Open quantum system identification

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Abstract. Engineering quantum systems offers great opportunities both technologically and scientifically for communication, computation, and simulation. The construction and operation of large scale quantum information devices presents a grand challenge and a major issue is the effective control of coherent dynamics. This is often in the presence of decoherence which further complicates the task of determining the behaviour of the system. Here, we show how to determine open system Markovian dynamics of a quantum system with restricted initialisation and partial output state information.

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1. Introduction

Recently, much effort has been put into the design and realization of large scale quantum devices operating in the coherent regime. This has been spurred by the possibilities offered by quantum communication and information processing, from secure transmission, simulation of quantum dynamics, and the solution of currently intractable mathematical problems [1]. Many different physical systems have been proposed as basic architectures upon which to construct quantum devices, ranging from atoms, ions, photons, quantum dots and superconductors. For large scale commercial applications, it is likely that this will involve scalable engineered and constructed devices with tailored dynamics requiring precision control.

Due to inevitable manufacturing tolerances and variation, each device will display different behaviour even though they may be nominally “identical”. For their operation, they will need to be characterised as to their basic properties, response to control fields, and noise or decoherence [2]. We may also need to know how ideal is the system in the first place, for instance the effective Hilbert space; what we may assume to be a qubit may have dynamics involving more than two effective levels [3]. Extracting this information efficiently and robustly is crucial.

In a laboratory setting, an experimentalist may have access to many tools with which to study a system, e.g. spectroscopy and external probes. In a production setting, provision of these extra resources may be difficult, expensive, or impossible to integrate with the device. It is therefore important to understand what sort of characterisation can be performed simply using what is available in situ. Ideally, we would also like to be able to characterise the performance of a device with as little prior parameter data, e.g. how it responds to control fields, if this is the information which we are trying to obtain in the first place. Characterisation using only the in situ resources of state preparation and measurement, even where it is possible, is challenging, due to the increasing complexity of the signals, number of parameters to be estimated and the complexity of reconstructing a valid Hamiltonian from the resulting signal parameters. Robust and efficient methods of data gathering and analysis, preferably in as an automated way as possible, are therefore essential.

System identification attempts to extract dynamics from minimal pre-existing system control resources. There is a trade-off between the universality of the dynamics that can be identified versus the resources available in terms of initialisation, access, and measurement. Here, we explore the issue of what can be extracted in practice, leaving aside the question of efficiency for future work. We show how we can extract the dynamics of an open quantum system with restricted state initialisation and only partial information of the evolving state. This relies on prior knowledge of the structure of the decoherence processes. Our results show that in some cases full state information without prior knowledge can lead to worse estimation than partial state information combined with limited a-priori knowledge about the expected model type.

1.1. Quantum Process Tomography and System Identification

In quantum process tomography (QPT) [4], what is determined is the discrete map between initial and final states. This requires in general the preparation of a complete set of input density operators, and quantum state tomography (QST) [5] of each of the output states, the result of which gives a completely positive map. However, this does not fully characterise the dynamical behaviour of the system such as the
In principle, by conducting QPT at various times, it is possible to construct a time dependent set of Kraus operators \([6]\), hence capturing the most general (not necessarily Markovian) open systems evolution but this is costly in both terms of initial state preparation and QST. We therefore look for methods which require fewer resources to determine the dynamics of a system, though perhaps at the expense of the ability to handle the most general evolutions, considering that for many systems the physics is sufficiently known so that the structure of the dynamics can be constrained, even if the precise values (which we are trying to determine) may not be known.

Previous work has examined several system identification scenarios. Hamiltonian identification for a single qubit was introduced in \([7, 8, 9]\), Hamiltonian identification in the presence of decoherence was examined in \([10]\), extension to higher dimensional systems and the use of Bayesian/Maximum Likelihood techniques in \([11]\) and \([12]\), and model-based system parameter reconstruction in \([13]\). Other work has also studied identification of system Hamiltonians for spin networks with restricted access \([15, 16]\) and limited system initialisation \([17]\).

In the setting where preparation and measurement are limited to a single fixed basis it was found that signal and parameter complexity proved to be a major challenge even for relatively small systems and Hamiltonian evolution \([11]\). Including open system behaviour magnifies the problem even further. Besides increasing the number of parameters to be estimated, damping reduces the signal length and limits the amount of information that can be extracted \([10]\). To make the problem tractable we can try to incorporate prior information about the structure of the dynamics \([18, 19]\). In this case we find that even when only partial projective measurement data is available the signal may contain sufficient information to enable Hamiltonian reconstruction \([13]\).

Here we examine problem of determining open quantum system dynamics based on restricted initial state preparation and incomplete state reconstruction, e.g., limited to measurements of a single observable. Using a combination of Bayesian/Maximum likelihood estimation of signal parameters \([14]\) coupled with analysis of the equations of motion in the Laplace domain we study the problem of identifiability of models, comparing scenarios involving different types and amounts of information available for reconstruction. The results are applied to the problem of identifying the dynamics of a qubit in a Markovian environment to reconstruct both Hamiltonian and decoherent processes in various settings.

### 2. Master equation for Markovian Case

The evolution of an \(N\)-level open quantum system in a Markovian environment is given by the dissipative master equation

\[
\frac{d}{dt} \rho(t) = -\frac{i}{\hbar} [H, \rho] + \sum_{n,m=1}^{N^2-1} f_{mn} \mathcal{D}(F_m, F_n) \rho(t)
\]  

(1)

where \(\rho(t)\) is the state of the system at time \(t\) and \(H\) is a Hermitian matrix representing the effective Hamiltonian. In the following we shall choose units such that \(\hbar = 1\) and drop \(\hbar\). The requirement of completely positive evolution necessitates that the super-operators \(\mathcal{D}(F_m, F_n) \rho(t)\) be of the form \([20, 21, 22]\)

\[
\mathcal{D}(F_m, F_n) \rho(t) = F_n \rho F_m^\dagger - \frac{1}{2} (\rho F_m^\dagger F_n + F_n F_m^\dagger \rho)
\]  

(2)
where \( \{ f_n \}_{n=1}^{N^2-1} \) is an orthonormal basis for all trace-zero operators on \( \mathcal{H} \), and the coefficient matrix \( (f_{mn}) \) is positive. The latter requirement implies \( f_{mn}^* = f_{nm} \), i.e., we can write \( f_{mn} = a_{mn} + ib_{mn} \), where \( (a_{mn}) \) is a symmetric real matrix and \( (b_{mn}) \) is a real-anti-symmetric matrix.

