Quantum gate control mechanism identification

Chakrabarti Group (*J. Quantum Information*)

Abstract

Quantum gates are usually executed by gate decomposition strategies that apply specifically designed Hamiltonians sequentially to generate the desired overall time evolution. However, the desired time evolution can also be achieved via optimal control methods, wherein shaped electromagnetic fields generate motion in the directions necessary to reach a target unitary gate. At present, optimal control approaches do not typically provide information on the directions generated by an optimal field, which is necessary for comparison to standard gate decomposition strategies. In this work we generalize and extend previously reported control mechanism identification methods in order to establish mechanism for diverse quantum information processing strategies. We assign different quantum systems to classes that display qualitatively similar gate control mechanisms, based on properties of the system Hamiltonian like *Lie algebraic depth*, and establish fundamental bounds that delineate the types of gate control strategies that can be analyzed with mechanism identification techniques.

I. INTRODUCTION

It has been shown over the past decade, exploiting the inherent quantum mechanical properties of any physical system for performing information processing could be very useful in a multitude of ways, the most prominent being the exponential speedup in computation. Quantum information processing uses at the most fundamental level the energy eigenstates of a physical system as quantum bits and processing of these qubits under appropriate controls corresponds to a time evolution that performs the logical operation at hand. In order to perform a desired logical operation by simply letting the system evolve, one has to manipulate time evolution, such that after a final time T, the initial energy eigenstates are transformed to a desired final state through an appropriate unitary operation.

Since $U(N)$ (and $SU(N)$) are compact Lie groups (ref), 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 $[0, T]$. This method of quantum (optimal) dynamical control requires manipulation of delicate wave interferences to achieve selective transfer from initial to final states. Such transfer generally involves multiphoton transitions.

Typically, bang-bang controllability requires a greater total evolution time T than control pulse shaping. Bang-bang control strategies are often preferred when bandwidth for pulse shaping is limited. However, in the presence of available bandwidth, optimal control theory (OCT) methods may be preferred, for several reasons including the shorter time evolution over which the system may decohere. Standard gate decomposition strategies may in fact be viewed as a special case of OCT. While the associated control problems cannot typically be analytically solved (there do not generally exist analytical control solutions for time-varying linear dynamical systems/bilinear control such as quantum control systems), once the optimal control is found, the mechanism by which it reaches the target gate can be understood.

Within the context of optimal control (ref), the number of quantum wave interferences required to achieve a control objective increases with the number of parameters of the dynamical propagator

being controlled. This results in the involvement of higher order terms in the Dyson series expansion for the propagator, which makes it increasingly difficult to understand control mechanisms even approximately through explicit perturbation theory, since the number of contributing terms is unclear *a priori*. An alternative approach is quantum control mechanism identification (MI) through Hamiltonian encoding (ref), which uses signal processing techniques to obtain the amplitudes of all contributing multiphoton terms simultaneously. [These methods provide analytical insight into the time-varying dynamical pathways, even though the control problem does not possess an analytical solution.].

Prior work on quantum control mechanism identification has focused on identifying contributing terms in the Dyson series representation of the unitary propagator for state-to-state population transfer problems. In the present work we interrogate control mechanisms for the synthesis of quantum gates rather than population transfer, in distinct classes of proposed systems for quantum computing(, which differ according to criteria such as dynamical Lie algebra depth (see below)). These systems are classified on the basis of their control theoretic properties, in particular the intensity and complexity of the fields required to drive them to target gates.

We show that MI methods previously developed for population transfer (quantum observable control) are generally inadequate for mechanism identification of gate control strategies in many classes of such systems, due to the instability of encoded quantum dynamics. Quantum systems are inherently stable, but encoded quantum systems are generally not; rather, they must typically be stabilized like general linear systems. Most Hamiltonian encoding schemes modulate the quantum system so its generators no longer have eigenvalues on the imaginary axis (stability limit) of the complex plane. By pushing the system away from the stability limit, it is possible to separate the contributions of different Dyson orders or pathways to the time evolution. However, as a result, the inherent stability of quantum dynamics is lost and like general linear systems, it is essential that the modulated dynamics remain bounded on $[0, T]$ for analysis to be possible.

In order to enable mechanism identification for diverse quantum gate control strategies, we introduce methods for stabilization of encoded (time-varying) quantum dynamics. These methods involve the use of a piecewise constant encoding function $A(t)$ that increases the dynamical time constants associated with unstable modes [modification of conventional Fourier-based encoding]. Such stabilization methods are required to interrogate the control mechanisms for complex objectives beyond population transfer. In particular, they are essential for mechanism identification of controlled quantum gate operations on multiple qubits, a central problem in quantum information processing. More generally, the stabilization strategies are essential for MI of medium-to-strong field quantum control problems. As shown in recent studies on the resource scaling of various

classes of quantum control problems, stronger fields are often required for quantum gate control (cite KM/RC), and the required field strength grows steeply as evolution time decreases (as is often desirable in order to reduce decoherence).

Using these methods, we compare mechanisms for several representative optimal quantum gate control strategies, some previously inaccessible through MI. Finally, we propose new techniques for gate control mechanism identification based on the Magnus rather than the Dyson expansion, which will enable direct comparison to standard gate decomposition strategies.

need more citations in intro, esp to oct for qip and mi - may ask ak to do this

II. HAMILTONIAN ENCODING SCHEMES AND MECHANISM IDENTIFICATION

The Hamiltonian of a system is described as $H = H_0 + V(t)$, where H_0 is called the drift or field-free Hamiltonian and $V(t)$ encodes various interactions the system might have. Operationally for the molecular system having a dipole interaction with the external field $\varepsilon(t)$, the interaction Hamiltonian $V(t) = -\mu \cdot \varepsilon(t)$ where μ is the dipole matrix that has the information of various possible transitions of energy levels. The energy levels correspond to the eigen functions and values of free Hamiltonian H_0 and can be obtained by solving the eigen value equation $H_0 \left|n_i\right\rangle = E_i \left|n_i\right\rangle$ for $i = 1, 2, \cdots, D$, D being the dimension of the system. The external electromagnetic field $\varepsilon(t)$, modelled using classical wave theory, triggers various transitions between that are embedded in the dipole matrix. The dynamical evolution of the system is determined by the Unitary propagator, $U(t)$ which is prescribed by Schrödinger equation

$$i\hbar \frac{dU(t)}{dt} = \left[H_0 - \mu\varepsilon(t)\right] U(t), \quad U(0) \equiv 1. \tag{1}$$

It is convenient to treat the problem in a rotating frame, called the interaction picture, which is acheived by making the transformation $V_I(t) = -exp(iH_0t/\hbar)\mu\varepsilon(t)exp(-iH_0t/\hbar)$ which leads to Schrödinger equation in the interaction picture

$$i\hbar \frac{dU_I(t)}{dt} = V_I U_I(t), \tag{2}$$

where $U_I(t)$ is the unitary propagator in the interaction picture and we will treat the problem in the interaction picture and drop the subscript I for brevity.

In reality a physical system evolving from an initial state $|i\rangle$ to a final state $|f\rangle$ will take several paths, i.e. via the intermediate states $|l_i\rangle$ and define a pathway. For example $|i\rangle \rightarrow |l_1\rangle \rightarrow |l_2\rangle \rightarrow \cdots \rightarrow |l_{n-1}\rangle \rightarrow |f\rangle$ define one particular path with n intermediate transitions. The mechanism identification aims at finding these paths by performing an encoding and we apply to the quantum gates.

The solution to Schrödinger equation 2 is given as a series expansion called Dyson series expansion

$$U(T) = I + \left(\frac{-i}{\hbar}\right)\int_0^T V_I(t_1)dt_1 + \left(\frac{-i}{\hbar}\right)^2 \int_0^T V_I(t_2)\int_0^{t_2} V_I(t_1)dt_1 dt_2 + \cdots \tag{3}$$

A transition $|i\rangle$ to $|f\rangle$ is prescribed by the matrix element $U_{if} = \langle f|U(T)|i\rangle$. The Dyson series in the interaction picture converges for any field strength.

In quantum computation, as stated earlier, a specific gate can be modeled as a unitary evolution under a pre-designed Hamiltonian, $H = H_0 - \mu\varepsilon(t)$. For a given physical systems,H_0 and μ are pre-defined and the design is only in finding the optimal $\varepsilon(t)$. This can be precisely achieved using the optimal control theory and the field is said to be an optimal field. An ideal optimal field is one such has only those specific transition elements of the unitary, $U_{jk} \neq 0$ and is zero for all other transitions. For instance consider a single qubit-Hadamard gate given as

$$W = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

When acted upon the ground state of a two level system $|1\rangle = [1 \quad 0]'$ would result in a 50-50 superposition of $|1\rangle$ and $|2\rangle$ given as: $\frac{1}{\sqrt{2}}[1 \quad 1]'$ that is although the initial state may be in a definite state, the final state consists a portion of initial state.

