# Non-Markovian Open Quantum Systems

zur Vorlesung

“Theorie der Quantensystemen im Nichtgleichgewicht” von Prof. Tobias Brandes

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# 1. Non-Markovian Propagation Methods

The Born and Markov approximations are valid in situations where the environment quickly recovers its original configuration regardless of what dynamics the system is undergoing. In physical situations where it is necessary to take into account the dynamics of the bath, this approximation is not suitable and non-Markovian methods of propagation are required. A plethora of approaches exists, and each method has its advantages and its drawbacks. We review some of them and attempt to provide general guidelines for their range of application.

## 1.1 Beyond Born-Markov: Polaron master equation

The simplest improvement beyond the Born-Markov master equation is to drop either the weak coupling or the fast-bath approximation.

For weak system-bath interactions, the first approach may be to drop the Markovian approximation. The resulting master equation is known as the Redfield master equation, which has the form

$$\frac{d}{dt}\tilde{\rho}\left(t\right) = Tr_B\left\{\mathcal{L}_t\rho\left(0\right)\otimes R_0\right\} + \int_0^t dt' Tr_B\left\{\mathcal{L}_t\mathcal{L}_{t'}\tilde{\rho}\left(t\right)\otimes R_0\right\},$$

so that non-Markovian effects of the system-bath interaction are encapsulated in a time-dependent dissipator. As with any method, it is necessary to handle the approximation regime appropriately, otherwise problems of positivity may arise.

When the coupling between the system and the bath is very strong, it may be possible to go beyond the Born approximation by use of polaron transformations, where the interaction Hamiltonian is eliminated by transforming into a suitable picture. The existence of such a transformation depends on the specific form of the Hamiltonian. Partial polaron transformations or generalized forms thereof may be helpful, but there is no general approach to the problem that works for any form of the system Hamiltonian. Nevertheless, there are few other practical approaches to treat the very strong coupling limit.

Let us consider a general total Hamiltonian consisting of a system, interaction and bath parts

$$\hat{\mathrm{H}} = \Delta\hat{\sigma}_z + J\hat{\sigma}_x + \hat{\sigma}_z \otimes \hat{\mathrm{X}} + \hat{\mathrm{H}}_{\mathrm{B}}, \tag{1.1}$$

$$\hat{\mathrm{H}}_{\mathrm{B}} = \sum_k \omega_k \hat{\mathrm{a}}_k^\dagger \hat{\mathrm{a}}_k. \tag{1.2}$$

$\hat{\mathrm{a}}_k$ and $\hat{\mathrm{a}}_k^\dagger$ are the usual bosonic or fermionic annihilation and creation operators for the mode $k$ and $\hat{\mathrm{X}} = \sum_k \gamma_k \left(\hat{\mathrm{a}}_k + \hat{\mathrm{a}}_k^\dagger\right)$. The initial state of the system and environment may be taken to be separable $\pi(0) = \rho(0) \otimes \frac{e^{-\beta\hat{\mathrm{H}}}}{\mathrm{Tr}\left\{e^{-\beta\hat{\mathrm{H}}}\right\}}$. The goal is to transform the Hamiltonian into a picture where the interaction between the system and the environment vanish. For that we will use the unitary transformation

$$S = e^{-i\hat{\sigma}_z\hat{\mathrm{P}}}$$

with $\hat{\mathrm{P}} = i\sum_k \frac{f_k}{\omega_k}\left(\hat{\mathrm{a}}_k - \hat{\mathrm{a}}_k^\dagger\right)$. The effect on the several operators is such that

$$S\hat{\mathrm{a}}_k S^\dagger = \hat{\mathrm{a}}_k - \frac{f_k}{\omega_k}\hat{\sigma}_z$$

$$S\hat{\sigma}_x S^\dagger = \hat{\sigma}^+ e^{-i\hat{\mathrm{P}}} + \hat{\sigma}^- e^{+i\hat{\mathrm{P}}}$$

