SYMMETRY PRINCIPLES IN OPTIMAL QUANTUM CONTROL WITH APPLICATIONS TO CLOSED AND OPEN SYSTEMS

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Abstract

Elucidating quantum systems theory in terms of symmetry principles has triggered us in a number of recent advances:

(1) it leads to a new handy controllability criterion,
(2) it guides the design of quantum hardware,
(3) it governs which quantum system can simulate another one given, and
(4) it specifies the limit between time-optimal control and relaxation-optimised control of open systems.

How principles turn into practice has been illustrated in the talk by a plethora of examples showing practical applications in solid-state devices, circuit-QED, and in spin systems. The algorithmic tools have been presented in a unified programming framework.

Key words

quantum systems theory, symmetry, optimal control, controllability, bilinear control systems, dynamic system Lie algebras.

1 Introduction

The purpose of my presentation summed up in this paper is to invite the well-established community of control engineers and *classical* physicists to exchange with the vibrant developments in the field of *quantum* systems and control [Dowling and Milburn, 2003] in view of future technologies. These may be triggered by precise controls for, e.g., quantum simulation in order to improve the understanding of quantum phase transitions [Sachdev, 1999] between normal conducting and superconducting phases, or ferromagentic vs. anti-ferromagnetic phases to name just a few. Needless to say an operative thorough picture of these phenomena will booster advanced material design.

More precisely, an important issue in *quantum simulation* [Feynman, 1982; Abrams and Lloyd, 1997; Bennett et al., 2002; Dodd et al., 2002; Jané et al., 2003; Bremner et al., 2005] is to manipulate all pertinent dynamical degrees of freedom of a system $\mathcal{A}$ of interest (which, however, all-to-often is experimentally not fully accessible) by another quantum system $\mathcal{B}$ that is in fact well controllable in practice and the dynamics of which are equivalent to those of $\mathcal{A}$. We will show how to characterise this situation algebraically in terms of quantum systems theory.

Besides the practical applications and implications, quntum systems should be of particular appeal to the (classical) control engineer, because nearly all sytems of interest boil down to the familiar standard form of *bilinear control systems* [Levine, 1996; Sontag, 1998; Elliott, 2009]

$$\dot{X}(t) = (A + \sum_j u_j B_j) X(t) \quad \text{with} \quad X_0 = X(0)\ . \tag{1}$$

Here one may take A, B as linear operators on the (finite-diemnsional) Hilbert space of quantum states $\{|\psi(t)\rangle\} \subseteq \mathcal{H}$. More precisely, A denotes the system or drift Hamiltonian iH_0, while the B_j are the control Hamiltonians iH_j governed by typically piecewise constant control amplitudes $u_j \in \mathbb{R}$ (which need not be bounded). Thus Eqn. (1) captures all of the following important scenarios

1. controlled Schrödinger eqn.
   $|\dot{\psi}(t)\rangle = -i(H_d + \sum_j u_j H_j)|\psi(t)\rangle$
2. quantum map of closed system
   $\dot{U}(t) = -i(H_d + \sum_j u_j H_j)U(t)$
3. quantum map of open quantum system
   $\dot{\rho}(t) = -(i\,\mathrm{ad}_{H_d} + i\sum_j u_j\,\mathrm{ad}_{H_j} + \Gamma_L)\,\mathrm{vec}(\rho(t))\ ,$
4. quantum map of open quantum system
   $\dot{F}(t) = -(i\,\mathrm{ad}_{H_d} + i\sum_j u_j\,\mathrm{ad}_{H_j} + \Gamma_L)F(t)\ ,$

where U denotes a unitary operator on $\mathcal{H}$ often used as a quantum gate, while F is the linear quantum map for open systems governed by the relaxation (super)operator Γ on $\mathcal{H} \otimes \mathcal{H}$ and ρ is the density operator.

