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IDENTIFICATION OF QUANTUM SYSTEMS

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Abstract:
An observer structure is presented which can be used to reconstruct the state and/or parameters of a quantum system using recorded data together with a model Hamiltonian which is assumed to have the same structure as the true Hamiltonian (except for the unknown parameters). The parameters are estimated using a gradient algorithm. A numerical simulation of a quantum spin system shows convergence of the algorithm in some, but not all, cases.

Keywords: system identification, quantum systems, control

1. INTRODUCTION

Quantum control of atomic and molecular motion has a long history, see, *e.g.*, [7], [10] and the references therein. Recent impetus has come from the hope of building a quantum computer, originally heralded by Feynman [5], and now grown into a very active area of theoretical and experimental research, *e.g.*, [12]. Quantum computers can perform tasks which are impossible for a classical computer. To make such a device will require very precise and reliable control of the quantum states.

Any real quantum system, no matter how well isolated, unavoidably interacts with the environment. This interaction makes evolution of a quantum system non-unitary and destroys coherence of quantum superpositions (entanglement), the key to quantum information and computation. This process, known as decoherence, is widely regarded as the most important and fundamental obstacle to the practical realization of quantum information processing. Active control of a quantum information processing machine, is a necessity for the effective management of decoherence processes. In recent years remarkable theoretical and experimental progress has been achieved in the area of control over quantum phenomena. Fortunately, the technology to achieve tailored pulses with femtosecond temporal resolution has developed significantly during the last decade and continues to improve.

In principle, although the most suitable pulse shape can be designed by means of optimal control theory, there are difficulties due to (1) the lack of precise knowledge of the system Hamiltonian, (2) inevitable experimental uncertainties and errors, and (3) the need to solve the associated design equations to adequate accuracy. These problems are especially acute for complex multi-particle physical systems, as likely to arise in realistic quantum information processing machines. In this paper we address problem (1) above by posing a model Hamiltonian of known structure with unknown parameters to be estimated using measurements from the actual system, *i.e.*, *quantum system identification*.

2. PROBLEM FORMULATION

From a systems view, quantum systems are bilinear: specifically jointly bilinear in control and state and parameters and state. Quantum systems are not alone in this category; two other examples include kinematic steering [13], and growth of thin films [14], [8], [6],

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In this paper we consider a quantum system modeled under the following assumptions: [2]

- the system is finite dimensional and represented in some basis by the Hamiltonian matrix, $H(t,\theta) \in \mathbf{C}^{n\times n}$ where $\theta \in \mathbf{R}^p$ are unknown parameters, and where t denotes time dependence due to external fields.
- The Hamiltonian is assumed affine in θ and is of the form,

$$H(t,\theta) = H_0(t) + \sum_{k=1}^{p} \theta_k \; H_k(t) \qquad (1)$$

where the time-dependent matrices $\{H_k(t) \in \mathbf{C}^{n\times n}\}$ are Hermitian and known affine functions of the external fields $\{\varepsilon_i(t) \in \mathbf{R}\}$, that is,

$$H_k(t) = G_{k0} + \sum_{i=1}^{q} \varepsilon_i(t)\, G_{ki},\; k = 0,\ldots,p \qquad (2)$$

- The system density matrix, $\rho(t) \in \mathbf{C}^{n\times n}$, then evolves according to,

$$i\hbar\dot{\rho}(t) = [H(t,\theta), \rho(t)] \qquad (3)$$

- The system has m possible outcomes, $\{\, y_\alpha \mid \alpha = 1,\ldots,m \,\}$, where the probability of measuring y_α at time t is given by,

$$p_\alpha(t) = \mathrm{tr}\,(M_\alpha \rho(t)) \qquad (4)$$

whre $\{M_\alpha\}$ are Hermitian and satisfy the *completion relation*, $\sum_\alpha M_\alpha = I_n$; equivalently, $\sum_\alpha p_\alpha(t) = 1,\; \forall \rho(t)$.

Before proceeding, first an important aside about how data can be recorded without effecting the state. As is well known, a postulate of quantum mechanics is "to observe is to disturb." To circumvent this dictum, numerous *identical* experiments are repeated at each of N uniformly spaced sample times in a specified interval, $0 \le t \le t_{\mathrm{f}}$, and then averaging the measurement results to obtain the outcome probabilities (4). For a sufficiently large number of eperiments the set of sample averages approximates the continuous recorded data,

$$\left\{ p_\alpha(t) \,\middle|\, \alpha = 1,\ldots,m,\; 0 \le t \le t_{\mathrm{f}} \right\} \qquad (5)$$

If in addition, the initial state of the system is random, which is likely the case, then the density $\rho(t)$ represents a *statistical state*, [2].

