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Simulation of open quantum dynamics in Markovian environment

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Abstract

Although conditions for controllability of quantum systems are well studied, most of them consider the infinite time horizon, i.e., whether certain operations are possible given enough time. In this article, I propose a framework studying all the possible operations one can generate at given finite time on a quantum system in Markovian environment. I give a complete characterization of the operations one can simulate at any given time on a qubit in unital Markovian environment and discuss possible extensions.

1. Introduction

Simulation of quantum systems have been an important subject since it was first suggested by Feynman in early 1980's [1]. Now for closed quantum system, the condition for universal quantum simulation and computation is well understood, basically for a finite-dimensional quantum system, the repeated application of a small set of basic coherent control operations allows one to enforce any desired unitary transformation on the system [2, 3]. However the real systems are usually coupled to the environment, which leads to the open quantum dynamics. One fundamental question thus is what coherent control can do on open systems, i.e., given a system coupled to the environment, what kind of operations one can generate on the system when one can only apply coherent control on the system? More specifically, considering the open system described by the Lindblad equation

$$\dot{\rho} = -i[H(t),\rho] + \sum_{\alpha\beta}\gamma_{\alpha\beta}(F_\alpha \rho F_\beta^\dagger - \frac{1}{2}\{F_\beta^\dagger F_\alpha, \rho\}), \quad (1)$$

where $H = H^\dagger$ is the effective system Hamiltonian(the natural Hamiltonian possibly renormalized by a Lamb-shift term), $\{F_\alpha\}$ are the basis for the space of bounded traceless operators on the system. $\Gamma = \Gamma^\dagger = \{\gamma_{\alpha\beta}\}$ is a positive semidefinite matrix. And suppose we have the ability to change the Hamiltonian $H(t)$ to generate any unitary operators on the system, then at a given time T, what is all the possible operations one can simulate on the system? This problem of finding all the possible operations one can simulate at any given time is closely related to the time optimal control problem, i.e., to find out the time optimal way generating a desired operator, which is another important subject and quite a few works have been done on closed quantum systems[6, 7, 8, 9, 10, 11, 12], and on state transferring of some open quantum systems[13, 14, 15]. In this article I will study the finite time simulation, i.e., to find all the possible operations one can simulate at any given time with open-loop coherent control. I will give a complete characterization of the operations that one can generate on a single qubit in unital[18] Markovian environment and discuss possible extension along this direction. The result is expected to be helpful for studying quantum noise processes [16] and quantum error correcting [17].

The article is organized as following: in section 2, some mathematics tools on majorization are reviewed; in section 3, the simulations of a qubit in unital Markovian environment is studied, and a complete characterization of the operations one can simulate by applying coherent control on the qubit is given; section 4 makes some extensions and concludes.

2. Preliminary

In this section, I give a brief review on majorization, interested readers can find more details in [25, 26].

For an element $x = (x_1,...,x_k)^T$ of $\mathbb{R}^k$ we denote by $x^\downarrow = (x_1^\downarrow,...,x_k^\downarrow)^T$ a permutation of x so that $x_i^\downarrow \geq x_j^\downarrow$ if $i < j$, where $1 \leq i,j \leq k$.

Definition 1 (majorization) A vector $x \in \mathbb{R}^k$ is majorized by a vector $y \in \mathbb{R}^k$ (denoted $x \prec y$), if

$$\sum_{j=1}^{d} x_j^\downarrow \leq \sum_{j=1}^{d} y_j^\downarrow \quad (2)$$

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for $d = 1, \ldots, k-1$, and the inequality holds with equality when $d = k$.

Proposition 1 $x \prec y$ iff x lies in the convex hull of y and all its permutations $P_i y$, where P_i are permutation matrices.

Proposition 2 (additive) If $x^{\downarrow} \prec y^{\downarrow}$ and $r^{\downarrow} \prec s^{\downarrow}$, then $x^{\downarrow} + r^{\downarrow} \prec y^{\downarrow} + s^{\downarrow}$.

