Projective and Typicality Approach to Transport and Relaxation in Quantum Systems

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Alternative methods: projection onto density waves

$$Dynamcis: \frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho} = i\hbar\left[\hat{\rho}, \hat{H}\right] \qquad Quantityofinterest, observableAA(t) := \mathrm{Tr}\{\hat{A}\hat{\rho}(t)\}$$

Direct integration in QM typicaly impossible. But “reduced information” may be obtained from projection techniques

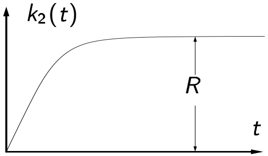
$$\mathcal{P}\hat{\rho} = \hat{1} + \mathrm{Tr}\{\hat{A}\hat{\rho}\}\hat{A} \quad \text{with} \quad \mathrm{Tr}\{\hat{A}^2\} = 1, \quad \mathrm{Tr}\{\hat{A}\} = 0 \Rightarrow \mathcal{P}^2\hat{\rho} = \mathcal{P}\hat{\rho}$$

Projection techniques are perturbative approaches

$$\hat{H} = \hat{H}_0 + \lambda\hat{V}, \quad [\hat{H}_0, \hat{A}] = 0, \quad \mathcal{P}\hat{\rho}(0) = \hat{\rho}(0) \tag{1}$$

TCL machinery

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

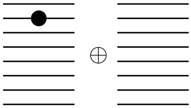


$$t < t_C \Rightarrow \quad \dot{A} = -\gamma A$$

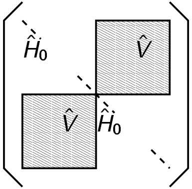
$$t_C < \frac{1}{\gamma} \quad \Rightarrow \text{Born-Markov} \Rightarrow \tag{2}$$

Truncate at second order?

"two-site hopping model"

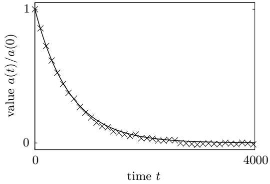


$$\hat{H}_0 = \sum_{i,\mu} \epsilon_i \; \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu,i}$$
$$\hat{V} = \sum_{ij} c_{ij} \; \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu+1,j} + \text{h.c.}$$
$$\hat{A} = \sum_i \; \hat{a}^\dagger_{1,i} \hat{a}_{1,i} - \sum_j \; \hat{a}^\dagger_{2,j} \hat{a}_{2,j}$$

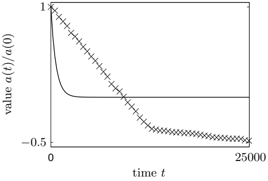


$t_C \approx 0.002$ in all examples below

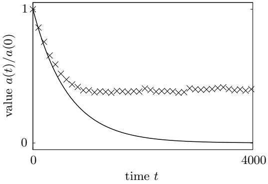
c_{ij} random



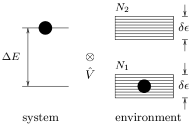
c_{ij} all equal



c_{ij} sparse



"spin finite environment model"



$$\hat{H}_0 = \sum_{i,\mu} \epsilon_i \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu,i}$$
$$\hat{V} = \sum_{ij} c_{ij} \, \hat{a}^\dagger_{\mu,i} \hat{a}_{\mu+1,j} + \text{h.c.}$$
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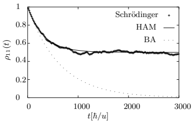


Basics and questions in transport theory

"microscopic"

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

$\Rightarrow ? \Rightarrow$

"macroscopic"

$$\vec{j} = \kappa\vec{F}, \quad \dot{n} = D\Delta n$$

"Fouriers Law: A challenge to theorists", Lebowitz et al., *World Scientific* (2000)

Boltzmann equation:
Adequate "Boltzmann-systems" show diffusive behavior

- Map the quantum system onto an adequate Boltzmann equation!
- Linearize the Boltzmann equation arround an equilibrium state
- Invert the scattering matrix to find D

Kubo formula:
Finite $\kappa(\omega = 0)$ indicates normal transport

- Derived on the basis of an external force $\Rightarrow D \propto T\kappa$?
- Requires diagonalization of the full Hamiltonian
- Result hard to interprete for finite (pieces of larger) systems

Alternative methods: projection onto density waves

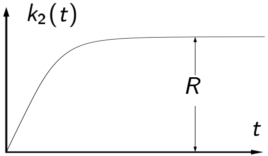
$$\hat{m}_q = \sum_x \cos(qx)\hat{n}(x) \quad \text{diff.:} \Rightarrow \mathrm{Tr}\{\hat{m}_q\hat{\rho}(t)\} \propto \mathrm{e}^{-q^2 Dt} \quad (\text{ball., e.g., :} \Rightarrow \propto \mathrm{e}^{-q^2 Dt^2})$$