so that the transformed Hamiltonian appears

$$S\hat{\mathrm{H}}S^\dagger = \Delta\hat{\sigma_{\mathrm{z}}} + J\left(\hat{\sigma}^+ e^{-i\hat{\mathrm{P}}} + \hat{\sigma}^- e^{+i\hat{\mathrm{P}}}\right) + \hat{\sigma}_z \otimes \sum_k \left(\gamma_k - f_k\right)\left(\hat{\mathrm{a}}_k + \hat{\mathrm{a}}_k^\dagger\right) + \hat{\mathrm{H}}_{\mathrm{B}},$$

and the remaining interaction can be adjusted to be a combination of the $J$ and the original term. By adjusting the transformation to a position where the weak coupling approximation applies, one can then perform the usual Born and possibly Markov approximations. One has to be careful with the fact that the average value of the coupling Hamiltonian does not necessarily vanish, since $\left\langle e^{-i\hat{\mathrm{P}}}\right\rangle \neq 0$. Adding this expected value to the system Hamiltonian and subtracting it from the interaction Hamiltonian recovers the usual situation.

## 1.2 Path Integral Methods

Equilibration or transport phenomena are usually modeled in terms of the interaction with an infinite ensemble of non-interacting particles. As shown in the appendix of the main lecture notes, be it bosons or fermions, their effect can be expressed formally in terms of an influence functional $\mathcal{F}$ that enters the path integral expression of the evolution of the open quantum system

$$\langle q|\,\rho\,(t)\,|q'\rangle = \int dq_0 dq_0' \,\langle q_0|\,\rho\,(0)\,|q_0'\rangle \int_{q_0}^{q} \mathcal{D}q \int_{q_0'}^{q'} \mathcal{D}^* q' \exp\left[i\left(S\left[q\right] - S\left[q'\right]\right)\right]\mathcal{F}\left[q\left(t\right), q'\left(t'\right)\right], \tag{1.3}$$

where $S$ is the action associated to the free evolution of the open quantum system and the influence functional has the form

$$\mathcal{F}\left[q\left(t\right), q'\left(t'\right)\right] = Tr\left\{U_B^{\dagger}\left[q'\right] U_B\left[q\right] R_0\right\} = \exp\left\{-\Phi\left[q, q'\right]\right\},$$

with the influence phase

$$\Phi\left[q, q'\right] = \int_0^t dt' \int_0^{t'} ds \left\{f\left[q_{t'}\right] - f\left[q'_{t'}\right]\right\}\left\{L\left(t'-s\right) f\left[q_s\right] - L^*\left(t'-s\right) f\left[q'_s\right]\right\} \tag{1.4}$$

and the correlation function

$$L\left(\tau\right) = \int d\Omega J\left(\Omega\right)\left(\coth\frac{\beta\Omega}{2}\cos\Omega\tau - i\sin\Omega\tau\right).$$

Propagation in terms of the influence functional may be implemented by the introduction of a time discretization that transforms the path integrals into high dimensional ordinary integrals. This is the underlying idea of an extended propagation method termed QUAPI (Quasiadiabatic path-integration).

Let us represent time in terms of an integer amount of steps $\Delta t$, $t = k\Delta t$. This allows us to rewrite the influence phase in Eq.(1.4) as

$$\Phi\left[q, q'\right] \simeq \sum_{k=0}^{N}\sum_{k'=0}^{k}\left\{f_k - f'_k\right\}\left\{\eta_{k-k'} f_{k'} - \eta^*_{k-k'} f'_{k'}\right\} \tag{1.5}$$

where $\eta_{\Delta k}$ are convenient bounded integrals of $L\left(\tau\right)$ and $f_k \equiv f\left[q\left(k\Delta t\right)\right]$, $f'_k \equiv f\left[q'\left(k\Delta t\right)\right]$. Under inspection of the correlation function, it may be possible to define a cutoff in terms of the index difference $\Delta k$ such that $\eta_{\Delta k_{max}} \simeq 0$. This can be seen as the introduction of a memory cutoff, and this is the basis for a large number of propagation methods that go beyond the Markovian approximation.