While the familiar *linear control systems*

$$\dot{x}(t) = Ax + Bu \quad \text{with} \quad x_0 = x(0) \tag{2}$$

are fully controllable [Kalman et al., 1969] if $\text{rank}\,[B, AB, A^2B, \ldots, A^{N-1}B] = N$ in the sense it has full rank N, *bilinear systems* of Eqn. (1) are fully controllable over the (compact) connected Lie group $\mathbf{G}$ (generated by its Lie algebra $\mathfrak{g}$ via $\mathbf{G} = \langle \exp \mathfrak{g} \rangle$) whenever they satisfy the so-called *Lie-algebra rank condition* [Sussmann and Jurdjevic, 1972; Jurdjevic and Sussmann, 1972; Brockett, 1972; Brockett, 1973]

$$\langle A, B_j \,|\, j = 1, 2, \ldots, m \rangle_{\text{Lie}} = \mathfrak{g} \quad .\mathfrak{su}(N) \quad . \tag{3}$$

For quantum systems of n spins-$\frac{1}{2}$, one has $\mathfrak{g} = \mathfrak{su}(N)$ with $N := 2^n$, which already shows the state space and thereby that the dyamic degrees of freedom in quantum systems scale *exponentially* in system size (as opposed to classical systems, where they scale linearly). Thus it is obvious that assessing controllability via an explicit Lie closure, though mathematically elegant, becomes dramatically more tedious in quantum systems, and beyond seven qubits it is mostly prohibitive.

2 Theory

Hence here we will sketch a particularly simple and powerful alternative to assessing the controllability of quantum systems by way of easy-to-visualise *symmetry arguments*.

2.1 Symmetry Conditions for Controllability

To begin with, it pays to envisage the bilinear control systems by graphs in the way illustrated in Fig. 1: while the vertices represent *local* qubits as controlled by typical control Hamiltonians $B_j = iH_j$ (represented by Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ acting on the qubit represented by the respective vertex), the edges stand for pair-wise *coupling* interactions as typically only occuring in the drift term $A = iH_0$ (represented by two-component tensor products of Pauli matrices as, e.g., $J_{zz} \cdot \sigma_z \otimes \sigma_z$ for the standard Ising interaction or $J_{XX} \cdot (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y)$ for the so-called Heisenberg-XX interaction. Here the Pauli operators act on the two qubits connected by the respective edge). Scenarios of this kind are illustrated in Fig. 1.

As a central notion in the subsequent arguments, we characterise a quantum bilinear control system by its *system Lie algebra*, which results from the Lie closure of taking nested commutators (until no new linear indepedent elements are generated)

$$\begin{aligned} \mathfrak{k} :&= \langle A, B_j \,|\, j = 1, 2, \ldots, m \rangle_{\text{Lie}} \\ &= \langle iH_0, iH_j \,|\, j = 1, 2, \ldots, m \rangle_{\text{Lie}} \end{aligned} \tag{4}$$

as well as by its (potential) symmetries, i.e. the *centraliser* to the system algebra collecting all terms that commute jointly with all Hamiltonian operators

$$\mathfrak{k}' := \{ s \in \mathfrak{su}(N) | [s, H_\nu] = 0 \quad \forall \nu = 0; 1, 2, \ldots, m \} \,. \tag{5}$$

If there are no symmetries, i.e. if the centraliser $\mathfrak{k}'$ is trivial (zero), then the system algebra $\mathfrak{k}$ is *irreducible*. This can easily be checked by determining the dimension of the nullspace (kernel) to the corresponding commutator superoperators (of dimension $N^2 \times N^2$)—so it boils down to solving a system of $m + 1$ homogeneous equations in N^2 dimensions. Moreover, in Ref. [Zeier and Schulte-Herbrüggen, 2011] we showed that a trivial centraliser plus a connected graph imply that the corresponding system algebra is *simple*. Since the largest possible Lie closure is $\mathfrak{su}(N)$, the system algebra $\mathfrak{k}$ of an irreducible connected qubit system has to be a (proper or improper) *simple subalgebra to* $\mathfrak{su}(N)$. By making heavy use of computer algebra, in Ref. [Zeier and Schulte-Herbrüggen, 2011] we have also classified all these simple subalgebras of $\mathfrak{su}(N)$ for $N = 2^n$ with $n \leq 15$ qubits as summarised by the branching diagrams in Fig. 2 thus extending the known results from $\mathfrak{su}(9)$ [MacKay and Patera, 1981; Polack et al., 2009] to $\mathfrak{su}(32768)$.

This figure also illustrates that every $\mathfrak{su}(N)$ with $N = 2^n$ has two canonical branches, a symplectic branch (shown in red) starting with $\mathfrak{sp}(N/2)$ and an orthogonal branch (blue) commencing with $\mathfrak{so}(N)$. Actually, for *odd* $n \leq 15$, these are the only ones (and we conjecture that this holds true even beyond 15 qubits). In contrast, for *even* n there are always subalgebras $\mathfrak{so}(2n + 2)$ of unitary spinor type (shown in black) plus potential others (observe the instances of $\mathfrak{su}(4)$). — Clearly, if the (non-trivial) system algebra $\mathfrak{k}$ of a dynamic system in question can be ruled out to be on any of these three branches, then corresponding control system is indeed *fully controllable* as will be shown next.