The problem addressed is to use the recorded data (5) to estimate the unknown parameters $\theta \in \mathbf{R}^p$ in the model (1)-(4).

[2] The mathematical representation used here for a quantum system is standard, *e.g.*, [2]. One exception is our use of the notation $H_0(t)$ in (1) which is normally preserved for the potential. Here we use it to represent that part of the Hamiltonian not dependent on unknown parameters. Thus, known parts of the potential are included in $H_0(t)$.

3. STATE ESTIMATION: KNOWN HAMILTONIAN

In this section a state observer is constructed for (3) under the assumption that θ is known. Thus, set $H(t) = H(t,\theta)$. Clearly the resulting system (3)-(4) is linear-time-varying. Hence, it is possible to construct a *time-varying* observer by utilizing standard optimal (Kalman) filtering design methods, or using fictitious noise variances as design variables. By analogy with this classical observer, consider the simpler *constant gain* quantum state observer:

$$\begin{aligned} i\hbar\dot{\widehat{\rho}} &= [H(t), \widehat{\rho}] + i\sum_{\alpha=1}^{m} \gamma_\alpha e_\alpha M_\alpha \\ e_\alpha &= p_\alpha - \mathrm{tr}\,(M_\alpha \widehat{\rho}) \end{aligned} \qquad (6)$$

Because of the error feedback terms $\{e_\alpha M_\alpha\}$, the observer state, $\widehat{\rho}$, may not be a density matrix, although it is Hermitian. Properties of the observer are enumerated in the following.

Lemma 1. From any initial state $\widehat{\rho}(0) \in \mathbf{C}^{n\times n}$:

(1) $\widehat{\rho}(t)$ is bounded for all t.
(2) $e_\alpha(t) \to 0$ as $t \to \infty$ for all $\alpha = 1,\ldots,m$.
(3) $\widehat{\rho}(t) \to \rho(t)$ exponentially as $t \to \infty$ if $\left\{ H(t), M_\alpha \,\middle|\, \alpha = 1,\ldots,m \right\}$ is **uniformly completely observable**, *i.e.*, if there exist finite constants $\delta > 0,\; \beta > 0$ such that for all $\tau \ge 0$,

$$\int_{\tau}^{\tau+\delta} N(t,\tau) N(t,\tau)^* dt \ge \beta\, I_{mn^2} \qquad (7)$$

where $N(t,\tau) \in \mathbf{C}^{mn^2}$ is,

$$N(t,\tau) = \begin{bmatrix} \mathrm{vec}\,(\, U(t,\tau)^* M_1 U(t,\tau)\,)^T \\ \vdots \\ \mathrm{vec}\,(\, U(t,\tau)^* M_m U(t,\tau)\,)^T \end{bmatrix} \qquad (8)$$

with $U(t,\tau) \in \mathbf{C}^{n\times n}$ the unitary transition matrix which solves:

$$i\hbar\dot{U}(t,\tau) = H(t)U(t,\tau),\; U(\tau,\tau) = I_n \qquad (9)$$

Proof Define the error state,

$$\widetilde{\rho} = \widehat{\rho} - \rho \qquad (10)$$

The observer expressed in the error state satisfies,

$$\begin{aligned} i\hbar\dot{\widetilde{\rho}} &= [H(t), \widetilde{\rho}] + i\sum_{\alpha=1}^{m} \gamma_\alpha e_\alpha M_\alpha \\ e_\alpha &= -\mathrm{tr}\,(M_\alpha \widetilde{\rho}) \end{aligned} \qquad (11)$$

Define the positive definite error measure,

$$V = \frac{1}{2}\mathrm{tr}\,(\widetilde{\rho}^2) \qquad (12)$$

Using the fact that $\mathrm{tr}\left(\widetilde{\rho}\left[H(t)\right),\widetilde{\rho}\right] = 0$, the rate of change of V along solutions of (11) becomes,

$$\dot{V} = -\sum_{\alpha=1}^{m} \gamma_\alpha e_\alpha^2$$

Since V is positive definite and $\dot{V}$ is negative semi-definite (in $\widetilde{\rho}$), it follows from Lyapunov stability theory that $\widetilde{\rho}(t) = 0$ is a globally stable solution and hence $\widetilde{\rho}(t)$ is bounded for bounded initial states. Since $\rho(t)$ is a density matrix, $\widehat{\rho}(t)$ is therefore bounded. It takes a few more steps to go from here to a proof of exponential stability – see [1, Ch.2] for all of them.