Insert description of original MI here Mitra and Rabitz proposed[**?**] (a field and dipole) (Hamiltonian) encoding mechanism, where in one can determine the most significant pathways during an evolution under a control field designed for a specific target state. This is a remarkable result as one can know which of the underlying transitions the system takes during the evolution. Briefly, this is achieved by encoding either the optimal electric field or the interacting dipole moment with a time like variable and taking the Fourier transform. **expand**

Consider the significant orders in the Dyson series given by Eq. 3. The interaction picture Hamiltonian V_I is multiplied by the modulation function $m(s)$:

$$V_I(t) \rightarrow V_I \exp(i\gamma s) \tag{4}$$

and due to which n^{th}-order pathway becomes

$$U_{fi}(s) = \sum_{n=1} \tilde{U}^n_{fi} \exp(in\gamma s) \tag{5}$$

where the n^{th}-order unmodulated pathway $\tilde{U}^n_{fi}(t)$ is given as

$$\tilde{U}^n_{fi} = \left(\frac{i}{\hbar}\right)^n \langle f| \int_0^T \cdots \int_0^{t_2} V_I(t_n)\cdots V_I(t_1)dt_1 \cdots dt_n|i\rangle \tag{6}$$

where the summation in Eq. 5 is due to the discretization of the integrals. Operationally speaking we need to solve the Schrödinger equation:

$$\frac{dU(t,s)}{dt} = \frac{-i}{\hbar} V_I(t,s) U(t,s) \tag{7}$$

treating the dummy frequency s as constant and the solution can be approximated as

$$U(t,s) \approx U(0,s) \exp(-iV_I(t,s) \approx \prod_{n=1}^{N} \exp\left(-iV_I(t_n,s)\Delta t\right). \tag{8}$$

After solving Eq. 7 for $s = 1, 2, 3 \cdots, N$ where N is chosen sufficiently large and an integral power of 2 such that the modulation function $m(s)$ is a discrete fourier transform function and in this case for decoding the orders $\gamma = 2\pi/N$ is a constant.

In order to decode the actual pathways we need use the modulation in a slightly different way. The modulation scheme proposed in [**?**] is to use a Fourier functions $m_{jk} = exp(i\gamma_{jk}s)$ multiplied to $V_{jk}(t)$. Thus with the modulation, the modulated Schrödinger equation for a d-dimensional system is

$$\frac{dU(t,s)}{dt} = \begin{pmatrix} v_{11}(t)m_{11}(s) & v_{12}(t)m_{12}(s) & \cdots & v_{1d}(t)m_{1d}(s) \\ v_{21}(t)m_{21}(s) & v_{22}(t)m_{22}(s) & \cdots & v_{2d}(t)m_{2d}(s) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ v_{d1}(t)m_{d1}(s) & v_{d2}(t)m_{d2}(s) & \cdots & v_{dd}(t)m_{dd}(s) \end{pmatrix} U(t,s) \tag{9}$$

and while integrating the above equation, the variable s is a constant. The idea is to find all the significant intermediate transitions as shown in Fig. 4 by choosing an appropriate value for γ_{ij} and then performing a Fourier transform on the resulting $U_{fi}(s)$. The choice of γ_{ij} is not unique and when $\gamma ij = -\gamma ji$ the encoding results in a Hermitian type which can be used to reveal the composite pathways and the solution to Eq. 9 is not too difficult. On the other hand when $\gamma ij \neq -\gamma ji$ we can find the actual pathways and this results in a non-Hermitian encoding.

While non-Hermitian encoding schemes provide the greatest mechanistic information about the controlled dynamics, they will generally destabilize the dynamical system, resulting in the possibility of unbounded outputs (matrix elements of the propagator) for bounded inputs (the control function $\varepsilon(t)$). This makes MI using the direct Fourier encoding schemes described above untenable for certain classes of quantum systems - **especially for gate control, and for systems controlled with stronger fields** - as discussed below.

III. OPTIMAL CONTROL FIELDS FOR QUANTUM GATES IN MOLECULAR SYSTEMS

To date, MI methods have only been applied to population transfer control problems. Extensive recent studies (ref) on the application of OCT to quantum gate control establishes a foundation for the development of methods for quantum gate control MI. We first review techniques for generating optimal gate control fields.

formulate the gate control problem w definition of F here:

The associated optimal control problems can be solved using so-called homotopy tracking algorithms [**?** **?**] [1] These algorithms follow a specified track F_s of objective function values, where s denotes algorithmic time, toward the global minimum of each objective (**??**). The following differential equation specifies the evolution of each control field ε_k in continuous algorithmic time:

$$\frac{\partial \varepsilon(s,t)}{\partial s} = f(s,t) + \frac{a(s,t)}{\gamma(s)} \left(\frac{\mathrm{d}F_s}{\mathrm{d}s} - \int_0^T a(s,t') f(s,t)\ dt \right).$$

Here $a(s,t)$ denotes the functional derivative (gradient) of the Hilbert-Schmidt distance with respect to the control $\varepsilon(t)$, $\gamma(s) = \int_0^T a^2(s,t)\mathrm{d}t$ is the norm square of the gradient, and $f(s,t)$ is a 'free" function that arises due to the fact that the control problem is underdetermined in the absence of a Lagrange cost [**?**]

Choice of $\frac{\mathrm{d}F_s}{\mathrm{d}s}$ determines the path followed in $U(N)$ from the initial propagator U_0 to the target gate W. We consider two cases: The choice of control optimization algorithm affects the fluence of the resulting optimal gate control field; following the shortest possible (geodesic) path from U_0 to W identifies higher fluence fields..Setting $\frac{\mathrm{d}F_s}{\mathrm{d}s} = 0$ after convergence to W allows exploration of the level set of control fields that drive the system to W at time T. The choice of free function $f(s,t) = ...$ seeks to reduce fluence while traversing the level set.

use these only after completion of 1st draft:

In this section we describe the physical system we consider, and classify them according to the control theoretic concepts of **the controllability rank condition and dynamical lie algebra depth**. We are specifically interested in 1) Rotational 2)Vibrational molecular systems, which have proposed as carriers of quantum information, and and 3)NMR **omit**. The common characteristic, from a quantum computing perspective, in these three systems is that there is an external control

[1] Dynamic optimization (optimal control) problems typically require specialized algorithms since the dynamical constraint is a differential equation that must be satisfied for each feasible control; homotopy tracking algorithms are ideal for multiobjective control problems [**?**].

field is employed to achirve a desired transformation of the states. Thus one can use the same methodology, OCT, to solve for such external controls. The application of OCT is especially common in proposed schemes for molecular quantum computing.

need to describe truncation of Hilbert space - argue w reference to GR's paper that leakage to higher states can be studied and effective dynamical dimension can be determined. For illustrate purposes we consider small N.

1.Rotational: One of the initial proposals towards physical quantum information processing, was to use the spin of electrons as qubits. Where spin-up, $|1\rangle$, can be mapped to 1 and spin-down, $|0\rangle$, to 0. Spin of an electron is intrinsic angular momentum, and the central point is to use the spin angular momentum vector as qubit. This prompts the use of rotational angular momentum vector of the entire molecule towards quantum computation. This may be particularly interesting because, rotational states have been extensively studied using spectroscopic methods and are also easy to be manipulated in lab with the existing technology within their relatively long dephasing times. **may mention GR's comments on scaling of degeneracy wrt N**

Use of Rotational modes of a molecular system as qubits and performing quantum information processing has been proposed [**?**], where in the authors make use of multi-target optimal control theory. A typical rotational system consists of a Diatomic molecule with a reduced mass m and seperated by a distance r. In the absence of external interactions such a molecule with N energy levels, will have the following form for the internal Hamiltonian in the rotational energy eigenbasis:

$$H_0 = \sum_{j=0}^{N-1} (j(j+1))|j\rangle\langle j|, \tag{10}$$

where j is the eigen value of the total angular momentum, $\hat{J}_0$. The z-component $\hat{J}_z$ with eigen value m takes $2j+1$ values.The qubits can be represented by any eigen state $|j,m\rangle$. For example for $j=1$, we have $m=-1,0,1$ and we can map $|1,0\rangle$ as $|0\rangle$ and $|1,1\rangle$ as $|1\rangle$.

In order to perform a quantum gate, we need to interact the system with a control feild designed for the specific gate. Such a molecular system interacts with external electromagnetic feild,$E(t)$ due to inherent dipole moment, which formally is represented by an $N\times N$ symmetric matrix μ. The symmetricity of this matrix is imposed due to the selection rules, where the transitions are only allowed to the neighboring states implying $\Delta j = \pm 1$ and leading to the matrix elements $\langle j|\mu|j'\rangle \propto \delta_{j,j\pm1}$. Thus the interaction Hamiltonian is $H_i = -\mu.E(t)$, where the minus sign implies that, due to the torque created by the feild, the dipole tends to align with the interacting electric field.