One may now extend the reduced density matrix so that it becomes a reduced density *tensor* of rank $\Delta k_{max}$

$$A\left(0\right) \equiv A^{\left(\Delta k_{max}\right)}\left(q_0, q_1, \ldots q_{\Delta k_{max}-1}; q'_0, q'_1, \ldots q'_{\Delta k_{max}-1}, 0\right) = \left\langle q_0\right|\rho\left(0\right)\left|q'_0\right\rangle,$$

so that expression (1.3) transforms into a tensor multiplication of the form

$$A\left(\Delta k_{max}\Delta t\right) = T^{\left(2\Delta k_{max}\right)} A(0),$$

where the propagation tensor is

$$T^{\left(2\Delta k_{max}\right)}\left(q_k, q_{k+1}, \ldots q_{2\Delta k_{max}+k-1}; q'_k, q'_{k+1}, \ldots q'_{2\Delta k_{max}+k-1}, 0\right) \equiv$$
$$\prod_{n=k}^{k+\Delta k_{max}-1} I_0\left(q_n, q'_n\right) I_1\left(q_n, q'_n, q_{n+1}, q'_{n+1}\right)\cdots I_{\Delta k_{max}}\left(q_n, q'_n, q_{n+\Delta k_{max}}, q'_{n+\Delta k_{max}}\right) K\left(q_n, q'_n, q_{n+1}, q'_{n+1}\right)$$

with

$$I_{\Delta k}\left(q_k, q'_k, q_{k+\Delta k}, q'_{k+\Delta k}\right) \equiv \exp\left\{\left(f_{k+\Delta k} - f'_{k+\Delta k}\right)\left(\eta_{\Delta k} f_k - \eta^*_{\Delta k} f'_k\right)\right\}$$

and $K$ the action associated to the free Hamiltonian of the system.

## 1.3 Memory Kernel Methods

An alternative for the design of generalized non-Markovian master equations is the use of projection operator techniques. Projection operators $\mathcal{P}$ have the property $\mathcal{P}^2 = \mathcal{P}$ and they define a complement $\mathcal{Q} = 1 + \mathcal{P}$. Let us derive a general equation for a partition of a closed system defined by projector $\mathcal{P}$. The evolution of a closed system is given by the Liouville equation

$$\frac{d}{dt}\rho = \mathcal{L}\rho,$$

and it can be decomposed into the two terms

$$\frac{d}{dt}\mathcal{P}\rho = \mathcal{P}\mathcal{L}\left(\mathcal{P}+\mathcal{Q}\right)\rho,$$
$$\frac{d}{dt}\mathcal{Q}\rho = \mathcal{Q}\mathcal{L}\left(\mathcal{P}+\mathcal{Q}\right)\rho.$$

Formal integration of the second equation provides

$$\mathcal{Q}\rho\left(t\right) = \exp\left(\mathcal{Q}\mathcal{L}t\right)\mathcal{Q}\rho\left(0\right) + \int_0^t \exp\left[\mathcal{Q}\mathcal{L}\left(t-t'\right)\right]\mathcal{Q}\mathcal{L}\mathcal{P}\rho\left(t'\right)dt'$$

and the introduction of the term into the equation for $\mathcal{P}\rho\left(t\right)$

$$\frac{d}{dt}\mathcal{P}\rho\left(t\right) = \mathcal{P}\mathcal{L}\mathcal{P}\rho\left(t\right) + \mathcal{P}\mathcal{L}\mathcal{Q}\exp\left(\mathcal{Q}\mathcal{L}t\right)\mathcal{Q}\rho\left(0\right) + \int_0^t \mathcal{P}\mathcal{L}\mathcal{Q}\exp\left[\mathcal{Q}\mathcal{L}\left(t-t'\right)\right]\mathcal{Q}\mathcal{L}\mathcal{P}\rho\left(t'\right)dt',$$

where we can distinguish three terms:

- the homogeneous term $\mathcal{P}\mathcal{L}\mathcal{P}\rho$,
- the inhomogeneous term $\mathcal{I}\left(t\right) \equiv \mathcal{P}\mathcal{L}\mathcal{Q}\exp\left(\mathcal{Q}\mathcal{L}t\right)\mathcal{Q}\rho\left(0\right)$ and
- the convolution over the memory kernel $\mathcal{K}\left(t\right) \equiv \mathcal{P}\mathcal{L}\mathcal{Q}\exp\left[\mathcal{Q}\mathcal{L}t\right]\mathcal{Q}\mathcal{L}\mathcal{P}$.