4. EXAMPLE: CHAIN OF SPIN SYSTEMS

Electron spin states are promising candidates for manifesting the qubits needed in a quantum computer. [3] Spin states are either "up" or "down," the direction determined by convention (and alignment of the measuring apparatus). Using the "ket" notation, the states are denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$. Sometimes it is simpler to write $\uparrow$ and $\downarrow$.

The example system we consider here is the interconnected chain of N-spin systems:

$$\boxed{\mathcal{Q}_1} \overset{\nu_1}{\Longleftrightarrow} \boxed{\mathcal{Q}_2} \overset{\nu_2}{\Longleftrightarrow} \cdots \overset{\nu_{N-1}}{\Longleftrightarrow} \boxed{\mathcal{Q}_N}$$

The Hamiltonian *operator* is,

$$\boldsymbol{H}/\hbar = \sum_{n=1}^{N} \frac{g_n}{2}\, \boldsymbol{B}_n(t)\cdot\boldsymbol{\sigma}_n + \sum_{n=1}^{N-1} \nu_n\, \boldsymbol{\sigma}_n\cdot\boldsymbol{\sigma}_{n+1} \quad (13)$$

where $\boldsymbol{B}_n(t) = (\boldsymbol{B}_{n,x}(t), \boldsymbol{B}_{n,y}(t), \boldsymbol{B}_{n,z}(t))$ is the external magnetic field, $\boldsymbol{\sigma}_n = (\boldsymbol{\sigma}_{n,x}, \boldsymbol{\sigma}_{n,y}, \boldsymbol{\sigma}_{n,z})$ the Pauli spin operator, $\{g_n\}$ the gyromagnetic ratios, and $\{\nu_n\}$ the spin couplings. The base states of each system are $(\uparrow\downarrow)$ with respect to that system. Since states of a collection of quantum systems are tensor products, the N-spin chain has 2^N-basis states formed from the tensor products of each individual system basis. A standard model yields the $2^N \times 2^N$ Hamiltonian matrix is given by,

$$H/\hbar = \sum_{n=1}^{N} \frac{g_n}{2}\left(I_{2^{n-1}} \otimes R_n(t) \otimes I_{2^{N-n}}\right) + \sum_{n=1}^{N-1} \nu_n \left(I_{2^{n-1}} \otimes S_n \otimes I_{2^{N-n-1}}\right)$$

with $R_n(t) \in \mathbf{C}^{2\times 2}$ and $S_n \in \mathbf{R}^{4\times 4}$ given by,

$$R_n(t) = \sum_{k=x,y,z} B_{n,k}(t)\,\sigma_k = \begin{bmatrix} B_{n,z}(t) & B_{n,x}(t) - iB_{n,y}(t) \\ B_{n,x}(t) + iB_{n,y}(t) & -B_{n,z}(t) \end{bmatrix}$$

$$S_n = \sum_{k=x,y,z} \sigma_k \otimes \sigma_k = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The probability that $\mathcal{Q}_k$ is in the state $\uparrow$ at time t is,

$$p_{\uparrow_k}(t) = \mathrm{tr}\left(M_{\uparrow_k}\rho(t)\right)$$

$$M_{\uparrow_k} = I_{2^{k-1}} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes I_{2^{N-k}}$$

Similarly,

$$p_{\downarrow_k}(t) = 1 - p_{\uparrow_k}(t) = \mathrm{tr}\left(M_{\downarrow_k}\rho(t)\right)$$

$$M_{\downarrow_k} = I_{2^{k-1}} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes I_{2^{N-k}}$$

A simulation was performed with,

$$N = 2,\ g = [1,\ 1],\ \nu = .1$$

external fields,

$$B_z(t) = [1,\ 1],\ B_x(t) = [\cos t,\ 0],\ B_y(t) = [\sin t,\ 0]$$

and normalization $\hbar = 1$. Suppose only the outputs of $\mathcal{Q}_1$ are recorded, thus, $y_1 = \uparrow,\ y_2 = \downarrow$ and

$$\begin{aligned} M_1 &= M_\uparrow = \mathrm{diag}(1,1,0,0) \\ M_2 &= M_\downarrow = \mathrm{diag}(0,0,1,1) \end{aligned} \quad (14)$$

