Quantum Control Robustness Analysis and Robust Control Algorithms

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Outline

Quantum robust control

- A challenge in model-based quantum control is to devise laser control strategies that are robust to parameter uncertainty and input noise

  1. *Input field noise*: noise in spectral amplitudes and phases associated with a frequency domain shaped laser pulse.
  2. *Parameter uncertainty*: uncertainty in the dipole matrix (control vector field) elements

- Approaches to combat noise and uncertainty in model-based quantum control:
  1. **Feedforward control**
  2. **Feedback control?** Feedback currently impossible for ultrafast dynamics.
  3. **Robust control:** $\varepsilon(t) = \varepsilon(\hat{\rho}(t))$ where $\hat{\rho}(t)$ is filtered from real-time measurement data, since $\rho(\hat{\theta}, t) \neq \rho(\theta_0, t)$; robust control: so $\rho(\hat{\theta}, t) \approx \rho(\theta_0, t)$. can exploit rich pulse shaping resources to minimize sensitivity to field and parameter uncertainty.
  4. **First-principles electronic structure theory** combined with efficient parameter estimators based on time-resolved quantum measurement data can reduce parameter uncertainty.

- *Classical vs quantum uncertainty*: input field noise and system parameter uncertainty are classical; the pdfs for observation outcomes given an exactly known wavefunction is quantum. We seek to combat the classical uncertainty.

Estimation of quantum states and Hamiltonians

- **State estimation**. Application: adaptive feedback (open loop) control of multiple output processes. Probabilities of observations $p_k = \mathrm{Tr}(\rho(\theta)|k\rangle\langle k|)$ are *linear* in parameters

$$\rho \equiv \rho(\theta) = \frac{1}{N} I_N + \frac{1}{2}\sum_{j=1}^{N^2-1} \theta_j \lambda_j,$$
$$(\theta_1, ..., \theta_{N^2-1}) \equiv \theta \in B_{N^2-1} \subset R^{N^2-1},$$

  where λ_j are generators of $SU(N)$.

- **Dynamical parameter estimation**. Application: robust control; assessment of worst case control performance for optimal control.

  Challenge: Probabilities of observations are nonlinear in Hamiltonian parameters.

Estimation of quantum Hamiltonians

- Assume H_0 known (from resonant frequencies). Parameterization of μ for Rb:

$$\mu(\theta) = \begin{bmatrix} 0 & \theta_1 & \theta_2 & 0 & 0 \\ \theta_1 & 0 & 0 & \theta_3 & 0 \\ \theta_2 & 0 & 0 & \theta_4 & 0 \\ 0 & \theta_3 & \theta_4 & 0 & \theta_5 \\ 0 & 0 & 0 & \theta_5 & 0 \end{bmatrix}$$

- For a constant field,

$$\rho(\theta, t_k) = \exp[-i(H_0 - \mu(\theta)\varepsilon)t_k]\rho(0)\exp[i(H_0 - \mu(\theta)\varepsilon)t_k]$$

- Unlike spectroscopic experiments used to obtain transition dipole elements for Rb, can be generalized to molecules

Asymptotically Efficient Parameter Estimators: MLE Theory

- *Likelihood function* of parameters: $L(\hat{\theta}|x)$ is joint density of observations x expressed as function of unknown parameter vector $\hat{\theta}$.

- Fisher information: $I(\theta) = -\mathrm{E}\left[\frac{\partial^2 \ln L(\theta|x)}{\partial\theta\partial\theta'}\right]$; $[I(\theta_0)]^{-1}$ is called the *Cramer-Rao lower bound (CRB)* for consistent estimators.

- Maximum likelihood estimator
$$\hat{\theta}_{ML} = \arg\max L(\hat{\theta}|x)$$
is asymptotically efficient estimator, achieves CRB

MLE Results: State Estimation

- Given measurement times $(t_1, \cdots, t_q)$; measure the energy through diagonal observable $H_0 = \sum_{i=1}^{N} E_i |i\rangle\langle i|$ at each time

- The FI can be maximized *prior* to collecting experimental data, so that we collect the most information possible about the state parameters from a given number of measurements
- Achieve by shaping control fields $\varepsilon(t)$: $\max\limits_{\varepsilon(\cdot)} ||\boldsymbol{I}(\hat{\theta})||$
- Applying fields $\varepsilon(t)$ that maximize Fisher information are found to improve the quality of parameter estimates

Optimal State estimation, dynamic

- For Hamiltonian estimation, likelihood function for constant field ε is

$$\ln L(\theta|x) = \sum_{k=1}^{N+1}\sum_{j=1}^{m_k} \ln p_{jk}(\theta)$$
$$= \sum_{k=1}^{N+1}\sum_{j=1}^{m_k} \ln \mathrm{Tr}[\rho(\theta, t_k)F_{i_j}]$$
$$\rho(\theta, t_k) = \exp[-i(H_0 - \mu(\theta)\varepsilon)t_k]\rho(0)\exp[i(H_0 - \mu(\theta)\varepsilon)t_k]$$

where x denotes the data, m_k is the number of observations made at time t_k for a time-independent Hamiltonian (constant control field $\varepsilon(t)$), and $F_i = |i\rangle\langle i|$ is the outcome of the $j - th$ observation.

MLE of atomic Hamiltonian parameters (cont'd)

- Covariance matrix of unknown dipole element parameters:

$$\Sigma = I^{-1}(\hat{\theta})$$

- Due to nonlinearity of likelihood for Hamiltonian estimation, choice of optimal measurement times important: choose the q measurement times or control the unitary propagators by (robust) laser fields to maximize Fisher information:

$$\max_{(t_1,\cdots,t_q)} ||I(\hat{\theta})|| \quad \text{or} \quad \max_{\varepsilon(\cdot)} ||I(\hat{\theta})||$$

  after an initial guess for θ is obtained from the first experiment or electronic structure theory and where

$$p_k(\theta, \varepsilon(\cdot)|F_r) = \mathrm{Tr}\left\{U(\varepsilon(\cdot), t_k, \theta)\rho(0)U^\dagger(\varepsilon(\cdot), t_k, \theta)F_r\right\}$$

- Adaptively update measurements given $\hat{\theta} = \arg\max L(\hat{\theta}|x_i)$, given measurement outcomes x_i from experiment i

Bayesian Estimation of Hamiltonian parameters

- The Hamiltonian identification problem is generally ill-posed - due to nonlinearity of likelihood, there are multiple solutions. Thus $\mu(\theta)$ is not *identifiable* by frequentist inference
- For nonlinear estimation, the parameter uncertainties returned by frequentist methods require the choice of one out of the many $\hat{\theta}$'s that may maximize the likelihood

- An alternative is *Bayesian Hamiltonian estimation*, which is based on the notion of a prior plausibility distribution on the space of parameters θ:

$$p\left(\theta \mid x \wedge I\right) d\theta = \frac{L\left(\theta \mid x\right) p\left(\theta \mid I\right) d\theta}{\int_{\Theta} L\left(\theta \mid x\right) p\left(\theta \mid I\right) d\theta},$$

- **Prospect**: In addition to parametric model, have *ab initio* estimates for parameters!

- *Bayesian Hamiltonian estimation* can a) use electronic structure calculations along with experimental data in constructing parameter estimates $\hat{\theta}$; b) render problem identifiable

Estimation of field noise

- Linear frequency domain analysis is common approach to robust controller design in engineering

- *Wiener-Khinchin Theorem*: a) Fourier transform of autocorrelation function gives noise power spectrum

$$|F(\omega)| = \int_0^\infty \exp(i\omega\tau)\mathrm{acf}(t, t+\tau)\ d\tau,$$

  where $|F(\omega)|$ denotes the power spectral density, τ is lag, and $f(t,t') \equiv \mathrm{acf}\ (t,t') \equiv \mathrm{E}[\delta u(t)\delta u(t+\tau)]$ is the noise autocorrelation function for a stationary, mean-zero noise process $\delta u(t)$

- For linear control systems, power spectrum can be used to assess robustness; for bilinear systems, must work directly in time-domain: sample field at different time lags τ to estimate acf or obtain from laser's known noise spectrum - if given noise power spectrum for a laser source, use W-K theorem to obtain autocorrelation function

Outline

Perturbation theory and the Dyson expansion

- The exact expression for the transition amplitude is $c_{ji}(t) = \langle j|U_I(t)|i\rangle$; if initial state is $|i\rangle$, $c_{ji}(t) = c_j(t)$
- To approximate it to arbitrary order, insert perturbation expansion for $U_I(t)$:

$$c_{ji}^1(t) = -\langle j|\lambda \frac{i}{\hbar} \int_0^t H_I(t')\ dt'|i\rangle$$

$$\vdots$$

$$c_{ji}^n(t) = \langle j|(-\lambda \frac{i}{\hbar})^n \int_0^t \cdots \int_0^{t^n-1} H_I(t') \cdots H_I(t^n)\ dt^n \cdots dt'|i\rangle$$

- Then, the total transition probability between states i and j at time t in n-th order perturbation theory is

$$|c_{ji}^1(t) + c_{ji}^2(t) + \cdots + c_{ji}^n(t)|^2 = \left[c_{ji}^1(t) + c_{ji}^2(t) + \cdots + c_{ji}^n(t)\right]^* \times \left[c_{ji}^1(t) + c_{ji}^2(t) + \cdots + c_{ji}^n(t)\right]$$

(which demonstrates the property of *quantum interference between paths* due to the presence of coherence terms $(c_{ji}^x(t))^* c_{ji}^y(t)$)

