# Non-Markovian Quantum Dynamics of Open Systems: Foundations and Perspectives

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**QCCC Workshop, Aschau, October 2007**

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- Quantum Markov processes
- Non-Markovian dynamics:
  Correlated projection superoperators
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# Quantum Markov processes

$$
\begin{array}{ccc}
\rho(0) = \rho_S(0) \otimes \rho_E & \xrightarrow{\text{unitary evolution}} & \rho(t) = U_t\left[\rho_S(0) \otimes \rho_E\right] U_t^\dagger \\
\mathrm{tr}_E \downarrow & & \downarrow \mathrm{tr}_E \\
\rho_S(0) & \xrightarrow{\text{dynamical map}} & \rho_S(t) = \Phi_t \rho_S(0)
\end{array}
$$

**Quantum dynamical map $\Phi_t$:**

$$
\rho_S(0) \longrightarrow \rho_S(t) = \Phi_t \rho_S(0) = \mathrm{tr}_E \left\{ U_t\left[\rho_S(0) \otimes \rho_E\right] U_t^\dagger \right\}
$$

**superoperator, quantum operation, quantum channel**

**CPT map**

# Quantum Markov processes

**Markov condition: Separation of time scales**

$$\tau_E \ll \tau_R$$

$\Longrightarrow$ **dynamical semigroup:**

$$\Phi_{t+s} = \Phi_t \cdot \Phi_s \Longrightarrow \Phi_t = e^{\mathcal{L}t}$$

$\Longrightarrow$ **Markovian master equation in Lindblad form:**

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}\rho_S(t)$$

$$\mathcal{L}\rho_S = -i\left[H_S, \rho_S\right] + \sum_\lambda \left( R_\lambda \rho_S R_\lambda^\dagger - \frac{1}{2}\left\{ R_\lambda^\dagger R_\lambda, \rho_S \right\} \right)$$

# Non-Markovian dynamics

## Features of non-Markovian dynamics:

- **Environmental correlations do not decay rapidly:**
  **Markov condition $\tau_E \ll \tau_R$ violated**
- **Higher-order correlation functions are important, strong memory effects**
- **Finite revival times (finite reservoirs)**
- **Initial correlations/non-factorizing initial states:**
  **No dynamical map $\Phi_t$**

**No master equation with Lindblad structure:**

$$\frac{d}{dt}\rho_S(t) \neq \mathcal{L}(t)\rho_S(t)$$

# Projection operator techniques

**Projection superoperator:**

**total state** $\rho(t)$ $\Longrightarrow$ **relevant part** $\mathcal{P}\rho(t)$

$$\mathcal{P}\rho(t) = \mathrm{tr}_E\{\rho(t)\} \otimes \rho_E = \rho_S \otimes \rho_E$$

$\Longrightarrow$ **Nakajima-Zwanzig (NZ) equation:**

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt_1 K(t,t_1)\mathcal{P}\rho(t_1)$$

$K(t,t_1) =$ **memory kernel**

**time integration over system's history**

# Time-convolutionless master equation

**Eliminating the memory kernel:**

$$\rho_S(t) = \Phi_t \rho_S(0) \quad \text{and} \quad \frac{d}{dt}\rho_S(t) = \dot{\Phi}_t \rho_S(0)$$

$\Longrightarrow$ **time-local master equation (TCL):**

$$\frac{d}{dt}\rho_S(t) = \left(\dot{\Phi}_t \Phi_t^{-1}\right)\rho_S(t) \equiv \mathcal{K}(t)\rho_S(t)$$

