Average quantum dynamics of closed systems over stochastic Hamiltonians

Li Yu and Daniel F. V. James

November 30, 2011

Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario M5S 1A7, Canada

Abstract

We develop a master equation formalism to describe the evolution of the average density matrix of a closed quantum system driven by a stochastic Hamiltonian. The average over random processes generally results in decoherence effects in closed system dynamics, in addition to the usual unitary evolution. We then show that, for an important class of problems in which the Hamiltonian is proportional to a Gaussian random process, the 2nd-order master equation yields exact dynamics. The general formalism is applied to study the examples of a two-level system, two atoms in a stochastic magnetic field and the heating of a trapped ion.

PACS number(s): 03.65.Ca, 03.65.Yz, 05.40.-a, 03.67.Lx

1 Introduction

The density operator encapsulates all the statistical information about the state of a quantum system. The evolution of the density operator of a closed system is governed by the Hamiltonian. In practice, the Hamiltonian can seldom be strictly determined or precisely controlled – it fluctuates both in a temporal sense and between repeated realizations, which can be mathematically described by random processes. Therefore, instead of treating any Hamiltonian as deterministic in an idealized manner, we would like to take such fluctuations into account explicitly when studying quantum dynamics. Our goal is to obtain the average dynamics in the following sense: Suppose an ensemble of systems are
prepared in some initial state and subsequently evolve under a randomly fluctuating Hamiltonian, how does the density matrix that describes the ensemble as a whole evolve?

Previous work on stochastic average dynamics was done by Budini [1] using a variational calculus method and Novikov’s theorem, and by Guha et al. [2] using a non-perturbative cluster cumulant method. A different kind of average dynamics over the time domain was studied by Gamel and James [3], assuming the deterministic (i.e. non-stochastic) Hamiltonian but taking into account the finite time-window of measurements. The master equation formalism is also widely used in the study of open systems dynamics [4]. It should be noted that, despite the formal similarity, our study is on the dynamics of closed quantum systems and no environment is involved.

In this paper, we will first adopt a series expansion approach and derive a time-local master equation that describes the ensemble-average dynamics of a general quantum system. The general formalism is then used to study a representative class of Hamiltonians obeying Gaussian statistics. Finally, we apply the master equation method to some physical examples and find interesting phenomena such as fluctuation-induced decoherence and decoherence-induced disentanglement. Throughout, our results are compared to exact dynamics and the validity of the master equation approach is discussed.

2 Theory

2.1 Ensemble-average density matrix

Consider a closed, but not isolated, system for which the Hamiltonian is determined by some classical stochastic quantity $x(t)$. Suppose an experiment is carried out repeatedly with each realization labelled by $\mu$. The evolution of the density matrix $\rho^\mu(t)$ that describes the quantum system in the $\mu$-th realization is governed by the Hamiltonian $\hat{H}^\mu(t) = \hat{H}[x^\mu(t)]$, and is given by

$$\rho^\mu(t) = \hat{U}^\mu(t, t_0) \rho_0 \hat{U}^{\mu\dagger}(t, t_0),$$

(1)

where $\rho_0$ is the initial density matrix, which is assumed to be uncorrelated with $x(t)$ and thus is the same in all realizations. The unitary evolution operator $\hat{U}^\mu(t, t_0)$ obeys the equation of motion,

$$i\hbar \frac{\partial}{\partial t} \hat{U}^\mu(t, t_0) = \hat{H}^\mu(t) \hat{U}^\mu(t, t_0).$$

(2)

The average density matrix $\bar{\rho}(t)$ is defined as follows,

$$\bar{\rho}(t) \equiv \lim_{N \to \infty} \frac{1}{N} \sum_{\mu=1}^{N} \rho^\mu(t).$$

(3)

It can be shown that $\bar{\rho}(t)$ is Hermitian, positive and of unit trace, which is ensured by the properties of the individual density matrices $\rho^\mu(t)$. Thus the op-
erator $\overline{\rho}(t)$ is indeed a physical density matrix, describing the average statistics of the ensemble of realizations as a whole.

The equation of motion for $\overline{\rho}(t)$ is formally given by

$$i\hbar \frac{\partial}{\partial t} \overline{\rho}(t) = \lim_{N \to \infty} \frac{1}{N} \sum_{\mu} i\hbar \frac{\partial}{\partial t} \rho(\mu)(t) = \lim_{N \to \infty} \frac{1}{N} \sum_{\mu} [\hat{H}(t), \rho(\mu)(t)] = [\overline{H}(t), \rho(t)].$$

(4)

However, since the right hand side cannot be written as a function of $\rho(t)$, the equation is not of a closed form and thus not very useful. With the goal of obtaining a closed equation for $\overline{\rho}(t)$, we resort to a series expansion approach.

2.2 Series expansion of the evolution operator

Following the standard recipe for perturbative expansion [5], the unitary operator $\hat{U}(t, t_0)$ in a particular realization $\mu$ can be written as a power series in $\lambda$ (a parameter controlling the “strength” of the Hamiltonian):

$$\hat{U}(t, t_0) = \sum_{n=0}^{\infty} \lambda^n \hat{U}(t, t_0)$$

where

$$\hat{U}(t, t_0) = i \frac{1}{\hbar} \int_{t_0}^{t} dt' \hat{H}(t') \hat{U}(t, t_0)$$

(7)

Thus $\overline{\rho}(t)$ can be expressed in terms of $\hat{U}(t, t_0)$ and $\lambda$:

$$\overline{\rho}(t) = \left( \sum_{m} \lambda^m \hat{U}(m, t_0) \right) \rho_0 \left( \sum_{n} \lambda^n \hat{U}(n, t_0) \right) = \sum_{k=0}^{\infty} \lambda^k \mathcal{E}_k[\rho_0] \equiv \mathcal{E}[\rho_0],$$

(8)

where $\mathcal{E}_k[\rho_0]$ is the time-dependent map defined as

$$\mathcal{E}_k[\rho_0] \equiv \sum_{j=0}^{k} \overline{U}_{k-j}(t, t_0) \rho_0 \overline{U}_j(t, t_0),$$

(9)

and $\mathcal{E}[\rho_0]$ is a completely positive linear map [6]. Although their argument is a density matrix in this instance, $\mathcal{E}_k$ and $\mathcal{E}$ can act on any operator in general.