This can be easily proved from the definition.

Definition 2 (log majorization) For $0 < x, y \in \mathbb{R}^k$, x is log majorized by y (denoted $x \prec_{log} y$), iff $logx \prec logy$. This is equivalent to requiring

$$\prod_{j=1}^{d} x_j^{\downarrow} \leq \prod_{j=1}^{d} y_j^{\downarrow} \tag{3}$$

for $d = 1, \ldots, k-1$, and the inequality holds with equality when $d = k$.

Proposition 3 (log additive) If $x^{\downarrow} \prec_{log} y^{\downarrow}$ and $r^{\downarrow} \prec_{log} s^{\downarrow}$, then $[(x^{\downarrow})_i (r^{\downarrow})_i] \prec_{log} [(y^{\downarrow})_i (s^{\downarrow})_i]$ (Here we use $[x_i]$ to denote a vector whose ith entry is x_i).

This is a direct extension of Proposition 2.

Proposition 4 *[21]* For any matrices M and N, $[s_i(MN)] \prec_{log} [s_i^{\downarrow}(M) s_i^{\downarrow}(N)]$, here we use $s_i(M)$ to denote the ith singular value of M.

3. Simulation of open quantum system

Let ρ denote the density matrix of an open quantum system, it evolves under the Lindblad equation, which takes the form

$$\dot{\rho} = -i[H(t), \rho] + L(\rho), \tag{4}$$

where $-i[H, \rho]$ is the unitary evolution of the quantum system and $L(\rho)$ is the dissipative part of the evolution. The term $L(\rho)$ is linear in ρ and takes the Lindblad form [20, 24]

$$L(\rho) = \sum_{\alpha\beta} \gamma_{\alpha\beta} (F_\alpha \rho F_\beta^\dagger - \frac{1}{2}\{F_\beta^\dagger F_\alpha, \rho\}),$$

where F_α, F_β are linear basis of traceless operators on the density matrix. For single qubit, we can take the basis $\{F_\alpha\}$ as normalized Pauli spin operators $\frac{1}{\sqrt{2}}\{\sigma_x, \sigma_y, \sigma_z\}$ and the coefficient matrix $\Gamma = \{\gamma_{\alpha\beta}\}$ known as the GKS(Gorini, Kossakowski and Sudarshan) matrix [23], is semi-positive definite. For the single qubit case, it takes the form

$$\Gamma = \begin{pmatrix} \gamma_{xx} & \gamma_{xy} & \gamma_{xz} \\ \gamma_{yx} & \gamma_{yy} & \gamma_{yz} \\ \gamma_{zx} & \gamma_{zy} & \gamma_{zz} \end{pmatrix}.$$

If the Markovian quantum dynamics is unital, i.e., $L(I) = 0$, then for the single qubit case, all the entries of Γ are real numbers[4].

Following [22], we assume that the action of the control Hamiltonian can be produced on a time scale fast compared with dissipation. If we denote τ_B as the time scale over which the reservoir correlation functions decay, and τ_C as the time scale for coherent control, and τ_R as the time scale of the dissipation, then we are working in the regime of $\tau_B << \tau_C << \tau_R$, for example, nuclear magnetic resonance satisfies this condition. We assume that the system is unitarily controllable, i.e., any unitary transformation $U \in SU(2)$ on the $2-$level system can be produced. Combining these two assumptions we have that any unitary transformation can be produced on the system in negligible time compared to the dissipation. It is convenient to rewrite the master equation (4) in terms of the Bloch vector $\overrightarrow{a} = (a_x, a_y, a_z)^T$, where

$$\rho = \frac{1}{2}I + \frac{1}{2}(a_x\sigma_x + a_y\sigma_y + a_z\sigma_z).$$

Substituting into the master equation (4) and taking the trace with σ_i then leads to the equivalent Bloch equation:

$$\frac{d}{dt}\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = [A(t) + B]\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} + p, \tag{5}$$

where $A(t)$ comes from the transformation of the unitary part $-i[H(t), \rho]$, since we assume we can produce any unitary matrix in negligible time, $A(t)$ can be chosen as any antisymmetric matrix. B and p comes from the dissipative part $L(\rho)$, if the dynamics is unital, i.e., $L(I) = 0$, then $p = 0$[4] and

$$B = \frac{\Gamma + \Gamma^T}{2} - Tr(\Gamma)I,$$

which is symmetric with eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3$:

$$\begin{aligned} \lambda_1 &= -(\mu_2 + \mu_3), \\ \lambda_2 &= -(\mu_1 + \mu_3), \\ \lambda_3 &= -(\mu_1 + \mu_2), \end{aligned} \tag{6}$$

where μ_i are eigenvalues of the GKS matrix Γ arranged in decreasing order.

The operator dynamics in the Bloch representation is just the uplift of the density matrix dynamics, for the unital case it takes the form

$$\dot{O} = [A(t) + B]O, \tag{7}$$

where O is now a 3×3 matrix. Now the problem is to find out all the possible operators O one can generate at time T under the dynamics [7].

Theorem 1 For unital markovian master equation as in Eq.(4), all the operators one can generate at time T, written in the Bloch representation (as in Eq.(7)), are

$$K_1 exp[diag(c_1, c_2, c_3)]K_2,$$

where $K_1, K_2 \in SO(3)$ and $(c_1, c_2, c_3) \prec (\lambda_1, \lambda_2, \lambda_3)T$.

To show this, first approximate the function $A(t)$ by a piece-wise constant function, and use the fact that

$$lim_{n\to\infty}[e^{\frac{A\delta t}{n}} e^{\frac{B\delta t}{n}}]^n = e^{(A+B)\delta t},$$

the evolution of the operator can then be approximated arbitrary close by alternating between the dissipative part and the unitary control

$$O(T) = S_{n+1}e^{Bt_n}S_n e^{Bt_{n-1}}S_{n-1}\cdots S_3 e^{Bt_2}S_2 e^{Bt_1}S_1 S_0,$$

where $S_i = e^{A\delta t_i} \in SO(3), i \in \{0, 1, \cdots, n\}$ are generated by the unitary part and takes negligible time.

Rearrange the above sequence

$$\begin{aligned}
O(T) =& S_{n+1}e^{Bt_n}S_n e^{Bt_{n-1}}S_{n-1}\cdots S_3 e^{Bt_2}S_2 e^{Bt_1}S_1 S_0 \\
=&(\prod_{i=1}^{n+1} S_i) e^{(\prod_{i=1}^{n} S_i)^T Bt_n (\prod_{i=1}^{n} S_i)} \\
& e^{(\prod_{i=1}^{n-1} S_i)^T Bt_{n-1} (\prod_{i=1}^{n-1} S_i)} \\
& \cdots e^{(S_2S_1)^T Bt_2 S_2 S_1} e^{S_1^T Bt_1 S_1} S_0 \\
=& S'_{n+1} e^{S_n'^T Bt_n S'_n} e^{S_{n-1}'^T Bt_{n-1} S'_{n-1}} \\
& \cdots e^{S_2'^T Bt_2 S'_2} e^{S_1'^T Bt_1 S'_1} S_0
\end{aligned} \tag{8}$$