**Expansion of the TCL generator (ordered cumulants):**

$$\mathcal{K}(t) = \sum_{n=1}^{\infty} \alpha^n \mathcal{K}_n(t)$$

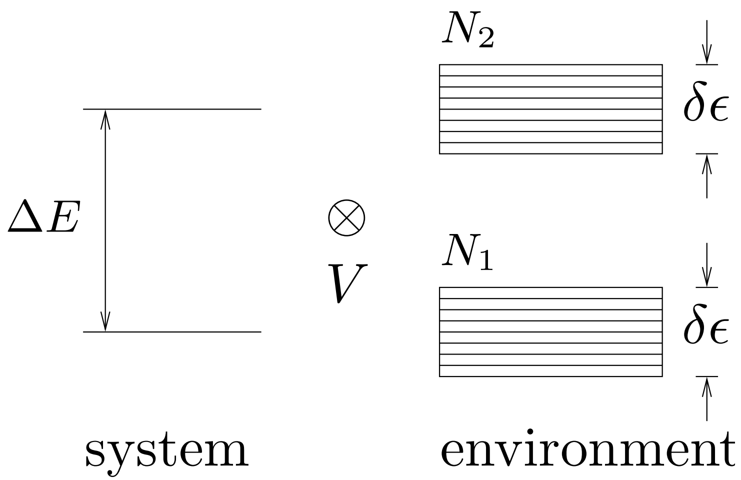
# Structured reservoirs

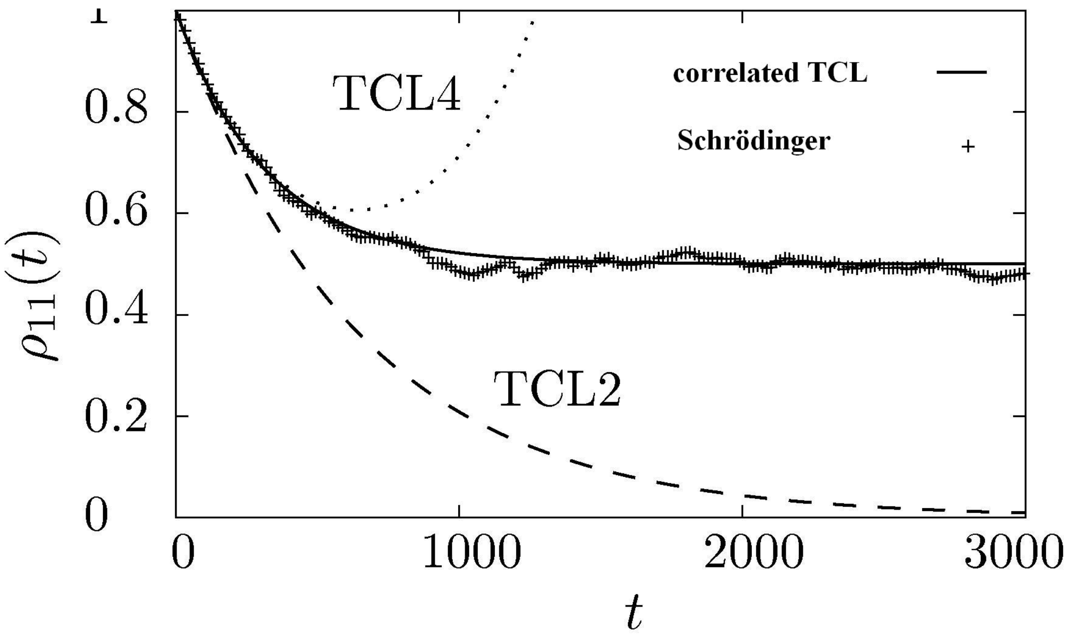
**Example:** **Interaction with finite reservoir**

$$H = H_S + H_E + V$$

$$\gamma/\delta\epsilon = 3 \cdot 10^{-3}$$

**Markov condition satisfied**




**H. P. B., J. Gemmer and M. Michel, Phys. Rev. E 73, 016139 (2006)**

# Correlated projection operators

**Standard projection:**

$$\mathcal{P}\rho = (\mathrm{tr}_E \rho) \otimes \rho_E = \text{uncorrelated tensor product state}$$