The projector that is relevant for the theory of open quantum systems can be expressed as $\mathcal{P}\rho(t) = Tr_B\left[\rho(t)\right]\otimes\rho_{B,eq}$, where $\rho_{B,eq}$ is the equilibrium state in the bath. Nevertheless, this is a general derivation where no assumption was taken, so this establishes a general approach for the propagation of open quantum systems.

## 1.4 Time Convolutionless equation

To avoid the integration over the history of the system, let us define the inverse propagation

$$\mathcal{P}\rho\left(t'\right) = \mathcal{P}\exp\left[-\mathcal{L}\left(t-t'\right)\right]\left(\mathcal{P}+\mathcal{Q}\right)\rho\left(t\right),$$

so that the object

$$\Sigma\left(t\right) = \int_0^t \exp\left[\mathcal{Q}\mathcal{L}\left(t-t'\right)\right]\mathcal{Q}\mathcal{L}\mathcal{P}\exp\left[-\mathcal{L}\left(t-t'\right)\right],$$

can be used to rewrite the formal solution of $\mathcal{Q}\rho\left(t\right)$

$$\left[1+\Sigma\left(t\right)\right]\mathcal{Q}\rho\left(t\right) = \exp\left(\mathcal{Q}\mathcal{L}t\right)\mathcal{Q}\rho\left(0\right) + \Sigma\left(t\right)\mathcal{P}\rho\left(t'\right).$$

## 1.5 Hierarchy of Equations Methods

Let us consider a general total Hamiltonian consisting of a system, interaction and bath parts

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_{\mathrm{S}} + \sum_{\nu} \hat{\mathrm{V}}_{\nu} \otimes \hat{\mathrm{B}}_{\nu} + \hat{\mathrm{H}}_{\mathrm{B}}, \tag{1.6}$$

$$\hat{\mathrm{H}}_{\mathrm{B}} = \sum_{\nu} \hat{\mathrm{H}}_{\nu} = \sum_{\nu,k} \omega_{\nu,k} \hat{\mathrm{a}}^{\dagger}_{\nu k} \hat{\mathrm{a}}_{\nu k}. \tag{1.7}$$

The index $\nu$ labels the baths, $\hat{\mathrm{a}}_{\nu,k}$ and $\hat{\mathrm{a}}^{\dagger}_{\nu,k}$ are the usual bosonic or fermionic annihilation and creation operators for the mode $k$ in bath $\nu$. The goal is to derive the full counting cumulant generating function of an observable $\hat{\mathrm{O}}$ of one of the baths which commutes with its free Hamiltonian $\hat{\mathrm{H}}_{\nu}$ and with the initial state of the system and baths $\pi(0) = \rho(0) \bigotimes_{\nu} \frac{e^{-\beta_{\nu}\hat{\mathrm{H}}_{\nu}}}{\mathrm{Tr}\left\{e^{-\beta_{\nu}\hat{\mathrm{H}}_{\nu}}\right\}}$. For simplicity, we will omit the explicit dependence on the thermodynamic constraint in the derivation, so that the two-measurement cumulant generating function takes the form

$$G(\chi, t) = \ln \mathrm{Tr} \left\{ e^{-i\hat{\mathrm{H}}\left[\frac{\chi}{2}\right]t} \pi(0) e^{i\hat{\mathrm{H}}\left[-\frac{\chi}{2}\right]t} \right\}, \tag{1.8}$$

where $\hat{\mathrm{A}}[\chi](t) = e^{i\chi\hat{\mathrm{O}}} \hat{\mathrm{A}}(t) e^{-i\chi\hat{\mathrm{O}}}$. This problem can be formulated in terms of the solution to a hierarchy of equations of motion for the counting field resolved density matrix

$$\rho(\chi, t) = \mathrm{Tr}_{\mathrm{B}} \left\{ e^{-i\hat{\mathrm{H}}\left[\frac{\chi}{2}\right]t} \pi(0) e^{i\hat{\mathrm{H}}\left[-\frac{\chi}{2}\right]t} \right\}, \tag{1.9}$$

and the equation $G(\chi, t) = \ln\left[\mathrm{Tr}\left\{\rho(\chi, t)\right\}\right]$ directly relates both quantities.

