Robust Control of Quantum Dynamics

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1. INTRODUCTION

- Theory of robust control of quantum dynamics in presence of noise/uncertainty in classical input variables or the quantum Hamiltonian
- Based on control of moments with respect to these sources of uncertainty relevant to control of components of the quantum state, unlike moments due to quantum uncertainty in the state of the system
- Such approaches are necessary foundations for model-based quantum control of molecular dynamics, or adaptive feedback approaches that combine model-based strategies with learning control

2. CONTROL SYSTEM

- For linear systems with additive noise, it is possible to obtain an analytical solution for the time evolution of the first and second moments of the state variables
- For example, linear Markovian diffusion process control (sde): $dy_t = Ay_t dt + Bu_t dt + Dd\omega_t$ (in the absence of $Bu_t dt$, this is the Ornstein-Uhlenbeck process)
- For bilinear systems (multiplicative noise) such an analytical solution does not exist

3. ROBUSTNESS OF CONTROLLED QUANTUM DYNAMICS

Here, we present an approach that can provide accurate estimates of the first and 2nd moments (and higher moments if desired) of δJ suitable for use in either distributional or worst-case robustness criteria for controlled quantum dynamics, along with bounds on the accuracy of those estimates. This approach is more accurate than methods for moment calculations based on leading order Taylor expansions.

3.1. Pathways

- **Expression for amplitude pathways**

$$U_{ji}^m(T) = \left(\frac{\imath}{\hbar}\right)^m \sum_{\vec{\alpha}\in\mathcal{M}} \prod_{k=1}^{K} A_k^{\alpha_k} \times \sum_{(k_1,\cdots,k_m)} \sum_{l_{m-1}}^{N} \mu_{jl_{m-1}} \int_0^T e^{i(\omega_{jl_{m-1}} t_m)} \cos(\omega_{k_m} t_m + \phi(\omega_{k_m}))\times \cdots \times \sum_{l_1}^{N} \mu_{l_1 1} \int_0^{t_2} e^{i(\omega_{l_1 i} t_1)} \cos(\omega_{k_1} t_1 + \phi(\omega_{k_1}))\, dt_1 \cdots dt_m$$

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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.

- **Dipole pathways**

$$
\begin{aligned}
U_{ji}^m(T) = \left(\frac{\imath}{\hbar}\right)^m \sum_{\vec{\alpha}\in\mathcal{M}} \prod_{p=1,q>p}^{N-1} \mu_{pq}^{\alpha_{pq}} \times \\
\sum_{(l_1,\cdots,l_{m-1})} \sum_{k_m=1}^{K} A_{k_m} \int_0^T e^{\imath(\omega_{jl_{m-1}} t_m)} \cos(\omega_{k_m} t_m + \phi(\omega_{k_m}))\times \\
\cdots \times \sum_{k_1=1}^{K} A_{k_1} \int_0^{t_2} e^{\imath(\omega_{l_1 i} t_1)} \cos(\omega_{k_1} t_1 + \phi(\omega_{k_1}))\ dt_1 \cdots dt_m
\end{aligned}
$$

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.

- **Phase pathways**

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

where $\vec{\alpha} \in \mathbb{Z}^K$, $1 \le |k_i| \le K$, $\omega_{-k_i} = -\omega_{k_i}$, $b_k(k_1,\cdots,k_m)$ 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.

- **Amplitude pathways in terms of encoding/decoding**

amplitude encoding:

$$
\begin{aligned}
A_k &\to A_k e^{\imath\gamma_k s}, \\
A_k^{\alpha_k} &\to A_k^{\alpha_k} e^{\imath(\alpha_k\gamma_k)s},
\end{aligned}
$$

where γ_k is the *modulating frequency* specific to the amplitude power α_k associated with a particular pathway ($\vec{\alpha}$). Using the modulation, the Schrödinger equation can be propagated in the time variable t and dummy variable s, for which the resulting *encoded* m-th order transition amplitude $U_{ji}^m(T,s)$ is comprised of the following terms:

$$
\begin{aligned}
U_{ji}^m(T,s) = \left(\frac{\imath}{\hbar}\right)^m \sum_{\vec{\alpha}\in\mathcal{M}} A_1^{\alpha_1} \cdots A_K^{\alpha_K} e^{\imath(\alpha_1\gamma_1+\cdots+\alpha_K\gamma_K)s} \times \\
\sum_{l_1=1}^{N} \cdots \sum_{l_{m-1}=1}^{N} \mu_{jl_{m-1}} \cdots \mu_{l_1 i} \times \cdots .
\end{aligned}
\tag{2}
$$

The encoded total transition amplitude contain the following terms:

$$
U_{ji}(T,s) = \sum_{m=1}^{M} \sum_{\vec{\alpha}\in\mathcal{M}} U_{ji}^m(T,\vec{\alpha}) e^{\imath(\alpha_1\gamma_1+\cdots+\alpha_K\gamma_K)s}. \tag{3}
$$

Deconvolution of the total transition amplitude leads to

$$
U_{ji}(T,\gamma) = \int_{-\infty}^{\infty} U_{ji}(T,s) e^{-i\gamma s}\ ds. \tag{4}
$$

where $\gamma \in [0, \cdots, \alpha_1\gamma_1 + \cdots + \alpha_K\gamma_K]$. This suggests that all amplitude pathways of different orders can be extracted through deconvolution of the encoded transition amplitude if all γ's associated with each pathway is uniquely known, i.e. $U_{ji}(T, \gamma = \alpha_1\gamma_1 + \cdots + \alpha_K\gamma_K) \to U^m_{ji}(T, \vec{\alpha})$. We can thus use 3 and 4 to concisely define amplitude pathways $\vec{\alpha}$ in **??**.

