Control of single spin in Markovian environment

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Control of single spin in Markovian environment

Haidong Yuan*

Abstract
In this article we study the control of single spin in Markovian environment. Given an initial state, we compute all the possible states to which the spin can be driven at arbitrary time, under the assumption that fast unitary operations on the single spin are available.

1. Introduction

In the last two decades, control theory has been applied to an increasingly wide number of problems in physics and chemistry whose dynamics are governed by the time-dependent Schrödinger equation (TDSE), including control of chemical reactions [1, 2, 3, 5, 6, 7, 8, 9], state-to-state population transfer [10, 11, 12, 13], shaped wavepackets [14], Bose-Einstein condensation [16, 17, 18], quantum computing [19, 20, 21], oriented rotational wavepackets [22], etc. [23, 24]. More recently, there has been vigorous effort in studying the control of open quantum systems which are governed by Lindblad equations, where the central object is the density matrix, rather than the wavefunction [25, 26, 27, 28, 29, 30, 31]. The Lindblad equation is an extension of the TDSE that allows for the inclusion of dissipative processes. In this article, we study two level systems governed by the controlled Lindblad equation, we will compute all the possible states to which the systems can be driven at arbitrary time, under the assumption that fast unitary operations on the system are available.

2. Setting up the control problem

2.1. The system equations of motion and the Lindblad formula for dissipation

Let $\rho$ denote the density matrix of an quantum system. The density matrix evolves under the Lindblad equation, which takes the form

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

(1)

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 $\rho$ and is given by the Lindblad form [32, 34],

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

where $F_\alpha, F_\beta$ are the Lindblad operators. Eq. (1) has the following three well known properties: 1) Tr$(\rho)$ remains unity for all time, 2) $\rho$ remains a Hermitian matrix, and 3) $\rho$ stays positive semi-positive definite, i.e. that $\rho$ never develops non-negative eigenvalues.

2.2. Formulation of the Control Problem

The problem we address in this paper is to compute all the density matrices the system can reach for the quantum dissipative system which evolves under the Lindblad equation of motion given by eq. (1). We assume that we can apply any desired sequence of unitary transformations to the system, over a time scale of its coupling to the bath. For the purpose of this paper, we will confine our attention to two level systems, such as, e.g., a two level atom where the Hamiltonian $H(t)$ is a time varying dipole term arising from a high bandwidth applied lase field. Our results will be largely generalizable to systems with arbitrary dimension.

3. Reformulation of the Problem in Terms of the Spectrum of $\rho$

In this section we develop a general formalism that highlights the cooperative interplay between Hamiltonian and dissipative dynamics. Following [27, 4], we assume that the action of the control Hamiltonian can be produced on a time scale fast compared with dissipation. We assume that the control Hamiltonian $H(t)$ can produce any unitary transformation $U \in SU(2)$ in the 2–level system, i.e. the system of interest is unitarily controllable. Combining these two assumptions we
have that any unitary transformation can be produced on the system in negligible time compared to the dissipation.

The above dynamical assumptions lead to another very important simplification. Since we have assumed that all unitary transformations in $SU(2)$ can be produced instantaneously, this includes bringing the density matrix into diagonal form. As a result, the different elements of each orbit can be considered redundant, and the orbit of $\rho$ can be completely represented by its diagonal form, or 'spectrum', $\lambda(\rho)$. This suggests reformulating the control problem entirely in terms of the spectrum, rather than in terms of $\rho$ itself. The key step in this reformulation is to replace the equation of motion for $\rho$, eq. (1), with an equation of motion for the spectrum. We do this in the next section. The controls will enter into the equation in a modified way that gives additional insight into the interplay of Hamiltonian and dissipative dynamics.

Let $\Lambda$ be its associated diagonal form of density matrix $\rho$.

Substitute $\rho(t) = U(t)\Lambda(t)U^\dagger(t)$ into Eq.(1), we get

$$\rho(t) = \dot{U}(t)\Lambda(t)U^\dagger(t) + U(t)\dot{\Lambda}(t)U^\dagger(t) + U(t)\Lambda(t)U^\dagger(t)\dot{U}(t) - U(t)\Lambda(t)U^\dagger(t)iH'(t)$$

$$= -i[H'(t), U(t)\Lambda(t)U^\dagger(t)] + U(t)\Lambda(t)U^\dagger(t)\dot{U}(t)$$

where $H'(t)$ is defined by $\dot{U}(t) = -iH'(t)U(t)$. We obtain

$$\dot{\Lambda}(t) = U^\dagger(t)\{ -i[H(t) - H'(t), U(t)\Lambda(t)U^\dagger(t)] + L[U(t)\Lambda(t)U^\dagger(t)]\}U(t)$$

$$= -i[U^\dagger(t)(H(t) - H'(t))U(t), \Lambda(t)] + U^\dagger(t)L[U(t)\Lambda(t)U^\dagger(t)]U(t)$$