For the sake of clarity, we will derive the equations of motion for Eq.(1.9). The matrix $\rho(\chi, t)$ satisfies the differential equation

$$\frac{d}{dt}\rho(\chi, t) = -i\, \mathrm{Tr}_{\mathrm{B}} \left\{ \hat{\mathrm{H}}\left[\frac{\chi}{2}\right] \pi(\chi, t) - \pi(\chi, t) \hat{\mathrm{H}}\left[-\frac{\chi}{2}\right] \right\}, \tag{1.10}$$

with $\pi(\chi, t) \equiv e^{-i\hat{\mathrm{H}}\left[\frac{\chi}{2}\right]t} \pi(0) e^{i\hat{\mathrm{H}}\left[-\frac{\chi}{2}\right]t}$. The formal solution of Eq.(1.10) in the interaction picture with respect to $\hat{\mathrm{H}}_{\mathrm{S}} + \hat{\mathrm{H}}_{\mathrm{B}}$ (denoted by an overhead tilde) can be obtained by means of Wick's theorem. For simplicity, we will focus on the derivation for the bosonic case, but all steps can be trivially generalized for the fermionic case. Wick's theorem simplifies the calculation of the partial trace of the bath by reducing products of 2n operators to n products of pairwise traces

$$\left\langle \hat{\mathrm{T}} \tilde{\hat{\mathrm{B}}}_{\nu}(t_{2n}) \tilde{\hat{\mathrm{B}}}_{\nu}(t_{2n-1}) \cdots \tilde{\hat{\mathrm{B}}}_{\nu}(t_2) \tilde{\hat{\mathrm{B}}}_{\nu}(t_1) \right\rangle = \sum_{app} \prod_{ij} \left\langle \hat{\mathrm{T}} \tilde{\hat{\mathrm{B}}}_{\nu}(t_i) \tilde{\hat{\mathrm{B}}}_{\nu}(t_j) \right\rangle,$$

where the sum is over all possible pairs (app) of indices up to $2n$, $\hat{\mathrm{T}}$ is the time ordering operator and the average may be performed over any Gaussian state. Therefore, the solution of Eq.(1.10) in the interaction picture is $\tilde{\rho}(\chi, t) = \tilde{\mathcal{U}}(\chi, t)\rho(0, 0)$, with

$$\tilde{\mathcal{U}}(\chi, t) = \prod_{\nu} \prod_{jk=0,1} \exp_{+} \left( \int_0^t \mathrm{ds}\, \tilde{\hat{\mathrm{W}}}^{jk}_{\nu}(\chi, s) \right), \tag{1.11}$$

where $\exp_+$ stands for the time ordered exponential and

$$\tilde{\hat{\mathrm{W}}}^{jk}_{\nu}(\chi,t) = -\int_0^t \mathrm{ds}\;\tilde{\hat{\mathrm{V}}}^{j}_{\nu}(t) C^{jk}_{\nu}(\chi, t-s)\,\tilde{\hat{\mathrm{V}}}^{k}_{\nu}(s). \tag{1.12}$$

Here we introduce the superoperator notation $\hat{\mathrm{A}}^0\rho \equiv \hat{\mathrm{A}}\rho$ and $\hat{\mathrm{A}}^1\rho \equiv \rho\hat{\mathrm{A}}$ and the bath correlation functions

$$C^{jk}_{\nu}(\chi,t) = (-)^{j+k}\left\langle \tilde{\hat{\mathrm{B}}}^{j}_{\nu}\left[(-)^j\frac{\chi}{2}\right](t)\,\tilde{\hat{\mathrm{B}}}^{k}_{\nu}\left[(-)^k\frac{\chi}{2}\right](0)\right\rangle, \tag{1.13}$$

where $\langle A\rangle = \mathrm{Tr}\left\{A\pi(0)\right\}$.

