Perturbative Master Equations for Open Quantum Systems and Decoherence

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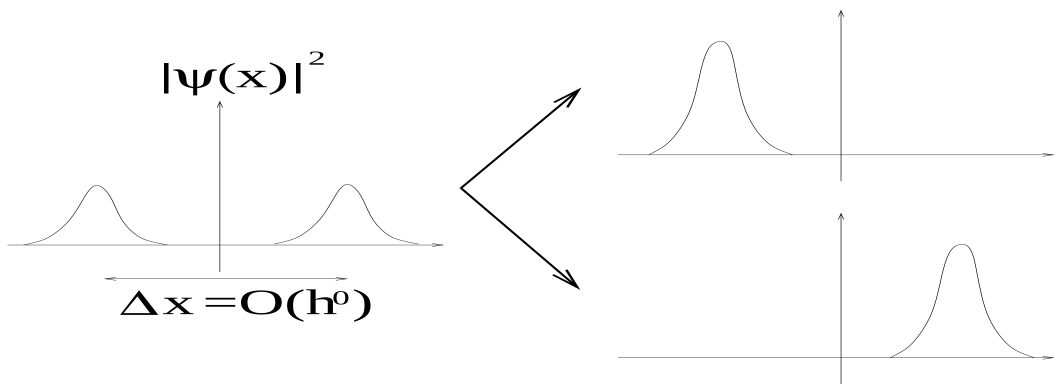
Outlines

- Motivation: decoherence vs dissipation
- Perturbative master equations
- Master equation for a Brownian quantum particle moving on a lattice $\mathbb{Z}^d$
- Perspectives, open problems

What is decoherence ?

Linear superposition of quantum states $|\psi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$

$\longrightarrow$ statistical mixture of the same states.



INTERFERENCES
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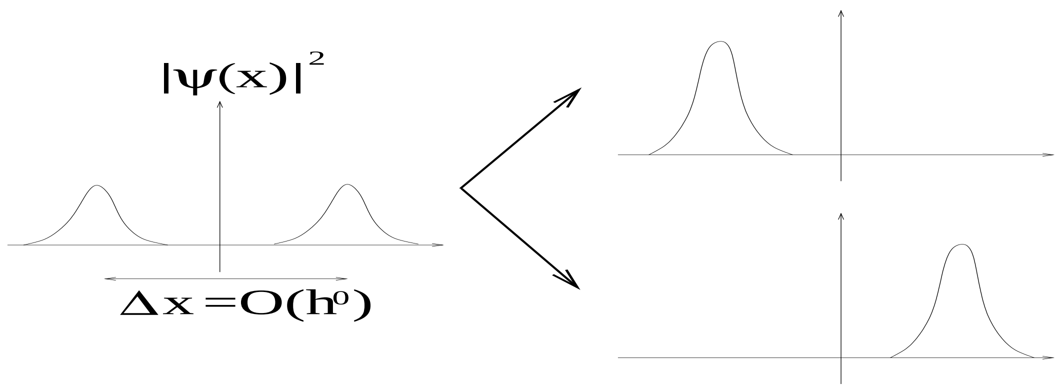

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Dynamical process characterized by a **decoherence time** t_{dec} (depending on φ_1, φ_2)