Taking \( \{ \sigma_k \}_{k=1}^{N^2} \) to be a basis for the Hermitian matrices on the Hilbert space \( \mathcal{H} \) the master equation (1) with dissipation term (2) can be written in coordinate form as a linear matrix differential equation (DE) \([23]\):

\[
\frac{d}{dt}\tilde{\mathbf{r}} = (\mathbf{L} + \mathbf{D})\tilde{\mathbf{r}},
\]

where \( \tilde{\mathbf{r}} = (r_n) \in \mathbb{R}^{N^2} \) with \( r_n = \text{Tr}(\sigma_n \rho) \) and \( \mathbf{L} \) and \( \mathbf{D} \) are \( N^2 \times N^2 \) (real) matrices with entries

\[
L_{mn} = \text{Tr}(iH[\sigma_m, \sigma_n]) = \sum_{n'} h_{n'} \text{Tr}(i\sigma_{n'}[\sigma_m, \sigma_n]),
\]

\[
D_{mn} = \sum_{m',n'} f_{m'n'} \text{Tr}(F_{m'}^\dagger \sigma_m F_{n'} \sigma_n - \frac{1}{2} F_{m'}^\dagger F_{n'} \{ \sigma_m, \sigma_n \}).
\]

Here \( \{ A, B \} = AB + BA \) and \( [A, B] = AB - BA \) are the usual matrix anti-commutator and commutator, respectively. If we choose a basis such that \( \sigma_{N^2} = \frac{i}{\sqrt{N}} \mathbf{1} \) and the remaining basis elements form a basis for the trace-zero Hermitian matrices then

\[
r_{N^2} = \frac{1}{\sqrt{N}} \text{Tr}(\rho) = \frac{1}{\sqrt{N}}
\]

is constant, i.e., \( \dot{r}_{N^2} = 0 \), and we can define a reduced so-called Bloch vector \( \mathbf{r} = (r_1, \ldots, r_{N^2-1})^T \) \([24]\), and rewrite the linear matrix DE for \( \tilde{\mathbf{r}} \) as affine-linear DE

\[
\dot{\mathbf{r}}(t) = A\mathbf{r}(t) + \mathbf{c},
\]

where \( A \) is an \( (N^2 - 1) \times (N^2 - 1) \) real matrix with \( A_{mn} = L_{mn} + D_{mn} \) and \( c_m = \frac{1}{\sqrt{N}} D_{mN^2} \). We can without loss of generality choose \( F_m = \sigma_n \).

The objective of complete identification of the dynamics is thus reduced to identifying the coefficients \( h_{n'} \) and \( f_{m'n'} \) of the \( N^2 \times N^2 \) (Hermitian) coefficient matrix. Positivity constraints restrict the parameter space further to a convex subset of \( \mathbb{R}^{N^4} \).

3. Identifiability given Complete State Information

The Bloch equation for dissipative quantum systems always has at least one steady state \( \mathbf{r}_{ss} \) \([25]\) for which we have

\[
0 = \dot{\mathbf{r}}_{ss} = A\mathbf{r}_{ss} + \mathbf{c}.
\]

This implies \( \mathbf{c} = -A\mathbf{r}_{ss} \) and shows that the Bloch vector \( \mathbf{r}(t) \) is given by

\[
\mathbf{r}(t) = \mathbf{r}_{ss} + e^{tA}(\mathbf{r}(0) - \mathbf{r}_{ss}).
\]

We note that if there are two steady states \( \mathbf{r}_{ss}^{(1,2)} \) then \( A\Delta \mathbf{r}_{ss} = A(\mathbf{r}_{ss}^{(1)} - \mathbf{r}_{ss}^{(2)}) = 0 \) shows that \( A\mathbf{r}_{ss}^{(1)} = A\mathbf{r}_{ss}^{(2)} \) and thus \( \mathbf{c} \) is well-defined and

\[
\mathbf{r}(t) = \mathbf{r}_{ss}^{(2)} + e^{tA}(\mathbf{r}(0) - \mathbf{r}_{ss}^{(2)}) = \mathbf{r}_{ss}^{(1)} + \Delta \mathbf{r}_{ss} + e^{tA}(\mathbf{r}(0) - \mathbf{r}_{ss}^{(1)} - \Delta \mathbf{r}_{ss}) = \mathbf{r}_{ss}^{(1)} + e^{tA}(\mathbf{r}(0) - \mathbf{r}_{ss}^{(1)})
\]
noting that $A x = 0$ implies $\exp(tA)x = 1x$.

Generically the superoperator $A$ has $d = N^2 - 1$ distinct eigenvalues $\lambda_n$ with corresponding eigenvectors $v_n$. The eigenvalues and eigenvectors may be complex but as $A$ itself is real, complex eigenvalues must occur in complex conjugate pairs. Suppose there are $p < d/2$ pairs of complex eigenvalues $\lambda_n = \gamma_n \pm i \omega_n$ and $d - 2p$ real eigenvalues $\lambda_n = \gamma_n$ for $n = p+1, \ldots, d - p$. Writing the corresponding eigenvectors as $v_n^\pm = x_n \pm i y_n$ for $n \in I_1 = \{1, \ldots, p\}$ and $v_n = x_n$ for $n \in I_2 = \{p+1, \ldots, d - p\}$ with $x_n, y_n \in \mathbb{R}^d$, and noting that $A^* = A$ shows that

$$A(x + i y) = (\gamma + i \omega)(x + i y) \quad \Rightarrow \quad A(x - i y) = (\gamma - i \omega)(x - i y).$$

The vectors $(x_n)_{n=1}^{d-p}$ and $(y_n)_{n=1}^p$ together form a (non-orthogonal) complete basis for $\mathbb{R}^d$ and we can expand the initial state $r_0$ and steady state $r_{ss}$ with respect to it

$$r_{ss} = \sum_{n=1}^{d-p} \beta_n x_n + \sum_{n=1}^p \beta_n y_n, \quad r_0 = \sum_{n=1}^{d-p} (\alpha_n + \beta_n) x_n + \sum_{n=1}^p (\alpha'_n + \beta'_n) y_n,$$

where $\alpha_n$ and $\beta_n$ are real coefficients. This yields

$$\Delta(t) = r_0 - r_{ss} = \sum_{n \in I_1} \alpha_n x_n + \alpha'_n y_n + \sum_{n \in I_2} \alpha_n x_n$$

$$= \sum_{n \in I_1} \frac{\alpha_n}{2} [v_n^+ + v_n^-] + \frac{\alpha'_n}{2} [v_n^+ - v_n^-] + \sum_{n \in I_2} \alpha_n v_n$$

$$= \sum_{n \in I_1} \frac{1}{2} (\alpha_n - i \alpha'_n) v_n^+ + \frac{1}{2} (\alpha_n + i \alpha'_n) v_n^- + \sum_{n \in I_2} \alpha_n v_n$$

$$= \sum_{n \in I_1} \xi_n (\tilde{v}_n^+ + \tilde{v}_n^-) + \sum_{n \in I_2} \xi_n \tilde{v}_n$$

where $\tilde{v}_n^\pm = \frac{1}{2} (\alpha_n \pm i \alpha'_n) v_n^\pm$ and $\tilde{v}_n = \alpha_n v_n$ and $\xi_n = 0$ if $\alpha_n = \alpha'_n = 0$ and $\xi_n = 1$ otherwise. Inserting the last expression into [8] and recalling $A v_n^\pm = (\gamma_n \pm i \omega_n) v_n^\pm$ we obtain

$$r(t) = a_0 + \sum_{n=1}^p \xi_n e^{\gamma_n t} [a_n \cos(\omega_n t) + b_n \sin(\omega_n t)] + \sum_{n=p+1}^{d-p} \xi_n a_n e^{\gamma_n t}$$

where the coefficient vectors are $a_0 = r_{ss}$, $a_n = 2 \tilde{x}_n$, $b_n = -2 \tilde{y}_n$ for $n \in I_1$, $a_n = \tilde{v}_n$ for $n \in I_2$, and $\tilde{v}_n^\pm = \tilde{x}_n \pm i \tilde{y}_n$ with $\tilde{x}_n = \frac{1}{2} (\alpha_n x_n + \alpha'_n y_n)$, $\tilde{y}_n = \frac{1}{2} (-\alpha'_n x_n + \alpha_n y_n)$.

