Lie algebraic quantum control mechanism analysis

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- Existing methods for quantum control mechanism identification do not exploit analytic features of control systems to delineate mechanism (or, they frame mechanism in terms of the unitary propagator, which does not have convenient interpretation in terms of directional motion induced by control)
- According to the CBH theorem, control mechanisms for bilinear systems work by generating new directions in the Lie group through commutators $[H_0, \mu], \cdots$
- These commutators must span the entire Lie algebra $u(N)$ for the system to be controllable; control mechanisms may be formally decomposed into contributions from each commutator
- For high-dimensional systems like those encountered in molecular control or composite gate spin control, (the amplitudes of) motion induced by the control $\varepsilon(t)$ in each direction $[H_0, \mu]$ cannot be determined analytically
- *Encoding* methods enable the extraction of the amplitudes associated with each Lie algebra direction by Fourier transforms into the domain of an auxiliary encoding parameter

1 Gate control mechanism and robustness classification

Since $U(N)$ (and $SU(N)$) are compact Lie groups, it is possible to generate any $U \in U(N)$ through sequential application of elements of a complete set of generators (see definition in Lie algebra rank below) $H_1, \cdots, H_k$ for $U(N)$, i.e., $W = \exp(H_k t_k) \cdots \exp(H_1 t_1)$. This strategy is now commonly applied in gate decomposition strategies wherein the unitary gate W on n qubits (2^n dimensional Hilbert space) is constructed through applications of various $U_i = \exp(H_i t_i)$ which each act on only 1-2 qubits.

Such *uniform finite generation* of the Lie group is sometimes referred to as "bang-bang controllability" (which is a more stringent criterion than full controllability). However, provided the system is controllable, it is also possible to generate any W through simultaneous applications of $H_2, \cdots, H_k$ at every time, by shaping *control functions* $\varepsilon(t_i),\ i = 2, k$ over $[0, T]$. Typically, bang-bang controllability requires a greater total evolution time T than control pulse shaping, as will be demonstrated below in the CBH section. Bang-bang control strategies are often preferred when bandwidth for pulse shaping is limited. However, in the presence of available bandwidth, the latter approach may be preferred, for several reasons including the shorter time evolution over which the system may decohere. The improved robustness to decoherence is counterbalanced by a decreased robustness to control field noise and uncertainty in the Hamiltonian parameters. While the associated control problems cannot be analytically solved, once the optimal control is found, the mechanism by which it reaches the target gate can be understood. The subject of our analysis is two-fold: (i) to interrogate control mechanisms for distinct classes of control systems that differ according to criteria such as dynamical Lie algebra depth (see below) (ii) to assess robustness to control field noise for such control strategies. Both (i) and (ii) will be assessed for various types of control systems (Hamiltonians), including those where the qubits are encoded in molecular vibrational states, molecular rotational states, and nuclear spin states, which constitute several of the most popular physical systems for encoding quantum computation.

1.1 Lie algebra rank condition for controllability

The rank condition for full controllability (i.e., any unitary matrix can be produced at some time T) is

$$\text{rank}\{[H_0, \mu], [H_0, [H_0, \mu]], [\mu, [H_0, \mu]], \cdots\}_{LA} = N^2.$$

The Lie algebra in brackets is called the *dynamical Lie algebra*. For $H_0, \mu \in u(N)$; for traceless Hermitian matrices, i.e., $H_0, \mu \in su(N)$, the rank must be N^2-1 for full controllability on $SU(N)$ (global phase irrelevant for most quantum gates). The set of skew-Hermitian matrices $[H_0,\mu], [H_0,[H_0,\mu]], \cdots$ are then said to span the Lie algebra. The *depth* of the dynamical Lie algebra is defined as the number of commutators required to span this algebra. Proposed gate control systems may differ considerably in Lie algebra depth. Control systems with similar dynamical Lie algebra depth may display common gate control mechanisms, a conjecture that may be interrogated by Lie algebraic mechanism analysis, but not unitary mechanism analysis based on the Dyson expansion.