**Projections onto correlated states:**

**1. $\mathcal{P}$ is a linear, positive and trace-preserving projection:**

$$\rho \mapsto \mathcal{P}\rho \quad \text{linear}$$

$$\rho \geq 0 \Longrightarrow \mathcal{P}\rho \geq 0, \quad \mathrm{tr}\{\mathcal{P}\rho\} = \mathrm{tr}\rho$$

$$\mathcal{P}^2 = \mathcal{P}$$

**2. $\mathcal{P}$ acts as a quantum channel on environment:**

$$\mathcal{P} = I_S \otimes \Lambda$$

$$\Lambda = \text{CPT map}$$

# Correlated projection operators

## Important physical implications:

- $\mathcal{P}$ maps product states to product states:

$$\mathcal{P}(A \otimes B) = A \otimes \Lambda B$$

- $\mathcal{P}$ maps separable states to separable states:

$$\rho_{\mathrm{sep}} = \sum_i p_i \rho_S^i \otimes \rho_E^i$$

$$\mathcal{P}\rho_{\mathrm{sep}} = \text{separable}$$

- Projection completely determines reduced density matrix:

$$\rho_S \equiv \mathrm{tr}_E \rho = \mathrm{tr}_E \{\mathcal{P}\rho\}$$

# Representation theorem

$$\mathcal{P}\rho = \sum_i \mathrm{tr}_E\{A_i\rho\} \otimes B_i = \sum_i \rho_i \otimes B_i$$

$\{A_i\}, \{B_i\} =$ **sets of linear independent observables**

## Hilbert-Schmidt orthogonal:

$$\mathrm{tr}_E\{B_i A_j\} = \delta_{ij}$$

## Normalization:

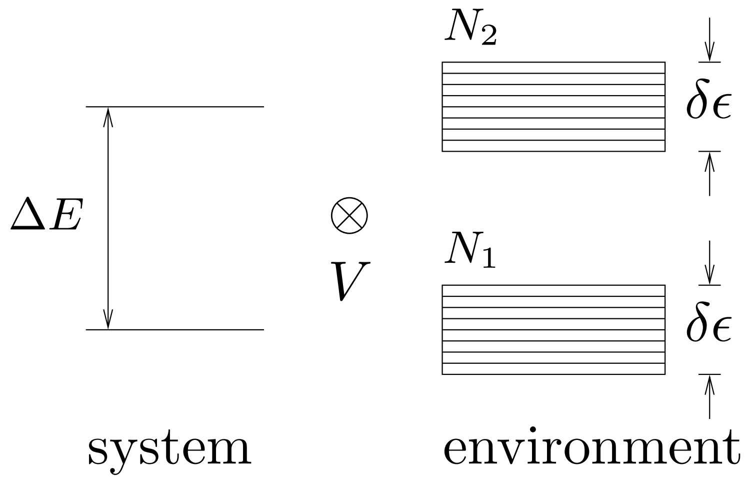
$$\sum_i (\mathrm{tr}_E B_i) A_i = I_E$$

