Model discrimination for dephasing two-level systems

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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.

Keywords: open quantum systems, dephasing, model discrimination, experiment design

1. Introduction

Control of quantum dynamics by means of Hamiltonian engineering is recognized as a crucial tool for the development of quantum technology from QIP applications to novel MRI pulse sequences \cite{1,2,3}. 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 a 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 \cite{4,5,6,7,8,9,10,11,12}.

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 quantum information processing \cite{13} to proton spins in magnetic resonance imaging (MRI) and spectroscopy \cite{14}, dephasing two-level systems are ubiquitous in many areas of physics and the ability to differentiate between decoherence models and identify of model parameters based on simple experimental paradigms for these basic building blocks is an important task.
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 $\rho$, whose evolution is governed by a Lindbladian master equation

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

with the usual Lindbladian dissipation superoperator

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

but with unknown Hermitian operators $\hat{H}$ and $V$. Broadly, we are interested in the determination of the operators $\hat{H}$ 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 $\hat{H}$ 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 $\hat{H}$, we further assume that $V$ has zero trace. Thus, $V$ has eigenvalues that occur in $\pm$ pairs and we can write

$$V = \sqrt{\gamma} \sigma_z, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

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

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

$$\hat{H}(t) = \frac{\hbar}{2} \left( \alpha I + \omega_z(t) \sigma_z + \omega_x(t) \sigma_x - \omega_y(t) \sigma_y \right),$$

where $I$ is the identity operator and

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

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

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

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

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

(8)

where $v_\alpha = \text{Tr}(\rho \sigma_\alpha)$ 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 $\omega_x$, $\omega_y$, $\omega_z$, and $\gamma$. 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 $H^\text{RWA} = \omega_z \sigma_z + \omega_x \sigma_x$ or $H^\text{RWA} = \omega_z \sigma_z + \omega_y \sigma_y$ where $\omega_z = \Delta \omega_0$ is the detuning of the field from the resonance frequency $\omega_0$ and $\omega_x$ or $\omega_y$ is the Rabi frequency $\Omega$ of the driving field. Thus, assuming that the field does not affect dephasing, the effective Hamiltonian $H^\text{RWA}$ 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 \( \rho_I \) 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 \( \rho_I \) 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

\[
|\Psi_I(0)\rangle = \cos \frac{\theta_I}{2} |0\rangle + \sin \frac{\theta_I}{2} |1\rangle
\]

and \( \{|0\rangle, |1\rangle\} \) denotes an eigenbasis of \( \mathcal{V} \) — 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 \( \theta_I \) may not be known initially and we shall see that such a priori knowledge of \( \theta_I \) 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 \( \pm 1 \) and write

\[
M = M_+ - M_- = |m_+\rangle \langle m_+| - |m_-\rangle \langle m_-|.
\]

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

\[
|m_+\rangle = \cos \frac{\theta_M}{2} |0\rangle + \sin \frac{\theta_M}{2} |1\rangle,
\]

\[
|m_-\rangle = \sin \frac{\theta_M}{2} |0\rangle - \cos \frac{\theta_M}{2} |1\rangle,
\]

so that the choice of the measurement can be reduced to suitable choice of the parameter \( \theta_M \), and we shall indicate this by writing \( M(\theta_M) \).

The problem considered here is similar to that considered in [6]. We still assume only a single initial state and single fixed measurement. Unlike in [6], however, the initial state and the measurement are not assumed to commute with the dephasing operator.

5. Solution of Bloch Equations

To address the model discrimination and parameter estimation problem we analytically solve the Bloch equation (8) for initial states of the form (9) and determine the predicted measurement outcomes for a measurement of type (10) for three different cases.
5.1. Case 1: $H = \omega \sigma_z$, $V = \sqrt{\frac{\sigma}{2}}\sigma_z$

In this case the Bloch equation (8) reduces to

$$\begin{pmatrix}
\dot{v}_x(t) \\
\dot{v}_y(t) \\
\dot{v}_z(t)
\end{pmatrix} =
\begin{pmatrix}
-\gamma & -\omega & 0 \\
\omega & -\gamma & 0 \\
0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
v_x(t) \\
v_y(t) \\
v_z(t)
\end{pmatrix}.$$  \hspace{1cm} (12)