The coefficient vectors $a_0$, $a_n$ and $b_n$ can be estimated along with the parameters $\omega_n$ and $\gamma_n$ using Bayesian estimation, choosing the basis functions

$$g_0 = 1 \quad (11a)$$

$$g_{2n-1}(t) = e^{\gamma_n t} \sin(\omega_n t) \quad n = 1, \ldots, p \quad (11b)$$

$$g_{2n}(t) = e^{\gamma_n t} \cos(\omega_n t) \quad n = 1, \ldots, p \quad (11c)$$

$$g_{2p+n}(t) = e^{\gamma_n t}, \quad n = 1, \ldots, N - 1. \quad (11d)$$

Thus, provided $\xi_n \neq 0$ for all $n$, we can determine all of the eigenvectors $\tilde{v}_n^\pm$ and eigenvalues of $A$, so that $A = SDS^{-1}$ with $S = (\tilde{v}_1^+, \tilde{v}_1^-, \tilde{v}_{p+1}^+, \tilde{v}_{p+1}^-, \tilde{v}_{2p+1}, \ldots, \tilde{v}_{p+d})$.
being a matrix whose columns are the complex eigenvalues of $A$ and $D = \text{diag}(\lambda_1^+, \lambda_1^-, \lambda_2^+, \lambda_2^-, \ldots, \lambda_p^+, \ldots, \lambda_{p+d}^+)$ is a diagonal matrix with the corresponding eigenvalues $\lambda_n^\pm = \gamma_n \pm i\omega_n$. $S$ will be invertible provided $\xi_n \neq 0$ for all $n$ so that we have determined all eigenvectors.

**Theorem 1** The trajectory $r(t)$ of an initial state uniquely determines the $A$ and $c = -Aa_0$ provided $r(0) - r_{ss}$, where $r_{ss}$ is a steady state, has non-zero overlap with all eigenvectors of $A$.

If $A$ has fewer than $N^2 - 1$ distinct eigenvalues then $\Delta(t) = r(t) - r_{ss}$ still satisfies a homogeneous linear equation $\dot{\Delta}(t) = A\Delta(t)$ and we have $A = SJS^{-1}$, where $S$ is a matrix determined by the (generalised) eigenvectors but $J = \text{diag}(J_n)$ is the Jordan normal form of $A$ consisting of irreducible Jordan blocks $J_n$ of dimension $k_n$ with some eigenvalue $\lambda_n$. In this case we have $\Delta(t) = Se^{Jt}S^{-1}\Delta(0)$, where $S$ is a matrix whose columns are generalised eigenvectors $v_{n,k}^\pm$ satisfying $(A - \lambda_n^\pm I)^k v_{n,k}^\pm = 0$, $(A - \lambda_n^\pm I)^{k-1} v_{n,k}^\pm \neq 0$. The generalised eigenvectors can be chosen such as to be span $\mathbb{R}^{N^2 - 1}$. The matrix exponential $e^{Jt}$ is block-diagonal with $k_n$ dimensional blocks

$$E_n(t) = e^{\gamma_n t} \begin{bmatrix} R_n & tR_n & \frac{1}{2}t^2 R_n & \frac{1}{6}t^3 R_n & \ldots \\ 0 & R_n & tR_n & \frac{1}{2}t^2 R_n & \ldots \\ 0 & 0 & R_n & tR_n & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

where

$$R_n = 1 \text{ for } \omega_n = 0, \quad R_n = \begin{pmatrix} \cos(\omega_n t) & -\sin(\omega_n t) \\ \sin(\omega_n t) & \cos(\omega_n t) \end{pmatrix} \text{ for } \omega_n \neq 0. \quad (13)$$

For non-generic $A$ there are many different subcases that arise even in the simplest case of a single qubit. These are discussed in detail in Appendix A. Most of these special cases rarely arise in practice and the nature of the positivity constraints impose further restrictions. Physically allowed examples of non-diagonalisable Bloch matrices do exist. For qubits they involve extremely high decoherence rates leading to overdamped dynamics [23], which are usually not of interest for quantum information. In higher dimensions there are more possibilities for $A$ to non-diagonalisable although generically $A$ is still diagonalisable. The analysis in the appendix suggests that the trajectory $r(t)$ of one initial state still uniquely determines $A$ and $c = -Aa_0$ even in the non-generic case provided (i) $A$ does not have two or more generalised eigenvectors of the same degree $k$ corresponding to the same eigenvalue $\lambda$, and (ii) $r(0) - r_{ss}$, where $r_{ss}$ is a steady state, has non-zero overlap with all (generalised) eigenvectors of $A$.

### 4. Identifiability given Partial State Information

A more interesting question is how much information about the dynamical generators we can obtain from partial state information such as measurement of a single observable. To address this problem it is useful to consider the identification problem in the Laplace domain [10]. The *Laplace Transform of the Bloch equation* [6] gives

$$s^2 R(s) - sr(0) = AR(s) + c = T\begin{pmatrix} sR(s) \\ 1 \end{pmatrix} \quad (14)$$
where $R(s)$ is the Laplace transform of $r(t)$ and $T = (A,c)$ is the matrix $A$ with the column vector $c$ appended. Thus, given $R(s)$ and $r(0)$ then $T$ and thus $A$ and $c$ are in principle fully determined. Indeed we only need to know $R(s)$ for $d + 1$ values of $s_k$ in general. Define the $d + 1 \times d + 1$ matrices

$$C = \begin{pmatrix} s_1R(s_1) & \cdots & s_{d+1}R(s_{d+1}) \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix},$$  

$$D = (s_1^2R(s_1) - s_1r(0), \ldots, s_{d+1}^2R(s_{d+1}) - s_{d+1}r(0)).$$

(15a)

(15b)

We have $D = TC$ and if $\det(C) \neq 0$ then $T = DC^{-1}$ and thus we have fully determined both $A$ and $c$. Thus if we could measure in the Laplace domain rather than the time domain only $d + 1$ measurements would be required to completely determine the dynamics although it not easy to see how to perform such measurements in practice.

But [14] can also be useful if we have incomplete information about the state, e.g., if we can only measure some components of the Bloch vector. We can use [14] to express the unknown components in terms of the known ones. For example, suppose we know only the last component $R_d(s)$. Let $R'(s)$, $r'(0)$ and $c'$ denote the first $d - 1$ components of $R(s)$, $r(0)$ and $c$, and partition the matrix $A$ as follows

$$A = \begin{pmatrix} A' & a \\ b^T & a_{dd} \end{pmatrix}.$$

(16)

Then [14] can be rewritten as

$$sR'(s) - r'(0) = A'R'(s) + aR_d(s) + c'/s$$

(17a)

$$sR_d(s) - r_d(0) = b^T R'(s) + a_{dd}R_d(s) + c_d/s.$$  

(17b)

If $s$ is not an eigenvalue of $A'$ then the first equation gives

$$R'(s) = (sI - A')^{-1}[sR'(0) + aR_d(s) + c'/s]$$

and inserting this into the second equation yields a non-linear equation in $s$ that depends only on $R_d(s)$.

$$0 = b^T(sI - A')^{-1}[sR'(0) + saR_d(s) + c'] - s^2R_d(s) + sr_d(0) + sa_{dd}R_d(s) + c_d,$$

(19)

which can be rewritten as

$$R_d(s) = \frac{b^T(sI - A')^{-1}[sR'(0) + c'] + sr_d(0) + c_d}{s^2 - s(b^T(sI - A')^{-1}a + a_{dd})}.$$  

(20)

The equation must be satisfied for all $s$. $R_d(s)$ is a rational function and we can therefore expand the numerator and denominator in terms of powers of $s$ and match the coefficients, leading to a set of algebraic equations for the coefficients. We can identify which parameters of $A$ contribute to the RHS of Eq. [20], hence determine what information can be extracted in principle.