## Positivity:

$$\sum_i A_i^T \otimes B_i \geq 0$$

**H. P. B., Phys. Rev. A 75, 022103 (2007)**

# Structured reservoir



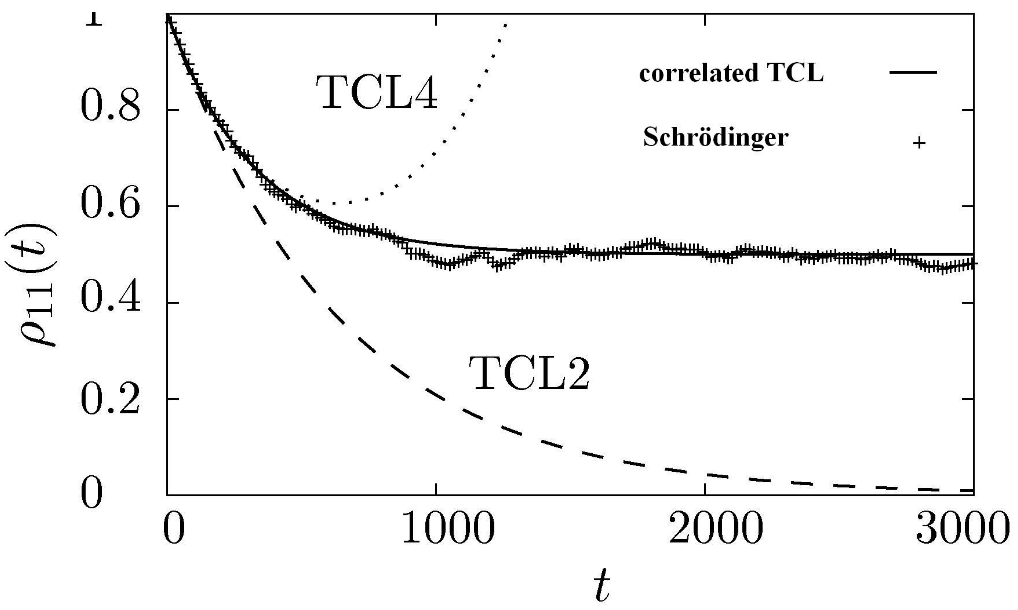

$$\mathcal{P}\rho = \rho_1 \otimes \frac{1}{N_1}\Pi_1 + \rho_2 \otimes \frac{1}{N_2}\Pi_2$$

$$\frac{d}{dt}\rho_1 = \gamma_1 \sigma_+ \rho_2 \sigma_- - \frac{\gamma_2}{2}\{\sigma_+\sigma_-, \rho_1\}$$
$$\frac{d}{dt}\rho_2 = \gamma_2 \sigma_- \rho_1 \sigma_+ - \frac{\gamma_1}{2}\{\sigma_-\sigma_+, \rho_2\}$$

$$\rho_S(t) = \rho_1(t) + \rho_2(t)$$

# Structured reservoir

$$\frac{\gamma}{\delta\epsilon} = 3 \cdot 10^{-3}$$




$$\frac{d}{dt}\rho_{11}(t) = -(\gamma_1 + \gamma_2)\rho_{11}(t) + \gamma_1\rho_{11}(0) + \gamma_2\langle 1|\rho_2(0)|1\rangle + \gamma_1\langle 0|\rho_2(0)|0\rangle$$

- **Not in Lindblad-Form, no semigroup, but CPT map**
- **Highly non-Markovian: System never forgets initial data**
- **Initial correlations $\Longrightarrow$ no quantum dynamical map**

# Generalization of Lindblad equation

## Correlated projection superoperator:

$$\mathcal{P}\rho(t) = \sum_{i=1}^{n} \rho_i(t) \otimes B_i$$

## Dynamical transformation:

$$\{\rho_i(0)\} \stackrel{V_t}{\Longrightarrow} \{\rho_i(t)\}$$

$$\Downarrow \qquad\qquad\qquad \Downarrow$$

$$\rho_S(0) = \sum_i \rho_i(0) \qquad\qquad \rho_S(t) = \sum_i \rho_i(t)$$

**no dynamical map on reduced state space**

# Generalization of Lindblad equation

**Representation in extended state space $\mathcal{H}_S \otimes \mathbb{C}^n$:**

$$\varrho(t) = \sum_i \rho_i(t) \otimes |i\rangle\langle i| = \begin{pmatrix} \rho_1(t) & 0 & \cdots & 0 \\ 0 & \rho_2(t) & \cdots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \cdots & \rho_n(t) \end{pmatrix}$$

**Embedding into Lindblad dynamics on extended state space:**

$$\varrho(t) = e^{\mathcal{L}t}\varrho(0)$$

$\Longrightarrow$ **Generalization of Lindblad equation:**

$$\frac{d}{dt}\rho_i = -i\left[H^i, \rho_i\right] + \sum_{j\lambda}\left(R_\lambda^{ij}\rho_j R_\lambda^{ij\dagger} - \frac{1}{2}\left\{R_\lambda^{ji\dagger}R_\lambda^{ji}, \rho_i\right\}\right)$$

H. P. B., Phys. Rev. A 75, 022103 (2007)

# Correlated projection operators

**Conserved quantity:**

$$[H, C] = 0$$

**Expectation values invariant under $\mathcal{P}$:**

$$\langle C \rangle \equiv \mathrm{tr}\{C\rho\} = \mathrm{tr}\{C\mathcal{P}\rho\} \qquad \Longleftrightarrow \qquad \mathcal{P}^{\dagger}C = C$$