- For bilinear systems, we can identify the contributions of each order in the Dyson series to the controlled time evolution by system-encoding and Fourier transform-based techniques. Let $V_I(t,s) = V_I(t)\exp(\imath\gamma s)$ for a specified parameter γ
- Operationally speaking we need to solve the Schrödinger equation:

$$\frac{dU_I(t,s)}{dt} = -iV_I(t,s)U_I(t,s) \tag{1}$$

- Deconvolute via inverse FT to obtain $U_I(T)$:

$$U_{fi}(T,\gamma) = \int_{-\infty}^{\infty} U_{ji}(T,s)\exp(-i\gamma s)\ ds$$

- The contribution of each m-th order pathway U_{ji}^m to the mechanism is obtained from $U_{fi}(\gamma)$; each pathway's contribution is encoded by a particular value of γ
- **Show some examples**

$$U_{ji}(T,\gamma=\gamma_0) = c_{ji}^1(T)$$
$$U_{ji}(T,\gamma=2\gamma_0) = c_{ji}^2(T)$$

MI of interferences

- $$c_{ji}^2 * c_{ji}^1 + c_{ji}^{1*} c_{ji}^2 = \langle j|U|i\rangle^{2*} \langle j|U|i\rangle^1 + \langle j|U|i\rangle^{1*} \langle j|U|i\rangle^2$$
- *Constructive interference:* $c_{ji}^2 * c_{ji}^1 + c_{ji}^{1*} c_{ji}^2 = 2\mathrm{Re}\left(c_{ji}^2 * c_{ji}^1\right) > 0$
- *Destructive interference:* $c_{ji}^2 * c_{ji}^1 + c_{ji}^{1*} c_{ji}^2 = 2\mathrm{Re}\left(c_{ji}^2 * c_{ji}^1\right) < 0$
- Obtain c_{ji}^1, c_{ji}^2's (with sums over all intermediate states) using the mechanism id transform techniques above
- Interferences between specific pathways can also be identified, using other mechanism id techniques reviewed below

Transition pathways for frequency domain-shaped fields: complex representation of field

- Now use the Fourier series representation of the field: $\varepsilon(t) = \int_{-\infty}^{\infty} d\omega\ A(\omega)\exp(i\phi(\omega))\exp(-i\omega t)$ and $H_I(t) = \exp(\frac{i}{\hbar}H_0 t)[-\mu\cdot\varepsilon(t)]\exp(-\frac{i}{\hbar}H_0 t)$
- $\langle j|\int_0^t H_I(t)\ dt|i\rangle = -\int_0^t \varepsilon(t)\langle j|\exp(\frac{i}{\hbar}H_0 t)\mu\exp(-\frac{i}{\hbar}H_0 t)|i\rangle\ dt$

$$
\begin{aligned}
c_{ji}^1(t) &= \frac{i}{\hbar}\langle j|\mu|i\rangle\int_0^t \varepsilon(t)\exp(\frac{i}{\hbar}(E_j - E_i)t)dt \\
&= \frac{i}{\hbar}\langle j|\mu|i\rangle\int_{-\infty}^{\infty} d\omega\ A(\omega)\exp(i\phi(\omega))\int_0^t \exp((\frac{i}{\hbar}(E_j - E_i) - i\omega)t)dt
\end{aligned}
$$

Transition amplitudes for frequency-domain shaped fields: one-photon path

$$\langle j|\exp(\imath H_0 t)\varepsilon(t)\mu\exp(-\imath H_0 t)|i\rangle = \langle j|\mu|i\rangle \sum_{k=1}^{m} A(\omega_k)\exp[\imath(E_j - E_i)t]\cos(\omega_j t + \phi(\omega_k))$$

- $$\int_0^T \exp[\imath(E_j - E_i)t]\cos(\omega_k t + \phi(\omega_k))\ dt = \frac{1}{2}\left\{\exp(\imath\phi_k)\int_0^T \exp\left[\imath(E_j - E_i + \omega_k)t\right]\ dt + \right. \left. + \exp(-\imath\phi_k)\int_0^T \exp\left[\imath(E_j - E_i - \omega_k)t\right]\ dt\right\}$$

$$c_{ji}^1(T) = \imath\langle j|\mu|i\rangle \sum_{k=1}^{n} A(\omega_k)\int_0^T \exp[\imath(E_j - E_i)t]\cos(\omega_k t + \phi(\omega_k))\ dt$$

$$= \frac{\imath}{2}\langle j|\mu|i\rangle \sum_{k=1}^{n} A(\omega_k)\{\exp(\imath\phi_k)\int_0^T \exp\left[\imath(E_j - E_i + \omega_k)t\right]\ dt + + \exp(-\imath\phi_k)\int_0^T \exp\left[\imath(E_j - E_i - \omega_k)t\right]\ dt\}$$

Dyson expansion of transition amplitude for frequency-domain shaped fields

$$\langle j|\exp(\imath H_0 t)\varepsilon(t)\mu\exp(-\imath H_0 t)|i\rangle = \langle j|\mu|i\rangle \sum_{k=1}^{n} A(\omega_k)\exp[\imath(E_j - E_i)t]\cos(\omega_k t + \phi(\omega_k))$$

- $$c_{ji}(T) = \sum_{m=1}^{\infty}(\imath)^m \sum_{l_1=1}^{N}\cdots\sum_{l_{m-1}=1}^{N}\langle j|\mu|l_{m-1}\rangle\langle l_{m-1}|\mu|l_{m-2}\rangle\cdots\langle l_1|\mu|i\rangle\times$$
$$\int_0^T \sum_{k_m=1}^{n} A(\omega_{k_m})\exp[\imath(E_j - E_{l_{m-1}})t_m]\cos(\omega_{k_m}t_m + \phi(\omega_{k_m}))\cdots$$
$$\cdots\int_0^{t_2}\sum_{k_1=1}^{n} A(\omega_{k_1})\exp[\imath(E_{l_1} - E_i)t_1]\cos(\omega_{k_1}t_1 + \phi(\omega_{k_1}))\; dt_1\cdots dt_m$$

- For bilinear systems, we can identify the contributions of each pathway to the controlled time evolution by system-encoding and Fourier transform-based techniques
- The elements $v_{jk}(t)$ of the interaction picture Hamiltonian $V_I(t)$ are multiplied by modulation functions $g_{jk} = \exp(i\gamma_{jk}s)$ to encode the dynamics and enable the extraction of pathway contributions. With the modulation, the modulated Schrödinger equation for a N-dimensional system is:

$$\frac{dU_I(t,s)}{dt} = -i \begin{pmatrix} v_{11}(t)g_{11}(s) & v_{12}(t)g_{12}(s) & \cdots & v_{1N}(t)g_{1N}(s) \\ v_{21}(t)g_{21}(s) & v_{22}(t)g_{22}(s) & \cdots & v_{2N}(t)g_{2N}(s) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ v_{N1}(t)g_{N1}(s) & v_{N2}(t)g_{N2}(s) & \cdots & v_{NN}(t)g_{NN}(s) \end{pmatrix} U_I(t,s), \quad (2)$$

due to which the modulated matrix elements of the interaction propagator become

$$U_{fi}(T,s) = \sum_{l_1,\cdots,l_{m-1}} U_{fi}^{l_1,\cdots,l_{m-1}}(T) \exp\left(\imath(\gamma_{fl_{m-1}} + \cdots + \gamma_{l_1 i})s\right), \quad (3)$$

where the unmodulated pathway $U_{fi}^{l_1,\cdots,l_{m-1}}(t)$ is given as

$$U_{fi}^{l_1,\cdots,l_{m-1}}(T) = (\imath)^m \int_0^T \cdots \int_0^{t_2} \langle f|V_I(t_m)|l_{m-1}\rangle \cdots \langle l_1|V_I(t_1)|i\rangle dt_1 \cdots dt_m \quad (4)$$

Dipole encoding and decoding

- *Dipole encoding* would reveal the contribution of the dipole moments in the transition amplitude. Here, each of the dipole matrix elements is encoded with a Fourier function:

$$\mu_{pq} \to \mu_{pq} e^{\imath \gamma_{pq} s},$$
$$\mu_{pq}^{\alpha_{pq}} \to \mu_{pq}^{\alpha_{pq}} e^{\imath (\alpha_{pq} \gamma_{pq}) s}, \tag{5}$$

  with $\gamma_{qp} = \gamma_{pq}$.
- The encoded and propagated unitary propagator consists of the different order dipole pathways with the encoded total transition amplitude:

$$U_{ji}(T, s) = \sum_{m=0}^{\infty} \sum_{\vec{\alpha} \in \mathcal{M}} U_{ji}(T, \vec{\alpha}) e^{i \left(\sum_{p<q} \alpha_{pq} \gamma_{pq} \right) s}. \tag{6}$$

- Deconvolution of the total transition amplitude leads to the decoded dipole pathway, i.e. $U_{ji}(T, \gamma = \sum_{p<q} \alpha_{pq} \gamma_{pq}) \to U_{ji}(T, \vec{\alpha})$.

