Physics Letters A 379 (2015) 272–278

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Model discrimination for dephasing two-level systems

Er-ling Gong [a,b], Weiwei Zhou [a], Sophie Schirmer [b,*]

[a] Department of Automatic Control, College of Mechatronic Engineering and Automation, National University of Defense Technology, Changsha, Hunan 410073, China

[b] College of Science (Physics), Swansea University, Singleton Park, Swansea, SA2 8PP, United Kingdom

ARTICLE INFO

Article history:
Received 26 August 2014
Received in revised form 19 November 2014
Accepted 20 November 2014
Available online 26 November 2014
Communicated by P.R. Holland

Keywords:
Open quantum systems
Dephasing
Model discrimination
Experiment design

ABSTRACT

The problem of model discriminability and parameter identifiability for dephasing two-level systems subject to Hamiltonian control is studied. Analytic solutions of the Bloch equations are used to derive explicit expressions for observables as functions of time for different models. This information is used to give criteria for model discrimination and parameter estimation based on simple experimental paradigms.

1. Introduction

Control of quantum dynamics by means of Hamiltonian engineering is recognized as a crucial tool for the development of quantum technology from quantum information processing (QIP) applications to novel pulse sequences for magnetic resonance imaging (MRI) [1–3]. The effectiveness of most quantum control strategies is conditional on the existence of accurate models for control design. The derivation of such models for systems subject to both control and decoherence is therefore crucial for the development of effective control strategies, and techniques for system identification based experimental data play an important role in finding such models. This is increasingly being realized and reflected by a rapidly growing body of literature in the field of quantum system identification [4–12].

In this Letter we specifically address the issue of distinguishability of different plausible models for dephasing two-level systems in the presence of a nontrivial Hamiltonian, via the time evolution of an observable. From qubits as building blocks for QIP [13] to proton spins in MRI and spectroscopy [14], two-level systems are ubiquitous in many areas of physics. Although, the Lindblad superoperator for a two-level system in a Markovian environment has 15 parameters, resulting in a complex identification problem for generic relaxation dynamics, the observed relaxation phenomena for many physical systems appear to be reasonably well approximated by a few parameters such as transverse and longitudinal relaxation rates associated with population relaxation and phase decoherence effects, respectively. Usually, it is assumed, often implicitly, that both population and phase relaxation occur in the eigenbasis of the system Hamiltonian. However, when control fields are applied, it is not necessarily clear which Hamiltonian basis one should use. The question therefore arises whether and how one can distinguish these models experimentally. Assuming that we can model the system as a dephasing two-level system, can we distinguish different cases and identify basic model parameters? We address this problem by deriving explicit analytic expressions for the time evolution of typical observables for the different models and discuss their distinguishing features.

2. Markovian master equation and Bloch equation

We study a two-level quantum system such as a spin-$\frac{1}{2}$ particle or qubit subject to Hamiltonian control and Markovian pure dephasing. The state of the system can be described by a density operator ρ, whose evolution is governed by a Lindbladian master equation

$$\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \rho] + \mathcal{D}[V](\rho), \tag{1}$$

with the usual Lindbladian dissipation superoperator

$$\mathcal{D}[V](\rho) = V\rho V^\dagger - \frac{1}{2}\left(V^\dagger V\rho + \rho V V^\dagger\right) \tag{2}$$

* Corresponding author.
E-mail address: sgs29@swan.ac.uk (S. Schirmer).

http://dx.doi.org/10.1016/j.physleta.2014.11.042
0375-9601/© 2014 Published by Elsevier B.V.

but with unknown Hermitian operators H and V. Broadly, we are interested in the determination of the operators H and V given limited or no prior knowledge of the system, with limited control and measurement resources. More specifically, we will be interested in the question of how to discriminate between two types of probable models and identify the relevant model parameters.

We note here that while Eq. (1) is a general model to describe a quantum system subject to Markovian dynamics, we have assumed a special form of the dissipation superoperator appropriate for modelling a two-level system subject to pure dephasing, which can be described by an Hermitian operator V. With these assumptions we can, without loss of generality, choose a basis so that either H or V is diagonal. We shall choose a basis so that V is diagonal. As V is a pure dephasing process and any component proportional to the identity can be incorporated into the Hamiltonian H, we further assume that V has zero trace. Thus, V has eigenvalues that occur in $\pm$ pairs and we can write

$$V = \sqrt{\frac{\gamma}{2}}\sigma_z, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

and $\gamma \geq 0$. Under these assumptions the dissipation super-operator simplifies

$$\mathcal{D}[\sigma_z](\rho) = \frac{\gamma}{2}(\sigma_z\rho\sigma_z - \rho). \tag{4}$$

We can further expand the control Hamiltonian with respect to the Pauli operator basis $\{I, \sigma_x, \sigma_y, \sigma_z\}$ for the 2×2 Hermitian matrices

$$H(t) = \frac{\hbar}{2}\big(\alpha I + \omega_z(t)\sigma_z + \omega_x(t)\sigma_x - \omega_y(t)\sigma_y\big), \tag{5}$$

where I is the identity operator and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{6}$$