Note that the left side of the above equation is a diagonal matrix, so for the right side we only need to keep the diagonal part. It is easy to see that the diagonal part is zero for the first term, thus we get

$$\dot{\Lambda}(t) = \text{diag}(U^\dagger(t)L[U(t)\Lambda(t)U^\dagger(t)]U(t))$$

where we use $\text{diag}(A)$ denote a diagonal matrix whose diagonal entries are the same as matrix $A$.

4. Reachable set for single spin

4.1. Examples

Let’s first work out two examples. We first study the single spin with pure decoherence in the $z$-basis. In this case,

$$L(\rho) = -\gamma[\sigma_z, [\sigma_z, \rho]]$$

So

$$\dot{\lambda}(t) = \text{diag}(U^\dagger L(U\Lambda U^\dagger)U)$$

$$= \text{diag}(-U^\dagger \gamma[\sigma_z, [\sigma_z, U\Lambda U^\dagger]]U)$$

$$= \text{diag}(-\gamma[U^\dagger \sigma_z U, [U^\dagger \sigma_z U, \Lambda]])$$

(8)

We can write

$$\Lambda(t) = \frac{1}{2}I + \lambda(t)\sigma_z$$

where $\lambda(t) \in [0, \frac{1}{2}]$, and

$$U^\dagger(t)\sigma_z U(t) = a_1(t)\sigma_x + a_2(t)\sigma_y + a_3(t)\sigma_z$$

where $\sum_{i=1}^3 a_i^2(t) = 1$. Substitute these into above equations, we get

$$\dot{\lambda}(t) = -4\gamma(a_1^2(t) + a_2^2(t))\lambda$$

(6)

So

$$\lambda(T) = \exp\int_0^T -4\gamma(a_1^2(t) + a_2^2(t))dt I \lambda(0)$$

Note that the quantity $a_1^2(t) + a_2^2(t) \in [0, 1]$, and by choosing appropriate $U(t)$, it can be any value in this interval. So at time $T$, $\lambda(T)$ can be any value in $[\exp(-4\gamma T)\lambda(0), \lambda(0)]$, i.e., the reachable set for the single spin in this case is

$$\rho(T) = \{ U(\frac{1}{2}I + \lambda(T)\sigma_z)U^\dagger |$$

$$\lambda(T) \in [\exp(-4\gamma T)\lambda(0), \lambda(0)], U \in SU(2) \}$$

(7)

Let’s look at another example with both longitudinal and transverse relaxation.

$$L(\rho) = -\gamma_1[\sigma_z, [\sigma_z, \rho]] - \gamma_2[\sigma_z, [\sigma_z, \rho]]$$

In this case

$$\dot{\lambda}(t) = \text{diag}(U^\dagger L(U\Lambda U^\dagger)U)$$

$$= \text{diag}(-U^\dagger \gamma_1[\sigma_z, [\sigma_z, U\Lambda U^\dagger]]U)$$

$$= \text{diag}(-\gamma_1[U^\dagger \sigma_z U, [U^\dagger \sigma_z U, \Lambda]])$$

$$= \text{diag}(-\gamma_2[U^\dagger \sigma_z U, [U^\dagger \sigma_z U, \Lambda]])$$

(8)
Again we write
\[ \Lambda(t) = \frac{1}{2} I + \lambda(t) \sigma_z \]
where \( \lambda(t) \in [0, \frac{1}{2}] \), and
\[ U^\dagger(t) \sigma_z U(t) = a_1(t) \sigma_x + a_2(t) \sigma_y + a_3(t) \sigma_z \]
where \( \sum_{i=1}^{3} a_i^2(t) = 1 \). Substituting these into the equation, we get
\[ \dot{\lambda}(t) = \gamma_1 (a_1^2(t) + a_2^2(t)) - 4 \gamma_2 (b_1^2(t) + b_2^2(t)) \lambda(t) \]  \hspace{1cm} (9)
As \( a_3 b_3 = -a_1 b_1 - a_2 b_2 \),
\[ (a_3 b_3)^2 = (a_1 b_1 + a_2 b_2)^2 \leq (a_1^2 + a_2^2)(b_1^2 + b_2^2) \]
\[ = (1 - a_3^2)(1 - b_3^2) \]  \hspace{1cm} (10)
We get \( a_3^2 + b_3^2 \leq 1 \), so
\[ 1 \leq a_3^2 + b_3^2 = (a_3^2 + b_3^2)(a_1^2 + a_2^2) \leq 2 \]
Assume \( \gamma_1 \geq \gamma_2 \), then
\[ 4 \gamma_1 (a_1^2(t) + a_2^2(t)) - 4 \gamma_2 (b_1^2(t) + b_2^2(t)) \leq (4 \gamma_2 (a_1^2(t) + a_2^2(t)) - 4 \gamma_2 (b_1^2(t) + b_2^2(t)) \leq [4 \gamma_2, 4 (\gamma_1 + \gamma_2)] \]

