Observer-based Hamiltonian identification for quantum systems

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Observer-based parameter estimation

Take $\frac{d}{dt}x = f(x, u(t), p)$ with output $y(t) = h(x)$ and control $u(t)$. The goal is to estimate p (and x) from noisy measurements of y.

State-parameter asymptotic observer Can we find g_1 and g_2 such that the solution $(\hat{x}(t), \hat{p}(t))$ of

$$\frac{d}{dt}\hat{x}(t) = f(\hat{x}, u(t), \hat{p}) + g_1(\hat{x}, u(t), \hat{p}, y(t))$$
$$\frac{d}{dt}\hat{p}(t) = g_2(\hat{x}, u(t), \hat{p}, y(t))$$

with an arbitrary initial state $(\hat{x}_0, \hat{p}_0)$ converges towards $(x(t), p)$ as $t \to \infty$?

Invariant asymptotic observers (Thesis of Silvère Bonnabel).

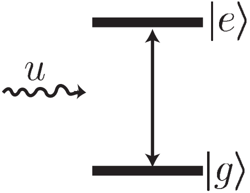
Outline

An invariant asymptotic observer for a 2-level system

Semi-local convergence proof

Possible extensions

The estimation problem for a two-level system



$$
\begin{aligned}
\frac{d}{dt}\rho &= -\imath\left[\frac{\Delta}{2}\sigma_z + \frac{u\mu}{2}\sigma_x, \rho\right] \\
y &= \mathrm{Tr}\left(\sigma_z \rho\right), \quad \text{(groud state population)}
\end{aligned}
$$

where:

- ρ is the density matrix: a 2×2 symmetric ≥ 0 matrix with $\mathrm{Tr}\left(\rho\right) = 1$ and $\mathrm{Tr}\left(\rho^2\right) = 1$ (here a projector).
- $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are the Pauli matrices: $\sigma_x^2 = 1$; $\sigma_x \sigma_y = \imath \sigma_z$..
- the two real parameters are Δ (the difference between the atomic frequency (transition $|g\rangle \leftrightarrow |e\rangle$) and the laser frequency of amplitude u) and $\mu > 0$ the dipole strength.
- $u\mu$ is the Rabi pulsation. This model is based on a singular perturbation of a Lindblad equation modelling the evolution of an ensemble of identical 3 level quantum systems.

Hamiltonian identification for quantum systems

Unknown parameters: μ and Δ.

Some previous methods:
Maximum-likelihood (Rabitz, Kosut, Walmsley, Paris, Mabuchi)
Maximum (Kullback) entropy (Buzek, Paris, Oliveras)
Optimal identification via least-square crieteria (Rabitz, Geremia)

Main issues: Robustness wrt uncertainties and noises, Computational cost, local minima.

Observer-based parameter identification (a previous result):

R.L. Kosut and H. Rabitz, 15th IFAC world congress, 2002.
Asymptotic state observer + iterative search algorithm to update the estimate of the parameters
Our approach: adptive observer