The solution for the initial state (9) is

$$\begin{pmatrix}
v_x(t) \\
v_y(t) \\
v_z(t)
\end{pmatrix} =
\begin{pmatrix}
e^{-\gamma t} \cos \omega t \sin \theta_I \\
e^{-\gamma t} \sin \omega t \sin \theta_I \\
\cos \theta_I
\end{pmatrix}.$$ \hspace{1cm} (13)

and applying the binary-outcome projective measurement $M(\theta_M)$ yields the measurement traces $p(t) = \text{Tr}[M \rho(t)]$.

$$p(t) = e^{-\gamma t} \cos \omega t \sin \theta_I \sin \theta_M + \cos \theta_I \cos \theta_M.$$ \hspace{1cm} (14)

5.2. Case 2: $H = \omega \sigma_x$, $V = \sqrt{\frac{\sigma}{2}}\sigma_z$

In this case the Bloch equation (8) reduces to

$$\begin{pmatrix}
\dot{v}_x(t) \\
\dot{v}_y(t) \\
\dot{v}_z(t)
\end{pmatrix} =
\begin{pmatrix}
-\gamma & 0 & 0 \\
0 & -\gamma & -\omega \\
0 & \omega & 0
\end{pmatrix}
\begin{pmatrix}
v_x(t) \\
v_y(t) \\
v_z(t)
\end{pmatrix}.$$ \hspace{1cm} (15)

The solution for the initial state (9) is

$$\begin{pmatrix}
v_x(t) \\
v_y(t) \\
v_z(t)
\end{pmatrix} =
\begin{pmatrix}
e^{-\gamma t} \sin \theta_I \\
\Phi_2^x(t) \cos \theta_I \\
\Phi_3^x(t) \cos \theta_I
\end{pmatrix}.$$ \hspace{1cm} (16)

where $\tilde{\omega} = \sqrt{\omega^2 - \frac{1}{4} \gamma^2}$ and

$$\Phi_2^x(t) = -e^{-\frac{\gamma}{2} t} \frac{\omega}{\tilde{\omega}} \sin \tilde{\omega} t,$$ \hspace{1cm} (17a)

$$\Phi_3^x(t) = e^{-\frac{\gamma}{2} t} \left[ \cos \tilde{\omega} t + \frac{\gamma}{2\tilde{\omega}} \sin \tilde{\omega} t \right].$$ \hspace{1cm} (17b)

If $\omega^2 < \frac{1}{4} \gamma^2$ then $\tilde{\omega}$ is purely imaginary and the sine and cosine terms above are replaced by the respective hyperbolic functions. If $\omega^2 = \frac{1}{4} \gamma^2$, the expression $\tilde{\omega}^{-1} \sin(\tilde{\omega} t)$ must be analytically continued. Applying the binary-outcome projective measurement $M(\theta_M)$ yields

$$p(t) = e^{-\gamma t} \sin \theta_I \sin \theta_M + \Phi_3^x(t) \cos \theta_I \cos \theta_M.$$ \hspace{1cm} (18)
5.3. Case 3: $H = \omega_0 \sigma_y$, $V = \sqrt{2} \sigma_z$

In this case the Bloch equation (8) reduces to

\[
\frac{d}{dt} \begin{pmatrix} v_x(t) \\ v_y(t) \\ v_z(t) \end{pmatrix} = \begin{pmatrix} -\gamma & 0 & -\omega \\ 0 & -\gamma & 0 \\ \omega & 0 & 0 \end{pmatrix} \begin{pmatrix} v_x(t) \\ v_y(t) \\ v_z(t) \end{pmatrix},
\]

(19)

The solution for the initial state (9) is

\[
\begin{pmatrix} v_x(t) \\ v_y(t) \\ v_z(t) \end{pmatrix} = \begin{pmatrix} \Phi^y_1(t) \sin \theta_I - e^{-\frac{\gamma}{2} t} \frac{\omega}{\sqrt{2}} \sin \tilde{\omega} t \cos \theta_I \\ 0 \\ \Phi^y_3(t) \cos \theta_I + e^{-\frac{\gamma}{2} t} \frac{\omega}{\sqrt{2}} \sin \tilde{\omega} t \sin \theta_I \end{pmatrix}
\]

(20)

where

\[
\tilde{\omega} = \sqrt{\omega^2 - \frac{\gamma^2}{4}}
\]

and

\[
\Phi^y_1(t) = e^{-\frac{\gamma}{2} t} [\cos \tilde{\omega} t - \frac{\gamma}{2\sqrt{2}} \sin \tilde{\omega} t]
\]

