Control Paradigms for Quantum Engineering

(Invited Paper)

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Abstract—We give an overview of different paradigms for control of quantum systems and their applications, illustrated with specific examples. We further discuss the implications of fault-tolerance requirements for quantum process engineering using optimal control, and explore the possibilities for architecture simplification and effective control using a minimum number of simple switch actuators.

II. PARADIGMS FOR QUANTUM CONTROL

Most quantum control strategies fall into one of three categories: feedback control based on feedback of classical information obtained from (weak) measurements of the system, coherent feedback control using quantum actuators, and open-loop Hamiltonian (and sometimes reservoir) engineering.

A. Open-loop Hamiltonian (and reservoir) engineering

The conceptually simplest, yet very important type of quantum control is open-loop control in the form of Hamiltonian [1] and sometimes reservoir engineering [2]. Considering that the evolution of a quantum system is governed by the Schrodinger equation (closed systems), or more generally, the quantum Liouville equation (with $h = 1$):

$$\dot{\rho}(t) = -i[H, \rho(t)] + \mathcal{L}_D \rho(t) \equiv -i(H\rho(t) - \rho(t)H) - \mathcal{L}_D \rho(t),$$

where $\rho(t)$ is a positive unit-trace operator (density operator) acting on a Hilbert space $\mathcal{H}$, which represents the state of the system, this approach involves basically engineering a Hamiltonian operator $H$, and possibly a (completely positive) superoperator $\mathcal{L}_D$ to achieve a desired evolution of the system. Hamiltonian engineering is usually achieved by applying suitable static or dynamic electromagnetic fields $f(t)$, that coherently interact with the system, thus modifying its intrinsic Hamiltonian $H_0 \rightarrow H[f(t)] = H_0 + H_C[f(t)]$. $\mathcal{L}_D$ is determined by the system’s interaction with its environment and can usually (at least for Markovian systems) be written as $\mathcal{L}_D[\rho(t)] = \sum_k \mathcal{D}[A_k] \rho(t)$, where $A_k$ are Hilbert space operators and the dissipative superoperators are [3]

$$\mathcal{D}[A_k] \rho(t) = A_k \rho(t) A_k^\dagger - (A_k^\dagger A_k \rho(t) + \rho(t) A_k^\dagger A_k)/2.$$

$\mathcal{L}_D$ can in principle be altered by environmental (reservoir) engineering, although this is usually challenging.

Open-loop Hamiltonian (and sometimes reservoir) engineering plays a crucial role in many applications including nuclear and electron spin engineering in nuclear magnetic resonance (NMR) [4] and electron spin resonance (ESR) applications, control of electronic [5], vibrational [6], rotational [7] and translational degrees of freedom of molecular systems, atomic vapours, trapped ions, Bose Einstein condensates [8], control of chemical reactions using photonic reagents in quantum chemistry [9], as well as control of artificial structures such as...
quantum well and quantum dots [10], cooper-pair boxes [11], and many other systems.

B. Measurement-based feedback control

Another important type of quantum control is measurement-based feedback control [12]. Typically, this approach also involves Hamiltonian engineering by applying suitable control fields, but in addition the system is monitored, usually via continuous weak measurements, and the information gained from these observations fed back to the actuators as shown in Fig. 1. Due to the nature of quantum measurements, this leads to stochastic evolution governed by a Master equation of the form

$$d\rho_c(t) = \{-i[H, \rho_c(t)] + \mathcal{L}_D\rho_c(t)\} dt + \mathcal{L}_M\rho_c(t) dW(t),$$

where $\rho_c(t)$ is a density operator now representing the conditional state (conditioned on the measurement record up to time $t$). $H$ and $\mathcal{L}_D$ are a Hamiltonian and positive superoperator as before, but in addition to these deterministic (drift) terms there is now a stochastic term $\mathcal{L}_M\rho_c(t) dW(t)$, which can usually be written in the from $\sum_k \mathcal{H}[B_k]\rho_c(t) dW(t)$ where

$$\mathcal{H}[B_k]\rho_c(t) = B_k\rho_c(t) + \rho_c(t)B_k^\dagger - Tr[B_k\rho_c(t) + \rho_c(t)B_k^\dagger]$$

for suitable Hilbert space operators $B_k$, which depend the measurement operators and feedback Hamiltonian, and $dW(t)$ is the Wiener element of the stochastic process.

