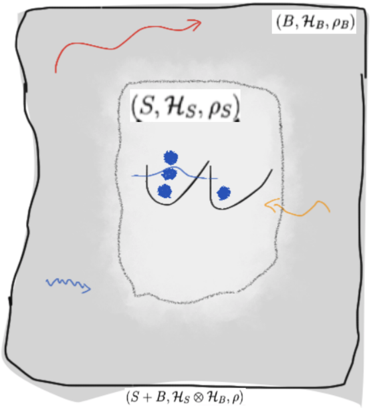
Approaching open quantum systems

July 4, 2018

Lindblad theorem

Open System

Master equation (ME): equation of motion for the density operator of an **open** system ρ_S.



Open System

An **open** system is a quantum system $\mathcal{S}$ which interacts with another system $\mathcal{B}$, called the **environment**

$$\mathbf{H} = \mathbf{H}_S \otimes \mathrm{Id}_B + \mathrm{Id}_S \otimes \mathbf{H}_B + \mathbf{H}_I \tag{1.1}$$

The interaction is described by $\mathbf{H}_I$. The full system dynamics is described by unitary evolution (von Neumann equation)

$$\frac{d\rho(t)}{dt} = \mathcal{L}\rho = -i[\mathbf{H}, \rho(t)] \tag{1.2}$$

Can be written in terms of Liouville super-operator

$$\rho(t) = \exp(\mathcal{L}t)\rho \tag{1.3}$$

Dynamical Map

Obtaining state of the open system by tracing out the environment after unitary evolution of the full system

$$\rho_S(t) = \mathrm{Tr}_B \left(\mathbf{U}(t)(\rho_S(0) \otimes \rho_B)\mathbf{U}^\dagger(t) \right) = \mathcal{V}(t)\rho_S(0) \qquad (1.4)$$

is described by dynamical map $\mathcal{V}(t)$. Here, at $t = 0$ the state of the total system is assumed to be in an **uncorrelated product state**.

The dynamical map can be described explicitly as a generalized quantum measurement process (see Chapter 3, The theory of open quantum system).

Define the family of quantum dynamical maps $\{\mathcal{V}(t) | t \geq 0\}$, with the identity $\mathcal{V}(0) = \mathrm{Id}_S$, to describe the dynamics. **Neglect memory effects** - if bath correlation functions decay much fast than typical system time scales

$$\mathcal{V}(t_1)\mathcal{V}(t_2) = \mathcal{V}(t_1 + t_2) \tag{1.5}$$

Quantum dynamical Semigroup

Quantum dynamical Semigroup

$$\mathcal{V}(t_1)\mathcal{V}(t_2) = \mathcal{V}(t_1 + t_2) \tag{1.6}$$

- No Memory-effects, e.g. $\mathcal{V}(\Delta t)\mathcal{V}(\Delta t) = \mathcal{V}(2\Delta t)\forall\Delta t$
- Physical approximations? What can QDSG implement?
- How to generate a QDS?

$$\rho_S(t) = \mathcal{V}(t)\rho_S(0) \stackrel{?}{=} \exp(\mathcal{L}t)\rho(0) \tag{1.7}$$

The most general form of the generator $\mathcal{L}$ of a quantum dynamical semigroup $\{\mathcal{V}(t)\}$ is given by the Lindblad master equation

$$\mathcal{L}\rho_S = -i[\mathbf{H}_u, \rho_S] + \sum_{l=1}^{N^2-1} \gamma_k \underbrace{\left(\mathbf{F}_k \rho \mathbf{F}_k^\dagger - \frac{1}{2}\{\mathbf{F}_k^\dagger \mathbf{F}_k, \rho_S\}\right)}_{=\mathcal{D}[\mathbf{F}_k] \text{ "dissipator"}} \tag{1.8}$$

Microscopic derivations

Summary

- Quantum dynamical Semigroups describe dynamics under certain approximations
- What are those Approximations?
- Approximations are not "unique"
- Microscopic derivations give insights

Start from full unitary evolutions, trace out environment, perform appropriate physical approximations, obtains Lindblad form $\rightarrow$ Quantum Dynamical Semigroup.