2.3 Inverse transformation

The map $\mathcal{E}$ is a linear transformation that maps $\rho_0$ to $\overline{\rho}$. Since both $\rho_0$ and $\overline{\rho}$ are operators in the same Hilbert space, and thus of the same dimension, it is
natural to postulate that an inverse transformation $F = E^{-1}$ exists that maps $\rho$ to $\rho_0$. That is, 

$$\rho_0 = E^{-1}[\rho] \equiv F[\rho].$$

Note that the meaning of “inverse” is purely mathematical here: the map $E^{-1}$ is not to be confused with an inverse dynamical evolution in the physical sense. According to the semigroup property, a completely positive, trace preserving (CPTP) linear map is physically invertible if and only if it is an unitary map (see Section 3.8 of Ref.[7]). Therefore, in general, a CPTP map $E : \rho_0 \rightarrow \rho$ does not have a physical inverse, that is, we cannot find another CPTP map that gives $\rho \rightarrow \rho_0$. However, the mathematical inverse $E^{-1}$ that serves our purpose here needs not be CPTP.

Since the composition of a transformation and its inverse is the identity transformation, the identity $F[E[\rho]] = I[\rho]$ holds for an arbitrary operator $\rho$. Following [3], we adopt the ansatz that $F$ can be expanded in powers of $\lambda$,

$$F[\rho] = \sum_{m=0}^{\infty} \lambda^m F_m[\rho].$$

Then we have

$$\sum_{m=0}^{\infty} \lambda^m F_m[\sum_{n=0}^{\infty} \lambda^n E_n[\rho]] = \sum_{k=0}^{\infty} \lambda^k \left( \sum_{j=0}^{k} F_j[E_{k-j}[\rho]] \right) = \lambda^0 I[\rho].$$

Collecting terms of like powers in $\lambda$, we obtain the set of equations involving $F_m$ and $E_n$:

$$F_0[E_0[\rho]] = I[\rho],$$

$$F_0[E_1[\rho]] + F_1[E_0[\rho]] = 0,$$

$$F_0[E_2[\rho]] + F_1[E_1[\rho]] + F_2[E_0[\rho]] = 0,$$

and so on. Solving for $F_m$ in terms of $E_n$, and making use of $E_0 = I$ as defined in Eq.(6), we have

$$F_0[\rho] = E_0[\rho] = I[\rho],$$

$$F_1[\rho] = -E_1[\rho],$$

$$F_2[\rho] = -E_2[\rho] + E_1[E_1[\rho]],$$

and so on.

2.4 Master equation

Differentiating Eq.(8) with respect to time and making use of the inverse relation in Eq.(10), we obtain the following equation:

$$i\hbar \frac{\partial}{\partial t} \rho(t) = i\hbar \dot{E}[\rho_0] = i\hbar \dot{E}[F[\rho(t)]] = \rho(t).$$

(18)
Here, the notation $\dot{\mathcal{E}}[\rho]$ means first taking time-derivative of the time-dependent transformation $\mathcal{E}$ to obtain a new transformation denoted by $\mathcal{E}'$ and then letting $\mathcal{E}'$ act on $\rho$: the argument $\rho$ is not differentiated whether or not it is time-dependent. Assuming the order of differentiation and summation can be switched, we have

$$\dot{\mathcal{E}}[\mathcal{F}(t)] = \sum_{n=0}^{\infty} \lambda^n \dot{\mathcal{E}}_n[\mathcal{F}(t)] = \sum_{k=0}^{\infty} \lambda^k \left( \sum_{j=0}^{k} \dot{\mathcal{E}}_{k-j}[\mathcal{F}(t)] \right); \quad (19)$$

thus the equation of motion can be written as

$$i\hbar \frac{\partial}{\partial t} \rho(t) = \sum_{k=0}^{\infty} \lambda^k \left( \dot{\mathcal{E}}_k[\mathcal{F}(t)] \right) \equiv \sum_{k=0}^{\infty} \lambda^k \mathcal{L}_k[\rho(t)]. \quad (20)$$

Evaluating $\mathcal{F}_m$ and $\dot{\mathcal{E}}_n$ explicitly, we find

$$\mathcal{L}_0[\rho] = i\hbar \dot{\mathcal{E}}_0[\rho_0] = 0, \quad (21)$$
$$\mathcal{L}_1[\rho] = i\hbar \dot{\mathcal{E}}_0[\mathcal{F}_1[\rho]] + i\hbar \dot{\mathcal{E}}_1[\mathcal{F}_0[\rho]] = \overline{H} \rho - \rho H, \quad (22)$$
$$\mathcal{L}_2[\rho] = i\hbar \dot{\mathcal{E}}_0[\mathcal{F}_2[\rho]] + i\hbar \dot{\mathcal{E}}_1[\mathcal{F}_1[\rho]] + i\hbar \dot{\mathcal{E}}_2[\mathcal{F}_0[\rho]]$$
$$= \overline{H} \rho U_1 \rho - \overline{H} \overline{U_1} \rho + \rho \overline{H} \overline{U_1} + \rho \overline{U_1} \rho$$
$$- \rho \overline{U_1} \overline{H} \rho + \rho \overline{H} \rho U_1, \quad (23)$$

and so on. Note again that the argument $\rho$ is not to be averaged or differentiated and that terms like $\overline{H}$ are time-dependent just as $\mathcal{L}_k[\rho]$ are time-dependent transformations.