= *time scale for the quantum-to-classical transition.*

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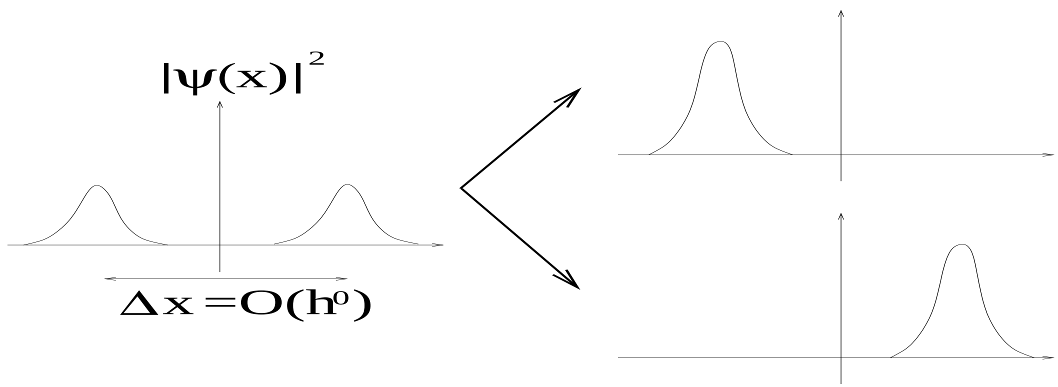

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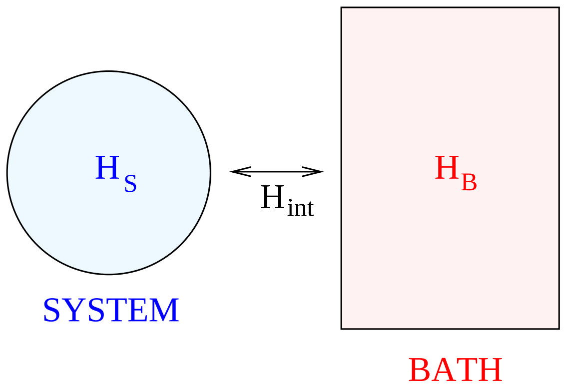
Cannot result from unitary dynamics $\Rightarrow$ irreversibility.

Open Quantum Systems

- A quantum system is coupled to its environment (e.g. a thermal bath).



Initially, $\rho = \underbrace{|\psi\rangle\langle\psi|}_{\text{SYSTEM}} \otimes \underbrace{\rho_B}_{\text{BATH}}$

with $|\psi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle$.

Reduced density matrix of the system at time $t \geq 0$:

$$\rho_S(t) = \mathrm{tr}_B(e^{-itH}\rho\, e^{itH}) \quad , \quad H = H_S + \lambda H_{\mathrm{int}} + H_B$$

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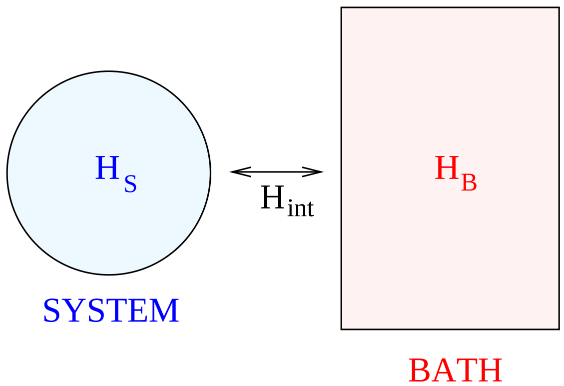

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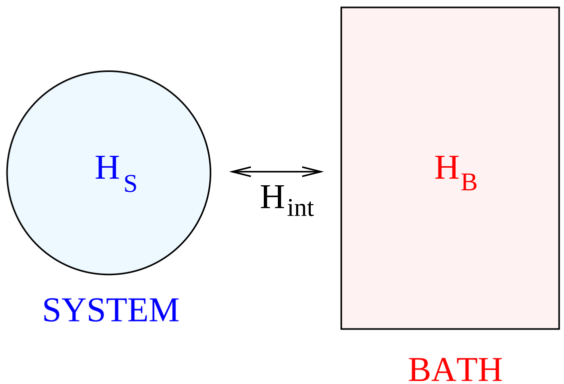

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$$\Rightarrow \quad \rho_S(t) = \sum_{i,j} c_i\overline{c_j}|\varphi_i\rangle\langle\varphi_j| \underbrace{\mathrm{tr}_B\left(e^{-it(s_iB+H_B)}\,\rho_B\, e^{it(s_jB+H_B)}\right)}_{\text{decoherence factor } K_t(s_i,s_j)}$$