Now let $M_2 = e^{S_2'^T Bt_2 S'_2}$ and $M_1 = e^{S_1'^T Bt_1 S'_1}$, apply theorem 4, we get

$$[s_i(M_2M_1)] \prec_{log} [s_i^{\downarrow}(M_2)s_i^{\downarrow}(M_1)],$$

where $[s_i^{\downarrow}(M_2)]$ and $[s_i^{\downarrow}(M_1)]$ are singular values of M_2 and M_1 respectively:

$$[s_i^{\downarrow}(M_2)] = (e^{\lambda_1 t_2}, e^{\lambda_2 t_2}, e^{\lambda_3 t_2}),$$

$$[s_i^{\downarrow}(M_1)] = (e^{\lambda_1 t_1}, e^{\lambda_2 t_1}, e^{\lambda_3 t_1}),$$

so $[s_i(M_2M_1)] \prec_{log} (e^{\lambda_1(t_1+t_2)}, e^{\lambda_2(t_1+t_2)}, e^{\lambda_3(t_1+t_2)})$. Using the log additive property of majorization(Proposition 3) and applying it recursively, we get

$$O(T) = S'_{n+1}CS_0,$$

where $[s_i(C)] \prec_{log} (e^{\lambda_1 T}, e^{\lambda_2 T}, e^{\lambda_3 T})$, where $T = \sum_i^n t_i$, i.e.,

$$C = K_1 \exp[diag(c_1, c_2, c_3)]K_2$$

while $K_1, K_2 \in SO(3)$ and

$$(c_1, c_2, c_3) \prec (\lambda_1, \lambda_2, \lambda_3)T.$$

Absorb S'_{n+1} and S_0 into K_1 and K_2 respectively, at time T the operators we can generate are of the form

$$K_1 \exp[diag(c_1, c_2, c_3)]K_2$$

where

$$(c_1, c_2, c_3) \prec (\lambda_1, \lambda_2, \lambda_3)T.$$

This is also a complete characterization, i.e., any operator satisfies this condition can be generated at time T: suppose $O = K_1 \exp[diag(c_1, c_2, c_3)]K_2$ while

$$(c_1, c_2, c_3) \prec (\lambda_1, \lambda_2, \lambda_3)T,$$

then (c_1, c_2, c_3) lies in the convex hull of the six permutations of $(\lambda_1, \lambda_2, \lambda_3)T$(Proposition 1), i.e.,

$$(c_1, c_2, c_3) = \sum_{i=1}^{6} \alpha_i(\lambda_{\pi_i(1)}, \lambda_{\pi_i(2)}, \lambda_{\pi_i(3)})T,$$

where $0 \le \alpha_1 \le 1$ and $\sum_{i=1}^{6} \alpha_i = 1$, π_i are permutations on $\{1, 2, 3\}$, one then can construct a sequence generating this operator:

$$O = K_1 e^{S_6^T Bt_6 S_6} e^{S_5^T Bt_5 S_5} \cdots e^{S_2^T Bt_2 S_2} e^{S_1^T Bt_1 S_1} K_2,$$

where we choose $S_i, i \in \{1, 2, 3, 4, 5, 6\}$ such that $S_i^T BS_i = diag(\lambda_{\pi_i(1)}, \lambda_{\pi_i(2)}, \lambda_{\pi_i(3)})$ and $t_i = \alpha_i T$, easy to see that this generates the desired operator, which concludes the proof.

The physics of this characterization is that basically the coherent controls are rotating the dissipative axis, at each time instant, one can use the coherent controls to change the dissipative axis thus change the dissipative rates on different subspaces, but the total effects lie in some convex hull which is captured by the majorization condition.

4. Possible extensions and further studies

4.1. Non-unital dynamics on single qubit

We have studied all the possible operators on a qubit one can simulate by using open-loop coherent controls in the unital open dynamics and given a simple and complete characterization. One immediate extension of this result is to consider a qubit in non-unital dynamics. There in the Bloch representation

$$\rho = \frac{1}{2}I + \frac{1}{2}(a_x\sigma_x + a_y\sigma_y + a_z\sigma_z),$$

the Lindblad equation will have an affine term, i.e.,

$$\frac{d}{dt}\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = [A(t)+B]\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} + p \tag{9}$$

