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Kraus Representation for the Density Operator of a Qubit

D. M. Tong[a], J. L. Chen[a], J. Y. Huang[b], L. C. Kwek[a, c], and C. H. Oh[a]

[a] *Department of Physics, National University of Singapore, 10 Kent Ridge Crescent, 119260 Singapore*
[b] *Wuxi Institute of Technology, 1 Gaolang West Road, University City, Wuxi, PRC 214121*
[c] *National Institute of Education, Nanyang Technological University, 1 Nanyang Walk, 639798 Singapore*
e-mail: phytdm@nus.edu.sg; phyohch@nus.edu.sg
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Abstract—We show that the time evolution of the density operator of a qubit can always be described in terms of the Kraus representation. A general scheme on how to construct the Kraus operators for an open qubit system is proposed, which can be generalized to open higher dimensional quantum systems.

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1. INTRODUCTION

It is well known that the time evolution of a closed quantum system can be described by a unitary operator. However, for an open system, the time evolution is not necessarily unitary. The evolution of an open system is often described by the Kraus representation [1]. Since a real physical system is generally entangled with its environment, the proper understanding of the nature of the Kraus representation for an open system is important and useful [1–10], especially in quantum information processing.

The Kraus representation of an open system is usually constructed by considering a larger closed system denoted as S_{ie}, comprising the system of interest S_i and its environment S_e. Let $\rho_{ie}(t)$, $\rho_i(t)$, and $\rho_e(t)$ be the density matrices of S_{ie}, S_i, and S_e, respectively, where $\rho_i(t) = \mathrm{tr}_e[\rho_{ie}(t)]$ and $\rho_e(t) = \mathrm{tr}_i[\rho_{ie}(t)]$, and $\rho_{ie}(0)$, $\rho_i(0)$, and $\rho_e(0)$ represent the corresponding initial states, respectively, at $t = 0$. Since the combined system is a closed one, its evolution is unitary:

$$\rho_{ie}(t) = U_{ie}(t)\rho_{ie}(0)U_{ie}(t)^+, \tag{1}$$

where $U_{ie}(t)$ is the unitary operator. The system of interest, as an open one, then evolves in the following way:

$$\rho_i(t) = \mathrm{tr}_e\{U_{ie}(t)\rho_{ie}(0)U_{ie}(t)^+\}. \tag{2}$$

If the above equation can be equivalently expressed in the form

$$\rho_i(t) = \sum_{\mu\nu} M_{\mu\nu}(t)\rho_i(0)M_{\mu\nu}(t)^+, \tag{3}$$

where $M_{\mu\nu}(t)$ satisfy

$$\sum_{\mu\nu} M_{\mu\nu}(t)^+ M_{\mu\nu}(t) = I, \tag{4}$$

then it is said that the evolution of $\rho_i(t)$ has the form of the Kraus representation.

It is obvious that $\rho_i(t)$ always has the Kraus representation for arbitrary $U_{ie}(t)$ if $\rho_{ie}(0)$ is *factorable* [5], i.e., $\rho_{ie}(0) = \rho_i(0) \otimes \rho_e(0)$, which means that there is no initial correlation between the open system and its environment. To show this, we can take $\rho_e(0) = \sum_\nu \sqrt{p_\nu}|\nu_e\rangle\langle\nu_e|$ and let

$$M_{\mu\nu}(t) = \langle\mu_e|\sqrt{p_\nu}U_{ie}(t)|\nu_e\rangle, \tag{5}$$

where $|\mu_e\rangle$, $|\nu_e\rangle$ ($\mu, \nu = 0, 1, \ldots, k-1$ are the orthonormal bases of S_e, and k is the dimension of S_e. One finds that $M_{\mu\nu}(t)$ defined by Eq. (5) satisfy Eqs. (3) and (4).