In practice we can use knowledge about $A$ to infer the structure of the expected signal. From Sec. [3] we know that in the generic case $A$ has $N^2 - 1$ distinct eigenvalues. More precisely, we expect $N - 1$ real eigenvalues and $(N^2 - N - 2)/2 = N(N-1)/2 - 1 =: p$ pairs of complex conjugate eigenvalues and thus a signal $r(t)$ of the form

$$r_d(t) = c_0 + \sum_{n=1}^{N-1} c_ne^{\gamma_n t} + \sum_{n=1}^p e^{\gamma_n t}[a_n \cos(\omega_n t) + b_n \sin(\omega_n t)].$$

(21)
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Given stroboscopic measurement data \( r_d(t_k) \) we can now use parameter estimation techniques to estimate \( \omega_n, \gamma_n \) and \( \gamma'_n \) and the coefficients \( a_n, b_n \) and \( c_n \).

The approach above can be generalised to arbitrary partitioning of the observed signals and in principle we could consider more general observables.

5. Application: Identification of Qubit Dynamics

We illustrate the ideas above by applying them to a qubit evolving under general Markovian dynamics. Taking

\[
\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(22)

to be the unnormalised Pauli matrices, we can expand the Hamiltonian \( H = h_0 I_2 + h_x \hat{\sigma}_x + h_y \hat{\sigma}_y + h_z \hat{\sigma}_z \), where \( h_j (j = 0, x, y, z) \) are real. Choosing \( F_n \) to be dissipation operators to be the normalised Pauli matrices, \( F_1 = \frac{1}{\sqrt{2}} \sigma_x, F_2 = \frac{1}{\sqrt{2}} \sigma_y, F_3 = \frac{1}{\sqrt{2}} \sigma_z, F_4 = \frac{1}{\sqrt{2}} I_2 \), and setting \( f_{mn} = f_{mn}^R + i f_{mn}^I \), where \( (f_{mn}^R) \) is a real symmetric matrix and \( (f_{mn}^I) \) are anti-symmetric matrix, the general Bloch operators take the form

\[
A = \begin{pmatrix} -f_{12}^R + f_{33}^R & f_{13}^R - 2h_z & f_{11}^R + f_{33}^R \\ f_{12}^R - 2h_z & -f_{13}^R + 2h_y & f_{11}^R - f_{33}^R \\ f_{11}^R + f_{33}^R & f_{13}^R - 2h_x & f_{12}^R + f_{33}^R \end{pmatrix}, \quad c = \sqrt{2} \begin{pmatrix} f_{13}^I \\ -f_{13}^I \\ f_{12}^I \end{pmatrix}.
\]

(23)

The anti-symmetric part of \( A \) determines the Hamiltonian while the symmetric part of \( A \) determines the real parts of the dissipation coefficients \( f_{mn} \) and the inhomogeneous part determines the imaginary part of \( f_{mn} \).

Generically, we expect one real eigenvalue \( -\delta \) and a pair of complex eigenvalues \( -\gamma \pm i\omega \) with \( \delta, \gamma \geq 0 \). Therefore we choose the basis functions for the Bayesian estimation

\[
g_0(t) = 1, \quad g_1(t) = e^{-\gamma t} \cos(\omega t), \quad g_2(t) = e^{-\gamma t} \sin(\omega t), \quad g_3(t) = e^{-\delta t},
\]

(24)
i.e., in particular the signal should be a linear combination of these basis functions

\[
s(t) = a_0 g_0(t) + a_1 g_1(t) + a_2 g_2(t) + a_3 g_3(t), \quad \text{and the Laplace transform of the signal should be the corresponding linear combination of}
\]

\[
G_0(s) = \frac{1}{s}, \quad G_1(s) = \frac{s + \gamma}{(s + \gamma)^2 + \omega^2}, \quad G_2(s) = \frac{\omega}{(s + \gamma)^2 + \omega^2}, \quad G_3(s) = \frac{1}{s + \delta}.
\]

The parameter estimation in all of the following cases uses a standard Bayesian estimation technique which involves orthogonal projections of the data onto the basis functions and optimisation to maximise the log-likelihood, this method being described more fully elsewhere \[11\] \[12\].

5.1. Identification given full Bloch vector information

We first consider a generic qubit system for which the Bloch matrix \( A \) has three distinct eigenvalues. The system is prepared in a fixed initial state \( r_0 \) and allowed to evolve under the unknown dynamics. After evolving for different times, \( t_k \), the components of the Bloch vector \( r_1(t_k) = \langle \hat{\sigma}_x(t_k) \rangle, r_2(t_k) = \langle \hat{\sigma}_y(t_k) \rangle, r_3(t_k) = \langle \hat{\sigma}_z(t_k) \rangle \) are measured. For each time point the experiment is repeated \( N_e \) times to determine
the relative frequency of measurement outcomes 0 and 1. If we can measure all three components of the Bloch vector (equivalent to QST of a qubit) then we obtain three data traces of a form shown in Figure 1.

From these data traces, we then estimate the underlying signal parameters and express the signal in the form (10) and consequently reconstruct the matrix $A$ and $c$ using the technique outlined in Section 3. Figure 2 shows the cumulative probability density of the relative root-mean-squared error of the reconstructed Bloch matrix $A$ and constant $c$ for a typical generic system, specifically (Model 1)

$$A = \begin{pmatrix} -0.0650 & -2.0000 & 2.0300 \\ 2.0000 & -0.0650 & -4.0000 \\ -1.9700 & 4.0000 & -0.0900 \end{pmatrix}, \quad c = \begin{pmatrix} -0.0424 \\ 0 \\ 0.0636 \end{pmatrix}, \quad r_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

for different choices of the signal length, number of samples $N$ and experiment repetitions $N_e$. A set of 100 randomly generated data traces were used for the reconstruction. Time samples for each run are chosen by low-discrepancy sampling [26]. As the figure shows the median error for $N = N_e = 1000$ is 1.5%; for $N = 1000, N_e = 5000$ the relative error of more than 95% of all runs is below 1%. There is an optimal range of the signal length around $T = 50$ for this system. The reconstruction error increases for substantially shorter or longer signals; in the latter case this is due to the signal vanishing. Comparing the results for $T = 50$ and $N = 2000, N_e = 1000$ and $N = 1000, N_e = 2000$ shows that there is virtually no difference in the probability density, suggesting that it makes little difference if we increase the number of time samples or the signal to noise ratio of the sample points.
Figure 2: Reconstruction-error cumulative probability density for model 1. We examined different sampling times, sampling points and experiment repetitions. As expected, as the noise of each data point decreases, and the number of time samples increases, the reconstruction accuracy diminishes. Different system models give similar error probability plots.

