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Bringing Quantum Systems under Control:

A Tutorial Invitation to Quantum Computing and Its Relation to Bilinear Control Systems

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Abstract— **Quantum computing comes with the potential to push computational boundaries in various domains including, e.g., cryptography, simulation, optimization, and machine learning. Exploiting the principles of quantum mechanics, new algorithms can be developed with capabilities that are unprecedented by classical computers. However, the experimental realization of quantum devices is an active field of research with enormous open challenges, including robustness against noise and scalabilty. While systems and control theory plays a crucial role in tackling these challenges, the principles of quantum physics lead to a (perceived) high entry barrier for entering the field of quantum computing.**

This tutorial paper aims at lowering the barrier by introducing basic concepts required to understand and solve research problems in quantum systems. First, we introduce fundamentals of quantum algorithms, ranging from basic ingredients such as qubits and quantum logic gates to prominent examples and more advanced concepts, e.g., variational quantum algorithms. Next, we formalize some engineering questions for building quantum devices in the real world, which requires the careful manipulation of microscopic quantities obeying quantum effects. To this end for N-level systems, we introduce basic concepts of (bilinear) quantum systems and control theory including controllability, observability, and optimal control in a unified frame. Finally, we address the problem of noise in real-world quantum systems via robust quantum control, which relies on a set-membership uncertainty description frequently employed in control.

A key goal of this tutorial paper is to demystify engineering aspects of quantum computing by emphasizing that its mathematical description mainly involves linear algebra (for quantum algorithms) and the handling of bilinear control systems (for quantum systems and control theory) but does not require too much detailed knowledge of quantum physics.

I. Introduction

Quantum computing holds high potential for solving certain computational problems faster than with classical computers [1]. Possible applications include integer factorization [2], which may be used to break current public-key encryption systems, unstructured search [3], and quantum simulation [4]. However, realizing these applications in experiments poses numerous challenges. In particular, in the current noisy intermediate-scale quantum (NISQ) era [5, 6], quantum devices are fragile such that noise and uncertainty may cause significant perturbations. While different approaches to address errors have been developed, in particular quantum error correction [7] and quantum error mitigation [8], they do not (yet) allow to fully resolve errors on current quantum computers.

Systems and control theory plays a crucial role in realizing quantum devices. In particular, experimental realizations require the development of specialized techniques for controlling quantum mechanical systems [9–13]. Also on the algorithmic level, various challenges in quantum computing are closely connected to control-theoretic concepts [14]. However, the principles of quantum physics lead to a (perceived) high entry barrier in particular also for the engineering community to enter the field of quantum computing, and more widely, quantum technology. This paper aims at lowering the barrier by providing a tutorial introduction to quantum systems. Here we address the subject from three different, complementary perspectives, covering not only the algorithmic framework of quantum computers but also doability questions connected to quantum systems theory and robust control that arise in their experimental realization. — Disclaimer: Naturally, there is a number of well-established important topics and results such a didactic line-of-thought will have to skip. E.g., for infinite-dimensional systems, linear quantum control has successfully been used [9, 13, 15]. In particular closed-loop feedback systems taking into account the backaction onto the quantum system via stochastic differential equations have been dwelled upon extensively in [16]. Most notably, they were put to good use in the Nobel-prize winning setup of a photon box, where a chosen number of photons could be entered and stabilized [17, 18]. For further reading see, e.g., the current European Quantum Control Roadmap [12] and the references therein.

For our goal, in Section II we first introduce the mathematical framework of quantum algorithms based on complex linear algebra. We cover qubits, which are the main building blocks of quantum computers and are mathematically described by complex unit vectors, and we explain how they are accessed and manipulated via measurements and quantum gates, respectively. Further, we discuss fundamental quantum algorithms, including variational quantum algorithms which

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are feedback interconnections of quantum and classical algorithms.

Next, in Section III, we sketch and exploit an emerging unified frame of quantum systems theory for the specific case of finite-dimensional bilinear quantum control systems connecting to N-level systems and their gates in quantum information. The frame is convenient and powerful for deciding engineering questions like controllability, observability, tomografiability etc. by common simple symmetry arguments. We use established tools of linear algebra to absorb intricacies (of Lie theory) so as to remain within a familiar 'matrix times vector' representation of linear maps now acting on operators (matrices) to exploit control on *orbits of quantum states*. All relevant symmetries naturally show up in this frame—and breaking them by controls is key to get quantum systems under control. This guideline matches with numerical quantum optimal-control algorithms and helps to steer concrete experimental quantum setups in an optimized way, where modulated noise can be incorporated as additional control resource. Bridges to powerful experimental settings are sketched.

Further, in Section IV, we show how noise occurring in real-world applications can be addressed using ideas from classical robust control. Specifically, we consider a set-membership uncertainty description for the underlying quantum system. Expanding upon the classic Method of Averaging, the standard "averaging transformation" is modified to be suitable for quantum systems. The resulting theory gives rise to an associated robust control optimization with two objectives, capturing a tradeoff between nominal performance and robustness. Further, we present a fundamental bound on the robust performance of uncertain quantum systems.

Finally, Section V (Conclusions) wraps up the paper.

II. Fundamentals of quantum algorithms

The development of powerful quantum algorithms has been a key driver behind the recent surge of research in quantum technologies. In this section, we provide a tutorial introduction to the mathematical framework of quantum algorithms based on complex linear algebra. In particular, we cover basic concepts such as qubits (Section II-A), measurement (Section II-B), and quantum gates (Section II-C). We then combine these concepts into quantum algorithms in Section II-D, introducing both the main mathematical concept as well as several important examples. Next, in Section II-E, we introduce variational quantum algorithms (VQAs) which are feedback interconnections of classical and quantum algorithms. Finally, we discuss density matrices which provide an alternative and often useful mathematical description of quantum states (Section II-F).

This section focuses on the fundamental basics of quantum algorithms and we refer to [14] for a more comprehensive introduction from the control perspective as well as to [1] for an excellent standard primer on quantum computing.

A. Qubits

Quantum bits (*qubits* in short) are the basic unit of computation on a quantum computer. Mathematically, a qubit is a complex unit vector $|\psi\rangle \in \mathbb{C}^2_{=1}$, where we use the standard *Dirac notation* $|\psi\rangle$ for quantum states. It is insightful to express a qubit in the *computational basis* as

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \tag{1}$$

for the basis states $|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}$, $|1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$. Here, α and β are commonly referred to as the probability amplitudes. Whereas a classical bit takes one of two values 0 or 1, a qubit lies in *superposition* of the basis states $|0\rangle$ and $|1\rangle$. A measurement of the qubit in the computational basis collapses this superposition onto one of two possible outcomes: either 0 or 1 with probability $|\alpha|^2$ and $|\beta|^2$, respectively (see Section II-B for details).

A quantum state composed of n qubits is a 2^n-dimensional complex unit vector, i.e., $|\psi\rangle \in \mathbb{C}^{2^n}_{=1}$. The computational basis for this space is formed by n-fold tensor products (i.e., Kronecker products) of the basis states $|0\rangle$ and $|1\rangle$ with themselves, i.e.,

$$|0\ldots00\rangle\,,\ \ |0\ldots01\rangle\,,\ \ \text{etc.,} \tag{2}$$

where we use the common notation $|ab\rangle = |a\rangle \otimes |b\rangle$ for bit strings a and b. A simple example of a 2-qubit quantum state is the tensor product of two single-qubit states $|\psi_1\rangle$ and $|\psi_2\rangle$, i.e., $|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$. States which can be written as the tensor product of two quantum states are called *separable*. It is an important fact that not all multi-qubit states are separable, e.g., the *Bell state*

$$|\Phi^+\rangle = \tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \tag{3}$$

cannot be decomposed into a tensor product of two single-quit states. States which are not separable are called *entangled*. Entanglement corresponds to a strong form of correlation which is unique to quantum systems and a key ingredient for computational speedups of quantum algorithms [19].

B. Projective Measurements

Contrary to classical physics, it is in general not possible to precisely determine the state of a quantum system. In the following, we introduce *projective measurements*, which allow to retrieve information about quantum states according to certain rules (see [1] for details and alternative forms of measurements).

Projective measurements are taken w.r.t. an *observable*, i.e., a Hermitian matrix $M = M^\dagger \in \mathbb{C}^{2^n \times 2^n}$, where we use $M^\dagger$ to denote the Hermitian transpose of a matrix M. Let us write M in its spectral decomposition

$$M = \sum_i \lambda_i P_i \tag{4}$$

with the different eigenvalues λ_i and the orthogonal projectors P_i onto the corresponding eigenspaces. When performing a projective measurement of the state $|\psi\rangle$ w.r.t. M, the

outcome is always one of the λ_i's. A particular λ_i is returned with probability

$$\langle\psi|P_i|\psi\rangle := \psi^\dagger P_i \psi. \tag{5}$$

Moreover, immediately after the measurement, the quantum state $|\psi\rangle$ *collapses*, i.e., it changes its value to the orthogonal projection on the corresponding eigenspace

$$\frac{P_i\,|\psi\rangle}{\langle\psi|P_i|\psi\rangle}. \tag{6}$$

The fact that quantum states possibly change their values due to a measurement poses unique challenges to the design and implementation of quantum algorithms.

Let us illustrate the concept of projective measurements with a simple example: Suppose we measure a single qubit $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ w.r.t. the Pauli matrix $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, an operation that is commonly referred to as measurement in the computational basis. According to the above exposition, the measurement can only return one of the two eigenvalues $\lambda_{1/2} = \pm 1$ of Z. The probability for measuring $\lambda_1 = +1$ or $\lambda_2 = -1$ is

$$\langle\psi|P_1|\psi\rangle = |\alpha|^2 \quad \text{and} \quad \langle\psi|P_2|\psi\rangle = |\beta|^2, \tag{7}$$

respectively, where $P_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and $P_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$. Moreover, if the measurement returns $+1$, then, immediately afterwards, the quantum state is equal to the corresponding eigenvector $|0\rangle$, and likewise for the measurement outcome -1 with the corresponding eigenvector $|1\rangle$.

In many practical scenarios, one is not interested in a particular measurement outcome but, instead, it is desirable to perform repeated measurements of the state $|\psi\rangle$ in order to determine the value of the quadratic form

$$\langle\psi|M|\psi\rangle = \psi^\dagger M \psi. \tag{8}$$

Since measurements affect the state in a possibly undesirable fashion, this requires the availability of independent copies of $|\psi\rangle$ which need to be generated separately. Assuming that such copies are available, a statistical estimate of (8) can be determined based on projective measurements. To be precise, suppose we have T independent copies of $|\psi\rangle$ and measure each state w.r.t. M, obtaining each outcome λ_i for T_i of these measurements. Then, we can form the approximation

$$\langle\psi|M|\psi\rangle \approx \frac{\sum_i \lambda_i T_i}{T}. \tag{9}$$

Projective measurements can be interpreted as sampling from a Bernoulli distribution. This allows to derive error bounds for the approximation in (9), which vanish when $T \to \infty$, see [20, Section 3.2.4] for details. To summarize, projective measurements can be interpreted as statistical estimates of the quadratic form (8).