Using the observer (6), Figure 1 shows a comparison of the actual and estimated probabilities using observer gain $\gamma = [2,2]$ with initial simulation states:

$$\begin{aligned} \rho(0) &= \mathrm{diag}(1,0,0,0) \\ \widehat{\rho}(0) &= \mathrm{diag}(0,0,0,1) \end{aligned} \quad (15)$$

Thus the initial state of $\mathcal{Q}_1$ is $\uparrow$ whereas the observer state presumes the opposite, *i.e.*, that $\mathcal{Q}_1$ is $\downarrow$.

5. OBSERVER BASED PARAMETER ESTIMATION

In this section the observer (6) is used for parameter estimation with an iterative search algorithm. The spin example is used to illustrate the efficacy of this approach.

[3] The physics of spin systems is described in many standard texts, see, *e.g.*, [4, III-12], [2, IV]. Their use in quantum computers is described in [12] and the references therein.

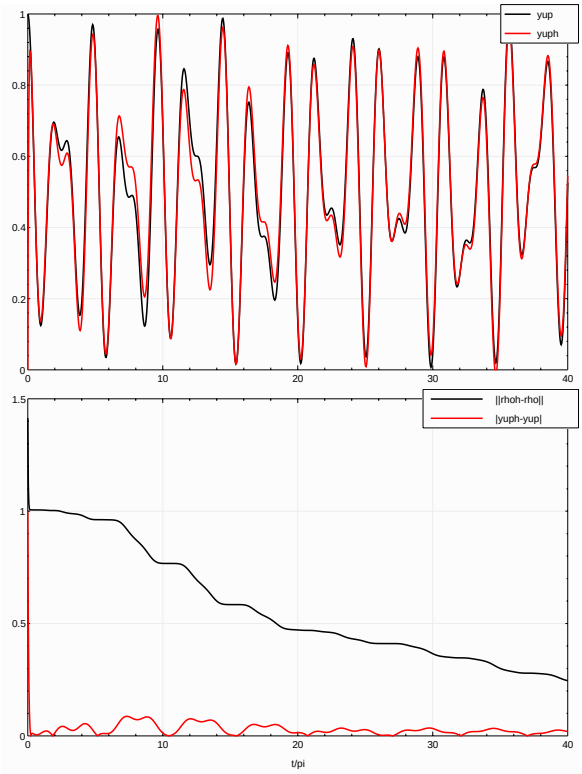

Fig. 1. Plots of true and estimated outputs and errors.
Row 1: black – $p_\uparrow(t)$, red – $\widehat{p}_\uparrow(t)$.
Row 2: black – $\mathrm{tr}\left(\widetilde{\rho}(t)^2\right)$, red – $|\widehat{p}_\uparrow(t) - p_\uparrow(t)|$.

Iterative search

To simplify the notation let p and $p(\theta)$ denote, respectively, the probability outcomes from the data and the model, *i.e.*,

$$p = \left\{ p_\alpha(t) \;\middle|\; \begin{array}{l} \alpha = 1\ldots, m \\ 0 \le t \le t_{\mathrm{f}} \end{array} \right\}$$
$$p(\theta) = \left\{ p_\alpha(t,\theta) = \mathrm{tr}\left(M_\alpha \widehat{\rho}(t,\theta)\right) \;\middle|\; \begin{array}{l} \alpha = 1:m \\ 0 \le t \le t_{\mathrm{f}} \end{array} \right\} \quad (16)$$

where $\widehat{\rho}(t,\theta)$ is the state of the observer (6). Consider the model selection criterion,

$$\text{minimize } V(\theta) = \|e(\theta)\|^2, \quad e(\theta) = p - p(\theta) \quad (17)$$

The general form of an iterative search algorithm is,

$$\theta^{(i+1)} = \theta^{(i)} + \epsilon^{(i)} \Gamma^{(i)}\, e(\theta^{(i)}) \quad (18)$$

where $\epsilon^{(i)}$ is a (typically) a small positive parameter, and $\Gamma^{(i)}$ reflects the particular method, *e.g.*,

Gradient search:

$$\Gamma^{(i)} = -G(\theta^{(i)}),\ G(\theta) = \nabla_\theta\, p(\theta) \quad (19)$$

Newton-Raphson search:

$$\Gamma^{(i)} = -\left[G(\theta^{(i)})G(\theta^{(i)})^T\right]^{-1} G(\theta^{(i)}) \quad (20)$$

Many other variants exist. The disadvantage with all of above methods is that, in general, there is no guarantee of global convergence to the optimum. The algorithms typically converge to a local minimum. However, for quantum systems, many good local minima are possible. As it is said, "Let not the best become the enemy of the good."