2 Lie algebraic representation of gate control pathways by Campbell-Baker-Hausdorff / Magnus expansion

Consider the CBH expansion of $\exp(A)\exp(B)\exp(C)$ for skew-Hermitian matrices A, B, C (put in Appendix):

$$
\begin{aligned}
&\exp(A)\exp(B)\exp(C) = \exp(A)\exp(B + C + \frac{1}{2!}[B,C] + \frac{1}{12}[B,[B,C]] + \frac{1}{12}[C,[B,C]]\cdots \\
&= \exp\Big\{A + (B + C + \frac{1}{2!}[B,C] + \frac{1}{12}[B,[B,C]] + \frac{1}{12}[C,[B,C]]\cdots) + \\
&\quad \frac{1}{2!}[A, B + C + \frac{1}{2!}[B,C] + \frac{1}{12}[B,[B,C]] + \frac{1}{12}[C,[B,C]]\cdots] + \cdots\Big\} \\
&= \exp\Big\{A + (B + C + \frac{1}{2}[B,C] + \frac{1}{12}[B,[B,C]] + \cdots) + \frac{1}{2!}[A,B] + \\
&\quad \frac{1}{2!}[A,C] + \frac{1}{4}[A,[B,C]] + \frac{1}{24}[A,[B,[B,C]]] + \frac{1}{24}[A,[C,[B,C]]]\cdots \\
&\quad + \frac{1}{12}([A,[A,B]] + [A,[A,C]] + \frac{1}{4}[A,[A,[B,C]]] + \frac{1}{24}[A,[A,[B,[B,C]]]] + \frac{1}{24}[A,[A,[C,[B,C]]]]\cdots)\Big\}
\end{aligned}
$$

Let $A = H(t_3)\Delta t, B = H(t_2)\Delta t, C = H(t_1)\Delta t$, with $t_2 = t_1 + \Delta t,\ \Delta t = \frac{t_n - t_1}{n}$. Generalize to

$$\mathbb{T}\exp\left[\int_0^t H(t')\ dt'\right] \equiv \lim_{n\to\infty} \exp(H(t_n)\ \Delta t)\cdots\exp(H(t_2)\ \Delta t)\exp(H(t_1)\ \Delta t).$$

Collecting terms like $[H(t_3), H(t_2)]\Delta t^2, [H(t_3), H(t_1)](\Delta t)^2$ and $[H(t_2), H(t_1)](\Delta t)^2$,(i.e., collecting all first-order commutators), we obtain in the argument of the exponential the integrals:

$$\int_0^t H(t') \int_0^{t'} H(t'')\ dt"dt' - \int_0^t \int_0^{t'} H(t")\ dt" H(t')\ dt'$$
$$= \frac{1}{2!} \int_0^t \int_0^{t'} [H(t'), H(t'')]\ dt"dt'$$

Whereas, collecting all "double commutators" such as

$$[H(t_3), [H(t_3), H(t_2)]], [H(t_3), [H(t_2), H(t_1)]], [H(t_2), [H(t_2), H(t_1)]],$$

etc provides the integrals

$$\frac{1}{12} \int_0^t H(t') \left(\int_0^{t'} H(t") \int_0^{t"} H(t''')\ dt'''dt" - \int_0^{t'} \int_0^{t"} H(t''')\ dt''' H(t")\ dt" \right)\ dt' -$$
$$- \int_0^t \left(\int_0^{t'} H(t") \int_0^{t"} H(t''')\ dt'''\ dt'' - \int_0^{t'} \int_0^{t"} H(t''')\ dt''' H(t")\ dt" \right) H(t')\ dt'$$
$$= \frac{1}{12} \int_0^t \int_0^{t'} \int_0^{t"} [H(t'), [H(t"), H(t''')]\ dt'''dt"dt'$$

and

$$\frac{1}{4} \int_0^t \int_0^{t'} \int_0^{t'} [[H(t'), H(t")], H(t''')]\ dt'''dt"dt'$$

In time-ordered exponential, the CBH theorem provides "commutators of multiple time integrals" that "map" to multiple integrals in Dyson expansion.