Integrate von Neumann equation

$$\rho(t) = \rho(0) - i \int_0^t ds [H_I(s), \rho(s)] \tag{2.1}$$

re-insert total integral form into von Neumann equation and trace out the environment

$$\frac{d\rho_S(t)}{dt} = -i \mathrm{Tr}_B [H_I(t), \rho(t)] = - \int_0^t ds \mathrm{Tr}_B [H_I(t), [H_I(s), \rho(s)]] \tag{2.2}$$

Born-Approximation / Weak Coupling: Environment is unaffected by the interaction with the system

$$\rho(t) \approx \rho_S(t) \otimes \rho_B \tag{2.3}$$

Markov-Approximation $\rho_S(s) \to \rho_S(t)$ "Only the current system state matters"

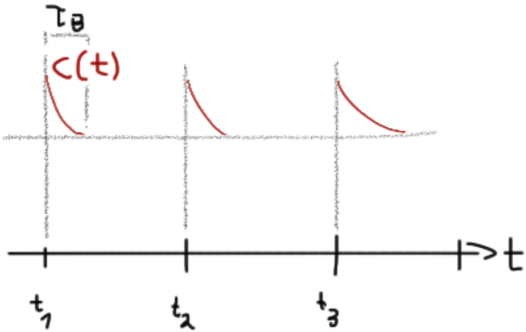
Redfield equation

$$\frac{d\rho_S(t)}{dt} = -\int_0^t ds \mathrm{Tr}_B[H_I(t), [H_I(s), \rho_S(t) \otimes \rho_B]] \tag{2.4}$$

Still depends on system preparation. Substitute $t - s$ and remove upper limit of integration.

Markovian Master Equation

$$\frac{d\rho_S(t)}{dt} = -\int_0^\infty ds \mathrm{Tr}_B[H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]] \tag{2.5}$$



τ_B
$c(t)$
t
t_1
t_2
t_3

Interaction with an optical bath

Model for single Josephson-Junction, two site Bose-Hubbard Model in photon field

$$\mathbf{H} = -J(\mathbf{a}_1^\dagger \mathbf{a}_2 \otimes e^{ia} + \mathbf{a}_2^\dagger \mathbf{a}_1 \otimes e^{-ia}) + \mathbf{H}_U \otimes \mathrm{Id}_B + \mathrm{Id}_S \otimes \mathbf{H}_B \in (\mathcal{H}_S \otimes \mathcal{H}_B) \tag{3.1}$$

where the phase a is the integrated vector potential **A** over the distance r_0 between the two sites

$$a = \frac{2\pi}{\Phi_0} \int_{r_0} dx \mathbf{A} = \frac{r_0 2\pi}{\Phi_0} \sum_{k\lambda} w(k) e_\lambda(k) \left(\mathbf{a}_\lambda(k) + \mathbf{a}_\lambda^\dagger(k) \right) \tag{3.2}$$

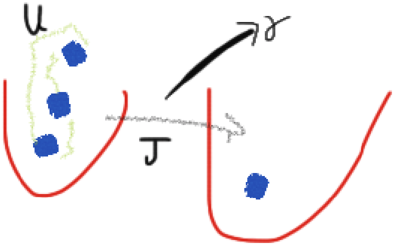


Figure: SJJ in interaction with photon field

The photon field contains polarized λ modes at frequency ω_k

$$\mathbf{H}_B = \sum_{\lambda k} \omega_k \mathbf{a}_\lambda^\dagger(k)\mathbf{a}_\lambda(k) \in \mathcal{H}_B \tag{3.3}$$

Bosons $[\mathbf{a}_\lambda(k), \mathbf{a}_{\lambda'}^\dagger(k')] = \delta_{\lambda\lambda'}\delta_{kk'}$

Polarization

$$\begin{aligned} k e_\lambda(k) &= 0 \\ e_\lambda(k) e_{\lambda'}(k) &= \delta_{\lambda\lambda'} \\ \sum_\lambda e_\lambda^i(k) e_\lambda^j(k) &= \delta_{ij} - \frac{k_j k_i}{|k|^2} \end{aligned} \tag{3.4}$$

Consider first order interaction

$$\begin{aligned}\mathbf{H} &\approx -J(\mathbf{a}_1^\dagger \mathbf{a}_2 \otimes (\mathrm{Id}_B + i\mathbf{a}) + \mathbf{a}_2^\dagger \mathbf{a}_1 \otimes (\mathrm{Id}_B - i\mathbf{a})) + \mathbf{H}_U \otimes \mathrm{Id}_B + \mathrm{Id}_S \otimes \mathbf{H}_B \\ &= \underbrace{\mathbf{j}_0 \otimes \mathbf{a}}_{H_I} + (\mathbf{H}_T^0 + \mathbf{H}_U) \otimes \mathrm{Id}_B + \mathrm{Id}_S \otimes \mathbf{H}_B\end{aligned} \tag{3.5}$$

The system Hamiltonian generates the unitary evolution while the non unitary part is described by the interaction

$$\mathbf{H}_I = \mathbf{j}_0 \otimes \mathbf{a} = \mathbf{j}_0 \otimes \frac{r_0 2\pi}{\Phi_0} \sum_{\lambda k} w(k) e_\lambda(k) (\mathbf{a}_\lambda(k) + \mathbf{a}_\lambda^\dagger(k)) \tag{3.6}$$