Keeping terms up to 2nd order and setting $\lambda = 1$ in Eq. (20), a time-local master equation is thus obtained for the evolution of $\rho(t)$:

$$i\hbar \frac{\partial}{\partial t} \rho(t) = \overline{H} \rho(t) - \rho \overline{H} + \dot{\rho}(t) \dot{A} + D[\rho(t)], \quad (24)$$

where $\dot{A} \equiv \overline{H} \dot{U_1} - \overline{H} \overline{U_1}$ and $D[\rho] \equiv \overline{H} \rho \dot{U_1} - \overline{H} \rho \overline{U_1} - \overline{U_1} \rho \overline{H} + \overline{U_1} \rho \overline{H}$. The effective Hamiltonian responsible for unitary evolution is

$$\dot{H}_{eff} \equiv \overline{H} + \frac{1}{2}(\dot{\hat{A}} + \hat{A}^\dagger), \quad (25)$$

with which the master equation can be written in a more insightful way,

$$i\hbar \frac{\partial}{\partial t} \rho(t) = [\dot{H}_{eff}, \rho(t)] + \frac{1}{2} \left\{ \hat{A} - \hat{A}^\dagger, \rho(t) \right\} + D[\rho(t)]. \quad (26)$$

It can be shown that the right-hand side of the equation can be put into the Lindblad form, which ensures Hermiticity, complete positivity and trace preservation of the evolution.
This result is formally similar to a previous work on average dynamics [3]. However, the physical meaning is different since the derivation in that case is for a time-average density matrix in a single realization. Incidentally, our result may also be reminiscent of some master equations for the reduced density matrix of open quantum systems. But it should be emphasized that our derivation is for a closed system and thus quantum entanglement with environment does not play a role here.

Note that the above results are formally applicable to an interaction-picture density matrix, though we implicitly assume the Schrödinger picture in the derivation. The only difference is in the interpretation of the density matrix: When we use the interaction-picture density matrix $\rho_I$, the expectation value of an observable $\hat{O}$ is given by $\langle \hat{O} \rangle = \text{Tr} (\hat{O} \rho_I)$, where $\hat{O}_I$ is the interaction-picture operator instead of the original operator in Schrödinger picture.

### 3 General applications

#### 3.1 Time-independent Hamiltonian

Let us first apply our general result to the simple case where the parameters in the Hamiltonian are time-independent. That is, $\hat{H} = \hat{H}(a)$, where $a$ represents random variable(s) instead of random process(es). Suppose further that $\hat{H}$ is of zero-mean, which implies a particular choice of “picture”: Any time-independent, deterministic part of the Hamiltonian plus the average component of the stochastic part can be removed by a gauge transformation, that is, by switching to a suitably chosen interaction picture [3]. Note that, in the case of time-independent random variables, $\hat{U}_1(t, t_0) = (t - t_0) \hat{H}/i\hbar$ and $\hat{U}_1^\dagger(t, t_0) = -\hat{U}_1^\dagger(t, t_0)$, thus $[\hat{U}_1, \hat{H}] = [\hat{U}_1^\dagger, \hat{H}] = 0$. So we have $\hat{A} + \hat{A}^\dagger = 0$ and thus $\hat{H}_\text{eff} = 0$. This result is special to the time-independent case, however. As we will see later, the effective Hamiltonian (to 2nd order) is in general non-zero, due to the non-commutativity of $\hat{U}_1$ and $\hat{H}$ in the time-dependent case. After simplification, the 2nd-order master equation in this particular case is

$$\frac{\partial}{\partial t} \hat{\rho}(t) = -\frac{t}{\hbar^2} \{ \hat{H}^2, \hat{\rho}(t) \} + \frac{2t}{\hbar^2} \hat{H} \hat{\rho}(t) \hat{H}.$$  

(27)

A class of problems of physical interest has a Hamiltonian of the form

$$\hat{H} = \hbar \sum_n a_n \hat{h}_n + a_n^* \hat{h}_n^\dagger,$$  

(28)

where $a_n$ are jointly circular complex Gaussian random variables of zero mean.\(^1\) Substituting Eq.(28) into Eq.(27), we find\(^2\)

---

\(^1\)According to the central limit theorem, Gaussian statistics is applicable when the random variables are due to the addition of many uncorrelated random sources.

\(^2\)For those readers who might be concerned about the factor $t$ on the right-hand side of Eq.(29): It is just a result of a time integral, as can be seen in the more general case of
\[ \frac{\partial}{\partial t} \tilde{\rho}(t) = i \sum_{k,l} \left\{ \Gamma_{kl} \left( -\hat{h}_k \hat{h}_l \tilde{\rho}(t) - \tilde{\rho}(t) \hat{h}_k \hat{h}_l + 2 \hat{h}_k^\dagger \tilde{\rho}(t) \hat{h}_l \right) ight. \\
+ \left. \Gamma_{kl}^* \left( -\hat{h}_l^\dagger \hat{h}_k \tilde{\rho}(t) - \tilde{\rho}(t) \hat{h}_k^\dagger \hat{h}_l + 2 \hat{h}_l \tilde{\rho}(t) \hat{h}_k^\dagger \right) \right\}, \] (29)

where \( \Gamma_{kl} = \langle a_k a_l^\dagger \rangle \) are the correlation functions. Note that the equation is of the familiar Lindblad form, which can be further simplified to a diagonal form through a linear transformation of the coefficients.