While open-loop Hamiltonian engineering usually involves control of non-equilibrium dynamics, often on nano-, pico or femtosecond timescales, measurement-based feedback control is very important for control of equilibrium dynamics, including steering the system to a steady state [13] with applications in quantum state reduction [14], laser cooling of atomic or molecular motion [15], control of solid-state qubits [16], decoherence control [17] and quantum metrology.

C. Coherent feedback and indirect control

A third major paradigm for quantum control is coherent feedback control [18], [19]. Unlike measurement-based feedback control, coherent feedback control does not (at least not directly) involve any classical actuators or measurements. Rather it relies on indirect control of a target quantum system $A$ through its coherent interaction with another quantum system $B$ acting as the controller. Unlike Hamiltonian/reservoir engineering and measurement-based feedback control, which are governed by generally complicated non-linear control equations, when the system and controller are both quantum-mechanical and their interaction is fully coherent, the resulting control system is often linear, and can be modelled using transfer functions [20], albeit with (stochastic) operators instead of real vectors representing the state of the system and controller.

This type of control is interesting in quantum photonics, for example, where one can use cavities, mirrors, beam splitters and waveguides to build optical networks that could control the state of atoms or quantum dots. Fig. 2 shows a very simple coherent feedback system involving a cavity and beam splitter. If an atom or quantum dot is put into the cavity, its state could be controlled though this coherent feedback. Another application of coherent feedback is indirect control, e.g., the control of nuclear spins by electron spins via the Heisenberg interaction, an example of which is shown in Fig. 3.

Quantum controllers cannot solve the problem of controlling quantum systems completely, however, as the quantum controller itself needs to be controlled in some form, and this usually requires interaction with a non-quantum system such as classical laboratory equipment at some stage, and thus control strategies such as Hamiltonian engineering or state preparation using measurement-based feedback. For instance, in the case of indirect control of nuclear spin dynamics, the electron spins need to be controlled using conventional Hamiltonian engineering techniques, e.g., by application of tailored control pulses as shown in Fig. 3 to achieve the desired effect on the nuclear spins. Indirect control therefore may seem to only complicate the problem—considering that nuclear spins can be controlled directly using radio-frequency fields, for example. Yet, the indirect approach is promising because
Fig. 3. Indirect control of a coupled electron-nuclear spin system: A modulated high-frequency control pulse applied to electron spin realizes a nuclear spin flip (swap gate). The trajectory of the Bloch vector corresponding to the nuclear spin system shows that the nuclear spin initially in the state $|↑\rangle$, indicated by $\bullet$, is flipped to $|↓\rangle$, indicated by $\ast$. The specific system considered here was a 1e1n (one electron, one nuclear spin) model of malonic acid described by the Hamiltonian $H_0/2\pi = \nu_n S_z + \nu_e I_z + A_{xx} S_x I_x + A_{zz} S_z I_z$, where $S_k$ and $I_k$ for $k \in \{x, y, z\}$ are the Pauli operators for the electron and nuclear spin, respectively, and the constants are $\nu_n = 11.885$ GHz, $\nu_e = 18.1$ MHz, $A_{xx} = 14.2$ MHz, $A_{zz} = -42.7$ MHz. Indirect control of nuclear spin dynamics using shaped pulses applied to the electron has been experimentally demonstrated for this system [21]. The shaped control pulse was calculated using a variational optimal control approach [22].

exploiting the strength of the quantum interaction between the spins and the fact that electron spins can be manipulated faster than nuclear spins, enables control of nuclear dynamics on shorter timescales than direct control. Moreover, for some systems direct control of certain degrees of freedom may not be possible at all.