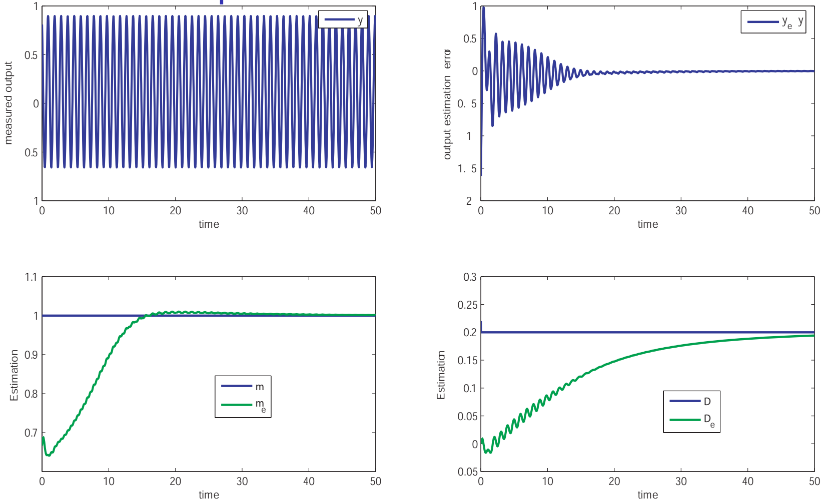
The non-linear asymptotic observer

$$\frac{d}{dt}\hat{\rho} = -\imath \left[\frac{\hat{\Delta}}{2}\sigma_z + \frac{u\hat{\mu}}{2}\sigma_x, \hat{\rho}\right]$$
$$- K_\rho(\text{Tr}(\sigma_z\hat{\rho}) - y)\ (\sigma_z\hat{\rho} + \hat{\rho}\sigma_z - 2\text{Tr}(\sigma_z\hat{\rho})\hat{\rho})$$
$$\frac{d}{dt}\hat{\mu} = -uK_\mu \text{Tr}\left(\sigma_y\hat{\rho}\right)\ (\text{Tr}(\sigma_z\hat{\rho}) - y)$$
$$\frac{d}{dt}\hat{\Delta} = -uK_\Delta \text{Tr}(\sigma_x\hat{\rho})\ (\text{Tr}(\sigma_z\hat{\rho}) - y)$$

with positive gains K_ρ, K_μ and K_Δ. Preservation of $\text{Tr}(\hat{\rho}) = 1$ and $\text{Tr}\left(\hat{\rho}^2\right) = 1$.
Convergence results from averaging consideration (RWA) under the following assumptions and gains design:

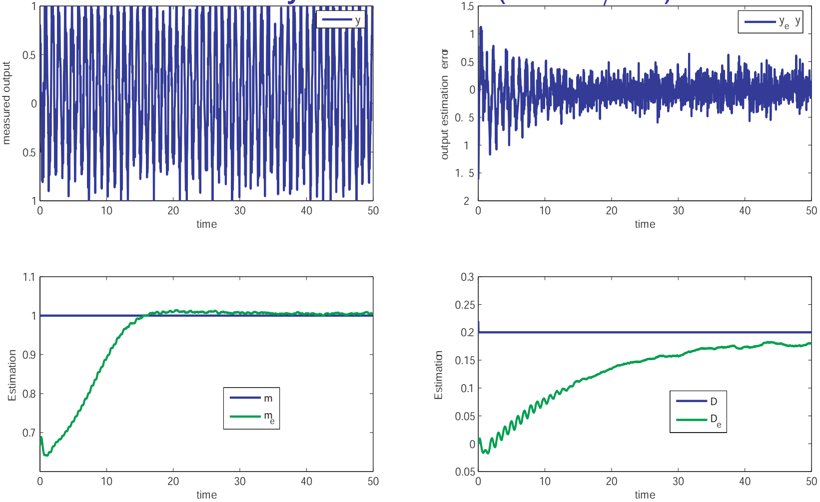
- slowly varying u versus Rabi pulsation $|u\mu|$: $|\dot{u}| \ll u^2\mu$.
- Small detuning $|\Delta|, |\hat{\Delta}| \ll |u|\mu$ and $|\hat{\mu}_{t=0} - \mu| \ll \mu$.
- Small gains: $K_\rho \ll |u|\mu$, $\sqrt{K_\mu} \ll \mu$, $K_\Delta \ll K_\mu\mu$.

Simulation with perfect measures



Initial conditions: $\rho_0 = \frac{1+\cos(\frac{\pi}{5})\sigma_x+\sin(\frac{\pi}{5})\cos(\frac{\pi}{1.4})\sigma_y+\sin(\frac{\pi}{5})\sin(\frac{\pi}{1.4})\sigma_z}{2}$,
$\mu = 1, \Delta = \frac{1}{5}$, $\hat{\rho}_0 = \sigma_x \rho_0 \sigma_x$
Control/gains: $u = 1$, $K_\rho = 2\varepsilon|u|\mu$, $K_\mu = 2\varepsilon^2\mu^2$ and $K_\Delta = 2\varepsilon^2|u|\mu^2$ with $\varepsilon = \frac{1}{5}$.

Simulation with noisy measures ($\sigma = 2/10$)



Initial conditions: $\rho_0 = \frac{1+\cos(\frac{\pi}{5})\sigma_x + \sin(\frac{\pi}{5})\cos(\frac{\pi}{1.4})\sigma_y + \sin(\frac{\pi}{5})\sin(\frac{\pi}{1.4})\sigma_z}{2}$,
$\mu = 1, \Delta = \frac{1}{5}$, $\hat{\rho}_0 = \sigma_x \rho_0 \sigma_x$
Control/gains: $u = 1$, $K_\rho = 2\varepsilon|u|\mu$, $K_\mu = 2\varepsilon^2\mu^2$ and
$K_\Delta = 2\varepsilon^2|u|\mu^2$ with $\varepsilon = \frac{1}{5}$.