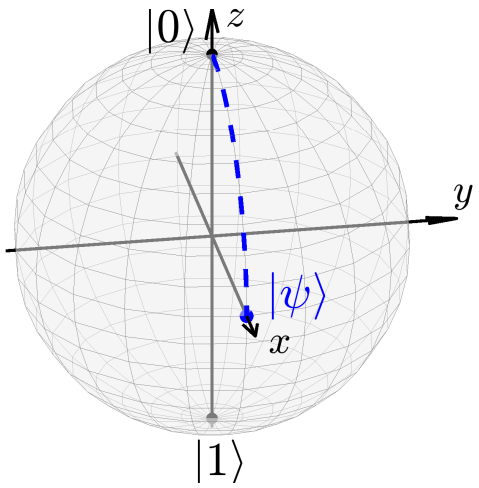

Fig. 1. Bloch-sphere representation of a single-qubit rotation $R_y(\frac{\pi}{2})$ applied to the qubit in state $|0\rangle$.

C. Quantum Gates

On a quantum computer, qubits are manipulated using *quantum gates*, which are the quantum analog to classical logical gates (AND, NOT, OR, etc.). Mathematically, quantum gates are unitary matrices $U \in \mathbb{C}^{2^n \times 2^n}$, i.e., they satisfy $U^\dagger U = I$. A quantum gate U acts on a qubit via multiplication, i.e., applying U to $|\psi\rangle$ produces $U\,|\psi\rangle$. Notable examples of quantum gates include the Pauli gates

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\ Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{10}$$

The Pauli-X gate is frequently referred to as NOT since $X\,|0\rangle = |1\rangle$ and $X\,|1\rangle = |0\rangle$. Intuitively, quantum gates can be thought of as rotations. To show this, we resort to the *Bloch sphere*, which is a useful graphical illustration of qubits. Since multiplication of a quantum state by a *global phase* $e^{-i\varphi}$ does not affect the outcome of a measurement (compare (5)), quantum states which only differ by a global phase are considered equivalent. Using additionally that $\||\psi\rangle\| = 1$, a qubit $|\psi\rangle$ has two free parameters, which can be mapped onto a sphere in $\mathbb{R}^3$, compare Figure 1. The north pole and south pole of this sphere is $|0\rangle$ and $|1\rangle$, respectively, whereas intermediate values are in superposition of these two basis states.

Figure 1 illustrates a simple quantum gate: the rotation around the y-axis by angle $\frac{\pi}{2}$, which corresponds to the unitary matrix $R_y(\frac{\pi}{2})$ for the *rotation gate*

$$R_y(\theta) = e^{-i\frac{\theta}{2}Y}. \tag{11}$$

To design a non-trivial quantum algorithm, multi-qubit gates are required. A popular example is the *controlled-NOT* gate (CNOT), which is a 2-qubit gate defined via the unitary matrix

$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{12}$$

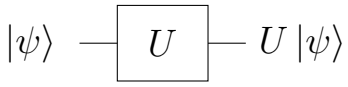

Fig. 2. Circuit representation of a quantum gate U acting on the input state $|\psi\rangle$ and leading to the output state $U|\psi\rangle$.

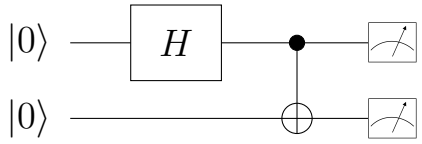

Fig. 3. Quantum circuit implementing the algorithm in (15) generating a Bell state $|\Phi^+\rangle$, followed by a measurement of each individual qubit w.r.t. the observable Z.

When applied to a quantum state of the form $|\psi_1\rangle \otimes |\psi_2\rangle$, the CNOT yields

$$|\psi_1\rangle \otimes |\psi_2\rangle \qquad \text{if } |\psi_1\rangle = |0\rangle \tag{13}$$

$$\text{and} \quad |\psi_1\rangle \otimes X|\psi_2\rangle \quad \text{if } |\psi_1\rangle = |1\rangle, \tag{14}$$

i.e., a Pauli-X gate (the NOT gate) is applied to the second qubit if the first qubit is in state $|1\rangle$. In quantum algorithms, the CNOT gate is typically used to generate entanglement. For example, when initializing two qubits in the computational basis state $|00\rangle$, applying the *Hadamard gate* $H = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$ to the first qubit and then applying a CNOT yields the prime example of an entangled state, the Bell state (3), i.e.,

$$|\Phi^+\rangle = \mathrm{CNOT}(H \otimes I_2)|00\rangle\,, \tag{15}$$

where I_2 is a two-dimensional identity matrix. Quantum gates are commonly illustrated in their circuit representation, compare Figure 2.

D. Quantum Algorithms

A quantum algorithm typically is a combination of qubits, quantum gates, and measurements. Quantum algorithms are commonly displayed in their circuit representation and are, therefore, also referred to as quantum circuits. Figure 3 illustrates the circuit implementing the operation in (15), i.e., converting the initial state $|00\rangle$ to the Bell state $|\Phi^+\rangle$, which is then measured. Measurements are generally depicted via the *meter* symbol on the right end of the circuit. If no observable is mentioned explicitly, then the measurement is understood as measurement in the computational basis, i.e., measuring each individual qubit w.r.t. Z.

By convention, quantum circuits are read from left to right. It is simple to show that a parallel and series interconnection of unitary matrices is, again, a unitary matrix. Hence, we obtain the following statement.[1]

[1]Throughout this tutorial paper, colored boxes contain key statements and takeaway messages.

Mathematical Core of Quantum Algorithms

In the *quantum-circuit model*, quantum algorithms can be concisely formulated as applying a (possibly large) unitary matrix U to an initial state $|\psi_0\rangle$ and performing a projective measurement w.r.t. an observable M afterwards. Often, the measurement has the purpose of estimating the quadratic form (8). In this case, the quantum algorithm outputs the expectation value

$$\langle\psi_0|U^\dagger M U|\psi_0\rangle\,. \tag{16}$$

In the following, we summarize and discuss several fundamental quantum algorithms.

Quantum Fourier Transform: The quantum Fourier transform (QFT) is one of the most important quantum algorithms, especially since it is frequently used as a subroutine (e.g., in Shor's algorithm). To define it, we use the decimal representation of the computational basis states in (2) such that, e.g., $|6\rangle = |110\rangle$. The QFT acts on a given initial state $|\psi_0\rangle$ by applying the discrete Fourier transform (DFT) on the probability amplitudes. More precisely, for $k = 0, \ldots, 2^n - 1$, the computational basis state $|k\rangle$ is mapped to

$$\frac{1}{2^{n/2}} \sum_{j=0}^{2^n-1} e^{2\pi i \frac{jk}{2^n}} |j\rangle\,. \tag{17}$$

The definition is extended to arbitrary states $|\psi_0\rangle$ via linearity. As shown in more detail in [1, Section 5], the above-defined operation is, in fact, unitary and can be implemented based on applying suitable quantum gates. At first glance, the QFT promises a remarkable speed-up over the classical DFT since it allows to Fourier transform 2^n values using only $\mathcal{O}(n^2)$ operations, whereas the DFT requires $\mathcal{O}(n2^n)$ operations. The main bottleneck is that the probability amplitudes of the resulting output state cannot be accessed directly but only via the principles of measurement as outlined in Section II-B.

Shor's Algorithm: Shor's algorithm allows to factorize integers into their prime factors in polynomial time. Integer factorization forms the backbone of the RSA public-key cryptosystem, i.e., the security of this system relies on the fact that, currently, no algorithm is known to factorize integers in polynomial time on a classical computer. Thus, a sufficiently large and reliable quantum computer could render RSA insecure. Shor's algorithm consists of two main steps: 1) translating the factorization problem into a period finding problem and 2) solving the latter problem using the QFT, compare [1, Section 5], [2] for further details.

Grover's Algorithm: On a classical computer, searching a single marked element in a list of overall N elements takes $\mathcal{O}(N)$ operations. Grover's algorithm [1, Section 5], [3] solves the same problem on a quantum computer in only $\mathcal{O}(\sqrt{N})$ operations, i.e., with a quadratic speedup. While a quadratic speedup is less powerful than an exponential one as in Shor's algorithm, Grover's algorithm has still become one of the most popular quantum algorithms since it can be

used to improve other quantum algorithms which are based on exhaustive search.

Quantum Simulation: Simulating the time evolution of a quantum system is a fundamental problem in various domains such as drug design, quantum chemistry, or material science. In fact, quantum simulation has inspired the original idea of a quantum computer by Richard Feynman [21]. Mathematically, quantum simulation boils down to solving the Schrödinger equation

$$|\dot{\psi}\rangle = -iH\,|\psi\rangle \tag{18}$$

for the quantum state $|\psi\rangle$ and the *Hamiltonian* $H = H^\dagger$. However, since the dimension of $|\psi\rangle$ scales exponentially with the number of qubits, quantum simulation is inherently challenging for classical computers. In quantum simulation, the key idea is to decompose the Hamiltonian H into a sum of Hamiltonians which only act non-trivially on a subset of the n qubits, i.e., $H = \sum_k H_k$ for sufficiently sparse matrices $H_k = H_k^\dagger$. The solution of (18) can then be approximated via the Lie-Trotter formula as

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle \approx \prod_k e^{-iH_k t}\,|\psi(0)\rangle\,, \tag{19}$$

where each of the unitary matrices $e^{-iH_k t}$ can be implemented (approximately) via suitable quantum gates. While this is only an approximation since $e^{A+B} \neq e^A e^B$ in general, the literature contains various results on bounding the resulting approximation error, see, e.g., [4, 22] and the references therein.