- Modulation scheme:

$$A_k \triangleq A(\omega_k) \to A(\omega_k)\exp(\imath\gamma_k s)$$
$$A^\alpha(\omega_k) \to A^\alpha(\omega_k)\exp(\imath\alpha\gamma_k s)$$

- The m-th order MI amplitude is comprised of terms of the following type:

$$(\imath^m)A(\omega_{k_1})A(\omega_{k_2})\cdots A(\omega_{k_m})\exp[\imath(\gamma_{k_1}+\cdots+\gamma_{k_m})s]\times$$
$$\times \sum_{l_1=1}^{N}\cdots\sum_{l_{m-1}=1}^{N}\langle j|\mu|l^{m-1}\rangle\langle l^{m-1}|\mu|l^{m-2}\rangle\cdots\langle l^1|\mu|i\rangle\times$$
$$\times\int_0^T \exp[\imath(E_j - E_{l_{m-1}})t_m]\cos(\omega_{k_m}t_m + \phi(\omega_{k_m}))\times$$
$$\times\int_0^{t_m} \exp[\imath(E_j - E_{l_{m-2}})t_{m-1}]\cos(\omega_{k_{m-1}}t_{m-1} + \phi(\omega_{k_m}))\cdots$$
$$\cdots\int_0^{t_1} \exp[\imath(E_j - E_{l_1})t_1]\cos(\omega_{k_1}t_1 + \phi(\omega_{k_1}))\ dt_1\cdots dt_{m-1}$$

- *Deconvolution*: $U_{ji}(T,\gamma) = \int_{-\infty}^{\infty} U_{ji}(T,s)\exp(-\imath\gamma s)\ ds$
- The above term can be extracted at frequency $\gamma_{k_1}+\cdots+\gamma_{k_m}$ if this frequency is unique:

$$U_{ji}(T,\gamma=\gamma_{k_1}+\cdots+\gamma_{k_m}) = (\imath^m)A(\omega_{k_1})A(\omega_{k_2})\cdots A(\omega_{k_m})\cdots$$

- Extract all terms containing $A_1^{\alpha_1}\cdots A_n^{\alpha_n}$, $\sum_i \alpha_i = m$, through amplitude $U_{ji}(T,\gamma=\alpha_1\gamma_1+\cdots+\alpha_n\gamma_n)$

- Modulation scheme:

$$\frac{1}{2}\sum_{k=1}^{n} A(\omega_k)\{\exp(\imath\phi_k)\exp(\imath\omega_k t) + \exp(-\imath\phi_k)\exp(-\imath\omega_k t)\} \rightarrow$$

$$\rightarrow \frac{1}{2}\sum_{k=1}^{n} A(\omega_k)\{\exp(\imath(\phi_k+\gamma_k))\exp(\imath\omega_k t) + \exp(-(\imath\phi_k+\gamma_k))\exp(-\imath\omega_k t)\}$$

- *Deconvolution:*

$$U_{ji}(T,\gamma) = \int_{-\infty}^{\infty} U_{ji}(T,s)\exp(-\imath\gamma s)\ ds$$

$$U_{ji}(T,\gamma=2\gamma_k) = -A^2(\omega_k)\exp(2\imath\phi_k)\left[\sum_l \langle j|\mu|l\rangle\langle l|\mu|i\rangle \int_0^T \cdots \int_0^t \cdots dt'\,dt\right]$$

$$U_{ji}(T,\gamma=-2\gamma_k) = -A^2(\omega_k)\exp(-2\imath\phi_k)\left[\sum_l \langle j|\mu|l\rangle\langle l|\mu|i\rangle \int_0^T \cdots \int_0^t \cdots dt'\,dt\right]$$

- For *phase encoding*, the modulation scheme is as follows:

$$e^{\pm\imath\phi_k} \to e^{\pm\imath(\phi_k+\gamma_k s)},$$
$$e^{\imath\alpha_k\phi_k} \to e^{\imath\alpha_k(\phi_k+\gamma_k s)}, \tag{7}$$

- The encoded transition amplitude is:

$$U_{ji}(T,s) = \sum_{\vec{\alpha}} \exp\left[\imath \sum_{k=1}^{K} \alpha_k\left(\phi_k+\gamma_k s\right)\right] \times$$
$$\sum_{m=m_{\min}}^{\infty} \left(\frac{\imath}{2\hbar}\right)^m \sum_{(k_1,\cdots,k_m)} \prod_{k=1}^{K} A_k^{b_k(k_1,\cdots,k_m)} \times$$
$$\sum_{l_{m-1}}^{N} \mu_{jl_{m-1}} \int_0^T e^{\imath(\omega_{jl_{m-1}}+\omega_{k_m})t_m} \cdots \times$$
$$\cdots \times \sum_{l_1=1}^{N} \mu_{l_1 i} \int_0^{t_2} e^{\imath(\omega_{l_1 i}+\omega_{k_1})t_1}\, dt_1 \cdots dt_m \tag{8}$$

where $m_{\min}$, b_k have been defined in (10).
$U_{ji}(T,s) = \sum_{\vec{\alpha}\in\mathbb{Z}^K} U_{ji}(T,\vec{\alpha}) \exp\left(\imath \sum_{k=1}^{K} \alpha_k\gamma_k s\right)$ along with (7) and (**??**) can therefore be used to define phase pathways $U_{ji}(T,\vec{\alpha})$.
- Deconvolution of the transition amplitude term yields *phase pathways* in a way analogous to the amplitude counterpart. Note that in the case of phase modulation, the encoding is H...

Outline

Converting moments of transition amplitudes into moments of observable expectation values

- Can obtain moments for expectation value of any quantum observable (including P_{ji} for any states j, i) given the moments of all transition amplitudes

Expression for amplitude pathways

$$U_{ji}^m(T) = \left(\frac{\imath}{\hbar}\right)^m \sum_{\vec{\alpha}\in\mathcal{M}} \prod_{k=1}^{K} A_k^{\alpha_k} \times$$

$$\sum_{(k_1,\cdots,k_m)} \sum_{l_{m-1}}^{N} \mu_{jl_{m-1}} \int_0^T e^{i(\omega_{jl_{m-1}} t_m)} \cos(\omega_{k_m} t_m + \phi(\omega_{k_m}))\times$$

$$\cdots \times \sum_{l_1}^{N} \mu_{l_1 1} \int_0^{t_2} e^{i(\omega_{l_1 i} t_1)} \cos(\omega_{k_1} t_1 + \phi(\omega_{k_1}))\; dt_1 \cdots dt_m$$

where the sum $\sum_{(k_1,\cdots,k_m)}$ is over all $1 \le k_i \le K,\;\; i = 1,\cdots,m$ such that mode k appears in the multiple integral α_k times.

- Denote by $c^m_{\alpha_1,\cdots,\alpha_n}$ the m-th order MI amplitude at frequency $\alpha_1\gamma_1+\cdots+\alpha_n\gamma_n$ divided by the product of field amplitudes appearing in that expression:

$$c^m_{\alpha_1,\cdots,\alpha_n} = U_{ji}(T,\gamma=\alpha_1\gamma_1+\cdots+\alpha_n\gamma_n)/(A_1^{\alpha_1}\cdots A_n^{\alpha_n})$$
$$\sum_i \alpha_i = m.$$

  We denote by $c_{\alpha_1,\cdots,\alpha_n}$ the analogous expression without the constraint on the α_i (i.e., without specification of the order of the amplitude).
- This MI amplitude is a sum of

$$\begin{pmatrix} & m & \\ \alpha_1 & \cdots & \alpha_n \end{pmatrix}$$

  distinct terms.

- Assuming $A_1, \cdots, A_n$ are independent random variables, $\mathrm{E}[c_{ji}(T)]$ can then be expressed as follows (written respectively for $\mathrm{Re}\ c_{ji}(T)$, $\mathrm{Im}\ c_{ji}(T)$):

$$\mathrm{E}[\mathrm{Re}, \mathrm{Im}\ c_{ji}(T)] = \sum_{(\alpha_1, \cdots, \alpha_n)} \mathrm{Re}, \mathrm{Im}\ c_{\alpha_1, \cdots, \alpha_n} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}]$$

- $\mathrm{var}\ c_{ji}(T)$ can be expressed:

$$\mathrm{var}\ (\mathrm{Re}, \mathrm{Im}\ c_{ji}(T)) = \mathrm{E}\left[\left\{\sum_{(\alpha_1, \cdots, \alpha_n)} \mathrm{Re}, \mathrm{Im}\ c_{\alpha_1, \cdots, \alpha_n} \left(A_1^{\alpha_1} \cdots A_n^{\alpha_n} - \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}]\right)\right\}^2\right]$$

$$= \sum_{(\alpha_1, \cdots, \alpha_n) \neq (\alpha'_1, \cdots, \alpha'_n)} \Big\{ 2\mathrm{Re}, \mathrm{Im}\ c_{\alpha_1, \cdots, \alpha_n} c_{\alpha'_1, \cdots, \alpha'_n} \times$$

$$\times \left(\mathrm{E}[A_1^{\alpha_1 + \alpha'_1}] \cdots \mathrm{E}[A_n^{\alpha_n + \alpha'_n}] - \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}] \mathrm{E}[A_1^{\alpha'_1}] \cdots \mathrm{E}[A_n^{\alpha'_n}]\right) \Big\} +$$

$$+ \sum_{(\alpha_1, \cdots, \alpha_n)} \mathrm{Re}, \mathrm{Im}\ c^2_{\alpha_1, \cdots, \alpha_n} \left(\mathrm{E}[A_1^{2\alpha_1}] \cdots \mathrm{E}[A_n^{2\alpha_n}] - \mathrm{E}^2[A_1^{\alpha_1}] \cdots \mathrm{E}^2[A_n^{\alpha_n}]\right)$$

- The above sums can be truncated to obtain approximations for the moments of the transition amplitude. An upper bound on the error in the moment calculations due to omission of terms in the sum with $\sum_i \alpha_i > m_{\max}$ will be provided

var U_{ji} (cont'd)

$$|\mathrm{var}\ (c_{ji}(T))\,|^2 = \sum_{(\alpha_1',\cdots,\alpha_n')<(\alpha_1,\cdots,\alpha_n)} 2\mathrm{Re}\ \left(c_{\alpha_1,\cdots,\alpha_n} c^*_{\alpha_1',\cdots,\alpha_n'}\right)\ \times\ \mathrm{E}[A_1^{\alpha_1+\alpha_1'}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha_n'}]+$$
$$+\sum_{(\alpha_1,\cdots,\alpha_n)} |c_{\alpha_1,\cdots,\alpha_n}|^2\mathrm{E}[A_1^{2\alpha_1}]\cdots\mathrm{E}[A_n^{2\alpha_n}]+$$
$$-\sum_{(\alpha_1',\cdots,\alpha_n')<(\alpha_1,\cdots,\alpha_n)} 2\mathrm{Re}\ \left(c_{\alpha_1,\cdots,\alpha_n} c^*_{\alpha_1',\cdots,\alpha_n'}\right)\ \times\ \mathrm{E}[A_1^{\alpha_1}]\cdots\mathrm{E}[A_n^{\alpha_n}]\mathrm{E}[A_1^{\alpha_1'}]\cdots$$
$$-\sum_{(\alpha_1,\cdots,\alpha_n)} |c_{\alpha_1,\cdots,\alpha_n}|^2\mathrm{E}^2[A_1^{\alpha_1}]\cdots\mathrm{E}^2[A_n^{\alpha_n}]$$