2.1 The Magnus expansion for the controlled propagator: systems with one control Hamiltonian

From the above we obtain

$$\mathbb{T}\exp\left\{ \int_0^t H(t')\ dt' \right\} = \exp\Bigg\{ \int_0^t H(t')\ dt' + \frac{1}{2!} \int_0^t \int_0^{t'} [H(t'), H(t'')]\ \ dt"dt' +$$
$$\frac{1}{12} \int_0^t \int_0^{t'} \int_0^{t'} [H(t'), [H(t"), H(t''')]]\ \ dt'''dt"dt' + \frac{1}{4} \int_0^t \int_0^{t'} \int_0^{t"} [[H(t'), H(t")], H(t''')]\ \ dt'''dt"dt' + \cdots \Bigg\}$$

which is called the Magnus series expansion [1] for the unitary propagator (note the domain of integration differs in the last two terms). The commutators ensure unitarity since $[A, B]$ is skew-Hermitian if A, B are skew-Hermitian, unlike the Dyson expansion. Approximation of this expression requires exponentiation of n-th order argument. Recursion formulas for the higher order terms are available [2, 3]. The recursion formula is, however, not necessary for the purposes of MI, as we will see below, since the MI algorithm automatically extracts the contributions of the relevant commutators given $A_T(s)$. When the control optimization is done in the frequency domain (particularly useful for systems that satisfy the rotating wave approximation), it is possible to analytically compute lower order integrals in the Magnus expansion, although we do not pursue this topic in the current work.

Now let $\varepsilon(t) \rightarrow -\varepsilon(t)$, and reexpress the 2nd order term in CBH with choice $H(t) = H_0 + \mu\varepsilon(t)$:

$$
\begin{aligned}
&\frac{1}{2!}\int_0^t\int_0^{t'} [H(t'), H(t'')]\ dt"dt' = \\
&\frac{1}{2!}\int_0^t (H_0+\mu\varepsilon(t'))\int_0^{t'}(H_0+\mu\varepsilon(t"))dt'"dt' - \int_0^t\int_0^{t'}(H_0+\mu\varepsilon(t"))\ dt"(H_0+\mu\varepsilon(t'))dt' \\
&= \frac{1}{2!}\int_0^t\int_0^{t'} H_0^2 + H_0\mu\varepsilon(t") + \mu H_0\varepsilon(t') + \mu^2\varepsilon(t")\varepsilon(t')\ dt"dt' - \int_0^t\int_0^{t'} H_0^2 + H_0\mu\varepsilon(t') + \mu H_0\varepsilon(t") + \mu^2\varepsilon(t")\varepsilon(t')\ dt"dt' \\
&= \frac{1}{2!}\int_0^t\int_0^{t'} [H_0,\mu]\varepsilon(t") - [H_0,\mu]\varepsilon(t')\ dt"dt' \\
&= \frac{1}{2!}[H_0,\mu]\int_0^t\int_0^{t'}(\varepsilon(t") - \varepsilon(t'))\ dt"dt' \\
&= \frac{1}{2!}[H_0,\mu]\int_0^t\left(\int_0^{t'}\varepsilon(t")\ dt" - t'\varepsilon(t')\right)\ dt' \\
&= \frac{1}{2!}[H_0,\mu]\left(\int_0^t\int_0^{t'}\varepsilon(t")\ dt"dt' - \int_0^t t'\varepsilon(t')\ dt'\right)
\end{aligned}
$$