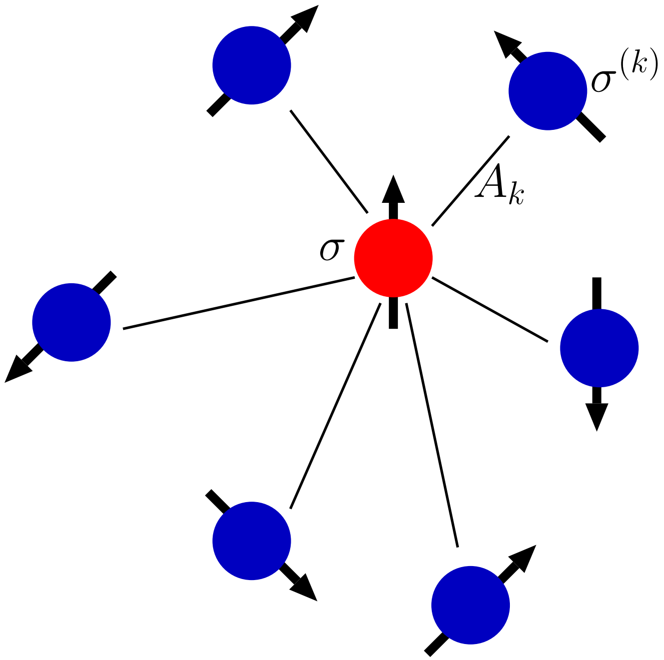
$\Longrightarrow$ **Master equation respects conservation law:**

$$\frac{d}{dt}\mathrm{tr}\{C\mathcal{P}\rho(t)\} = 0$$

**Example:**

$$C = \sigma_{+}\sigma_{-} + \Pi_2$$

# Hyperfine interaction




$$H = \frac{\omega_0}{2}\sigma_3 + \sum_{k=1}^{N} A_k \vec{\sigma} \cdot \vec{\sigma}^{(k)}$$

**spin star**

## Conserved quantity: 3-component of total spin

$$J_3 = \frac{1}{2}\sigma_3 + \frac{1}{2}\sum_k \sigma_3^{(k)} \qquad \Longrightarrow \qquad [H, J_3] = 0$$