The HEOM formalism uses an approximate representation of the correlation functions by means of linear combinations of decaying exponential functions. The extended version generalizes the framework to more involved functional bases [?]. In our case, the coefficients of the linear combination are functions dependent on the counting field $\chi$, so that we approximate $C^{jk}_{\nu}(\chi,t) = \sum_r c^{jk}_{\nu r}(\chi)\phi_r(t)$ by means of a set of functions $\{\phi_r(t)\}$ whose derivatives are well defined within the set by $\frac{\mathrm{d}}{\mathrm{d}t}\phi_r(t) = \sum_n \eta_{rs}\phi_s(t)$, where $\eta$ is a matrix with complex entries. The form of $c^{jk}_{\nu r}(\chi)$ is general and depends on the specific observable of interest $\hat{\mathrm{O}}$. For instance, in the case $\hat{\mathrm{O}} = \mathrm{H}_{\nu}$ and $\hat{\mathrm{B}}_{\nu} = \sum_k \gamma_{\nu k}\left(\hat{\mathrm{a}}_{\nu k} + \hat{\mathrm{a}}^{\dagger}_{\nu k}\right)$, $C^{jk}_{\nu}(\chi,t) = C^{jk}_{\nu}(\chi \pm t)$ and the dependence is expected to be similar to that of $\phi_r(t)$. With this representation, it is possible to define the auxiliary objects

$$\tilde{\rho}^{\{n\}}(\chi,t) = \hat{\mathrm{T}}\prod_{\nu,r;k=0,1}\left(\int_0^t \mathrm{ds}\,\phi_r(t-s)\;\tilde{\hat{\mathrm{V}}}^{k}_{\nu}(s)\right)^{n^k_{\nu r}}\tilde{\mathcal{U}}(\chi,t)\rho(0,0),$$

where $\{n\} \equiv \left\{\ldots, n^k_{\nu r},\ldots\right\}$ is a rank-three tensor of non-negative integer entries which sum up to $n$ and $n$ is the so-called *hierarchic level*. It is clear that $\tilde{\rho}^{\{0\}}(\chi,t) = \tilde{\rho}(\chi,t)$ and the auxiliary fields satisfy the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^{\{n\}}(\chi,t) = -i\hat{\mathrm{H}}^{\times}_{S}\rho^{\{n\}}(\chi,t) + \sum_{\nu,r;k=0,1}\left(\bar{\hat{\mathrm{V}}}^{k}_{\nu r}\,\rho^{\left\{\ldots,n^k_{\nu r}+1,\ldots\right\}}(\chi,t)\right. \tag{1.14}$$

$$+\sum_s n^k_{\nu r}\eta_{rs}\rho^{\left\{\ldots,n^k_{\nu r}-1,\ldots,n^k_{\nu s}+1,\ldots\right\}}(\chi,t) \tag{1.15}$$

$$\left.+\,n^k_{\nu r}\phi_r(0)\hat{\mathrm{V}}^{k}_{\nu}\rho^{\left\{\ldots,n^k_{\nu r}-1,\ldots\right\}}(\chi,t)\right),$$

where we have used the notation $\hat{\mathrm{A}}^{\times}\rho \equiv \hat{\mathrm{A}}\rho - \rho\hat{\mathrm{A}}$ and $\bar{\hat{\mathrm{V}}}^{k}_{\nu r} \equiv \sum_{j=0,1} c^{jk}_{\nu r}(\chi)\hat{\mathrm{V}}^{j}_{\nu}$.

### 1.5.1 Hierarchy of equations of motion for high order statistical moments

Although Eq.(1.14) can be used on its own to obtain the generating function, in the case where one is interested in specific statistical moments, a specialized hierarchy can be derived. Let us define the object

$$\tilde{\sigma}_m(t) \equiv \frac{\partial^m}{\partial(i\chi)^m}\tilde{\rho}^{\{0\}}(\chi,t)\Big|_{\chi=0} = \hat{\mathrm{T}}\ \frac{\partial^m}{\partial(i\chi)^m}\tilde{\mathcal{U}}(\chi,t)\Big|_{\chi=0}\rho(0,0),$$

so that the moment $m$ of the full counting distribution may be obtained by tracing: $\mathrm{Tr}\left\{\tilde{\sigma}_m(t)\right\}$. It contains correlation functions of the form $\frac{\partial^q}{\partial(i\chi)^q}C^{jk}_{\nu}(\chi,t)\Big|_{\chi=0} \equiv C^{jk}_{\nu q}(t)$, which are well defined in terms of the approximate representation as $C^{jk}_{\nu q}(t) = \sum_r c^{jk}_{\nu rq}\phi_r(t)$ with $c^{jk}_{\nu rq} \equiv \frac{\mathrm{d}^q}{\mathrm{d}(i\chi)^q}c^{jk}_{\nu r}(\chi)\Big|_{\chi=0}$. In a procedure analogous to the one followed for the obtention of Eq.(1.14), we define