Similarly for the two 3rd-order terms in the Magnus expansion:

$$
\begin{aligned}
&\frac{1}{12}\int_0^t (H_0+\mu\varepsilon(t'))\left([H_0,\mu]\int_0^{t'}\int_0^{t'}(\varepsilon(t''') - \varepsilon(t"))\ dt'''dt"\right)\ dt' \\
&\qquad - \frac{1}{12}\int_0^t\left([H_0,\mu]\int_0^{t'}\int_0^{t'}(\varepsilon(t''') - \varepsilon(t"))dt'''dt''\right)(H_0+\mu\varepsilon(t'))\ dt' = \\
&= \frac{1}{12}\left\{[H_0,[H_0,\mu]]\int_0^t\int_0^{t'}\int_0^{t'}(\varepsilon(t''') - \varepsilon(t"))\ dt'''dt''dt' + [\mu,[H_0,\mu]]\int_0^t\varepsilon(t')\int_0^{t'}\int_0^{t'}(\varepsilon(t''') - \varepsilon(t"))\ dt'''dt"dt'\right\},
\end{aligned}
$$

$$\frac{1}{4}[H_0,\mu]\int_0^t\int_0^{t'}(\varepsilon(t")-\varepsilon(t'))\left(\int_0^{t"}H_0+\mu\varepsilon(t''')\,dt'''\right)dt"\,dt'$$
$$-\frac{1}{4}\int_0^t\int_0^{t'}(\varepsilon(t")-\varepsilon(t'))\left(\int_0^{t"}H_0+\mu\varepsilon(t''')dt'''\right)[H_0,\mu]\,dt"\,dt'=$$
$$=-\frac{1}{4}\left\{[H_0,[H_0,\mu]]\int_0^t\int_0^{t'}(\varepsilon(t")-\varepsilon(t'))\int_0^{t"}dt'''dt''dt'+[\mu,[H_0,\mu]]\int_0^t\int_0^{t'}(\varepsilon(t")-\varepsilon(t'))\int_0^{t"}\varepsilon(t''')\,dt'''dt"dt'\right\}.$$

The same field power appears in all n-th order Magnus expansion terms containing the same power of μ.

The reason that bang-bang control strategies generally require longer time (and hence are more susceptible to decoherence) than control function pulse shaping strategies is that in the latter case, all directions in the Lie group tangent bundle (parameterized by skew-Hermitian matrices) can be generated in arbitrarily small time (although this does not imply that any U can be generated in arbitrarily small time). By contrast, bang-bang strategies require finite time to generate all group directions. In other words, the control functions are constrained in bang-bang control strategies.

The above analysis may be directly extended to systems with multiple control Hamiltonians.

2.1.1 Convergence of the Magnus expansion

Various studies have addressed the radius of convergence of the Magnus expansion [4, 5, 2]. The series does not always converge to the time ordered exponential, especially for strong fields and long evolution times T. The tightest bound on the radius of convergence derived thus far is [5]

$$\int_0^t\sqrt{\mathrm{Tr}[H^\dagger(t')H(t')]}\,dt'\le\pi.$$

The bound is not sharp, in that the radius of convergence is greater for many systems, but it may suffice for the purposes of MI. After finding the optimal control $\bar{\varepsilon}(t)$, we compute $t_i,\ i=0,\cdots,n-1$ such that

$$\int_{t_i}^{t_{i+1}}\sqrt{\mathrm{Tr}[(H_0-\bar{\varepsilon}(t'))^\dagger(H_0-\bar{\varepsilon}(t'))]}\,dt'=\pi.$$

with $t_0=0$ and $t_n=T$ and carry out MI on each time interval $[t_i,t_{i+1}]$ corresponding to propagator $U(t_{i+1},t_i)$. The total controlled propagator is $U(T,0)=\prod_{i=0}^{n-1}U(t_{i+1},t_i)$.

2.1.2 Lie algebraic encoding/decoding theory

Now letting $-\varepsilon(t) \to \varepsilon(t)$, the controlled evolution can be represented in the form $U_T(\varepsilon(t)) = \exp[A_T(\varepsilon(t)]$, with