6. EXAMPLE: GRADIENT ALGORITHM

Suppose the parameters to be estimated are:

$$\theta = (\eta, \nu) \quad (21)$$

with ν as previously defined (spin coupling in (13)) and η defined via:

$$g_1 B_1 = [\eta \cos\omega t,\ \sin\omega t,\ \omega] \quad (22)$$

(The choice here is illustrative.) Suppose, further, that the data is generated from the system,

$$i\hbar\dot{\rho} = [H(t,\theta_0), \rho],\ \theta_0 = (\eta_0, \nu_0) = (1, 0.2)$$
$$p_\alpha = \mathrm{tr}\left(M_\alpha \rho\right),\ \alpha = \uparrow, \downarrow$$

with $\mathcal{Q}_1$ intially measured in the $\uparrow$ state. The initial state of the complete system, $\rho(0)$, is randomly selected to satisfy $\mathrm{tr}\left(M_\uparrow \rho(0)\right) = 1$. (We return to this assumption later). The observer with parameter estimate $\widehat{\theta}$ is,

$$i\hbar\dot{\widehat{\rho}} = [H(t,\widehat{\theta}), \widehat{\rho}] + i\sum_\alpha \gamma_\alpha e_\alpha M_\alpha$$
$$\widehat{\rho}(0) = [1,1,0,0]^T/\sqrt{2}$$
$$e_\alpha = p_\alpha - \mathrm{tr}\left(M_\alpha \widehat{\rho}\right),\ \gamma_\alpha = 1$$

For comparison, suppose we are able to measure *all* the states, *i.e.*, $\mathcal{Q}_1$ and $\mathcal{Q}_2$ are both observed. Hence, $y_1 = \uparrow\uparrow$, $y_2 = \uparrow\downarrow$, $y_3 = \downarrow\uparrow$, $y_4 = \downarrow\downarrow$ from which it follows that,

$$\begin{array}{l} M_1 = M_{\uparrow\uparrow} = \mathrm{diag}[1,0,0,0] \\ M_2 = M_{\uparrow\downarrow} = \mathrm{diag}[0,1,0,0] \\ M_3 = M_{\downarrow\uparrow} = \mathrm{diag}[0,0,1,0] \\ M_4 = M_{\downarrow\downarrow} = \mathrm{diag}[0,0,0,1] \end{array} \quad (23)$$

For purposes of distinction, we refer to these measurements as *full information* and to the measurements (14) as *partial information*.

The first set of results using the gradient search algorithm (19) are shown in Figure 2 for various initial values and adaptation gains – ϵ in (19). The algorithm is modified with a projection scheme so that if the parameters get outside a prescribed region, the new parameter is randomly located nearby, but inside the region. The initial values of the estimates all start from the four corners of the box $\{0.1 \le \widehat{\nu} \le .3,\ .5 \le \widehat{\eta} \le 1.5\}$. The true parameter (shown in the big black dot) is $(\eta_0, \nu_0) = (0.2, 1)$. The full information case (23) shows convergence from all

corners. The more realistic case with partial information shows no global convergence to the true value. In fact, the best results only converge to a neighborhood of the true value. The trajectories clearly depend on the starting value of the iteration. In one case the algorithm heads to a "blob" just inside the boundary due to the projection scheme. Without this projection the estimates would move outside the box, possibly becoming negative which is not physical in this case.