To this end, it is convenient to exclude the symplectic and orthogonal subalgebras in the first place. It is a task that can again be readily accomplished (after having made sure $\mathfrak{k}$ is irreducible) by determining the dimension of the joint null space (over S) to the following equations for each H_ν with $\nu = 0; 1, 2, \ldots, m$

$$SH_\nu^t + H_\nu S = 0 \tag{6}$$

or in its superoperator form

$$(H_\nu \otimes \mathbb{1} + \mathbb{1} \otimes H_\nu)\,\text{vec}(S) = 0 \;, \tag{7}$$

where by Schur's Lemma one must have $S\bar{S} = \pm\mathbb{1}$ [Obata, 1958]. If there is a non-trivial solution for the (+)-variant, then $\mathfrak{k} \subseteq \mathfrak{so}(N)$ is of orthogonal type, if there is for the (-)-variant, then $\mathfrak{k} \subseteq \mathfrak{sp}(N/2)$ is of symplectic type. So if the solution space for both cases $(\pm)$

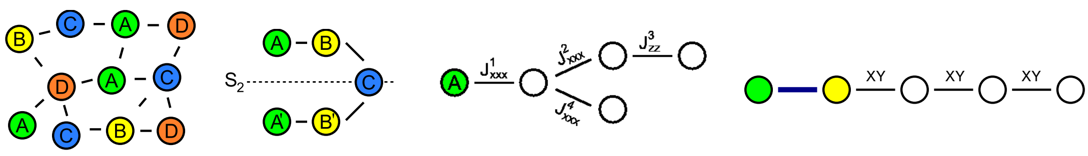

Figure 1. Graph representation of quantum dynamical control systems: vertices represent two-level systems (qubits), where common colour and letter code denotes joint local action, while the edges stand for pairwise coupling interactions. White vertices are qubits that are just coupled to the dynamic system without allowing to be controlled locally. The first and the last graph show no symmetries and their underlying control system is fully controllable. In contrast, the interior two graphs do exhibit symmetries: the left interior one has a mirror symmetry, while the right interior one leaves the Pauli operator σ_z on the upper terminal qubit invariant. These constants of the motion clearly preclude full controllability.