The issue is whether $\rho_i(t)$ still has the form of the Kraus representation when $\rho_{ie}(0)$ is *not factorable*, which means that the initial correlations between S_i and S_e are present. Or, in other words, can one always find the Kraus representation of an open system for an arbitrary given initial state $\rho_{ie}(0)$ and arbitrary unitary operator $U_{ie}(t)$? Recently, some papers [8–10] have contributed to the issue. Štelmachovič and Bužek [8] investigated the role of the initial correlations between the open system and its environment and showed that a map based on the reduced dynamics in the presence of initial correlations cannot be described by the form of the Kraus representation, because an additional inhomogeneous part appears. Salgado and Sánchez-Gómez [9] pointed out that $\rho_i(t)$ still has the Kraus representation even in the presence of any initial correlation if the evolution is local, namely, $U_{ie}(t) = U_i(t) \otimes U_e(t)$. In a very recent paper [10], Hayashi et al. examined the validity of the Kraus representation in the presence of initial correlations and concluded that the dynamical map for an open system reduced from a combined system with an arbitrary initial correlation takes the form of the Kraus representation if and only if the joint dynamics is locally unitary.

To arrive at the above conclusion, an operator $\rho_{cor}(0)$, called the correlation operator, was introduced through the definition $\rho_{cor}(0) \equiv \rho_{ie}(0) - \rho_i(0) \otimes \rho_e(0)$. Equation (2) can then be recast to the following form:

$$\begin{aligned}\rho_i(t) &= \mathrm{tr}_e\{U_{ie}(t)\rho_i(0)\otimes\rho_e(0)U_{ie}(t)^+\} \\ &\quad + \mathrm{tr}_e\{U_{ie}(t)\rho_{cor}(0)U_{ie}(t)^+\} \\ &= \sum_\mu M_{\mu\nu}(t)\rho_i(0)M_{\mu\nu}(t)^+ + \delta\rho_i(t),\end{aligned} \tag{6}$$

where

$$\delta\rho_i(t) = \mathrm{tr}_e\{U_{ie}(t)\rho_{cor}(0)U_{ie}(t)^+\}. \tag{7}$$

The analysis in [8–10] is based on the idea that $\rho_i(t)$ has the Kraus representation if and only if $\delta\rho_i(t) = 0$. Clearly, $\rho_i(t)$ has the form of Eq. (3) if $\delta\rho_i(t) = 0$ and the Kraus operators are given by Eq. (5). However, noticing that Kraus operators are highly nonunique, one may start wondering whether $\rho_i(t)$ has an alternative form of the Kraus representation even if $\delta\rho_i(t) \neq 0$, because there may exist Kraus operators $\tilde{M}_{\mu\nu}(t)$ such that

$$\begin{aligned}\rho_i(t) &= \sum_\mu M_{\mu\nu}(t)\rho_i(0)M_{\mu\nu}(t)^+ + \delta\rho_i(t) \\ &= \sum_\mu \tilde{M}_{\mu\nu}(t)\rho_i(0)\tilde{M}_{\mu\nu}(t)^+,\end{aligned} \tag{8}$$

and $\sum_{\mu\nu}\tilde{M}_{\mu\nu}(t)^+\tilde{M}_{\mu\nu}(t) = I$. $\tilde{M}_{\mu\nu}$ may not be calculated from Eq. (5), but they need to have the properties of Kraus operators, which ensure that the map defined by them is Hermitian, trace-preserving, and positive.

We consider this problem in the present paper. Our investigation focuses on the open qubit system. The paper is organized as follows. In Section 2, an example is provided to show that the alternative Kraus representation really exists even if $\delta\rho_i(t) \neq 0$. In Section 3, we propose a general approach on how to construct Kraus operators for an arbitrary open qubit system. We end with some discussions in the final section.

2. KRAUS REPRESENTATION WITH NONZERO $\delta\rho_i(t)$

In this section, by providing an example, we show that $\rho_i(t)$ may still have an alternative form of the Kraus representation even if $\delta\rho_i(t) \neq 0$. We choose the same model as that used in [10]. That is, we consider a combined system composed of two spin-1/2 subsystems with the interaction Hamiltonian $H_{ie} = \sigma_x \otimes \frac{1}{2}(\mathbf{1} - \sigma_z) + \mathbf{1} \otimes \frac{1}{2}(1 + \sigma_z)$, where σ_x and σ_z are Pauli spin operators. In this model, the first qubit plays the role of the open system, while the second qubit plays the role of the environment. The interaction described by the Hamiltonian corresponds to the well-known controlled-NOT gate [2, 8]. The unitary evolution operator is given by $U_{ie}(t) = e^{-iH_{ie}t}$; explicitly,

$$U_{ie}(t) = \begin{pmatrix} e^{-it} & 0 & 0 & 0 \\ 0 & \cos t & 0 & -i\sin t \\ 0 & 0 & e^{-it} & 0 \\ 0 & -i\sin t & 0 & \cos t \end{pmatrix}. \tag{9}$$