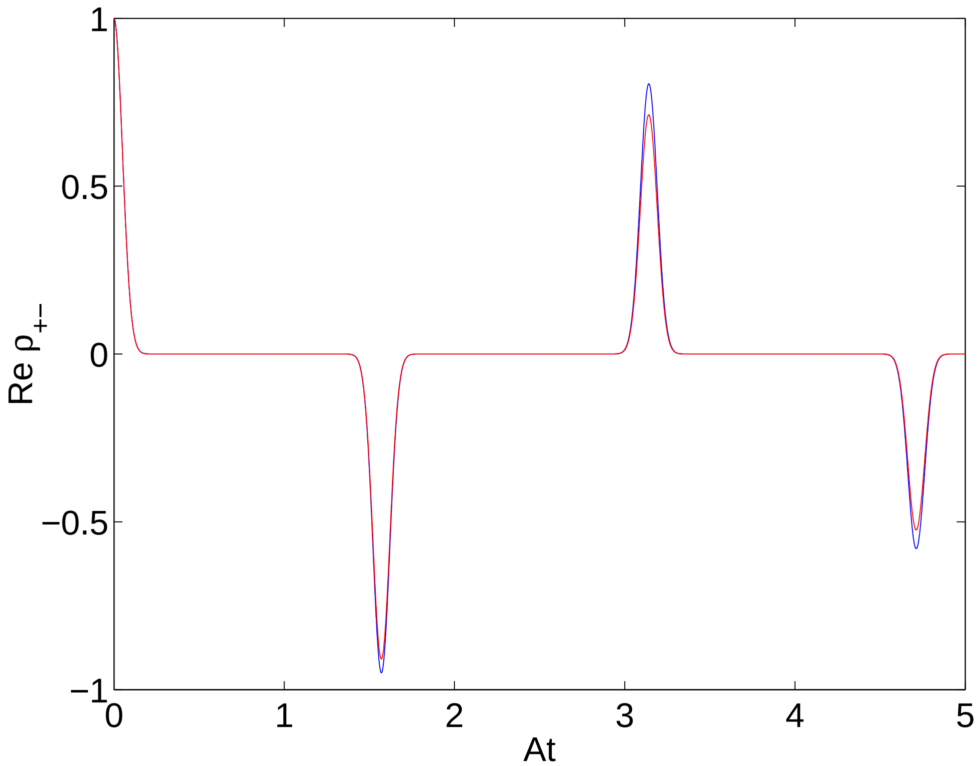

**H. P. B. and F. Petruccione, Phys. Rev. E 76, 016701 (2007)**

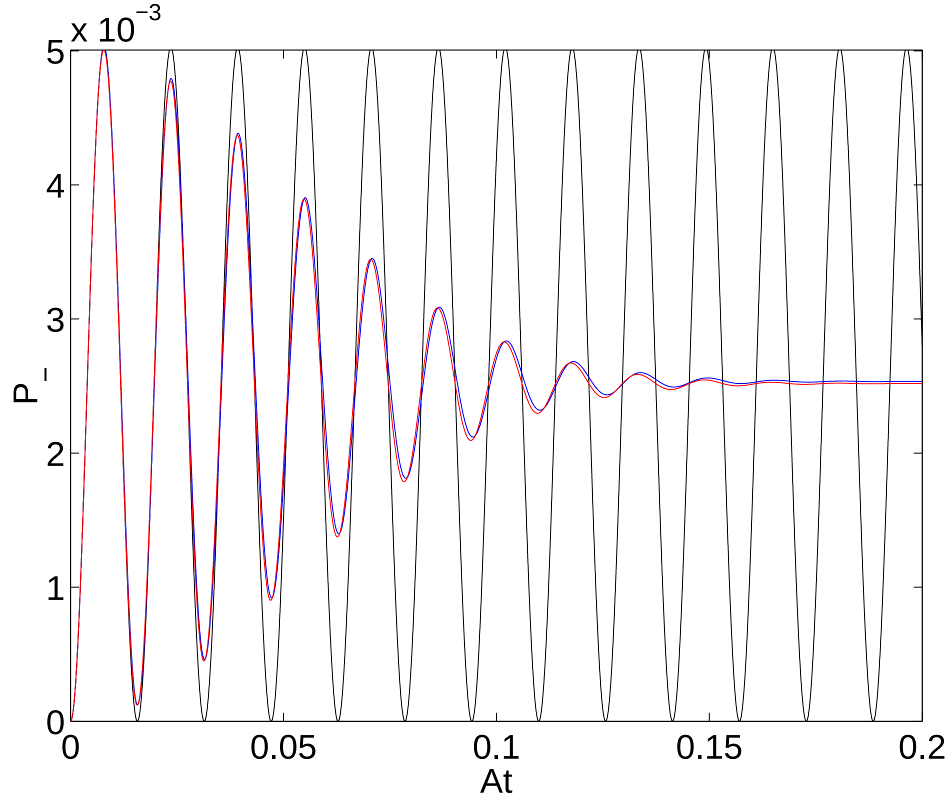
**H. P. B., D. Burgarth and F. Petruccione, Phys. Rev. B 70, 045323 (2004)**

# Hyperfine interaction

$\Longrightarrow$ **Construct projection that leaves invariant $J_3$: $\mathcal{P}^\dagger J_3 = J_3$**

$$\mathcal{P}\rho = \sum_m \mathrm{tr}_E\{\Pi_m \rho\} \otimes \frac{1}{N_m}\Pi_m \equiv \sum_m \rho_m \otimes \frac{1}{N_m}\Pi_m$$



