Interplay of multiple environments in open quantum systems: breakdown of common approximations

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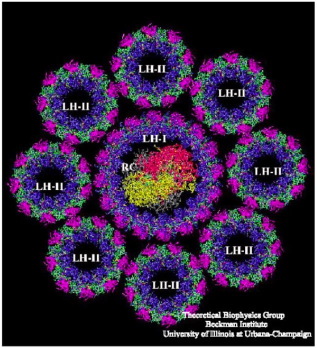
Gathering on Non-Hermitian Quantum Systems
Cuernavaca, November 4–8, 2019

Outline

1. *Non-Hermitian Hamiltonian for decay channels*
   - motivation and origin of the model
   - the energy-independent approximation
2. *Limits of validity*
   - problems for very short and long times
   - approximation is good if the relevant physics is at intermediate times
   - interplay of decay with static disorder
3. *Interplay with other baths*
   - the presence of noise or a thermal bath influences the decay properties
   - noise and decay can be modeled independently only if noise is small

Motivation



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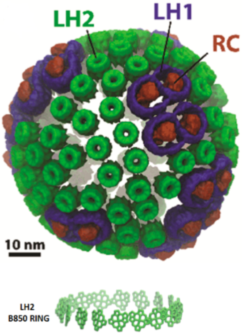
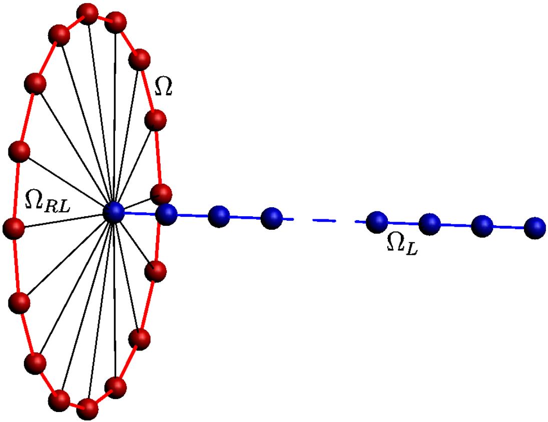


$$\textit{Reaction Center} \quad \longleftrightarrow \quad -\mathrm{i}\gamma$$
$$\textit{Chromophore Fluorescence} \quad \longleftrightarrow \quad -\mathrm{i}\gamma_{\mathrm{fl}}$$

Is it really so simple?

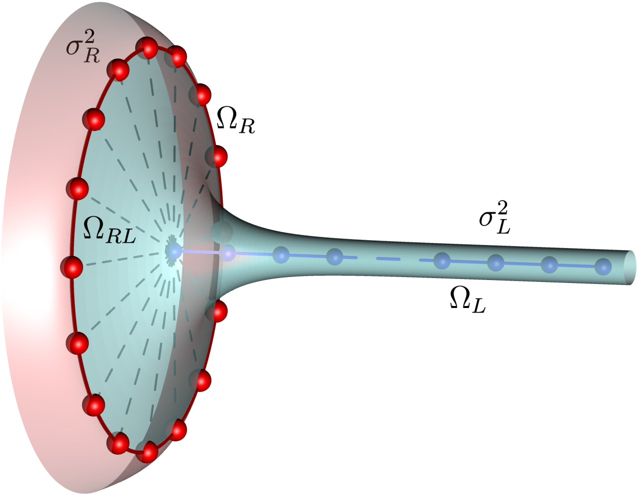
Start with a Hermitian system . . .