In the model considered, ρ_{ie} is a 4×4 matrix while ρ_i and ρ_e are 2×2 matrices. For simplicity, we take the initial state of the combined system as

$$\rho_{ie}(0) = \begin{pmatrix} \frac{1-r_0}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1+r_0}{2} \end{pmatrix}, \tag{10}$$

where $r_0 \in (0, 1)$ is a real parameter. Noting that, at $r_0 = 0$ or 1, $\rho_{ie}(0)$ is *factorable*, and the Kraus representation certainly exists, we need not consider these two cases. It is easy to obtain the initial reduced density matrices of S_i and S_e as

$$\begin{aligned}\rho_i(0) &= \mathrm{tr}_e\rho_{ie}(0) = \frac{1}{2}(\mathbf{1} - r_0\sigma_z), \\ \rho_e(0) &= \mathrm{tr}_i\rho_{ie}(0) = \frac{1}{2}(\mathbf{1} - r_0\sigma_z),\end{aligned} \tag{11}$$

and the correlation operator is

$$\rho_{cor}(0) = \frac{1}{4}(1 - r_0^2)\sigma_z \otimes \sigma_z. \tag{12}$$

From Eqs. (2), (9), and (10), we get the density matrix of the system S_i:

$$\rho_i(t) = \frac{1}{2}\begin{pmatrix} 1 + \sin^2 t - r_0\cos^2 t & -i(1+r_0)\sin t\cos t \\ i(1+r_0)\sin t\cos t & (1+r_0)\cos^2 t \end{pmatrix}. \tag{13}$$

Substituting Eqs. (9) and (12) into Eq. (7), one gets

$$\delta\rho_i(t) = \frac{1}{4}(1 - r_0^2)\begin{pmatrix} 2\sin^2 t & -i\sin 2t \\ i\sin 2t & -2\sin^2 t \end{pmatrix}. \tag{14}$$

We see that $\delta\rho_i(t)$ is, in general, nonzero. However, the Kraus representation of $\rho_i(t)$ still exists. One can verify that the following expressions hold:

$$\rho_i(t) = \sum_{\mu=0}^{1} M_\mu(t)\rho_i(0)M_\mu(t)^+, \tag{15}$$

$$\sum_{\mu=0}^{1} M_\mu(t)^+ M_\mu(t) = I, \tag{16}$$

with

$$M_0(t) = \frac{1}{\sqrt{2r_t(1+r_0)}}\begin{pmatrix} -\sqrt{(1+r_0)(r_t+\sin^2 t - r_0\cos^2 t)} & i\sqrt{(1-r_t)(r_t-\sin^2 t + r_0\cos^2 t)} \\ -i\sqrt{(1+r_0)(r_t-\sin^2 t + r_0\cos^2 t)} & \sqrt{(1-r_t)(r_t+\sin^2 t - r_0\cos^2 t)} \end{pmatrix},$$
$$M_1(t) = \frac{\sqrt{r_t+r_0}}{\sqrt{2r_t(1+r_0)}}\begin{pmatrix} 0 & \sqrt{r_t+\sin^2 t - r_0\cos^2 t} \\ 0 & i\sqrt{r_t-\sin^2 t + r_0\cos^2 t} \end{pmatrix}, \tag{17}$$

where $r_t = \sqrt{\sin^2 t + r_0^2\cos^2 t}$ and $M_0(t)$ and $M_1(t)$ are the Kraus operators.