5.2. Identification based on single component of Bloch vector

Suppose we can only measure one component of the Bloch vector in a fixed measurement basis. This is typically the case where there is a physically preferred or engineered mechanism and before coherent rotations of the state are possible. Without loss of generality assume we measure \( r_z(t) \), for instance by atomic population measurement by fluorescence shelving [27]. We can write the Laplace transform of the signal as

\[
R_d(s) = \frac{a_0}{s} + \frac{a_1(s + \gamma) + a_2 \omega}{(s + \gamma)^2 + \omega^2} + \frac{a_3}{s + \delta} = \frac{C_3 s^3 + C_2 s^2 + C_1 s + C_0}{s^4 + D_3 s^3 + D_2 s^2 + D_1 s},
\]

(25)

Assuming we have estimated the coefficients \( a_0, a_1, a_2, a_3 \) as well as \( \omega, \gamma \) and \( \delta \) using signal parameter estimation, the constants \( C_k, D_k \) for \( k = 0, 1, 2 \) are determined from
the observed signal

\[ C_0 = a_0 \delta (\gamma^2 + \omega^2) \]  
\[ C_1 = a_0 (\gamma^2 + 2\gamma \delta + \omega^2) + a_1 \delta \gamma + a_2 \delta \omega + a_3 (\gamma^2 + \omega^2) \]  
\[ C_2 = a_0 (\delta + 2\gamma) + a_1 (\gamma + \delta) + a_2 \omega + a_3 \gamma \]  
\[ C_3 = a_0 + a_1 + a_3 \]  
\[ D_1 = \delta (\gamma^2 + \omega^2) \]  
\[ D_2 = 2\gamma \delta + \gamma^2 + \omega^2 \]  
\[ D_3 = 2\gamma + \delta \]

Comparing with (20) for a generic single-qubit Bloch matrix \( A = (a_{mn}) \) shows that the constants must satisfy

\[ C_0 = (a_{21} a_{32} - a_{22} a_{31}) c_1 + (a_{12} a_{31} - a_{11} a_{32}) c_2 + (a_{11} a_{22} - a_{12} a_{21}) c_3 \]  
\[ C_1 = a_{31} c_1 + a_{32} c_2 - (a_{11} + a_{22}) c_3 + (a_{32} a_{21} - a_{31} a_{22}) r_x(0) + (a_{31} a_{12} - a_{32} a_{11}) r_y(0) + (a_{11} a_{22} - a_{12} a_{21}) r_z(0) \]  
\[ C_2 = c_3 + a_{31} r_x(0) + a_{32} r_y(0) - (a_{11} + a_{22}) r_z(0) \]  
\[ D_1 = a_{13} a_{31} a_{22} - a_{12} a_{32} a_{31} - a_{13} a_{21} a_{32} + a_{11} a_{23} a_{32} + a_{12} a_{21} a_{33} - a_{11} a_{22} a_{33} \]  
\[ D_2 = -a_{12} a_{21} - a_{13} a_{31} - a_{23} a_{32} + a_{22} a_{33} + a_{11} (a_{22} + a_{33}) \]  
\[ D_3 = -a_{11} - a_{22} - a_{33} \]

As the constants \( C_k \), \( D_k \) and the initial state \( r_x(0), r_y(0) \) and \( r_z(0) \) are known, we have a system of six non-linear algebraic equations for the coefficients of \( A \) and \( c \). Given that \( A \) in general has 9 coefficients and \( c \) has three, these equations do not determine \( A \) uniquely, although we may be able to effectively identify all unknown parameters if we have prior information about the dominant types of dissipation, effectively restricting the form of \( A \) and \( c \). This may be derived from physically motivated grounds or from prior measurements of similar systems. We apply this to some examples below.

5.2.1. Dephasing in a general basis

Consider the special case of a qubit subject to a fixed but unknown Hamiltonian \( H = \frac{i}{2} (h_x \sigma_x + h_y \sigma_y + h_z \sigma_z) \) and dephasing operator \( V = \frac{1}{\sqrt{2}} (\alpha \sigma_x + \beta \sigma_y + \gamma \sigma_z) \), which corresponds to dephasing in an arbitrary basis. In this case the master equation can be written in Lindblad form

\[ \frac{d}{dt} \rho(t) = -\frac{i}{\hbar} [H, \rho] + V \rho(t) V^\dagger - \frac{1}{2} \{ V^\dagger V, \rho(t) \} \]  

and expanding with respect to the normalised Pauli matrices, the corresponding terms in the Bloch equation are

\[ A = \begin{pmatrix} -(\beta^2 + \gamma^2) & -h_z + \alpha \beta & h_y + \alpha \gamma \\ h_z + \alpha \beta & -(\alpha^2 + \gamma^2) & -h_x + \beta \gamma \\ -h_y + \alpha \gamma & h_x + \beta \gamma & -(\alpha^2 + \beta^2) \end{pmatrix}, \quad c = 0. \]  

i.e., we have a total of six parameters. We see from (27) that for \( c = 0 \) there are only five non-trivial signal parameters. Thus, a single trace is not sufficient to completely determine all of the model parameters. If the system is initialised in a measurement
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Figure 3: Comparison of cumulative probability density for the relative Hilbert-Schmidt error of estimated Bloch matrix $A$ for Model 2. We examined different starting states and reconstructions based on full or partial observable information. The reconstruction based on full XYZ information did not assume any particular decoherence model, unlike the reconstruction based on only partial observables. Initial states were either $r_0 = (1,0,0)^T$ or $r_0 = (0,0,1)^T$. Partial observation was either the $z$ trace only, $y$ and $z$, $x$ and $z$, or $x$ and $y$ traces.

basis state $r_0 = (0,0,1)^T$ then (26) and (27) give explicitly

$$C_0 = 0$$

$$C_1 = h_z^2 + \gamma^2(\alpha^2 + \beta^2 + \gamma^2)$$

$$C_2 = \alpha^2 + \beta^2 + 2\gamma^2$$

$$D_1 = h_z^2 (\alpha^2 + \beta^2) + h_y^2 (\alpha^2 + \gamma^2) + h_x^2 (\beta^2 + \gamma^2) - 2 h_x h_z \alpha \gamma - 2 h_y h_x \alpha \beta - 2 h_z h_y \beta \gamma$$

$$D_2 = h_x^2 + h_y^2 + h_z^2 + (\alpha^2 + \beta^2)^2 + \gamma^2 (2\alpha^2 + 2\beta^2 + \gamma^2)$$

$$D_3 = 2(\alpha^2 + \beta^2 + \gamma^2) = 2(C_2 - \gamma^2)$$

We cannot determine all 6 model parameters, the observed signal is invariant under a rotation around the $z$-axis, hence we cannot determine the azimuthal components of the Hamiltonian and dephasing simultaneously, only their relative orientation. This is similar to the original situation of Hamiltonian identification where there is a “gauge symmetry” which exists due to only being able to initialise and measure in a fixed basis, i.e. we do not have a phase reference to measure the $x$ and $y$ components of the dynamics separately. However, we can determine $h_z^2 + h_y^2$ and $\alpha^2 + \beta^2$. We can “gauge fix”, e.g. $h_y = 0$, and define $\alpha$ and $\beta$ in reference to the projection of the Hamiltonian onto the $x - y$ plane.
Figure 4: Comparison of probability density for the relative Hilbert-Schmidt norm error of estimated Bloch matrix $A$ for Model 3. Reconstruction procedures as in Figure 3. The optimum sampling time is shorter than for Model 2 as the signal decays faster.