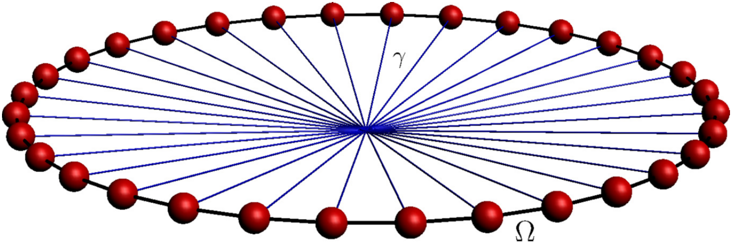
Eigenvectors of the Hamiltonian with real eigenvalues E_i evolve as

$$|\varepsilon_i(t)\rangle = e^{-\frac{i}{\hbar}E_i t}|\varepsilon_i(0)\rangle$$

. . . forget about part of it . . .



. . . focus on what is left



Eigenvectors with complex eigenvalues $E_i - \mathrm{i}\Gamma_i/2$ evolve as

$$|\varepsilon_i(t)\rangle = e^{-\frac{\mathrm{i}}{\hbar}(E_i - \mathrm{i}\Gamma_i/2)}|\varepsilon_i(0)\rangle \quad \text{with} \quad \langle\varepsilon_i(t)|\varepsilon_i(t)\rangle = e^{-\frac{\Gamma_i}{\hbar}t}$$

The effective non-Hermitian Hamiltonian

Consider two subsystems A and B and the following projectors:

$$P_A = \sum_{i=1}^{N_A} |i\rangle\langle i|, \quad P_B = \sum_{c=1}^{M} \sum_{E=1}^{N_B} |c, E\rangle\langle c, E| \,.$$

Under the orthogonality conditions $\langle i|j\rangle = \delta_{i,j}$, $\langle c, E|c', E'\rangle = \delta_{c,c'}\delta_{E-E'}$, $\langle i|c, E\rangle = 0$, we can rewrite the total Hamiltonian of the system as

$$H = H_0 + V = \begin{pmatrix} H_{AA} & 0 \\ 0 & H_{BB} \end{pmatrix} + \begin{pmatrix} 0 & H_{AB} \\ H_{BA} & 0 \end{pmatrix} ,$$

where

$$H_{AA} = P_A H P_A \,, \quad H_{AB} = P_A H P_B \,, \quad H_{BA} = P_B H P_A \,, \quad H_{BB} = P_B H P_B .$$

We can now define the unperturbed and total Green functions $G_0(x) = (x - H_0)^{-1}$ and $G(x) = (x - H)^{-1}$, related by Dyson's equation

$$G(x) = G_0(x) + G_0(x) V G(x)\,,$$

which gives rise to the following coupled equations for $G_{AA} = P_A G P_A$ and $G_{BA} = P_B G P_A$:

$$\begin{cases} G_{AA} = G^0_{AA} + G^0_{AA} H_{AB} G_{BA}\,, \\ G_{BA} = G^0_{BB} H_{BA} G_{AA}\,. \end{cases}$$

taking into account that $G^0_{BB} = (x - H_{BB})^{-1}$, we have

$$G_{AA}(x) = \frac{1}{x - H_{AA} - H_{AB} \frac{1}{x - H_{BB}} H_{BA}}\,.$$

From this expression we obtain an effective Hamiltonian, which defines the propagator over the subspace A and takes the form

$$H_{\mathrm{eff}}(x) = H_{AA} + H_{AB} \frac{1}{x - H_{BB}} H_{BA}\,.$$

The effective non-Hermitian Hamiltonian

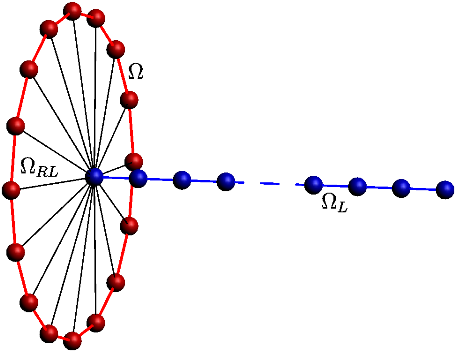
The general structure of an effective Hamiltonian describing the opening towards decay channels is then given by

