Self-consistent non-Markovian theory of a quantum state evolution for quantum information processing

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It is shown that the operator sum representation for non-Markovian dynamics and the Lindblad master equation in Markovian limit can be derived from a formal solution to quantum Liouville equation for a qubit system in the presence of decoherence processes self-consistently. Our formulation is the first principle theory based on projection-operator formalism to obtain an exact reduced density operator in time-convolutionless form starting from the quantum Liouville equation for a noisy quantum computer. The advantage of our approach is that it is general enough to describe a realistic quantum computer in the presence of decoherence provided details of the Hamiltonians are known.

PACS number(s): 03.67.-a, 89.70.+c

Dynamics of a quantum system coupled to an environment has been studied extensively for potential applications to quantum computing and quantum information processing recently [1–4]. The key element of the studies is the reduced-density-operator which is a solution to quantum Liouville equation (QLE). The QLE would involve Hamiltonians for systems representing qubits, reservoir, and mutual interaction between the system and reservoir that causes decoherence [5]. The presence of decoherence would be the most important obstacle to the ideal operations of quantum gates or quantum channels [6]. To overcome this difficulty, the quantum error correcting codes [7] and the decoherence free subspaces [8] of multiple qubit systems have been suggested. For both quantum error correcting codes and decoherence free subspaces the knowledge of the reduced density operator of the qubit system is essential.

Up to now the information about the reduced density operator is obtained from Lindblad master equation [3,9] in Markovian approximation or an operator sum representation (OSR) [10] in the non-Markovian case which is also known as Kraus representation. Even though the OSR provides better information about the qubit system than the Markovian formalism, somewhat surprisingly, as pointed out by Bacon et al. [11], the former is obtained in the language of gates, i.e., the unitary transformation, rather than from the solution to the QLE itself in the Hamiltonian formulation. In other words, most of the proposals for quantum computers or quantum gates have assumed particular forms of the unitary transformations beforehand. In our opinion, it would be desirable if there is a way to obtain the direct solution for the reduced density operator from the QLE to model physical implementations of the quantum computers.

The QLE is an integro-differential equation and, in general, it is nontrivial to obtain the solution of the form

$$\dot{\rho} = \mathcal{E}[\rho]$$

where $\rho$ is the reduced density operator and $\mathcal{E}$ is the superoperator of linear mapping. The superoperator $\mathcal{E}$ is not necessarily a unitary transformation if one considers an open system interacting with a reservoir in the presence of decoherence processes. Sometime ago we studied the time-convolutionless reduced density operator formulation to model quantum devices [12,13] and noisy quantum channels [14]. In this theory the memory kernels of the Volterra-type integral equation are solved self-consistently using the superoperator formalism and it was shown that both non-Markovian decoherence process and renormalization of the memory effects can be incorporated.

In this paper we formulate a general non-Markovian theory based on a QLE and show that the OSR for the non-Markovian case and the Lindblad master equation approach within the Markov approximation can be derived self-consistently.

The Hamiltonian of the total system is assumed to be

$$\hat{H}_t(t) = \hat{H}_s(t) + \hat{H}_b + \hat{H}_{\text{int}},$$

where $\hat{H}_s(t)$ is the Hamiltonian of the system, $\hat{H}_b$ the reservoir, and $\hat{H}_{\text{int}}$ the Hamiltonian for the interaction of the system with the reservoir. Note that the system Hamiltonian $\hat{H}_s(t)$ may contain time-dependent external field terms to control the qubit system. The equation of motion for density operator $\hat{\rho}_t$ of the total system is given by a QLE as