2.Vibrational: Tesch *et. al* [**?**] have proposed the use of vibrational modes of the molecule towards quantum information processing. In this case, the vibrionic excitations, which corresponds

normal modes are used to define th qubit. Each such modes will have several excitations, and two such, preferably the two lowest energy excitations can be used to represent $|0\rangle$ and $|1\rangle$. The implementation of logic gates is performed by interacting the molecule with pre-designed laser pulses, which are calculated using the OCT. Although the formal method of finding the optimal pulse shapes will be the same, the physical implementation will be done using different frequencies of the electromagnetic spectrum. In the case of vibrational, usually the IR frequency is used, whereas in the case of rotaional states, microwave frequencies may be needed. **need to motivate these systems based on depth - should systems be introduced later w 3d depth plots shown? Mention scaling wrt N of degeneracy**

A generic description of the vibrational modes is extensively studied since inception of quantum mechanics, as harmonic oscillator, and now is included in any introductory quantum mechanics course. The idea of using harmonic oscillator eigenstates is described in Ref.However the harmonic oscillator potential is superseded by what is called as Morse potential, which is a more realistic description of molecular interactions. Morse potential can be formally written as $V(r-r_e) = D_e(1-e^{-\beta(r-r_e)})^2$, where r is the inter-nuclear distance of the molecules, and r_e is the equillibrium distance. The constant D_e is called as dissociation energy and $\beta = \omega_0\sqrt{\frac{m}{2D_e}}$ where ω_0 is the charecteristic angular frequency of the oscillator. It can be seen that for small values of $r-r_e$, Morse potential can be written as $V(r-r_e) = m\omega_0^2(r-r_e)^2/2$, which is the harmonic oscillator potential. Solving the Schrodinger equation, which for the case of Morse potential is not a trivial, allows us to write the Hamiltonian in the energy eigen basis as

$$H_0 = \sum_{\nu=0}^{N-1}\left[\hbar\omega_0(\nu+\frac{1}{2}) - \frac{\hbar^2\omega_0^2}{4D_e^2}(\nu+\frac{1}{2})^2\right]|\nu\rangle\langle\nu|\,, \tag{11}$$

where $|\nu\rangle$ is the eigen function, which are in written in terms of Laguerre Polynomials are explicitly given in Ref. [**?**]. The dipole interaction matrix for such a system is also provided analytically in Ref. [**?**] for a dipole function $\mu(r) = q(r-r_e+x_0)\exp(-(r-r_e)/x_1)$ and is written as,

$$\langle\nu|\mu(r)|\nu'\rangle = \frac{\mu_{perm}\mathcal{N}_\nu\mathcal{N}_{\nu'}}{\beta r_e}\frac{\Gamma(2K-2\nu'+1)\ \ \Gamma(2K-2\nu+1)}{(2K+1)^\xi\ \ \Gamma(2K-\nu'+1)}\sum_{n=0}^{\nu}A_n \tag{12}$$

where,

$$A_n = \frac{(-\nu)_n}{n!}\frac{\Gamma(2K-\nu-\nu'+n+\xi)\Gamma(\nu-n+1-\xi)}{\Gamma(2K-2\nu+n+1)\Gamma(\nu-\nu'-n+1-\xi)}$$
$$\times\left[\psi(\nu-n+1-\xi) - \psi(2K-\nu-\nu'+n+\xi) - \psi(\nu-\nu'-n+1-\xi) + \ln(2K+1) + \beta x_0\right] \tag{13}$$

and the normalization,

$$\mathcal{N}_\nu = \sqrt{\frac{(2K-2\nu)\Gamma(2K-\nu+1)}{\nu!\ \ \Gamma(2K-2\nu+1)^2}}.$$

where $\xi = 1/\beta x_1$ and $(-\nu)_n = \Gamma(-\nu+n)/\Gamma(-\nu)$ is the Pochhammer symbol. The parameters x_0 and x_1 can be fit to experimental data.

3.NMR: **check what we have done with this** NMR has shown to be one of the most promising approach towards a practical realization of quantum information processing. In NMR, the nuclear spins of a molecule are treated as qubits and generally there will be an ensemble of protons each with spin-1/2. The desired unitary transformation is achieved using a sequence of radio-frequency pulses. The design of optimal pulses that generate a particualr unitary transformation, is not a trivial task and relies on OCT. A generic description of such an ensemble, can be imagined as a network of n interacting spin-1/2 particles, where each spin has a coupling with all the other spins in the ensemble. The quantum gate, which is a unitary evolution is described by an element of $SU(2^n)$ [**?**], which are represented by Pauli matrices:

$$I_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; I_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; I_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These matrices have eigen values ± 1 and the prefix $\frac{1}{2}$ indicates the spin has a 50% probability to be in either of the orthogonal eigen vectors. The internal Hamiltonian, H_0 is then written as [**?**]

$$H_0 = 2\pi \sum_i \nu_i I_{iz} + 2\pi \sum_{ij} J_{ij} I_{iz} I_{jz}, \tag{14}$$

where ν_i represents Larmor frequencies for individual spins and J_{ij} represents coupling between spins and the values of both the quantities depend on the particular molecule being used. $I_{iz} = I_z \otimes I_2$ which generated the z rotation of the i^{th} qubit and I_2 is the identity. In a frame rotating about the z axis with the pins at respective frequencies ν_i, Eq. (14) simplifies to

$$H_0 = 2\pi \sum_{ij} J_{ij} I_{iz} I_{jz}. \tag{15}$$

When this Hamiltonian interacts with the controls in the x-y plane, which are pre-designed radio-frequency pulses, the total Hamiltonian is

$$H = 2\pi \sum_{ij} J_{ij} I_{iz} I_{jz} + 2\pi \sum_i (u_{ix}(t) I_{ix} + u_{iy}(t) I_{iy}) \tag{16}$$

where $u(t)$ is a time dependent control field. Appropriate fields may be designed using OCT [**?**]. In contrast to rotational and vibrational systems, the interaction of spins with external (magnetic) field is with the operators I_{ix} and I_{iy} as indicated in the above equation.

FIG. 1.

FIG. 2. Signal: Evolution of the element $U_{21}(t)$ for the vibrational system described in the text

IV. MECHANISM IDENTIFICATION OF WEAK-FIELD QUANTUM GATE CONTROL

The encoding strategies described above in Section II suffice for weak-field quantum gate control problems.

Rotor N=4 T=400 W1; Rotor N=4 T=400 W2; Rotor N=8 T=800 W5

Morse N=4 T=800 W1, n=9

Morse N=4 T=400 W1, n=9: this is stable - must generate another unstable candidate by either further decreasing T or increasing fluence starting from this

However, for the shorter evolution times that are desirable for reduction of decoherence in gate control, previously reported methods for MI fail for systems (...).

We illustrate the **issue of instability** in the basic methodology developed in [**?**] by applying it to single qubit Hadamard **replace vibrational 2-qubit hamiltonian** gate. The physical system under consideration is vibrational molecular system with the following values:

$$H_0 = \begin{pmatrix} 0.0227 & 0 \\ 0 & 0.0677 \end{pmatrix}; \quad \mu = \begin{pmatrix} 0 & 0.3736 \\ 0.3736 & 0 \end{pmatrix}$$

and the optimal $\varepsilon(t)$ are calculated employing the optimal control theory where the objective function is to mimize the norm $\|W - U(T)\|$. From the initial condition of the Schrödinger equation 2, $U(0) = 1$, the matrix elements $U_{1,2}(0) = 0 = U_{2,1}$. Upon the application of the OCT, we found that for the system under consideration, the dynamics are timed out at $T = 220$, where the norm $\|W - U(T)\| = 0.0049$. Now consider the time series of $U_{1,2}(t)$, which is now the signal and is shown in Fig. 2. As can be seen from the figure the $U_{1,2}(T) \approx 0.707$.

Figures: a) optimal fields; b) path of one matrix element in time series; c) path of largest and smallest eigenvalues.

FIG. 3. The significant orders in the Dyson series in Eq. 3. The frequency on the X-axis is the modulating frequency and should not be confused with the frequency of the optimal $\varepsilon(t)$

order	Amplitude
2	-1.5329
6	0.887
10	-0.148
Total	-0.7810

TABLE I. Significant orders contributing to the Unitary propagator in Eq. 3. The modulus of the total expected is 0.72646 and as indicated the sum of significant orders is 0.7810.

FIG. 4. Different pathways that are possible due to the constructive interferences of pathways. The initial state is $|E_1\rangle$. The different paths are as shown

V. CONTROLLABILITY AND LIE ALGEBRA DEPTH

To understand why the vibrational system (11) generally requires stronger fields or longer evolution times than the rotational system (10) to control quantum gates, we consider the differences between these model systems from the perspective of control(lability) theory.

repeat degeneracy analysis from GR paper?

Tasks 2,3: will determine whether to mention role of integrals associated w higher order brackets in destabilizing (since field strengths for vibrational above not much higher than for rotational) or only mention field strength/time in context of destabilization

Controllability of a physical system implies that, there always exists a control, such that the system can be driven from an initial state to any given final state [**?**]. Operationally this can be checked using Lie Algebra Rank Condition(LARC), which states that a system is controllable if the associated Lie-Algebra has a rank, which for *U(n)* system is n^2 and for *SU(n)* systems is n^2-1. 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*. A consequence of Lie Algebra Rank Condition is that, one can generate the underlying basis of the corresponding Lie-Algebra as discussed in Ref. [**?**].