E. Variational Quantum Algorithms

In the current NISQ era [5, 6], quantum devices are of limited size and significantly affected by noise. VQAs [23] have emerged as a promising class of algorithms to address these challenges. The key idea is to design quantum algorithms that are smaller but adapt to potential inaccuracies in the hardware. This is made possible by introducing parametrized quantum algorithms, where the individual unitary matrices depend on real-valued parameters. To be precise, for a set of matrices $H_j = H_j^\dagger$ and parameters $\theta \in \mathbb{R}^N$, define

$$U(\theta) = U_1(\theta_1)\cdots U_N(\theta_N) \tag{20}$$

with each $U_j(\theta_j) = e^{-i\theta_j H_j}$ for $j = 1, \ldots, N$. Inserting $U(\theta)$ into the equation (16) characterizing a generic quantum algorithm, we obtain a map $f : \mathbb{R}^N \to \mathbb{R}$ with

$$f(\theta) = \langle\psi_0|U(\theta)^\dagger M U(\theta)|\psi_0\rangle \tag{21}$$

for some initial state $|\psi_0\rangle$ and observable $M = M^\dagger$. In a VQA, the main idea is to iteratively adapt the parameters θ via a classical parameter update rule

$$\theta^+ = g(\theta, f(\theta)), \tag{22}$$

in order to find a minimizer θ^* of the function $f(\theta)$. Here, the map $g : \mathbb{R}^{N+1} \to \mathbb{R}^N$ is typically defined via some classical optimization routine, e.g., based on gradient descent [24]. Note that executing (22) requires the execution of the quantum algorithm $f(\theta)$ as well as the classical computation $g(\theta, f(\theta))$, which is why VQAs are frequently referred to as hybrid quantum-classical algorithms. From a control viewpoint, VQAs are especially interesting.

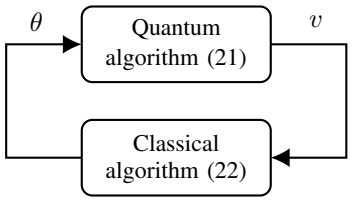

Fig. 4. Variational quantum algorithm (VQA) as feedback interconnection of the quantum algorithm (21) (a static nonlinearity) and the classical algorithm (22) (a dynamical system).

VQAs As Feedback Interconnections

VQAs are feedback interconnections of a dynamical system (the classical algorithm) and a static nonlinear function (the quantum algorithm), compare Figure 4. Mathematically, this means

$$\theta^+ = g(\theta, v) \quad \text{with} \quad v = f(\theta). \tag{23}$$

While VQAs have received significant attention in recent years, they face a number of open challenges, in particular the design of the classical optimization scheme g as well as the corresponding convergence analysis [23]. Given that they are, in fact, Lur'e systems, they lend themselves naturally to a theoretical analysis via systems-theoretic tools such as dissipativity [25, 26].

Let us conclude by mentioning several examples of VQAs. The variational quantum eigensolver (VQE) [27] aims to determine the minimum eigenvalue of a matrix H, which is a challenging problem of central importance in various domains, in particular in quantum chemistry. The quantum approximate optimization algorithm (QAOA) [28], on the other hand, tackles combinatorial optimization problems. Given that many relevant problems arising in control involve integer optimization, the QAOA is an interesting candidate for using quantum computers in control, see [29–31]. Finally, in variational quantum machine learning, the function f in (21) is employed as a function approximator for supervised learning [32–36].

F. Density Matrices

Density matrices are an alternative representation of quantum states that emerge naturally from the following thought experiment: Suppose we are given an ensemble of quantum state vectors $|\psi_i\rangle$, $i = 1, \ldots, q$. It is unknown in which of these states a given quantum system is, but we have a set of probabilities p_i, $i = 1, \ldots, q$, such that the system is in state $|\psi_i\rangle$ with probability p_i. This information can be conveniently summarized via the *density matrix*

$$\rho = \sum_{i=1}^{q} p_i\,|\psi_i\rangle\,\langle\psi_i|\,. \tag{24}$$

The density matrix description of quantum states is equivalent (up to phases, cf. below) to the state vector picture employed in the previous sections. Density matrices can be mathematically more convenient to use, in particular in the context of quantum error correction [1] as well as in quantum systems and control theory, compare Section III. To provide a specific example, recall that multiplication of a quantum state by a global phase $e^{-i\varphi}$ does not affect the measurement outcome and therefore, strictly speaking, any quantum state $|\psi\rangle$ gives rise to an equivalence class $\{e^{-i\varphi}|\psi\rangle \mid \varphi \in \mathbb{R}\}$. In the density matrix picture, on the other hand, global phase factors cancel out in forming the products

$$|\psi_i\rangle e^{i\varphi} e^{-i\varphi} \langle\psi_i| = |\psi_i\rangle \langle\psi_i| . \tag{25}$$

All operations defined in the previous sections can be equivalently formulated for density matrices. The action of a quantum gate U on ρ can be easily computed by acting on each of the states $|\psi_i\rangle$ individually, i.e.,

$$\rho \mapsto \sum_{i=1}^{q} p_i U |\psi_i\rangle \langle\psi_i| U^\dagger = U\rho U^\dagger. \tag{26}$$

Further, a projective measurement w.r.t. an observable $M = \sum_i \lambda_i P_i$ yields the outcome λ_i with probability

$$\mathrm{tr}(P_i\rho). \tag{27}$$

If the measurement returns λ_i, then the state collapses to

$$\rho' = \frac{P_i \rho P_i}{\mathrm{tr}(P_i\rho)}. \tag{28}$$

It is simple to verify that, in the special case where ρ represents one quantum state vector $|\psi\rangle$ with certainty, i.e., $\rho = |\psi\rangle\langle\psi|$, the above formulas reduce to those presented in Section II-B. States ρ for which $\rho = |\psi\rangle\langle\psi|$ holds with some $|\psi\rangle$ are called *pure states*, whereas states as in (24) with $q > 1$ are called *mixed states*. The trace of ρ^2 provides a simple criterion to distinguish between pure states ($\mathrm{tr}(\rho^2) = 1$) and mixed states ($\mathrm{tr}(\rho^2) < 1$). For single-qubit states $\rho \in \mathbb{C}^{2\times 2}$, this difference can be nicely illustrated via the Bloch sphere. Here, pure states are all the points on the sphere whereas mixed states lie within the unit ball. Intuitively, states that are closer to the center of the ball possess a higher level of uncertainty. The state at the center has the maximum possible uncertainty and is, therefore, referred to as the *maximally mixed* state. Mathematically, it lies in equal superposition of the computational basis states $|0\rangle$ and $|1\rangle$ such that

$$\rho = \tfrac{1}{2}|0\rangle\langle 0| + \tfrac{1}{2}|1\rangle\langle 1| = \tfrac{1}{2} I_2. \tag{29}$$

III. Exploiting a Unified Lie Frame for Quantum Systems Theory and Control Engineering

The amount of oversimplification when reading this section under the overarching motto '*Break the symmetries of your (bilinear) quantum control system by choosing the right controls (or observables) in order to bring it under control (or observation)!*' is—of course not quite negligible but—in no way criminal. The reader is invited to bear with us when making the motto more precise step by step in the sequel. In so doing, we wrap up Lie-theoretical intricacies in adapted matrix representations, so the reader may keep the familiar 'matrix times vector' picture.

Finite-dimensional dynamical sytems pertinent to quantum-control engineering of, e.g., N-level quantum gates often boil down to the standard form of *bilinear control systems* [37–40]

$$\dot{X}(t) = -(A + \textstyle\sum_j u_j(t) B_j) X(t) \quad \text{with} \quad X(0) = X_0 \ \ (\Sigma)$$

as exemplified in the summarizing Tab. I. E.g., in a controlled Schrödinger equation $|\dot{\psi}(t)\rangle = -i(H_0 + \sum_j u_j(t) H_j)|\psi(t)\rangle$ A, B are linear operators on a (finite-dimensional) Hilbert space $\mathcal{H}$ and $X(t) = |\psi(t)\rangle$ is a pure quantum state. In these closed systems, the non-switchable *drift term* A is given by the system Hamiltonian iH_0, while the B_j are the *control Hamiltonians* iH_j governed by typically piece-wise constant control amplitudes $u_j(\tau) \in \mathbb{R}$. In such a time interval, the time evolution is $|\psi(\tau)\rangle = e^{-i\tau H}|\psi(0)\rangle =: U(\tau)|\psi(0)\rangle$. Compiling quantum gates as in Section II-C can be thought of (and done!) via solving an optimal-control problem for the system (Σ) with variables as in Tab. I (1').

In general and for open dissipative systems, states are described by *density operators* $\rho(t) = \sum_k p_k |\psi_k\rangle\langle\psi_k|$, i.e. convex combinations of pure-state projectors as in Section II-F. Then taking $X(t) = |\rho(t)\rangle$ as vectorised density operator, and conveniently moving to (super)operators in Liouville space now with drift term $i\widehat{H}_0 + \widehat{\Gamma}$ (including possible relaxation $\widehat{\Gamma}$) *versus* controls as $u_j(t) i\widehat{H}_j$ recovers the simple bilinear pattern of Eqn. (Σ). For the Hamiltonian part, $\widehat{H}|\rho\rangle$ corresponds to the commutator $[H, \rho] := H\rho - \rho H$ also written as $\mathrm{ad}_H(\rho)$ in the sequel.

In the respective operator lift of a closed system, $X(t)$ takes the form of a unitary conjugation map $\widehat{U}(t)$ acting on density operators $|\rho\rangle$ corresponding to $U(t)\rho U^\dagger(t)$ denoted $\mathrm{Ad}_{U(t)}(\rho)$—see the remark on tools and notations below.

For deciding the feasibility of quantum engineering tasks, in the sequel we introduce core definitions and systems-theoretical concepts for (Σ) like controllability, reachabilty, observability etc. The concrete implementation can then be relegated, e.g., to numerical optimal-control algorithms as sketched in Sec. III-E.