(21a)

\[
\Phi^y_3(t) = e^{-\frac{\gamma}{2} t} [\cos \tilde{\omega} t + \frac{\gamma}{2\sqrt{2}} \sin \tilde{\omega} t]
\]

(21b)

Applying the binary-outcome projective measurement $M(\theta_M)$ yields

\[
p(t) = \alpha_1 e^{-\frac{\gamma}{2} t} \cos \tilde{\omega} t + \alpha_2 e^{-\frac{\gamma}{2} t} \sin \tilde{\omega} t
\]

(22)

where the coefficient functions are

\[
\alpha_1 = \cos(\theta_I - \theta_M)
\]

(23a)

\[
\alpha_2 = \frac{\gamma}{2\sqrt{2}} \cos(\theta_I + \theta_M) + \frac{\gamma}{\sqrt{2}} \sin(\theta_I - \theta_M)
\]

(23b)

As before, if $\omega^2 < \frac{1}{4} \gamma^2$ then $\tilde{\omega}$ will be purely imaginary and the sine and cosine terms above turn into their respective hyperbolic sine and cosine equivalents, and if $\omega^2 = \frac{1}{4} \gamma^2$, the expression $\tilde{\omega}^{-1} \sin(\tilde{\omega} t)$ must be analytically continued.

6. Discussion of Model Discrimination

The results of the preceding section show that given the same initialization and measurement procedures, the different cases lead to different measurement outcomes:

\[
p^{(1)}(t) = e^{-\gamma t} \cos \omega t \sin \theta_I \sin \theta_M + \cos \theta_I \cos \theta_M
\]

(24a)

\[
p^{(2)}(t) = e^{-\gamma t} \sin \theta_I \sin \theta_M + \Phi^y_1(t) \cos \theta_I \cos \theta_M
\]

(24b)

\[
p^{(3)}(t) = \alpha_1 e^{-\frac{\gamma}{2} t} \cos \tilde{\omega} t + \alpha_2 e^{-\frac{\gamma}{2} t} \sin \tilde{\omega} t.
\]

(24c)

This shows that the models are in principle distinguishable except in a few special cases. If $\sin \theta_I \sin \theta_M = \cos \theta_I \cos \theta_M = 0$ models 1 and 2 are indistinguishable as the measurement traces for both vanish identically. This can only
Figure 1: Model discrimination problem for $x$-control: Evolution of system state on the Bloch sphere and projection onto measurement axis for $H \propto \sigma_x$, $\theta_I = \pi/4$, $\theta_M = 0$ and $V \propto \sigma_x$ (left) and $V \propto \sigma_x$ (right).

Figure 2: Model discrimination problem for $y$-control: Evolution of system state on the Bloch sphere and projection onto measurement axis for $H \propto \sigma_y$, $\theta_I = \pi/4$, $\theta_M = \pi/2$ and $V \propto \sigma_y$ (left) and $V \propto \sigma_z$ (right).
happen if either \( \theta_I = m\pi \) and \( \theta_M = \frac{\pi}{2} + n\pi \) or vice versa, where \( m \) and \( n \) are integers. Models 1 and 3 are always distinguishable with the given initialization and measurement procedure.

Applied to the problem of distinguishing whether the dephasing acts in the original basis or the eigenbasis of the new effective Hamiltonian, a driving field applied in the \( x \)-direction (\( y \)-direction) with dephasing acting in the original (\( \sigma_z \)) basis corresponds to Case 2 (Case 3) above. Dephasing acting in the basis of the new effective system Hamiltonian corresponds to Case 1 above in that both \( H \) and \( V \) are simultaneously diagonalizable. However, we must be careful here as the basis in which both operators are diagonal depends on the control field applied, while in the derivation of Case 1 above it was assumed that both \( H \) and \( V \) were diagonal in the \( \sigma_z \)-basis. Therefore a basis change is necessary depending on the direction of the control field applied. We explicitly consider the resulting discrimination problems for three cases.

1(a): If no field is applied or the field is acting in the \( z \)-direction then no change of basis is necessary, and the model discrimination problem is trivial as the effective Hamiltonian acts in the same basis as the original Hamiltonian.