The map defined by Eq. (17) ensures $\rho_i(t)$ is Hermitian, trace-preserving, and positive. The evolution of the system S_i obeys Eq. (15), while the combined system evolves under the unitary operator $U_{ie}(t)$ given by Eq. (9). This example shows that, even if $\delta\rho_i(t) \neq 0$, $\rho_i(t)$ can still be written in the form of the Kraus representation.

3. KRAUS REPRESENTATION FOR ARBITRARY DENSITY OPERATOR

From Eq. (6), we see that the state $\rho_i(t)$ cannot be written in the form of the Kraus representation with the Kraus operators defined by Eq. (5) if $\delta\rho_i(t) \neq 0$. However, the example in Section 2 illustrates that there may exist an alternative form of the Kraus representation even if $\delta\rho_i(t) \neq 0$. This encourages us to conjecture that the time evolution of the density operator can always have the Kraus representation irrespective of the forms of initial state and evolution path. In this section, we will prove that it is true that $\rho_i(t)$ can always be connected with its initial state $\rho_i(0)$ by Kraus operators.

Let us begin by considering an arbitrary evolution of an open qubit system with an arbitrary initial state. The most general initial state for an open qubit system can be written as

$$\rho_i(0) = \frac{1}{2}(1+\mathbf{r}_0\cdot\sigma)$$
$$= \frac{1}{2}\begin{pmatrix} 1+r_0\cos\theta_0 & r_0\sin\theta_0 e^{-i\phi_0} \\ r_0\sin\theta_0 e^{i\phi_0} & 1-r_0\cos\theta_0 \end{pmatrix}, \tag{18}$$

and the most general evolution of the system is

$$\rho_i(t) = \frac{1}{2}(1+\mathbf{r}\cdot\sigma)$$
$$= \frac{1}{2}\begin{pmatrix} 1+r\cos\theta & r\sin\theta e^{-i\phi} \\ r\sin\theta e^{i\phi} & 1-r\cos\theta \end{pmatrix}, \tag{19}$$

where $r = r(t)$, $\theta = \theta(t)$, $\phi = \phi(t)$, depending on time t, and $r(0) = r_0$, $\theta(0) = \theta_0$, $\phi(0) = \phi_0$. $0 \le r \le 1$, $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$. We want to show that there always exist Kraus operators $M_\mu(t)$ such that

$$\rho_i(t) = \sum_\mu M_\mu(t)\rho_i(0)M_\mu(t)^+, \tag{20}$$

$$\sum_\mu M_\mu(t)^+ M_\mu(t) = I, \tag{21}$$

where we have used $M_\mu(t)$ instead of $M_{\mu\nu}(t)$ to denote the Kraus operators. To find the Kraus operators, one may write $M_\mu(t)$ as 2×2 matrices with undetermined elements, and one may then directly solve Eqs. (20) and (21) to determine the matrices. However, it is too difficult to do it in that way. Since a diagonal matrix is, in general, easier to handle than a nondiagonal ones, we first diagonalize the density matrices $\rho_i(0)$ and $\rho_i(t)$ by unitary transformations:

$$\rho_i(0) = U_1\rho_i'(0)U_1^+, \quad \rho_i(t) = U_2(t)\rho_i'(t)U_2(t)^+. \tag{22}$$

The eigenvalues of $\rho_i(0)$ and $\rho_i(t)$ make up the entries of the diagonalized matrices $\rho_i'(0)$ and $\rho_i'(t)$, respectively, and their orthogonal vectors make up the columns of the unitary matrices U_1 and U_2, respectively. In this way, the diagonalized matrices can be written as

$$\rho'_i(0) = \frac{1}{2}(1 + \mathbf{r}'_0 \cdot \sigma) = \frac{1}{2}\begin{pmatrix} 1 - r_0 & 0 \\ 0 & 1 + r_0 \end{pmatrix}, \quad (23)$$

$$\rho'_i(t) = \frac{1}{2}(1 + \mathbf{r}' \cdot \sigma) = \frac{1}{2}\begin{pmatrix} 1 + r & 0 \\ 0 & 1 - r \end{pmatrix}, \quad (24)$$

where $\mathbf{r}'_0$ and $\mathbf{r}'$ are defined as $\mathbf{r}'_0 = (0, 0, -r_0)$ and $\mathbf{r}' = (0, 0, r)$, respectively, and the corresponding unitary transformation matrices are