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

where $\mathcal{L}_t(t) = \mathcal{L}_s(t) + \mathcal{L}_b + \mathcal{L}_{\text{int}}$ is the Liouville operator. The Liouville operators are in one-to-one correspondence with the Hamiltonians. Here we use a unit of
where \( U \) substituting Eq. (9) can be put into time-convolutionless form by sub-
olution operator \( H \). The projected propagator by [12–14]
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and \( Q \) are defined as
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and \( Q \) are defined as
h = 1. The reservoir is assumed to be in the thermal
state. However, the assumption may be extended to any
time-independent reservoir states which commutes with
the reservoir Hamiltonian, i.e., \( \mathcal{L}_b \hat{\rho}_b = 0 \). In order to
derive and to solve an equation for the system alone, we
employ the projection-operators [15,16] that decompose
the total system by eliminating the degrees of freedom for
the reservoir. Time-independent projection-operators \( P \)
and \( Q \) are defined as
\[
\mathcal{P} \hat{X} = \hat{\rho}_b \text{Tr}_b(\hat{X}), \quad \mathcal{Q} = 1 - \mathcal{P},
\]
for any dynamical variable \( \hat{X} \). Here \( \text{Tr}_b \) indicates a par-
tial trace over the quantum reservoir. The information of
the system is contained in the reduced density operator
\( \hat{\rho}(t) \) given by
\[
\hat{\rho}(t) = \text{Tr}_b \hat{\rho}_b(t) = \text{Tr}_b \mathcal{P} \hat{\rho}_b(t).
\]
After some mathematical manipulations, the time convo-
lutionless equation of motion for \( \mathcal{P} \hat{\rho}_b(t) = \hat{\rho}_b \hat{\rho}(t) \) is given by [12–14]
\[
\frac{d}{dt} \mathcal{P} \hat{\rho}_b(t) = -i \mathcal{P} \mathcal{L}_t(t) \mathcal{P} \hat{\rho}_b(t) + i \mathcal{P} \mathcal{L}_t(t) (\mathcal{N}(t) - 1) \mathcal{P} \hat{\rho}_b(t),
\]
where
\[
\mathcal{N}^{-1}(t) = 1 + i \int_0^t d\tau \mathcal{H}(t, \tau) \mathcal{Q} \mathcal{L}_t(\tau) \mathcal{P} \mathcal{G}(t, \tau).
\]
The projected propagator \( \mathcal{H}(t, \tau) \) and the anti-time evolu-
tion operator \( \mathcal{G}(t, \tau) \) of the total system are defined as
\[
\mathcal{H}(t, \tau) = T \exp \left\{ -i \int_\tau^t d\tau ' \mathcal{Q} \mathcal{L}_t(\tau) \mathcal{P} \right\},
\]
and
\[
\mathcal{G}(t, \tau) = T^c \exp \left\{ i \int_\tau^t d\tau ' \mathcal{L}_t(\tau) \mathcal{P} \right\},
\]
where \( T \) and \( T^c \) denote the time ordering and the anti-
time ordering operators respectively. The formal solution
to Eq. (6) is given by [14]
\[
\mathcal{P} \hat{\rho}_b(t) = \mathcal{U}(t, 0) \mathcal{P} \hat{\rho}_b(0) - i \int_0^t d\tau \, \mathcal{U}(t, \tau) \mathcal{P} \mathcal{L}_t(\tau) \mathcal{N}(s) \mathcal{P} \hat{\rho}_b(s),
\]
where the projected propagator \( \mathcal{U}(t, \tau) \) of the system is
defined by
\[
\mathcal{U}(t, \tau) = T \exp \left\{ -i \int_\tau^t d\tau ' \mathcal{P} \mathcal{L}_t(\tau) \right\}.
\]
Eq. (9) can be put into time-convolutionless form by sub-
stituting
\[
\hat{\rho}_b(s) = \mathcal{G}(t, s) \hat{\rho}_b(t)
\]
and after some mathematical manipulations, we obtain the
reduced density operator \( \hat{\rho}(t) \), which is an exact
solution to the QLE, given in the form of Eq. (1),
\[
\hat{\rho}(t) = \mathcal{E}(t) \hat{\rho}(0) = \mathcal{W}^{-1}(t) \mathcal{U}_s(t, 0) \hat{\rho}(0),
\]
with
\[
\mathcal{W}(t) = 1 + i \int_0^t ds \, \mathcal{U}_s(s, t) \mathcal{P} \mathcal{L}_t(s) \mathcal{Q} \mathcal{L}_t(0) \mathcal{P} \hat{\rho}(0) \mathcal{G}(t, 0) \mathcal{L}_t(0) \mathcal{P} \mathcal{G}(t, s) \mathcal{P} \hat{\rho}(s).
\]
Here, we define
\[
\mathcal{Z}(t) = 1 - N^{-1}(t),
\]
\[
\mathcal{U}_s(t, \tau) = T \exp \left\{ i \int_\tau^t d\tau ' \mathcal{L}_s(\tau) \mathcal{P} \right\},
\]
\[
\mathcal{U}_0(t, \tau) = \exp \left\{ -i (t - \tau) \mathcal{L}_b \mathcal{P} \right\},
\]
and
\[
\mathcal{R}(t, \tau) = T^c \exp \left\{ i \int_\tau^t d\tau ' \mathcal{L}_0^{-1}(\tau) \mathcal{L}_s(0) \mathcal{L}_t \mathcal{P} \right\},
\]
where \( \mathcal{U}_0(t, \tau) \) is the non-interacting time-evolution
operator of the system and the reservoir and \( \mathcal{R}(t, \tau) \) is the
anti-time evolution operator of the total system in the
interaction picture [13,14].