- **Dipole pathways in terms of encoding/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:

$$\begin{gathered}\mu_{ij} \to \mu_{ij} e^{\imath\gamma_{ij}s},\\ \mu_{ij}^{\alpha_{ij}} \to \mu_{ij}^{\alpha_{ij}} e^{\imath(\alpha_{ij}\gamma_{ij})s},\\ i < j \in [1, N].\end{gathered}$$

  The encoded and propagated unitary propagator consists of the different order dipole pathways with the encoded total transition amplitude:

$$U_{ji}(T, s) = \sum_{m=1}^{M} \sum_{\vec{\alpha}\in\mathcal{M}} U^m_{ji}(T, \vec{\alpha}) e^{i(\alpha_{12}\gamma_{12}+\cdots+\alpha_{N(N-1)}\gamma_{N(N-1)})s}. \tag{5}$$

  Deconvolution of the total transition amplitude leads to the decoded dipole pathway, i.e. $U_{ji}(T, \gamma = \alpha_{12}\gamma_{12} + \cdots + \alpha_{N(N-1)}\gamma_{N(N-1)}) \to U^m_{ji}(T, \vec{\alpha})$. We can similarly use 5 to define dipole pathways in **??**.

- **Phase pathways in terms of encoding/decoding**

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

$$\begin{gathered}e^{\imath\phi_k} \to e^{\imath(\phi_k+\gamma_k s)},\\ e^{\imath\alpha_k\phi_k} \to e^{-\imath\alpha_k(\phi_k+\gamma_k s)},\end{gathered} \tag{6}$$

  and the transition amplitude consists of:

$$\begin{aligned}U^m_{ji}(T) = &\left(\frac{\imath}{\hbar}\right)^m \sum_{(\alpha_1,\cdots,\alpha_K)} \frac{1}{2}\left(e^{\imath(\alpha_1(\phi_1+\gamma_1)+\cdots+\alpha_k(\phi_K+\gamma_K))} + c.c.\right) \times\\ &A_1^{\alpha_1}\cdots A_K^{\alpha_K} \sum_{l_{m-1}=1}^{N} \mu_{jl_{m-1}} \int_0^T \cdots \sum_{l_1=1}^{N} \mu_{l_1 i} \int_0^{t_2} \cdots\\ &dt_1 \cdots\ dt_m.\end{aligned} \tag{7}$$

  Deconvolution of the transition amplitude term yields m^{th} order *phase pathways* in a way identical to the amplitude counterpart. Note that in the case of phase modulation, the encoding is Hermitian. Similarly,

3.2. First Moments

- Assuming $\theta_1, \cdots, \theta_n$ are independent random variables, $\mathrm{E}[c_{ji}(T)]$ can then be expressed as follows (written respectively for $\mathrm{Re}\ c_{ji}(T),\ \mathrm{Im}\ c_{ji}(T)$):

$$\mathrm{E}[\mathrm{Re}, \mathrm{Im}\ c_{ji}(T)] = \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re}, \mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n} \mathrm{E}[\theta_1^{\alpha_1}]\cdots\mathrm{E}[\theta_n^{\alpha_n}]$$

- In some cases we will use the notation θ to denote the vector of uncertain or noisy parameters (either input or Hamiltonian parameters)

- First moment for arbitrary quantum observables: general expression

$$\begin{aligned}\tilde{\rho}_0 &= R^\dagger \rho_0 R = diag\,(\lambda_1, \cdots, \lambda_N)\\ \tilde{O} &= S^\dagger O S = diag\,(\gamma_1, \cdots, \gamma_N)\\ \tilde{U} &= S^\dagger U R\end{aligned}$$

- Let $W(t) = \exp\left(\frac{i}{\hbar} H_0 t\right)$
- Then

$$\begin{aligned}
\mathrm{E}\left[J(\tilde{U})\right] &= \mathrm{E}\left[\mathrm{Tr}\left(\tilde{U}\tilde{\rho}_0 U^\dagger \tilde{O}\right)\right] \\
&= \mathrm{E}\left[\sum_{i,j} |\tilde{U}_{ij}|^2 \gamma_i \lambda_j\right] \\
&= \sum_{i,j} \gamma_i \lambda_j \mathrm{E}\left[|\tilde{U}_{ij}|^2\right] \\
&= \sum_{i,j} \gamma_i \lambda_j \mathrm{E}\left[|(S^\dagger U R)_{ij}|^2\right] \\
&= \sum_{i,j} \gamma_i \lambda_j \mathrm{E}\left[|(S^\dagger W^\dagger U_I R)_{ij}|^2\right]
\end{aligned}$$

- Define $\tilde{U}_{ij}^{\vec{\alpha}}$ and $\tilde{c}_{ij}^{\vec{\alpha}}$'s in terms of expansion of elements $\tilde{U}_{ij}(T)$
- Decode $\tilde{U}(T,s) = S^\dagger W^\dagger(T) U_I(T,s) R$ directly to obtain $\tilde{U}_{ij}^{\vec{\alpha}}$'s

$$\mathrm{E}\left[\sum_{i,j} |\tilde{U}_{ij}|^2 \gamma_i \lambda_j\right] = \sum_{i,j}\left(\sum_{\vec{\alpha}} \mathrm{E}\left[\tilde{U}_{ij}^{\vec{\alpha}}\right] + 2\mathrm{Re}\sum_{\vec{\alpha}'<\vec{\alpha}} \mathrm{E}\left[\tilde{U}_{ij}^{\vec{\alpha}} \tilde{U}_{ij}^{\vec{\alpha}',*}\right]\right)\gamma_i \lambda_j$$