$$H_{\mathrm{eff}}(x) = H_s + \Delta(x) - \mathrm{i}Q(x),$$

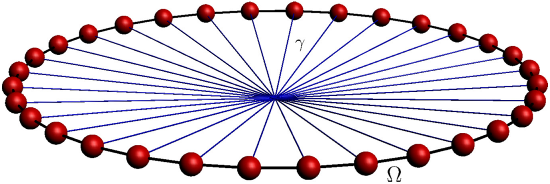
with H_s, Δ and Q real symmetric and Q positive semidefinite, with $Q_{ik} \propto \sum_c A_i^c A_k^c$, where A_i^c is the coupling amplitude between site i and the decay channel c.
The *exact propagator* for the open system is given by

$$\mathcal{U}(t,t_0) = -\frac{1}{2\pi i}\int_{-\infty}^{+\infty} \frac{\exp\left[-\frac{i}{\hbar}x(t-t_0)\right]}{x - H_{\mathrm{eff}}(x)}\, dx\,,$$

that can be turned into a conventional propagator with the *energy-independent approximation*.



Compared with $\gamma = \frac{2\Omega_{RL}^2}{\Omega_L}$



Giusteri, Mattiotti, Celardo, Phys. Rev B, 91, 094301 (2015)

The open ring model

For this system we have

$$Q_{rr'}(x) = \begin{cases} \frac{\gamma}{2}\sqrt{1 - \frac{x^2}{4\Omega_L^2}} & \text{for } x \in [-2\Omega_L, 2\Omega_L]\,, \\ 0 & \text{otherwise,} \end{cases}$$

where we introduced the opening strength $\gamma = \frac{2\Omega_{RL}^2}{\Omega_L}$, and

$$\Delta_{rr'}(x) = \frac{\gamma}{2\pi}\mathrm{Pv}\int_{-2\Omega_L}^{2\Omega_L} \frac{\sqrt{1-(E/2\Omega_L)^2}}{x-E}\,dE\,.$$

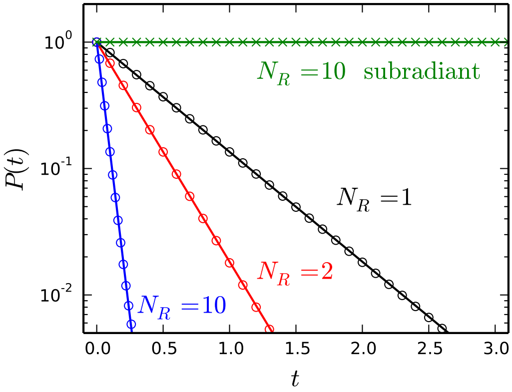
There is only one super-radiant state with

$$\Gamma_{\mathrm{sr}}(x) = \begin{cases} N_R\gamma\sqrt{1 - \frac{x^2}{4\Omega_L^2}} & \text{for } x \in [-2\Omega_L, 2\Omega_L]\,, \\ 0 & \text{otherwise,} \end{cases}$$

Energy-independent approximation

This can be obtained by setting $\Delta(x) \approx 0$ and $Q(x) \approx Q(0)$ and implies $\Gamma_{\mathrm{sr}} = N_R\gamma$. It is *exact* only if $\Omega_L = +\infty$.

The decay width is *unevenly* distributed among the eigenstates determining the presence of super- and sub-radiant eigenstates.



Agreement is lost for very short and long times

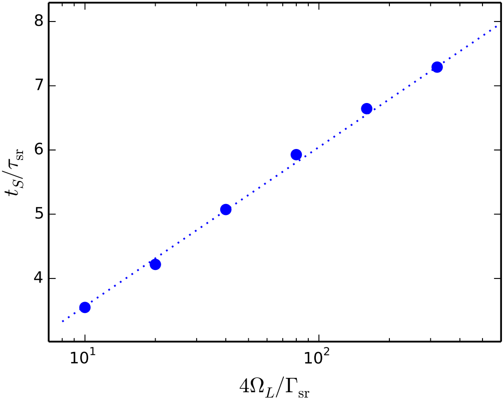
For the superradiant state, the decay of $P(t) = \langle\psi(t)|\psi(t)\rangle$ is exponential between two time-scales t_0 and t_S and we have:

$$P(t) \approx \begin{cases} 1 - \frac{N_R \Omega_{RL}^2}{\hbar^2} t^2 & \text{for } t < t_0 \,, \\ e^{-\Gamma_{\mathrm{sr}} t/\hbar} & \text{for } t_0 < t < t_S \,, \\ \mathrm{const.}/t^3 & \text{for } t > t_S \,. \end{cases}$$

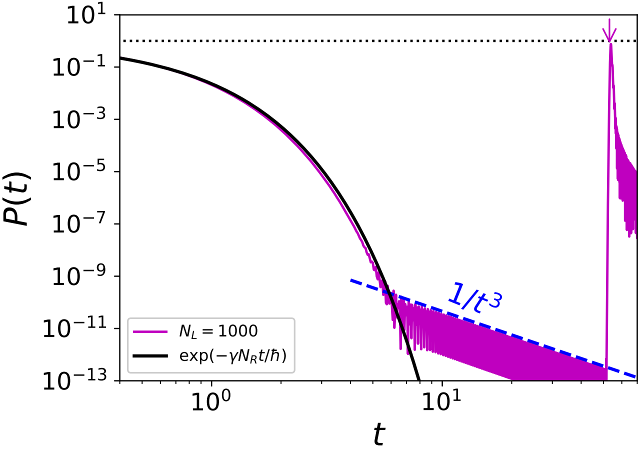
- From perturbation theory we have $t_0 = \frac{\hbar}{2\Omega_L}$

Agreement is lost for very short and long times

- From the asymptotics of the propagator we have $\frac{t_S}{\tau_{\rm sr}} \propto \ln \frac{4\Omega_L}{\Gamma_{\rm sr}}$, with $\Gamma_{\rm sr} = N_R\gamma$ and $\tau_{\rm sr} = \frac{\Gamma_{\rm sr}}{\hbar}$