$$A_T(\varepsilon(t)) = H_0 - \mu\varepsilon(t) - \frac{1}{2!}[H_0,\mu]\int_0^t\int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt"dt - \frac{1}{12}[H_0,[H_0,\mu]]\int_0^t\int_0^{t'}\int_0^{t"} \varepsilon(t''') - \varepsilon(t")\ dt'''dt"dt' +$$
$$-\frac{1}{4}[H_0,[H_0,\mu]]\int_0^t\int_0^{t'}\int_0^{t'} \varepsilon(t''') - \varepsilon(t")\ dt'''dt"dt' +$$
$$+\frac{1}{12}[\mu,[H_0,\mu]]\int_0^t \varepsilon(t')\int_0^{t'}\int_0^{t"} \varepsilon(t''') - \varepsilon(t")\ dt'''dt"dt' +$$
$$+\frac{1}{4}[\mu,[H_0,\mu]]\int_0^t \varepsilon(t')\int_0^{t'}\int_0^{t'} \varepsilon(t''') - \varepsilon(t")\ dt'''dt"dt' + \cdots$$

and the encoded controlled evolution may be represented $U_T(\varepsilon(t), s) = \exp[A_T(\varepsilon(t), s)]$. The structure of the Hermitian matrix $A_T(\varepsilon(t), s)$ depends on the encoding strategy, and several forms are enumerated below.

Numerically, $A_T(s)$ is computed via

$$A_{ij}(s) = \{\mathrm{logm}[U(s)]\}_{ij}$$

Due to the fact that the matrix logarithm is not injective (it is a one-to-many mapping), we choose $A_T(s)$ so that its eigenvalues lie on the principal branch. This assumption may be validated by direct computation of lower order integrals, e.g. $\int_0^t\int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt"dt'$. An alternative, computationally less expensive approach is to follow the evolution of the eigenvalues $(\exp(i\theta_1), \cdots, \exp(i\theta_N))$ of $U(t)$ during the evolution of the system over $t \in [0, T]$; assign each eigenvalue $i\theta_j$ of $A_T(s)$ to an appropriate branch according to the number of times that $\exp(i\theta_j)$ has wrapped around the circle. Explicitly, for all $t \in [0, T]$, we have $U(t) = \exp(A(t))$, with

$$A(t) = \mathrm{logm}\left\{ V(t)\begin{bmatrix} \exp(i\theta_1(t)) & & \\ & \ddots & \\ & & \exp(i\theta_N(t)) \end{bmatrix} V^\dagger \right\} = V(t)\begin{bmatrix} i\theta_1(t) & & \\ & \ddots & \\ & & i\theta_N(t) \end{bmatrix} V^\dagger(t). \quad (1)$$

where $V(t)$ is a unitary matrix and $\theta_i(0) = 0,\ i = 1, \cdots, N$. The principal branch of the logarithm is defined as $-\pi \le \theta_i(t) \le \pi,\ \forall\ i$. An equivalence relation maps $\theta_i(t) = \pi + x$ and $\theta_i(t) = -\pi + x$

to the same unitary matrix, but the skew-Hermitian logarithms are inequivalent. However, since each $\theta_i(t),\ t \in [0, T]$ is a smooth function of time, each $\theta_i(t)$ may be assigned to the appropriate branch by following its time evolution.

We briefly compare unitary MI based on the Dyson expansion

$$\mathbb{T}\exp\left[-\frac{i}{\hbar}\int_0^t H(t')\ dt'\right] = I + \frac{i}{\hbar}\int_0^t H(t')\ dt' + \left(\frac{i}{\hbar}\right)^2 \int_0^t H(t') \int_0^{t'} H(t")\ dt" dt' + \\ + \int_0^t H(t') \int_0^{t'} H(t") \int_0^{t"} H(t''')\ dt''' dt" dt' + \cdots$$

to Lie algebraic MI. First, note that truncation of Dyson series to any finite order is not unitary. Second, consider the second order term in Dyson series (for comparison to the CBH derivation, we use $\varepsilon(t) \to -\varepsilon(t)$):

$$H_0^2 \int_0^t \int_0^{t'} dt" dt' + H_0\mu \int_0^t \int_0^{t'} \varepsilon(t")\ dt" dt' + \mu H_0 \int_0^t \varepsilon(t') \int_0^{t'} dt" dt' + \mu^2 \int_0^t \varepsilon(t') \int_0^{t'} \varepsilon(t"))\ dt" dt'$$

The integrals in the second two terms appear in the CBH matrix exponential argument at second order. However, note that the Magnus expansion has an additional integral (with coefficient $\frac{1}{12}$) associated with this commutator. Since the Magnus series appears in the exponent, it may be expected that this expansion converges more quickly, but the convergence should be compared numerically in any given case by explicit MI in both representations.