- See RC notes 11/2013 for $\mathrm{E}[P_{ji}]$
- Note the similarity between the $\mathrm{var}\ U_{ji}$ and $\mathrm{E}\ [P_{ji}]$ expressions
- Expressions were originally written separately in terms of real, imaginary parts to simplify coding of both simultaneously, since $\mathrm{var}\ U_{ji}$ must be separated into real and imaginary parts
- $|\mathrm{var}\ U_{ji}|^2$ can be written in a form similar to $\mathrm{E}\ [P_{ji}]$:
- (This form of the expression for P_{ji} was previously provided in RC's quantum pathway interference notes)
- $\mathrm{var}\ U_{ji}$ is the second classical moment of a quantum transition amplitude; $\mathrm{E}\ [P_{ji}]$ is the first classical moment of a quantum expectation
- $|\mathrm{var}\ U_{ji}|^2$ has applications to quantum gate control; consider Pareto minimization $\mathrm{var}\ \mathrm{Re}\ U_{ji}$ / maximization of $|\mathrm{E}\ [U_{ji}]|^2$ (or simply $\mathrm{E}\ [\mathrm{Re}\ U_{ji}]$) toward the maximum value of 1 (assuming that is the target value of a quantum gate matrix element)
- Allows interpretation of Pareto tradeoffs in terms of interference moments

- First moment of transition probability:

$$\mathrm{E}\left[P_{ji}(T)\right] = \mathrm{E}\left[\left(\mathrm{Re}\ c_{ji}(T)\right)^2\right] + \mathrm{E}\left[\left(\mathrm{Im}\ c_{ji}(T)\right)^2\right]$$

- which is comprised of the following terms:

$$\mathrm{E}\left[\left(\mathrm{Re},\mathrm{Im}\ c_{ji}(T)\right)^2\right] = \mathrm{E}\left[\left\{\sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n} A_1^{\alpha_1}\cdots A_n^{\alpha_n}\right\}^2\right]$$

$$= \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha_1',\cdots,\alpha_n')} 2\mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n} c_{\alpha_1',\cdots,\alpha_n'}\ \mathrm{E}[A_1^{\alpha_1+\alpha_1'}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha_n'}] +$$

$$\sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c^2_{\alpha_1,\cdots,\alpha_n}\mathrm{E}[A_1^{2\alpha_1}]\cdots\mathrm{E}[A_n^{2\alpha_n}]$$

$$
\begin{aligned}
\mathrm{var}\ P_{ji} &= \mathrm{E}\Bigg[\left(\left(\sum_{\alpha}|U_{ji}^{\alpha}|^2 + 2\sum_{\alpha'<\alpha}\mathrm{Re}\,(U_{ji}^{\alpha}U_{ji}^{\alpha'*})\right) - \mathrm{E}\,[P_{ji}]\right) * \\
&\quad * \left(\left(\sum_{\alpha''}|U_{ji}^{\alpha''}|^2 + 2\sum_{\alpha'''<\alpha''}\mathrm{Re}\,(U_{ji}^{\alpha''}U_{ji}^{\alpha'''*})\right) - \mathrm{E}\,[P_{ji}]\right)\Bigg] \\
&= \mathrm{E}\Bigg[\left(\sum_{\alpha}|U_{ji}^{\alpha}|^2 + 2\sum_{\alpha'<\alpha}\mathrm{Re}\,(U_{ji}^{\alpha}U_{ji}^{\alpha'*})\right) * \\
&\quad * \left(\sum_{\alpha''}|U_{ji}^{\alpha''}|^2 + 2\sum_{\alpha'''<\alpha''}\mathrm{Re}\,(U_{ji}^{\alpha''}U_{ji}^{\alpha'''*})\right)\Bigg] - \mathrm{E}^2\,[P_{ji}]
\end{aligned}
$$

$$\text{var } P_{ji} = \mathrm{E}\left[\sum_{\alpha''}\sum_{\alpha}|U_{ji}^{\alpha}|^2|U_{ji}^{\alpha''}|^2\right] + \\ + 4\mathrm{E}\left[\sum_{\alpha'''<\alpha''}\sum_{\alpha}|U_{ji}^{\alpha}|^2\mathrm{Re}\left(U_{ji}^{\alpha''}U_{ji}^{\alpha'''*}\right)\right] + \\ + 4\mathrm{E}\left[\sum_{\alpha'''<\alpha''}\sum_{\alpha'<\alpha}\mathrm{Re}\left(U_{ji}^{\alpha}U_{ji}^{\alpha'*}\right)\mathrm{Re}\left(U_{ji}^{\alpha''}U_{ji}^{\alpha'''*}\right)\right] + \\ - \mathrm{E}^2[P_{ji}]$$

$$
\begin{aligned}
\mathrm{var}\ P_{ji} = & \sum_{\alpha''}\sum_{\alpha} \mathrm{E}\left[\prod_k A_k^{2(\alpha_k+\alpha''_k)}\right] |c_{ji}^{\alpha}|^2 |c_{ji}^{\alpha''}|^2 + \\
& + 4 \sum_{\alpha'''<\alpha''}\sum_{\alpha} \mathrm{E}\left[\prod_k A_k^{2\alpha_k+\alpha''_k+\alpha'''_k}\right] |c_{ji}^{\alpha}|^2 \mathrm{Re}\ \left(c_{ji}^{\alpha''} c_{ji}^{\alpha'''}*\right) + \\
& + 4 \sum_{\alpha'''<\alpha''}\sum_{\alpha'<\alpha} \mathrm{E}\left[\prod_k A_k^{\alpha_k+\alpha'_k+\alpha''_k+\alpha'''_k}\right] \mathrm{Re}\left(c_{ji}^{\alpha} c_{ji}^{\alpha'}*\right) \mathrm{Re}\left(c_{ji}^{\alpha''} c_{ji}^{\alpha'''}*\right) + \\
& - \mathrm{E}^2[P_{ji}]
\end{aligned}
$$

var P_{ji} (cont'd)

- The first term above captures (classical) correlations between single pathway transition probabilities
- The second term above captures (classical) correlations between single pathway transition probabilities and interferences
- The third term captures (classical) correlations between interferences

- First moment of interference between all pathways of order m and order m':

$$\mathrm{E}[U_{ji}^{m} U_{ji}^{m' *} + U_{ji}^{m*} U_{ji}^{m'}] = E[2\mathrm{Re}\; U_j i^{m} U_j i^{m' *}]$$
$$= E[2\mathrm{Re} \left(\sum_{(\alpha_1,\cdots,\alpha_n)} c_{\alpha_1,\cdots,\alpha_n} A_1^{\alpha_1} ... A_n^{\alpha_n} \right) \left(\sum_{(\alpha_1',\cdots,\alpha_n')} c^*_{\alpha_1',\cdots,\alpha_n'} A_1^{\alpha_1'} ... A_n^{\alpha_n'} \right)]$$
$$= \sum_{(\alpha_1,\cdots,\alpha_n),\; (\alpha_1',\cdots,\alpha_n')} 2\mathrm{Re} c_{\alpha_1,\cdots,\alpha_n} c^*_{\alpha_1',\cdots,\alpha_n'} \; E[A_1^{\alpha_1+\alpha_1'}] .... E[A_n^{\alpha_n+\alpha_n'}]$$

where $\sum_{\alpha_k} = m, \;\; \sum_{\alpha_k'} = m'$.

- This expression will be the basis for the plot of 1st moment of interferences expected below
- We expect the expression and corresponding plots to help explain the downstream figures representing the robust vs. non-robust interference pattern

- Assume $A(\omega_k) \sim \mathcal{N}(\bar{A}_k, \sigma_k^2)$
- Then we have

$$\mathrm{E}[A] = \bar{A}$$
$$\mathrm{E}[A^2] = \sigma^2 + \bar{A}^2$$

and

$$\mathrm{E}[A^\alpha] = \mathrm{E}[(A-\bar{A})^\alpha] - \sum_{i=0}^{n} \begin{pmatrix} & \alpha & \\ i & & (\alpha - i) \end{pmatrix} \mathrm{E}[A^i](-\bar{A})^{(n-i)}$$

where the coefficients are binomial coefficients,

$$\mathrm{E}[(A-\bar{A})^\alpha] = \begin{cases} 0, & \alpha \text{ odd} \\ (\alpha-1)\sigma^\alpha, & \alpha \text{ even} \end{cases}$$

and the $\mathrm{E}[A^i]$ can be obtained recursively using the above expression starting with $i = 3$.