The procedure for generating the basis[**?**] involves repeated commutators, also called as *repeated Lie bracket* such as $[[H_0, H_1], H_2]$ and many such permutations of the free Hamiltonian H_0, the interacting Hamiltonian H_i, where the subscript i represents the multiple interacting components of the Hamiltonian. The maximum number of such nested commutators is not known a priori and the procedure becomes very tedious as the dimension of the Hilbert space grows and as the number of interacting components increases. 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. Each commutator generates a matrix of dimension of the Hilbert space at hand. The algorithm presented in Ref. [**?**] indicates that one has to repeat the commutators until there are no more *linearly independent* basis (matrices) and so a quantity called as *depth* is introduced. Formally, *depth* is associated with the order of the commutators, i.e. $depth(H_i)$=1, $depth([H_i, H_j])$=2, $depth([[H_i, H_j], H_k])$=3 and so on. The *depth* of the dynamical Lie algebra is defined as the number of commutators required to span this algebra. The *depth* may differ considerably for different physical system.

The molecular system's interaction with the external field is mediated by a symmetric dipole moment μ as given by Eq. (**??**). The interaction dipole moment μ is associated with the external field and consequently the Dyson series expansion of the unitary propagator which involves the various integrals of the electric field are associated with the order of μ. Based on our **conjecture - change; place in context of controllability literature**, in the context of controllability, we need at least the commutators that span the Lie algebra. This implies that the order of μ within these nested commutators reveals the sensibility of the molecular system to the external electromagnetic field. Thus from the above analysis one can theoretically find the "photo-sensibility" of a given molecule. Lower number of μ means the molecule responds easily and requires less energy to control and in general may be easier to control. On the other hand higher order of μ means the molecule is inert to the external field and requires more energy to control and in general may be difficult to steer the molecule.

The algorithm presented in Ref. [**?**] suggests how to find the basis that span the Lie Algebra, but does not reveal the order of μ, i.e does not allow to know how many $\mu's$ are involved in a given nested commutator. Here we present an algorithm that can reveal the number of $\mu's$ involved in the basis.

Algorithm:

1. Calculate the comm. $[H_0, \mu] = R_1$(say).

2. Calculate all the commutators with $R_1 : [H_0, \cdots [H_0, R_1]]$ until all the linearly independent basis are found .

3. Now increase the order of $\mu : [\mu, R_1] = R_2$(say).

4. Repeat step 2 and 3 with $R_2 : [H_0, \cdots [H_0, R_2]]$.

5. Stop once the number of basis$= N^2$.

This could imply that in the search of optimal solution, one would require different energy to locate the solution in different direction. It may also be possible in few cases (**give an example?**) two different directions may not differ significantly and so to distinguish these directions requires more energy.

Before we classify the physical systems we describe how the depth **is relevant - edit** for the Unitary propagator. Very often the solution to Eq. **??** is given in terms of the power series known as Dyson series expansion, whose roots lie in the perturbation theory of quantum mechanics and is represented as given in Eq. **??**. Upon expanding we get,

$$\hat{U}(t) = \mathbb{I} + \left(\frac{-i}{\hbar}\right)\int_0^t H(t_1)dt_1 + \left(\frac{-i}{\hbar}\right)^2 \int_0^t H(t_2)\int_0^{t_2} H(t_1)dt_1 dt_2 + \cdots\cdots + \left(\frac{-i}{\hbar}\right)^n \int_0^t \int_0^{t'} \cdots \int_0^{t^{n-1}} H(t')H(t'')\cdots H(t^{t^n})dt'\cdots dt^n. \tag{17}$$

One can use CBH theorem as discussed in the appendix and obtain an expansion of Eq. **??** in terms of *commutators* by letting letting Let $A = H(t_3)\Delta t, B = H(t_2)\Delta t, C = H(t_1)\Delta t$, with $t_2 = t_1 + \Delta t,\ \Delta t = \frac{t_n - t_1}{n}$. It turns out that the CBH theorem is equivalent to a more generalized expansion called *magnus expansion* as shown in Ref. [**?**], according to which Eq.**??** can be written as,

$$\hat{U}(t) = \mathbb{T}\exp\left\{\int_0^t H(t')\ dt'\right\} = \exp\Bigg\{\int_0^t H(t')\ dt' + \tfrac{1}{12}\int_0^t H(t')\left(\int_0^{t'} H(t")\int_0^{t"} H(t"')\ dt"'dt" - \int_0^{t'}\int_0^{t"} H(t"')\ dt"'H(t")\ dt"\right) - \int_0^t \left(\int_0^{t'} H(t")\int_0^{t"} H(t"')\ dt"'\ dt' - \int_0^{t'}\int_0^{t"} H(t"')\ dt"'H(t")\ dt"\right) H(t')\ dt' + \cdots\Bigg\}$$

This is elaborated below in the Magnus MI description; may reduce Since the Hamiltonians at different times do not necessarily commute, and theintegration is only with respect to time implies that the integrands in each integral is the external interacting electric field. Therefore for $H = H_0 + \mu\varepsilon(t)$, we immediately get by letting $\varepsilon(t) \to -\varepsilon(t)$ and the unitary propagator at a

final time $U_T(\varepsilon(t)) = exp[A_T(\varepsilon(t))]$,

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

Our goal in this work is to decode the **strength** associated with various commutators up to the *depth* which is calculated numerically **may remove and rephrase - requires Magnus MI**.

Insert depth 3d plots: Figures ... show the Lie algebraic depth for the rotational and vibrational Hamiltonians from Section III, for various values of the Hilbert space dimension N.

compare depth figs to MI for stable weak field rotational systems here or only later?

VI. (INSTABILITY AND) STABILIZATION OF MODULATED QUANTUM DYNAMICS

The analysis above shows that some quantum systems (those with higher Lie algebraic depth) generally require stronger fields (or longer evolution times) to reach arbitrary gates. We have seen that a consequence of this requirement is that standard Hamiltonian encoding strategies are insufficient for gate control mechanism identification in such systems, due to instability of the encoded dynamics.

To understand why Hamiltonian encoding generally leads to unstable dynamical systems, let us start by considering the most general form of orders-based encoding, for which the stability analysis is most direct. Let $V_I(t_j)$ denote the interaction picture Hamiltonian at time t_j. The most general whole matrix (orders) encoding at any given s will look like

$$V_I(t_j)|A(s)|\exp(i\phi(s)),$$

where $|A|$ is the amplitude and $\exp(i\phi)$ contributes the complex phase. Generally we write $A = A(s)$ and $\phi = \phi(s)$, such that the encoded matrix may be written $V_I(t_j)m(s)$ with $m(s) = A(s)\exp(i\phi(s))$, but we will drop the s for simplicity. For the special case of Mitra-Rabitz Fourier encodings, $|A| = 1$, and the complex number multiplying $V_I(t_j)$ is always of modulus 1.

Now since $V_I)t_j|A(s)|\exp(i\phi(s))$ is skew-Hermitian, we can write $V_I(t_j)m(s) = Y(t_j)D(s)Y^\dagger(t_j)$,

where $Y(t_j)$ denotes the matrix of eigenvectors of $V_I(t_j)$. Now consider the form of the matrix D:

$$D = i \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{bmatrix} \tag{19}$$

where all the $\lambda_i \in \mathbb{R}$ (since a Hermitian matrix has only real eigenvalues) and hence the eigenvalues of $V_I(t_j)$ are all purely imaginary. Note that the λ_i can be either positive or negative. Thus a skew-Hermitian matrix is always at the stability limit, i.e., its eigenvalues lie on the imaginary axis on the complex plane between the left (stable, damped) and right (unstable) half planes, and the eigenvalues of the unitary propagator exhibit undamped oscillation with time (over the time interval Δt). As such the matrix exponential

$$\exp(V_I \Delta t) = \exp(Y D \Delta t Y^\dagger) = Y(t_j) \begin{bmatrix} \exp(i\lambda_i \Delta t) & & \\ & \ddots & \\ & & \exp(i\lambda_N \Delta t) \end{bmatrix} Y^\dagger(t_j)$$

where will always have norm (squared) equal to N for an unmodulated interaction or for any modulation that preserves skew-Hermiticity (we will refer to such simply as Hermitian encodings).

Since $V_I(t_j)$ is skew-Hermitian, $V_I(t_j)|A|\exp(i\phi) = Y(t_j)D|A|\exp(i\phi)Y^\dagger(t_j)$. Thus, any whole matrix encoding necessarily produces an encoded interaction Hamiltonian that is diagonalizable for all s, and moreover its eigenvectors are mutually orthogonal - the left and right eigenvectors of $Bm(s)$ are identical, such that it is a normal matrix (as skew-Hermitian and unitary matrices also are). For more general encodings, $Bm(s)$ may in principle be defective; whether this is likely can be studied for various alternate encodings. For these encodings, $V_I(t_j)m(s)$ will generally have left and right eigenvectors and can be written

$$V_I(t, s) = Y E X^\dagger$$

where $X^\dagger Y = I$ and

$$E = \begin{bmatrix} \delta_1 & & \\ & \ddots & \\ & & \delta_N \end{bmatrix},$$

where $\delta_N \in \mathbb{C}$. In such cases, for low-dimensional systems (e.g. $N = 2, N = 4$) the matrix can be diagonalized analytically (or in Mathematica) and the analytical expression for the $\delta_i(s)$ can be used to derive stability limits, analogously to the below.