3.3. Generalized expression for moments of quantum observables

- Review of encoding scheme (above)
- Let $F(U(T,s)) = \mathrm{Tr}\left[U(T,s)\rho_0 U^\dagger(T,s)\Theta\right] = \mathrm{Tr}\left[U_I(T,s)\rho_0 U_I^\dagger(T,s)\Theta_I\right] = F_I(U_I(T,s))$ denote the encoded quantum observable expectation value. Alternatively, for robustness of quantum gate control, let $F(U(T,s)) = ||W - U(T,s)||^2$, where W is the target gate. For robustness of a single transition amplitude, let $F(U(T,s)) = \mathrm{Re}, \mathrm{Im}\ U_{ji}(T,s)$.
- For simplicity we drop the subscript I on both F and U; both are understood to refer to the interaction picture
- Let $\gamma' = \vec{\gamma} \cdot \vec{\alpha}$ and $\vec{\alpha}(\gamma') = \vec{\alpha}'$. Under a suitable encoding scheme (described above), $\vec{\alpha}(\cdot)$ then induces the following bijection: $U(T,\gamma) \leftrightarrow U(T,\vec{\alpha})$
- The upper limit $s_{\max}$ on s is determined by the maximum series order $m_{\max}$, which is in turn determined by the specified level of accuracy of the moment calculations according to the theory above. Let $\Gamma = \{0, ..., \gamma_f\}$ denote the set of encoding frequencies corresponding to the significant pathways (which is an infinite set for the exact solution).
- Then the exact expression for the observable expectation value can be written in terms of the inverse FT with respect to the encoding variable as follows in the case of amplitude noise:

$$\mathrm{E}[F(U(T))] = \sum_{\gamma' \in \Gamma} \int_{-\infty}^{\infty} F(U(T,s)) \exp(-i\gamma s)\ ds\ \cdot \delta(\gamma, \gamma') \cdot \frac{\mathrm{E}\left[\prod_k A_k^{\alpha_k(\gamma')}\right]}{\prod A_k^{\alpha_k(\gamma')}}$$

- Note that an uncertain initial state estimate ρ_0 (i.e., $\hat{\rho}_0$ and Σ_{ρ_0}) can be accommodated within the framework by replacing ρ_0 with $\rho_0(s)$, where the latter is any function of s such that the first and second moments match $\hat{\rho}_0$ and Σ_{ρ_0}.
- Covariances of $U_{ij}(T)$ can also be obtained

- For amplitude or dipole uncertainty, the FT can be restricted to the positive timelike axis, with the upper limit of integration set to s_f for the specified error tolerance on the moment calculation:

$$\mathrm{E}[F(U(T))] = \sum_{\gamma' \in \Gamma} \int_0^{s_f} F(U(T,s)) \exp(-i\gamma s)\ ds \ \cdot \delta(\gamma,\gamma') \cdot \frac{\mathrm{E}\left[\prod_k A_k^{\alpha_k(\gamma')}\right]}{\prod A_k^{\alpha_k(\gamma')}}$$

- The same treatment can be applied to moments of transition amplitudes. The above formulation applies to any F. E.g., when $F(U(T,s)) = \mathrm{Re},\mathrm{Im}(U_{ji}^n(T,s))$,

$$\mathrm{E}[\mathrm{Re},\mathrm{Im}\ U_{ji}(T)] = \sum_{\gamma' \in \Gamma} \int_0^{s_f} \mathrm{Re},\mathrm{Im}\ U_{ji}(T,s) \exp(-i\gamma s)\ ds \ \cdot \delta(\gamma,\gamma') \cdot \frac{\mathrm{E}\left[\prod_k A_k^{\alpha_k(\gamma')}\right]}{\prod A_k^{\alpha_k(\gamma')}}$$

- Expressions are analogous for dipole operator (control Hamiltonian) uncertainty
- The nth moment of $F(U(T,s))$ can be computed using the binomial expansion relating the moment to the expectations of the first n powers of $F(U(T,s))$
- The expectation of the nth power of $F(U(T))$ can be written

$$\mathrm{E}[F^n(U(T))] = \sum_{\gamma' \in \Gamma} \int_0^{s_f} F^n(U(T,s)) \exp(-i\gamma s)\ ds \ \cdot \delta(\gamma,\gamma') \cdot \frac{\mathrm{E}\left[\prod_k A_k^{\alpha_k(\gamma')}\right]}{\prod A_k^{\alpha_k(\gamma')}}$$

- We obtain any moment $\langle (J-\bar{J})^n\rangle = \langle (F(U(T)) - \bar{F}(U(T)))^n\rangle$ through the binomial expansion:

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

- Once the state equations are solved in t,s to provide $U(t,s)$ over $[0,T]$ and $[0,s_f]$, any moment of $F(U(T))$ can be calculated (within an error tolerance depending on s_f)
- The above formulations provide moments of the observables and quantum interferences
- Expressions can also be provided in terms of quantum pathways
- For example, first moment of transition probability:

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

- which is comprised of the following terms:

$$\mathrm{E}\left[(\mathrm{Re},\mathrm{Im}\ c_{ji}(T))^2\right] = \mathrm{E}\left[\left\{\sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n} A_1^{\alpha_1}\cdots A_n^{\alpha_n}\right\}^2\right]$$
$$= \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha_1',\cdots,\alpha_n')} 2\mathrm{Re},\mathrm{Im}\ c_{\alpha_1,\cdots,\alpha_n} c_{\alpha_1',\cdots,\alpha_n'}\ \mathrm{E}[A_1^{\alpha_1+\alpha_1'}]\cdots \mathrm{E}[A_n^{\alpha_n+\alpha_n'}] +$$
$$\sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{Re},\mathrm{Im}\ c^2_{\alpha_1,\cdots,\alpha_n} \mathrm{E}[A_1^{2\alpha_1}]\cdots \mathrm{E}[A_n^{2\alpha_n}]$$

3.4. General noise and uncertainty distributions

- Expressions above for $\mathrm{E}[c_{ji}]$, 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

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

- 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

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

- 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 (**may omit**):

$$\langle x^3 \rangle = 3\mu\sigma^2 + \mu^3$$
$$\langle x^4 \rangle = 3\sigma^4 + 6\mu^2\sigma^2 + \mu^4$$

- Applying the binomial expansion, we obtain any moment $\langle (x - \bar{x})^n \rangle$
- 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 $\langle (x - \bar{x})^n \rangle = 0$.

3.5. A generating function for quantum observable moment calculations

- The characteristic or moment-generating function provides moments of a distribution in terms of derivatives of its Fourier transform
- It is possible to express the moments of quantum observables in terms of a type of generating function, through two Fourier transforms
- Defining

$$\phi_k(s') = \langle \exp(\imath s' A_k) \rangle = \int_{-\infty}^{\infty} p(A_k) \exp(\imath s' A_k)\ dA_k$$

and assuming amplitude noise that is uncorrelated between modes, the generating function for the expectation of the nth power of $F(U(T))$ can be written

$$f(\gamma,\gamma',s') = \int_0^{s_f} F^n(U(T,s))\exp(-i\gamma s)\ ds \cdot \frac{\prod_k \phi_k(s')}{\prod A_k^{\alpha_k(\gamma')}}$$

with the expectation expressed in terms of the generating function as

$$\mathrm{E}[F^n(U(T))] = \sum_{\gamma'\in\Gamma} \int_0^{s_f} F^n(U(T,s))\exp(-i\gamma s)\ ds\ \cdot \delta(\gamma,\gamma') \cdot \frac{\prod_k (-\imath)^{\alpha_k(\gamma')} \left[\frac{\partial^{\alpha_k(\gamma')}}{\partial s'^{\alpha_k(\gamma')}}\phi_k(s')\right]_{s'=0}}{\prod A_k^{\alpha_k(\gamma')}}$$

- Note that by changing the $\sum'_\gamma$ to run over a subset of Γ, we can extract expectations of specified interferences (in the case $n=1$) or any other subset of terms
- Similarly, the PMP first-order conditions for optimality for moments (see below) can be expressed in this form as well

4. ROBUST CONTROL OF QUANTUM DYNAMICS

4.1. Pontryagin Maximum Principle for Quantum Robust Control

- The PMP for quantum control can be extended to control of moments
- For linear systems with additive noise, it is possible to obtain an analytical solution for the time evolution of the first and second moments of the state variables (e.g. for the Ornstein-Uhlenbeck process)
- This is the basis for the linear quadratic (Gaussian) regulator (LQR/LQG) problems in feedback control, where the first and second moments are generally controlled
- The LQG is derived in terms of the Hamilton-Jacobi-Bellman partial differential equations
- The LQG formulation is used in the theory of linear quantum filtering and real-time feedback control
- For bilinear systems (multiplicative noise) such an analytical solution does not exist
- However, it is possible to derive a PMP for quantum control of moments of any objective function in the presence of field or Hamiltonian uncertainty, starting from the robustness analysis theory developed above
- This provides the theoretical foundation for model-based robust control of molecular quantum systems.
- It also has applications to the robust control of other bilinear systems with multiplicative noise.
- The state and costate equations for the robust qc PMP are partial differential equations.
- Both state and costate are functions of t and the timelike variable s
- A generalized expression for the moments of quantum observables is required in order to derive the PMP (see above)
- The costate equation and PMP (first-order conditions for optimality) for quantum robust control can be derived analogously to the deterministic quantum control PMP (**derivation to be inserted**)
- The costate equation for quantum robust control is a partial differential equation in t, s:

$$\frac{\partial}{\partial t}\phi(t,s) = -\frac{\imath}{\hbar}H_I(t,s)\phi(t,s),$$

subject to the terminal boundary condition $\phi(T,s) = \nabla_U F(U(T,s))$

- Analogously to $\mathrm{E}[U(T)]$, the expectation of the quantum control costate at the final time, $\phi(T)$, can be obtained as follows for amplitude noise:

$$\mathrm{E}[\phi(T)] = \sum_{\gamma'\in\Gamma} \int_0^{s_f} \nabla_U F(U(T,s)) \exp(-i\gamma s)\ ds\ \cdot \delta(\gamma,\gamma') \cdot \frac{\mathrm{E}\left[\prod_k A_k^{\alpha_k(\gamma')}\right]}{\prod A_k^{\alpha_k(\gamma')}}$$

- Note $\mathrm{E}[\phi(T)] \neq \nabla_U \mathrm{E}[F(U(T))]$
- The PMP-Hamiltonian function for a state variable function of t, s (no Lagrange cost) is

$$\mathcal{H}(x(t,s),\phi(t,s),u(t)) = \langle \phi(t,s), f(x(t,s),u(t))\rangle$$