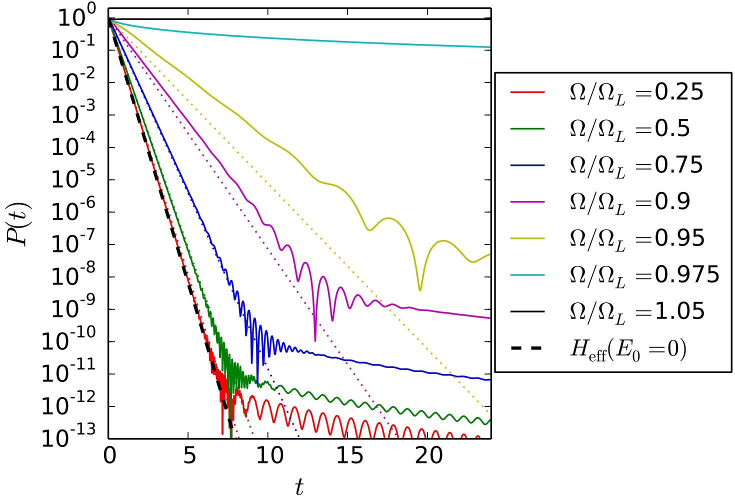


Power-law decay and reflection for long times

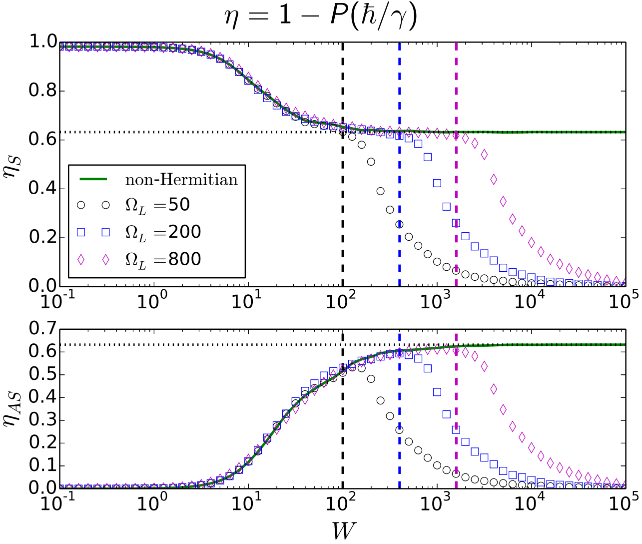


Reflection from the end of the lead (arrow) is another obvious effect

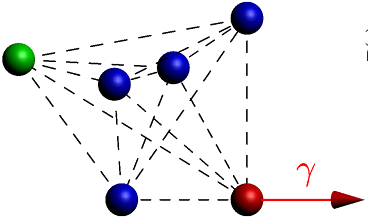
Going off-resonance

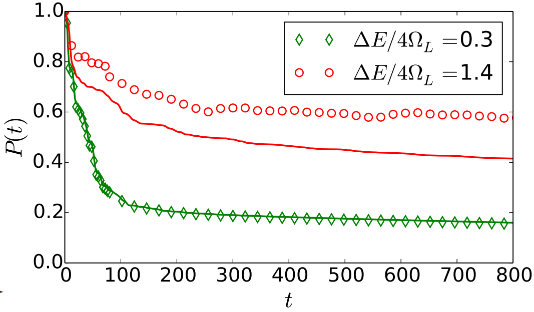


Static disorder inhibits decay: a finite-bandwidth effect



The limits are rather generic

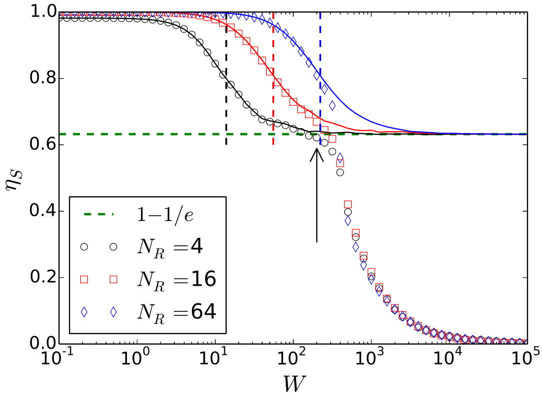




The non-Hermitian dynamics follows the full Hermitian model as long as the energy band of the system fits within that of the decay channel

Cooperative robustness to disorder

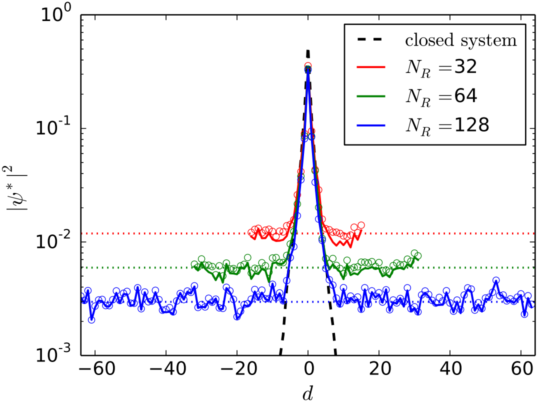
$$W_{\rm sr} = \sqrt{\frac{48\Omega^2(N_R-1)}{\sum_{q=1}^{N_R-1}\frac{1}{\left(\cos\frac{2\pi q}{N_R}-1\right)^2+\frac{N_R^2\gamma^2}{16\Omega^2}}}} \approx \sqrt{3}N_R\gamma \quad \text{for } N_R\gamma \gg 4\Omega.$$



The size N_R of the ring has been varied, keeping fixed $\Omega = 1$, $\Omega_{RL} = 10$, $\Omega_L = 100$, and $N_L = 100$.