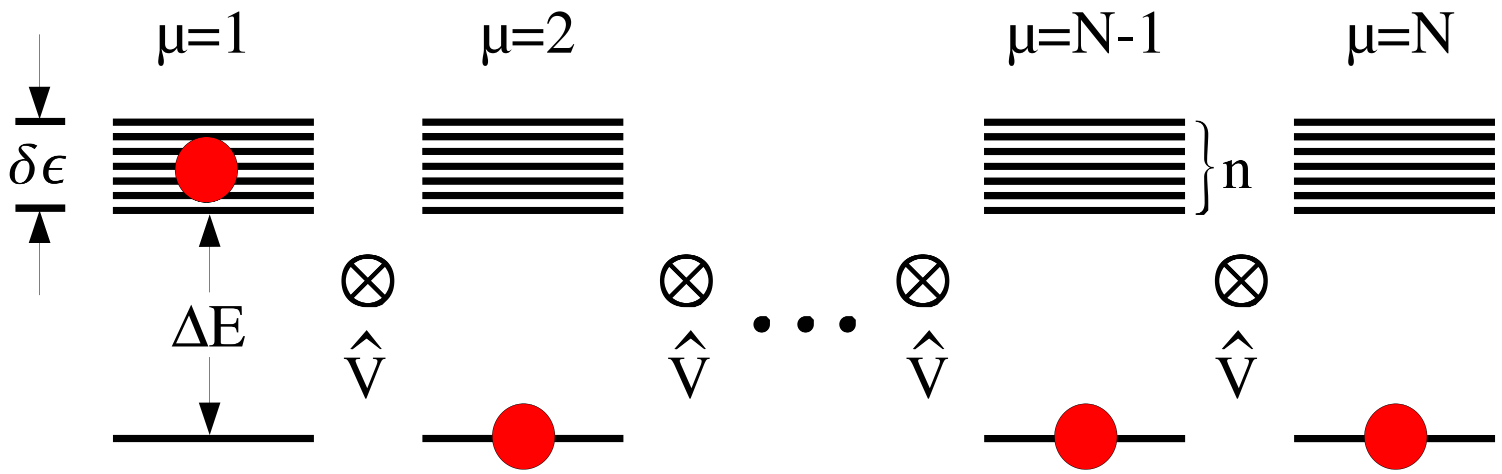




**J. Fischer and H. P. B., Phys. Rev. A, to appear (2007)**

# Transport in modular quantum systems

$$\boldsymbol{H_0} = \sum_{\mu} \sum_{i} \epsilon_i \, |\mu, i\rangle \langle \mu, i|$$

$$\hat{\boldsymbol{V}} = \sum_{\mu} \sum_{i,j} c_{ij} \, |\mu, i\rangle \langle \mu + 1, i| + \text{h.c.}$$