Expression for dipole pathways

$$U_{ji}^m(T) = \left(\frac{\imath}{\hbar}\right)^m \sum_{\vec{\alpha}\in\mathcal{M}} \prod_{p=1,q>p}^{N-1} \mu_{pq}^{\alpha_{pq}} \times$$

$$\sum_{(l_1,\cdots,l_{m-1})} \sum_{k_m=1}^{K} A_{k_m} \int_0^T e^{i(\omega_{jl_{m-1}} t_m)} \cos(\omega_{k_m} t_m + \phi(\omega_{k_m}))\times$$

$$\cdots \times \sum_{k_1=1}^{K} A_{k_1} \int_0^{t_2} e^{i(\omega_{l_1 i} t_1)} \cos(\omega_{k_1} t_1 + \phi(\omega_{k_1}))\ dt_1 \cdots dt_m$$

where the sum $\sum_{(l_1,\cdots,l_{m-1})}$ is over all $1 \le l_i \le N,\ i = 1,\cdots,m-1$ such that frequency $\pm\omega_{pq}$ corresponding to dipole parameters μ_{pq}, μ_{qp} appears in the multiple integral α_{pq} times.

- For simplicity, assume all elements of the dipole operator μ are real and the diagonal elements are all zero, so that μ is parameterized by $\frac{N^2-N}{2}$ parameters.
- The vector of these parameters can be denoted $\vec{\theta} = [\mu_{12}, \cdots, \mu_{(N-1)N}]^T$.
- Now let $U_{ji}(T, \alpha_1, \cdots, \alpha_{\frac{N^2-N}{2}})$ be the sum of all terms in expression (..) for the transition amplitude that contain $\mu_{12}^{\alpha_1}, \cdots, \mu_{(N-1)N}^{\alpha_{\frac{N^2-N}{2}}}$.
- Then

$$c_{\alpha_1, \cdots, \alpha_{\frac{N^2-N}{2}}} = \frac{U_{ji}(T, \alpha_1, \cdots, \alpha_{\frac{N^2-N}{2}})}{(\mu_{12}^{\alpha_1} \cdots \mu_{(N-1)N}^{\alpha_{\frac{N^2-N}{2}}})} \tag{9}$$

  and the expressions for $\mathrm{E}[c_{ji}]$ and $\mathrm{var}\ c_{ji}$ are identical to those for amplitude noise, with $\mathrm{E}[A_i^{\alpha_i}]$ replaced by $\mathrm{E}[\theta_i^{\alpha_i}]$
- In the encoding, it is necessary to set $\gamma_{ji} = \gamma_{ij}$ in order to have $U_{ji}(T, \gamma = \alpha\gamma_1 + \cdots + \alpha_{\frac{N^2-N}{2}}\gamma_{\frac{N^2-N}{2}}) = U_{ji}(T, \alpha_1, \cdots, \alpha_{\frac{N^2-N}{2}})$ as required, because the corresponding dipole parameters are equal due to Hermiticity (under the assumption above of a real dipole)

Moments of $c_{ji}(T)$ - Hamiltonian uncertainty

- See above

Gaussian Hamiltonian uncertainty (e.g., ML estimation)

- Let $\theta_k \sim \mathcal{N}(\bar{\theta}_k, \sigma_k^2)$ (see above)

$$U_{ji}(T,\vec{\alpha}) = \exp\left(\imath\sum_{k=1}^{K}\alpha_k\phi_k\right)\sum_{m=m_{\min}}^{\infty}\left(\frac{\imath}{2\hbar}\right)^m \times$$
$$\sum_{(k_1,\cdots,k_m)}\prod_{k=1}^{K}A_k^{b_k(k_1,\cdots,k_m)}\sum_{l_{m-1}}^{N}\mu_{jl_{m-1}}\int_0^T e^{\imath(\omega_{jl_{m-1}}+\omega_{k_m})t_m}\times$$
$$\cdots\times\sum_{l_1=1}^{N}\mu_{l_1 i}\int_0^{t_2}e^{\imath(\omega_{l_1 i}+\omega_{k_1})t_1}\,dt_1\cdots dt_m \tag{10}$$

where $\vec{\alpha}\in\mathbb{Z}^K$, $1\leq|k_i|\leq K$, $\omega_{-k_i}=-\omega_{k_i}$, $b_k(k_1,\cdots,k_m)$ denotes the number of times mode k appears in the multiple integral, and $m_{\min}=\sum_{k=1}^{K}|\alpha_k|$. Note that a particular combination of phases in a phase pathway does not uniquely specify the pathway order, unlike amplitude and dipole pathways.

Moments of $c_{ji}(T)$ - phase noise

- In progress

Gaussian phase noise

-

General noise and uncertainty distributions

- Expressions above for $\mathrm{E}[c_{ji}]$, $\mathrm{var}\ c_{ji}$ require expressions for higher moments of noisy/uncertain manipulated input and system parameters like A_k, μ_{ij}
- Higher moments can be provided in closed form for any uncertainty distribution for which there exists an analytical Fourier transform
- Apply the characteristic (moment-generating) function $\phi(s)$ of the probability distribution function $p(x)$ of the manipulated input or system parameter:

$$\phi(s) = \langle \exp(\imath s x) \rangle = \int_{-\infty}^{\infty} p(x) \exp(\imath s x)\ dx$$

- If $\phi(s)$ is available in closed form, the moments of x are obtained via

$$\langle x^n \rangle = (-\imath)^n \left[\frac{\partial^n}{\partial s^n} \phi(s) \right]_{s=0}$$

Example: Gaussian noise distribution

- Consider Gaussian noise: i.e., $p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{(x-\mu)^2}{2\sigma^2}\right]$
- Then

$$\phi(s) = \int_{-\infty}^{\infty} p(x) \exp(\imath sx)\ dx = \exp\left(\imath\mu s - \frac{\sigma^2 s^2}{2}\right)$$

- Moments:

$$\langle x^n \rangle (-\imath)^n \left[\frac{\partial^n}{\partial s^n} \exp\left(\imath\mu s - \frac{\sigma^2 s^2}{2}\right)\right]_{s=0}$$

- Examples:

$$\begin{aligned} \langle x^3 \rangle &= 3\mu\sigma^2 + \mu^3 \\ \langle x^4 \rangle &= 3\sigma^4 + 6\mu^2\sigma^2 + \mu^4 \end{aligned}$$

- Applying the binomial expansion, we obtain any moment $\langle (x - \bar{x})^n \rangle$ via

$$\langle (x - \bar{x})^n \rangle = \langle x^n \rangle - \sum_{i=0}^{n} \begin{pmatrix} & n & \\ i & & (n-i) \end{pmatrix} \langle x^i \rangle (-\mu)^{n-i}$$

- For any odd moment, we find

$$\langle x^n \rangle = \sum_{i=0}^{n} \begin{pmatrix} & n & \\ i & & (n-i) \end{pmatrix} \langle x^i \rangle (-\mu)^{n-i}$$

and hence $\langle (x - \bar{x})^n \rangle = 0$.

Sensitivity to field noise

- The transition probability is one objective function that can be expressed in terms of the amplitudes c_{ji}. Here we consider leading order Taylor approximations for its moments (note these can be obtained more accurately using the expressions above)
- We have

$$\mathrm{E}[\delta J] \approx \frac{1}{2}\int_0^T \int_0^T \mathcal{H}(t,t')\mathrm{E}\left[\delta u(t)\delta u(t')\right] \; dt \; dt' \quad = \frac{1}{2}\int_0^T \int_0^T \mathcal{H}(t,t')\mathrm{acf}(t,t') \; dt \; dt'$$

- Consider Hessian nullspace; $\mathcal{H}(t,t')$ is finite rank kernel:

$$\mathcal{H}(t,t') = \mathrm{Tr}\left\{\rho\Theta(T)[\mu(t),\mu(t')]_+ - \Theta(T)(\mu(t)\rho\mu(t') + \mu(t')\rho\mu(t))\right\}$$

which has rank $2N-2$, where N is Hilbert space dimension, for state-to-state population transfer.

Prospect: Thus to second order, field noise at most frequencies does not affect population transfer

- To second order, laser noise can only decrease $\mathrm{E}[J_{\mathrm{nom}} + \delta J]$ since Hessian is negative semidefinite

Field noise (time-domain amplitude noise): $\mathrm{var}\ J$, first order

- A first-order approximation to the variance of population transfer fidelity due to field noise can be found in closed form:

$$\begin{aligned}\mathrm{var}\ J &\approx \int_0^T \int_0^T \mathrm{E}\left[\delta\varepsilon(t)\delta\varepsilon(t')\right] \frac{\delta J}{\delta\varepsilon(t)} \frac{\delta J}{\delta\varepsilon(t')}\ dt\ dt', \\ &= \int_0^T \int_0^T \mathrm{acf}(t,t') \frac{\delta J}{\delta\varepsilon(t)} \frac{\delta J}{\delta\varepsilon(t')}\ dt\ dt'\end{aligned}$$

  where

$$\frac{\delta J}{\delta\varepsilon(t)} = \mathrm{Tr}\left\{[\rho_0, \Theta(T)]\mu(t)\right\}$$

Hamiltonian uncertainty: $\mathrm{var}\ J$, first order

- A first-order approximation to the variance of population transfer fidelity due to Hamiltonian parameter uncertainty can be found in closed form:

$$\mathrm{var}\ J \approx \mathrm{Tr}\left[\Sigma \nabla_\theta J (\nabla_\theta J)^T\right],$$

where

$$[\nabla_\theta J]_i = -i\mathrm{Tr}\left\{[\rho_0, \Theta(T)] \int_0^T U^\dagger(t) X_i \varepsilon(t) U(t)\ dt\right\}$$

and X_i is the Hermitian matrix obtained by setting $\theta_i = 1,\ \ \theta_j = 0,\ j \neq i$ in $\mu(\theta)$.