A. Controllability and Reachability in Closed Systems

While a *linear control system* $\dot{x}(t) = Ax(t) + Bu$ with $x_0 = x(0)$ is fully controllable [38, 42] provided its reachability matrix $[B, AB, A^2B, \ldots, A^{N-1}B]$ has full rank, controllability of a *bilinear system* of the form Eqn. (Σ) (henceforth on a compact connected Lie group $\mathbf{K}$ with Lie algebra $\mathfrak{k}$, so $\mathbf{K} = \langle \exp \mathfrak{k} \rangle$) depends on its *system algebra*

$$\mathfrak{k}_\Sigma := \langle A, B_j \mid j = 1, 2, \ldots, m \rangle_{\mathrm{Lie}} , \tag{30}$$

where $\langle\cdot\rangle_{\mathsf{Lie}}$ denotes the *Lie closure* of taking the real span over nested commutators until no new linearly indepedent elements are generated. So the system algebra $\mathfrak{k}_\Sigma$ takes the

TABLE I

SCENARIOS OF BILINEAR QUANTUM CONTROL SYSTEMS [41]

Setting and Task $\dot{X}(t) = -\big(A + \sum_j u_j(t) B_j\big) X(t)$	'State' $X(t)$	Drift A	Controls B_j
closed systems:			
(1) pure-state transfer (fixed global phase)	$\lvert\psi(t)\rangle$	iH_0	iH_j
(1') gate synthesis (fixed global phase)	$U(t)$	iH_0	iH_j
(2) state transfer (modulo global phase)	$\lvert\rho(t)\rangle$	$i\widehat{H}_0$	$i\widehat{H}_j$
(2') gate synthesis (modulo global phase)	$\widehat{U}(t)$	$i\widehat{H}_0$	$i\widehat{H}_j$
open systems:			
(3) state transfer I	$\lvert\rho(t)\rangle$	$i\widehat{H}_0{+}\widehat{\Gamma}$	$i\widehat{H}_j$
(3') quantum-map synthesis I	$F(t)$	$i\widehat{H}_0{+}\widehat{\Gamma}$	$i\widehat{H}_j$
(4) state transfer II	$\lvert\rho(t)\rangle$	$i\widehat{H}_0$	$i\widehat{H}_j, \widehat{\Gamma}$
(4') quantum-map synthesis II	$F(t)$	$i\widehat{H}_0$	$i\widehat{H}_j, \widehat{\Gamma}$

$\lvert\psi\rangle$ is a pure-state vector, $\lvert\rho\rangle$ a vectorised density operator, $\widehat{H}$ is the Hamiltonian adjoint action generating unitary conjugation $\widehat{U}$ see notational remark below

form of a Lie algebra.[2] It is the fingerprint of the dynamic system and it decides its controllability as follows.

Controllability of Bilinear Systems

The bilinear control system (Σ) is *controllable* on $\mathbf{K}$, if its system Lie algebra $\mathfrak{k}_\Sigma$ of Eqn. (30) satisfies the celebrated *Lie-algebra rank condition* $\mathfrak{k}_\Sigma = \mathfrak{k}$ [43–47] and thus generates the entire Lie group $\mathbf{K}$ by way of exponentiation $\mathbf{K} = \langle \exp \mathfrak{k}_\Sigma \rangle$.

In closed quantum systems (no dissipation) with N levels (dimensions), first take $\mathfrak{k}_\Sigma$ as a subalgebra of $\mathfrak{su}(N)$, the latter comprising the $N \times N$ skew-hermitian (traceless) matrices. Each element can be thought of as (i times) a Hamiltonian direction 'iH' where $H{=}H^\dagger$ is some Hamiltonian (i.e. 'energy operator'). So—at first sight in the scenario (1 or 1') of Tab. I—for a (closed) N-level quantum bilinear control system to be fully controllable on the pure-state vectors $|\psi\rangle$, it suffices that $\mathbf{K} = SU(N)$, i.e. the system algebra comprises all the unitaries $\mathfrak{k}_\Sigma = \mathfrak{su}(N)$. For quantum information, this means that every unitary quantum gate can be generated as $SU(N) = \exp \mathfrak{k}_\Sigma$. Such a system is *universal* as it allows to implement a universal quantum computer.

Recall that, by Eqn. (8), a quantum mechanical expectation value of an observable $A{=}A^\dagger$ w.r.t. to a state $|\psi\rangle$ is of scalar-product form $\langle A \rangle_\psi = \langle \psi | A \psi \rangle$, hence all states $\{e^{i\phi} |\psi\rangle \mid \phi \in \mathbb{R}\}$ share the same expectation value and are thus operationally indistinguishable. Therefore, fixed *global* phases are artificial and do not correspond to any physically relevant degree of freedom[3]. The same holds for global phases of unitary time-evolutions $\{e^{i\alpha} U(t) \mid \alpha \in \mathbb{R}\}$. Most conveniently, by projective construction they neither appear in the density operator $\rho(t) = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ nor in its time evolution under unitary conjugation $\rho(t) = \mathrm{Ad}_{U(t)}(\rho_0) = U(t)\rho_0 U^\dagger(t)$.

That's why—see (2 or 2') of Tab. I—it is natural to work with *density operators* ρ and their time evolutions $\rho(t)$ henceforth as control problems on the *unitary orbit* $\mathcal{O}_U(\rho) := \{U\rho_0 U^\dagger \mid U \in SU(N)\}$.

Tutorial Remark on Tailored Toolbox and Notations:
To solve matrix equations as $[H, X] = HX - XH = 0$ for X, it is convenient to vectorise the matrix X to the vector $|X\rangle$ defined as the stacked column of all columns of X. In this convention, one gets the useful formula $|AXB\rangle = (B^\top \otimes A)\,|X\rangle$, see Chp. 4. of [48]. Then the solution sets to $[H, X] = 0$ and $(\mathbb{1}\otimes H - H^\top \otimes \mathbb{1})\,|X\rangle = |0\rangle$ interrelate, as the kernel of $\widehat{H} := (\mathbb{1}\otimes H - H^\top \otimes \mathbb{1})$ represents the *commutant* of H in vectorised form. Likewise, the *joint commutant* of a set $\{H_j\}$ with, e.g., $j = 1, 2$ can conveniently be read from the joint kernel of the stacked matrix $\left[\begin{smallmatrix}\widehat{H}_1\\ \widehat{H}_2\end{smallmatrix}\right]$.

With H hermitian, $i\widehat{H}$ may be thought of as representing $i\,\mathrm{ad}_H$. Therefore, $\exp(-it\,\mathrm{ad}_H) = \mathrm{Ad}_{U(t)} = U(t)(.)U^\dagger(t)$ (where $U(t) := e^{-itH}$) can be represented in the vectorised picture by $\widehat{U}(t) = \exp(-it\widehat{H}) = \bar{U} \otimes U$. For staying in the familiar 'matrix times vector' representation, think of $\mathrm{Ad}_U(\rho)$ as $\widehat{U}\,|\rho\rangle$ and of $\mathrm{ad}_H(\rho)$ as $\widehat{H}\,|\rho\rangle$.

A set of square matrices like $\{iH_j\}_{j=0}^m$ is called *irreducible* if and only if, as linear operators, they have no common non-trivial invariant linear subspaces (other than the full space or the zero-space). This is guaranteed if their *joint commutant is trivial* (i.e. just consists of multiples of the identity), since then there is no common reducing projector.

A key to the following symmetry considerations is that irreducibility of $\{iH_j\}_{j=0}^m$ does *not* necessarily imply irreducibility[4] of $\{i\widehat{H}_j\}_{j=0}^m$, unless the $\{iH_j\}_{j=0}^m$ *generate the entire Lie algebra* $\mathfrak{su}(N)$ by $\langle iH_j \mid j = 0, 1, 2, \ldots, m\rangle_{\mathrm{Lie}}$, which means *the corresponding bilinear control system is fully controllable* [49].

Now we have the proper operational setting for the following controllability condition.

Full Controllability (in Closed Quantum Systems)

A closed N-level *quantum* bilinear control system (also comprising mixed states) is fully controllable on density operators ρ if and only if its system algebra is $\mathfrak{k}_\Sigma = \mathrm{ad}_{\mathfrak{su}(N)}$. It also generates the entire group of unitary conjugation $\mathbf{K}_\Sigma = \mathrm{Ad}_{SU(N)}$ by $\exp \mathfrak{k}_\Sigma = \mathrm{Ad}_{SU(N)} = \{U(.)U^\dagger \mid U \in SU(N)\}$ and thus all unitary gates.

As an immediate consequence, in fully controllable systems one has the following reachable set of states ρ.

[2] A *Lie algebra* $\mathfrak{g}$ (here over finite-dim. square matrices) is closed under the commutator $[A, B] := AB - BA$, and it is (i) bilinear in its arguments, (ii) antisymmetric ($[A, B] = -[B, A]$) and (iii) satisfying JACOBI's identity $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$ $\forall A, B, C \in \mathfrak{g}$. NB: all square matrices $\mathbb{C}^{N\times N}$ form the Lie algebra $\mathfrak{gl}(N, \mathbb{C})$, while $\mathfrak{su}(N)$ is a subalgebra comprising its traceless skew-hermitian ($A^\dagger{=}{-}A$) part.

[3] in contrast to *relative* phases of one *sub*system w.r.t. other subsystems as, e.g., in the Aharanov-Bohm experiment

[4] In the adjoint representation the 2 trivial symmetries are $\mathbb{1}^{\otimes 2}$ and $|\mathbb{1}\rangle\langle\mathbb{1}|$.

Reachable Sets in Fully Controllable Systems

The reachable set to an initial state ρ_0 of a *fully controllable* closed quantum bilinear control system (Σ) with system algebra $\mathfrak{k}_\Sigma = \mathrm{ad}_{\mathfrak{su}(N)}$ corresponds to the entire unitary orbit $\mathrm{Reach}_\Sigma(\rho_0) = \mathcal{O}_U(\rho_0) = \{U\rho_0 U^\dagger \,|\, U \in SU(N)\}$. It thus equals the *isospectral set of* ρ_0 defined as the set of all density operators ρ sharing the same eigenvalues with the initial state ρ_0.

Shifting back to quantum gates one arrives at the following result in the general (not necessarily fully controllable) case.

Reachable Gates

The reachable set of gates $\{K(.)K^\dagger\}$ of a closed quantum bilinear control system (Σ) with system algebra $\mathfrak{k}_\Sigma$ is given by $\mathbf{K}_\Sigma := \exp \mathfrak{k}_\Sigma$.

Accordingly one gets the following general reachability result for quantum states ρ.

Reachable Sets

The reachable set to an initial state ρ_0 of a closed quantum bilinear control system (Σ) with system algebra $\mathfrak{k}_\Sigma$ is given by the orbit $\mathrm{Reach}_\Sigma(\rho_0) = \{K\rho K^\dagger \,|\, K(.)K^\dagger \in \mathbf{K}_\Sigma\}$ determined by the system algebra via $\mathbf{K}_\Sigma = \exp \mathfrak{k}_\Sigma$.

Thus in closed systems a reachable set of states $\mathrm{Reach}_\Sigma(\rho_0)$ is always a subset of the full unitary orbit $\mathcal{O}_U(\rho_0)$.

Application: Can Specific Gates be Engineered?
For quantum engineering of unitary gates, the following result is of practical relevance. Even if a quantum system (Σ) is *not fully controllable* so that it does not allow for implementing all unitary quantum gates, it may still serve to implement specific gates. And, e.g., on a dedicated quantum chip it may even do so in a faster or more robust fashion than a fully controllable universal setup. By way of the system algebra $\mathfrak{k}_\Sigma$, the system theoretic setting here allows for the following straightforward feasibility check:

Let $\hat{L}_t$ be a (negative) matrix logarithm of a desired target unitary gate $\hat{U}_t$ (in adjoint representation), i.e. $\hat{U}_t = e^{-\hat{L}_t}$. Then it can be realised by the control system (Σ) if $\hat{L}_t$ can be spanned by the matrices in its system algebra $\mathfrak{k}_\Sigma$, which in turn can be checked by vectorising the matrices to test whether $\mathrm{rank}\ (\mathfrak{k}_\Sigma) = \mathrm{rank}\ (\mathfrak{k}_\Sigma, \hat{L}_t)$. — This is an example of how in our Lie frame of quantum systems theory, engineering questions can often be broken down to simple linear algebra.