III. PARADIGMS FOR OPTIMAL CONTROL DESIGN

Regardless of the specifics of the system and control paradigm, it is always desirable to optimise the control. But as with control paradigms for quantum systems in general, there are many paradigms for optimal control. In many applications in quantum chemistry, optimal control is understood to mean finding photonic reagents, typically shaped pulses, to maximise the yield of some observable, or reaction product, subject to constraints. Similarly, in quantum information processing the aim is often to find controls to maximise the fidelity of a quantum process, subject to constraints. In the latter area, it has been argued that beside optimising the overall fidelity, time-optimality is crucial, as shorter control pulse sequences mean shorter gate operation times, and the rate of decoherence is roughly constant, less decoherence, and thus higher gate fidelities. However, some proposed approaches to circuit optimisation appear incompatible with fault-tolerant designs, which in the context of robust, scalable architectures may be a more important consideration. The implementation of non-trivial gates (such as Toffoli or T-gates) on encoded logical qubits in fault-tolerant designs requires a large number of ancilla qubits, multiple verification measurements and classical feed-forward in the standard model, and it could be argued that eliminating or reducing some of these cumbersome require-
ments should be an important paradigm for optimal control. Another important issue are design constraints. While a large number of sophisticated actuators may be desirable for reasons of flexibility, robustness and possibilities for optimisation, in practice, simplicity of a design is often a crucial factor, and may be the difference between a physically realistic device and a practically infeasible one.

A. Time-optimality vs Fault-tolerance

An interesting and important application of optimal control has been in the area of quantum circuit design. In the conventional circuit model of quantum computing, quantum operations are constructed from a small set of elementary gates. Although any quantum operation on $n$ qubits can be constructed from a universal set of gates, a major drawback of this approach is that, even if the overhead is polynomial, a very large number of gates is required to implement any non-trivial operation, and standard sets of elementary gates such as the Hadamard, phase, or CNOT gates, are often no easier to implement physically than arbitrary single or twqubit gate. This approach therefore seems quite inefficient and it appears sensible to decompose quantum circuits into larger modules that can be implemented efficiently for a particular architecture using optimal control theory instead. It has been shown that the implementation time for the quantum Fourier transform circuit, for example, can be improved by (at least) a factor of eight in this way [23].

A potential problem of this approach, however, is its compatibility with fault-tolerant architectures. No matter how effective the control, realistic quantum circuits will require redundancy, error correction and fault-tolerant designs to mitigate errors caused not only by imperfect control but also by environmental noise and decoherence. A standard approach to fault-tolerant design is encoding information into logical qubits formed by groups of physical qubits using error correction codes [24]. In all existing proposals, fault-tolerant gates on encoded qubits are constructed from single and two-qubit logic gates. It is not clear therefore that optimisation of larger circuit blocks acting on physical qubits is compatible with fault-tolerant designs. Furthermore, when implementing quantum logic gates on encoded qubits in general, overall fidelity and time-optimality are not the only considerations, but we may wish to explicitly minimise errors that cannot be corrected vs errors that can be corrected for a given encoding.

To illustrate some of the ideas, consider the popular [[7,3,1]] CSS code [25], which uses seven physical qubits to define one logical qubit, where the logical basis states are superpositions of codewords containing an odd and even number of ones, respectively,

\[
|0\rangle_L = |0000000\rangle + |1111000\rangle + |1100110\rangle + |1010101\rangle + |0011110\rangle + |0101101\rangle + |0110011\rangle + |0110100\rangle.
\]

\[
|1\rangle_L = |1111111\rangle + |0000111\rangle + |0011001\rangle + |0100111\rangle + |0110001\rangle + |1010010\rangle + |1001100\rangle + |0110100\rangle.
\]
Assuming we can at least perform measurements of the observables \(X\) and \(Z\) given by the Pauli matrices
\[
X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]
(6)
on individual physical qubits, we can extract an error syndrome by performing parity checks, which project arbitrary states into the \(\pm 1\) eigenstates of the stabiliser operators, e.g.,
\[
\mathcal{G}_S = \{ \text{IIIxxxx, IXiXxx, XIXIXI, } \}
\]
for the CSS code. On clean code word states errors act to switch the eigenstate, which can be detected via the parity check and correctly via local operations on the physical qubits. The \([7,3,1]\) code can correct only a single bit or phase flip error. If more than one error occurs then the code fails. Thus, for the code to be effective, no more than one error should occur per error correction block, and a single error should not propagate, i.e., if we apply a gate to a state with a single error, the output state should not contain more than a single error.