Tracing out the commutators of MME

$$\frac{\rho_S}{dt} = -\int ds \mathrm{Tr}_B[H_I(t), [H_I(t-s), \rho_S \otimes \rho_B]] \qquad (3.7)$$

leads to two-time bath correlation function as a prefactor

$$\mathrm{Tr}_B[H_I(t), [H_I(t-s), \rho_S \otimes \rho_B]] = \underbrace{\mathrm{Tr}(\mathbf{a}(t)\mathbf{a}(t-s)\rho_B)}_{=\langle \mathbf{a}(t)\mathbf{a}(t-s)\rangle_B \equiv C(s)}[\mathbf{j}_0, [\mathbf{j}_0, \rho_S] \qquad (3.8)$$

$(a(t) = e^{iH_B t} a e^{-iH_B t})$

Assumption Stationary ρ_B.

Two Time Correlation / "How much coupling we can expect at a certain energy $\hbar\omega_k$".

$$
\begin{aligned}
X(s) = \langle \mathbf{A}(s)\mathbf{A} \rangle_B = \sum_{kk'} \sum_{\lambda\lambda'} w(k) w(k') e_\lambda(k) e'_\lambda(k') \Bigg(& \\
& \left\langle \underbrace{e^{iH_B s} \mathbf{a}_\lambda(k) e^{-iH_B s}}_{e^{-i\omega_k s}\mathbf{a}_\lambda(k)} \mathbf{a}_{\lambda'}(k') \right\rangle \\
& + \left\langle e^{iH_B s} \mathbf{a}_\lambda(k) e^{-iH_B s} \mathbf{a}^\dagger_{\lambda'}(k') \right\rangle \\
& + \left\langle e^{iH_B s} \mathbf{a}^\dagger_\lambda(k) e^{-iH_B s} \mathbf{a}_{\lambda'}(k') \right\rangle \\
& + \left\langle e^{iH_B s} \mathbf{a}^\dagger_\lambda(k) e^{-iH_B s} \mathbf{a}^\dagger_{\lambda'}(k') \right\rangle \Bigg)
\end{aligned}
\tag{3.9}
$$

e.g. $\left\langle \mathbf{a}^\dagger_\lambda(k) \mathbf{a}_{\lambda'}(k') \right\rangle = \delta_{\lambda\lambda'} \delta_{kk'} N(\omega_k)$ Bose-Einstein-Statistics $\rightarrow$ "the bath has a temperature"

At this point the master equation is

$$\frac{\rho_S}{dt} = -i[\mathbf{H}_S^0, \rho_S] - \int ds X(s)\Big([\mathbf{j_0}(t), \mathbf{j_0}(t-s)\rho_S] + h.c\Big) \quad (3.10)$$

How to evaluate $\mathbf{j}_0(t) = \exp(i\mathbf{H}_S t)\mathbf{j}_0 \exp(-i\mathbf{H}_S t)$?
Baker-Hausdorff: no luck

The following operators rotate in the interaction picture

$$\mathbf{j}_0(\Omega) = \sum_{ab} \delta(\omega_{ba} - \Omega) \left| a \right\rangle \underbrace{\left\langle a \right| \mathbf{j}_0 \left| b \right\rangle}_{=j_{ab}} \left\langle b \right| \tag{3.11}$$

meaning $\mathbf{j}_0(\Omega, t) = e^{-i\Omega t}\mathbf{j}_0(\Omega)$ and $\mathbf{j}_0^\dagger(\Omega, t) = e^{+i\Omega t}\mathbf{j}_0^\dagger(\Omega)$.

$\mathbf{j}_0(\Omega)$ Lets current flow thru the junction such that the system emits $\hbar\Omega$ to the bath

$$
\begin{aligned}
\mathbf{H}_S \mathbf{j}_0(\Omega) \left| c \right\rangle &= \mathbf{H}_S \sum_{ab} \delta(\omega_{ba} - \Omega) \left| a \right\rangle \left\langle a \right| \mathbf{j}_0 \left| b \right\rangle \delta_{bc} \\
&= \sum_{a} \delta(\omega_{ca} - \Omega) \epsilon_a \left| a \right\rangle \left\langle a \right| \mathbf{j}_0 \left| c \right\rangle \\
&= (\epsilon_c - \Omega) \mathbf{j}_0(\Omega) \left| c \right\rangle
\end{aligned}
\tag{3.12}
$$

Junction is an antenna of length r_0.