We have solved for the analytic solutions of (30) but due to signal noise, these may not be exactly consistent. We therefore implemented the non-linear system of equations by minimising the least-squares errors using numerical optimisation starting with an initial guess derived from the analytic solutions. We plot the cumulative probability distribution for the errors in Figure 3 for Model 2, $A = \begin{pmatrix} -0.08 & -1.98 & 0.02 \\ 2.02 & -0.05 & -1.96 \\ 0.02 & 2.04 & -0.05 \end{pmatrix}$, $c = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$, which corresponds to $h_x = h_z = 2$, $h_y = 0$ and $\alpha = 0.1$, $\beta = \gamma = 0.2$. We implemented various initial states, observables and prior knowledge.

5.2.2. Dephasing and Relaxation in Measurement basis We also consider the special case of a qubit subject to a fixed but unknown Hamiltonian $H = \frac{1}{2}(h_x\hat{\sigma}_x + h_y\hat{\sigma}_y + h_z\hat{\sigma}_z)$, and relaxation and decoherence along the measurement basis governed by the Lindblad equation

$$\frac{d}{dt} \rho(t) = -\frac{i}{\hbar}[H, \rho] + \sum_{k=1}^{3} V_k(t)\rho(t)V_k^\dagger - \frac{1}{2}\{V_k^\dagger V_k, \rho(t)\}$$  \hspace{1cm} (31)$$

with dephasing operator $V_1 = \sqrt{T}\hat{\sigma}_y$, and relaxation operators $V_2 = \sqrt{\gamma_1}|0\rangle\langle 1|$ and $V_3 = \sqrt{\gamma_2}|1\rangle\langle 0|$ where we include both spontaneous emission and absorption. Again, expanding with respect to the normalised Pauli basis the Bloch operators take the
Figure 5: Error histogram plot (Model 3, $r_0 = (0, 0, 1)^T$, $z$-trace, $N = N_e = 1000$, $T = 15$). The absolute errors in the elements of matrix $A$ were comparable with each other, but as the Hamiltonian parameters are much larger than the decoherence parameters, the relative errors of the latter are commensurately greater. Due to rotational symmetry around $z$, we can only determine $\sqrt{h_x^2 + h_y^2}$.

Analytical solutions to these have also been found but as in the previous case, numerical optimisation is required due to signal noise. Again, we can only determine $h_x^2 + h_y^2$ and not $h_x$ and $h_y$ individually if we start off with $r_0 = (0, 0, 1)^T$ and measure $r_z$. If we start off with $r_0 = (1, 0, 0)^T$, we obtain the same expressions as in (33) except for the two equations

$$C_2 = \Delta \gamma - h_y$$

$$C_1 = 2\Gamma_{\text{eff}} \Delta \gamma + h_x h_z - h_y \Gamma_{\text{eff}},$$
which allow us in principle to identify all six parameters. However, the equations appear to be sensitive to noise and often lead to incorrect model parameters. This behaviour is a subject for further research. The results for Model 3

\[
A = \begin{pmatrix}
-0.25 & -3.00 & 2.0 \\
3.00 & -0.25 & -1.0 \\
-2.00 & -1.00 & 0.1
\end{pmatrix}, \quad c = \begin{pmatrix}
0 \\
0 \\
0.1/\sqrt{2}
\end{pmatrix},
\]

are shown in Figure 4 for various initial states, observables, and prior knowledge. Figure 5 shows the histogram of the error distribution of the model parameters for one reconstruction setting.

5.3. Identification given two components of the Bloch vector

In some systems, e.g. bulk nuclear magnetic resonance, determination of the \(x\) and \(y\) components of the Bloch vector is easy to measure. In this case, we assume we can measure both \(r_x(t)\) and \(r_y(t)\). Inserting (18b) into (18a) gives

\[
sR'(s) - r'(0) = A'R'(s) + a|b^T R'(s) + a_{dd}r_d(s) + c_d/s + r_d(0)| + c'/s.
\]

Solving for \(R'(s)\) gives

\[
R'(s) = [sI' - A' - ab^T/(s - a_{dd})]^{-1}(r'(0) + c'/s + a(c_d/s + r_d(0))/(s - a_{dd})
\]

from which we can obtain two explicit rational equations for \(R_x(s)\) and \(R_y(s)\). The denominators of both are the same and the coefficients of the polynomials on the top and bottom can be related to the observed signals as before.

For the two examples in sections 5.2.1 and 5.2.2 we implemented the reconstruction procedure, the results of which are presented in Figures 3 and 4. For the sake of comparison we considered not only \(x\) and \(y\) but different combination of two traces including \(y\) and \(z\), and \(x\) and \(z\) observable information for the reconstruction. The general observation is that for the systems considered the \(z\)-trace appeared to be the best choice for the reconstruction. The addition of the extra information in the form of the \(x\) or \(y\) trace did not improve the reconstruction accuracy over reconstruction using the \(z\) trace alone for these examples, and using the \(x\) and \(y\) traces instead appear to result in substantially worse reconstruction results. There are also initial state effects with initialisation in the \(z\)-eigenstate being decided preferable compared to initialisation in the \(x\)-eigenstate in the second case, for example.

6. Summary and Discussion

We have studied the problem of identification of the dynamics of open systems in a Markovian environment without recourse to quantum process tomography. By utilising stroboscopic measurements over time we showed that the system dynamics is completely determined by the evolution of a single initial state, at least in the generic case when \(A\) has distinct eigenvalues and the initial state has overlap with all eigenspaces of \(A\), i.e., we can in principle fully determine the Bloch operator \(A\) and inhomogeneous term \(c\) from stroboscopic measurements of the state at different times. Analysis of non-generic cases suggests that this result basically still holds in most cases and we can give specific conditions under which full information about the dynamics can be obtained. For systems governed by Markovian evolution this
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approach is preferable to process tomography for several reasons. First, it does not require initialisation in a large set of different basis states. Second, it avoids the rather messy procedure of extracting the dynamical generators from process tomography data, which is susceptible to noise. Third, it is more efficient than performing process tomography at numerous different times.

By going to the Laplacian domain, we can identify algebraic equations relating the observed signals to the models parameters. In the absence of a mechanism of directly sampling in the Laplacian domain, we can use Bayesian signal estimation in the time domain to find a functional representation of the measurements more amenable to Laplacian domain analysis. The most important advantage of this approach is that it shows that in many cases most or all model parameters can be obtained from far less data, i.e., we do not even require full state tomography. Rather we can extract the same information from measurements of a smaller set of observables. This approach is especially useful if there is physical information restricting the type of decoherence model we expect, and the dynamical generators depend on fewer parameters. Our analysis of the qubit cases shows that not only is it possible to extract all of the system parameters from this restricted data but often this even leads to better reconstruction results than using full state reconstruction.