3.2 Single real Gaussian random process

Now consider the case of a time-dependent Hamiltonian

\[ \hat{H}(t) = \hbar a(t) \hat{h}, \] (30)

where \( a(t) \) is a (real) Gaussian random process. This is representative of a wide class of problems, for example, the Zeeman effect, where \( a(t) \) is proportional to the external magnetic field and \( \hat{h} \) is the \( z \)-component of the total angular momentum [9]. The random process in this section is taken to be the most general case, that is, we do not assume any additional property like zero-mean or stationarity.

The ensemble-average dynamics under this Hamiltonian is exactly solvable, so let us first work out the exact, analytic result. The unitary evolution operator in a particular realization \( \mu \) is

\[ \hat{U}^\mu(t, t_0) = \exp \left( -it^\mu(t) \hat{h} \right), \] (31)

where

\[ t^\mu(t) \equiv \int_{t_0}^t dt' a^\mu(t'). \] (32)

For an initial state \( \rho(t_0) = \sum_{k,l} \rho_{kl}(t_0) |k\rangle \langle l| \), where \( \{|n\rangle\} \) is the energy-eigenbasis with \( \hat{h}|n\rangle = E_n |n\rangle \), the evolution in a particular realization is

\[ \rho^\mu(t) = \hat{U}^\mu(t, t_0) \rho(t_0) \hat{U}^{\mu\dagger}(t, t_0) = \sum_{k,l} \rho_{kl}(t_0) \exp \left\{ -it^\mu(t) (E_k - E_l) \right\} |k\rangle \langle l|, \] (33)

thus the ensemble-average is

time-dependent Hamiltonians later. Note that the trace-preserving property of the equation is guaranteed by the Lindblad form.
\[ \rho(t) = \sum_{k,l} \rho_{kl}(t_0) \exp \{-i(v(t)(E_k - E_l))\} |k\rangle \langle l|. \quad (34) \]

Invoking the special properties of Gaussian statistics\(^3\) it can be shown that

\[ \exp \{-i(v(t)(E_k - E_l))\} = \exp \left\{ -i(E_k - E_l)v(t) - \frac{(E_k - E_l)^2}{2} \left[v(t)^2 - \bar{v}(t)^2\right] \right\}. \tag{35} \]

Thus, the exact ensemble-average dynamics is given by the elements of the average density matrix:

\[ \rho_{kk}(t) = \rho_{kk}(t_0), \quad (36) \]
\[ \rho_{kl}(t) = \rho_{kl}(t_0) \exp \left\{ -i(E_k - E_l)v(t) - \frac{(E_k - E_l)^2}{2} \left[v(t)^2 - \bar{v}(t)^2\right] \right\}. \tag{37} \]

Now let us solve the same problem by the master equation approach. Using the results from Eqs.\((25-26)\), the following expression is obtained,

\[ i\hbar \frac{\partial}{\partial t} \rho(t) = [\hat{a}(t)\hat{\rho}, \rho(t)] \]
\[ + i\hbar \left[ \int_{t_0}^{t} dt' \hat{a}(t') - \int_{t_0}^{t} dt' \hat{a}(t')\hat{a}(t') \right] \left( \hat{\rho}^2(t) + \rho(t)\hat{\rho}^2 \right) \]
\[ + 2i\hbar \left[ \int_{t_0}^{t} dt' \hat{a}(t')\hat{a}(t') - \hat{a}(t)\int_{t_0}^{t} dt' \hat{a}(t') \right] \hat{\rho}(t)\hat{\rho}, \tag{38} \]

which can be simplified to

\[ \frac{\partial}{\partial t} \rho(t) = -i\bar{a}(\bar{a})(\hat{\rho}, \rho(t)) + D(t) \left[ \hat{\rho}, [\hat{\rho}, \rho(t)] \right], \tag{39} \]

where

\[ D(t) \equiv \bar{a}(\bar{a}) \int_{t_0}^{t} dt' \hat{a}(t') - \int_{t_0}^{t} dt' \hat{a}(t')\hat{a}(t'). \tag{40} \]

To find the solution to this differential equation, we first write it down in terms of the matrix elements in the \(\hat{a}\)-eigenbasis:

\(^3\)Since \(v(t)\) is a linear filtered Gaussian random process, it is a Gaussian random process itself. (See page 83 of Ref.\([10]\).)
\[
\frac{\partial}{\partial t} \rho_{kk}(t) = 0, \quad (41)
\]
\[
\frac{\partial}{\partial t} \rho_{kl}(t) = \left[-ia(t)(E_k - E_l) + D(t)(E_k - E_l)^2\right] \rho_{kl}(t), \quad (k \neq l). \quad (42)
\]
Now we have a set of (de-coupled) linear ordinary differential equations (ODE’s), which is easily solvable,

\[
\rho_{kk}(t) = \rho_{kk}(t_0), \quad (43)
\]
\[
\rho_{kl}(t) = \rho_{kl}(t_0) \exp \left\{ \int_{t_0}^{t} dt' \left[ -ia(t')(E_k - E_l) + D(t')(E_k - E_l)^2 \right] \right\} = \rho_{kl}(t_0) \exp \left\{ -i(E_k - E_l)\bar{v}(t) - \frac{(E_k - E_l)^2}{2} \left[ \bar{v}(t)^2 - v(t)^2 \right] \right\}. \quad (44)
\]

The second equality in Eq.(44) is obtained after some calculation, where \(v(t)\) is given by Eq.(32). Thus we find the dynamics generated by the 2nd-order master equation coincides with the exact dynamics in this case.

We observe that the energy population is conserved during the evolution while the coherence between different energy levels decays. Thus the evolution of the average dynamics is pure decoherence, with the “pointer basis” \([12]\) being the energy-eigenbasis. Note that, although the Hamiltonian varies with time and across different realizations, the energy-eigenbasis is the same throughout. In the case where some energy level is degenerate, we readily have a “decoherence-free subspace”, in which quantum information can be stably stored \([14]\). Incidentally, a derivation in the context of open systems also suggests that energy eigenstates can emerge as “pointer states” in the so-called “quantum limit of decoherence” \([15]\). In that case, however, the decoherence results from small environmental perturbation to the system, not from the fluctuation of the system Hamiltonian itself.