From this, it is easy to see that at time \( T \),
\[ \lambda(T) \in [\exp(-4(\gamma_1 + \gamma_2) T) \lambda(0), \exp(-4 \gamma_2 T) \lambda(0)] \]
so the reachable set for the single spin in this case is
\[ \rho(T) = \{ U \left( \frac{1}{2} I + \lambda(T) \sigma_z \right) U^\dagger \lambda(T) \in [\exp(-4(\gamma_1 + \gamma_2) T) \lambda(0), \exp(-4 \gamma_2 T) \lambda(0)], U \in SU(2) \} \]

4.2. General case

The examples above are just two special cases of the following general result.

Take the general expression of the master equation
\[ \rho = -i[H, \rho] + L(\rho) \]
where
\[ L(\rho) = \sum_{a\beta} a_{a\beta} (F_a \rho F_{a\beta} - \frac{1}{2} \{F_{a\beta}, F_a, \rho\}) \]

For the single spin, we can take the basis \( \{ F_a \} \) as normalized Pauli spin operators \( \frac{1}{\sqrt{2}} \{ \sigma_x, \sigma_y, \sigma_z \} \). The coefficient matrix
\[ A = \begin{pmatrix} a_{xx} & a_{xy} & a_{xz} \\ a_{yx} & a_{yy} & a_{yz} \\ a_{zx} & a_{zy} & a_{zz} \end{pmatrix} \]

known as the GKS(Gorini, Kossakowski and Sudarshan) matrix [33], is semi-positive definite. For the moment assume that the Markovian quantum dynamics is unital, just means \( L(t) = 0 \). In the single spin case, this is equivalent to the condition that all the entries of the GKS matrix are real numbers[40].

\[ \dot{\lambda}(t) = \text{diag}(U^\dagger L(U \Lambda U^\dagger)) \]
\[ = \text{diag}(\sum_{a\beta} a_{a\beta} (F_a \Lambda F_{a\beta} - \frac{1}{2} \{F_{a\beta}, F_a, \Lambda\})) \] \hspace{1cm} (11)
\[ = \text{diag}(\sum_{a\beta} a_{a\beta} (F_a \Lambda F_{a\beta} - \frac{1}{2} \{F_{a\beta}, F_a, \Lambda\})) \]

For the last step we just used the fact that \( F_{a\beta} \) is a Pauli matrix which is Hermitian. Now
\[ U^\dagger F_a U = c_{a\gamma} F_{\gamma} \]
where
\[ C = \begin{pmatrix} c_{xx} & c_{xy} & c_{xz} \\ c_{yx} & c_{yy} & c_{yz} \\ c_{zx} & c_{zy} & c_{zz} \end{pmatrix} \] \hspace{1cm} (12)
is the transformed GKS matrix, i.e.,
\[ A' = C^T A C \]

Substituting \( \Lambda(t) = \frac{1}{2} I + \lambda(t) \sigma_z \) into equation (12), we obtain
\[ \dot{\lambda}(t) = \text{diag}(\sum_{a\beta} a'_{a\beta} (F_a \Lambda F_{a\beta} - \frac{1}{2} \{F_{a\beta}, F_a, \Lambda\})) \]
where
\[ a'_{a\beta} = c_{\gamma a} c_{\beta \mu} c_{\mu \beta} \] is the transformed GKS matrix, i.e.,
\[ A' = C^T A C \]

Using Schur and Horn’s theorem on majorization (see appendix), we obtain
\[ \mu_3 + \mu_2 \leq a'_{xx} + a'_{yy} \leq \mu_2 + \mu_1 \]
where \( \mu_1 \geq \mu_2 \geq \mu_3 \) are eigenvalues of the GKS matrix. From this it is easy to see that at time \( T \), all the values \( \lambda(T) \) can be are
\[ [e^{-((\mu_1 + \mu_2) T) \lambda(0)}, e^{-((\mu_2 + \mu_3) T) \lambda(0)}] \]
So the reachable set for the single spin under unital master quantum dynamics is
\[ \rho(T) = \{ U \left( \frac{1}{2} + \lambda(T) \right) 0 \} U^\dagger \lambda(T) \in \{ e^{-(\mu_1 + \mu_3)T} \lambda(0), e^{-(\mu_2 + \mu_3)T} \lambda(0) \}, U \in SU(2) \}

Important examples of unital master equation includes phase damping and depolarizing, whose GKS matrix is just \( \gamma I \) (I is the identity matrix). But there is another important decoherence mechanism which is not unital—amplitude damping, which models the spontaneous emission from \( |1\rangle \) to \( |0\rangle \), we will study it in the next section.