B. Symmetry Assessment of Controllability and Simulability

Although the system algebra $\mathfrak{k}_\Sigma$ is a highly useful fingerprint encapsulating the capabilities of the parent bilinear control system (Σ), it may be tedious to come by via calculating the entire Lie closure of Eqn. (30).

So, how can we simplify the assessment? Often the properties of a control system may already be read from its *symmetries*, which mirror invariances under controls. It is intuitively obvious that a control system with non-trivial symmetries comes with invariant 'constants of the motion' that preclude full controllability. It just takes a few steps to make these symmetry arguments rigorous:

Definition: Dynamic Symmetries of Bilinear Systems
Let (Σ) be an N-level bilinear control system with system algebra $\mathfrak{k}_\Sigma = \langle i\,\mathrm{ad}_{H_j} \,|\, j = 0, \ldots, m\rangle_{\mathsf{Lie}}$, where the adjoint representation is crucial. Then its *symmetries* are defined by the commutant of $\mathfrak{k}_\Sigma$, i.e. the set S_Σ of all matrices simultaneously commuting with the entire system algebra.

Now the beauty of Lie theory comes in handy: Since $\mathfrak{k}_\Sigma$ carries the structure of a Lie algebra, one simply[5] gets its entire symmetries just by the symmetries of the few(!) drift and control terms (as generators of the system Lie algebra) by $S_\Sigma := \{S \in \mathrm{Mat}(N^2) \,|\, [S, i\,\mathrm{ad}_{H_j}] = 0 \;\forall\; j = 0, 1, \ldots, m\}$[6].

Trivial Symmetry Guarantees Controllability

A closed *quantum* bilinear control system is fully controllable on density operators ρ (or on gates of unitary conjugation) if and only if its system algebra $\mathfrak{k}_\Sigma$ just shows trivial symmetries, i.e. $\dim(S_\Sigma) = 2$.

The core insight can be made lucid by a standard group-theory argument[7]: if the system algebra $\mathfrak{k}_\Sigma$ (adjoint representation) is irreducible in the sense of trivial symmetries, then there is no non-trivial invariant subspace supporting control-invariant states ρ other than multiples of the identity.

The symmetry assessment is very powerful and readily extends to quantum simulation. In quantum simulation one picks a well controllable system (Σ) realized in an experimentally handable setup in order to simulate the dynamics of another system (Σ') of interest similar in dynamics, which, however, is difficult to control experimentally, cp. Sec. II-D.

Definition: Simulability in Bilinear Control Systems
A bilinear quantum control system (Σ) with system algebra $\mathfrak{k}_\Sigma$ can *simulate* another one (Σ') with system algebra $\mathfrak{k}_{\Sigma'}$ if the simulating dynamics encapsulate the simulated dynamics, i.e. if and only if (up to isomorphism) $\mathfrak{k}_{\Sigma'} \subseteq \mathfrak{k}_\Sigma$ [49].

Again, the explicit system algebras $\mathfrak{k}_\Sigma$ and $\mathfrak{k}_{\Sigma'}$ may be tedious to come by via the respective Lie closure of Eqn. (30). Now let S_Σ and $S_{\Sigma'}$ denote the respective symmetries of the simulating and the simulated quantum bilinear control system. The powerful intuitive symmetry argument that the *simulated* system may not break the symmetries of the *simulating* system can be expressed as a necessary condition $S_{\Sigma'} \supseteq S_\Sigma$, which was generalised to arbitrary compact cases and made precise in [52] by also taking into account the

[5] i.e. by JACOBI's identity

[6] JACOBI's identity likewise endows the symmetries S_Σ themselves with the structure of a Lie algebra.

[7] although the original rigorous proof of this fact was rather involved [49] in relating back to DYNKIN's work [50] reproduced in [51]

dimensions of central projections (adding up to the necessary condition above the sufficient condition) not discussed here.

C. Symmetry Assessment of Observability, Accessibility, and Tomografiability

Recall that a *linear control system* $\dot{x}(t) = Ax(t) + Bu$ with $x_0 = x(0)$ and observed by $y(t) = Cx(t)$ is *observable* if its observability matrix $[C, AC, A^2C, \ldots, A^{N-1}C]^\top$ has full rank. On the other hand, observability of the *bilinear control system* (Σ)[8] *in quantum dynamics* comes with an observation term in form of a scalar product for the expectation value of C w.r.t. the state $X(t)$ as $Y(t) = \mathrm{tr}\,\{CX(t)\}$ brought about by an *observable* C=$C^\dagger$. In accordance with scenario (2) of Tab. I, it pays to represent the observation term in vectorised form so as to give the control system (on the orbit) as

$$\begin{aligned} |\dot{X}(t)\rangle &= -(\widehat{A} + \textstyle\sum_j u_j \widehat{B}_j)\,|X(t)\rangle \text{ with } |X(0)\rangle = |X_0\rangle \\ Y(t) &= \langle C\,|\,X(t)\rangle \end{aligned} \qquad (\Sigma')$$

In this setting one gets the following definitions modified from [53, 54].

Definition: Observability Space of Quantum Bilinear Systems Let (Σ') be an N-level bilinear control system observed by C and with system algebra $\mathfrak{k}_{\Sigma'}$ as in Eqn. (30). Denote the traceless part[9] of C as $\tilde{C}$ and let $k^{(\nu)}(\tilde{C}) := k_1 k_2 \cdots k_\nu(\tilde{C})$ be the set of all products of adjoint actions from the system algebra $k_i \in \mathfrak{k}_{\Sigma'}$ $(i = 1, \ldots, \nu)$ with $\tilde{C}$ of order ν. Then the *observability space* of (Σ') w.r.t. the observable C is defined

$$\mathcal{O}_{\Sigma'}(C) := \mathrm{span}_{\mathbb{R}}\left\{\tilde{C}, k^{(1)}(\tilde{C}), k^{(2)}(\tilde{C}), \ldots, k^{(N^2-1)}(\tilde{C})\right\}. \qquad (31)$$

Definition: Observability in Quantum Bilinear Systems Let (Σ') be an observed N-level bilinear control system. Then (Σ') *is observable by* C if for any pair of states X_1, X_2 the equality of their expectation values $\mathrm{tr}\,\{CX_1(t)\} = \mathrm{tr}\,\{CX_2(t)\}$ for all $t \in \mathbb{R}$ and joint controls $u_j(t)$ implies the equality of the states $X_1 = X_2$. — This is the case if and only if $\mathcal{O}_{\Sigma'}(C)$ comprises *all hermitian matrices* [53, 54], as such an observability space is *informationally complete*.

Note that a fully controllable bilinear control system is always observable as well by any non-trivial C, which gives a sufficient condition that in turn is not necessary: systems that fall short of full control may still be observable w.r.t. a specific observable C_1, while for other observables C_2 they are not—see the worked example below.

Again, it may be tedious to calculate the entire observability space of Eqn. (31). Hence yet again symmetry assessment helps: Intuition suggests that the dynamic symmetries $S_{\Sigma'}$ of an observed bilinear quantum control system (Σ') with system algebra $\mathfrak{k}_{\Sigma'}$ (if any) have to be broken by the observable C. The following makes this argument rigorous.

[8] again on a compact connected Lie group $\mathbf{K}$ with Lie algebra $\mathfrak{k}$

[9] $\tilde{C} := C - \frac{\mathrm{tr}\,C}{N}\mathbb{1}_N$

Trivial Symmetry Guarantees Observability

A closed *quantum* bilinear control system (Σ') with system algebra $\mathfrak{k}_{\Sigma'}$ is *observable* by C if and only if for its projector $P_C := |\tilde{C}\rangle\langle\tilde{C}|$ the joint commutant to $\mathfrak{k}_{\Sigma'}$ and P_C is again two-dimensional.

Worked Example:

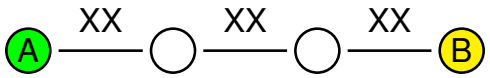

Fig. 5. XX-coupled 4-qubit chain with local controls on the ends.

Take a linear chain consisting of four spin-1/2 qubits. In the basis of Pauli operators written as strings[10], let the drift term be what the physicists call nearest-neighbour XX-coupling, i.e. $H_0 := (xx11 + yy11 + 1xx1 + 1yy1 + 11xx + 11yy)$. The local control Hamiltonians $H_1 := x111, H_2 := y111$ acting as x- and y-controls on qubit (A) and $H_3 := 111x, H_4 := 111y$ as controls on qubit (B) make the coloured ends in Fig. 5 controllable, while the white qubits are uncontrolled.

This system has non-trivial symmetries[11]. When choosing the observable to be $C_1 := xxx1$, the symmetries are preserved and thus the system fails to be observable[12] because it is taken from a $\mathfrak{k}_{\Sigma'}$-invariant subspace. The proper choice in order to get full observability is, e.g., to make it $C_2 := xxx1 + 1z11$, which breaks the symmetry of $\mathfrak{k}_{\Sigma'}$-invariant subspaces—as corroborated by trivial joint commutants.

[For the expert: in $\mathfrak{g} = \mathfrak{su}(N)$ we take the orthogonal decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{m}$ with $\mathrm{ad}_{\mathfrak{k}}(\mathfrak{k}) \subseteq \mathfrak{k}$ and $\mathrm{ad}_{\mathfrak{k}}(\mathfrak{m}) \subseteq \mathfrak{m}$, where (by mild abuse of language) we identify the system algebra $\mathfrak{k}_{\Sigma'}$ in its adjoint representation with $\mathrm{ad}_{\mathfrak{k}}$ to see $\mathfrak{k}$ and $\mathfrak{m}$ as $\mathfrak{k}_{\Sigma'}$-invariant subspaces.]

Observability Limited to Symmetry Sectors

A closed quantum bilinear control system (Σ') with system algebra $\mathfrak{k}_{\Sigma'}$ is called *partially observable* by C if it is observable only for those A whose (non-trivial) $\mathfrak{k}_{\Sigma'}$-invariant support is included in that of C. This requires the joint commutant to $\mathfrak{k}_{\Sigma'}$, $P_{\tilde{A}}$ and $P_{\tilde{C}}$ to contain a (non-trivial) projector $P_{\mathfrak{n}}$ so that

$$P_{\mathfrak{n}}\,|\tilde{A}\rangle = |\tilde{A}\rangle \text{ and } P_{\mathfrak{n}}\,|\tilde{C}\rangle = |\tilde{C}\rangle\,.$$

NB: In the trivial case of $P_{\mathfrak{n}} = \mathbb{1}^{\otimes 2} - |\mathbb{1}\rangle\langle\mathbb{1}|$ full observability is recovered.