- For quantum control,

$$\begin{aligned}\mathcal{H}(U(t,s),\phi(t,s),\varepsilon(t)) &= \langle \phi(t,s), -\frac{i}{\hbar} H_I(t,s)U(t,s)\rangle \\ &= -\frac{i}{\hbar}\mathrm{Tr}\left\{\phi(t,s)H_I(t,s)U(t,s)\right\} \\ &= -\frac{i}{\hbar}\mathrm{Tr}\left\{U^\dagger(T,s)\nabla_U F(U(T,s))U^\dagger(t,s)\mu_I\varepsilon(t)U(t,s)\right\}\end{aligned}$$

- Using the PMP-Hamiltonian function we can obtain first-order conditions for optimality of moments
- Expressing the Lagrangian in terms of $\mathcal{H}$ and integrating $\langle \phi(t), \frac{dU(t)}{dt}\rangle$ by parts, we get

$$\bar{J} \;=\; F(U(T)) \;-\; i\mathrm{Tr}(\phi(T)U(T)) \;+\; \frac{i}{\mathrm{Tr}}(\phi(0)U(0))) \;+\; \int_0^T \mathcal{H}(U(t),\phi(t),\varepsilon(t)) \;+\; \mathrm{Tr}\left(\frac{d\phi(t)}{dt}U(t)\right)\quad dt,$$

- The first-order variation of this Lagrangian is

$$\begin{aligned}\mathrm{E}\left\{\delta\bar{J}\right\} = \mathrm{Tr}\left(\mathrm{E}\left[\nabla_{U(T)}F(U(T)) - \phi^\dagger(T)\right]\delta U^\dagger(T)\right) + \mathrm{Tr}\left(\mathrm{E}\left[\phi^\dagger(0)\right]\delta U^\dagger(0)\right) + \\ + \int_0^T \mathrm{Tr}\left[\mathrm{E}\left[\nabla_{U(t)}\mathcal{H} + \frac{d\phi^\dagger(t)}{dt}\right]\delta U^\dagger(t)\right] + \mathrm{E}\left[\nabla_{\varepsilon(t)}\mathcal{H}\right]\cdot\delta\varepsilon(t)\ dt.\end{aligned}$$

- This expression can be evaluated by first writing the s-evolved Lagrangian $\bar{J}$ and then considering its first-order variation

$$\begin{aligned}\delta\bar{J} = \mathrm{Tr}\left(\left[\nabla_{U(T,s)}F(U(T,s)) - \phi^\dagger(T,s)\right]\delta U^\dagger(T)\right) + \mathrm{Tr}\left(\left[\phi^\dagger(0,s)\right]\delta U^\dagger(0)\right) + \\ + \int_0^T \mathrm{Tr}\left[\left[\nabla_{U(t,s)}\mathcal{H} + \frac{\partial\phi^\dagger(t,s)}{\partial t}\right]\delta U^\dagger(t)\right] + \left[\nabla_{\varepsilon(t)}\mathcal{H}\right]\cdot\delta\varepsilon(t)\ dt.\end{aligned}$$

- The corresponding first-order conditions (Euler-Lagrange equations) follow from the requirement that $\delta\mathrm{E}\left[\bar{J}\right] = 0$ for any specified *deterministic* variation $\delta\varepsilon$, and hence for any deterministic variation $\delta U(t)$.
- If the uncertainty is in the system Hamiltonian, $\mathrm{E}\left[\nabla_{\varepsilon(t)}\mathcal{H}\right] = \nabla_{\varepsilon(t)}\mathrm{E}\left[\mathcal{H}\right]$
- For control Hamiltonian uncertainty with parameter vector θ,

$$\begin{aligned}\mathrm{E}[\frac{\partial}{\partial\varepsilon(t)}\mathcal{H}(U,\phi,\varepsilon)] &= \frac{\partial}{\partial\varepsilon(t)}\mathrm{E}[\mathcal{H}(U,\phi,\varepsilon)] \\ &= \frac{\partial}{\partial\varepsilon(t)}\sum_{\gamma'\in\Gamma}\langle\phi(t,s), -\frac{i}{\hbar}H_I(t,s)U(t,s)\rangle\ \exp(\imath\gamma s)\ ds\ \delta(\gamma,\gamma')\frac{\mathrm{E}[\prod_k\theta_k^{\alpha_k(\gamma')}]}{\prod_k\theta_k^{\alpha_k(\gamma')}} \\ &= -\frac{i}{\hbar}\sum_{\gamma'\in\Gamma}\mathrm{Tr}\left\{U^\dagger(T,s)\nabla_U F(U(T,s))U^\dagger(t,s)\mu_I U(t,s)\right\}\ \exp(-\imath\gamma s)\ ds\ \times \\ &\quad\times\ \delta(\gamma,\gamma')\frac{\mathrm{E}[\prod_k\theta_k^{\alpha_k(\gamma')}]}{\prod_k\theta_k^{\alpha_k(\gamma')}}\end{aligned}$$

which can be written in terms of the t- and s-evolved dipole operator $\mu_I(t,s) = U^\dagger(t,s)\mu_I U(t,s)$

- **The explicit forms of $\nabla_U F(U)$ for observables and gates can be substituted above**
- The first-order condition is $\mathrm{E}[\frac{\partial}{\partial\varepsilon(t)}\mathcal{H}(U,\phi,\varepsilon)] = 0, \ \forall t \in [0,T]$
- Note that the first-order conditions are above are written for direct optimization of $\varepsilon(t)$ in the time domain, but the first-order condition can also be written in the frequency domain
- Using the PMP-Hamiltonian function we can obtain first-order conditions for optimality of moments
- For amplitude uncertainty,

$$\mathrm{E}[\frac{\partial}{\partial A(\omega)}\mathcal{H}(U,\phi,A] =$$
$$= -\frac{i}{\hbar}\sum_{\gamma'\in\Gamma}\int_0^{s_f}\mathrm{Tr}\left\{U^\dagger(\omega_f,s)\nabla_U F(U(\omega_f,s))U^\dagger(\omega,s)\mu_I U(\omega,s)\right\}\ \exp(-\imath\gamma s)\ ds\ \times$$
$$\times\ \delta(\gamma,\gamma')\frac{\mathrm{E}[\prod_k A_k^{\alpha_k(\gamma')}]}{\prod_k A_k^{\alpha_k(\gamma')}}$$