2nd order distributional results: $E[J]$, Hamiltonian parameter uncertainty

- The leading term in the expansion for $E[\delta J]$ due to parameter uncertainty is of 2nd order:

$$\begin{aligned} \mathrm{E}[\delta J] &\approx \frac{1}{2}\mathrm{E}[\delta\theta^T \mathcal{H}(\theta,\theta')\delta\theta] \\ &\approx \frac{1}{2}\mathrm{Tr}\left(\Sigma\mathcal{H}(\theta,\theta')\right) \end{aligned}$$

  where $\mathcal{H}(\theta,\theta') = \frac{d^2 J}{d\theta d\theta'}$ denotes the Hessian matrix with respect to Hamiltonian parameters

- Parameter uncertainty can improve $\mathrm{E}[J]$; consider overlap:

$$\begin{aligned} \mathrm{Tr}\left(\Sigma\mathcal{H}(\theta,\theta')\right) &= \mathrm{Tr}\left(V\Lambda V^T W\Gamma W^T\right) \\ &= \mathrm{Tr}\left(\Lambda\tilde{V}\Gamma\tilde{V}^T\right) \end{aligned}$$

  where $\Lambda \geq 0$, and $\tilde{V}$ is an orthogonal matrix

- How to search for fields where, given uncertainty spectrum, overlap with the directions in parameter space associated with largest positive eigenvalues maximized

2nd order distributional results: $E[J]$, Hamiltonian parameter uncertainty

- $\mathcal{H}(\theta, \theta') = \frac{d^2 J}{d\theta d\theta'}$:

$$\begin{aligned}\mathcal{H}(i,j) = \mathrm{Tr}\{\rho\Theta(T) &\int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt \int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt + \\ &\Theta(T)\rho \int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt \int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt - \\ &\int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\ \rho \int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt\ \Theta(T) - \\ &\int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt\ \rho \int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\ \Theta(T) + \\ &[\rho, \Theta(T)] \int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t) \int_0^t iU^\dagger(t')X_j\varepsilon(t')U(t')\ dt' dt\} + \\ &-[\rho, \Theta(T)] \int_0^T \int_0^t iU^\dagger(t')X_j\varepsilon(t')U(t')\ dt'\ iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\end{aligned}$$

Gradients and Hessians

$$\frac{\delta}{\delta\varepsilon(t)}U(T) = U(T)\mu(t)$$

$$\begin{aligned}
\frac{\delta}{\delta\varepsilon(t)}U(T) &= U(T)\mu(t) \\
\frac{\delta J}{\delta\varepsilon(t)} &= \langle \nabla_U F(U(T)), \frac{\delta}{\delta\varepsilon(t)}U(T)\rangle \\
&= \mathrm{Tr}\left\{[\rho_0, \Theta(T)]U^\dagger(T)\frac{\delta}{\delta\varepsilon(t)}U(T)\right\} \\
&= \mathrm{Tr}\left\{[\rho_0, \Theta(T)]U^\dagger(T)U(T)\mu(t)\right\} \\
&= \mathrm{Tr}\left\{[\rho_0, \Theta(T)]\mu(t)\right\}
\end{aligned}$$

Gradients and Hessians (cont'd)

$$\mathcal{H}(t,t') = -i\mathrm{Tr}\{\rho_0\Theta(T)\frac{\delta}{\delta\varepsilon(t')}U^\dagger(t)\mu U(t) +$$
$$\frac{\delta}{\delta\varepsilon(t')}\left(\rho_0 U^\dagger(T)\Theta U(T)\right)U^\dagger(t)\mu U(t)\} +$$
$$+ i\mathrm{Tr}\{\Theta(T)\rho_0\frac{\delta}{\delta\varepsilon(t')}U^\dagger(t)\mu U(t)$$
$$- \frac{\delta}{\delta\varepsilon(t')}\left(U^\dagger(T)\Theta U(T)\rho_0\right)U^\dagger(t)\mu U(t)\}$$

$$\mathcal{H}(t,t') = \mathrm{Tr}\{\rho\Theta(T)\mu(t')\mu(t) + \Theta(T)\rho\mu(t)\mu(t') - \mu(t)\rho\mu(t')\Theta(T)$$
$$- \mu(t')\rho\mu(t)\Theta(T) + [\rho,\Theta(T)][\mu(t),\mu(t')]\}$$

$$[\nabla_\theta U(t)]_j = -iU(t)\int_0^t U^\dagger(t')X_j\varepsilon(t')U(t')\ dt'$$

$$\begin{aligned}\mathcal{H}(i,j) = \mathrm{Tr}\{\rho\Theta(T)\int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt\ \int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt + \\ \Theta(T)\rho\int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\ \int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt - \\ \int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\ \ \rho\int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt\ \Theta(T) - \\ \int_0^T iU^\dagger(t)X_j\varepsilon(t)U(t)\ dt\ \ \rho\int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\ \Theta(T) + \\ [\rho,\Theta(T)]\int_0^T iU^\dagger(t)X_i\varepsilon(t)U(t)\ \int_0^t iU^\dagger(t')X_j\varepsilon(t')U(t')\ dt'dt + \\ -[\rho,\Theta(T)]\int_0^T\int_0^t iU^\dagger(t')X_j\varepsilon(t')U(t')\ dt'\ iU^\dagger(t)X_i\varepsilon(t)U(t)\ dt\end{aligned}$$

Worst-case quantum control robustness analysis

- Worst-case robustness analysis can also be carried out based on constrained maximization of the distance between the nominal and worst-case values of the performance measure. These approaches are based on leading order Taylor expansions. In a first-order formulation, the problem can be expressed as

$$\max_{\delta\theta\in\Theta} |\delta J|^2 \approx \delta\theta^T (\nabla_\theta J)^T \nabla_\theta J \delta\theta, \tag{11}$$

where

$$\Theta = \{\delta\theta \mid \delta\theta^T \Sigma^{-1} \delta\theta \ \leq \ \chi^2_K(c)\},$$
$$\delta\theta = \theta - \hat{\theta}, \tag{12}$$

Worst-case quantum control robustness analysis (cont'd)

- Let $x = \chi_K^{-1}(c) Q^{-1} \delta\theta$, where $Q^T Q = \Sigma$. Then under this change of variables the constrained maximization problem (11) is mapped:

$$\max_{\delta\theta \in \Theta} |\delta J|^2 \to \max_{x^T x \leq 1} \chi_K^2(c) x^T Q^T (\nabla_\theta J)^T (\nabla_\theta J) Q x. \tag{13}$$

- This problem has the form of a Rayleigh quotient [**?**], which has an analytical solution for J_{wc} and $\theta_{wc} = \hat{\theta} + \delta\theta_{wc}$, with $\delta\theta_{wc} = \arg\max |\delta J|^2$ written in terms of a singular value decomposition with appropriately chosen sign.

Outline

Software implementation

- Precalculation of required amplitude, Hamiltonian parameter and phase moments: higher moments of the manipulated inputs like $\mathrm{E}[A_k]$ and system parameters θ should be computed once and reused in all transition amplitude expressions wherein they appear above.
- Either specify a maximum series order $m_{\max}$ arbitrarily, or choose it based on a required moment accuracy, using the upper bounds on moment approximation errors that will be provided. Then precalculate all moments of the manipulated input or system parameters that appear in the transition amplitude moment expressions up to order m
- Testing of the expressions for specified values (changes) in amplitudes, Hamiltonian parameters, and phases: the first test for implementation of the MI-based robustness analysis methods is to compute the value of c_{ji} for a specified (deterministic) change in the A_k or θ using e.g.

$$c_{ji}(T) = \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n} A_1^{\alpha_1} \cdots A_n^{\alpha_n}$$

  and verify the approximation with direct MI
- Even without implementing amplitude, phase and full dipole MI, it is possible to do some preliminary tests with just orders MI (the simplest type of MI). This however requires the development of additional code that retrieves the $c_{\alpha_1,\cdots,\alpha_n}$ with the help of orders MI and some linear algebra. The computational complexity of this method is greater.

Computational complexity of quantum control robustness calculations

- The transform-based techniques above greatly reduce the complexity of quantum control robustness calculations, which would otherwise require direct evaluation of a very large number of multiple integrals
- Generality: these methods for robustness analysis (and associated robust control algorithms below) can be applied to any bilinear control system - general methodological contribution for robust control of bilinear systems
- Need for stabilization: Most of the above MI formulations are non-Hermitian. Non-Hermitian MI suffers from instability, especially for stronger fields and larger systems. There exists a maximum evolution time beyond which the $c_{\alpha_1,\cdots,\alpha_n}$ cannot be retrieved. For such systems the time domain must be subdivided into many small subdomains; the $c_{\alpha_1,\cdots,\alpha_n}$ must then be computed from the MI amplitudes on each subdomain. This is computationally expensive
- Complexity of robustness calculations vis-a-vis MI stabilization: *Stabilization* of MI can alleviate this problem, by reducing MI amplitudes and hence the number of time-domain subdivisions required
- Even prior to implementing amplitude, phase and full dipole MI, it is possible to do some preliminary tests of robustness analysis with just orders MI (the simplest type of MI). This however requires the development of additional code that retrieves the $c_{\alpha_1,\cdots,\alpha_n}$ with the help of orders MI and some linear algebra. The computational complexity of this method is greater.