Invariance versus $SU(2)$ action

For any $U \in SU(2)$, the transformation ((u, y, Δ, μ) unchanged)

$$\rho \mapsto \varpi =\mapsto U\rho U^\dagger, \sigma_x \mapsto \varsigma_x = U\sigma_x U^\dagger, \dots$$

leaves

$$\frac{d}{dt}\rho = -\imath \left[\frac{\Delta}{2}\sigma_z + \frac{u(t)\mu}{2}\sigma_x, \rho \right], \quad y = \mathrm{Tr}\left(\sigma_z \rho\right)$$

unchanged:

$$\frac{d}{dt}\varpi = -\imath \left[\frac{\Delta}{2}\varsigma_z + \frac{u(t)\mu}{2}\varsigma_x, \varpi \right], \quad y = \mathrm{Tr}\left(\varsigma_z \varpi\right),$$

and ς_x,ς_y,ς_z are new Pauli matrices.

$SU(2)$ invariance of the non-linear observer

For any $U \in SU(2)$, the transformation ($(\hat{\Delta}, \hat{\mu})$ unchanged)

$$\hat{\rho} \mapsto \hat{\varpi} = \mapsto U\hat{\rho}U^{\dagger}, \sigma_x \mapsto \varsigma_x = U\sigma_x U^{\dagger}, \ldots$$

leaves the asymptotic observer

$$\begin{aligned}
\frac{d}{dt}\hat{\rho} &= -\imath \left[\frac{\hat{\Delta}}{2}\sigma_z + \frac{u\hat{\mu}}{2}\sigma_x, \hat{\rho} \right] \\
&\quad - K_\rho(\mathrm{Tr}(\sigma_z\hat{\rho}) - y)\ (\sigma_z\hat{\rho} + \hat{\rho}\sigma_z - 2\mathrm{Tr}(\sigma_x\hat{\rho})\hat{\rho}) \\
\frac{d}{dt}\hat{\mu} &= -uK_\mu \mathrm{Tr}\left(\sigma_y\hat{\rho}\right)\ (\mathrm{Tr}(\sigma_z\hat{\rho}) - y) \\
\frac{d}{dt}\hat{\Delta} &= -uK_\Delta \mathrm{Tr}(\sigma_x\hat{\rho})\ (\mathrm{Tr}(\sigma_z\hat{\rho}) - y)
\end{aligned}$$

unchanged.

Assumptions

In

$$\frac{d}{dt}\hat{\rho} = -\imath \left[\frac{\hat{\Delta}}{2}\sigma_z + \frac{u\hat{\mu}}{2}\sigma_x, \hat{\rho} \right] - K_\rho (\mathrm{Tr}(\sigma_z\hat{\rho}) - y) \, (\sigma_z\hat{\rho} + \hat{\rho}\sigma_z - 2\mathrm{Tr}(\sigma_z\hat{\rho})\hat{\rho})$$

$$\frac{d}{dt}\hat{\mu} = -uK_\mu \mathrm{Tr}\left(\sigma_y\hat{\rho}\right) \, (\mathrm{Tr}(\sigma_z\hat{\rho}) - y)$$

$$\frac{d}{dt}\hat{\Delta} = -uK_\Delta \mathrm{Tr}(\sigma_x\hat{\rho}) \, (\mathrm{Tr}(\sigma_z\hat{\rho}) - y)$$

we assume that u is constant and that

$$\hat{\Delta} = \epsilon\hat{d}, \quad K_\rho = 4k_\rho\epsilon|u|\mu, \quad K_\mu = 2k_\mu\epsilon^2\mu^2, \quad K_\Delta = 2k_\Delta\epsilon^2|u|\mu^2$$

for $\epsilon > 0$ small $\epsilon \ll 1$, $k_\rho, k_\mu, k_\Delta \sim 1$.
Convergence based on perturbation techniques (Rotating Wave Approximation (RWA)) but up to order 2 in ϵ.