- Here, $A_k = A(\omega_k)$ denotes a subset of noisy amplitude modes
- Note that use of the PMP for amplitude noise implies that the control optimization is executed in the frequency domain through modification any of the amplitudes $A(\omega)$, of which the above subset is subject to noise

5. LEADING ORDER TAYLOR EXPANSIONS

The eventual goal of robustness analysis is to understand how a control field achieves robust transition amplitude and probability when distribution is present in the control or system parameters. We consider robustness of the control performance measure (e.g., transition probability) to variations $\delta\theta$ in the parameters. Assuming the covariance matrix of parameter estimates is available as in (**??**), the posterior distribution of $\delta\theta$ is modeled as a multivariate normal distribution, i.e., $\theta \sim \mathcal{N}(\hat{\theta},\Sigma)$. Through choice of a confidence level c, we can specify the set of possible realizations of $\delta\theta$ corresponding to that confidence level as:

$$\Theta = \{\delta\theta \mid \delta\theta^T\Sigma^{-1}\delta\theta \ \leq \ \chi^2_K(c)\}$$
$$\delta\theta = \theta - \hat{\theta}, \tag{8}$$

where χ^2_K denotes the chi-square distribution with K degrees of freedom, K denoting the number of noisy or uncertain parameters. The distribution of $\delta\theta$ can be used to estimate the corresponding distribution of the control performance measure J. Let $J = P_{ji}$, the transition probability between states i and j, and consider the case of dipole operator uncertainty as an example. With a 1st order Taylor expansion, the only distribution function that can be derived is a normal distribution with variance

$$\sigma_J^2 \approx \mathrm{Tr}\left[\Sigma\nabla_\theta J(\nabla_\theta J)^T\right], \tag{9}$$

where

$$[\nabla_\theta J]_i = -\imath\mathrm{Tr}\Bigg\{|i\rangle\langle i|, U^\dagger(T)|j\rangle\langle j|U(T)\times \int_0^T U^\dagger(t)X_i\varepsilon(t)U(t)\ dt\Bigg\}, \tag{10}$$

and X_i is the Hermitian matrix obtained by setting $\theta_i = 1,\ \theta_j = 0,\ j \neq i$ in $\mu(\theta)$. Then assuming a normal distribution for J with variance σ_J^2, the worst case deviation of the performance measure can be defined as the lower boundary of the c-confidence interval, i.e.

$$J \sim \mathcal{N}(J(\hat{\theta}),\sigma_J^2), \tag{11}$$
$$\delta J = -\sqrt{2}\sigma_J\ \mathrm{erf}^{-1}(c), \tag{12}$$
$$J_{wc} = J(\hat{\theta}) - \sqrt{2}\sigma_J\ \mathrm{erf}^{-1}(c). \tag{13}$$

With higher order Taylor expansions, one cannot derive a distribution function for δJ analytically; one cannot obtain higher moments from higher order Taylor expansions.

- 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

$$\begin{aligned}
\mathrm{E}[\delta J] &\approx \frac{1}{2}\int_0^T \int_0^T \mathcal{H}(t,t')\mathrm{E}\left[\delta u(t)\delta u(t')\right]\ dt\ dt'\mathcal{O}(||\Sigma||^3) \\
&= \frac{1}{2}\int_0^T \int_0^T \mathcal{H}(t,t')\mathrm{acf}(t,t')\ dt\ dt'
\end{aligned}$$

- 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

- 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

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

- 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 $\mu(\theta)$.

- 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

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

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

6. WORST-CASE ROBUSTNESS ANALYSIS AND CONTROL

As noted above, 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. For example, in a first-order formulation, the problem can be expressed as

$$\max_{\delta\theta\in\Theta} |\delta J|^2 \approx \delta\theta^T(\nabla_\theta J)^T\nabla_\theta J\delta\theta, \tag{14}$$

where Θ was defined in (8) and $\nabla_\theta J$ in (10) (assuming $J = P_{ji}$). If we let $x = \chi_K^{-1}(c)Q\delta\theta$, where $Q^TQ = \Sigma$, then:

$$|\delta J|^2 = \chi_K^2(c)x^TQ^T(\nabla_\theta J)^T\nabla_\theta JQx. \tag{15}$$

Under this change of variables, the constraints are mapped as:

$$\delta\theta^T\Sigma^{-1}\delta\theta \le \chi_K^2(c) \to x^Tx \le 1, \tag{16}$$

and the constrained maximization problems are mapped as follows:

$$\max_{\delta_\theta\in\Theta} |\delta J|^2 \to \max_{x^Tx\le 1} \chi^2(c)x^TQ^T(\nabla_\theta J)^T(\nabla_\theta J)Qx. \tag{17}$$

This problem has the form of a Rayleigh quotient [**?**], which has an analytical solution for J_{wc} and θ_{wc} written in terms of a singular value decomposition. However, since the formulation is first order, it is subject to the same issues of accuracy noted above. Future work will compare the accuracy of these various approaches to estimation of J_{wc} for quantum control systems.