Outline

Bounds on amplitude robustness analysis series expansion terms

- Need bound on norm of $c_{\alpha_1,\cdots,\alpha_n} = \frac{U_{ji}(T,\alpha_1,\cdots,\alpha_n)}{A_1^{\alpha 1}\cdots A_n^{\alpha n}}$
- $|\langle x|\mu|y\rangle| < d,\ 1 \leq x,y \leq N$

$$
\begin{aligned}
|c_{\alpha_1,\cdots,\alpha_n}| = \Bigg| & \sum_{l_1=1}^{N}\cdots\sum_{l_{m-1}=1}^{N} \langle j|\mu|l^{m-1}\rangle\langle l^{m-1}|\mu|l^{m-2}\rangle\cdots\langle l^1|\mu|i\rangle\times \\
& \times \int_0^T \exp[\imath(E_j - E_{l_{m-1}})t_m]\cos(\omega_{k_m}t_m + \phi(\omega_{k_m}))\times \\
& \times \int_0^{t_m} \exp[\imath(E_{l_{m-1}} - E_{l_{m-2}})t_{m-1}]\cos(\omega_{k_{m-1}}t_{m-1} + \phi(\omega_{k_{m-1}}))\cdots \\
& \cdots\int_0^{t_2} \exp[\imath(E_{l_1} - E_i)t_1]\cos(\omega_{k_1}t_1 + \phi(\omega_{k_1}))\ dt_1\cdots dt_m\Bigg| \\
& \leq \sum_{l_1=1}^{N}\cdots\sum_{l_{m-1}=1}^{N} d^m \Bigg|\int_0^T \exp[\imath(E_j - E_{l_{m-1}})t_m]\cos(\omega_{k_m}t_m + \phi(\omega_{k_m}))\times \\
& \times \int_0^{t_m} \exp[\imath(E_{l_{m-1}} - E_{l_{m-2}})t_{m-1}]\cos(\omega_{k_{m-1}}t_{m-1} + \phi(\omega_{k_{m-1}}))\cdots \\
& \cdots\int_0^{t_2} \exp[\imath(E_{l_1} - E_i)t_1]\cos(\omega_{k_1}t_1 + \phi(\omega_{k_1}))\ dt_1\cdots dt_m\Bigg|
\end{aligned}
$$

Bounds on amplitude robustness analysis series expansion terms (cont'd)

$$
\begin{aligned}
|c_{\alpha_1,\cdots,\alpha_n}| \leq \sum_{l_1=1}^{N} \cdots \sum_{l_{m-1}=1}^{N} d^m \int_0^T | \exp[\imath(E_j - E_{l_{m-1}})t_m]| |\cos(\omega_{k_m} t_m + \phi(\omega_{k_m}))| \times \\
\times \cdots \int_0^{t_2} | \exp[\imath(E_{l_1} - E_i)t_1]| |\cos(\omega_{k_1} t_1 + \phi(\omega_{k_1}))| \; dt_1 \cdots dt_m \\
\leq \sum_{l_1=1}^{N} \cdots \sum_{l_{m-1}=1}^{N} d^m \frac{T^m}{m!} \\
\leq N^{m-1} d^m \frac{T^m}{m!} = \frac{(NdT)^m}{Nm!}.
\end{aligned}
$$

- Use either d^m or sum of product of μ matrix elements (latter tighter bound, but more computationally intensive to calculate); former preferred
- **Check this bound numerically and plot vs m**

Bounds on amplitude robustness analysis series expansion terms and maximum series order computation

- $U_{ji}(T) \approx \sum_{m=1}^{m_{\max}} U_{ji}^m(T)$
- $U_{ji}^m(T) = \sum_{\vec{\alpha}} c_{\alpha_1,\cdots,\alpha_n} A_1^{\alpha_1} \cdots A_n^{\alpha_n}, \;\; \sum_k \alpha_k = m, \;\; m \in [1, m_{max}]$
- $\mathrm{E}[U_{ji}(T)] \approx \sum_{m=1}^{m_{\max}} \mathrm{E}[U_{ji}^m(T)]$
- $|\mathrm{E}[U_{ji}^m(T)]| \leq \frac{(NdT)^m}{Nm!} \left(\sum_{\vec{\alpha}} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}]\right), \;\; \sum_k \alpha_k = m, \;\; m \in [1, m_{max}]$
- **Check this bound numerically and plot vs m**
- $m_{\max} = \max \; m \mid \frac{(NdT)^m}{Nm!} \left(\sum_{\vec{\alpha}} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}]\right) \geq \epsilon, \;\; \sum_k \alpha_k = m$
- Bound on accuracy: $\mathrm{E}[U_{ji}(T)] - \sum_{m=1}^{m_{\max}} \mathrm{E}[U_{ji}^m(T)] = \sum_{m=m_{\max}}^{\infty} \mathrm{E}[U_{ji}^m(T)]$;

$$\left| \sum_{m=m_{\max}}^{\infty} \mathrm{E}[U_{ji}^m(T)] \right| \leq \sum_{m=m_{\max}}^{\infty} \frac{(NdT)^m}{Nm!} \left(\sum_{\vec{\alpha}} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}] \right)$$

$$\sum_{m=m_{\max}}^{\infty} \frac{(NdT)^m}{Nm!} \left(\sum_{\vec{\alpha}} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}] \right) \approx \sum_{m=m_{\max}}^{m_{eps}} \frac{(NdT)^m}{Nm!} \left(\sum_{\vec{\alpha}} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}] \right),$$

  where m_{eps} denotes the smallest m such that $\frac{(NdT)^m}{Nm!} \left(\sum_{\vec{\alpha}} \mathrm{E}[A_1^{\alpha_1}] \cdots \mathrm{E}[A_n^{\alpha_n}]\right) \leq \mathrm{eps}$, eps denoting the smallest floating point number that can be represented on the computer
- **Compute $m_{\max}$ and bound on error for specified ϵ**
- Note, it is possible to derive an analytical bound on the error, but it is less accurate and not necessary

Bounds on series expansion terms for first moment of the transition probability

$$\left|\mathrm{E}\left[\left(\mathrm{Re},\mathrm{Im}\ c_{ji}(T)\right)^2\right]\right| \leq \sum_{m=2}^{m_{\max}} \sum_{m'<m} \left\{ 2\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha'_n}] \right\} +$$

$$+ \sum_{m=1}^{m_{\max}} \frac{(NdT)^{2m}}{(Nm!)^2} \left\{ \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{E}[A_1^{2\alpha_1}]\cdots\mathrm{E}[A_n^{2\alpha_n}] \right\},$$

$$\sum_k \alpha_k = m, \sum_{k'} \alpha'_k = m',\ \ m, m' \ \in\ [1, m_{max}]$$

- $\mathrm{E}\left[\left(\mathrm{Re},\mathrm{Im}\ c_{ji}(T)\right)^2\right] = \sum_{m=1}^{m_{\max}} \mathrm{E}\left[\left(\mathrm{Re},\mathrm{Im}\ c_{ji}(T)\right)_m^2\right]$

$$\left|\mathrm{E}\left[\left(\mathrm{Re},\mathrm{Im}\ c_{ji}(T)\right)_m^2\right]\right| \leq \sum_{m'<m} 2\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha'_n}] +$$

$$+ \frac{(NdT)^{2m}}{(Nm!)^2} \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{E}[A_1^{2\alpha_1}]\cdots\mathrm{E}[A_n^{2\alpha_n}],$$

$$\sum_k \alpha_k = m, \sum_{k'} \alpha'_k = m',\ \ m, m' \ \in\ [1, m_{max}]$$

- **Check this bound numerically and plot vs m**

Bounds on series expansion terms for first moment of the transition probability

$$\left|\mathrm{E}\left[P_{ji}^{m}(T)\right]\right| \leq \sum_{m'<m} 4\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha'_n}]+$$

$$+2\frac{(NdT)^{2m}}{(Nm!)^2} \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{E}[A_1^{2\alpha_1}]\cdots\mathrm{E}[A_n^{2\alpha_n}],$$

$$\sum_k \alpha_k = m, \sum_{k'} \alpha'_k = m', \; m, m' \in [1, m_{max}]$$

Maximum series order computation: first moment of the transition probability

- $m_{\max} = \max \; m$ such that

$$\sum_{m'<m} 4\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha_1',\cdots,\alpha_n')} \mathrm{E}[A_1^{\alpha_1+\alpha_1'}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha_n'}]+$$
$$+2\frac{(NdT)^{2m}}{(Nm!)^2}\sum_{(\alpha_1,\cdots,\alpha_n)}\mathrm{E}[A_1^{2\alpha_1}]\cdots\mathrm{E}[A_n^{2\alpha_n}] \geq \epsilon,$$
$$\sum_k \alpha_k = m, \sum_{k'} \alpha_k' = m'$$

- Bound on accuracy: $\mathrm{E}[P_{ji}(T)] - \sum_{m=1}^{m_{\max}} \mathrm{E}[P_{ji}^m(T)] = \sum_{m=m_{\max}}^{\infty} \mathrm{E}[P_{ji}^m(T)]$;

  where m_{eps} denotes the smallest m such that $\leq \mathrm{eps}$, eps denoting the smallest floating point number that can be represented on the computer

- **Compute $m_{\max}$ and bound on error for specified ϵ**
- Note, it is possible to derive an analytical bound on the error, but it is less accurate and not necessary

Outline

Pareto Tradeoffs in Robust Control

Figure : Pareto frontier of solutions to mean-variance optimal control problems.

- *Pareto frontier* of robust control solutions:

$$\{\bar{\varepsilon}(t) \;\mid\; J_1(\varepsilon(t)) \leq J_1(\bar{\varepsilon}(t)) \quad \vee \quad J_2(\varepsilon(t)) \leq J_2(\bar{\varepsilon}(t)), \;\; \forall \varepsilon(t) \neq \bar{\varepsilon}(t)\}$$

- E.g., $J_1(\varepsilon(t)) = \mathrm{E}[J(\varepsilon(t)]]$, $J_2(\varepsilon(t)) = -\mathrm{std}\; J(\varepsilon(t))$ or $J_2(\varepsilon(t)) = J_{wc}(\varepsilon(t))$
- Importance/interpretation of user preferences: would one prefer lower expected performance with more reliability?