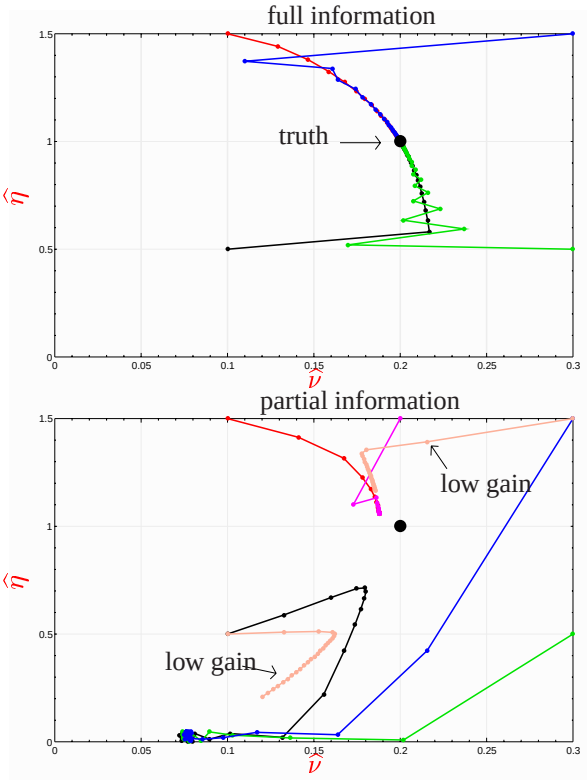

Fig. 2. Gradient algorithm with observer

Part of the reason for the difference in the convergence behavior of two cases is due to differences between the initial state of the "true" system and of the estimator. With full information (23), the initial state is known because it is measured. As previously mentioned, the system is therefore known to start in the state $\uparrow\uparrow$, *i.e.*,

$$\psi(0) = \widehat{\psi}(0) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

With partial information (14), the system state of $\mathcal{Q}_1$ reads $\uparrow$ but the state of $\mathcal{Q}_2$ is random, *i.e.*,

$$\psi(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes b$$

with $b \in \mathbf{C}^2$ randomly chosen such that $\|b\| = 1$. The estimator state is chosen to nominally reflect the fact that $\uparrow$ is read from $\mathcal{Q}_1$, *i.e.*,

$$\widehat{\psi}(0)^T = [1\ 1\ 0\ 0]\,/\sqrt{2}$$

With partial information, the discrepancy in the initial states of the system and estimator causes the gradient algorithm to be slightly incorrect even when the estimated parameters are close to the true values. Because the data length is finite, the observer states may not have yet converged to the true state, and in fact, they may never if there is not sufficient excitation. With full information there is no initial condition error to cause a bias in the algorithm, assuming it converges.

In our example with partial information, $c = a \otimes b$, with $a \in \mathbf{C}^m$, $\|a\| = 1$ known because it is measured from $\mathcal{Q}_1$, whereas the state $b \in \mathbf{C}^\ell$, $\|b\| = 1$ is not known (in our example $m = \ell = 2$). If it is assumed that b be a random variable, then

$$\rho(0) = aa^* \otimes \langle bb^* \rangle$$

In most cases $\langle bb^* \rangle$ can be determined from the underlying physics. For example, if the spins of $\mathcal{Q}_2$ weakly interact with the applied field, and the interaction is smaller than the thermal energy, the thermal limit forms a statistical population which is reasonably approximated by $\langle bb^* \rangle \approx I_\ell/\ell$. (This also gives $\langle \|b\|^2 \rangle \approx 1$.) This random population limit corresponds to the high temperature limit in a thermal bath. Mathematically, this approximation is exact when b is given by $b = x/\|x\|$ with each element of x drawn from an independent zero mean gaussian or uniform distribution with equal variance.

If we make the assumption that $\langle bb^* \rangle$ is known, or can be reasonably approximated, then we know the initial state. In our simulation we set $\langle bb^* \rangle = I_\ell/\ell$. The gradient algorithm applied to the full information case is shown in Figure 3. The parameter estimate trajectories converge to the true value. The partial information case is shown in Figure 4. Comparing 4 with 3 shows that convergence is more rapid with full information as might be expected.

7. CONCLUDING REMARKS

Despite some of the positive simulation results shown here, it is not clear if a gradient model based algorithm will work, *i.e.*, provide *global* convergence to the optimum for quantum system identification in the laboratory. Perhaps this is asking too much. Certainly if a parametric physics based model is posed, nominal parameter values may also be available. If these are not far from the "true" values, then gradient algorithms will most likely be adequate. The question then, is are there better approaches to identification of these physics based models? Or are we facing a fundamental problem as for example in *output error identification*, which is known to have many local minima, [11].