Consider now the general expression for the non-Hermitian propagator $U(s, T)$ for whole matrix

encoding:

$$U(s,T) = \mathbb{T}\exp[\int_0^T V_I(t)m(s)\ dt] \approx \exp[iV_I(t_{n-1}m(s)\Delta t]\cdots\exp[V_I(t_0)m(s)\Delta t]$$
$$= Y(t_{n-1})\exp[i|A(s)|\exp(i\phi(s))Y(s,t_{n-1})\Delta t]Y^\dagger(t_{n-1})\cdots Y(t_0)\exp[i|A(s)|\exp(i\phi(s))D(s,0)\Delta t]Y^\dagger(t_0)$$

where there are n discrete time steps. Consider the j-th such non-Hermitian matrix $\exp[iV_I(t_j)m(s)\Delta t] = Y(t_j)\exp[i|A(s)|\exp(i\phi(s))D(s,t_{n-1})\Delta t]Y^\dagger(t_j)$. Simplifying,

$$\exp(V_I(t_j)|A|\exp(i\phi)\Delta t) = \tag{20}$$
$$= Y(t_j)\begin{bmatrix}\exp[i\lambda_1|A|(\cos\phi + i\sin\phi)\Delta t)] & & \\ & \ddots & \\ & & \exp[i\lambda_N|A|(\cos\phi + i\sin\phi)\Delta t)]\end{bmatrix}Y^\dagger(t_j). \tag{21}$$

The *condition for stability* of the modulated dynamical system is that all the eigenvalues of $C = B|A|\exp(i\phi)$ (poles of the linear dynamical system) lie on the left complex half plane, or, $\Re\{i\lambda_i|A|(\cos\phi + i\sin\phi)\Delta t\} \leq 0,\ i = 1,\cdots,N$. Since there are n such matrices in the above discrete representation, they must all satisfy this property. Moreover, for the modulated dynamical system to be numerically stable for all s, irrespective of Δt, this condition must hold for all the matrices $B|A(s)|\exp(i\phi(s))$. Solving for the admissible values of A and $\exp(i\phi)$, we have

$$|A|\Re\{i\lambda_i(\cos\phi + i\sin\phi)\} \leq 0$$

where $\lambda_i \in \mathbb{R}$ and hence $-\lambda_i\sin\phi \leq 0$. There are two cases: i) $\lambda_i \geq 0$, for which the condition is $M\pi \leq \phi \leq (M+1)\pi$, $M = 0,2,4,\cdots$; ii) $\lambda_i < 0$, for which we require $M\pi \leq \phi \leq (M+1)\pi$, $M = 1,3,5,\cdots$. Since the matrices D will generally have both positive and negative diagonal elements λ_i, there will generally not exist a complex encoding that will satisfy the stability criterion for all t and all s. (Note that real-valued whole matrix encoding functions, or composite pathway encodings do maintain skew-Hermiticity and stability, since $\Re\{i\lambda_i(\cos\phi + i\sin\phi)\} = 0$; alternatively, encodings operating on individual eigenvalues of $V_I(t_j)$ are a possible means of enforcing stability, although they would rely on these eigenvalues changing only slowly over all t). However, it is possible to design encodings that maintain boundedness of $||U(s,t)||$ over $s \in [0,s_f]$ and $t \in [0,T]$.

However, note that stability alone is not a sufficient condition for accurate mechanism identification. An eigenvalue of C of the form $\Re\{i\lambda_i|A|(\cos\phi + i\sin\phi)\} < 0$ will result in damped oscillation of the associated eigenvalue of $U(s,T)$, and the norm of this eigenvalue will rapidly decrease according to $\exp[-\lambda_i|A|\sin\phi\Delta t]$ toward the lower limits of machine precision, possibly compromising the accuracy of MI since the inverse transform will be subject to numerical errors. This issue of a lower bound on $|A|$ will be addressed below in terms of the Dyson series expansion.

Note that the competing requirements of both bounded and nonnegligible $\exp[-\lambda_i|A|\sin\phi\Delta t]$ can only be universally satisfied for ϕ at the stability limits (i.e., Hermitian encoding). However, the amplitude A can play an important role in maintaining numerical precision, as shown below.

VII. DESIGN OF STABLE HAMILTONIAN ENCODINGS

possibly combine w Sect 3; may put some of this in appendix:

We now derive bounds on $||U(s,T)||$ that can be used to design encodings. Applying the Cauchy-Schwarz inequality $|\langle A,B\rangle| \leq ||A|| * ||B||$ (where A, B are matrices and $||\cdot||$ denotes the matrix norm $[\mathrm{Tr}(A^\dagger A)]^{1/2}$) to the norm of the product XY of two matrices, we have

$$\begin{aligned}
||XY||^2 &= \langle XY, XY\rangle = \mathrm{Tr}[(XY)^\dagger XY] \\
&= \mathrm{Tr}[YY^\dagger X^\dagger X] \\
&= \langle YY^\dagger, X^\dagger X\rangle \\
&\leq ||Y^\dagger Y||||X^\dagger X|| = [\mathrm{Tr}(Y^\dagger YY^\dagger Y)]^{1/2}[\mathrm{Tr}(X^\dagger XX^\dagger X)]^{1/2}.
\end{aligned}$$

Letting $X = \exp[V_I(t_{j+1})m(s)]$, $Y = \exp[V_I(t_j)m(s)]$, we have

$$\begin{aligned}
||\exp[V_I(t_{j+1})m(s)]\exp[V_I(t_j)m(s)]||^2 \leq ||\exp[V_I(t_{j+1})m(s)]\exp^\dagger(V_I(t_{j+1})m(s))]||* \\
* ||\exp[V_I(t_j)m(s)]\exp^\dagger[V_I(t_j)m(s)]||.
\end{aligned}$$

Diagonalizing the V_I's, we find

$$\begin{aligned}
&||\exp[V_I(t_{j+1})\Delta t]\exp[V_I(t_j)m(s)\Delta t]||^2 \leq \\
&\leq ||\exp[Y(t_{j+1})D(s,t_{j+1})\Delta tY^\dagger(t_{j+1})]\exp^\dagger[Y(t_{j+1})D(s,t_{j+1})\Delta tY^\dagger(t_{j+1})]||* \\
&\quad * ||\exp[Y(t_j)D(t_j)\Delta tY^\dagger(t_j)]\exp^\dagger[Y(t_j)D(t_j)\Delta tY^\dagger(t_j)]|| \\
&= \left\{\sum_{i=1}^N [\exp[i\lambda_{ij+1}|A|(\cos\phi + i\sin\phi)\Delta t)] * \exp^*[i\lambda_{ij+1}|A|(\cos\phi + i\sin\phi)\Delta t]]^2\right\}^{\frac{1}{2}} \\
&\qquad \left\{\sum_{i=1}^N [\exp[i\lambda_{ij}|A|(\cos\phi + i\sin\phi)\Delta t)] * \exp^*[i\lambda_{ij}|A|(\cos\phi + i\sin\phi)\Delta t]]^2\right\}^{\frac{1}{2}} \\
&= \left\{\sum_{i=1}^N \exp[-4\lambda_{ij+1}|A|\sin\phi\Delta t]\right\}^{\frac{1}{2}} \left\{\sum_{i=1}^N \exp[-4\lambda_{ij}|A|\sin\phi\Delta t]\right\}^{\frac{1}{2}}
\end{aligned}$$

where superscript $*$ denotes the complex conjugate. Extending to all j, we have

$$||U(s,T)||^2 \leq \Pi_{j=1}^n \left\{\sum_{i=1}^N \exp[-4\lambda_{ij}|A|\sin\phi\Delta t]\right\}^{1/2}. \tag{22}$$

This is the worst case bound. The condition that MI does not become numerically inaccurate due to instabilities is

$$\Pi_{j=1}^{n}\left\{\sum_{i=1}^{N}\exp[-4\lambda_{ij}|A|\sin\phi\Delta t]\right\}^{1/2} \leq (\alpha * d)^2, \tag{23}$$

where d denotes the largest floating point number that can be represented on the computer and $\alpha < 1$ is a scaling constant (dividing the above expression by N^2 provides a bound in terms of the average magnitude of a matrix element of U). To obtain the $|A|_{\max}$ that saturates the above bound, one may apply Newton's method for both $\phi = \frac{\pi}{2}$ and $\phi = -\frac{\pi}{2}$, and choose the smallest root.

