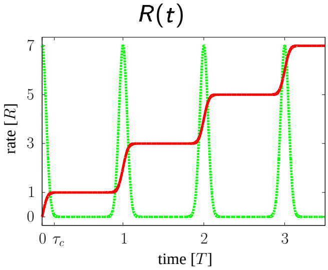
$$\Gamma_q(t) \approx -q^2 D \quad \Rightarrow \quad A_q(t) \propto e^{-q^2 Dt} \quad \Rightarrow \text{diffusive}$$

$$\Gamma_q(t) \approx -q^2 Dt \quad \Rightarrow \quad A_q(t) \propto e^{-q^2 Dt^2} \quad \Rightarrow \text{ballistic}$$

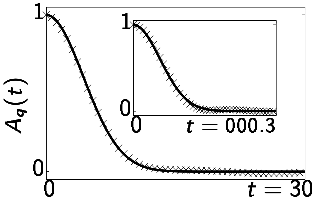
$$\Gamma_q(t) \to 0 \quad \Rightarrow \quad A_q(t) \to \text{const} \quad \Rightarrow \text{localized}$$

Systems featuring translational invariance $\Rightarrow$
second order scales as $\Gamma_q(t) = q^2\lambda^2 R(t)$

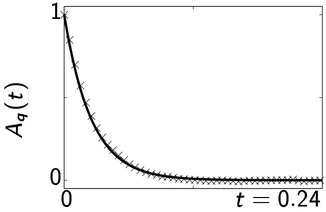
lengthscale dependent "diffusive - ballistic transition"



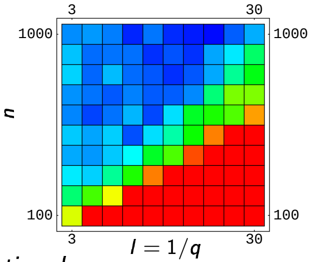
long/short wavelength



intermediate wavelength

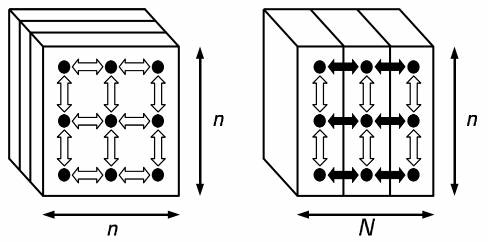


Deviation from diffusion:



Second order description seems to hold for all times!

3d-Anderson model

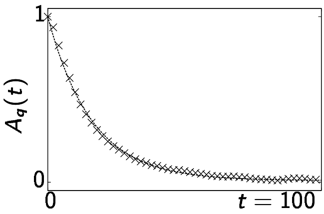


$$\hat{H}=\sum_{\mathbf{r}}\epsilon(\mathbf{r})\,\hat{a}^\dagger(\mathbf{r})\,\hat{a}(\mathbf{r})+\sum_{\mathrm{NN}}\hat{a}^\dagger(\mathbf{r})\,\hat{a}(\mathbf{r}')+\mathrm{h.c.}$$

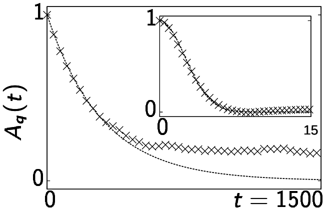
$\epsilon(\mathbf{r})$: Gaussian random numbers, σ $\Rightarrow$

$$\hat{H}=\sum_{\mu=0}^{N-1}\hat{h}_0(\mu)+\lambda\sum_{\mu=0}^{N-1}\hat{v}(\mu,\mu+1)$$

intermediate wavelength



long/short wavelength



$n=30,\ N=42,\ \sigma=1$

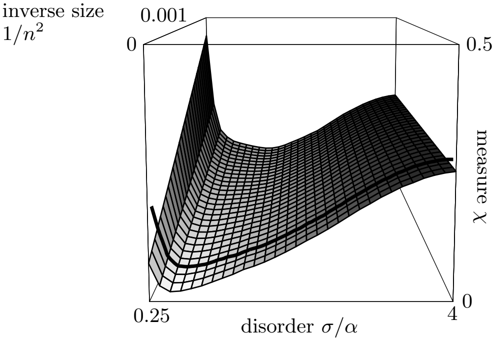
loclization appears as fourth order effect

localization: effect of higher order terms in the projection expansion

Evaluating fourth order terms is an art. We work with a feasible estimation based on the fact that there is Van Hove structure.

t_C: transition to ballistic lengthscale, $\Gamma_{q,4}$: transition to localized lengthscale

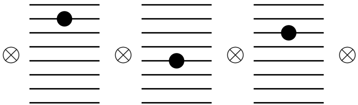
We compute $\sqrt{1/\chi}$: "range" (maximum ratio) of diffusive wavelengths in between ballistic (short) and localized (long) wavelengths.