5. Two level dissipative system

The Lindblad form for two level system with spontaneous emission from \( |1\rangle \) to \( |0\rangle \) is given by

\[ \dot{L}(\rho) = 2\gamma \sigma_- \rho \sigma_+ - \gamma \{ \sigma_+, \rho \sigma_- \} = \gamma \{ \sigma_- \rho, \sigma_+ \} \]  

where

\[ \sigma_+ = \sigma_x + i \sigma_y = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \]  

\[ \sigma_- = \sigma_x - i \sigma_y = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix} \]

Similarly we write \( \Lambda(t) = \frac{1}{2} I + \lambda(t) \sigma_z \), \( 0 \leq \lambda(t) \leq \frac{1}{2} \), and

\[ U^\dagger(t) \sigma_z U(t) = a_1(t) \sigma_x + a_2(t) \sigma_y + a_3(t) \sigma_z \]

\[ U^\dagger(t) \sigma_y U(t) = b_1(t) \sigma_x + b_2(t) \sigma_y + b_3(t) \sigma_z \]

where \( \sum_{i=1}^3 a_i^2(t) = 1, \sum_{i=1}^3 b_i^2(t) = 1 \) and \( \sum_{i=1}^3 a_i b_i = 0 \).

Substituting these into the equation

\[ \dot{\lambda}(t) = \text{diag}(U^\dagger L(U \Lambda U^\dagger) U) \],

we obtain

\[ \dot{\lambda}(t) = \gamma \{ -4(a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t)) \lambda + 4(a_2(t)b_1(t) - a_1(t)b_2(t)) \} \]  

(16)

It is convenient to study the dynamics of \( \frac{1}{2} + \lambda(t) \):

\[ \frac{d}{dt} \left( \frac{1}{2} + \lambda(t) \right) = \gamma \{ -4(a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t)) \times \]

\[ (\frac{1}{2} + \lambda(t)) + 2[a_2(t) + b_1(t)]^2 + 2[a_1(t) - b_2(t)]^2 \}

Let’s look at the right side of the above equation to see what value it can take. As we have shown before,

\[ 1 \leq a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t) \leq 2 \]

So

\[ -8 \left( \frac{1}{2} + \lambda(t) \right) \leq -4(a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t)) \times \]

\[ (\frac{1}{2} + \lambda(t)) \]  

\[ \leq -4 \left( \frac{1}{2} + \lambda(t) \right) \]

And \( 2[a_2(t) + b_1(t)]^2 + 2[a_1(t) - b_2(t)]^2 \geq 0, \) so

\[ \gamma \{ -4(a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t)) \left( \frac{1}{2} + \lambda(t) \right) \}

\[ + 2[a_2(t) + b_1(t)]^2 + 2[a_1(t) - b_2(t)]^2 \} \leq -8 \gamma \left( \frac{1}{2} + \lambda(t) \right) \]

and the equality is achievable at \( a_1 = b_1 = a_2 = b_2 = 0 \), which gives the upper bound of \( \frac{d}{dt} \left( \frac{1}{2} + \lambda(t) \right) \).

Now let’s find the upper-bound. Suppose

\[ a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t) = c \]

where \( c \in [1,2] \), as

\[ (a_2 + b_1)^2 + (a_1 - b_2)^2 \leq 2(a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t)) \]

\[ = 2c \]

We get

\[ \gamma \{ -4(a_1^2(t) + a_2^2(t) + b_1^2(t) + b_2^2(t)) \times \]

\[ \left( \frac{1}{2} + \lambda(t) \right) + 2(a_2(b_1(t) - a_1(t)b_2(t)) \}

\[ \leq \gamma \{ -4c \left( \frac{1}{2} + \lambda(t) \right) + 4c \} \]

\[ = 4 \gamma c \left( \frac{1}{2} - \lambda(t) \right) \]

\[ \leq 8 \gamma \left( \frac{1}{2} - \lambda(t) \right) \]

The equality is achievable at \( a_2 = b_1 = a_1 = b_2 = 0 \), which gives the upper bound.