Consider the simplest case of implementing an arbitrary single qubit gate \(U_T\) on a logical qubit, i.e., a unitary operator on \(n\) physical qubits \((n = 7\) for \([7,3,1]\) CSS code\), in a single step using optimal control. Even if the control is very effective, the operator actually implemented will not be exactly \(U_T\) but an operator \(U_R\) related to \(U_T\) by an error operator \(U_E = U_T^\dagger U_R\), which is the identity exactly if \(U_R = U_T\). Since \(U_E\) is an operator acting on \(n\) physical qubits, we can expand it with respect to the \(n\)-qubit Pauli group \(P_n = P^{\otimes n} = \{I, X, Y, Z\}^{\otimes n}\). If we define the weight of an operator in \(P^{\otimes n}\) as the number of non-identity operations, then the errors we can correct in the standard \([7,3,1]\) CSS encoding are the contributions of the terms in the expansion that have weight 1, corresponding to single bit or phase flip errors.

Hence, to maintain a fault-tolerant circuit design we must ensure at least \(W_1(U_E) \gg W_2(U_E) \gg W_3(U_E) \ldots\), where \(W_k(U_E)\) indicates the contribution of terms with weight \(k\) in the Pauli expansion of \(U_E\). In practice this could be archived by adding constraint terms to the functional to be optimised. For example, instead of maximising the (normalised) fidelity \(\mathcal{F}(U) = 2^{-n} \text{Tr}(U^\dagger U)\), one might consider maximising \(\mathcal{F}(U) = \sum_{k \geq 1} \lambda_k W_k(U_E)\), where \(\lambda_k\) are suitable weighting factors satisfying \(\lambda_2 \ll \lambda_3 \ll \ldots\). Although preliminary calculations for very simple systems suggest that we can find controls that minimise projections of \(U_E\) onto certain subspaces, it is not clear at this stage to which extent it is possible to suppress the projections onto multi-error subspaces for realistic physical systems, and if circuits composed of larger modules implemented using optimal control can be made fault-tolerant in general.

### B. Architecture Simplification vs Control Sophistication

Many quantum systems can be controlled by external electromagnetic fields generated by actuators capable of creating complicated pulses. For example, optical fields generated by lasers, as well as coherent microwave or radio-frequency pulses used in ESR and NMR, can be shaped either using spectral pulse shaping or temporal modulation to create complex control fields, offering considerable potential for optimisation. Optimal control in a quantum setting is therefore often understood to mean optimisation of control pulse shapes. However, this type of optimal control is not appropriate in all settings. An important case are nano-scale systems such as quantum dots controlled electronically using gate electrodes. Although there is some scope for optimising voltage profiles, for example, a more important consideration for these systems is often design optimisation, in particular, minimising the number of actuators required, and using the simplest actuators that can accomplish the desired task.

As a specific example, consider the Kane proposal for a solid-state quantum computer \([26]\). The original design involves \(2n - 1\) voltage gates, as pictured in Fig. 4, to selectively tune \(n\) quantum dots, in this case the nuclear spins of phosphorus donors in silicon, into resonance with a globally applied transverse AC magnetic field, and to control the interactions between them. This design suffers from various problems, among them the high density of nanometer-scale control electrodes required for a scalable architecture, which poses a serious challenge for current manufacturing techniques. Furthermore, even if fabrication techniques improve, the presence of a large number of closely spaced control electrodes creates fundamental physical problems including substantial crosstalk \([27]\) between the actuators and the potential for significant decoherence of the quantum information stored in the quantum dots via incoherent interaction with the control electrodes, which is highly detrimental to device performance. Thus, it is highly desirable in this setting to minimise the number of control electrodes (i.e., actuators) and to keep the actuators simple. A control scheme that requires only binary switch actuators, for example, will be advantageous because switching between two fixed voltage settings is far simpler than producing complicated temporal voltage profiles, and it is easier to experimentally characterise (and compensate) crosstalk effects in this setting. This raises the question of how many of the actuators are really necessary.