Hybrid sub-radiant states

Probability of being on a ring site at distance d from site 1, obtained by the long-time evolution of an excitation initially localized on site 1. The wave function ψ^* is re-normalized while increasing time.



Disorder strength $W = 10$ in a regime where Anderson localization should be achieved, while Superradiance is not yet destroyed, that is $W_{\rm loc} < W < W_{\rm sr}$.

Adding a thermal bath: white noise with intensity σ_R^2

The evolution is described in terms of a Hermitian density matrix ρ.

Equations including the effect of white noise can be written as

$$\dot{\rho}_{ik} = -\frac{\mathrm{i}}{\hbar}(H\rho - \rho H^{\dagger})_{ik} - (1 - \delta_{ik})\frac{\sigma_i^2 + \sigma_k^2}{2\hbar}\rho_{ik}$$

that adds a decay of the off-diagonal terms (dephasing) to the dynamics induced by the Hamiltonian structure.

The Haken–Strobl master equation can be derived for both Hermitian and complex symmetric Hamiltonians stating from a stochastic Schrödinger equation for the single-excitation network.

Giusteri, Recrosi, Schaller, Celardo, Phys. Rev. E, 96, 012113 (2017)

Infinite temperature: stochastic Schrödinger equation

$$d\psi^\alpha = \left(-\frac{\mathrm{i}}{\hbar}H^\alpha{}_\beta - \frac{1}{2\hbar}\sum_j \sigma_j^2 \delta^\alpha{}_{\beta j}\right)\psi^\beta dt \\ - \frac{\mathrm{i}}{\sqrt{\hbar}}\sum_j \sigma_j \delta^\alpha{}_{\beta j} dW_j \psi^\beta \,.$$

The white-noise terms

$$V_j(t)^\alpha{}_\beta \equiv \sigma_j \delta^\alpha{}_{\beta j}\, dW_j(t)\,, \quad \text{for} \quad j = 1, \ldots, N\,,$$

represent the random fluctuations of the energy of each site (j) with intensity given by $\sigma_j^2 dt$.

Average master equation at infinite temperature

By taking the expected value of the QSME, recalling that terms proportional to dW_j have zero mean, we obtain the equation for ρ:

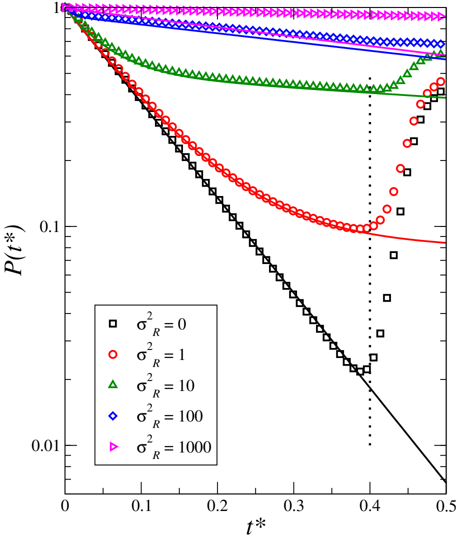
$$
\begin{aligned}
d\langle(\psi^\gamma\psi^*_\lambda)\rangle = &-\frac{\mathrm{i}}{\hbar}\Big\langle {H^\gamma}_\beta\psi^\beta\psi^*_\lambda - \psi^\gamma\psi^*_\beta {H^{*\beta}}_\lambda\Big\rangle dt \\
&- \frac{1}{2\hbar}\Big\langle \sum_j \sigma_j^2\Big({\delta^\beta}_{\lambda j}\psi^\gamma\psi^*_\beta + {\delta^\gamma}_{\beta j}\psi^\beta\psi^*_\lambda\Big)\Big\rangle dt \\
&+ \frac{1}{2\hbar}\Big\langle \sum_j \sigma_j^2\Big({\delta^\gamma}_{\tau j}{\delta^\rho}_{\lambda j}\psi^\tau\psi^*_\rho + {\delta^\gamma}_{\tau j}{\delta^\rho}_{\lambda j}\psi^{*\tau}\psi_\rho\Big)\Big\rangle dt\,.
\end{aligned}
$$