We could have worked out the higher-order terms (i.e. \(L_n[\rho]\) for \(n \geq 3\)) explicitly to see how accurate the 2nd-order approximation is. However, since the solution to the 2nd-order master equation coincides with the exact dynamics, we can readily conclude that all higher-order terms must sum up to zero without actually carrying out further calculations.

Note that when deriving Eq.(39) we do not assume anything about the nature of the random process \(a(t)\), not even the Gaussian statistics. In other words, the solution to the 2nd-order master equation is given by Eqs.(43-44) in all cases. On the other hand, the exact dynamics Eqs.(36-37) is based on the assumption of Gaussian statistics. If \(a(t)\) is not a Gaussian random process, then the exact dynamics will be different. \(^4\) The implication is that, for \(a(t)\) being non-Gaussian, the 2nd-order master equation is not exact.

\[^{4}\text{It may not be exactly solvable, but we know for sure that the solution is different from that in the Gaussian case.}\]
3.3 Multiple jointly circular complex Gaussian random processes

Let us briefly present the results for the more general Hamiltonian \( \hat{H}(t) = \hbar \sum_n \left( a_n(t) \hat{h}_n + a_n^*(t) \hat{h}_n^\dagger \right) \), where \( a_n(t) \) are jointly circular complex Gaussian random processes of zero mean. The 2nd-order master equation in Lindblad form is found to be

\[
\frac{\partial}{\partial t} \rho(t) = - \sum_{k,l} \alpha_{kl}(t) \left[ [\hat{h}_k, \hat{h}_l^\dagger], \rho(t) \right] + \sum_{k,l} \beta_{kl}(t) \\
\times \left\{ - \hat{h}_k \hat{h}_l^\dagger \rho(t) - \rho(t) \hat{h}_k \hat{h}_l^\dagger + 2 \hat{h}_l \hat{h}_k \rho(t) \hat{h}_l^\dagger - \rho(t) \hat{h}_l^\dagger \hat{h}_k - \hat{h}_l^\dagger \hat{h}_k \rho(t) - \rho(t) \hat{h}_k \hat{h}_l + 2 \hat{h}_k \hat{h}_l \rho(t) \hat{h}_k^\dagger \right\},
\]

(45)

where

\[
\alpha_{kl}(t) \equiv \frac{1}{2} \int_{t_0}^t dt' \left( a_k(t)a_l^\dagger(t') - a_k^\dagger(t)a_l(t') \right), \hspace{1cm} (46)
\]

\[
\beta_{kl}(t) \equiv \frac{1}{2} \int_{t_0}^t dt' \left( a_k(t)a_l^\dagger(t') + a_k^\dagger(t)a_l(t') \right). \hspace{1cm} (47)
\]

By comparing with Eq. (29) for the time-independent Hamiltonian case, we notice a major difference in this case is that the effective Hamiltonian is non-zero despite \( \hat{H}(t) = 0 \). This effective unitary evolution results from the fact that the Hamiltonian operators at different times do not commute with each other in general.

The 2nd-order master equation yields exact dynamics only for the special case of a single real Gaussian random process. In this more general case, Eq. (45) does not lead to exact dynamics in general. This can be shown by explicitly evaluating higher-order terms like \( \mathcal{L}_4[\rho] \) to find that they do not vanish in general.

Despite the lack of perfect agreement, the master equation is nevertheless of great use in such cases, because the exact dynamics is generally not obtainable and the 2nd-order master equation serves as a good approximation when the higher-order terms (e.g. \( \mathcal{L}_4[\rho] \)) are small compared to \( \mathcal{L}_2[\rho] \).

4 Physical examples

We will illustrate the general results by applying them to a few examples. The findings will then be used to gain physical insights, and the validity of the master equation approach will be examined by comparing to the exact dynamics.
4.1 Two-level system

First consider a two-level system (e.g. spin-1/2) subject to the Hamiltonian
\[ \hat{H}(t) = \hbar \omega(t) \hat{Z}, \]
where \( \hat{Z} \) is the \( z \)-component of Pauli operator and \( \omega(t) \) a stationary Gaussian random process of zero mean. This falls into the category of Hamiltonians (30). Using Eq.(39), the 2nd-order master equation is obtained,
\[ \frac{\partial}{\partial t} \rho(t) = -\frac{1}{4} d(t) \left[ \hat{Z}, [\hat{Z}, \rho(t)] \right], \]
where \( d(t) \equiv 4 \int_{t_0}^{t} dt' \omega(t)\omega(t') \). Assuming an auto-correlation function of the form \( \omega(t)\omega(t') = \overline{\omega^2} \exp \left( -|t-t'|/T \right) \), where \( \overline{\omega^2} \equiv \overline{\omega(t)^2} \), we have \( d(t) = 4\overline{\omega^2} T \left( 1 - e^{-(t-t_0)/T} \right) \) for \( t > t_0 \).