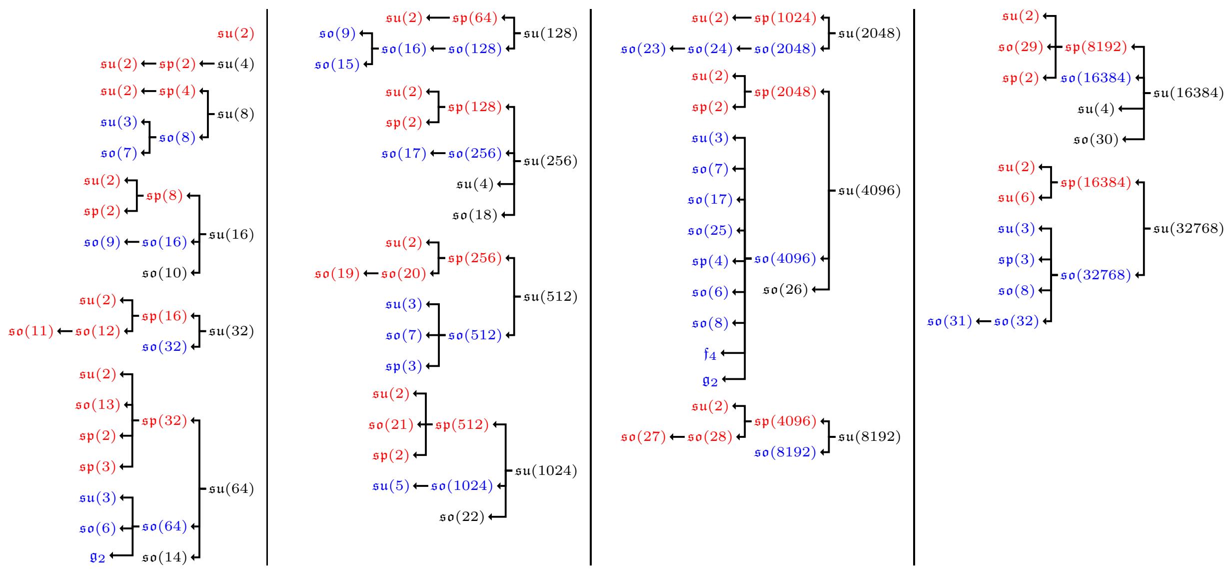

Figure 2. Branching diagrams showing all the irreducible simple subalgebras of $\mathfrak{su}(N)$ with $N := 2^n$ for n-qubit systems with $n \leq 15$ as given in [Zeier and Schulte-Herbrüggen, 2011]. Note that for *odd* n only the two canonical branches with orthogonal (blue) and symplectic (red) subalgebras occur. In contrast, for *even* n there always are unitary spinor-type subalgebras $\mathfrak{so}(2n+2)$ and in some instances $\mathfrak{su}(4)$. The orthogonal subalgebras are related to fermionic quantum systems, while the symplectic ones relate to bosonic ones as desribed in the text and shown in Tabs. I and II.

is zero-dimensional (corrresponding to the only solution being trivial) then $\mathfrak{k}$ is neither of orthogonal nor symplectic type.

For odd $n \leq 15$, this does in fact already ensure full controllability, since only n even allows for spinor-type simple subalgebras. However, these may finally be excluded by the following powerful theorem of Ref. [Zeier and Schulte-Herbrüggen, 2011]:

Theorem: A bilinear control system governed by Hamiltonians $\{iH_\nu \,|\, \nu = 0; 1, 2, \ldots, m\}$ with system algebra $\mathfrak{k} := \langle iH_0, iH_j \,|\, j = 1, 2, \ldots, m\rangle_{\rm Lie}$ is fully controllable if and only if the joint centraliser to $\{(iH_\nu) \otimes \mathbb{1} + \mathbb{1} \otimes (iH_\nu) \,|\, \nu = 0; 1, 2, \ldots, m\}$ in $\mathfrak{u}(N^2)$ has dimension two.

To sum up, a bilinear (n-qubit) control system as in Eqn. (1) is fully controllable if and only if all of the following conditions are satisfied

(1) the system has no symmetries, i.e. $\mathfrak{k}'$ is trivial;
(2) the system has a connected coupling graph;
(3) the system algebra $\mathfrak{k}$ is neither of orthogonal nor of symplectic type, and finally
(4) the system algebra is not of unitary or spinor-type or of exceptional type.

While we gave a rigorous proof in Ref. [Zeier and Schulte-Herbrüggen, 2011], the key arguments can easily be made intuitive as follows:

(1) symmetries would entail conserved entities (invariant one-parameter groups) thus precluding full controllability;
(2) coupling graphs with several connected components preclude that these components can be coherently coupled, which, however, is necessary for full controllability;
(3) orthogonal or symplectic subalgebras are proper subalgebras to $\mathfrak{su}(N)$ (for $N > 2$) and therefore do not explore all dynamic degrees of freedom of $\mathfrak{su}(N)$, and finally
(4) the same holds for unitary or spinor-type or exceptional subalgebras of $\mathfrak{su}(N)$.

By the branching diagrams in Fig. 2 it is immediately obvious: establishing full controllability boils down to ensuring the dynamic system is governed by a system algebra that is irreducible (no symmetries), and simple (connected coupling graph) and *top of the branch*. This shifts the paradigm from the Lie-algebra rank-condition to easily verifiable symmetry conditions.

2.2 Connection to Quantum Simulation

Recall that fermionic quantum systems relate to orthogonal system algebras, while bosonic ones relate to symplectic system agebras. Then the link from controlled quantum systems to quantum simulation becomes obvious: the branching diagrams of Fig. 2 also illustrate that an (irreducible and connected) n-qubit quantum system is fully controllable if and only if it can simulate *both bosonic* as well as *fermionic* systems.