This can be rearranged in the more familiar Haken–Strobl form

$$
\frac{d{\rho^j}_k}{dt} = -\frac{\mathrm{i}}{\hbar}\Big(H\rho - \rho H^\dagger\Big)^j{}_k - (1-{\delta^j}_k)\left(\frac{\sigma_j^2+\sigma_k^2}{2\hbar}\right){\rho^j}_k\,.
$$

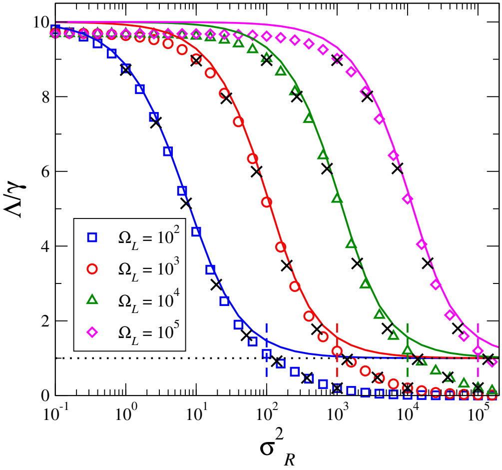
Note that no Hermiticity assumption was made on H.

Hindered super-radiant decay



$$t^* = \frac{\gamma t}{\hbar}$$

Finite bandwidth effect with white noise



The noise intensity at which the reduced model departs from the full system dynamics scales again with Ω_L

Breakdown of the additive approximation

The Haken–Strobl equation for the non-Hermitian effective Hamiltonian corresponds to an approximation in which the effects of the probability-absorbing lead and of the thermal bath *act on the system in an additive way*.

$$\dot{\rho}_{ik} = -\frac{\mathrm{i}}{\hbar}[H_R, \rho]_{ik} - \frac{\mathrm{i}}{\hbar}\{Q, \rho\}_{ik} - (1 - \delta_{ik})\frac{\sigma_i^2 + \sigma_k^2}{2\hbar}\rho_{ik}$$

Using the appropriate super-operator formalism, we show that *eliminating the degrees of freedom of the lead and of the thermal bath are non-commuting operations*, except when the bandwidth of the lead is larger than the energy band spanned, on average, by the system subject to the fluctuations induced by the noise.

Reduction in the superoperator formalism

$$\mathcal{H}_0\rho = \frac{\mathrm{i}}{\hbar}[H_0, \rho]\,, \qquad \mathcal{V}_{RL}\rho = \frac{\mathrm{i}}{\hbar}[H_{RL}, \rho]\,,$$

$$[\mathcal{D}_0\rho]_{ik} = \begin{cases} (1-\delta_{ik})\dfrac{\sigma_R^2}{\hbar}\rho_{ik} & \text{if } i,\ k \leq N_R\,, \\ 0 & \text{otherwise,} \end{cases}$$

$$[\mathcal{D}_{RL}\rho]_{ik} = \begin{cases} \dfrac{\sigma_R^2}{2\hbar}\rho_{ik} & \text{if } i(k) \leq N_R,\ k(i) > N_R, \\ 0 & \text{otherwise.} \end{cases}$$

The master equation in super-operator form reads now

$$\dot{\rho} = -(\mathcal{H}_0 + \mathcal{D}_0)\rho - (\mathcal{V}_{RL} + \mathcal{D}_{RL})\rho\,,$$

where $(\mathcal{H}_0 + \mathcal{D}_0)$ is the non-interacting super-operator. The interaction super-operators are $\mathcal{V}_{RL}$, proportional to the coupling Ω_{RL}, and $\mathcal{D}_{RL}$, due to the noise terms.