Since it is difficult for most encodings to restrict $\phi(s)$ to a domain such that the system is stable for all s, $|A|$ can instead be scaled in order to maintain this bound. Moreover, $|A|$ can be tuned to reduce damping effects for poles on the left half plane; smaller $|A|$ will generally reduce numerical inaccuracies due to either excessive damping or instability[2]. An alternative approach to constructing an upper bound on $|A|$ is to choose the $B(s,t_j)$ that has the eigenvalue with the largest $\Re(\lambda_{ij})$ of all, and then use the bound

$$\left\{\sum_{i=1}^{N}\exp[-2\lambda_{ij}|A|\sin\phi\Delta t]\right\}^{n} \leq (\alpha * d)^2.$$

Note that these expressions do not have closed form solutions for $|A|$. The following approximation, which may apply in cases where $Y(t)$ is slowly varying, enables such an analytical solution (**may eliminate**). Then,

$$\begin{aligned}
&||\exp[Y(s,t_{j+1})D(s,t_{j+1})\Delta t]Y^{\dagger}(s,t_{j+1})]\exp[Y(s,t_j)D(s,t_j)\Delta tY^{\dagger}(s,t_j)]|| \approx \\
&\approx ||\exp[Y(s,t_j)D(s,t_j)\Delta tY^{\dagger}(s,t_j)]\exp[Y(s,t_j)D(s,t_j)\Delta tY^{\dagger}(s,t_j)]|| \\
&= \sum_{i=1}^{N}\left\{\prod_{j=1}^{n}\exp[i\lambda_{ij}|A|(\cos\phi + i\sin\phi)\Delta t]\right\}\left\{\prod_{j=1}^{n}\exp[i\lambda_{ij}|A|(\cos\phi + i\sin\phi)\Delta t]\right\}^{*} \\
&= \sum_{i=1}^{N}\exp[-2\sum_{j}\lambda_{ij}|A|\sin\phi\Delta t] \\
&\leq N\exp[-2\sum_{j}\lambda_{i\max,j}|A|\sin\phi\Delta t] \leq (\alpha d)^2,
\end{aligned}$$

where $\lambda_{i\max,j}$ denotes the largest positive eigenvalue[3] of the modulated interaction Hamiltonian at

[2] To ensure that the eigenvalues of the modulated propagator on each time step remain bounded from below by the machine precision of the computer, one may choose $|A|_{\max}$ such that $\exp[-\lambda_{ij,\max}|A|\sin\phi\Delta t] = \text{eps}$, where $-\lambda_{ij,\max}$ denotes the eigenvalue of greatest absolute magnitude and $\phi = \frac{\pi}{2}$ or $-\frac{\pi}{2}$ depending on whether $\lambda_{ij,\max}$ is positive or negative.

[3] Strictly, whether the positive or negative eigenvalue of the greatest magnitude is chosen depends on whether the norm is larger for $\phi = \pi/2$ or $\phi = -\pi/2$; the norm can be evaluated for both choices.

time step j. The solution is

$$|A| \leq \frac{\ln((\alpha d)^2/N)}{2\Delta t \sum_j \lambda_{i\,\max,j}}, \tag{24}$$

where we have chosen $\phi = -\pi/2$ such that the inequality holds for all ϕ. $|A|$ may be chosen as large as possible to maximize the peak amplitudes upon inverse Fourier transform. **end eliminate**

A simple version of this stabilization strategy would entail the use of Fourier encoding schemes $m(s) = |A| \exp(i\gamma s)$ where A is chosen to satisfy the above bounds for all s. Then, after the inverse transform, powers of $|A|$ will be eliminated as follows. (Note that the alternative approach of scaling $B = V_I(t)$ would require inverse scaling of T, which would not fix the problem). The encoded propagator in the Dyson series representation is

$$U(s,t) = I + |A| \exp(i\gamma_0 s) \int_0^t V_I(t_1)\ dt_1 + |A|^2 \exp(2i\gamma_0 s) \int_0^t V_I(t_1) \int_0^{t_1} V_I(t_2) dt_2 dt_1 + \cdots,$$

with inverse FFT giving the spectrum[4]

$$\begin{aligned} U(\gamma,t) &= \int_{-\infty}^{\infty} \exp(-i\gamma s) U(s,t)\ ds \\ &= \delta(\gamma,\gamma_0)|A| \int_0^t V_I(t_1) dt_1 + \delta(\gamma,2\gamma_0)|A|^2 \int_0^t V_I(t_1) \int_0^{t_1} V_I(t_2) dt_2 dt_1 + \cdots, \end{aligned} \tag{25}$$

such that

$$\int_0^t V_I(t_1) dt_1 = U(\gamma_0,t)/|A|, \quad \int_0^t \int_0^{t_1} V_I(t_2) dt_2 dt_1 = U(2\gamma_0,t)/|A|^2, \quad \cdots \tag{26}$$

(i.e., since a strict Fourier modulation was not used for the encoding, an inverse Fourier transform will not retrieve the correct amplitudes by orthonormality of Fourier modes alone). Note that the m-th order pathway will be scaled by $|A|^m$ in $U(s,t)$.

We now show how to obtain bounds on the range of $|A|$ that can be used to extract all relevant mechanistic information about the matrix element $\langle x|V_I(t)|y\rangle$. For any finite-d quantum system, it is possible to identify an upper bound $k_{\max}$ on the orders in the Dyson expansion that contribute to the terminal propagator $U(T)$, within a specified tolerance ϵ. Let $|\langle x|\varepsilon(t)V^\dagger(t)\mu V(t)|y\rangle| < c,\ 1 \leq x,y \leq N$, for some positive constant c. (Note that c does not depend on the field-free Hamiltonian

[4] The upper and lower frequency limits in the discrete transform will be determined by the number of sampled time points j according to the Nyquist critical frequencies.

H_0.) Then

$$\left|\sum_{x_1=1}^{N}\cdots\sum_{x_{k-1}=1}^{N}\int_0^T\langle x|V_I(t)|x_1\rangle\cdots\int_0^{t_{k-1}}\langle x_{k-1}|V_I(t_k)|y\rangle\ dt_k\cdots dt\right|$$

$$\leq\sum_{x_1=1}^{N}\cdots\sum_{x_{k-1}=1}^{N}\int_0^T|\langle x|V_I(t)|x_1\rangle|\cdots\int_0^{t_{k-1}}|\langle x_{k-1}|V_I(t_k)|y\rangle|\ dt_k\cdots dt$$

$$\leq\sum_{x_1=1}^{N}\cdots\sum_{x_{k-1}=1}^{N}c^k\int_0^T\cdots\int_0^{t_{k-1}}dt_k dt \tag{27}$$

$$\leq N^{k-1}\frac{c^kT^k}{k!}=\frac{(NcT)^k}{Nk!}. \tag{28}$$

Then we have as a worst case bound on the k-th order contribution to the norm of the propagator[5]:

$$||U_k(t)||\leq N^2*N^{k-1}\frac{c^kT^k}{k!}=N^{k+1}\frac{c^kT^k}{k!}. \tag{29}$$

This result can be used as follows. Set a tolerance ϵ for convergence of the Dyson series. (A reasonable choice is the floating point (machine) precision of the computer, denoted eps). Then, find numerically the largest integer k such that $\frac{(NcT)^k}{Nk!}\leq\epsilon$, and denote it by $k_{\max}$. This is the maximum order in the Dyson series for $\langle x|U(T)|y\rangle$ that will be considered mechanistically relevant. [6] As noted above, there exists a minimum value $|A|_{\min}$ below which the inverse scaling according to equation (25) will be numerically inaccurate. This is because the amplitudes of orders $k\leq k_{\max}$ can be pushed below machine precision due to the modulation by $|A|$. We can compute $|A|_{\min}$ using the bound on the amplitude of Dyson series term $k_{\max}$. We require that all contributing orders $1,\cdots,k_{\max}$ maintain amplitudes above machine precision. According to (25), then, combined with (27),

$$|A|_{\min}^k N^{k-1}\frac{c^kT^k}{k!}>\text{eps},\ \forall k\leq k_{\max},$$

which can be solved numerically for $|A|_{\min}$. If we choose $c=\max_t\varepsilon(t)*||\mu||$, $|A|_{\min}$ will guarantee that the contributing orders of all matrix elements of $U(T)$ will have amplitudes maintained above machine precision.

Similarly, it is possible to obtain an upper bound $|A|_{\max}$ on the modulus of $m(s)$ using the Dyson series rather than the time-ordered exponential approach that led us to (22). In this approach, $|A|_{\max}$ is the largest value of $|A|$ such that the modulus of each order with $k<=k_{\max}$ in (the

[5] It is also possible to obtain a bound by applying the Cauchy-Schwarz inequality on each term in the product of sums rather than integrals in a discrete time representation of (27), and writing the norm of each $V_I(t_j)$ in terms of its eigenvalues; however this does not lead to a significant improvement over (29).