Basic controllability analysis of various model systems suggests that most of the actuators are not necessary, and for certain model systems it can be shown that a single, local actuator such as a control electrode is theoretically sufficient for complete controllability of the system \([28]\). For instance, a spin chain of length \(N\) with isotropic Heisenberg interaction decomposes into \(N\) excitation subspaces with \(n\) excitations \((n = 1, \ldots, N)\). Assuming nearest neighbour coupling, the Hamiltonian of the first excitation subspace is tridiagonal
\[
H_0 = \begin{pmatrix} E_1 & d_1 & 0 & \ldots & 0 \\ d_1 & E_2 & d_2 & \ldots & 0 \\ 0 & d_2 & E_3 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & E_N \end{pmatrix}
\]
where $d_n > 0$ defines the strength of the interaction between the spins $n$ and $n + 1$ in the chain for $n = 1, \ldots, N - 1$ and $E_n$ are the energy levels. It can be shown using Lie algebraic techniques that a single local actuator that allows us to modulate the coupling between spins $r$ and $r + 1$ only, is sufficient in this case for complete controllability of the entire excitation subspace. This result also holds for spin chains with isotropic XY or dipole-dipole coupling. In fact, the controllability result is generic for any type of system with a nearest neighbour coupling Hamiltonian of the form (7), and similar results can be proved for other types of systems.

Although there are many open questions—such as the exact conditions for a single actuator to suffice, or the minimum number of actuators required for complete controllability for a particular system, these preliminary controllability results are encouraging from the point of view of architecture simplification—but can we actually find constructive control schemes for systems such as the spin chain with a single local actuator above? Suppose we have a single actuator that has $M$ distinct states. If the interaction with system is fully coherent and the system dynamics is therefore Hamiltonian, each of the $M$ actuator states is associated with a system Hamiltonian $H_m$ for $m = 1, \ldots, M$. Since the only control we have is the ability to switch between these $M$ Hamiltonians, the unitary operators we can implement are of the form

$$U(m, t) = U^{(m_1)}(t_1) \ldots U^{(m_{K-1})}(t_{K-1})U^{(m_K)}(t_K)$$

(8)

where $m$ and $t$ are vectors of length $K$ with $m_k \in \{1, \ldots, M\}$ and $t_k \in \mathbb{R}^+_0$, and $U^{(m_k)}(t_k) = \exp(-it_kH^{(m_k)})$ are the elementary evolution operators. The vector $m$ determines the switching sequence and $t$ the switching times, i.e., length of time the system evolves under a particular Hamiltonian $H_m$. The $t_k$ can be regarded as generalised Euler angles. For $M = 2$, i.e., a binary switch controller, Eq. (8) can be simplified. Noting that $U^{(m)}(t_1)U^{(m)}(t_2) = U^{(m)}(t_1 + t_2)$, we see that the elements of $m$ must alternate between 1 and 2, and we have without loss of generality

$$U(t) = U^{(1)}(t_1)U^{(2)}(t_2) \ldots U^{(1)}(t_{2\ell-1})U^{(2)}(t_{2\ell})$$

(9)

if we set $K = 2\ell$ and allow the possibility of $t_1 = 0$ or $t_\ell = 0$.