$$\text{With } J(E') = \begin{cases} \frac{\Omega_{RL}^2}{\pi\hbar^2\Omega_L}\sqrt{1-\left(\frac{E'}{2\Omega_L}\right)^2} & \text{for } E \in [-2\Omega_L,\, 2\Omega_L]\,, \\ 0 & \text{otherwise.} \end{cases}$$

the partial trace on the lead becomes

$$\mathrm{tr}_L\left\{\int_0^t \mathcal{V}_{RL}(t)\mathcal{V}_{RL}(t')\rho_R^I(t') \otimes |0_L\rangle\langle 0_L|\; dt'\right\} =$$

$$= -\int_0^t dt' \sum_{i,k=1}^{N_R} \boldsymbol{r}_{ik} \int dE'\, J(E') e^{\alpha_{ik} t} \times$$

$$\times \sum_{r,s=1}^{N_R} \left(e^{-\frac{\mathrm{i}}{\hbar}E'(t-t')}\delta_{ks}\rho_{rs}(t') + e^{\frac{\mathrm{i}}{\hbar}E'(t-t')}\delta_{ir}\rho_{rs}(t')\right)$$

$$+\, 2\int_0^t dt' \boldsymbol{r}_{00} \int dE'\, J(E') \sum_{r,s=1}^{N_R} \rho_{rs}(t') \cos\frac{E'(t-t')}{\hbar}\,.$$

Wide-band limit

To understand better what are the crucial approximations, we first simplify the kernel $J(E')$ by setting $J(E') \equiv J(0)$ for $E' \in [-2\Omega_L, 2\Omega_L]$, and zero otherwise. Then we obtain

$$\mathrm{tr}_L \left\{ \int_0^t \mathcal{V}_{RL}(t)\mathcal{V}_{RL}(t')\rho_R^I(t') \otimes |0_L\rangle \langle 0_L| \, dt' \right\} =$$

$$= - \int_0^t \sum_{i,k=1}^{N_R} dt' \boldsymbol{r}_{ik} \frac{2\pi\hbar J(0) \sin(2\Omega_L(t-t')/\hbar)}{\pi(t-t')} \times \sum_{r,s=1}^{N_R} e^{\alpha_{ik} t}(\delta_{ks} + \delta_{ir})\rho_{rs}(t')$$

$$+ \int_0^t dt' \boldsymbol{r}_{00} \frac{4\pi\hbar J(0) \sin(2\Omega_L(t-t')/\hbar)}{\pi(t-t')} \sum_{r,s=1}^{N_R} \rho_{rs}(t') \, .$$

Wide-band limit

We consider the characteristic time of the ring dynamics given by $\hbar/\sigma_R^2$ and introduce the dimensionless interval $\tau = \sigma_R^2(t - t')/\hbar$. Since

$$\lim_{\omega\to\infty} \frac{\sin(\omega\tau)}{\pi\tau} = \delta(\tau)$$

in the sense of distributions, we can obtain a local-in-time equation by substituting τ in the previous expression and taking $\Omega_L/\sigma_R^2 \to \infty$.

Note that the wide-band limit is not performed with respect to the energy scale of the ring, which is always assumed negligible compared to Ω_L in our argument. What we are comparing here is the bandwidth of the probability-absorbing bath with the energy scale of the dephasing bath. This operation is responsible for removing back-action effects between the two baths.

Take-home messages

1. When using non-Hermitian models we must be aware of their limits
2. They are good if the relevant physics is at intermediate times
3. The interplay between probability-absorbing baths and thermal baths or disorder affects the decay properties of the system
4. When multiple environments act on a system they can interfere with each other, so that additivity/linearity assumptions may breakdown
5. Decay channels must allow the necessary room, in space and energy, to be modeled with simple non-Hermitian terms

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Thanks for your attention!