Next, let us address accessibility, which in open systems is strictly weaker than full controllability: A quantum bilinear

[10] so $1xx1$ stands for $\mathbb{1} \otimes \sigma_x \otimes \sigma_x \otimes \mathbb{1}$

[11] The commutant to its system algebra $\mathfrak{k}_\Sigma$ in adjoint representation is 3-dimensional and the system algebra is (the adjoint representation of) the orthogonal algebra $\mathfrak{so}(10)$ embedded in the one for the four-qubit unitary algebra $\mathfrak{su}(16)$ as elaborated on in [49].

[12] The observability space of C_1 under $\mathfrak{k}_\Sigma$ has just 210 dimensions, being the orthocomplement to $\mathfrak{so}(10)$ in $\mathfrak{su}(16)$, while for C_2 it exhausts all the 255 dimensions of traceless (skew)hermitian 16×16 matrices as in $\mathfrak{su}(16)$.

control system (Σ) is *accessible* from a given initial state X_0, if the reachable set $\mathrm{Reach}_\Sigma(X_0)$ has non-empty interior. Roughly speaking 'it has to touch all dimensions'. In closed systems the reachable set of states takes the form of a $\mathbf{K}$-orbit as above. While in closed systems controllability and accessibility coincide, in *open Markovian* systems (where controllability is lost), symmetry arguments may be used to decide accessibility as sketched in the outlook.

Combining these notions suggests that given an initial state X_0, its dynamics under a quantum bilinear control system (Σ') is (fully) *tomografiable* by an observable C, if the system is both *accessible* from X_0 and (fully) *observable* by C. The respective weakening to symmetry sectors of non-trivial $\mathfrak{k}_{\Sigma'}$-invariant support is obvious.

Tomografiability would also lend itself as a feasibility criterion for Kalman filtering.

D. Outlook: Reachability in Open Quantum Systems

Open Markovian [55, 56] quantum bilinear control systems can be treated similarly by scenarios (3, 3') and (4, 4') in Tab. I[13]. In N-level systems, the system algebra $\mathfrak{g}_\Sigma$ then becomes a subalgebra of the $N^2 \times N^2$ matrices $\mathfrak{gl}(N^2, \mathbb{R})$, while the reachable sets change from Lie-group orbits (as in the closed systems above) to Lie-*semigroup* orbits as shown in [56] by 1:1 correspondence between Lie and Markov properties in the rich structure of Markovian quantum systems (sparked by the seminal works around Kossakowski and Lindblad [57–59]).

Depending on the sets of fixed points in such open systems, there are two families: in the *unital* case, the maximally mixed state $\rho = \frac{1}{N}\mathbb{1}$ counts among the fixed points, whereas in the *non-unital* case it does not.

Motivated by earlier results [41], the *symmetry assessment* of reachability elaborated on above seems to extend to *Markovian* open bilinear quantum control systems of scenarios (3',4'): ongoing research reveals that n-qubit unital bilinear control systems with a system algebra $\mathfrak{g}_\Sigma$ the symmetries to which are just two-dimensional[14] are (map)accessible, while in non-unital n-qubit bilinear control systems, (map)accessibility comes with one-dimensional trivial symmetry of the system algebra $\mathfrak{g}_\Sigma$.

Thus engineering questions of controllability, reachability, accessibility, observability, and tomografiability can be answered in the emerging unified Lie frame of quantum systems theory. The doability (existence) problems often break down to decision or membership problems in linear algebra related to the respetive dynamic system Lie algebras.

Separating existence questions from constructive proofs makes the methods more general and more versatile. On the other hand, it invites *numerical methods* to address optimal-control engineering in the specific scenario of an experiment taking into account its parameters and constraints without need of (over)simplification or approximation making paper-and-pen constructions viable.

[13] if Γ in Tab. I is of Lindblad form [57–59]

[14] and coincide with the trivial ones in the closed systems above

E. Implementations: Numerical Quantum Optimal Control

For devising control pulses for experimental quantum setups, numerical optimal-control methods play a key role see, e.g., the European Roadmap to Quantum Control Engineering [12]. Here variants of gradient-assisted methods like GRAPE [60] (incl. quasi-Newton extensions [61]) are established as widely applicable and popular. They embrace the important PRONTRYAGIN Maximum Principle [62], which comes into play whenever running costs are taken into account [60]. For robustness in numerical optimal quantum control and its roots in *ensemble controllability* also see [63], Chp. 4.3 in [13], and [64–67], respectively as well as Sec. IV.

F. Exploiting Thermal Resources

With numerical methods at hand, one can easily go beyond the scenarios (3 and 3') in Tab. I and even use (Markovian) noise terms (Γ) as additional controls (4 and 4'). Experimentally, this is made possible in the context of superconducting qubits (GMONs) coupled—in a switchable way(!)—to an open transmission line as, e.g., in [68, 69], among them a former group at Google.

Coupling a (coherently fully controllable) quantum bilinear system in a switchable way to the open transmission line acts when seen from within the quantum system[15] as standard amplitude-damping noise [1], now time-modulated as additional control. In the language of quantum thermodynamical resources it serves as a switchable coupling to a temperature-zero bath. This is an extremely powerful resource, because any N-level coherently fully controllable system coupled via (at least) one qubit to such a bath acts transitively on the set of now mixed quantum states (density operators ρ): it can transform any given initial state ρ_0 in to *any* desired target state ρ_T in the sense that the (closure[16] of the) reachable set to any initial state exhausts the entire set of density operators on that Hilbert space. So $\overline{\mathrm{Reach}_{\Sigma_T}(\rho_0)} = D(\mathcal{H})$ as has been shown in [70] for the concrete parameter setting of [68]—in accordance with the symmetry considerations of Sec. III-D.

These findings have also initiated to exploit the limits of Markovian thermal relaxation seen as an additional resource in a more fundamental way [71, 72].

Conclusion: As to symmetries in systems theory, the initial motto is a *natural guideline* to be taken over to numerical approaches. To get a quantum system with drift term A under control, the more the control terms B_j (Hamiltonians) can be chosen such as to *break the symmetries of the drift term*, the more control one gets over the system. This has been elucidated, e.g., for controlling atoms in a cavity in an (*infinite-dimensional*) Jaynes-Cummings model, where the control terms on the atom break the symmetry of the oscillator [73]. The same concept can be readily extended to couple a system of an atom and cavity to a mechanical oscillator for obtaing non-classical mechanical states with high accuracy [74] using GRAPE-based numerical optimal control in a concrete experimental setup.

[15] i.e. by projection onto the system

[16] since one may have to wait for thermal exponential decay

IV. Robust Synthesis of Quantum Gates

A. Robustness

As explained in Section II, quantum algorithms consist of a combination of qubits, quantum gates, and measurements. In experimental realizations of quantum computers, perturbations due to noise pose a key challenge as they may affect the (ideal) outcome of the computation to an extent that the overhead required for error correction becomes out of reach in the near-term, *e.g.*, [75]. To address this problem, robustness is key, meaning that, despite imperfections or perturbations, each *actual* gate operation should be as close as possible to its ideal. In this section, we introduce a recently proposed robust quantum control approach [76] which borrows ideas from the control community by modeling Hamiltonian uncertainty using a set-membership approach, *e.g.*, [77–82]. We also establish a limit of robust performance if certain conditions are met. This is not *the* limit, that is not known.

There is much written on the subject of perturbed systems. Of special note are the classic works of Bellman, Coppel, and Hale [83–85]. These works show how to transform certain classes of systems to a standard perturbation form, and secondly, show how system properties are maintained as long as the perturbation has a small effect in a well-defined sense. Similar theory follows for robustness of feedback systems via the *Small-Gain Theorem*, *e.g.*, [77, 78], and generalizations for multiple and various uncertainty models, *e.g.*, [81, 82].

Expanding upon the *Method of Averaging* in [85] we modify the standard "averaging transformation" to be suitable for quantum systems. This resulting theory can be viewed through the lens of the Small Gain Theorem as well as an optimization-based approach whose underlying mechanism is supported by several known control design methods similar to dynamical decoupling, *e.g.*, see [86–91] and the references therein. These approaches, and the one presented here, differ from the typical quantum optimal control formulation where the objective is to minimize fidelity error. In contrast, the optimization problem here is posed with *two* objectives: fidelity error along with a term dependent on the size of an interaction representation derived from the characteristics of the sources of uncertainty. In the simplest case, this *regularization* part of the objective function is the first term in the Magnus expansion of a transformed system unitary: *the interaction unitary.*

B. Optimization

The robust quantum control objective is typically formulated as an optimization problem to maximize a worst-case or average case fidelity (compare Section IV-F) with respect to a set of uncertainties represented by bounded sets, and subject to constraints on the optimization variables. For model-based control optimization, although the details vary, and are very important, most problems fit the following formulation:

$$\begin{array}{ll} \text{maximize} & \begin{cases} \text{worst-case} & F = \min_\delta \ F(\theta,\delta) \\ \text{or} & \\ \text{average-case} & F = \langle F(\theta,\delta)\rangle_\delta \end{cases} \\ \text{subject to} & \theta \in \Theta,\ \delta \in \Delta \end{array} \tag{32}$$

Here, F denotes the fidelity [1], which quantifies the overlap between a given to-be-realized quantum gate and the actually realized, imperfect quantum gate, i.e., the deviation of F from 1 quantifies their difference, compare (39). The optimization variables θ typically include control amplitudes and phases produced by a field generator, or commands to the field generator if generator dynamics are of concern. Other design variables can include parameters corresponding to different circuit/gate layouts, material properties, etc. The design variables typically reside in a convex set Θ. The uncertain variables δ are in a set Δ which may not be convex, though often well represented as such depending upon the specific physical implementation, i.e., the uncertainty set can be combinations of deterministic and random variables. Even if all the constraints are convex, the bilinear control nature of the quantum evolution means that the control problem in any form is not a convex optimization problem. As a result all solutions are iterative.

Fortunately, however, the control landscape topology is favorable, *i.e.*, almost always no traps, only saddles [92]. One route is via *sequential convex programming* (SCP) [93] where robust performance can be attained in the presence of a list of inequalities associated with each uncertainty set. In addition to control parameters, the optimization can be used to select any physical adjustable parameters such as Hamiltonian couplings, material parameters, geometry of the qubit layout (an important consideration for QEC involving sparsely connected processor architectures), etc. For "small" deterministic and/or probabilistic perturbations, local approximations by convex functions will suffice rather than lists of inequalities.