$$U_1 = \begin{pmatrix} -\sin\frac{\theta_0}{2} & \cos\frac{\theta_0}{2}e^{-i\phi_0} \\ \cos\frac{\theta_0}{2}e^{i\phi_0} & \sin\frac{\theta_0}{2} \end{pmatrix}, \quad (25)$$

$$U_2 = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2}e^{-i\phi} \\ \sin\frac{\theta}{2}e^{i\phi} & \cos\frac{\theta}{2} \end{pmatrix}. \quad (26)$$

If we can find operators $M'_\mu(t)$ that satisfy $\rho'_i(t) = \sum_\mu M'_\mu(t)\rho'_i(0)M'_\mu(t)^+$ and $\sum_\mu M'_\mu(t)^+ M'_\mu(t) = I$, then the Kraus representation of $\rho_i(t)$ can be realized by letting

$$M_\mu(t) = U_2 M'_\mu(t) U_1^+. \quad (27)$$

Since $\rho'_i(t)$ and $\rho'_i(0)$ are diagonal, the operators $M'_\mu(t)$ are easy to find. There are an infinite number of choices of this kind of Kraus operator. Without loss of generality, we may choose them as

$$M'_0(t) = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{\frac{1-r}{1+r_0}} \end{pmatrix}, \quad M'_1(t) = \begin{pmatrix} 0 & \sqrt{\frac{r+r_0}{1+r_0}} \\ 0 & 0 \end{pmatrix}. \quad (28)$$

Substituting Eqs. (25), (26), and (28) into Eq. (27), we obtain the Kraus operators $M_\mu(t)$

$$M_0(t) = \begin{pmatrix} -\cos\frac{\theta}{2}\sin\frac{\theta_0}{2} - \sqrt{\frac{1-r}{1+r_0}}\sin\frac{\theta}{2}\cos\frac{\theta_0}{2}e^{i(\phi_0-\phi)} & \cos\frac{\theta}{2}\cos\frac{\theta_0}{2}e^{-i\phi_0} - \sqrt{\frac{1-r}{1+r_0}}\sin\frac{\theta}{2}\sin\frac{\theta_0}{2}e^{-i\phi} \\ -\sin\frac{\theta}{2}\sin\frac{\theta_0}{2}e^{i\phi} + \sqrt{\frac{1-r}{1+r_0}}\cos\frac{\theta}{2}\cos\frac{\theta_0}{2}e^{i\phi_0} & \sin\frac{\theta}{2}\cos\frac{\theta_0}{2}e^{i(\phi-\phi_0)} + \sqrt{\frac{1-r}{1+r_0}}\cos\frac{\theta}{2}\sin\frac{\theta_0}{2} \end{pmatrix},$$

$$M_1(t) = \sqrt{\frac{r+r_0}{1+r_0}}\begin{pmatrix} \cos\frac{\theta}{2}\cos\frac{\theta_0}{2}e^{i\phi_0} & \cos\frac{\theta}{2}\sin\frac{\theta_0}{2} \\ \sin\frac{\theta}{2}\cos\frac{\theta_0}{2}e^{i(\phi+\phi_0)} & \sin\frac{\theta}{2}\sin\frac{\theta_0}{2}e^{i\phi} \end{pmatrix}. \quad (29)$$

$M_0(t)$ and $M_1(t)$ satisfy Eqs. (20) and (21). The Kraus representation given by $M_0(t)$ and $M_1(t)$ in expression (29) ensures that $\rho_i(t)$ is Hermitian, trace-preserving, and positive. So, no matter what the forms of $U_{ie}(t)$ and $\rho_{ie}(0)$ are, there always exist Kraus operators connecting $\rho_i(t)$ with $\rho_i(0)$. For any given $\rho_{ie}(0)$ and $U_{ie}(t)$, the Kraus operators $M_\mu(t)$ can be calculated by diagonalizing the reduced matrices $\mathrm{tr}_e\{U_{ie}(t)\rho_{ie}(0)U_{ie}(t)^+\}$ and $\mathrm{tr}_e\rho_{ie}(0)$. One general expression of the Kraus operators is given by Eq. (29), with which the Kraus representation of $\rho_i(t)$ is obtained by Eq. (20).