Written in the \( \hat{Z} \)-eigenbasis \( \{ |0\rangle, |1\rangle \} \), the master equation becomes a set of linear ODE's:
\[
\begin{align*}
\frac{\partial}{\partial t} \varrho_{00}(t) & = 0, \\
\frac{\partial}{\partial t} \varrho_{11}(t) & = 0, \\
\frac{\partial}{\partial t} \varrho_{01}(t) & = -d(t)\varrho_{01}(t), \\
\frac{\partial}{\partial t} \varrho_{10}(t) & = -d(t)\varrho_{10}(t); 
\end{align*}
\]
the solutions to which are
\[
\begin{align*}
\varrho_{00}(t) & = \rho_{00}(t_0), \\
\varrho_{11}(t) & = \rho_{11}(t_0), \\
\varrho_{01}(t) & = \rho_{01}(t_0) \exp \left\{ -4\overline{\omega^2} T^2 \left( \frac{t-t_0}{T} + e^{-(t-t_0)/T} - 1 \right) \right\}, \\
\varrho_{10}(t) & = \rho_{10}(t_0) \exp \left\{ -4\overline{\omega^2} T^2 \left( \frac{t-t_0}{T} + e^{-(t-t_0)/T} - 1 \right) \right\}. 
\end{align*}
\]
As already discussed in the general case of a single Gaussian random process, the energy population remains constant while the coherence decays. This can be understood from a more physical perspective. Quantum coherence depends on the relative phase between the two components \( |0\rangle \) and \( |1\rangle \). In an individual realization, the relative phase factor is \( \exp \left\{ 2i \int_{t_0}^{t} dt' \omega(t') \right\} \). Since \( \omega(t) \) is a random process, the quantity \( \int_{t_0}^{t} dt' \omega(t') \) becomes increasingly randomized with the passage of time. When the average is taken over an ensemble, these randomly distributed relative phase factors cancel out, thus suppressing the coherence. This suggests that quantum interference is difficult to observe because random fluctuation is ubiquitous.
As has been shown in the more general case Eqs. (43-44), the 2nd-order master equation gives exact dynamics. When we work out the exact dynamics directly, the result is indeed found to be consistent, though such a direct calculation is more demanding. Clearly, calculational convenience is one advantage of the master equation approach.

4.2 A pair of two-level systems in magnetic field

Next consider an example of two atoms in magnetic field, each atom being a two-level system. The interaction of the spin with the B-field is given by

\[ \hat{H}(t) = \hbar \Omega(t) \left( \hat{Z}^I \otimes \hat{Z}^II + \hat{Z}^I \otimes \hat{Z}^II \right) \equiv \hbar \Omega(t) \hat{Z}_{\text{total}}, \]

where \( \hat{Z}^j \) is the usual Pauli \( z \)-operator of the \( j \)-th atom. Suppose that the frequency \( \Omega(t) \), which is proportional to the B-field strength, is a stationary Gaussian random process of zero mean and that its auto-correlation is of a Markovian type

\[ \Omega(t)\Omega(t') = \frac{1}{8} \gamma \delta(t-t'), \]

where the constant \( \gamma \) has dimension of inverse-time. Applying Eq. (39), it can be shown that the 2nd-order master equation is

\[ \frac{\partial}{\partial t} \rho(t) = -\frac{1}{16} \gamma \left[ \hat{Z}_{\text{total}}, \left[ \hat{Z}_{\text{total}}, \rho(t) \right] \right]. \quad (57) \]

Suppose the system starts in an entangled state between two atoms \( | \Psi(t_0) \rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \). Since it is an eigenstate of \( \hat{Z}_{\text{total}} \), the right-hand side of Eq. (57) is identically zero, thus the system does not evolve (except possibly to an unobservable global phase). So the two atoms remain entangled over time. Indeed, notice that \( |01\rangle \) and \( |10\rangle \) are degenerate eigenstates with the same energy. Thus any arbitrary superposition state of \( |01\rangle \) and \( |10\rangle \) will remain unchanged over time; in particular, the coherence between them does not decay. Thus, any state in this degenerate subspace is immune to decoherence, making it a good place to store quantum information [14].

Let us see what happens if the 2-atom system starts in a different entangled state like \( | \Psi(t_0) \rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \). Writing the master equation in the energy eigenbasis \( \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \} \), we obtain a set of decoupled linear ODE’s as usual. The solutions are found to be

\[ \rho_{00,00}(t) = \rho_{11,11}(t) = \frac{1}{2}, \quad (58) \]

\[ \rho_{00,11}(t) = \rho_{11,00}(t) = \frac{1}{2} \exp \{-\gamma(t-t_0)\}, \quad (59) \]

while the rest of the matrix elements are identically zero. Note that decoherence occurs here, as is expected, since the initial state does not lie in the decoherence-free subspace. Furthermore, as \( t \to \infty \), the coherence is suppressed to zero and \( \rho(t) \to \frac{1}{2} |00\rangle \langle 00| + \frac{1}{2} |11\rangle \langle 11| = \frac{1}{2} |0\rangle \langle 0| \otimes |0\rangle \langle 0| + \frac{1}{2} |1\rangle \langle 1| \otimes |1\rangle \langle 1|. \) Interestingly, the two atoms become disentangled, as there is no quantum correlation between them. In contrast to the general belief that entanglement leads to decoherence, as is widely studied for open quantum systems, here we find that decoherence can result in disentanglement in the case of a closed system.
4.3 Heating of a trapped ion

Consider an ion with mass $M$ and charge $e$ in a harmonic binding potential with characteristic frequency $\omega_0$. The ion is driven by a classical electric field $E(t)$, which is a stationary Gaussian random process of zero mean. It is more convenient to work in the interaction picture, in which the easily solvable, deterministic evolution induced by the harmonic potential is treated separately.

The interaction-picture Hamiltonian\footnote{Throughout this section we work in the interaction picture. The subscripts to denote interaction-picture operators are dropped for notational simplicity.} is given by $\hat{H}(t) = i\hbar \left[ u(t)\hat{a}^\dagger - u^*(t)\hat{a} \right]$, where $u(t) = ieE(t)e^{i\omega_0 t}/\sqrt{2M\hbar\omega_0}$ and $\hat{a}$ ($\hat{a}^\dagger$) being the zero-time annihilation (creation) operator for the harmonic oscillator. The evolution is exactly solvable and the analytic results are given in [11].