In the interaction frame

Consider the following time-varying transformation

$$\rho = e^{-\imath \frac{u\mu t \sigma_x}{2}} \xi e^{\imath \frac{u\mu t \sigma_x}{2}}, \qquad \hat{\rho} = e^{-\imath \frac{u\mu t \sigma_x}{2}} \hat{\xi} e^{\imath \frac{u\mu t \sigma_x}{2}}.$$

The dynamics reads:

$$\frac{d}{dt}\xi = -\imath \left[\frac{\Delta}{2} e^{\imath u\mu t\sigma_x}\sigma_z, \xi\right]$$

$$\frac{d}{dt}\hat{\xi} = -\imath \left[\frac{\hat{\Delta}}{2} e^{\imath u\mu t\sigma_x}\sigma_z + \frac{u(\hat{\mu}-\mu)}{2}\sigma_x, \hat{\xi}\right] - K_\rho \operatorname{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z(\hat{\xi}-\xi)\right)$$

$$\ldots \left(e^{\imath u\mu t\sigma_x}\sigma_z\hat{\xi} + \hat{\xi} e^{\imath u\mu t\sigma_x}\sigma_z - 2\operatorname{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z\hat{\xi}\right)\hat{\xi}\right)$$

$$\frac{d}{dt}\hat{\mu} = -uK_\mu \operatorname{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_y\hat{\xi}\right) \operatorname{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z(\hat{\xi}-\xi)\right)$$

$$\frac{d}{dt}\hat{\Delta} = -uK_\Delta \operatorname{Tr}\left(\sigma_x\hat{\xi}\right) \operatorname{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z(\hat{\xi}-\xi)\right).$$

First order secular approximation

By assumption the frequency $u\mu$ is large and the integration of $e^{\imath u\mu t\sigma_x}$ will produce terms of small amplitude. We neglect terms rotating at $u\mu$ and also $2u\mu$ (first order in ε):

$$
\begin{aligned}
\frac{d}{dt}\xi &= 0 \\
\frac{d}{dt}\hat{\xi} &= -\imath \left[\frac{u(\hat{\mu}-\mu)}{2}\sigma_x, \hat{\xi}\right] \\
&\qquad - \frac{K_\rho}{2}\operatorname{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)\left(\sigma_y\hat{\xi}+\hat{\xi}\sigma_y - 2\operatorname{Tr}\left(\sigma_y\hat{\xi}\right)\hat{\xi}\right) \\
&\qquad - \frac{K_\rho}{2}\operatorname{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right)\left(\sigma_z\hat{\xi}+\hat{\xi}\sigma_z - 2\operatorname{Tr}\left(\sigma_z\hat{\xi}\right)\hat{\xi}\right) \\
\frac{d}{dt}\hat{\mu} &= -\frac{uK_\mu}{2}\left(\operatorname{Tr}\left(\sigma_y\hat{\xi}\right)\operatorname{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right) - \operatorname{Tr}\left(\sigma_z\hat{\xi}\right)\operatorname{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)\right) \\
\frac{d}{dt}\hat{\Delta} &= 0.
\end{aligned}
$$

Convergence of $\hat{\xi}$ and $\hat{\mu}$

Up to second order terms, $\hat{\xi}$ and $\hat{\mu}$ obey an autonomous differential system where ξ is a parameter:

$$\begin{aligned}\frac{d}{dt}\hat{\xi} = -\imath \; & \left[\frac{u(\hat{\mu}-\mu)}{2}\sigma_x, \hat{\xi}\right] \\ & - \frac{K_\rho}{2}\mathrm{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)\left(\sigma_y\hat{\xi}+\hat{\xi}\sigma_y - 2\mathrm{Tr}\left(\sigma_y\hat{\xi}\right)\hat{\xi}\right) \\ & - \frac{K_\rho}{2}\mathrm{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right)\left(\sigma_z\hat{\xi}+\hat{\xi}\sigma_z - 2\mathrm{Tr}\left(\sigma_z\hat{\xi}\right)\hat{\xi}\right)\end{aligned}$$

$$\frac{d}{dt}\hat{\mu} = -\frac{uK_\mu}{2}\left(\mathrm{Tr}\left(\sigma_y\hat{\xi}\right)\mathrm{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right) - \mathrm{Tr}\left(\sigma_z\hat{\xi}\right)\mathrm{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)\right)$$