So far, we have proved that the time evolution of the density operator of an open qubit system always has the Kraus representation. At the same time, we have put forward a general approach for constructing the Kraus operators for arbitrary evolution. From the physical point of view, the above process of finding the Kraus operators means that we first align the Bloch vectors $\mathbf{r}$ and $\mathbf{r}_0$ in the Bloch sphere along the z axis by using U_1 and U_2, respectively, to find the Kraus representation of $\mathbf{r}'$ with $\mathbf{r}'_0$ and then reverse $\mathbf{r}'$ and $\mathbf{r}'_0$, back to $\mathbf{r}$ and $\mathbf{r}_0$, to obtain the Kraus representation of $\mathbf{r}$ with $\mathbf{r}_0$. The model in Section 2 is just an example of applying this approach to solve the Kraus representation. In fact, expression (17) is calculated in this way.

4. DISCUSSION

We have shown that the time evolution of the density operator of an open qubit system can always have the Kraus representation. A scheme on how to construct the

Kraus representation is proposed. One general expression of the Kraus representation for an arbitrary evolution is provided by Eqs. (20), (21), and (29). Since the expressions of the Kraus operators are not unique, the form given by Eq. (29) is only one kind of them. The equivalent expressions of the Kraus operators can be written as $\tilde{M}_\mu(t) = \sum_\nu M_\nu(t) V_{\mu\nu}$, where $V_{\mu\nu}$ are the elements of an arbitrary unitary matrix.

In [8–10], the possibility of the Kraus representation for an open system with initial correlations between the system and its environment is investigated and some important conclusions are derived. As a supplement, the present paper studies the existence of an operator-sum representation for an arbitrary given evolution of density operator. Our result shows that an arbitrary evolution of the state can always be written in the form of the Kraus representation in theory. The Kraus operators can be calculated by Eq. (5) if $\delta\rho_i(t) = 0$, while they cannot be expressed explicitly in the form of Eq. (5) if $\delta\rho_i(t) \neq 0$. For the latter case, they can still be obtained by the approach described in the current paper. Moreover, $M_\mu(t)$ in the latter case are generally dependent on the initial state, and there does not exist a universal form of Kraus operators for all different initial states.

An interesting corollary of our result is that one can always construct a CP map between any two quantum states of a qubit, and the map can be represented through two Kraus operators. This corollary is obvious, because any two states can be connected by the Kraus operators M_μ ($\mu = 0, 1$) and the CP maps can then be defined by them. The corollary shows that even for two such states ρ and ρ', where ρ' is obtained from ρ by a non-CP map $\$: \rho \longrightarrow \rho'$, one can still find an alternative map $\tilde{\$}$ that is completely positive, satisfying $\tilde{\$} : \rho \longrightarrow \rho'$. Note that the Kraus operators are not unique, and expression (29) is only one of them. The other equivalent expressions of the Kraus operators can be obtained by $\tilde{M}_\mu(t) = \sum_\nu M_\nu(t) V_{\mu\nu}$, where $V_{\mu\nu}$ are the elements of an arbitrary unitary matrix V.

This approach can be generalized to higher dimensional quantum systems. The procedure for higher dimensional systems is similar to the qubit case but may be more complicated. In fact, the density matrix $\rho_i(t)$ with the parameter t and $\rho_i(0)$ can always be diagonalized by unitary transformations U_1 and U_2, respectively, regardless of the dimensions of the density matrices. It is easy to find the Kraus operators $M'_\mu(t)$ of the diagonal density matrix $\rho'_i(t)$ with the diagonal initial density matrix $\rho'_i(0)$, although it is difficult to find the Kraus representation of an arbitrary density matrix with arbitrary initial conditions. Using Eq. (27) and U_1, U_2, and $M'_\mu(t)$, the Kraus representation of $\rho_i(t)$ is obtained. Certainly, as the dimensions of the density matrices become larger, solving for the Kraus operator may become more a formidable task.

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