Environment-induced decoherence

Decoherence factor

$$K_t(s_i, s_j) = \mathrm{tr}_B(e^{-it(H_B+s_iB)}\rho_B\, e^{it(H_B+s_jB)})$$

Quantum CLT *[Goderis & Vets '90, Verbeure, DS]. Assume:*

(i) *bath initially in a Gibbs state at temperature* $\beta^{-1} > 0$

(ii) $B = N^{-\frac{1}{2}} \sum_{\nu=1}^{N} B_\nu$, B_ν *acts on* $\mathcal{H}_\nu$, B *acts on* $\otimes_{n=1}^N \mathcal{H}_\nu$

(iii) *no long-range correlations:* $\mathrm{tr}_B(B_\mu B_\nu \rho_B) \to 0$ *faster than* $1/|\mu - \nu|$ *as* $|\mu - \nu| \to \infty$.

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(iii) *no long-range correlations:* $\mathrm{tr}_B(B_\mu B_\nu \rho_B) \to 0$ *faster than* $1/|\mu-\nu|$ *as* $|\mu-\nu| \to \infty$. *Then for fixed times* t,

$$\lim_{N\to\infty} |K_t(s_i, s_j)| = \exp\left\{-\frac{(s_i-s_j)^2}{2} \underbrace{\int_0^t \mathrm{d}\tau \int_0^t \mathrm{d}\tau' h_B(\tau-\tau')}_{\geq 0}\right\}$$

If $s_i \neq s_j$, $\lim_{N\to\infty} |K_t(s_i, s_j)|$ **decreases to** 0 **as** $t \to \infty$.

$h_B(\tau)$ = *2-point bath correlator* $= \mathrm{tr}_B(e^{-i\tau H_B} B\, e^{i\tau H_B}\, B\, \rho_B)$.

Decoherence vs relaxation times

Main question: how is the decoherence time

$$t_{\mathrm{dec}}(\varphi_i, \varphi_j) = \min\{t_d \geq 0; |K_t(s_i \neq s_j)| \leq e^{-1} \; \forall \; t \geq t_d\}$$

related to the time scale t_{rel} of the relaxation to the steady state (if any)?

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In our model: $t_{\rm dec}$ *decreases with the distance* $|s_i - s_j|$ *between the components of the initial superposition.*

$\hookrightarrow t_{\rm dec} \ll t_{\rm rel}$ for “macroscopic superpositions” ($|s_1 - s_2| \gg \hbar$)

$\hookrightarrow t_{\rm dec}$ can be smaller than the bath correlation time ($\Rightarrow$ Markov approximation is not justified!).

LARGE TIME ASYMPTOTICS OF THE DYNAMICS (given e.g. by spectral properties of the Liouvillian or Lindblad generator) PROVIDES LITTLE INFORMATION ABOUT DECOHERENCE

(see however [Merkli, Sigal & Berman, ’07]).

Limitations of the model

1. The system's proper dynamics (generated by H_S) has not been taken into account:

   OK only if the time scale of this dynamics is much larger than t_{dec} (as is the case e.g. in quantum dots, in nanocircuits with Josephson junctions, and for ideal quantum measurements).

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   OK only if the time scale of this dynamics is much larger than $t_{\rm dec}$ (as is the case e.g. in quantum dots, in nanocircuits with Josephson junctions, and for ideal quantum measurements).