1(b): If the control is applied in the \( x \)-direction then the new effective Hamiltonian is proportional to \( \sigma_x \), and the eigenbasis in which \( H \) and \( V \) are diagonal is \(|\pm_x\rangle = \frac{1}{\sqrt{2}} [|0\rangle \pm |1\rangle] \). We must express the initial state in this basis

\[
|\Psi_I(0)\rangle = \cos(\theta_I/2)|0\rangle + \sin(\theta_I/2)|1\rangle
= \cos(\theta_I/2)\frac{|+x\rangle + |−x\rangle}{\sqrt{2}} + \sin(\theta_I/2)\frac{|+x\rangle − |−x\rangle}{\sqrt{2}}
= \frac{1}{\sqrt{2}}[\cos(\theta_I/2) + \sin(\theta_I/2)]|+x\rangle + \frac{1}{\sqrt{2}}[\cos(\theta_I/2) − \sin(\theta_I/2)]|−x\rangle
= \cos(\theta'_I)|+x\rangle + \sin(\theta'_I)|−x\rangle
\]

with \( \theta'_I = \frac{\pi}{2} − \theta_I \), and similarly for the measurement basis states

\[
|m_{\pm}\rangle = \cos(\theta'_M)|+x\rangle \pm \sin(\theta'_M)|−x\rangle
\]

with \( \theta'_M = \frac{\pi}{2} − \theta_M \), i.e., \( \theta_I \) and \( \theta_M \) must be replaced by \( \theta'_I \) and \( \theta'_M \).

The model discrimination problem for \( x \)-control, i.e., the problem of discriminating whether dephasing acts in the original Hamiltonian (\( \sigma_z \)) basis or in the new \( \sigma_x \) basis is thus equivalent to distinguishing

\[
p^{(1x)}(t) = e^{−\gamma t}\cos\omega t\cos\theta_I\cos\theta_M + \sin\theta_I\sin\theta_M
p^{(2)}(t) = e^{−\gamma t}\sin\theta_I\sin\theta_M + \Phi_3(t)\cos\theta_I\cos\theta_M.
\]

The differences in the evolution and measurement traces between both cases are illustrated in Fig. 1. In the first case, when \( H \) and \( V \) both act in the \( x \)-basis, the trajectories follow a spiral path around the \( x \)-axis in a plane perpendicular to the \( x \)-axis through the point on the sphere defining the initial state, while in the second case the trajectory follows a spiral path on a cone around the \( x \)-axis. In both cases the measurement signal corresponds to a damped oscillation but the traces are clearly distinguishable.
If a resonant control field is applied in the $y$-direction then $H\text{RWA}\propto \sigma_y$ and the eigenbasis in which $H$ and $V$ are diagonal is $|\pm_y\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm i|1\rangle)$. We must express the initial state in this basis to be able to apply the results from Case 1 above:

$$|\Psi_I(0)\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)|1\rangle$$

and similarly the measurement basis states $|m_{\pm}\rangle = \exp\left(-\frac{\theta_M}{2}\right)|+y\rangle \pm \exp\left(+\frac{\theta_M}{2}\right)|-y\rangle$.

Solving the Bloch equation (15) for the initial state (28), which has the Bloch vector representation $v = (\cos\theta_I, \sin\theta_I, 0)^T$ in the $\sigma_y$ basis, gives

$$\begin{pmatrix} v_x(t) \\ v_y(t) \\ v_z(t) \end{pmatrix} = \begin{pmatrix} e^{-\gamma t} \cos(\omega z t + \theta_I) \\ e^{-\gamma t} \sin(\omega z t + \theta_I) \\ 0 \end{pmatrix}$$

and applying the binary-outcome projective measurement $M(\theta_M)$ yields the measurement traces

$$p^{(1)}(t) = \Tr[M \rho(t)] = e^{-\gamma t} \cos(\omega t + \theta_I - \theta_M).$$

The model discrimination problem for $y$-control, i.e., the problem of discriminating whether dephasing acts in the original Hamiltonian ($\sigma_z$) basis or in the new $\sigma_y$ basis is therefore equivalent to distinguishing

$$p^{(1y)}(t) = e^{-\gamma t} \cos(\omega t + \theta_I - \theta_M)$$

and

$$p^{(2)}(t) = e^{-\gamma t} \sin \theta_I \sin \theta_M + \Phi_{\phi}(t) \cos \theta_I \cos \theta_M.$$}

The differences in the evolution and measurement traces between both cases are illustrated in Fig. 2. As before, in the first case, when $H$ and $V$ both act in the $y$-basis, the trajectories follow a spiral path, this time around the $y$-axis in a plane perpendicular to the $y$-axis through the point on the sphere defining the initial state, while in the second case the trajectory follows a more complex spiral path. In both cases the measurement signal corresponds to a damped oscillation but the traces are again clearly distinguishable.