[6] Note the present method can also be used to decrease ϵ below the floating point precision.

modulated series) does not exceed the maximum accurate integer d. Note that since modulation by the complex phase $\exp(i\phi)$ does not change the modulus of each integrand in (27) - i.e.,

$$|\langle x|\varepsilon(t_k)V^\dagger(t_k)\mu\exp(i\phi)V(t_k)|y\rangle| = |\langle x|\varepsilon(t_k)V^\dagger(t_k)\mu V(t_k)|y\rangle|$$

the bounds on these moduli are identical. Thus, these bounds do not depend on s.

The machine precision of the computer is determined by the number of bits used to store floating point numbers. IEEE standard double precision floating point arithmetic has eps $= 2^{-53} \approx 10^{-16}$ unit roundoff (machine precision). [7] The maximum precise integer according to the IEEE standard is $2^{53} = \text{eps}^{-1}$. There will only be 16 significant digits even for higher numbers (there may be a limit to the exponent as well but it is less important). Thus we use eps $= 10^{-16}$ and $d = 10^{16}$. (For further details on finite precision arithmetic, see N. J. Higham, Accuracy and Stability of Numerical Algorithms, SIAM, Philadelphia, 1996.)

For non-Hermitian matrices, higher order terms in the Dyson series can contribute more to the $U(s,t)$ even if they have negligible contribution to $U(T)$. Introducing and tuning $|A|$ aims to eliminate these terms so they do not propagate through the MI procedure (while preserving the important terms).

To apply these results numerically, thus first check the eigenvalue spectrum of each $V_i(t_j)m(s)$ by diagonalizing the $V_I(t_j)\exp(i\gamma s)$ at each j for any whole matrix (orders) Hamiltonian encoding problem. The magnitudes of the real parts of the eigenvalues on the right half plane will determine stability, and the magnitudes of those on the left half plane will determine overdamping. Compute (22) and determine if it exceeds d, the largest integer than can be represented on the computer. If so, apply the following algorithm:

1. Determine the upper bound c on (all matrix elements of) the interaction Hamiltonian, c, numerically by

   $$c = \max_t |\langle x|V_I(t)|y\rangle.$$

   For simplicity, let $c = \max_t \varepsilon(t) * ||\mu||$, which is conservative.

2. Numerically, find $k_{\max} \mid \frac{(NcT)^k}{Nk!} \leq \epsilon,\ \forall k \leq k_{\max}$.

[7] This is because, according to the standard, 64 bits are allocated to storing a double precision number - 52 bits are used to rep the decimal fraction of the floating point number (the relevant part for our purposes), 1 bit is sign, 11 bits are exponent (for single precision arithmetic, 32 bits are allocated, with only 23 bits used to represent the decimal part).

3. Check if $\frac{(NcT)^k}{Nk!} < d$, where d is the maximum accurate integer that can be represented on the computer (generally eps^{-}1), $\forall k \leq k_{\max}$. If so, apply orders MI with modulating function $m(s) = \exp(i\gamma s$ and stop. If not, choose a $|A| < 1$ in the MI modulating function $m(s) = |A| \exp(i\gamma s)$.

4. Find $|A|_{\min}$ by
$$|A|_{\min} = \frac{(\text{eps } Nk_{\max}!)^{1/k_{\max}}}{NcT}.$$

5. Find $|A|_{\max}$ numerically by
$$|A|_{\max} = \min_{k<k_{\max}} \frac{(dNk!)^{1/k}}{NcT}$$
and also by equation (22) and choose the smaller value.

6. Then, check if $|A|_{\max} > |A|_{\min}$. If so, apply orders MI with modulating function $m(s) = |A| \exp(i\gamma s)$, scanning over $|A|_{\min} \leq |A| \leq |A|_{\max}$ until one satisfies the sumcheck. If not, divide T by 2 and apply MI on $[0, T/2)$, $[T/2, T]$ separately (return to 1 and let $T \to T/2$).

Apply stabilization to $N = 4$ vibrational system: Task 2

use Morse N=4 T=400 W1, W2 w fluence increased to a level determined by constant field analysis in Task 3; possibly T=800 w higher fluence generated by geodesic dm. Figure:

compare Morse depth figs reported earlier to MI sig orders. Decide whether to mention theory in Dyson 'necessary conditions' draft to indicate that relationship can be understood more rigorously - or put next to Magnus MI below

Since $|A|$ is a single parameter, it is likely for strong fields that $|A|_{\max} < |A|_{\min}$, as seen in the above example (check). This implies that the system cannot be properly bounded on the time interval $[0, T]$. Applying steps 5 and 6 above,...**fill in results if we subdivide T in any case**

This approach provides a picture of mechanism as a product of controlled evolutions over $i = 1, m$. In each interval $[t^i, t^{i+1}]$, multiple generators are being applied simultaneously, resulting in multiphoton pathways. By expanding the product of Dyson series on each subinterval, we retain all information that would have been obtained via standard MI, and in fact obtain new information about pathways that is lost in orders-based encoding. As long as the $m << n$ (the number of time steps), it is straightforward to multiply out the corresponding propagators $U(t^{i+1}, t^i)$ and

enumerate these pathways **fix indices**:

$$U(t_{i+1},t_i)U(t_i,t_{i-1}) = (I + \int_{t^i}^{t^{i+1}} V_I(t_1)\ dt_1 + \int_{t^i}^{t^{i+1}} V_I(t_1) \int_{t^i}^{t_1} V_I(t_2) dt_2 dt_1 + \cdots) *$$
$$(I + \int_0^{t^i} V_I(t_1)\ dt_1 + \int_0^{t^i} V_I(t_1) \int_0^{t_1} V_I(t_2) dt_2 dt_1 + \cdots)$$
$$= I + \int_{t^i}^{t^{i+1}} V_I(t_1)\ dt_1 \int_0^{t^i} V_I(t_1)\ dt_1 + \int_{t^i}^{t^{i+1}} V_I(t_1)\ dt_1 \int_0^{t^i} V_I(t_1) \int_0^{t_1} V_I(t_2) dt_2 dt_1 +$$
$$+ \int_{t^i}^{t^{i+1}} V_I(t_1) \int_{t^i}^{t_1} V_I(t_2) dt_2 dt_1 + \cdots$$

VIII. CONTRIBUTIONS OF LIE BRACKETS TO STABILITY OF ENCODED QUANTUM DYNAMICS

this method (incl computing contributions of Lie brackets to destabilization) may be used prior to those in prev sections, given H_0, μ and c from OCT; then apply $|A|$ stabilization for cases w large c using methods in prev sections and determine what orders can be retrieved accurately

Task 3 will determine whether constant field analysis can be used to predict which systems are likely to be unstable - otherwise mention here that contribution of higher order brackets to destabilization cannot be done through constant field analysis (although it provides insights) and Magnus MI needed in follow up work

The analysis in previous sections has employed the Dyson expansion for the unitary propagator, which has foundations in standard perturbation theory. By contrast the approach of geometric control theory focuses on the notion of directions generated by sequential application of drift and control Hamiltonians; these directions are termed Lie brackets. In this section, we study the effects of Hamiltonian encoding on the Lie brackets of quantum control systems. In order to obtain closed form solutions, we consider the case of a control field with constant amplitude, $\varepsilon(t) = c$.

Interaction propagator is related to the Schrodinger propagator through

$$U_I(t) = \exp(iH_0 t)U(t)$$

If $H(t) = H = H_0 - c\mu$ (constant field),

$$U_I(t) = \exp(iH_0 t)\exp\{-i(H_0 - c\mu)t\}$$

According to the CBH theorem,

$$\exp(iH_0 t)\exp\{-i(H_0 - c\mu)t\} = \exp\{iH_0 t - i(H_0 - c\mu)t - \frac{i^2}{2}[H_0, c\mu]t + \frac{i^3}{12}[H_0,[H_0,c\mu]] + \frac{i^3}{12}[c\mu,[H_0,c\mu]] + \cdots\}$$

Now let $V_I(s,t) = -\exp(iH_0t)\mu\varepsilon(t)|A|\exp(i\phi(s))\exp(-iH_0t)$. With $H(t) = H$, $V_I(s,t) = -\exp(iH_0t)\mu c|A|\exp(i\phi(s))\exp(-iH_0t)$ and setting $|A| = 1$,

$$U_I(s,t) = \exp(iH_0t)\exp[i(H_0 - c\exp(i\phi(s))\mu)t].$$

Let γ_i, $i = 1,\cdots,N$ denote the eigenvalues of $(\cos\phi(s) + i\sin\phi(s))i\mu$ (list them for a given μ). Since $i\mu$ has purely imaginary eigenvalues, $\phi(s) = \frac{\pi}{2}$ or $\phi(s) = -\frac{\pi}{2}$ provides the largest $\max_i \mathrm{Re}(\gamma_i) = \max_i \gamma_i$.

$$\begin{aligned} U_I(s_{\pi/2},t) &= \exp(iH_0t)\exp\{-(iH_0 \pm c\mu)t\} \\ &= Y(t)\tilde{U}_I(s_{\pi/2},t)Y^\dagger(t) \end{aligned} \tag{30}$$

where $s_{\pi/2} \equiv s|\phi(s) = \pm\frac{\pi}{2}$ and where $\tilde{U}_I$ is the matrix of eigenvalues of U_I. Given $t = T$, compute $\tilde{U}_I(s_{\pm\pi/2},T)$. Find $c_{\max}$ or T such that eigenvalues don't overflow. E.g., given c from dmorph, apply MI on $[0,T],\cdots,[(n-1)T,nT]$.