$$\tilde{\sigma}^{\{n\}}_{\{m\}}(t) = \hat{\mathrm{T}}\prod_{\nu,k;j=0,1}\left(\int_0^t \mathrm{d}s\,\phi_k\left(t-s\right)\,\tilde{\bar{\mathrm{V}}}^j_{\nu}(s)\right)^{n^j_{\nu k}}\prod_q\left(\int_0^t \mathrm{d}s\ \tilde{\bar{\mathrm{W}}}_{\nu q}(s)\right)^{m_q}\tilde{\mathcal{U}}(0,t)\rho(0,0),$$

where $\{m\} \equiv \{\ldots,m_q,\ldots\}$ is a vector of non-negative integer entries such that $\sum_q m_q q = m$ and $\tilde{\bar{\mathrm{W}}}_{\nu q}(t) \equiv \sum_{j,k=0,1} - \int_0^t \mathrm{d}s\ \tilde{\bar{\mathrm{V}}}^j_{\nu}(t)C^{jk}_{\nu q}(t-s)\,\tilde{\bar{\mathrm{V}}}^k_{\nu}(s)$. This object satisfies the equation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\sigma^{\{n\}}_{\{m\}}(t) = &-i\hat{\mathrm{H}}^{\times}_S\sigma^{\{n\}}_{\{m\}}(t) + \sum_{\nu,r;k=0,1}\Bigg(\bar{\bar{\mathrm{V}}}^k_{\nu r}\,\sigma^{\{\ldots,n^k_{\nu r}+1,\ldots\}}_{\{m\}}(t) + \sum_s n^k_{\nu r}\eta_{rs}\sigma^{\{\ldots,n^k_{\nu r}-1,\ldots,n^k_{\nu s}+1,\ldots\}}_{\{m\}}(t)\\ &+ n^k_{\nu r}\phi_r(0)\hat{\mathrm{V}}^k_{\nu}\sigma^{\{\ldots,n^k_{\nu r}-1,\ldots\}}_{\{m\}}(t) + \sum_q m_q\,\bar{\bar{\mathrm{V}}}^k_{\nu rq}\,\sigma^{\{\ldots,n^k_{\nu r}+1,\ldots\}}_{\{\ldots,m_q-1,\ldots\}}(t)\Bigg),\end{aligned}$$

where $\bar{\bar{\mathrm{V}}}^k_{\nu rq} \equiv \sum_{j=0,1} c^{jk}_{\nu rq}\hat{\mathrm{V}}^j_{\nu}$. The structure is identical to the usual hierarchy (Eq. 1.14) but for the last term, which connects it to the next tier elements of the hierarchy associated to the previous moment. This can be interpreted as an additional driving that each moment exerts on the next one. This naturally defines a cascade of hierarchies that can be exploited for parallel simulation of several moments with reduced overhead.

The relationship between $\tilde{\sigma}_m(t)$ and the set of $\tilde{\sigma}^{\{n\}}_{\{m\}}(t)$ follows

$$\tilde{\sigma}_m(t) = \sum_{\{m\}} a_{\{m\}}\tilde{\sigma}^{\{0\}}_{\{m\}}(t). \tag{1.16}$$

where the sum is over all partitions $\{m\}$ of $m$ (all vectors $m_q$ with the property $\sum_{q=1}^m m_q q = m$) and

$$a_{\{m\}} \equiv \prod_{q=1}^{m}\prod_{j=1}^{m_q}\frac{1}{j}\begin{pmatrix} m - \sum_{r=q}^m r m_r + jq \\ k\end{pmatrix}$$

is the number of permutations associated to that partition.

## 1.6 Stochastic Methods

Direct evaluation of the path integral formulation for the evolution of open quantum systems is not practical. But it is possible to use Montecarlo techniques to implement that evaluation.