Let us derive the 2nd-order master equation for this case. Note that it does not fall into the category of a single real Gaussian random process as in Eq.(30).

Since $\hat{H} = 0$, applying Eq.(25), the effective Hamiltonian is found to be

$$\hat{H}_{\text{eff}} = \frac{1}{2} \int_{t_0}^{t} dt' \left( u(t)u^*(t') - u^*(t)u(t') \right) [\hat{a}, \hat{a}^\dagger]$$

$$= -\frac{e^2}{2M\omega_0} \int_{t_0}^{t} dt' E(t)E(t') \sin [\omega_0(t - t')] \hat{I}. \quad (60)$$

In this case, the 2nd-order contribution to the effective Hamiltonian is non-zero, a consequence of the non-commutativity of $\hat{H}(t)$ and $\hat{U}_1(t)$. However, since $\hat{H}_{\text{eff}}$ is proportional to $\hat{I}$, the unitary part of the equation of motion results only in an unobservable global phase in this case. For more general cases, $\hat{H}_{\text{eff}}$ can be different from the identity $\hat{I}$ and can well lead to non-trivial dynamics. Evaluating the remaining terms in Eq.(23) for this example, we find the following master equation:

$$\frac{\partial}{\partial t} \hat{p}(t) = -\mathcal{C}(t) \left( \hat{a}^\dagger \hat{a} \hat{p}(t) + \hat{p}(t)\hat{a}^\dagger \hat{a} - 2\hat{a} \hat{p}(t)\hat{a}^\dagger \right)$$

$$-\mathcal{C}(t) \left( \hat{a}^\dagger \hat{a} \hat{p}(t) + \hat{p}(t)\hat{a}^\dagger \hat{a} - 2\hat{a} \hat{p}(t)\hat{a}^\dagger \right)$$

$$-e^{2i\omega_0 t} \left[ \mathcal{C}(t) - iS(t) \right] \left( (\hat{a}^\dagger)^2 \hat{p}(t) + \hat{p}(t)\hat{a}^\dagger \hat{a}^\dagger - 2\hat{a}^\dagger \hat{p}(t)\hat{a}^\dagger \right)$$

$$-e^{-2i\omega_0 t} \left[ \mathcal{C}(t) + iS(t) \right] \left( \hat{a}^2 \hat{p}(t) + \hat{p}(t)\hat{a}^\dagger \hat{a}^\dagger - 2\hat{a} \hat{p}(t)\hat{a} \right), \quad (61)$$

where $\mathcal{C}(t)$ ($S(t)$) are proportional to the incomplete cosine (sine) transform of...
the field correlation function, viz

\[
C(t) \equiv \frac{e^2}{2M\hbar\omega_0} \int_{t_0}^{t} dt' E(t)E(t') \cos[\omega_0(t-t')],
\]

(62)

\[
S(t) \equiv \frac{e^2}{2M\hbar\omega_0} \int_{t_0}^{t} dt' E(t)E(t') \sin[\omega_0(t-t')].
\]

(63)

Assuming \( E(t)E(t') = E(0)^2 \exp(-|t-t'|/T) \) and setting \( t_0 = 0 \) for convenience, we find \( C(t) = (1/2\tau_1) \{ e^{-t/T} [\omega_0 T \sin(\omega_0 t) - \cos(\omega_0 t)] + 1 \} \) and \( S(t) = -(1/2\tau_1) \{ e^{-t/T} [\sin(\omega_0 t) + \omega_0 T \cos(\omega_0 t)] - \omega_0 T \} \), where \( \tau_1 \) is the heating time defined as \( 1/\tau_1 = (e^2 E(0)^2/M\hbar\omega_0) (T/(1 + \omega_0^2 T^2)) \).

Unlike the case of Eq. (30), the 2nd-order master equation does not generate exact dynamics in this case. To get an approximation of the heating from the ground state (i.e. \( \rho_{00}(0) = 1 \)) for a short period of time, let us write the master equation in the energy eigenbasis of the harmonic oscillator,

\[
\frac{\partial}{\partial t} \bar{\rho}_{00}(t) = -2C(t)\bar{\rho}_{00}(t) + 2C(t)\bar{\rho}_{11}(t)
- \sqrt{2}e^{2i\omega_0 t} \left( C(t) - iS(t) \right) \bar{\rho}_{02}(t)
- \sqrt{2}e^{-2i\omega_0 t} \left( C(t) + iS(t) \right) \bar{\rho}_{20}(t).
\]

(64)

Since \( \bar{\rho}_{11}(t) \), \( \bar{\rho}_{02}(t) \) and \( \bar{\rho}_{20}(t) \) are all negligibly small for \( t \ll T, 1/\omega_0 \), we have \( \frac{\partial}{\partial t} \bar{\rho}_{00}(t) \cong -2C(t)\bar{\rho}_{00}(t) \) to the lowest order. In the same manner, since the depopulation \( 1 - \bar{\rho}_{00}(t) \) is perturbatively small, we have \( \bar{\rho}_{00}(t) \cong 1 \) to the lowest order on the right-hand side. Thus an approximate differential equation is obtained as \( \frac{\partial}{\partial t} \bar{\rho}_{00}(t) \cong -2C(t) \). Solving this ODE, we find, to lowest order \(^6\)

\[
1 - \bar{\rho}_{00}(t) \cong 2 \int_{0}^{t} dt' C(t') \cong \frac{e^2 E(0)^2}{2M\hbar\omega_0} t^2,
\]

(65)

which holds for short times and agrees with the analytic result in \([11]\).