7. QUANTUM ROBUST CONTROL ALGORITHMS

- Pareto Tradeoffs in Robust Control

- *Pareto frontier* of robust control solutions:

$$\{\bar\varepsilon(t)\ \mid\ J_1(\varepsilon(t)) \le J_1(\bar\varepsilon(t))\ \ \vee\ \ J_2(\varepsilon(t)) \le J_2(\bar\varepsilon(t)),\ \ \forall\varepsilon(t)\ne\bar\varepsilon(t)\}$$

- 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 var J, E$[\delta J]$ are approximations: inaccuracies can reduce fidelity if 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 $J_{\text{nom}}^{\max}$ and find fields $\varepsilon(t)$ that minimize var J or maximize E$[\delta J]$.
- Alternatively, use robust optimization with the accurate expressions for moments obtained with MI

7.1. Deterministic algorithms

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

$$\int_0^T \frac{\delta J}{\delta\varepsilon(t)}\delta\varepsilon(t)\; dt = 0, \tag{18}$$

  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 $\delta\varepsilon(t) = f(t) - [\int_0^T \left(\frac{\delta J}{\delta\varepsilon(t')}\right)^2 \; dt']^{-1}\frac{\delta J}{\delta\varepsilon(t)}\int_0^T f(t')\frac{\delta J}{\delta\varepsilon(t')}\; dt'$
- The following equations can be derived by extension of the approaches described in Chakrabarti, Wu and Rabitz, Quantum Multiobservable Control (2008).
- To explore fields holding constant high values of J and E$[\delta J]$ while reducing var J, let

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

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

- 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

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

$$\begin{aligned} a(s,t) &= \frac{\delta J}{\delta\varepsilon(s,t)} + \frac{\delta \mathrm{E}[\delta J]}{\delta\varepsilon(s,t)} \\ f(s,t) &= \frac{\delta\ \mathrm{var}\ J}{\delta\varepsilon(s,t)} \end{aligned}$$

- 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

- Approximate gradient with Dyson series via MI methods described above

- For example,

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

  where the latter two expressions follow from the fact that E is a linear operator. encoding and apply one additional FFT of $\int U_I^\dagger(s,t)\mu U_I(s,t)\exp(\imath\omega t)\ dt$ into γ domain; would need to write expressions for each term in modulated Dyson series, divide by amplitudes to obtain time-domain integrals, then update amplitudes with fixed integrals until amplitudes exceed a specified tolerance

- Less expensive to evaluate - reevaluation of time-domain integrals not needed at each iteration

- Update MI periodically given tolerance setting

- Compare to the expression provided by the PMP for quantum robust control

- 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 $f(s,\omega), g(s,\omega)$

8. NUMERICAL IMPLEMENTATION

8.1. Fourier Encoding

- Encoding of subset of parameters subject to uncertainty

$$\theta_k \to \theta_k \exp(i\gamma_k s), k = 1, ..., n;\ n \leq n_{\max}.$$

Here, unlike the fully encoded equations previously reported, $n_{\max}$ denotes the total number of parameters.

- Assumes uncertainty is in parameters 1,...,n only; without loss of generality, can renumber the parameters so the ones subject to uncertainty are the first n parameters.
- Extract all terms containing $\theta_1^{\alpha_1}....\theta_n^{\alpha_n}$, through amplitude $U_{ji}(T, \gamma = \alpha_1\gamma_1 + ... + \alpha_n\gamma_n)$ (compare analogous expressions from previously reported robustness analysis above, where there was no sum over unencoded parameters):

$$\begin{aligned} &U_{ji}(T, \gamma = \alpha_1\gamma_1 + ... + \alpha_n\gamma_n) = \\ &= \theta_1^{\alpha_1}...\theta_n^{\alpha_n}\Bigg[(i^{m1})\sum_{k_1=n+1}^{n_{\max}}\theta_{k_1}...\sum_{k_{m1}=n+1}^{n_{\max}}\theta_{k_{m1}}...+ \\ &\quad + (i^{m_2})\sum_{k_1=n+1}^{n_{\max}}\theta_{k_1}...\sum_{k_{m2}=n+1}^{n_{\max}}\theta_{k_{m_2}}... + ...\Bigg] \end{aligned}$$

- The coefficient $c_{\alpha_1,...,\alpha_n}$, which is written without specification of a constraint on the α_i's, contains contributions from many different orders
- Hence note for subset encoding $m = \sum_i \alpha_i$ is not a Dyson series order. However, it plays an important role in determining the effect of noise on the pathway norm and interferences involving that pathway, since the ratio $\frac{\mathrm{E}[\prod_k \theta_k]}{\prod_k \theta_k}$ depends on m not the Dyson series order.
- Effect on scaling of required memory - replace nmodes or $n_{\max}$ with the –number of encoded modes–.