A driving field applied in an arbitrary direction in the $xy$-plane, i.e., at an arbitrary angle $\phi_f$ to the $x$-axis, could be similarly accommodated by a suitable basis change.

7. Parameter Identifiability

Once the model type has been identified the next question is if and how we can identify the parameters in relevant models.
Figure 3: Evolution of system state on the Bloch sphere and projection onto measurement axis for $H = V$. The measurement trace contains information about both $H$ and $V$ (left), provided the initial state is not stationary, and the measurement axis does not coincide with the $H, V$-axis. In the latter case, although the system state is not stationary, no information about the system parameters can be obtained (right).

7.1. Model 1a – Hamiltonian and dephasing in $\sigma_z$-basis

Recalling that the observable in case of model (1a) takes the form

$$p^{(1)}(t) = e^{-\gamma t} \cos \omega t \sin \theta_I \sin \theta_M + \cos \theta_I \cos \theta_M$$

(33)

shows that we can obtain information about the system parameters $\omega$ and $\gamma$ if and only if $\sin \theta_I \neq 0$ and $\sin \theta_M \neq 0$, i.e., if neither the initial state preparation $\Pi(\theta_I)$ nor the measurement $M$ commutes with $H$ and $V$ as illustrated in Fig. 3. In this case the measurement traces also yield information about $\theta_I$ and $\theta_M$, i.e., we can determine the relative angles between the initialization and measurement axis and the fixed Hamiltonian / dephasing axis if they are not known a priori. We also see that the visibility is maximized if $\sin \theta_I \sin \theta_M = 1$, which will be the case if the initialization and measurement axis are orthogonal to the joint Hamiltonian and dephasing axis.

We can physically understand these results as follows. As $[H, V] = 0$, if the initial state preparation $\Pi(\theta_I)$ commutes with $H$ and $V$ then the initial state is a stationary state of the dynamics and the measurement outcome is constant in time $c_\pm = \frac{1}{2}(1 \pm 1)$. If $\sin \theta_I \neq 0$ then the initial state is not stationary and the state follows a spiral path towards the joint Hamiltonian and dephasing axis but as both $H$ and $V$ are proportional to $\sigma_z$, $\text{Tr}[\sigma_z \rho(t)]$ is a conserved quantity of the dynamics. Hence, if $\sin \theta_M = 0$ then the measurement commutes with $\sigma_z$, and as $\text{Tr}[\sigma_z \rho(t)]$ is a conserved quantity, we are unable to identify the system parameters $\gamma$ and $\omega_0$, illustrated in Fig. 3 (right). In both cases the constant measurement result still uniquely identifies the joint eigenbasis of the dephasing and Hamiltonian operators.

7.2. Model 1b – Hamiltonian and dephasing in $\sigma_z$-basis

If the initial state preparation and measurement operators are projectors onto states in the $xz$-plane as assumed here then our derivation above showed
that the measurement signal is of the form
\[ p^{(1x)}(t) = e^{-\gamma t} \cos \omega t \cos \theta_I \cos \theta_M + \sin \theta_I \sin \theta_M. \]
This case is similar to the previous case and the change of basis simply requires adjustment of the initial state and measurement parameters \( \theta_I \) and \( \theta_M \).

7.3. Model 1c – Hamiltonian and dephasing in \( \sigma_y \)-basis

If the initial state preparation and measurement operators are projectors onto states in the \( xz \)-plane as we have assumed then the initial state in this case is always orthogonal to the joint Hamiltonian and dephasing axis. This ensures that the model parameters \( \omega \) and \( \gamma \) in
\[ p^{(1y)}(t) = e^{-\gamma t} \cos(\omega t + \theta_I - \theta_M) \]
can be identified for any \( \theta_I \) and \( \theta_M \) and we always have maximal visibility.