To investigate the evolution of the system for longer times, we write down the master equation in the same basis and solve it numerically. Since the Hilbert space is of infinite dimensions, it is not possible to write down the complete set of ODE's for the matrix elements. Instead, we truncate it to a set of 5 \times 5 coupled ODE's that includes only the matrix elements of the five lowest energy-eigenstates and their coherence\(^7\). The numerical solutions of \( F(t) \equiv \bar{\rho}_{00}(t) \)

\(^6\)The same result can be obtained by working out the evolution of \( \bar{\rho}_{11}(t) \) for \( t \ll T, 1/\omega_0 \) using approximation to the same order.

\(^7\)Since the system is of continuous nature, we could have solved the master equation in the Wigner representation. However, that approach is not analytically solvable either and is not computationally economical. Furthermore, even in that case, we still have to accept the imperfection of truncation since the numerics can only be done on a finite region of the “phase space”.

14
(i.e. fidelity of the ground state) are shown in Figure 1 for different sets of parameters. It can be seen that, as $\omega_0\tau_1$ (i.e. the dimensionless heating time) increases with $\omega_0 T$ (i.e. the dimensionless coherence time of $E(t) E(t')$) fixed, the numerical result gives better approximation to the exact dynamics. Also note that, for larger values of $\omega_0 T$, the ground state population shows temporary revival against its general trend of decrease.

Despite the artificial defect caused by the truncation of the set of ODE’s, it is of more interest to know the validity of the 2nd-order master equation itself in approximating the exact dynamics. This is done by comparing the size of higher-order terms to that of the 2nd-order term. Using the Gaussian moment theorem\[10\], it is easy to show that $\mathcal{L}_n[\rho] = 0$ for all odd numbers $n$, so we are interested in the ratios between the even-number-order terms. Assuming $\omega_0 T$ is fixed, it can be shown that $\mathcal{L}_4[\rho] \propto 1/\tau_1^2\omega_0$ as opposed to $\mathcal{L}_2[\rho] \propto 1/\tau_1$, so $\mathcal{L}_4[\rho]/\mathcal{L}_2[\rho] \propto 1/\omega_0\tau_1$. The same ratio holds for $\mathcal{L}_6[\rho]/\mathcal{L}_4[\rho]$, etc. Therefore, as long as $1/\omega_0\tau_1$ is small, the higher-order terms become progressively small, lending legitimacy to the 2nd-order approximation. This is also consistent with the previous observation from the numerical results. Physically, this can be better understood by switching to the Schrödinger picture: The external field $H_{\text{field}} \propto 1/\tau_1$ is treated as a perturbation to the self-Hamiltonian of the system $H_{\text{self}} \propto \omega_0$. Naturally, as the relative size of the perturbing Hamiltonian
$H_{\text{self}}/H_{\text{field}} \propto 1/\omega_0 \tau_1$ becomes smaller, a perturbative method such as the 2nd-order master equation gives better approximation to the exact dynamics.

5 Conclusion

In this paper we have presented the derivation of a master equation for closed systems driven by stochastic Hamiltonians from an ensemble-average perspective. The principal result is given in Eqs. (25-26). The validity of this approach is examined and 2nd-order master equation is found to yield either exact dynamics or good approximations to exact dynamics.

Applying the formalism to various physical examples, we find the ensemble-average dynamics usually contains decoherence terms in addition to the unitary evolution. Decoherence plays an important role in the foundational problems of quantum mechanics, as it gives insights in two aspects of the measurement problem, namely the absence of observable superposition and the problem of preferred basis [12]. Extensive research has been done on how environmental entanglement causes decoherence in open systems. However, as our findings suggest, decoherence could also be attributed to the random fluctuations of physical quantities in closed systems. If this is true, then the tension between the classicality of our experience and the quantumness of the underlying laws of physics could be reconciled in some degree by the ubiquitous random fluctuations. Further investigation is needed to find out (a) to what extent decoherence is actually caused by random fluctuations and (b) whether/how we can distinguish it from the usual entanglement-induced decoherence through physical observation.

Acknowledgements

The authors would like to thank O. Gamel for valuable discussions and C.-H. Chang for comments on the manuscript. This work is supported by Natural Sciences and Engineering Research Council of Canada (NSERC) through CREATE and by University of Toronto through UTEA-NSE.

References

[1] A. A. Budini, Phys. Rev. A 64, 052110 (2001).
[2] S. Guha, G. Sanyal, S. H. Mandal, and D. Mukherjee, Phys. Rev. E 47, 2336 (1993).
[3] O. Gamel and D. F. V. James, Phys. Rev. A 82, 052106 (2010).
[4] H.-P. Breuer and F. Petruccione, The Theory of Open Quantum Systems (Oxford University Press, 2002).
[5] R. Shankar, Principles of Quantum Mechanics (Springer, 2nd edition, 1994), p. 488.
[6] M. Choi, Linear Algebra and Its Applications, 10, 285-290 (1975).

[7] J. Preskill, Quantum computation, Lecture Notes, available at [http://www.theory.caltech.edu/people/preskill/ph229/](http://www.theory.caltech.edu/people/preskill/ph229/) California Institute of Technology, Pasadena, CA, 1998.

[8] A. Messiah, Quantum Mechanics (Dover, 1999), p. 321.

[9] B. H. Bransden and C. J. Joachain, Physics of Atoms and Molecules (Benjamin Cummings, 2 edition, 2003), p. 469.

[10] J. W. Goodman, Statistical Optics (John Wiley and Sons, New York, 1985).

[11] D. F. V. James, Phys. Rev. Lett. 81, 317-320 (1998).

[12] M. Schlosshauer, Decoherence and the Quantum-to-Classical Transition (Springer, 2007).

[13] M. B. Plenio and P. L. Knight, Rev. Mod. Phys. 70, 101 (1998).

[14] D. A. Lidar, I. L. Chuang, and K. B. Whaley, Phys. Rev. Lett. 81, 2594 (1998).

[15] J. P. Paz and W. H. Zurek, Phys. Rev. Lett. 82, 5181-5185 (1999).