Although the latter unhappy possibility is persuasive, there are other methods available for identification. For example, recent efforts in subspace identification

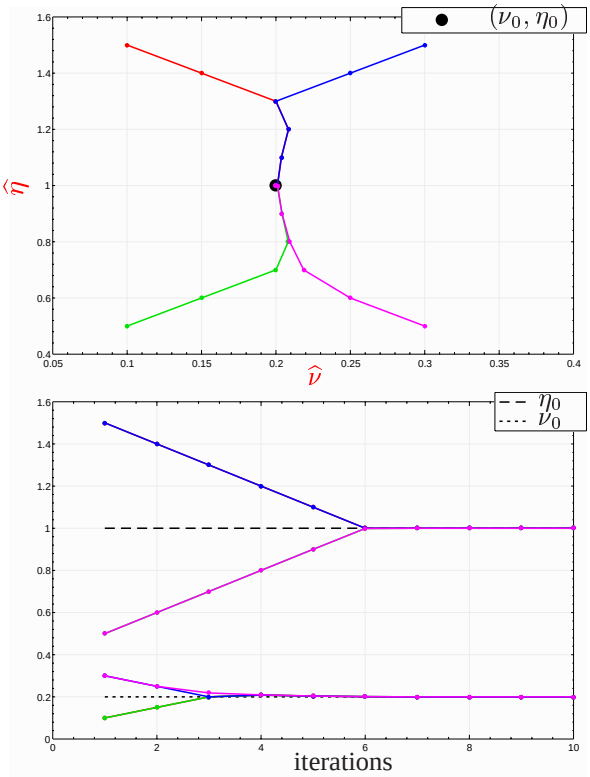

Fig. 3. Trajectories of parameter estimate with full information. Upper: in parameter space. Lower: per iteration.

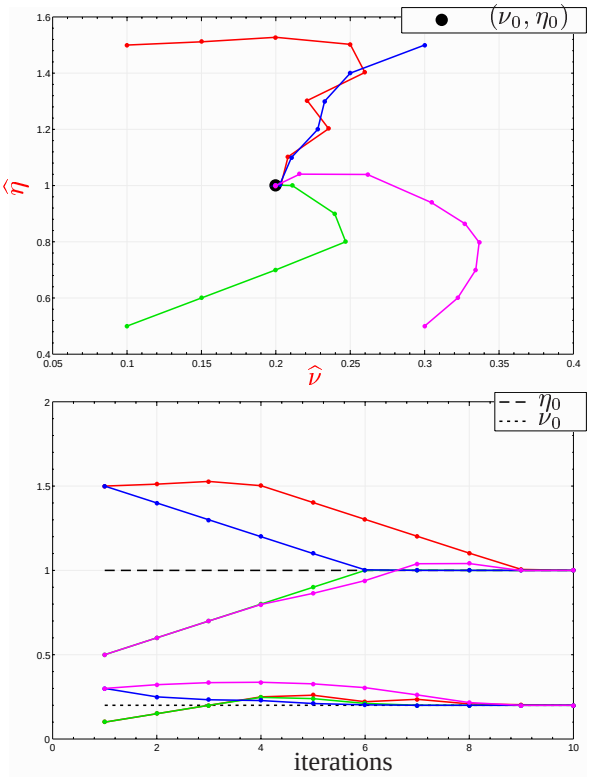

Fig. 4. Trajectories of parameter estimate with partial information. Upper: in parameter space. Lower: per iteration.

of bilinear systems holds promise, *e.g.*, [3]. In this approach a *canonical* bilinear system is identified from the data. The particular state which is identified has no physical meaning except as a vehicle for matching the input/output data. A topic of our current research is to see if it is possible to add constraints consistent with quantum mechanics. Even if this is possible, the use of such a canonical model would likely be for control design rather than system design or physical understanding as would be accrued from the Hamiltonian identification methods examined here.

Another class of approaches is based on learning algorithms. For example, data directed selection of the gain matrix, Γ, in (18) can be accomplished using the unfalsified control adaptive concept [9]. The method of closed-loop laboratory learning control [7] can be modified to become an identification algorithm. Both of these require further development. However, these approaches can take advantage of a number of unique special features: (i) the quantum system solves its own Schrödinger equation in real time, (ii) the high-duty cycle of pulse shaping is a rapidly evolving practical technology, and (iii) in favorable cases (*e.g.*, laser fields) literally millions of experiments can be performed under full automation in a short period of time (*e.g.*, an hour or less).

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