In part these results can be explained by overfitting, i.e., trying to fit the most general model given noisy data when the actual dynamics is determined by a smaller set of parameters leads to fitting the noise and results in worse model over all. However, overfitting does not appear to explain the peculiar dependence of the results on the choice of initial state or observables noted earlier. For many of the systems considered the success of the reconstruction showed a strong dependence on the choice of the initial state and the type of measurement, with initialisation in a $z$-eigenstate of measurement of $\langle \sigma_z \rangle$ being distinctly preferable over other combinations such as measuring $\langle \sigma_x \rangle$ or initialising in an $x$-eigenstate. This effect was most pronounced for system subject to relaxation in the measurement basis. In this case the choice of the initial state $(1,0,0)^T$ in principle breaks the rotational symmetry, allowing the determination of all six model parameters, instead of the five using the initial state $(0,0,1)^T$. However, in the former case the reconstruction often fails, converging to a model which is distinctly different from the actual model. There appears to be a trade-off between the breadth of the information one versus the quality of the information gathered but the issue of the optimal choice of the initial state and observables warrants further study, as do the choice of optimal signal lengths, adaptive sampling, stability of reconstruction algorithms in the presence of noise among others.

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Appendix A. Non-diagonalisable Bloch matrices for $N = 2$

As the complex eigenvalues of the Bloch matrix $A$ must occur in pairs $\gamma \pm i\omega$, we can only have a non-trivial Jordan block for a qubit system if $\omega = 0$, i.e., the eigenvalues are real, and there are five cases: $A = SJS^{-1}$ with

$$J_1 = \begin{pmatrix} \gamma_1 & 1 \\ 0 & \gamma_1 \end{pmatrix}, \quad J_2 = \begin{pmatrix} \gamma_1 & 0 \\ 0 & \gamma_1 \end{pmatrix}, \quad J_3 = \begin{pmatrix} \gamma & 1 \\ 0 & \gamma \end{pmatrix}, \quad J_4 = \begin{pmatrix} \gamma & 1 \\ 0 & 0 \end{pmatrix},$$

and $J_5 = \gamma I$. The corresponding time evolution operators are $e^{tA} = Se^{tJ}S^{-1}$ with

$$e^{tJ_1} = \begin{pmatrix} e^{t\gamma_1} & te^{t\gamma_1} \\ 0 & e^{t\gamma_1} \end{pmatrix}, \quad e^{tJ_2} = \begin{pmatrix} e^{t\gamma_1} & 0 \\ 0 & e^{t\gamma_1} \end{pmatrix},$$

$$e^{tJ_3} = \begin{pmatrix} e^{t\gamma} & t^2 e^{t\gamma} \\ 0 & e^{t\gamma} \end{pmatrix}, \quad e^{tJ_4} = \begin{pmatrix} e^{t\gamma} & 0 \\ 0 & e^{t\gamma} \end{pmatrix}, \quad e^{tJ_5} = e^{t\gamma} I.$$

**Case 1.** There are two proper eigenvectors $x_{11}$, $x_2$ and one generalised eigenvector $x_{12}$ satisfying $(A - \gamma_1 I)x_{11} = 0$ for $n = 1, 2$ and $(A - \gamma_1 I)^2x_{12} = 0$. Expanding with respect to these $\Delta(0) = \alpha_{11}x_{11} + \alpha_{12}x_{12} + \alpha_2x_2$ and using the Jordan form of $A$ above gives

$$r(t) = r_{ss} + e^{t\gamma_1}(\alpha_{11} + \alpha_{12}t)x_{11} + e^{t\gamma_1}\alpha_{12}x_{12} + e^{t\gamma_2}\alpha_2x_2$$

$$= r_{ss} + e^{t\gamma_1}t\alpha_{12}x_{11} + e^{t\gamma_1}(\alpha_{11}x_{11} + \alpha_{12}x_{12}) + e^{t\gamma_2}\alpha_2x_2$$

$$= a_0 + te^{t\gamma_1}a_1 + e^{t\gamma_1}a_2 + e^{t\gamma_2}a_3$$

Using parameter estimation we can in principle estimate $\gamma_n$, $n = 1, 2$, as well as the coefficient vectors $a_n$ for $n = 0, 1, 2, 3$. $a_0$ determines the steady state and $a_1$ and $a_3$ determine the two proper eigenvectors as we can absorb the factors $\alpha_{12}$ and $\alpha_2$. $a_2$ is a generalised eigenvector as $(A - \gamma_1 I)(\alpha_{11}x_{11} + \alpha_{12}x_{12}) = (A - \gamma_1 I)\alpha_{12}x_{12} \neq 0$, $(A - \gamma_1 I)^2(\alpha_{11}x_{11} + \alpha_{12}x_{12}) = 0$. Thus we have $S = (a_1, a_2, a_3)$ and both eigenvalues and $A$ is completely determined.

**Case 2.** There are two proper eigenvectors $x_1, x'_1$ with eigenvalue $\gamma_1$ and one proper eigenvector $x_2$ with eigenvalue $\gamma_2$. Expanding with respect to these eigenvectors $\Delta(0) = \alpha_1x_1 + \alpha_1'x'_1 + \alpha_2x_2$ and

$$r(t) = r_{ss} + e^{t\gamma_1}(\alpha_1x_1 + \alpha_1'x'_1) + e^{t\gamma_2}\alpha_2x_2$$

$$= a_0 + e^{t\gamma_1}a_1 + e^{t\gamma_2}a_2$$

Using parameter estimation we can estimate $\gamma_n$ as well as the coefficient vectors $a_n$ for $n = 0, 1, 2$. $a_0$ determines one steady state and $a_1$ and $a_2$ determine two of the proper eigenvectors of $A$ but without further information we cannot determine the third eigenvector.

**Case 3.** In this case there is only one eigenvalue $\gamma$ and one proper eigenvector $x_{11}$ and two generalised eigenvectors $x_{12}$, $x_{13}$. Expanding with respect to these generalised
eigenvectors, $\Delta(0) = \alpha_1 x_{11} + \alpha_2 x_{12} + \alpha_3 x_{13}$, and using the Jordan form gives

$$r(t) = r_{ss} + e^{\gamma t}[(\alpha_1 + \alpha_2 t + \frac{1}{2} \alpha_3 t^2)x_{11} + e^{\gamma t}(\alpha_1 x_{11} + \alpha_2 x_{12} + \alpha_3 x_{13})$$

$$= r_{ss} + \frac{1}{2} \alpha_3 t^2 e^{\gamma t} x_{11} + te^{\gamma t}(\alpha_1 x_{11} + \alpha_2 x_{12} + \alpha_3 x_{13})$$

$$= a_0 + t^2 e^{\gamma t} a_1 + te^{\gamma t} a_2 + e^{\gamma t} a_3$$

Using parameter estimation we can estimate $\gamma$ as well as the coefficient vectors $a_n$ for $n = 0, 1, 2, 3$. Again $a_0$ determines a steady state. $a_1 = \frac{1}{2} \alpha_1 x_{11}$ is a proper eigenvector of $A$, $a_2$ and $a_1$ are generalised eigenvectors with $(\hat{A} - \gamma I)^2 a_2 = 0$ and $(\hat{A} - \gamma I)^3 a_3 = 0$, respectively. $S = (a_1, a_2, a_3)$ and $\gamma$ and $A$ is completely determined.