A related route to robust quantum control which can handle uncertainties more efficiently is to view the system through the lens of an *interaction representation*, e.g., the basis for filter function formulations [89–91, 94, 95], our recent approach based on the method of averaging [76], and dynamical decoupling (see below)

C. Nominal and perturbed system

To illustrate the main ideas we assume a quantum system of dimension n whose *nominal* (uncertainty-free) dynamics produces the unitary and state evolution for $t \in [0, T]$ given by

$$\begin{aligned} &i\dot{U}_{\rm nom}(t) = \bar{H}(t)U_{\rm nom}(t), \quad U_{\rm nom}(0) = I_n \\ &|\psi_{\rm nom}(t)\rangle = U_{\rm nom}(t)\,|\psi_{\rm nom}(0)\rangle \end{aligned} \tag{33}$$

These dynamics correspond to the bilinear control system (Σ) with $X = U_{\rm nom}$ and $\bar{H} = A + \sum_j u_j B_j$ comprising both the drift as well as the control terms (compare scenario (1') in

Tab. I). Similarly the *perturbed* (uncertain) system evolves according to

$$\begin{aligned} i\dot{U}_{\rm pert}(t) &= \Big(\bar{H}(t) + \tilde{H}(t)\Big)U_{\rm pert}(t) \\ |\psi_{\rm pert}(t)\rangle &= U_{\rm pert}(t)\,|\psi_{\rm pert}(0)\rangle \end{aligned} \tag{34}$$

The nominal and perturbed Hamiltonians are assumed to be members of known sets:

$$\begin{aligned} \Big\{\bar{H}(t), t\in[0,T]\Big\} &\in \mathcal{H}_{\rm nom} \\ \Big\{\tilde{H}(t), t\in[0,T]\Big\} &\in \mathcal{H}_{\rm unc} \end{aligned} \tag{35}$$

The nominal Hamiltonian, $\bar{H}(t)$, typically depends in part on the control variables with control constraints in $\mathcal{H}_{\rm nom}$. Since the control signal generator is also subject to uncertainties, if these are included then the control variables will also appear in the uncertain Hamiltonian, $\tilde{H}(t)$. Though $\tilde{H}(t)$ is uncertain, the set $\mathcal{H}_{\rm unc}$ has specific known characteristics, *e.g.*, parameters or dynamics that are "unknown but bounded."

D. Interaction Hamiltonian

An alternate representation of the perturbed unitary system (34) which exposes the robustness issues is the *interaction unitary*

$$R(t) = U_{\rm nom}(t)^\dagger U_{\rm pert}(t) \tag{36}$$

whose evolution is given by

$$\begin{aligned} i\dot{R}(t) &= G(t)R(t) \\ G(t) &= U_{\rm nom}(t)^\dagger \tilde{H}(t) U_{\rm nom}(t) \end{aligned} \tag{37}$$

where $G(t)$ is the *interaction Hamiltonian*. The latter shows how the controls, acting to produce the nominal unitary, can affect the uncertain Hamiltonian. Note that, if $R(0) = I$ and $G(t)$ is sufficiently small (in a suitable sense), then $R(t) \approx I$ for all t, i.e., $U_{\rm nom}(t)$ is close to $U_{\rm pert}(t)$ at all times. Thus, the deviation of the interaction unitary $R(t)$ from identity quantifies the error and will, therefore, be used to formulate robustness in the following.

E. Open bipartite system

In general the perturbed system is assumed to be in a *bipartite* Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ with system space S of dimension N_S and bath-space B of dimension N_B. The resulting Hilbert space has dimension $n = N_S N_B$. This means that any state can be described as a linear combination of the tensor product of an N_S-system basis set and an N_B-bath basis set.

The term "bath' is used to denote an inaccessible environment, that is, the bath system is very difficult to measure. Conversely, the S-system is accessible by measurement. The system-bath ($S-B$) combination is referred to as an *open system*, and without the bath, a *closed-system*. Though the SB system is unitary, and hence periodic, with a large enough bath the time to return is so large as to appear irreversible. Thus the bath is a principal source of *decoherence*, *i.e.*, from the viewpoint of the accessible S-system, information is lost, and in effect, the dynamics change from quantum to classical.

A general form of the complete Hamiltonian is,

$$H(t) = H_S(t)\otimes I_B + I_S \otimes H_B(t) + H_{SB}(t) \tag{38}$$

where $H_S(t)$ is typically the accessible part of the system, and which includes the controls, $H_B(t)$ is the sel-dynamics of the bath, and $H_{\rm SB}(t0$ is the couping term between the system and the bath. If we take the nominal (uncertainty-free) Hamiltonian as $\bar{H}(t) = H_S(t)\otimes I_B$, then all the uncertainty is in $\tilde{H}(t) = I_S \otimes H_B(t) + H_{SB}(t)$. There could of course be uncertainties in $H_S(t)$ as well (*e.g.*, control noise and other imperfections), and these would then be included in $\tilde{H}(t)$.

F. Fidelity

Measures of quantum computing performance are typically evaluated at a final time $t = T$ corresponding to completion of the intended operation. Hence, for ease of notation in this section, unless otherwise stated, we drop the time dependence, *e.g.*, for unitaries set $U_{\rm pert} \equiv U_{\rm pert}(T), R \equiv R(T), U_{\rm nom} \equiv U_{\rm nom}(T)$, *etc.*, and for states, set $\psi_{\rm in} \equiv |\psi_{\rm pert}(0)\rangle$ and $\psi_{\rm out} \equiv |\psi_{\rm pert}(T)\rangle$.

Let $U_{\rm des}$ denote the final-time desired unitary. The Uhlmann-Josza fidelity [96, 97] comparing the desired output state $\psi_{\rm des} = U_{\rm des}\psi_{\rm in}$ with the actual output state $\psi_{\rm out} = U\psi_{\rm in}$ is

$$F(\psi_{\rm in}) = |\psi_{\rm des}^\dagger \psi_{\rm out}|^2 = |\psi_{\rm in}^\dagger U_{\rm des}^\dagger U \psi_{\rm in}|^2 \tag{39}$$

In this case $F(\psi_{\rm in})$ is identical to the probability of obtaining the desired output state for a given input state $\psi_{\rm in}$. Mathematically, $F(\psi_{\rm in})$ is equal to 1 if and only if $|\psi_{\rm des}\rangle = |\psi_{\rm out}\rangle$.

G. Performance goals

To evaluate performance we will use the fidelity measure (39) for both the nominal (uncertainty-free) system (33) and for the perturbed system (34). For the perturbed system there are two goals:

- *Robust performance* – The final-time unitary $U_{\rm pert}$ should be close to the final-time nominal (uncertainty-free) unitary,

$$U_{\rm pert} \approx U_{\rm nom} = U_S \otimes I_B \tag{40}$$

- *Nominal performance* – Let W be the S-channel target unitary for U_S. Then the desired final-time unitary is,

$$U_{\rm des} = \phi W \otimes I_B \tag{41}$$

with global phase $|\phi| = 1$. Thus the desired unitary is uncorrelated with the bath. A more general form is $U_{\rm des} = \phi W \otimes \Phi_B$ for any unitary Φ_B. As shown in [76, 98], adding this term does allow some additional design flexibiity.

H. Interaction unitary

Expressing these goals using the final-time interaction unitary,

$$R = U_{\rm nom}^\dagger U_{\rm pert} = (U_S \otimes I_B)^\dagger U_{\rm pert} \tag{42}$$

gives the fidelity (39),

$$F_{\rm pert}(\psi_{\rm in}) = |\psi_{\rm in}^\dagger (W^\dagger U_S \otimes I_B) R \psi_{\rm in}|^2 \tag{43}$$

Since by definition there is no uncertainty in the model of the nominal system, then $R_{\rm nom} = I$ and the nominal fidelity becomes,

$$F_{\rm nom}(\psi_{\rm in}) = |\psi_{\rm in}^\dagger (W^\dagger U_S \otimes I_B) \psi_{\rm in}|^2 \tag{44}$$

If the target unitary W is achieved by the nominal (uncertainty-free) system, that is, $U_S = \phi W$ with global phase $|\phi| = 1$, then from (42):

$$\left\{ \begin{array}{ll} \text{nominal fidelity} & F_{\rm nom}(\psi_{\rm in}) = |\psi_{\rm in}^\dagger \psi_{\rm in}|^2 = 1 \\ \text{perturbed fidelity} & F_{\rm pert}(\psi_{\rm in}) = |\psi_{\rm in}^\dagger R \psi_{\rm in}|^2 \\ \text{interaction unitary} & R = (W \otimes I_B)^\dagger U \end{array} \right\} \tag{45}$$

I. Limit of robust performance via averaging

Clearly deviations from the nominal fidelity are captured by a deviation of $R(T)$ from identity, *i.e.*, if $R(T) \approx I_n$ then $F_{\rm pert} \approx F_{\rm nom}$. This approximation was made precise in [76] using the classic *method of averaging* [85] and extended in [98]. Define the robustness measure as the worst-case size of the time-averaged interaction Hamiltonian in (37):

$$J_{\rm rbst} = \max_{\mathcal{H}_{\rm unc}} \|\langle G \rangle\|, \quad \langle G \rangle = \frac{1}{T} \int_0^T G(t) dt \tag{46}$$

Assume the following:

- The uncertain perturbation Hamiltonian is bounded in the induced two-norm (the maximum singular value)

$$\|\tilde{H}(t)\|_2 \leq \delta_{\rm unc} \tag{47}$$

- Simultaneously the uncertainty-free fidelity is maximized while the robustness measure is minimized, *i.e.*,

$$\begin{aligned} &F_{\rm nom}(\psi_{\rm in}) = 1 \text{ iff } U_S(T) = \phi W, \ |\phi| = 1 \\ &J_{\rm rbst} = \min_{\mathcal{H}_{\rm nom}} \max_{\mathcal{H}_{\rm unc}} \|\langle G \rangle\| \end{aligned} \tag{48}$$

Robust Performance Bound

Under the conditions in (47)-(48), as shown in [98], the perturbed fidelity is bounded below by $F_{\rm low-bnd}$, *i.e.*,

$$F_{\rm pert}(\psi_{\rm in}) = |\psi_{\rm in}^\dagger R(T) \psi_{\rm in}|^2 \geq F_{\rm low-bnd} \tag{49}$$

provided that,

$$T(\delta_{\rm unc} + J_{\rm rbst}) \leq \sqrt{4 \ln \left(1 + \sqrt{2 \left(1 - \sqrt{F_{\rm low-bnd}} \right)} \right)} \tag{50}$$

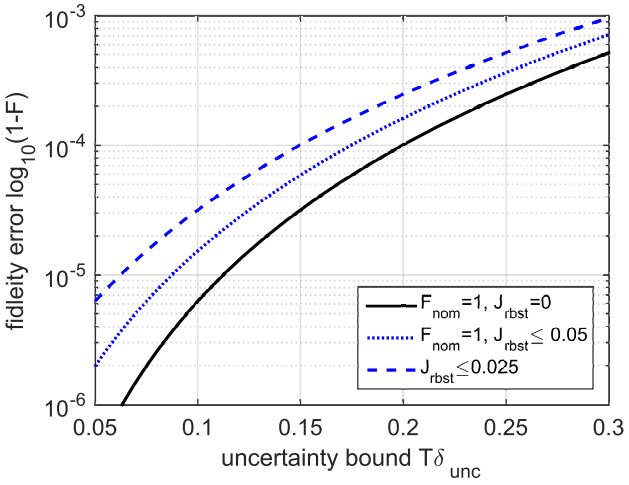

Fig. 6. Performance limit curves from (50) shown at two uncertainty error scales and with a few selected robustness measures: solid $J_{\rm rbst} = 0$, dots $J_{\rm rbst} = 0.025$, and dashes $J_{\rm rbst} = 0.05$.