Determine $\mathrm{Tr}\{\hat{m}_q\hat{\rho}(t)\} =: m_q$ with a **projection operator method**, e.g., "TCL"

$$\hat{H} = \hat{H}_0 + \lambda\hat{V}, \quad [\hat{H}_0, \hat{m}_q] = 0, \quad \hat{\rho}(0) = \sum_q C_q \hat{m}_q, \qquad \text{translational invariance}$$

$$\Rightarrow \dot{m}_q = \sum_n \lambda^n K_{n,q}(t) m_q \quad (n : \text{even}), \quad K_{2,q}(t) \approx q^2 k_2(t)$$

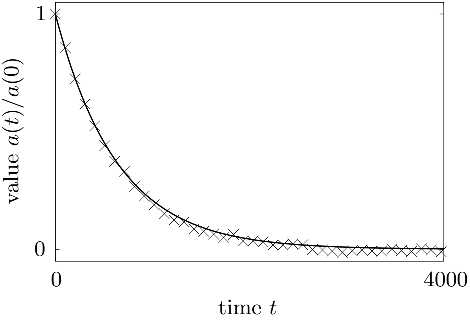
Assume higher orders are negligible and $k_2(t)$ looks like this:



$$\Rightarrow \quad \dot{m}_q = -q^2\lambda^2 R m_q$$

- divide $\hat{H}$ into $\hat{H}_0$ and $\hat{V}$
- diagonalize $\hat{H}_0$
- calculate $k^2(t)$ and estimate higher order terms

"one particle" modular quantum system:



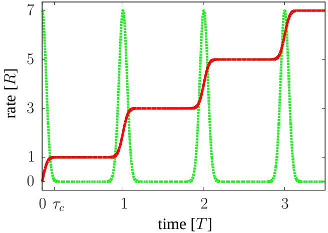
$$\hat{H}_0 = \sum_{\mu=1}^{N} \hat{h}_\mu$$
$$\hat{V} = \sum_{\mu=1}^{N} \hat{v}_\mu$$

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

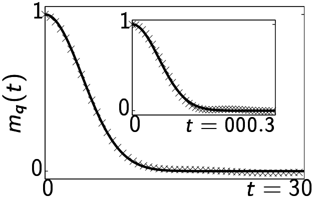
- This may be viewed as a model for: a particle moving on lattice sites, energy exchange between molecules, etc.
- The model features: no particle-particle interaction, nearest neighbor random interband hoppings, no disorder, a finite amount of sites
- Exploiting the Bloch theorem the dynamics of this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

Results of the projection onto density waves:

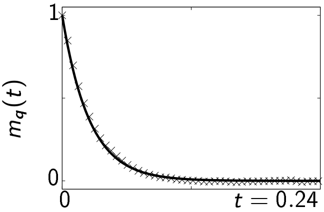
corr. function and $k_2(t)$



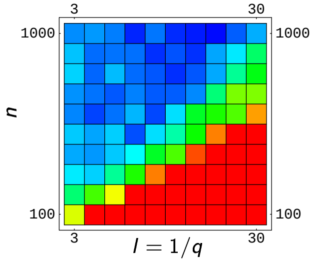
long/short wavelength



intermediate wavelength

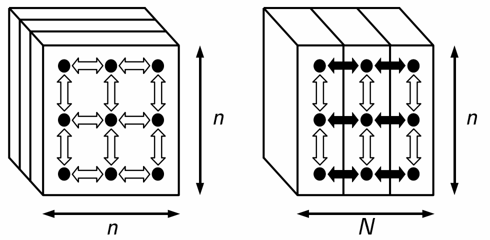


Deviation from diffusion:



There is a lenghtscale dependent "diffusive - ballistic transition"

3d-Anderson models: projection onto density waves

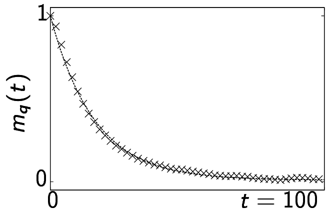


$$\hat{H}=\sum_{\mathbf{r}}\epsilon(\mathbf{r})\,\hat{a}^\dagger(\mathbf{r})\,\hat{a}(\mathbf{r})+\alpha\sum_{\mathrm{NN}}\hat{a}^\dagger(\mathbf{r})\,\hat{a}(\mathbf{r}')+\mathrm{h.c.}$$