In the context of unitary process control, constructive control requires therefore that we find vectors $m$ and $t$ such that

$$\|U_T - U(m, t)\| < \epsilon$$

(10)

for a given target operator $U_T$ and tolerance $\epsilon$. For very special classes of Hamiltonians, e.g., Hamiltonians that are mutually orthogonal with respect to the Hilbert-Schmidt norm, $\text{Tr}[H_m^\dagger H_n] \propto \delta_{mn}$, there are various explicit decomposition algorithms to compute the switching sequence $m$ and generalised Euler angles $t$. In practice, we are seldom so lucky, however. Indeed for a system with $H_0$ as in Eq. (7) and a local binary switch actuator that annuls the coupling between spins $r$ and $r + 1$, we have $H_r = -d_r(e_{r,r+1} + e_{r+1,r})$, where $e_{r,r+1}$ is a matrix that is zero everywhere except for a 1 in the $(r, r + 1)$ position, and

$$\text{Tr}[H_0^\dagger(H_0 + H_r)] = 2\|d - d_r\|^2 + \|E\|^2,$$

(11)

where $d = (d_1, \ldots, d_{N-1})$, $E = (E_1, \ldots, E_N)$ and $d_r = (d_{rt})$ with $d_{rt} = d_{t_r}$, $E_{rt} = E_{t_r}$. Thus, we see that the available Hamiltonians $H_0$ and $H_0 + H_r$ corresponding to the off and on position of the switch, respectively, are never orthogonal, except when all the parameters vanish. In general

$$\cos \alpha = \frac{\text{Tr}[H_0^\dagger(H_0 + H_r)]}{\text{Tr}[H_0^\dagger H_0] \text{Tr}[H_0 + H_r]^2]}$$

(12)

is close to 1 in this case, and thus the angle $\alpha$ between the Hamiltonians is very small. Although it is difficult to derive explicit expressions for the generalised Euler angles and to prove the optimality of a particular switching sequence, the vectors $t$ and $m$ can be determined numerically using general optimisation techniques.

As an example, we consider a spin chain of length 4 with uniform isotropic Heisenberg coupling and a single actuator as shown in Fig. 4(b). Using the natural identification

$$|0\rangle = |00\rangle, \ |1\rangle = |01\rangle, \ |2\rangle = |10\rangle, \ |3\rangle = |11\rangle$$

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of the 1st excitation subspace states, our goal is to implement the six "two-qubit" gates
\[ U_T^{(s)} \in \{ I \otimes I, \text{Had} \otimes I, T \otimes I, I \otimes \text{Had}, I \otimes T, \text{CNOT} \} , \]
where I is the identity operator on a single two-level subspace (qubit), T = \exp(-i\pi/8\sigma_z) is a π/8 phase gate,
\[ \text{Had} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad \text{CNOT} = e^{-i\pi/4} \begin{pmatrix} 1 & 0 \\ 0 & X \end{pmatrix} . \]
Fig. 5 shows a possible solution switching sequences, which was obtained using an optimisation routine that took into account only the number of switches and overall gate operation times required to achieve the target fidelity of 99.99%. In practice, it may be desirable to consider other factors such as penalties for rapid switching, etc. to obtain the most robust and experimentally feasible solutions.

IV. CONCLUSION

We have shown that there are different paradigms for quantum control from open-loop Hamiltonian and reservoir engineering, to measurement-based feedback control and coherent (quantum) feedback using quantum systems as controllers, all of which have important applications, and different paradigms may be combined, as in the case of indirect control of one quantum system such as nuclear spins by another such as electron spins, the latter being itself subject to open-loop or measurement-based feedback control via external fields. An important objective for control engineering is optimal control. In the context of quantum systems the term has often come to mean control via shaped pulses designed to optimise certain quantities such as the expectation value of an observable, yield of a chemical reaction, or fidelity of a quantum process. Especially in the latter type of applications, time-optimality has often been considered to be of paramount importance beside ensuring high fidelity. However, we have seen that there are other paradigms for optimal control. In particular in the context of quantum information processing, but not necessarily limited to this application, fault-tolerance is an important consideration for optimal control that has received little attention so far. Another important paradigm for optimisation is simplifying architectures with a view to eliminating unnecessary actuators and replacing complicated actuators by simple switches, for instance, while still maintaining the ability to effectively control the system. Naturally, there are many open questions, in particular in novel areas such as optimal control and fault-tolerant circuit design, or minimalist control using the simplest possible actuators, ranging from the compatibility of optimal control and fault-tolerant networks to the optimal switching sequences for binary switch actuators.

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