Terms proportional to the identity give rise only to a global phase and can be neglected. Similarly expanding ρ with respect to the standard Pauli basis

$$\rho = \frac{1}{2}(I + v_x\sigma_x + v_y\sigma_y + v_z\sigma_z), \tag{7}$$

we can recast Eq. (1) in the common Bloch equation formulation

$$\begin{pmatrix} \dot{v}_x(t) \\ \dot{v}_y(t) \\ \dot{v}_z(t) \end{pmatrix} = \begin{pmatrix} -\gamma & -\omega_z(t) & -\omega_y(t) \\ \omega_z(t) & -\gamma & -\omega_x(t) \\ \omega_y(t) & \omega_x(t) & 0 \end{pmatrix} \begin{pmatrix} v_x(t) \\ v_y(t) \\ v_z(t) \end{pmatrix}, \tag{8}$$

where $v_\alpha = \mathrm{Tr}(\rho\sigma_\alpha)$ and we have assumed units are chosen such that $\hbar = 1$.

3. Model discrimination and parameter estimation problem

The general system identification problem for Eq. (8) is to find all model parameters ω_x, ω_y, ω_z, and γ. This general identification problem may be difficult to solve, especially when the parameters are time-dependent. However, there are interesting special cases.

One such special case is when dephasing acts in the same basis as the Hamiltonian, i.e., H and V commute, and $\omega_x = \omega_y = 0$. This is the case that is usually assumed without justification. When no control is applied and H is simply a static system Hamiltonian H_0 then this is a reasonable assumption. However, when control fields are applied the assumption that H and V commute may not be valid. Suppose we have a two-level system with $H_0 = \frac{1}{2}\omega_0\sigma_z$ that is driven by a constant amplitude control field giving rise to a control Hamiltonian $H_C = f(t)\sigma_x$ or $H_C = f(t)\sigma_y$, for example. Transforming to a rotating frame and neglecting counter-rotating terms, this gives an effective Hamiltonian $H^{\mathrm{RWA}} = \omega_z\sigma_z + \omega_x\sigma_x$ or $H^{\mathrm{RWA}} = \omega_z\sigma_z + \omega_y\sigma_y$ where $\omega_z = \Delta\omega_0$ is the detuning of the field from the resonance frequency ω_0 and ω_x or ω_y is the Rabi frequency Ω of the driving field. Thus, assuming that the field does not affect dephasing, the effective Hamiltonian H^{RWA} and V no longer commute.

From a model identification perspective, an interesting question is whether the control affects dephasing — for example, does V act in the original system Hamiltonian basis, or the new effective Hamiltonian basis, and to determine the model parameters. The first question can be regarded as a model discrimination problem while the latter is a parameter estimation problem. Specifically, we are interested in whether we can discriminate the different cases by performing a series of simple experiments, and what the best experimental protocols are. Motivated by the discussion above, we specifically consider three different cases:

(1) $\omega_z \neq 0$, $\omega_x = \omega_y = 0$;
(2) $\omega_x \neq 0$, $\omega_y = \omega_z = 0$;
(3) $\omega_y \neq 0$, $\omega_x = \omega_z = 0$,

where (a) can be regarded as the case of a two-level system with no driving fields applied and (b) and (c) as a two-level system resonantly driven by a constant amplitude field in the x-direction and y-direction, respectively.

4. Experimental design and assumptions

Lack of precise knowledge about the system typically precludes precise and sophisticated control. Therefore experimental protocols for system identification must be kept simple. In general minimal requirements for system identification include (1) the ability to prepare the system in *some* state ρ_I and (2) the ability to measure some observable M to obtain information about the system. With regard to assumption (1) we may not know a priori what the state ρ_I is but it should be possible to repeatedly initialize the system in the same state by following the same preparation procedure. In this spirit we make the following assumptions.

(1) Initialization. We assume that we are able to prepare the system in some initial state. For simplicity we take this to be a pure state $\rho_I = |\Psi_I(0)\rangle\langle\Psi_I(0)|$, where $|\Psi_I(0)\rangle$ takes the form

$$\big|\Psi_I(0)\big\rangle = \cos\frac{\theta_I}{2}|0\rangle + \sin\frac{\theta_I}{2}|1\rangle \tag{9}$$

and $\{|0\rangle, |1\rangle\}$ denotes an eigenbasis of V — although this assumption will be relaxed later. In practice this preparation might correspond to letting the system relax to its ground state and applying a short control pulse. In the absence of precise knowledge of the ground state, the resonance frequency of the system and the coupling strength, the effective rotation angle θ_I may not be known initially and we shall see that such a priori knowledge of θ_I is not necessary. We can formally represent the initialization procedure by the operator $\Pi(\theta_I)$, which is the projector onto the state $|\psi_I\rangle$.

(2) Measurement. We assume the ability to perform a two-outcome projective measurement. Without loss of generality we can assume the eigenvalues of the measurement operator to be ± 1 and write

$$M = M_+ - M_- = |m_+\rangle\langle m_+| - |m_-\rangle\langle m_-|. \tag{10}$$

We shall assume that the measurement basis states $|m_\pm\rangle$ can be written as

$$|m_+\rangle = \cos\frac{\theta_M}{2}|0\rangle + \sin\frac{\theta_M}{2}|1\rangle, \tag{11a}$$

$$|m_-\rangle = \sin\frac{\theta_M}{2}|0\rangle - \cos\frac{\theta_M}{2}|1\rangle, \tag{11b}$$