where $p = 2(\mathrm{Im}(\gamma_{zy}), \mathrm{Im}(\gamma_{xz}), \mathrm{Im}(\gamma_{yx}))^{\mathrm{T}}$, which is not zero for non-unital dynamics. In this case, we can include $\frac{1}{2}I$ into the Bloch equation to get a homogenous linear equation, denote $a_0 = \frac{1}{2}I$, then

$$\frac{d}{dt}\begin{pmatrix} a_0 \\ a_x \\ a_y \\ a_z \end{pmatrix} = \left[\begin{pmatrix} 0 & 0 \\ 0 & A(t) \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ p & B \end{pmatrix}\right]\begin{pmatrix} a_0 \\ a_x \\ a_y \\ a_z \end{pmatrix}$$

And the operator dynamics is just the uplift of this equation,

$$\frac{d}{dt}N(t) = \left[\begin{pmatrix} 0 & 0 \\ 0 & A(t) \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ p & B \end{pmatrix}\right]N(t) \tag{10}$$

The solution of this equation is

$$N(T) = \begin{pmatrix} 1 & 0 \\ \int_0^T O(T-s)pds & O(T) \end{pmatrix} \tag{11}$$

where $O(t)$ is the solution of equation (7), and has to satisfy the majorization constrain, here $O(T)$ and $O(T-s)$ are correlated.

4.2. Higher dimension systems

For higher($m \geq 3$) dimensional systems, consider a basis for traceless operators $\{F_\alpha\}$ that is Hermitian and trace orthonormal. Then we can express a density matrix as $\rho = \rho_0 I + \sum_\alpha \rho_\alpha F_\alpha$ where ρ_0, ρ_α are real numbers. If we put ρ_α into a vector $\vec{a}$, then the master equation becomes

$$\frac{d}{dt}\vec{a}(t) = [A(t)+B]\vec{a} + p \tag{12}$$

where $A(t)$ and B are $(m^2-1)\times(m^2-1)$ matrices, $A(t)$ is antisymmetric, lies in $\mathfrak{so}(m^2-1)$ and B is symmetric, p is a (m^2-1)-dimension vector. First consider the case that $p = 0$, in this case, the operator dynamics can be obtained by uplifting the dynamics of $\vec{a}$,

$$\frac{d}{dt}O(t) = [A(t)+B]O \tag{13}$$

Using the same argument, one can show that

$$O(T) = S_1 \exp[diag(c_1, c_2, \cdots, c_{m^2-1})]S_0$$

where $S_1, S_0 \in SO(m^2-1)$ and

$$(c_1, c_2, \cdots, c_{m^2-1}) \prec (\lambda_1, \lambda_2, \cdots, \lambda_{m^2-1})T,$$

λ_i are eigenvalues of B. For the case of $p \neq 0$, one can get a similar expression as equation (11). This gives a necessary condition on what operators one can simulate at time T for high dimensional systems, but different from single qubit case, this is not a complete characterization, i.e., not all the operators satisfy this condition can be generated, as for higher($m \geq 3$) dimension, coherent controls can not generate the whole group of $SO(m^2-1)$ (as opposed to the single qubit case, coherent controls can generate the whole $SO(3)$ in the Bloch representation), so it is not always possible to diagonalize B and permuting the diagonal entries. Further studies are needed for a complete characterization for higher dimensional systems.

4.3. Beyond open-loop coherent control

While in this article I consider open-loop coherent controls, one can also consider the closed loop controls and other possible resources, which is beyond the scope of this article, interested readers are referred to some works[4, 5] on those directions.

5. Conclusion

In this article I considered simulation of open quantum system in Markovian environment, particularly simulation of single qubit for unital quantum dynamics. With coherent control on system, I studied the possible operations one can simulate on the system at any given time. A simple and complete characterization is found for single qubit in unital quantum dynamics, and possible extensions on general systems are discussed along this direction. I hope this result will be helpful in better understanding open quantum dynamics.

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