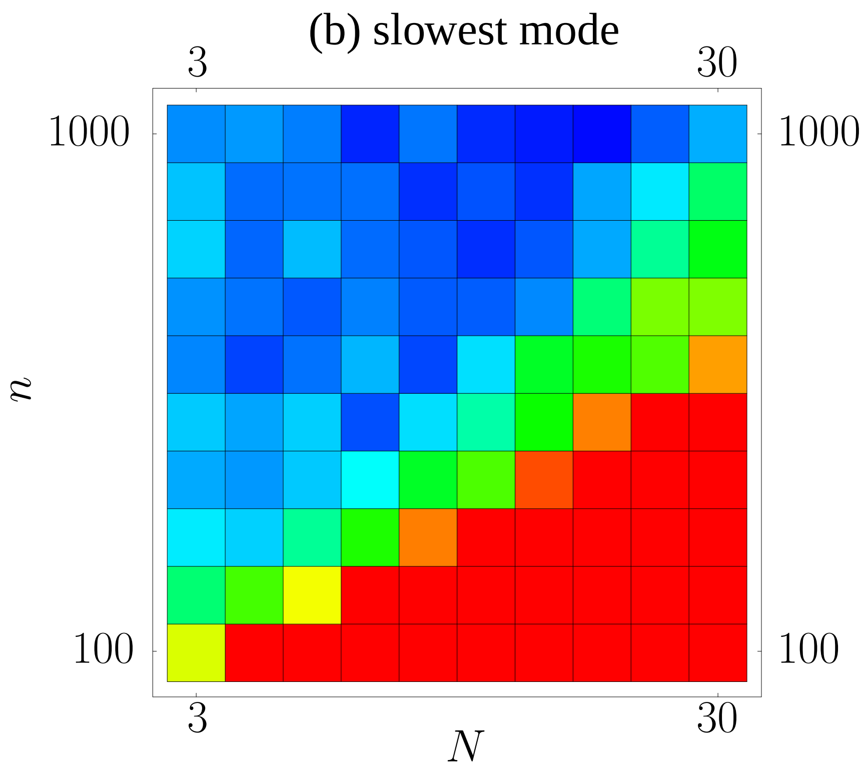


# Projection onto Fourier modes

$$\mathcal{P}\rho = \sum_{q} \mathrm{tr}\left[\Phi_q \rho\right] \Phi_q = \sum_{q} F_q(t) \Phi_q \qquad \Phi_q = C_q \sum_{\mu} \cos(q\mu) \Pi_\mu$$

**Diffusive transport:** $F_q(t) \propto \exp[-at]$

**Ballistic transport:** $F_q(t) \propto \exp[-bt^2]$




R. Steinigeweg, H. P. B. and J. Gemmer, Phys. Rev. Lett. 99, 150601 (2007)

# Perspectives

**Projection onto entangled quantum states?**

$$\mathcal{P}\rho = \sum_i \mathrm{tr}_E\{A_i\rho\} \otimes B_i = \text{entangled state}$$

- **Methods of quantum information theory**
- **Entanglement criteria and measures**
- **Dynamical significance of entanglement**

# Perspectives

## Combination of TCL and NZ?

**TCL master equation:**

$$\frac{d}{dt}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t)$$

$\Longrightarrow$ **exact on average for transport model**

**NZ master equation:**

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt_1 \mathcal{K}(t,t_1)\mathcal{P}\rho(t_1)$$

$\Longrightarrow$ **exact for populations of spin star**

# Monte Carlo methods

- **Stochastic representation of Lindblad dynamics:**

$$\rho_S(t) = \mathbb{E}\big(|\psi(t)\rangle\langle\psi(t)|\big)$$
$$|\psi(t)\rangle = \text{stochastic process in Hilbert space}$$

- **TCL master equation:**

$$\rho_S(t) = \mathbb{E}\big(|\psi_1(t)\rangle\langle\psi_2(t)|\big)$$

- **Generalized Lindblad equation:**

$$\rho_S(t) = \sum_i \mathbb{E}\big(|\psi_i(t)\rangle\langle\psi_i(t)|\big)$$

# Exact Monte Carlo methods?

**First ansatz:**

$$\rho(t) = \mathbb{E}\Big(|\Phi(t)\rangle\langle\Phi(t)|\Big)$$
$$|\Phi(t)\rangle = \psi(t) \otimes \chi(t) = \text{stochastic product state}$$

**Does not work because of:**

$$\rho(t) = \sum_{\lambda} p_{\lambda} |\Phi_{\lambda}\rangle\langle\Phi_{\lambda}| = \text{separable state}$$

$\Longrightarrow$ **no representation of entangled states possible**

# Exact Monte Carlo methods?

**Use a pair of stochastic states:**

$$|\Phi_i(t)\rangle = |\psi_i(t)\rangle \otimes |\chi_i(t)\rangle \qquad i = 1, 2$$

- **Any state can be represented as:**

$$\rho(t) = \mathbb{E}\Big(|\Phi_1(t)\rangle\langle\Phi_2(t)|\Big)$$

- **'Bra' and 'Ket' evolve independently**
- **Reproduces the exakte non-Markovian dynamics**
- **Problem: exponential growth of fluctuations**

H. P. B., Phys. Rev. A 69, 022115 (2004); Phys. Rev. A 70, 012106 (2004)

# Summary

- **Correlated projection operator techniques**
  - Highly non-Markovian dynamics (infinite memory times)
  - Correlations in initial state
  - Non-perturbative
  - Generalization of Lindblad theory
  - Stochastic representations
- **Further investigations:**
  - Projections onto entangled quantum states
  - Time-dependent generators
  - Combination of TCL and NZ: New expansion techniques