By CBH, for phase angle $\phi = \pm\frac{\pi}{2}$,

$$\begin{aligned} &\exp(iH_0t)\exp\{(-iH_0 \pm c\mu)t\} = \\ &\quad = \exp\{-iH_0t + (iH_0 \pm c\mu)t - \frac{1}{2}[iH_0,\pm c\mu]t^2 + \frac{1}{12}[iH_0,[iH_0,\pm c\mu]]t^3 + \\ &\qquad - \frac{1}{12}[\pm c\mu,[iH_0,\pm c\mu]]t^3 + \cdots\} \\ &\quad = \exp\{\pm c\mu t - \frac{1}{2}[iH_0,\pm c\mu]t^2 + \frac{1}{12}[iH_0,[iH_0,\pm c\mu]]t^3 - \frac{c^2t^3}{12}[\mu,[iH_0,\mu]] + \cdots\} \end{aligned} \tag{31}$$

Note that the Lie bracket (commutator) of a skew-Hermitian matrix with a Hermitian matrix is Hermitian, whereas the Lie bracket of a Hermitian matrix with a Hermitian matrix is skew-Hermitian. Generators of the modulated dynamical system are hence either skew-Hermitian or Hermitian at $\phi = \pm\frac{pi}{2}$; the modulated system does not evolve on a classical matrix Lie group (besides $GL(N,\mathbb{C})$). Lie brackets of the modulated system that contain odd powers of control Hamiltonian μ are Hermitian, and hence have real eigenvalues and can destabilize the system, whereas those containing even powers of μ are skew-Hermitian, and hence have (marginally stable) imaginary eigenvalues. At $\phi \neq \pm\frac{\pi}{2}$, even order terms can also destabilize the system, but for moderate or strong field strengths (common in gate control) the maximum destabilization will generally occur $\phi = \pm\frac{\pi}{2}$, since the real parts of the eigenvalues of the brackets are scaled by $\sin^n(\phi)$ where n is the power with which μ appears in the bracket.

Recall Lie brackets can be defined (cite) in terms of time-derivatives of

$$\begin{aligned} V_I(t) &= -\exp(iH_0t)c\mu\exp(-iH_0t) \\ &= -c\mu - ct[iH_0,\mu] + \frac{1}{2!}c^2t^2[iH_0,[iH_0,\mu]] + \cdots \end{aligned}$$

i.e., the interaction picture control Hamiltonian where the control vector field is constant. Application of the Magnus expansion described in Section V to this expression gives the above formula for $U_I(t) = \exp(iV_I(t))$.

More generally, for time-varying control vector fields, contributions to destabilization can be found through the Magnus expansion, as discussed below.

may place examples in this section rather than next

IX. LIE BRACKETS VIS-A-VIS STABILITY OF HAMILTONIAN ENCODING FOR COMMON MOLECULAR GATE CONTROL SYSTEMS

Task 3: For each of the molecular control systems introduced in Section III, the eigenvalue matrix $\tilde{U}_I(s_{\pm\frac{\pi}{2}}, T)$ in equation (30) was computed for various choices of constant field amplitude c and evolution time $t = T$. **The results are presented in Table/Fig ...**

Task 4: All possible Lie brackets of H_0, μ of order $1, \cdots, x$ were computed for rotor and Morse systems for $N = 4, 8$. For specified values of c, T in each case, the corresponding modulated Lie bracket terms in equation ([**?**]) were computed, and summed. **Figure .... (a,b,c; three traces in each subfig) plots the magnitude of the largest three eigenvalues of the resulting matrix for each system, for these values of c, T.**

Find $c_{\max}$ or T such that eigenvalues don't overflow. Then, e.g., given mean field amplitude c from dmorph, apply MI on corresponding intervals $[0, T], \cdots, [(n-1)T, nT]$. Unlike the analysis in Section VII, however, this method cannot identify the MI orders that can be accurately computed with encodings that employ $|A|$ stabilization.

insert summary of proposed Magnus MI (in Schrödinger picture) possibly in new sect 'Dynamical Lie algebra depth and Lie algebraic mechanism identification"; may replace directly from magnus mi draft:

connect to definition of depth above However their **mitra/rabitz** study does not focus on **strength** of different commutators in the unitary propagator. We study this aspect and for different control systems and since each commutator is associated with certain power of the dipole matrix, we use the dipole encoding. It is worth mentioning that one can also perform the following encoding to the Hamiltonian H_0 instead of the dipole μ.

Dipole encoding simply is multiplying with a Fourier function: $\mu \rightarrow \mu exp(i\gamma s)$, where γ, which is a frequency like parameter should be carefully chosen while performing the numerical simulations and s is a time like variable and taking an inverse Fourier transform and checking for the amplitudes

corresponding to $\gamma, 2\gamma, 3\gamma \cdots$. Thus the commutators now become,

$$\mu \longrightarrow \mu exp(i\gamma s), [H_0, \mu] \longrightarrow [H_0, \mu] exp(i\gamma s), \tag{32}$$
$$[H_0, [H_0, \mu]] \longrightarrow [H_0[H_0, \mu]] exp(i\gamma s), [\mu, [H_0, \mu]] \longrightarrow [\mu, [H_0, \mu]] exp(2i\gamma s).$$

Thus in this representation, the encoded hermitian generator becomes:

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

which makes the Unitary propagator, $U_T(s, \varepsilon(t)) = A_T(s, \varepsilon(t))$. By taking the inverse Fourier transform and identifying the Fourier amplitudes corresponding to $\gamma, 2\gamma, 3\gamma \cdots$ will give the **strength** of different commutators. It is straight forward to see from the above that this method does not distinguish commutators with the same powers of μ. **may therefore omit**

Due to indistinguishability between the commutators of the same power of μ, it might be more useful to have a full system encoding. Since the system is basically composed of H_0 and μ, we may use two frequency like variables and write

$$H_0 \longrightarrow H_0 exp(i\alpha s), \mu \longrightarrow \mu exp(i\gamma s). \tag{33}$$

Hence the commutators become,

$$[H_0, \mu] \longrightarrow [H_0, \mu] \exp(i(\alpha + \gamma)s) \tag{34}$$
$$[H_0, [H_0, \mu]] \longrightarrow [H_0[H_0, \mu]] \exp(i(2\alpha + \gamma)s), [\mu, [H_0, \mu]] \longrightarrow [\mu, [H_0, \mu]] \exp(i(\alpha + 2\gamma)s).$$

so we can distinguish different commutators and associated **strength**. Proceeding in this way the argument of the unitary, $A_T(\varepsilon(t), s)$ is given by

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

By performing the Fourier transform, we can identify the **strength**, which is the Fourier amplitude associated with frequencies $n\alpha + m\gamma$ where n and m could take values $0, 1, 2, \cdots$.

may mention how this can be applied to also determine contributions of brackets to destabilization

X. CONCLUSION

three possible concluding themes

following applies to stabilization for dyson mi: Analogously to classical controller tuning, $|A|$ tunes the time constant τ associated with each response mode/eigenvector of the system, pushing poles closer to the imaginary axis. More generally, encodings that maintain $\phi(s)$ near the stability limit (skew-Hermiticity) may give more accurate numerical results.

Because each $C = V_I(t_j)m(s)$ is a normal matrix, it can be accurately exponentiated by diagonalization followed by exponentiation of the matrix of eigenvalues. This method may be more accurate than exponentiation by Pade approximants for whole matrix encodings. In fact, since each $V_I(t_j)$ has to be diagonalized in order to apply the above bounds, one may simply multiply D by $|A|\exp(i\phi)$ to get the diagonal form of C.

The methods presented herein are not limited to quantum control, and have applications to high-order perturbation theory for general linear time-varying dynamical systems (operator control for general bilinear control systems), which may be inherently unstable. Within the domain of quantum control, the methods can be used to interrogate the control mechanisms for quantum gates operating on multiple qubits. In a separate work we evaluate these mechanisms for a variety of systems (H_0, μ) commonly proposed for quantum information processing.

following pertains to reasons for / generality of using oct for gate synthesis:

The notion of bang-bang controllability is also intimately related to the issue of the complexity of gate decomposition schemes for n qubit transformations, i.e., the problem of determining the minimum number of one- and two-qubit unitary transformations required to produce a given n qubit gate; for algorithms where this scaling is poor, the application of pulse shaping may simplify the construction.

The improved robustness to decoherence is counterbalanced by a decreased robustness to control field noise and uncertainty in the Hamiltonian parameters. assess robustness to control field noise for such control strategies.

following pertains to future lie algebraic mi work; connect to eqns in last section above 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

Lie algebraic encoding methods enable the extraction of the amplitudes associated with each Lie algebra direction by Fourier transforms into the domain of the auxiliary encoding parameter