7.4. Model 2 – \( \sigma_x \)-Hamiltonian, \( \sigma_z \)-dephasing

As the expression \( \Phi^x_3(t) \) in the measurement signal
\[ p^{(2)}(t) = e^{-\gamma t} \sin \theta_I \sin \theta_M + \Phi^x_3(t) \cos \theta_I \cos \theta_M \]
depends on both \( \omega \) and \( \gamma \) we can obtain full information about the system parameters if and only if \( \cos \theta_I \neq 0 \) and \( \cos \theta_M \neq 0 \). If \( \cos \theta_I = 0 \) or \( \cos \theta_M = 0 \), we can identify \( \gamma \) but not \( \omega \). Both cases are illustrated in Fig. 4 and can be understood as follows.

\( \cos \theta_I = 0 \) for \( \theta_I = \frac{\pi}{2} \), i.e., if the initial state is an eigenstate of the Hamiltonian. Since \( [H, V] \neq 0 \) in this case, eigenstates of \( H \) are not stationary. However, since the Hamiltonian and dephasing axis are orthogonal, the initial state remains in a plane orthogonal to the dephasing axis, the \( z = 0 \) plane in
our case, following the path \( x(t) = e^{-\gamma t} \). Thus we have \([H, \rho(t)] = 0\) for all times, and we can therefore not obtain any information about the Hamiltonian parameter \( \omega \) but we can still obtain information about the dephasing parameter \( \gamma \). If the Hamiltonian and dephasing axis were different but not orthogonal then we would be able to identify both the Hamiltonian and dephasing parameters even if the initial state was an eigenstate of \( H \) as in this case it would not remain an eigenstate of \( H \) under the evolution.

If \( \cos \theta_I \neq 0 \) but \( \cos \theta_M = 0 \) then the measurement commutes with the Hamiltonian. Transforming to the Heisenberg picture,

\[
\dot{M}(t) = -i[M(t), H] - \frac{\gamma}{2} D[s_z]M(t),
\]

and one can show that \( M(t) \) remains orthogonal to the dephasing axis and \( \text{Tr}[M(t)\rho_0] = \text{Tr}[M\rho(t)] \) is independent of the Hamiltonian \( H \), explaining why we cannot obtain any information about \( H \) in this case.

7.5. Model 3 – \( \sigma_y \)-Hamiltonian, \( \sigma_z \)-dephasing

It is impossible to find \( \theta_I \) and \( \theta_M \) such that \( \cos(\theta_I - \theta_M) = \sin(\theta_I - \theta_M) = \cos(\theta_I + \theta_M) = 0 \). Hence, we identify both model parameters for any \( \theta_I \) and \( \theta_M \) from the measurement signal

\[
p^{(2)}(t) = e^{-\gamma t} \sin \theta_I \sin \theta_M + \Phi^x_s(t) \cos \theta_I \cos \theta_M.
\]

The reason for this is that the initial state preparation and measurement operator in this case always project the system into state in the \( xz \)-plane which is orthogonal to the Hamiltonian axis, regardless of the choice of \( \theta_I \) and \( \theta_M \). As \([M, H] \neq 0\), there are no conserved quantities and the only stationary state of the system is the completely mixed state.

8. Conclusions

We have studied the problem of model identification for two-level quantum systems subject to Hamiltonian evolution and simultaneous dephasing assuming a simple experimental paradigm of repeated initialization and measurement after a delay. Analytic solutions of the Bloch equations were used to derive explicit expressions for the measured observables for different models. The latter were used to elucidate differences between different models and the ability to discriminate between them experimentally as well as the ability to identify model parameters from the measurement traces. The explicit solutions show that model discrimination and estimation of model parameters in general do not require a priori knowledge of the initial state or measurement operators as these can be learned along with the system parameters from the measurement traces except for a few very special (degenerate) cases.

There are practical advantages to formulating the general system identification problem as a model discrimination problem to decide whether dephasing acts in the original Hamiltonian basis or the new effective Hamiltonian basis.
These options appear physically most plausible, the resulting models are analytically tractable, and reducing the general model this way, reduces the number of parameters to be estimated. Thus, in practice one may wish to start with this assumption and generalize the problem to allow dephasing in an arbitrary basis if neither model proves to be a good fit to the data.

More work remains to be done to develop efficient algorithms for model discrimination and parameter identification based on noisy experimental data. However, the analytic solutions provide a basis for the development of optimal experimental protocols and numerical algorithms. These tools pave the way for experimental tests of the validity and accuracy of commonly used models for driven, dephasing two-level systems, and facilitate the development of more sophisticated decoherence models to more accurately describe environmental effects and their interaction with coherent control as necessary.

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