**Case 4.** In this case there is again only one eigenvalue $\gamma$ but there are two proper eigenvectors $x_1, x^\prime_1$ and one generalised eigenvector $x_{12}$ with $(\hat{A} - \gamma I)x_{12} \neq 0$ but $(\hat{A} - \gamma I)^2 x_{12} = 0$. Expanding with respect to these generalised eigenvectors, $\Delta(0) = \alpha_1 x_{11} + \alpha_1^\prime x_{11} + \alpha_2 x_{12}$, and using the Jordan form gives

$$r(t) = r_{ss} + e^{\gamma t}[(\alpha_1 + \alpha_2 t + \frac{1}{2} \alpha_3 t^2)x_{11} + e^{\gamma t}(\alpha_1 x_{11} + \alpha_2 x_{12} + \alpha_3 x_{13})$$

$$= r_{ss} + te^{\gamma t}(\alpha_1 x_{11} + \alpha_2 x_{12} + \alpha_3 x_{13})$$

$$= a_0 + te^{\gamma t} a_1 + e^{\gamma t} a_2$$

Using parameter estimation we can estimate $\gamma$ as well as the coefficient vectors $a_n$ for $n = 0, 1, 2, 3$. Again $a_0$ determines a steady state. $a_1 = \frac{1}{2} \alpha_1 x_{11}$ is a proper eigenvector of $A$, $a_2$ determines another generalised eigenvector but the third eigenvector can again not be determined.

**Case 5.** In this case any vector is an eigenvector with eigenvalue $\gamma$ and we have $r(t) = r_{ss} + e^{\gamma t} \Delta(0)$. Using parameter estimation we can determine $\gamma, a_0$ and $\Delta(0)$ and in this case this information is sufficient to determine $A$ and $c$ — if it is known that we have case 5.

Cases 1 and 3 can clearly be identified from the structure of the observed signal. A signal of the form observed in case 2 can also arise if $A$ has three distinct (real) eigenvalues but the initial state is such that $\Delta(0)$ has no overlap with one of the eigenvectors. Case 4 can also arise if $A$ has two real eigenvalues, one of which corresponding to a Jordan block of size 2 but the initial state is such that $\Delta(0)$ has no overlap with one of the proper eigenvectors. Finally, a signal of the form observed in Case 5 can arise not only when $A$ is a scalar matrix but also when $\Delta(0)$ does not have overlap with all (generalised) eigenvectors of $A$.

**References**

[1] Special issue on quantum coherence, Nature 453, 1008-1049 (2008)

[2] Physics-based mathematical models for quantum devices via experimental system identification, S. G. Schirmer, D. K. L. Oi, S. J. Devitt, Institute of Physics: Conferences Series 107, 012011 (2008).

[3] Subspace Confinement: How good is your qubit?, S. J. Devitt, S. G. Schirmer, D. K.L. Oi, J. H. Cole, L. C. L. Hollenberg, New J. Phys. 9, 384 (2007)

[4] Quantum Process Tomography: Resource Analysis of Different Strategies, M. Mohseni, A. T. Rezakhani, D. A. Lidar, Phys. Rev. A 77, 032322 (2008)

[5] Symmetric Informationally Complete Quantum Measurements, J. M. Renes, R. Blume-Kohout, A. J. Scott, C. M. Caves, J. Math. Phys. 45, 2171 (2004)

[6] Procedures for Converting among Lindblad, Kraus and Matrix Representations of Quantum Dynamical Semigroups Timothy F. Havel, J. Math. Phys. 44, 534-557 (2003)

[7] Experimental Hamiltonian identification for controlled two-level systems, S. G. Schirmer, A. Kolli, D. K. L. Oi, Phys. Rev. A 69, 050306 (2004)
[8] Experimental Hamiltonian Identification for Qubits subject to Multiple Independent Control Mechanisms, S. G. Schirmer, D. K. L. Oi, A. Kolli, J. H. Cole, AIP Conf. Proc. 734 (AIP, New York, 2004), ISBN 0-7354-0216-7
[9] Identifying an Experimental Two-State Hamiltonian to Arbitrary Accuracy, J. H. Cole, S. G. Schirmer, A. D. Greentree, C. J. Wellard, D. K. L. Oi, L. C. L. Hollenberg, Phys. Rev. A 71, 062312 (2005)
[10] Identifying a Two-State Hamiltonian in the Presence of Decoherence, J. H. Cole, A. D. Greentree, D. K. L. Oi, S. G. Schirmer, C. J. Wellard, L. C. L. Hollenberg, Phys. Rev. A 73, 062333 (2006)
[11] Two-Qubit Hamiltonian Tomography by Bayesian Analysis of Noisy Data, S. G. Schirmer, D. K. L. Oi, Phys. Rev. A 80, 022333 (2009).
[12] Quantum system identification by Bayesian analysis of noisy data: Beyond Hamiltonian tomography, Laser Physics 20, 1203-1209 (2010)
[13] Quantum system characterization with limited resources, D. K. L. Oi and S. G. Schirmer, arXiv:12.025779, Philosophical Transactions A: In Press.
[14] Bayesian Spectrum Analysis and Parameter Estimation, G. Larry Bretthorst (Springer, Berlin, 1998)
[15] Coupling strength estimation for spin chains despite restricted access, D. Burgarth, K. Maruyama, F. Nori, Phys. Rev. A 79, 020305(R) (2009)
[16] Indirect Quantum Tomography of Quadratic Hamiltonians, D. Burgarth, K. Maruyama, F. Nori, New J. Phys. 13, 013019 (2011)
[17] Bypassing state initialization in Hamiltonian tomography on spin-chains, C. Di Franco, M. Paternostro, M. S. Kim, Int. J. Quant. Inf. 9, Supp. 1, 181 (2011)
[18] Quantum System Identification: Hamiltonian Estimation using Spectral and Bayesian Analysis, S. G. Schirmer, F. C. Langbein, Proc. 4th ISCCSP 2010, Limassol, Cyprus, 3-5 March 2010.
[19] Parameter estimation of a 3-level quantum system with a single population measurement, Z. Leghtas, M. Mirrahimi, P. Rouchon, 48th IEEE Conf. CDC 2009, Shanghai, China (2009)
[20] On the generators of quantum dynamical semigroups, G. Lindblad, Comm. Math. Phys. 48 119 (1976)
[21] Completely positive semigroups of N-level systems, Gorini V., Kossakowski A. and Sudarshan E. C. G., J. Math. Phys. 17, 821 (1976)
[22] The Theory of Open Quantum Systems, Breuer, H.-P. and Petruccione, F., 2002. Oxford University Press.
[23] Evolution matrix in a coherence vector formulation for quantum Markovian master equations of N-level systems, K. Lendi, J. Phys. A: Math. Gen. 20, 15 (1987)
[24] The Bloch Vector for N-Level Systems, Gen Kimura, Phys. Lett. A 314, 339 (2003)
[25] S. G. Schirmer and Xiaoting Wang, Phys. Rev. A 81, 062306 (2010)
[26] H. Niederreiter, Random Number Generation and Quasi-Monte Carlo Methods (SIAM Review, 1992)
[27] A. H. Myerson et al., High-fidelity readout of trapped-ion qubits, Phys. Rev. Lett. 100, 200502 (2008)