The inequality (50) establishes a limit of performance for robust quantum control. This is not *the* limit – that is not known. This performance bound does establish what is achievable under the given conditions in (47) and (48). Figure 6 shows a plot of fidelity error $\log_{10}(1 - F_{\rm pert})$ vs. uncertainty error $T\delta_{\rm unc}$ for $J_{\rm rbst} = 0$ (solid curve), $J_{\rm rbst} = 0.025$ (dotted curve), and $J_{\rm rbst} = 0.05$ (dashed curve). Some general remarks about the bound:

- The performance bounding relationship (50) is based on three assumptions:
  - the nominal fidelity is at the maximum of $F_{\rm nom} = 1$
  - the *fact* that a (hopefully small) bound on $J_{\rm rbst}$ has been obtained, not *how*.
  - the induced two-norm of the time-bandwidth product $T\tilde{H}(t)$ is bounded by $\delta_{\rm unc}$, equivalently, a bound on the product of the operation time and the maximum instantaneous frequency of the uncertain Hamiltonian.
- Under these conditions, the bounding relationship is:
  - agnostic to *how* the assumptions on $F_{\rm nom}$ and $J_{\rm rbst}$ are achieved, *e.g.*, by control, material selection, circuit layout, *etc.*
  - independent of dimension.
- Ensuring that the robustness measure is at a minimum, or at the absolute limit of $J_{\rm rbst} = 0$, clearly must account for the specifics of the uncertainty set $\mathcal{H}_{\rm unc}$.

J. Example

To illustrate the bounding relationship consider a single-qubit system with no drift, under control in σ_x and σ_z with an uncertain σ_z coupling c_z to a constant uncertain bath B_z. The system Hamiltonian is then,

$$H(t) = (v_x(t)\sigma_x + v_z(t)\sigma_z) \otimes I_B + c_z \sigma_z \otimes B_z \tag{51}$$

Suppose all the uncertainty is due to coupling with the bath,

$$\left\|\tilde{H}\right\|_2 = \|c_z B_z\|_2 \leq \delta_{\rm unc} \tag{52}$$

Set a normalized final time to $T = 1$ with 4 piece-wise-constant (PWC) control pulses each for $v_x(t)$ and $v_z(t)$. Figure 7 shows the fidelity error and optimized control pulses to make the Hadamard gate $W = (\sigma_x + \sigma_z)/\sqrt{2}$. The solid curve is the limit-bound and the squares show the actual worst-case fidelity from random samples of the bath using the robust pulses. The optimization protocol is described in the next section.

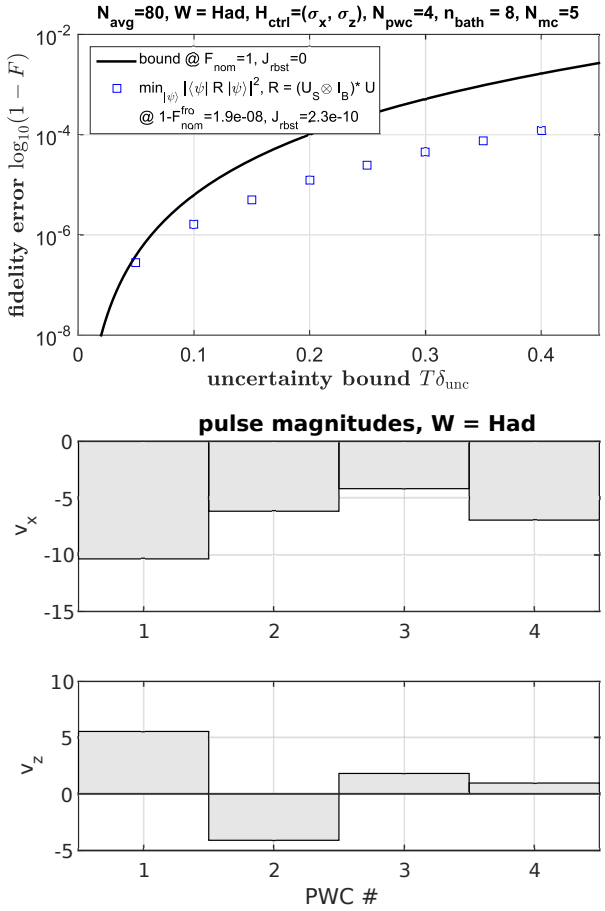

Fig. 7. **Single-qubit system** (51). Final time $T = 1$, number of PWC pulses per control is 4 to make Hadamard. **Top:** Solid curve is bound from (50). Blue squares are actual fidelity from (45) from 5 random samples of the bath. **Bottom:** control pulses.

K. Landscape Topology: Two-Stage Optimization

The Averaging Theorem [85] shows that robustness can be achieved by minimizing the size of the time-averaged Hamiltonian: the first term in the Magnus expansion of $R(T)$. In general the *trajectory* of the nominal propagator, if properly tailored, can achieve a high fidelity nominal response *and* simultaneously minimize the robustness measure. This latter freedom is known to arise from the ability to roam over the null space at the top of the fidelity landscape [92, 99–103].

In effect, the Averaging Theorem provides design criteria to *synthesize* a robust control. Specifically, the final time nominal unitary $U_{\rm nom}(T)$ should be very close to the target W, and the result of its evolution over $t \in [0, T]$ is that $J_{\rm rbst} \approx 0$ or as small as possible. These two goals, which place simultaneous demands on the *nominal trajectory*, $U_{\rm nom}(t), t \in [0, T]$, has been presented in various forms in [89–91, 94, 104–107].

Multicriterion Optimization

Cast as an optimization problem in the control variables:

$$\begin{aligned} \text{minimize} \quad & J_{\rm rbst} = \max_{\mathcal{H}_{\rm unc}} \|G_{\rm avg}\| \\ \text{subject to} \quad & F_{\rm nom} \geq f_0 \end{aligned} \tag{53}$$

As described in [76], one path to finding a solution to (53) is to first maximize only the nominal fidelity $F_{\rm nom}$. When this fidelity crosses a high threshold, $f_0 \approx 1$, then switch to minimizing the robustness measure $J_{\rm rbst}$ while keeping the fidelity above f_0. Specifically, we utilize the following two stage algorithm in the control variables v:

$$\begin{aligned} &\textbf{Stage 1} \text{ maximize } \textbf{only } F_{\rm nom}(v) \textbf{ until } F_{\rm nom}(v) \geq f_0 \\ &\textbf{Stage 2} \text{ minimize } J_{\rm rbst}(v) \textbf{ while } F_{\rm nom}(v) \geq f_0 \end{aligned} \tag{54}$$

The uncertainty-free optimization in Stage 1 can be done by many different gradient ascent methods. For Stage 2, when $F_{\rm nom}(v) \geq f_0$, we show in [76] that at each iteration finding an optimal control increment can be recast as a convex optimization problem, [108, App.B].

L. Concluding Remarks & Outlook

The approach to robust quantum control presented here follows [76] which rests on the theoretical foundation provided by the classic method of averaging [85]. A direct result is a multicriterion optimization problem consisting of the uncertainty-free fidelity competing with a generic robustness measure, the latter being a time-domain product of a function of the controls and the character of the uncertainty. Such a product form is ubiquitous in the many applications of classical robust control. These require a product in a feedback loop to be small: an uncertainty bound and an uncertainty-free (closed-loop) map. From the averaging theory there naturally arises a quantitative norm measure of a time-averaged Hamiltonian reflective of the interaction between the uncertain perturbation and the uncertainty-free unitary evolution. This term is equivalent to the first term in a Magnus expansion of the interaction unitary, a term that has been used extensively as an objective for dynamical decoupling control protocols. If this term is sufficiently small, then at most, only second order error effects can accrue. In the case of quantum information sciences for established realizations, the tacit assumption is that the (possibly known or unknown) perturbations are small.

The bound developed in [98] and reproduced here in (50) establishes a limit of robust control performance in the presence of Hamiltonian set-membership uncertainty. Depending on specifics of the uncertainty set, this limiting

bound – *the* limiting bound is not known – relates an upper bound on fidelity error to a bound on uncertainty magnitude (a time-bandwidth product) as shown in Figures 6 and 7. In general the upper bound is agnostic to *how* it is obtained, *e.g.*, by control, circuit layout, material selection, *etc*. The information required to make full use of the bound may require new experiments. The goal is to expand the boundary of quantum control to get the best performance possible.

V. Conclusion

This paper introduced algorithmic, systems- and control theoretical as well as experimental aspects of quantum engineering for quantum computing from three complementary perspectives. In Section II, we covered the framework of quantum algorithms, which are formulated in the language of linear algebra as a combination of unit vectors, unitary matrices, and quadratic forms. Many experimental realizations towards a quantum computer or other high-end quantum technolgies (in finite dimensions) require to control (bilinear) systems with high accuracy. With this motivation, Section III presented a unified systems and control framework for such quantum systems, using their symmetries to simplify rigorous treatment of decision problems such as controllability, simulability, and observability. Finally, current quantum devices are severely affected by noise, which requires the development of robust techniques. To this end, Section IV introduced a robust quantum-control framework based on a set-membership uncertainty description and an optimal control objective trading off performance and robustness.

The main goal of this tutorial is to introduce basic concepts to understand and solve engineering problems in quantum systems. Throughout the paper, we have encountered various open challenges in quantum computing which are closely connected to control-theoretic concepts. We hope that addressing these challenges based on principles outlined in this tutorial will contribute towards *bringing quantum systems under control*.

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