Scaling the matrix elements of H_0, μ and the field amplitudes can ensure that the eigenvalues of A will lie on the principal branch, and may allow discrimination of mechanism classes between systems of differing Lie algebra depth, but such scaling cannot be used to extract the true mechanism (without commensurate scaling of T).

If the eigenvalues of $A_T(s)$ are not placed on the appropriate branches, the inverse FT for decoding will not properly identify control mechanisms. Possible *numerical* issues with Lie algebraic encoding/decoding include distortion of the harmonic characteristic functions upon the matrix logarithm operation, which may compromise the accuracy of the inverse FT; finer s-discretization may be required. The length of the s-domain interval $[0, s_f]$ must be set in conjunction with the s-step length in order to maximize discrimination of pathways while minimizing computational expense. These issues must be studied in simulations.

Note that unlike $U_T(s)$ in unitary MI, contributions to the matrix elements of $A_T(s)$ obtained from Lie algebraic MI cannot be physically interpreted as state-to-state transition amplitudes; rather the interest is in the commutator/directional contributions.

check method by explicit computation of some integrals

3 Time-independent Hamiltonian encoding

3.1 H_0, μ element encoding

- Here the matrix elements of H_0 and μ are each individually encoded

$$H0_{ij} \rightarrow H0_{ij} \exp(i\gamma_{ij} s)$$

$$\mu_{ij} \rightarrow \mu_{ij} \exp(i\beta_{ij} s)$$

  such that the matrix elements of the commutators are encoded e.g. as follows:

$$[H_0, \mu]_{ij} \rightarrow [H_0(s), \mu(s)]_{ij} = \sum_k \{H_{ik}\mu_{kj} \exp[i(\gamma_{ik} + \alpha_{kj})s] - \mu_{ik} H_{kj} \exp[i(\alpha_{ik} + \gamma_{kj})s]\}$$

- For $[H_0, \mu]$-based encoding, the encoded Hermitian generator of controlled dynamics is

$$[A_T(s, \varepsilon(t))]_{ij} = H0_{ij} \exp[i(\gamma_{ij} s] - \mu_{ij} \exp[i(\gamma_{ij} s]\varepsilon(t) -$$
$$\frac{1}{2} \sum_k \{H0_{ij}\mu_{kj} \exp[i(\gamma_{ik} + \alpha_{kj})s] - \mu_{ik} H0_{kj} \exp[i(\alpha_{ik} + \gamma_{kj})s]\} \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt" dt' +$$
$$- [H_0(s), [H_0(s), \mu(s)]]_{ij} \left\{ \frac{1}{12} \int_0^t \int_0^{t'} \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' - \frac{1}{4} \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t') \int_0^{t"}\ dt''' dt" dt' \right\}$$
$$+ [\mu(s), [H_0(s), \mu(s)]]_{ij} \left\{ \frac{1}{12} \int_0^t \varepsilon(t') \int_0^{t'} \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' - \frac{1}{4} \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t') \int_0^{t"} \varepsilon(t''')\ dt''' dt" dt' \right\}$$

  where the second order and higher terms have not been expanded. To truncate the Magnus expansion to include only contributions from a selected set (order) of commutators, eliminate the corresponding modes after the FT and then execute an inverse FT back into the s-domain.

- Encoding only μ_{ik}'s is also possible: $\sum_i \sum_k H0_{ik}\mu_{kj}\exp[i\alpha_{kj}s]$ Note that these amplitudes should not be interpreted as n-photon paths, as in the Dyson formulation. For this reason, element-by-element encoding of H_0, μ is not as useful as in standard unitary MI. However such encoding strategies may be useful for extracting commutator contributions directly from unitary MI, as discussed above (to be treated later if necessary).