With

$$\sum_{\Omega} \mathbf{j}_0(\Omega) = \mathbf{j}_0 \tag{3.13}$$

the the commutators in the MME get

$$[\mathbf{j}_0(t), \mathbf{j}_0(t-s)\rho_S] = \sum_{\Omega\Omega'} e^{i\Omega' s} e^{i(\Omega-\Omega')t} [\mathbf{j}_0^\dagger(\Omega), \mathbf{j}_0(\Omega')\rho_S] \tag{3.14}$$

The dissipative part gets

$$\sum_{\Omega\Omega'} e^{+i(\Omega-\Omega')t} \Big(\int_0^\infty ds X(s) e^{i\Omega' s}\Big) \left([\mathbf{j}_0^\dagger(\Omega), \mathbf{j}_0(\Omega')\rho_S] + h.c \right) \tag{3.15}$$

- Still not Lindblad form. (In general, Markovian Master equation is not guaranteed to define a Quantum dynamical Semigroup).
- Secular approximation: Average fast rotating terms in the equation (Rotating Wave approximation)

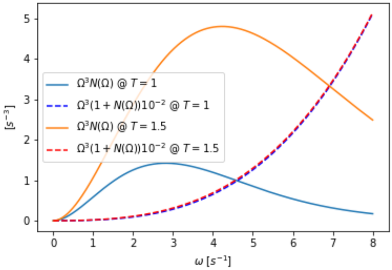
$$\sum_{\Omega}\Big(\int_0^{\infty} dsX(s)e^{i\Omega s}\Big)\left([\mathbf{j}_0^{\dagger}(\Omega), \mathbf{j}_0(\Omega)\rho_S] + h.c\right) \tag{3.16}$$

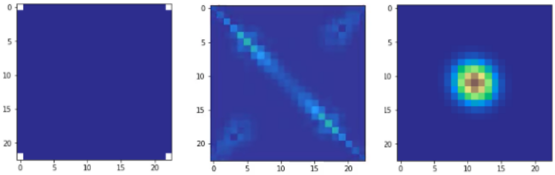
Obtain Lindblad Form (99%)

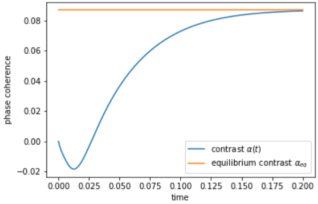
$$-2\sum_{\Omega}\Big(\int_0^{\infty} dsX(s)e^{i\Omega s}\Big)\left(\mathbf{j}_0(\Omega)\rho_S\mathbf{j}_0^{\dagger}(\Omega) - \frac{1}{2}\{\mathbf{j}_0^{\dagger}(\Omega)\mathbf{j}_0(\Omega), \rho_S\}\right) \tag{3.17}$$

Optical Lindblad master equation, coupling via. current

$$\dot{\rho_S} = -i[\mathbf{H}_S^0 + \mathbf{H}_{\mathrm{LS}}, \rho_S] + \overbrace{\gamma \sum_{\Omega>0} \Omega^3(1+N(\Omega))\mathcal{D}[\mathbf{j}_0(\Omega)]\rho_S}^{\text{dissipation}} + \underbrace{\gamma \sum_{\Omega>0} \Omega^3 N(\Omega)\mathcal{D}[\mathbf{j}_0^\dagger(\Omega)]\rho_S}_{\text{heating}} \tag{3.18}$$




0
5
10
15
20


phase coherence
time
contrast $\alpha(t)$
equilibrium contrast α_{eq}

Summary

- **Separability**: No correlations at $t = 0$: $\rho = \rho_S(0) \otimes \rho_B(0)$.
- **Born-Approximation**: State of the bath does not change significantly due to interaction: $\rho(t) = \rho_S(t) \otimes \rho_B$.
- **Markov approximation**: Bath correlation time τ_B is much smaller then the smallest system dynamics time scale τ_S: $\tau_B \ll \tau_S$.
- **Secular approximation**: Drop elements with non secular terms having $|\omega_{ab} - \omega_{cd}| \ll 1/\tau_S$

Upcoming / Outlook

Non-Markovian Dynamics

Dynamics beyond Markovian Master equation, e.g. non-pertubative approach?

- What about Low temperatures and strong coupling?
- What assumptions must be dropped in order to describe the latter?
- Initial state entangled? Initial Sweeping? $\rho_0 = \exp(-\beta(H_B + H_S + H_I))$
- Quantum Dynamical Semigroup assumption of disentangled initial state may not be appropriate.
- Many non-Markovian equations have a long-time behaviour that can be appoximated by Markovian equations.

Reduced hierarchical equations of motion (HEOM)

But... Next time... Thanks!

- Quantum Dynamical Semigroups and Applications [Robert Alicki Karl Lendi]
- Invitation to quantum dynamical semigroups [Robert Alicki]
- Proof Redfield equation: Quantum Theory of Open Systems [E.B. Davis]
- Yoshitaka Tanimura: Reduced hierarchical equations of motion in real and imaginary time: Correlated initial states and thermodynamic quantities
- Quantum Dissipative Systems [Ulrich Weiss]
- Master equation - Tutorial approach [S.Kryszewski, J.C.Kryskz]
- Quantum Field Theory of Many-Body Systems [Xiao-Gang Wen]