2. For more realistic interaction Hamiltonians $H_{\rm int}$:

   - A saturation of $t_{\rm dec}$ as $|s_1 - s_2|$ increases occurs for translation-invariant Hamiltonians

     [Gallis & Fleming '90, Hornberger & Sipe '03]

   - In specific physical situations such as in a Bose Josephson junction, $t_{\rm dec}$ is independent of $|s_1 - s_2|$

     [Ferrini, DS, Minguzzi & Hekking '09]

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- Perturbative master equations

Lindblad master equation

$$\frac{d\rho_S}{dt} = -i[H_S, \rho_S(t)] + \frac{\gamma}{2}\Big([L, \rho_S(t)L^*] + \mathrm{h.c.}\Big)$$

$\hookrightarrow$ can be derived from the unitary (system+bath) dynamics with Hamiltonians

(a) $H = H_S + H_B + \lambda S \otimes B$ for $\lambda \to 0$ and $t = \tau\lambda^{-2} \to \infty$, τ fixed *(Weak Coupling Limit)*

(b) $H = \lambda^2 H_S + H_B + \lambda S \otimes B$, same limits *(Singular Coupling)*

However, the W.C. limit in (a) is *not well-defined* if H_S has continuous spectrum. *Many physical processes* (spin relaxation in NMR, decoherence in solid state devices,...) are *not correctly described by the Lindblad equation!*

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Reason: W.C.L. contains a local time averaging (= rotating wave approximation), valid for $t_{\text{rel}}^{-1} \ll$ spectral gap ΔE between neighboring eigenvalues of H_S.

Born-Markov approximation

$$H = H_S + H_B + \lambda S \otimes B$$

Bath correlation function: $h_B(\tau) = \mathrm{tr}_B(e^{-i\tau H_B} B e^{i\tau H_B} B\, \rho_B)$.

Davies's 1$^{\mathrm{st}}$ theorem *[Math. Ann. '76]*: *Assume* $\|S\| < \infty$ *and* $\int d\tau\, \tau\, h_B(\tau) < \infty$. *Then, for a fixed* $\tau > 0$,

$$\sup_{0 \le t \le \lambda^{-2}\tau} \Big\| \underbrace{\rho_S(t)}_{\text{exact}} - \underbrace{e^{(-i[H_S,\cdot]+\lambda^2 K_D)t}\big(\rho_S(0)\big)}_{\text{approximate semigroup}} \Big\|_1 = \mathcal{O}(\lambda^2)$$

with $K_D(\rho_S) = \int_{-\infty}^{0} \mathrm{d}\tau \left\{ h_B(t) \left[e^{-i\tau H_S} S e^{i\tau H_S}, \rho_S\, S \right] + \mathrm{h.c.} \right\}$.

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Remarks: 1. K_D is not unique: another generator K_R leads to a similar approximation of $\rho_S(t)$.

2. K_D is not a Lindblad generator $\Rightarrow$ the approximate semigroup is not positivity conserving!

3. $2^{\rm nd}$ order perturbation but error of order λ^2...

Redfield Master Equation

[Redfield '57]

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Then for any $0 \leq t \leq \lambda^{-2}\tau$,

$$\Big\| \underbrace{\rho_S(t)}_{\text{exact}} - \underbrace{\widehat{\rho}_S(t)}_{\text{approximate}} \Big\|_1 = \mathcal{O}(\lambda^4 t + \lambda^6 t^2)$$

where $\widehat{\rho}_S(t)$ *is the solution of the time-dependent Redfield eq.*

$$\frac{\mathrm{d}\widehat{\rho}_S}{\mathrm{d}t} = -i[H_S, \widehat{\rho}_S(t)] + \lambda^2 \int_{-t}^{0} \mathrm{d}\tau \left\{ h_B(\tau) \left[S, \widehat{\rho}_S(t) e^{i\tau H_S} S e^{-i\tau H_S} \right] + \mathrm{h.c.} \right\}$$

Moreover, if $[H_S, S] = 0$ *then* $\widehat{\rho}_S(t) = \rho_S(t)$ *for all* λ *and* t.

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Remarks: 1. Going to higher orders in perturbation theory does not help for large times $t \ge t_{\mathrm{rel}} \propto \lambda^{-2}$, but leads to smaller errors for $t \ll t_{\mathrm{rel}}$.

2. As in Davies's theorem, the master eq. is not unique $\longrightarrow$ *which is the best one?*

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Model

- Consider a free particle on the lattice $\mathbb{Z}^d$ with Hamiltonian $H_S = -\lambda^2 \Delta$ on $\ell^2(\mathbb{Z}^d)$ (Δ = discrete Laplacian).