- Decoding: FT into frequency domain conjugate to s-variable, check frequency-domain amplitudes of $(\gamma_{ik} + \alpha_{kj}), (\alpha_{ik} + \gamma_{kj})$ modes; subtract as above

3.2 Full matrix encodings

These are the preferred time-independent Hamiltonian encoding implementations.

3.2.1 μ encoding

- Simultaneously extract all $[H_0, \mu],\ [H_0, [H_0, \mu]],\ \cdots$ by encoding only μ and with a single s domain parameter

- Does not distinguish pathways or field mode contributions

- Encoded Hermitian generator:

$$[A_T(s, \varepsilon(t))]_{ij} = H_0 - \mu\exp[i\gamma s]\varepsilon(t) - [H_0, \mu]\exp[i\gamma s]\int_0^t\int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt" dt' -$$
$$- [H_0, [H_0, \mu]]\exp[i\gamma s]\left\{\frac{1}{12}\int_0^t\int_0^{t'}\int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' - \frac{1}{4}\int_0^t\int_0^{t'}\int_0^{t"} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt'\right\}$$
$$+ [\mu, [H_0, \mu]]\exp[2i\gamma s]\left\{\frac{1}{12}\int_0^t \varepsilon(t')\int_0^{t'}\int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' - \frac{1}{4}\int_0^t\int_0^{t'} \varepsilon(t") - \varepsilon(t')\int_0^{t"} \varepsilon(t''')\ dt''' dt" dt'\right\}$$

- Decoding: Check Fourier modes $\gamma, 2\gamma, 3\gamma, \cdots$

For any finite T, commutators $[H_0, \cdots, [H_0, \mu]]$ cease to contribute above some finite order; we are interested in determining comparing this order for different control systems and comparing to Lie algebra depth.

3.2.2 H_0, μ encoding

- Here we make the substitutions

$$H_0 \to H_0 \exp(i\gamma s)$$

$$\mu \to \mu \exp(i\beta s)$$

- Then

$$[A_T(s, \varepsilon(t))]_{ij} = H0 \exp[i\gamma s] - \mu \exp[i\alpha s]\varepsilon(t) +$$
$$[H_0, \mu] \exp[i(\gamma+\alpha)s] \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt" dt' +$$
$$- [H_0, [H_0, \mu]] \exp[i(2\gamma+\alpha)s] \left\{ \frac{1}{12} \int_0^t \int_0^{t'} \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' - \frac{1}{4} \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t') \int_0^{t"}\ dt''' dt" dt' \right\} +$$
$$+ [\mu, [H_0, \mu]] \exp[i(\gamma+2\alpha)s] \left\{ \frac{1}{12} \int_0^t \varepsilon(t') \int_0^{t'} \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' - \frac{1}{4} \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t') \int_0^{t"} \varepsilon(t''')\ dt''' dt$$

4 Field encoding

- $\varepsilon(t) = \sum_{m=1}^{M} \frac{b_m}{2} [\exp(i\omega_m t + \phi_m) + \exp(-i\omega_m t - \phi_m)] \to \varepsilon(s,t) = \sum_{m=1}^{M} \frac{b_m}{2} [\exp(i\gamma_m s + i\omega_m t + \phi_m) - \exp(-i\gamma_m s - i\omega_m t - \phi_m)] = \sum_{m=1}^{M} b_m \cos(i\gamma_m s + i\omega_m t + \phi_m)$
- Does not distinguish between control pathways
- Does not distinguish between Lie algebra directions that contain same power of control Hamiltonian μ (these share same characteristic function)
- Provides info on amplitude of each field mode combination contribution to each direction (commutator)
- Isolates contributions of all commutators with same field power:

$$[H_0, \mu] \int_0^t \int_0^{t'} \varepsilon(t") - \varepsilon(t')\ dt" dt' \quad (2)$$

$$[H_0, [H_0, \mu]] \int_0^t \int_0^{t'} \int_0^{t"} \varepsilon(t") - \varepsilon(t')\ dt''' dt" dt' \quad (3)$$

- Given a uniform bound $|\varepsilon(t)| \leq c$ on the control, **the contribution of the integral** in (2) (with the constant series prefactor) to $A_T(s)$ scales as $\frac{cT^2}{2}$ whereas that of (3) scales as $\frac{cT^3}{12} = \frac{cT^3}{2!\cdot 3!}$.