It is straightforward to obtain the time-convolutionless
equation of motion for a reduced density operator \( \hat{\rho}(t) \). From
Eq. (6), we get
\[
\frac{d}{dt} \hat{\rho}(t) = -i \mathcal{L}_s(\hat{\rho}(t) + \mathcal{C}(t) \hat{\rho}(t),
\]
with
\[
\mathcal{C}(t) = -i \text{Tr}_b \left\{ \mathcal{L}_t \mathcal{Z}(t) (1 - \mathcal{Z}(s))^{-1} \hat{\rho}_b \right\}
\]
where \( \mathcal{C}(t) \) is a generalized collision operator and we use
an anzatz \( \mathcal{P} \mathcal{L}_t \mathcal{P} = 0 \) which is equivalent to neglect
renormalization of the unperturbed energy of the system
[16].

In the following, we first show that the time-
convolutionless equation of motion (19) becomes the
Lindblad master equation in the Markov approximation.
The lowest-order Born approximation, which is valid up
to the order \( (\mathcal{H}_\text{int})^2 \), is used subsequently. The effect of
\( \mathcal{C}(t) \) on \( \hat{\rho}(t) \) up to the second-order expansion becomes
\[
\mathcal{C}^{(2)}(t) \hat{\rho}(t) = - \int_0^t d\tau \, \text{Tr}_b \left\{ \mathcal{H}_\text{int}, \left[ \mathcal{H}_\text{int}(\tau - t), \hat{\rho}_b \hat{\rho}(t) \right] \right\},
\]
and
where $\hat{H}_{\text{int}}(t)$ is the Heisenberg transformation of $\hat{H}_{\text{int}}$ defined by $U_0(t)\hat{H}_{\text{int}}$. For the specific form of the interaction Hamiltonian, we assume a Caldeira-Leggett-type model [17,18] given by

$$\hat{H}_{\text{int}} = \sum_{\alpha} \hat{v}_\alpha \otimes \hat{b}_\alpha$$

(22)

where $\hat{v}_\alpha$ is the Hermitian operator acting on the system and $\hat{b}_\alpha = \sum_k (g_{\alpha k} \hat{a}_k^\dagger + g_{\alpha k}^* \hat{a}_k)$ is a fluctuating bosonic quantum field whose unperturbed motion is governed by the harmonic oscillator Hamiltonian for the reservoir,

$$\hat{H}_b(t) = \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k.$$  

(23)

The set of operators $\{\hat{v}_\alpha\}$ describes the various decoherence processes and sometimes they are denoted as the error generators. From Eqs. (21) and (22), we obtain

$$C^{(2)}(t)\hat{\rho}(t) = \sum_{\alpha,\beta} \int_0^t d\tau \chi_{\alpha\beta}(\tau-t)[\hat{v}_\beta(\tau-t)\hat{\rho}(t),\hat{v}_\alpha]$$

$$+ \sum_{\alpha,\beta} \int_0^t d\tau \chi_{\alpha\beta}(t-\tau)[\hat{v}_\alpha,\hat{\rho}(t)\hat{v}_\beta(\tau-t)]$$

(24)

where

$$\chi_{\alpha\beta}(t) = \text{Tr}_b \hat{b}_\alpha(t) \hat{b}_\beta \hat{\rho}_b = \text{Tr}_b \hat{b}_\alpha \hat{b}_\beta(-t) \hat{\rho}_b.$$  

(25)

The characteristic function $\chi_{\alpha\beta}(t)$ for the heat bath satisfies $\chi_{\alpha\beta}(t) = \chi_{\beta\alpha}^*(t)$. In the Markovian limit, it becomes

$$\chi_{\alpha\beta}(t) \approx \frac{1}{2} \gamma_{\alpha\beta} \delta(t).$$

(26)

Then, we get

$$C^{(2)}(t)\hat{\rho}(t) \approx \frac{1}{2} \sum_{\alpha,\beta} \gamma_{\alpha\beta} \{[\hat{v}_\alpha,\hat{\rho}(t),\hat{v}_\beta] + [\hat{v}_\alpha,\hat{\rho}(t)\hat{v}_\beta]\}$$

(27)

where $\gamma_{\alpha\beta}$ contains the information about the physical decoherence parameters. It is now obvious that Eq. (27) is equivalent to the Lindblad term $L_D$ described in Ref. [3], which takes into account the nonunitary, decohering dynamics.