Problems with unconstrained optimization approaches

- Expressions above for $\mathrm{var}\ J$, $\mathrm{E}[\delta J]$ are approximations: inaccuracies can reduce fidelity if $\mathrm{E}[J]$ used at each step of $\varepsilon(t)$ optimization
- Instead i) maximize nominal population transfer J_{nom} using only true value θ_0; ii) constrain $J_{\mathrm{nom}}^{\mathsf{max}}$ and find fields $\varepsilon(t)$ that minimize $\mathrm{var}\ J$ or maximize $\mathrm{E}[\delta J]$.
- Alternatively, use robust optimization with the accurate expressions for moments obtained with MI

Constrained nonlinear control optimization

- To obtain an expression for $\delta\varepsilon(t)$ that maximize or minimize auxiliary costs while holding $J_{\mathrm{nom}}^{\mathrm{max}}$, solve the Fredholm integral equation of the first kind

$$\int_0^T \frac{\delta J}{\delta\varepsilon(t)}\delta\varepsilon(t)\ dt = 0, \tag{14}$$

  with kernel $\frac{\delta J}{\delta\varepsilon(t)}$, for $\delta\varepsilon(t)$.

- Since this integral equation has a separable kernel, it can be solved by writing the unknown vector function $\delta\varepsilon(t)$ in terms of $\frac{\delta J}{\delta\varepsilon(t)}$; then $\delta\varepsilon(t) = c\frac{\delta J}{\delta\varepsilon(t)} + f(t)$ (where $f(t)$ is a free function, since the integral equation is underspecified) and we have

$$\int_0^T \left(\frac{\delta J}{\delta\varepsilon(t)}\right)^2\ dt + \int_0^T f(t)\frac{\delta J}{\delta\varepsilon(t)}\ dt = 0.$$

- Solving for c, we find $c = -[\int_0^T \left(\frac{\delta J}{\delta\varepsilon(t)}\right)^2\ dt]^{-1}\ \int_0^T f(t)\frac{\delta J}{\delta\varepsilon(t)}\ dt]$.

- Then $\delta\varepsilon(t) = f(t) - [\int_0^T \left(\frac{\delta J}{\delta\varepsilon(t')}\right)^2\ dt']^{-1}\frac{\delta J}{\delta\varepsilon(t)}\int_0^T f(t')\frac{\delta J}{\delta\varepsilon(t')}\ dt'$

Formulations of relevance to robust control (cont'd)

- To explore fields holding constant high values of J and $\mathrm{E}[\delta J]$ while reducing $\mathrm{var}\ J$, let

$$a(s,t) = \frac{\delta J}{\delta\varepsilon(s,t)} = -i\mathrm{Tr}\{[\rho_0, O(T)]\mu(s,t)\}$$
$$g(s,t) = \frac{\delta \mathrm{E}[\delta J]}{\delta\varepsilon(s,t)}$$
$$f(s,t) = \frac{\delta \mathrm{var}\ J}{\delta\varepsilon(s,t)}$$

- Then propagate

$$\frac{\partial\varepsilon(s,t)}{\partial s} = f(s,t) - \left[\int_0^T [a(s,t') \ \ g(s,t')] f(s,t')\ dt'\right]^T \Gamma_s^{-1}[a(s,t'), g(s,t')]$$

where $\Gamma_s = \int_0^T [a(s,t') \ \ g(s,t')][a(s,t') \ \ g(s,t')]^T\ dt'$.

Exploring robust control fields

- Setting $f(t)$ to the functional derivative of the appropriate auxiliary cost, and choosing $\varepsilon(0,t) = \bar{\varepsilon}(t)$, one can then solve the constrained optimization problem by iteratively solving for $\delta\varepsilon(s,t)$, with iterations indexed by algorithmic parameter s.
- To explore fields holding a constant high value of $\mathrm{E}[J]$ while reducing $\mathrm{var}\ J$, solve

$$\frac{\partial \varepsilon(s,t)}{\partial s} = f(s,t) - \frac{a(s,t)}{\int_0^T a^2(s,t')\ dt'} \int_0^T f(s,t')a(s,t')\ dt'$$

$$a(s,t) = \frac{\delta J}{\delta\varepsilon(s,t)} + \frac{\delta \mathrm{E}[\delta J]}{\delta\varepsilon(s,t)}$$

$$f(s,t) = \frac{\delta\ \mathrm{var}\ J}{\delta\varepsilon(s,t)}$$

- To maximize $\mathrm{E}[J]$ for given risk level ($\mathrm{var}\ J$ or J_{wc}), switch the definitions of $a(s,t)$ and $f(s,t)$

Joint field/parameter-based robust control approaches

- **Prospect:** Multiplicity of control solutions and flexible pulse shaping permits formulation of Hamiltonian parameter uncertainty robustness criteria as constraints

- Since field uncertainty less severe, minimize $\mathrm{var}\ J$ or maximize $\mathrm{E}[J]$ due to field pdf among fields obtained above

- To explore fields holding a constant high value of $\mathrm{E}_{\varepsilon(t)}\ [J]$ while reducing $\mathrm{var}_{\theta}\ J$, formulation is analogous to above

Frequency domain gradient

$$\delta U(T) = -\imath U(T) \int_0^T U^\dagger(t)\mu\delta\varepsilon(t)U(t)\; dt$$

$$= -\frac{\imath}{2} U(T) \int_{-\infty}^{\infty} d\omega\; \delta A(\omega) \int_0^T \mu(t)[\exp(\imath\omega t)\exp(\imath\phi(\omega)) + \exp(-\imath\omega t)\exp(-\imath\phi(\omega))]\; dt$$

$$\frac{\delta U(T)}{\delta A(\omega)} = -\frac{\imath}{2} U(T) \int_0^T \mu(t)[\exp(\imath\omega t)\exp(\imath\phi(\omega)) + \exp(-\imath\omega t)\exp(-\imath\phi(\omega))]\; dt$$

$$= -\frac{\imath}{2} U(T) \left\{ \exp(\imath\phi(\omega)) \int_0^T \mu(t)\exp(\imath\omega t)\; dt + \exp(-\imath\phi(\omega)) \int_0^T \mu(t)\exp(-\imath\omega t)\; dt \right\}$$

- Compute time-domain integrals efficiently through FFT of $\mu(t)$ ($N(N+1)/2$ FFTs of complex functions - N diagonal elements are real-valued) - Fourier transform provides both 1st and 2nd integrals above via $\mu(\omega)$ at all frequencies ω
- For a given J, only need to compute FFT of one scalar function of time.

Dyson series approximation of frequency domain gradient, $\frac{\delta \mathrm{E}[J]}{\delta A(\omega)}$, $\frac{\delta \mathrm{var}\ J}{\delta A(\omega)}$

- Alternatively, to avoid FFT's at each iteration, approximate with Dyson series via MI methods described above
- For example,

$$\frac{\delta}{\delta A_1}\mathrm{Re},\mathrm{Im}\ c_{ji}(T) = \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n}\alpha_1 A_1^{\alpha_1-1}\cdots A_n^{\alpha_n}$$

$$\frac{\delta}{\delta A_1}\mathrm{E}[\mathrm{Re},\mathrm{Im}\ c_{ji}(T)] = \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n}\alpha_1 \mathrm{E}[A_1^{\alpha_1-1}]\cdots \mathrm{E}[A_n^{\alpha_n}]$$

$$\frac{\delta}{\delta A_1}\mathrm{var}\left(\mathrm{Re},\mathrm{Im}\ c_{ji}(T)\right) = \mathrm{E}\Bigg[\Bigg\{\sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n}\times \times\left(\alpha_1 A_1^{\alpha_1-1}\cdots A_n^{\alpha_n} - \alpha_1\mathrm{E}[A_1^{\alpha_1-1}]\cdots\mathrm{E}[A_n^{\alpha_n}]\right)\Bigg\}^2\Bigg]$$

where the latter two expressions follow from the fact that E is a linear operator.

- Less expensive to evaluate - reevaluation of time-domain integrals not needed at each iteration
- Update MI periodically given tolerance setting

Frequency domain robust control optimization

- All the above expressions for deterministic robust control optimization algorithms carry over to the frequency domain with time-domain gradient $a(s,t)$ replaced by frequency-domain gradient $a(\omega,t)$, $f(s,t), g(s,t)$ replaced by $f(s,\omega), g(s,\omega)$

- The above expressions for moments of J (amplitude and phase noise) can be used in robust optimization algorithms that ensure that the worst case values of the field parameters in a given iteration do not lie within a specified confidence interval of these parameters at the next iteration
- This approach is most useful if one is solving a single objective minimax problem using J_{wc} rather than sampling the mean-variance frontier
- To be implemented after implementation of the above deterministic and below stochastic algorithms

MOEA algorithms for sampling the mean-variance frontier

- Instead of controlling quantum expectation values of multiple observables, control classical moments of expectation value of a single observable
- Use the above MI expressions for the moments $\mathrm{E}[J]$, $\mathrm{var}\ J$
- AK to provide more details on the GA algorithms used

Outline

1. Quantum robust control
2. Quantum control mechanism identification
3. Quantum control robustness analysis: moments of the transition amplitude
   - Field amplitude noise
   - Hamiltonian uncertainty
   - Phase noise
   - Obtaining amplitude, phase and Hamiltonian parameter moments for robustness analysis
   - Moments of the transition probability: leading order Taylor approximations
   - Worst-case analysis
4. Implementation of robustness analysis methods and use of alternate MI formulations
5. Bounds on series expansion terms and accuracy of robustness analysis
6. Quantum robust control algorithms
   - Deterministic algorithms
   - Robust optimization
   - Stochastic algorithms
7. Results: atomic Rb

- AK preliminary results

Comparing robust and nonrobust quantum control mechanisms

(a)(b)

Figure : **Left:** Amplitudes of pathways contributing to the mechanism of a robust control field for population transfer to $5D3/2$ in atomic Rb. **Right:** Amplitudes of pathways for a comparatively nonrobust field inducing the same transition.

- Robust fields generally exploit fewer pathways, quantum interferences
- For multilevel systems, multipathway interferences nonetheless required
- Robustness of each pathway/interference to parameter uncertainty can be computed