- For field-based encoding, the encoded Hermitian generator of controlled dynamics is

$$
\begin{aligned}
&A_T(\varepsilon(s,t)) = H_0 - \mu \sum_{m_1=1}^{M} b_{m_1} \cos(\omega_{m_1} t' + \phi_{m_1} + \gamma_{m_1} s) \\
&+ [H_0, \mu] \sum_{m_1=1}^{M} b_{m_1} \int_0^t \int_0^{t'} \cos(\omega_{m_1} t" + \phi_{m_1} + \gamma_{m_1} s) - \cos(\omega_{m_1} t' + \phi_{m_1} + \gamma_{m_1} s)\ dt" dt' + \\
&- [H_0, [H_0, \mu]] \Bigg\{ \frac{1}{12} \sum_{m_1=1}^{M} b_{m_1} \int_0^t \int_0^{t'} \int_0^{t'} \cos(\omega_{m_1} t''' + \phi_{m_1} + \gamma_{m_1} s) - \cos(\omega_{m_1} t'' + \phi_{m_1} + \gamma_{m_1} s)\ dt''' dt" dt' \\
&- \frac{1}{4} \sum_{m_1=1}^{M} b_{m_1} \int_0^t \int_0^{t'} \cos(\omega_{m_1} t" + \phi_{m_1} + \gamma_{m_1} s) - \cos(\omega_{m_1} t' + \phi_{m_1} + \gamma_{m_1} s) \int_0^{t"} \ dt''' dt" dt' \Bigg\} \\
&+ [\mu, [H_0, \mu]] \Bigg\{ \frac{1}{12} \sum_{m_1=1}^{M} b_{m_1} \int_0^t \cos(\omega_{m_1} t' + \phi_{m_1} + \gamma_{m_1} s) \\
&\qquad \sum_{m_2=1}^{M} b_{m_2} \int_0^{t'} \int_0^{t'} \cos(\omega_{m_2} t''' + \phi_{m_2} + \gamma_{m_2} s) - \cos(\omega_{m_2} t'' + \phi_{m_2} + \gamma_{m_2} s)\ dt''' dt" dt' \\
&\qquad - \frac{1}{4} \sum_{m_1=1}^{M} b_{m_1} \int_0^t \sum_{m_2=1}^{M} b_{m_2} \int_0^{t'} \cos(\omega_{m_2} t" + \phi_{m_2} + \gamma_{m_2} s) - \cos(\omega_{m_2} t' + \phi_{m_2} + \gamma_{m_2} s) \\
&\qquad \int_0^{t"} \cos(\omega_{m_1} t''' + \phi_{m_1} + \gamma_{m_1} s)\ dt''' dt" dt' \Bigg\} + \cdots
\end{aligned}
$$

- Characteristic functions: $\exp(i\gamma_{m_1} + \cdots + i\gamma_{m_n})$ (sums all n-order pathways). Decoding: Check s-domain amplitude of $(\gamma_{m_1} + \cdots + \gamma_{m_n})$-th mode

- Characteristic function frequencies for commutator with n-th power of μ are sums of $\gamma_{m_1}, \cdots, \gamma_{m_n}$

Noise sensitivity analysis:

- We consider colored (frequency-dependent) noise in $\varepsilon(t)$

- For an infinitesimal variation $\delta A_T(s)$,

$$\delta J = \frac{1}{N} \Re \mathrm{Tr}[(W^\dagger U(T) - U^\dagger(T) W) \delta A_T(s)]$$

- However, the noisy perturbations need not be infinitesimal; instead we simply compute the expected mechanism using field-based encoding by sampling noisy fields according to a frequency dependent distribution function

5 Joint H_0, field encoding

- To distinguish contributions of each combination of field modes to each commutator, can combine $H_0, \varepsilon(t)$ encoding; use only one γ s-frequency to encode whole H_0
- To be completed

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