This suggests: diffusive behavior only between l_{min}, l_{max} with $l_{max}/l_{min} \approx 7$ for infinitely sized systems and "optimum" disorder

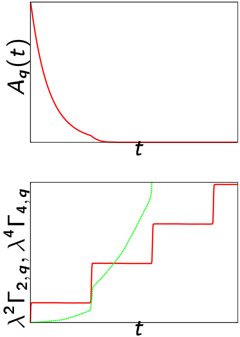
"many particle" modular quantum system:

defined on the full product space of the subunits, random NN-interactions, translational invariance, 1-d

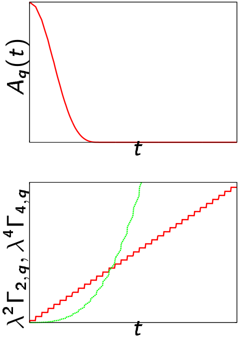


consider transport of local energy:

intermediate wavelength:

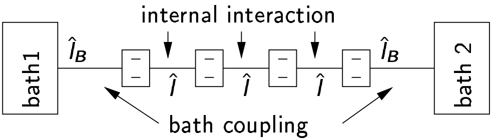


long wavelength:

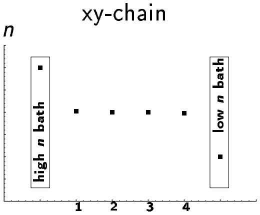


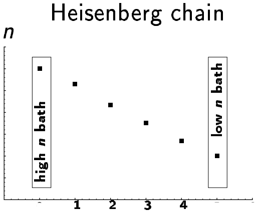
This indicates a lenghtscale dependent "diff.-ball.-transition" in a (strongly) interacting, 1-d, quantum chaotic system

Modeling of coupled reservoirs:



$$i\hbar \frac{d}{dt}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right] + \mathcal{L}(\mu_1, \mu_2)\hat{\rho}$$

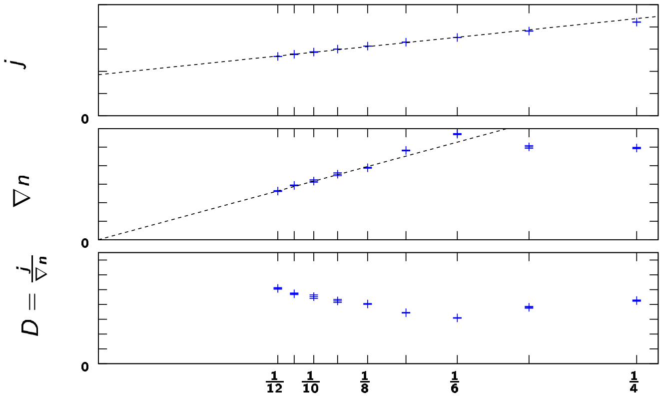




- find some $\mathcal{L}$ that adequately models the reservoirs
- find the null-space ($\hat{\rho}_0$) of an non-Hermitian matrix of dimension d^2
- compute $j = \mathrm{Tr}\{\hat{\rho}_0 \hat{j}\}$ and $\nabla n = \mathrm{Tr}\{\hat{\rho}_0 \nabla \hat{n}\}$ to construct $D = j/\nabla n$

Reservoirs coupled to the Heisenberg chain, $\Delta = 1$:

$$\hat{H} = \sum_{\mu} B\hat{\sigma}^z_\mu + \lambda(\hat{\sigma}^x_\mu\hat{\sigma}^x_{\mu+1} + \hat{\sigma}^y_\mu\hat{\sigma}^y_{\mu+1} + \Delta\hat{\sigma}^z_\mu\hat{\sigma}^z_{\mu+1}) \qquad \hat{n}(x) = \hat{n}_\mu = \hat{\sigma}^z_\mu$$



Find null-space of a $2^{24}x2^{24}$ non-Hermitian matrix? Here we used "stochastic unravelling". $\Rightarrow$ Probably ballistic transport in the limit of long chains.

The "take home message":
Alternative approaches to quantum transport may help to get more detailed information on transport behavior with respect to the lengthscale. Furthermore quantitative analysis of strongly interacting 2d or 3d systems may possibly become feasible.

More information: ask me or visit our webpage.

Many thanks to M. Michel, R. Steinigeweg, H. Wichterich, H.-P. Breuer, C. Bartsch, ... and the audience!