We now proceed to prove that the OSR or the Kraus representation can be derived from the formal solution given in Eqs. (12) and (13). The evolution superoperator $\mathcal{E}(t)$ becomes

$$\mathcal{E}(t) = \left\{ 1 - i \int_0^t ds \ U_s(t,s) \text{Tr}_b \left[ L_{\text{int}} \mathcal{Z}^{(1)}(s) \hat{\rho}_b \right] U_s^{-1}(t,s) \right\} \times U_e(t,0)$$

(28)

with

$$\mathcal{Z}^{(1)}(s) = -i \int_0^s d\tau \ U_0(s,\tau) \mathcal{L}_{\text{int}} U_0^{-1}(s,\tau),$$

(29)

within the Born approximation. Substituting Eqs. (22) and (25) into Eq. (28), Eq. (12) becomes

$$\hat{\rho}(t) = U_e(t,0)\hat{\rho}(0) - U_e(t,0) \sum_{\alpha,\beta} \int_0^t ds \ \int_0^s d\tau$$

$$\times \left\{ \chi_{\alpha\beta}(\tau - s) [\hat{\rho}(0)\hat{v}_\beta(\tau)\hat{v}_\alpha(s) - \hat{v}_\alpha(s)\hat{\rho}(0)\hat{v}_\beta(\tau)]$$

$$+ \chi_{\alpha\beta}^*(\tau - s) [\hat{v}_\alpha(s)\hat{v}_\beta(\tau)\hat{\rho}(0) - \hat{v}_\beta(\tau)\hat{\rho}(0)\hat{v}_\alpha(s)] \right\}$$

(30)

The superoperator $\mathcal{E}^{(2)}(t)$ satisfies the following conditions: (i) trace-preserving, (ii) Hermiticity-preserving, and (iii) complete positivity. As a result, there exists a corresponding OSR [10]. We will find the OSR for $\mathcal{E}^{(2)}(t)$ in Eq. (28) although any order of perturbation is applicable based on our formulation. Let $\{\hat{K}_\alpha\}$ be the set of Kraus operators for $\hat{\rho}(t)$ described in Eq. (30), then

$$\hat{\rho}(t) = \mathcal{E}^{(2)}(t)\hat{\rho}(0) = \sum_{\alpha} \hat{K}_\alpha(t)\hat{\rho}(0)\hat{K}_\alpha^\dagger(t)$$

(31)

with the completeness relation, independent of the evolving time $t$,

$$\sum_{\alpha} \hat{K}_\alpha^\dagger(t)\hat{K}_\alpha(t) = 1.$$  

(32)

In order to derive explicit expressions for the superoperator $\mathcal{E}^{(2)}$, we employ the interaction picture for the time evolution of the system state as

$$\hat{\rho}(t) = \mathcal{E}^{(2)}(t)\hat{\rho}(0)$$

$$= U_s^{-1}(t,0)\mathcal{E}^{(2)}(t)\hat{\rho}(0)$$

$$= \sum_{\alpha} \hat{K}_\alpha(t)\hat{\rho}(0)\hat{K}_\alpha^\dagger(t).$$

(33)

To derive the set of Kraus operators $\{\hat{K}_\alpha\}$, we adopt a matrix representation for them. Then,

$$\mathcal{E}^{(2)} = \sum_{ab} \mathcal{E}_{nm}^{ab} \hat{e}_{ab},$$

(34)

with

$$\mathcal{E}_{nm}^{ab} = \langle \hat{e}_{ab}, \mathcal{E}^{(2)} \hat{e}_{nm} \rangle$$

(35)

where $\{\hat{e}_{ab}\}$ is an orthonormal basis set which spans the Hilbert-Schmidt space of reduced density operators. The Kraus operator is expanded in this basis as

$$\hat{K}_\alpha = \sum_{ab} \kappa_{ab} \hat{e}_{ab},$$

(36)

then,
Comparing Eqs. (34) and (37), we obtain
\[ \mathcal{E}_{nm}^{ab} = \sum_{\alpha} \kappa_{\alpha}^{an} \kappa_{\alpha}^{bm} \epsilon_{ab}. \]  

(38)

The conversion to \( \mathcal{E}^{(2)} \) is straightforward since \( \mathcal{U}(t) \) is unitary. From Eqs. (30) and (35), we get
\[ \mathcal{E}_{nm}^{ab} = \delta_{an} \delta_{bm} - B_{an} \delta_{bm} - \delta_{an} B_{bm} + A_{an, bm} \]  