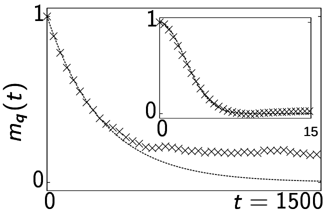
$\epsilon(\mathbf{r})$: Gaussian random numbers, σ $\Rightarrow$

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

intermediate wavelength



long/short wavelength



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

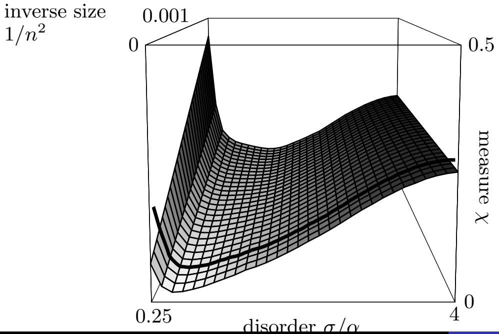
The diffusive wavelength regime appears to be rather small.

Influence of higher order terms in the projection expansion

$\lambda^2 K_q^2(t) \approx (q\lambda)^2 k^2(t)$ and $k^2(t)$ may be evaluated straightforward

$K^4(t)$ cannot be evaluated straightforward but we think we found a valid feasible estimation, which scales as $\lambda^4 K_q^4(t) \approx (q\lambda)^4 k^4(t)$ as long its influence is "small"

(This only holds for interactions having "van Hove structure" which is the case for all models considered here)

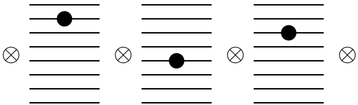


$\sqrt{1/\chi}$: range of diffusive wavelengths in between ballistic (short) and localized (long) wavelength.

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

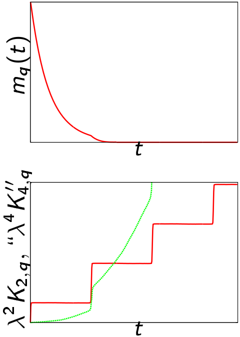
"many particle" modular quantum system:

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

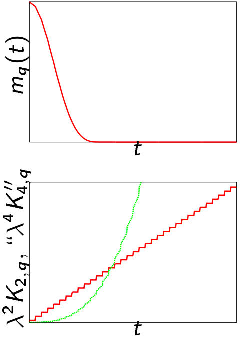


consider transport of local energy:

intermediate wavelength:

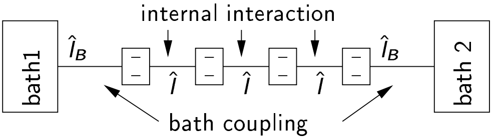


long wavelength:

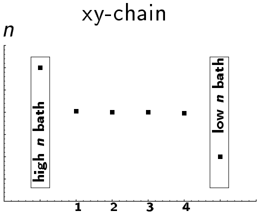


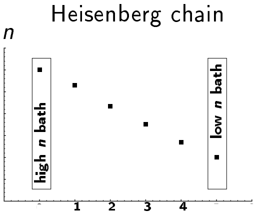
This indicates a lenghtscale dependent "diff.-ball.-transition" in a (strongly) interacting, 1-d, quantum chaotic system

Modeling of coupled reservoirs:



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

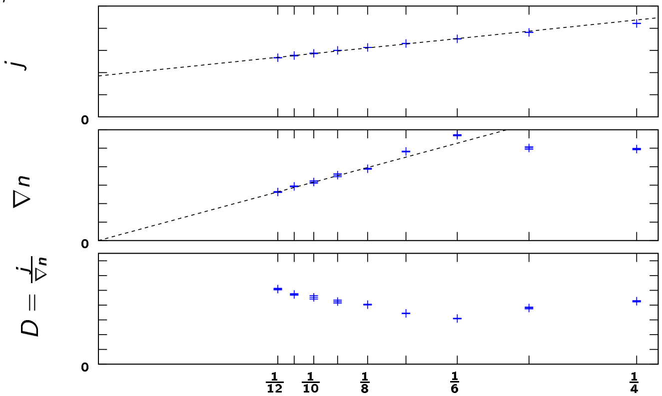




- find some $\mathcal{L}$ that adequately models the reservoirs
- find the null-space ($\hat{\rho}_0$) of an non-Hermitian matrix of dimension d^2
- compute $j = \mathrm{Tr}\{\hat{\rho}_0 \hat{j}\}$ and $\nabla n = \mathrm{Tr}\{\hat{\rho}_0 \nabla \hat{n}\}$ to construct $D = j/\nabla n$

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!