By connecting property, we know that \( \frac{d}{dt} \left( \frac{1}{2} + \lambda(t) \right) \) can take any value in

\[ [-8 \gamma \left( \frac{1}{2} + \lambda(t) \right), 8 \gamma \left( \frac{1}{2} - \lambda(t) \right)] \]

With this, we can find the reachable set for \( \lambda(T) \).

First for the lower bound, we always take the right side of eq. (17) to be the smallest:

\[ \frac{d}{dt} \left( \frac{1}{2} + \lambda(t) \right) = -8 \gamma \left( \frac{1}{2} + \lambda(t) \right) \]
So 
\[ \frac{1}{2} + \lambda(T) = \exp(-8\gamma T)\left(\frac{1}{2} + \lambda(0)\right) \]
\[ \lambda(T) = \exp(-8\gamma T)\left(\frac{1}{2} + \lambda(0)\right) - \frac{1}{2} \]

Similarly for the upper bound:
\[ \frac{d}{dt}\left[\frac{1}{2} + \lambda(t)\right] = 8\gamma\left[\frac{1}{2} - \lambda(t)\right] \]
\[ = -8\gamma\left[\frac{1}{2} + \lambda(t)\right] + 8\gamma \quad (19) \]

The solution in this case is
\[ \frac{1}{2} + \lambda(T) = \exp(-8\gamma T)\left(\frac{1}{2} + \lambda(0)\right) + \exp(-8\gamma T)\int_0^T 8\gamma\exp(8\gamma t)dt \quad (20) \]
\[ = \exp(-8\gamma T)\left(\frac{1}{2} + \lambda(0)\right) + 1 - \exp(-8\gamma T) \]
So
\[ \lambda(T) = \exp(-8\gamma T)\left(-\frac{1}{2} + \lambda(0)\right) + \frac{1}{2} \]

Thus the reachable set for this system is
\[ \rho(T) = \{U\left[\frac{1}{2}I + \lambda(T)\sigma_z\right]U^\dagger | U \in SU(2), \lambda(T) \in [\max\{0,\exp(-8\gamma T)\left(-\frac{1}{2} + \lambda(0)\right) - \frac{1}{2}\}, \exp(-8\gamma T)\left(-\frac{1}{2} + \lambda(0)\right) + \frac{1}{2}\}\} \quad (21) \]

The intuitive interpretation of this is as follows. For times short compared with \(\frac{1}{T}\), the reachable spectra are close to the original spectrum. For longer times, however, one can play the tendency of the system to relax off against the ability to perform unitary control to manipulate the spectrum in any desired faction, so that for \(T >> \frac{1}{T}\), essentially all possible states can be reached.

6. Conclusion

Control of open quantum systems is an important problem for a wide variety of physics, chemistry, and engineering applications. This paper analyzed the problem of controlling open quantum systems in cases where full, high-bandwidth coherent control of the system is available. This coherent control can be used to ‘present’ various aspects of the system’s state to the environmental interaction. Because of the presence of fast coherent control, the quantity of interest under control is the spectrum of the density matrix. We analyzed the reachability of various spectral forms for two-level systems and derived general formulae for reachability in the presence of pure decoherence, and of decoherence and relaxation. In the presence of pure decoherence, the time evolution is unital, and tends inevitably towards the fully mixed state. Coherent control can only delay this process and achieve a variety of less than fully mixed states at various times along the way. The presence of relaxation in addition to decoherence allows a richer set of states to attained by playing decoherence (which drives the system to a fully mixed state) and relaxation (which drives the system to a pure state) off against each other.

A. Majorization

For an element \(x = (x_1, ..., x_k)^T\) of \(\mathbb{R}^k\) we denote by \(x_i^\dagger = (x_1^\dagger, ..., x_k^\dagger)^T\) a permutation of \(x\) so that \(x_i^\dagger \geq x_j^\dagger\) 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 \(x < y\)), if
\[ \sum_{j=1}^d x_j^\dagger \leq \sum_{j=1}^d y_j^\dagger \]

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

Proposition 1 (Schur, Horn [39, 41]) For an element \(\lambda = (\lambda_1, ..., \lambda_n)^T\), let \(D_\lambda\) be a diagonal matrix with \((\lambda_1, ..., \lambda_n)\) as its diagonal entries, let \(a = (a_1, ..., a_n)^T\) be the diagonal entries of matrix \(A = K^T D_\lambda K\), where \(K \in SO(n)\). Then \(a < \lambda\). Conversely for any vector \(a < \lambda\), there exists a \(K \in SO(n)\), such that \((a_1, ..., a_n)^T\) are the diagonal entries of \(A = K^T D_\lambda K\).

References