8.2. Fourier Decoding

9. RESULTS: EXAMPLE

9.1. Comparison of robustness analysis and robust control based on PMP to leading order and worst-case approximations

10. SUMMARY AND PROSPECTIVE

11. APPENDIX

The upper bound of pathway calculation is:

$$\begin{aligned} |c_{\vec{\alpha}}| &\leq \sum_{l_1=1}^{N}\cdots\sum_{l_{m-1}=1}^{N} d^m \Bigg| \int_0^T e^{\imath\left(\omega_{jl_{m-1}}t_m\right)}\cos(\omega_{k_m}t_m + \phi(\omega_{k_m}))\times \\ &\cdots\times\int_0^{t_{m-1}} e^{\imath\left(\omega_{l_1 i}t_1\right)}\cos(\omega_{k_1}t_1 + \phi(\omega_{k_1}))\ dt_1\cdots dt_m\Bigg| \\ &\leq \sum_{l_1=1}^{N}\cdots\sum_{l_{m-1}=1}^{N} d^m\frac{T^m}{m!} \leq N^{m-1}d^m\frac{T^m}{m!} = \frac{(NdT)^m}{Nm!} \end{aligned}$$

where $|\langle j|\mu|i\rangle| < d$, and $i, j \in [1, N]$. Correspondingly, the upper bound of the Dyson term is given as:

$$|\mathrm{E}[U_{ji}^m(T)]| \leq \frac{(NdT)^m}{Nm!} \sum_{\vec{\alpha}} \prod_{k=1}^{K} \mathrm{E}[A_k^{\alpha_k}]$$

The upper bound on the error associated with the robustness calculations can in turn be determined:

$$\mathrm{E}[U_{ji}(T)] - \sum_{m=1}^{M} \mathrm{E}[U_{ji}^m(T)] = \sum_{m=M}^{\infty} \mathrm{E}[U_{ji}^m(T)]$$

where

$$\left| \sum_{m=m_{max}}^{\infty} \mathrm{E}[U_{ji}^m(T)] \right| \leq \sum_{m=m_{max}}^{\infty} \frac{(NdT)^m}{Nm!} \sum_{\vec{\alpha}} \prod_{k=1}^{K} \mathrm{E}[A_k^{\alpha_k}]$$

$$\sum_{m=m_{max}}^{\infty} \frac{(NdT)^m}{Nm!} \sum_{\vec{\alpha}} \prod_{k=1}^{K} \mathrm{E}[A_k^{\alpha_k}] \approx \sum_{m=m_{max}}^{m_{eps}} \frac{(NdT)^m}{Nm!} \sum_{\vec{\alpha}} \prod_{k=1}^{K} \mathrm{E}[A_k^{\alpha_k}] \tag{19}$$

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

$$\left|\mathrm{E}\left[(\mathrm{Re}, \mathrm{Im}\ c_{ji}(T))^2\right]\right| \leq \sum_{m=2}^{m_{\max}} \sum_{m'<m} \left\{ 2\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots \mathrm{E}[A_n^{\alpha_n+\alpha'_n}] \right\} +$$
$$+ \sum_{m=1}^{m_{\max}} \frac{(NdT)^{2m}}{(Nm!)^2} \left\{ \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{E}[A_1^{2\alpha_1}]\cdots \mathrm{E}[A_n^{2\alpha_n}] \right\},$$
$$\sum_k \alpha_k = m, \sum_{k'} \alpha'_k = m',\ m, m' \in [1, m_{max}]$$

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

$$\left|\mathrm{E}\left[(\mathrm{Re}, \mathrm{Im}\ c_{ji}(T))_m^2\right]\right| \leq \sum_{m'<m} 2\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots \mathrm{E}[A_n^{\alpha_n+\alpha'_n}] +$$
$$+ \frac{(NdT)^{2m}}{(Nm!)^2} \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{E}[A_1^{2\alpha_1}]\cdots \mathrm{E}[A_n^{2\alpha_n}],$$
$$\sum_k \alpha_k = m, \sum_{k'} \alpha'_k = m',\ m, m' \in [1, m_{max}]$$

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

$$\left|\mathrm{E}\left[P_{ji}^m(T)\right]\right| \leq \sum_{m'<m} 4\frac{(NdT)^{m+m'}}{N^2 m! m'!} \sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots \mathrm{E}[A_n^{\alpha_n+\alpha'_n}] +$$
$$+ 2\frac{(NdT)^{2m}}{(Nm!)^2} \sum_{(\alpha_1,\cdots,\alpha_n)} \mathrm{E}[A_1^{2\alpha_1}]\cdots \mathrm{E}[A_n^{2\alpha_n}],$$
$$\sum_k \alpha_k = m, \sum_{k'} \alpha'_k = m',\ m, m' \in [1, m_{max}]$$

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

$$\sum_{(\alpha_1,\cdots,\alpha_n)\neq(\alpha'_1,\cdots,\alpha'_n)} \mathrm{E}[A_1^{\alpha_1+\alpha'_1}]\cdots\mathrm{E}[A_n^{\alpha_n+\alpha'_n}]\Bigg\}+$$

$$\mathrm{E}[A_n^{2\alpha_n}]\Bigg\},$$

where m_{eps} denotes the smallest m such that $\leq$ 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
- Frequency domain gradient

$$\begin{aligned}
\delta U(T) &= -\imath U(T)\int_0^T U^\dagger(t)\mu\delta\varepsilon(t)U(t)\ dt \\
&= -\frac{\imath}{2}U(T)\int_{-\infty}^{\infty} d\omega\ \delta A(\omega)\int_0^T \mu(t)[\exp(\imath\omega t)\exp(\imath\phi(\omega)) + \exp(-\imath\omega t)\exp(-\imath\phi(\omega))]\ dt \\
\frac{\delta U(T)}{\delta A(\omega)} &= -\frac{\imath}{2}U(T)\int_0^T \mu(t)[\exp(\imath\omega t)\exp(\imath\phi(\omega)) + \exp(-\imath\omega t)\exp(-\imath\phi(\omega))]\ dt \\
&= -\frac{\imath}{2}U(T)\left\{\exp(\imath\phi(\omega))\int_0^T \mu(t)\exp(\imath\omega t)\ dt + \exp(-\imath\phi(\omega))\int_0^T \mu(t)\exp(-\imath\omega t)\ dt\right\}
\end{aligned}$$

- 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.