Local exponential convergence for any ξ (excepted some isolated values) and for any $K_\rho, K_\mu > 0$ via the Lyapounov function:

$$\frac{1}{2}\mathrm{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)^2 + \frac{1}{2}\mathrm{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right)^2 + \frac{1}{K_\mu}(\hat{\mu}-\mu)^2.$$

Second order secular approximation

We use Kapitsa short-cut method to compute these second order terms particularly important for ξ and $\hat{\Delta}$ since the first order secular terms vanish.
We can decompose $\xi = \bar{\xi} + \delta\xi$: $\bar{\xi}$ is the no-oscillatory part, whereas $\delta\xi$ is the oscillatory one with zero mean and small amplitude $\|\delta\xi\| \ll \|\bar{\xi}\|$. Since $\frac{d}{dt}\xi = -\imath \left[\frac{\Delta}{2} e^{\imath u \mu t \sigma_x} \sigma_z, \xi\right]$ we have approximatively:

$$\delta\xi = \frac{\imath\Delta}{2u\mu}\left[\frac{\Delta}{2} e^{\imath u \mu t \sigma_x} \sigma_y, \bar{\xi}\right] + \ldots$$

Plugging this relation into the true dynamics of ξ and taking the secular terms yields up to the third order:

$$\frac{d}{dt}\xi = -\imath \frac{\Delta^2}{2u\mu}[\sigma_x, \xi] + \ldots$$

the term $\frac{\Delta^2}{2u\mu}$ corresponds exactly to Bloch-Siegert frequency shift.

Second order secular approximation (continued)

Since $\frac{d}{dt}\hat{\Delta} = -uK_\Delta \mathrm{Tr}\left(\sigma_x \hat{\xi}\right)\ \mathrm{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z(\hat{\xi}-\xi)\right)$ the secular effect can only comes from the part of $\delta\xi$ and $\delta\hat{\xi}$ with frequency $u\mu$: terms of double frequency $2u\mu$ have no secular effect. In the $\hat{\xi}$ dynamics

$$\frac{d}{dt}\hat{\xi} = -\imath\ \left[\frac{\hat{\Delta}}{2}e^{\imath u\mu t\sigma_x}\sigma_z + \frac{u(\hat{\mu}-\mu)}{2}\sigma_x, \hat{\xi}\right] - K_\rho \mathrm{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z(\hat{\xi}-\xi)\right)$$
$$\ldots \left(e^{\imath u\mu t\sigma_x}\sigma_z\hat{\xi} + \hat{\xi}e^{\imath u\mu t\sigma_x}\sigma_z - 2\mathrm{Tr}\left(e^{\imath u\mu t\sigma_x}\sigma_z\hat{\xi}\right)\hat{\xi}\right)$$

the $u\mu$ frequency oscillatory term, denoted by $\delta_1\hat{\xi}$, comes only from $-\imath\ \left[\frac{\hat{\Delta}}{2}e^{\imath u\mu t\sigma_x}\sigma_z, \hat{\xi}\right]$. Thus

$$\delta_1\hat{\xi} = \frac{\imath\hat{\Delta}}{2u\mu}\left[e^{\imath u\mu t\sigma_x}\sigma_y, \hat{\xi}\right] \quad \text{and} \quad \delta\xi = \delta_1\xi = \frac{\imath\Delta}{2u\mu}\left[e^{\imath u\mu t\sigma_x}\sigma_y, \xi\right]$$

Second order secular approximation (end)

We have the following triangular and locally convergent dynamics:

$$
\begin{aligned}
\frac{d}{dt}\hat{\xi} \overset{\text{order 1}}{=} & -\imath \left[\frac{u(\hat{\mu}-\mu)}{2}\sigma_x, \hat{\xi}\right] \\
& - \frac{K_\rho}{2}\mathrm{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)\left(\sigma_y\hat{\xi}+\hat{\xi}\sigma_y - 2\mathrm{Tr}\left(\sigma_y\hat{\xi}\right)\hat{\xi}\right) \\
& - \frac{K_\rho}{2}\mathrm{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right)\left(\sigma_z\hat{\xi}+\hat{\xi}\sigma_z - 2\mathrm{Tr}\left(\sigma_z\hat{\xi}\right)\hat{\xi}\right) \\
\frac{d}{dt}\hat{\mu} \overset{\text{order 1}}{=} & -\frac{uK_\mu}{2}\left(\mathrm{Tr}\left(\sigma_y\hat{\xi}\right)\mathrm{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right) - \mathrm{Tr}\left(\sigma_z\hat{\xi}\right)\mathrm{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right)\right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}\xi \overset{\text{order 2}}{=} & -\imath\frac{\Delta^2}{2u\mu}[\sigma_x, \xi] \\
\frac{d}{dt}\hat{\Delta} \overset{\text{order 2}}{=} & -\frac{K_\Delta}{\mu}\left(\mathrm{Tr}\left(\sigma_x\hat{\xi}\right)^2\hat{\Delta} - \mathrm{Tr}\left(\sigma_x\hat{\xi}\right)\mathrm{Tr}\left(\sigma_x\xi\right)\Delta\right) \\
& + \frac{K_\Delta\hat{\Delta}}{2\mu}\left(\mathrm{Tr}\left(\sigma_y\hat{\xi}\right)\mathrm{Tr}\left(\sigma_y(\hat{\xi}-\xi)\right) - \mathrm{Tr}\left(\sigma_z\hat{\xi}\right)\mathrm{Tr}\left(\sigma_z(\hat{\xi}-\xi)\right)\right).
\end{aligned}
$$

Gain design via linear tangent approximation

With

$$\hat{\xi} - \xi = \frac{1 + \tilde{x}\sigma_x + \tilde{y}\sigma_y + \tilde{z}\sigma_z}{2}, \quad \tilde{\mu} = \hat{\mu} - \mu, \quad \tilde{\Delta} = \hat{\Delta} - \Delta$$

we have, around $\rho = \frac{1-\sigma_z}{2}$;

$$\frac{d}{dt}\tilde{y} = -u\tilde{\mu} - K_\rho \tilde{y}, \qquad \frac{d}{dt}\tilde{\mu} = uK_\mu \tilde{y}/2$$

and around $\rho = \frac{1-\sigma_x}{2}$

$$\frac{d}{dt}\tilde{\Delta} = -\frac{K_\Delta}{\mu}\tilde{\Delta}.$$

To respect the scaling, choose $0 < \varepsilon \ll 1$ and set

$$K_\rho = 2k_\rho \varepsilon |u| \mu, \quad K_\mu = 2\varepsilon^2 \mu^2, \quad K_\Delta = k_\Delta \varepsilon^2 |u| \mu^2$$

with k_ρ, k_Δ around 1.

N-level system

The system is ($\Delta^{kl} = 0$, no laser de-tuning here)

$$\frac{d}{dt}\rho = -\imath \left[\sum_{kl} \frac{u^{kl}\mu^{kl}}{2}\sigma_x^{kl}, \rho\right], \quad y_k = \mathrm{Tr}\left(P_k \rho\right)$$

with $P_k = |k\rangle\langle k|$ and its asymptotic observer reads:

$$\frac{d}{dt}\hat{\rho} = -\imath \left[\sum_{kl} \frac{u^{kl}\hat{\mu}^{kl}}{2}\sigma_x^{kl}, \hat{\rho}\right] - \sum_k K_\rho^k (\mathrm{Tr}\left(P_k\hat{\rho}\right) - y_k)\ (P_k\hat{\rho} + \hat{\rho}P_k - 2\mathrm{Tr}\left(P_k\hat{\rho}\right)\hat{\rho})$$

$$\frac{d}{dt}\hat{\mu}^{kl} = -\sum_{kl} K_\mu^{kl} \mathrm{Tr}\left(u\sigma_y^{kl}\hat{\rho}\right)\ (\mathrm{Tr}\left(\sigma_z^{kl}\hat{\rho}\right) - y_k + y_l)$$

where $\sigma_x^{kl} = |k\rangle\langle l| + |l\rangle\langle k|, \ldots$
Such extensions are possible since we start with an invariant observer for the 2-level system, i.e. we exploit the geometry.

Previous works

- Identifiability for quantum systems: see, e.g., C. Lebris et al (COCV) where it is shown that resonant controls are sufficiant.
- Asymptotic observers and symmetries: few references (Aghannan, Bonnabel, Martin, R., Dayawansa and coworkers). See the preprint on Symmetry preserving Observers: `http://arxiv.org/abs/math.OC/0612193` IEEE TAC Jan 2009

Measurement process