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  The mass of the particle diverges like λ^{-2} with the coupling constant.
- The particle is coupled to a phonon bath initially in a Gibbs state ρ_{ph} with $\beta^{-1} > 0$ and $h_{\text{ph}} : \varphi(q) \mapsto |q|\varphi(q)$.
  The coupling Hamiltonian is translation-invariant,

$$
\begin{aligned}
H_{\text{int}} &= \int_{\mathbb{T}^d} d^d q \, g(q) \, e^{iqX} \otimes (a_q^\dagger + a_{-q}) \\
&= \sum_{x \in \mathbb{Z}^d} |x\rangle\langle x| \otimes \underbrace{\left(a^*(g_x) + a(g_x)\right)}_{\text{creation/annihilation op.}} \;, \; g_x(q) = g(q)\, e^{iqx}
\end{aligned}
$$

$\{|x\rangle\}_{x\in\mathbb{Z}^d}$ = canonical basis of $\ell^2(\mathbb{Z}^d)$, X = position op.,

$g(q) = g(|q|)$ form factor (analytic in a strip around $\mathbb{R}$-axis).

Main result

Let $\rho_S(t) = \operatorname*{tr}_B\Big(e^{-it[-\lambda^2\Delta+\Gamma_s(h_{\rm ph})+\lambda H_{\rm int},\,\cdot\,]}\big(\rho_S(0)\otimes\rho_{\rm ph}\big)\Big)$.

Space-dependent phonon correlation function

$$h_{x-y}(t-s) = \operatorname*{tr}_B\Big(\big(a^*(e^{ith_{\rm ph}}g_x) + a(e^{ith_{\rm ph}}g_x)\big)\big(a^*(g_y)+a(g_y)\big)\rho_{\rm ph}\Big)$$

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$$\lim_{n\to\infty} \frac{1}{n} \int_0^\infty dt \sup_{x\in\mathbb{Z}^d} |h_x(t)| e^{-\kappa|x|/n} < \infty \text{ for some } \kappa > 0.$$

Then for any $\tau > 0$ *and any trace-class op.* $\rho_S(0)$ *on* $\ell^2(\mathbb{Z}^d)$,

$$\Big\| \underbrace{\rho_S(t)}_{\text{exact}} - \underbrace{e^{\tau\mathcal{L}}\big(\rho_S(0)\big)}_{\text{approx. semigroup}} \Big\|_1 \to 0 \quad \text{as } \lambda \to 0, \text{ with}$$

$$\mathcal{L}(\rho_S) = i\big[\Delta, \rho_S\big] + \int dt \sum_{x,y\in\mathbb{Z}^d} h_{y-x}(t) |x\rangle\langle x| \rho_S |y\rangle\langle y| - \int dt\, h_0(t)\, \rho_S$$

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Remarks: 1. Hypothesis fulfilled for $d\geq 2$, but not for $d=1$.

2. $\mathcal{L}$ is a Lindblad generator.

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Perspectives & Open problems

- *Convolutionless master eq.* for a system-bath coupling Hamiltonian $H_{\rm int} = \lambda_{\|} S_{\|} \otimes B_{\|} + \lambda_{\perp} S_{\perp} \otimes B_{\perp}$ with $[H_S, S_{\|}] = 0$, *non-perturbative in* $\lambda_{\|}$ and $2^{\rm nd}$ order in $\lambda_{\perp}$.
- *Does the time-dependent Redfield equation and/or its higher-order versions conserve positivity? What are the asymptotic states?*
- *Translation-invariant Hamiltonians:* Gallis & Fleming's model of a Brownian particle coupled to light particles, W.C.L. for an electron in a random potential coupled to a phonon bath (Anderson localization regime).
- *Decoherence vs entanglement losses.*
- *Decoherence in Bose-Einstein condensates* & link with experiments.