(39)

where \( \delta_{an} \) is a Kronecker delta,
\[ B_{an} = \sum_{\alpha, \beta} \int_{0}^{t} d\tau \int_{0}^{s} d\tau' \chi_{\alpha \beta}^*(\tau - s) \langle a| \hat{v}_{\alpha}(s) \hat{v}_{\beta}(\tau)|n\rangle, \]  

(40)

\[ A_{an, bm} = \sum_{\alpha, \beta} \int_{0}^{t} d\tau \int_{0}^{s} d\tau' \chi_{\alpha \beta}(\tau - s) \times \langle a| \hat{v}_{\alpha}(s)|n\rangle \langle b| \hat{v}_{\beta}(\tau)|m\rangle^*. \]  

The set of Kraus operators are not unique and can be generated from a canonical set by an extended unitary matrix [10, 19, 2, 20]. We will obtain the canonical set of Kraus operators. The superoperator \( \mathcal{E}_{nm}^{ab} \) can be regarded as a positive and Hermitian matrix with \((a, n)\) being the row index and \((b, m)\) the column index [2]. Then, there exists some unitary matrix \( U_{an, \alpha} \) which diagonalizes \( \mathcal{E}_{nm}^{ab} \) as
\[ \mathcal{E}_{nm}^{ab} = \sum_{\alpha} U_{an, \alpha} d_{\alpha} U_{\alpha, bm}^*. \]  

(42)

Since all eigenvalues \( d_{\alpha} \) are positive, \( d_{\alpha} = \sqrt{d_{\alpha}} \sqrt{d_{\alpha}} \), and Eq. (42) is in the form of Eq. (38). One may choose \( \kappa_{\alpha}^{an} \) as
\[ \kappa_{\alpha}^{an} = \sqrt{d_{\alpha}} U_{an, \alpha}. \]  

(43)

All equivalent sets of Kraus operators for the given superoperator can be generated by “unitary remixing” of the canonical set with the eigenvalue vector \( d' \) extended by some arbitrary number of zeros as \( d' = (d, 0, ..., 0) \) [19].

In addition to the derivation from the canonical set, when the superoperator is already in the form of Eq. (38), the Kraus operators can be obtained more explicitly. As an example, let us consider a simple dephasing channel for a single qubit system where Hamiltonian is given by [21]
\[ \hat{H}_t = \frac{1}{2} \epsilon_0 \hat{\sigma}_z + \sum_{k} \omega_k \hat{a}_k^\dagger \hat{a}_k + \hat{\sigma}_z \hat{b} \]  

(44)

where \( \hat{b} = \sum_{k} g_k \hat{a}_k^\dagger + g_k^* \hat{a}_k \). From Eqs. (25), (40), and (41), we obtain
\[ \chi(t) = Tr_b(\hat{b}(t) \hat{\rho}_b) \]  

(45)

\[ B_{an} = \delta_{an} f(t), \]  

(46)

\[ A_{an, bm} = 2 Re f(t) \lambda_{an} \lambda_{bm} \delta_{an} \delta_{bm} \]  

(47)

where \( \lambda_{an} \) is an eigenvalue of \( \hat{\sigma}_z \), and \( f(t) = \int_0^t ds \int_0^s d\tau \chi^*(\tau - s) \). Note that the eigenvectors \(|n\rangle\) of \( \hat{\sigma}_z \) was used for the basis to obtain \( B \) and \( A \). If we set \( \kappa_{an}^{an} = \delta_{an}[1 - f(t)] \) and \( \kappa_{1an}^{an} = \sqrt{2Re f(t) - |f(t)|^2} \lambda_{an} \), then the resulting Kraus operators are
\[ \hat{K}_0 = [1 - f(t)] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \]  

(48)

\[ \hat{K}_1 = \sqrt{2Re f(t) - |f(t)|^2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]  

(49)

It is obvious that the Kraus operators (48) satisfy the completeness relation (32).

In summary, we have shown that the OSR for the non-Markovian case and the Lindblad master equation for the Markov case can be derived from the formal solution to the QLE for the qubit system in the presence of decoherence provided that details of the Hamiltonians for the system, reservoir, and the mutual interaction are known.

ACKNOWLEDGMENTS

This work was supported by the Korean Ministry of Science and Technology through the Creative Research Initiatives Program under Contract No. 00-C-CT-01-C-35.