This is because–clearly–a controlled bilinear dynamic system $\mathcal{A}$ can simulate another system $\mathcal{B}$ if and only if for the system algebras one has $\mathfrak{k}_A \supseteq \mathfrak{k}_B$. Moreover, given a fixed Hilbert space $\mathcal{H}$, $\mathcal{A}$ simulates $\mathcal{B}$ *efficiently* (i.e. with least state-space overhead in $\mathcal{H}$) if for any interlacing system $\mathcal{I}$ with system algebra $\mathfrak{k}_I$ satisfying $\mathfrak{k}_A \supseteq \mathfrak{k}_I \supseteq \mathfrak{k}_B$ one must have either $\mathfrak{k}_I = \mathfrak{k}_A$ or $\mathfrak{k}_I = \mathfrak{k}_B$ or (trivially) both.

For illustration, consider an n-qubit nearest-neighbour coupled Heisenberg-XX spin chain with single local controls. Then Tab. I shows that a single controllable qubit at one end suffices to simulate a fermionic system with quadratic interactions on n levels (governed by $\mathfrak{so}(2n+1)$, while local controls on both ends are required to simulate quadratic fermionic systems on $n+1$ levels with system algebra $\mathfrak{so}(2n+2)$. Most remarkably, if the controllable qubit is shifted to the second position, one gets dynamic degrees of freedom scaling *exponentially* in the number of qubits in the chain. This is by virtue of the system algebras $\mathfrak{so}(2^n)$ or $\mathfrak{sp}(2^{n-1})$, which most noticeably result depending on the length of the n-qubit chain: if $n (\mathrm{mod}\, 4) \in \{0, 1\}$ the system is fermionic ($\mathfrak{so}(2^n)$), while for $n (\mathrm{mod}\, 4) \in \{2, 3\}$ the system is bosonic ($\mathfrak{sp}(2^{n-1})$) [Zeier and Schulte-Herbrüggen, 2011]. It is not until *two adjacent* qubits can be coherently controlled (as $\mathfrak{su}(4)$) that the Heisenberg-XX spin chains become fully controllable [Burgarth et al., 2009].

Moreover, Tab. II illustrates the power of classifying dynamic systems by symmetries and thereby in terms of their system Lie algebras: it turns out that joint controls on all the local qubits simultaneously suffice to even simulate effective three-body interactions (usually never occuring naturally), provided the Ising-ZZ coupling in odd-membered spin chains can be designed to have opposite signs on the two branches reaching out from the central spin.

2.3 Open Systems

While in closed systems there is a particularly simple characterisation of reachable sets in terms of the system algebra $\mathfrak{k}$ generating the Lie group $\mathbf{K} := \langle \exp(\mathfrak{k}) \rangle$ and the corresponding group orbit reading

$$\mathrm{Reach}\, \rho_0 = \mathcal{O}_{\mathbf{K}}(\rho_0) := \{K \rho_0 K^\dagger \,|\, K \in \mathbf{K} \subseteq SU(N)\} \tag{8}$$

in open quantum systems it is considerably more intricate to estimate the rechable sets. Just for unital systems (i.e. those with fixed point proportional to $\mathbb{1}$) which are further simplified by the (hopelessly idealising) assumption that all coherent controls are infinitely fast in the sense of

$$\langle iH_j \,|\, j = 1, 2, \ldots, m \rangle_{\mathrm{Lie}} = \mathfrak{su}(N) \tag{9}$$

one finds by the seminal work of [Uhlmann, 1971] and [Ando, 1989] on majorisation that

$$\mathrm{Reach}\, \rho_0 \subseteq \{\rho \in \mathfrak{pos}_1 \,|\, \rho \prec \rho_0\} \tag{10}$$

as recently pointed out more explicitly in [Yuan, 2010]. However, this simple characterisation becomes hopelessly inaccurate in all physically more realistic scenarios, where the drift Hamiltonian H_0 is necessary to ensure full controllability in the sense of

$$\langle \mathbf{iH_0}, iH_j \,|\, j = 1, 2, \ldots, m \rangle_{\mathrm{Lie}} = \mathfrak{su}(N)\;. \tag{11}$$

In these experimentally more realistic and hence highly relevant cases, we have recently characterised the dynamic system in terms of the underlying Lie wedge $\mathfrak{w}$, i.e. the generating set of the dynamic system *Lie semigroup* $\mathbf{S}$ of irreversible (Markovian) time evolution in Refs. [Dirr et al., 2009; O'Meara et al., 2011]. Here the reachable sets can be conveniently and more accurately be approximated by

$$\begin{aligned} \mathrm{Reach}\, \rho_0 = \mathbf{S}\, \mathrm{vec}\, \rho_0 \quad \text{where} \\ \mathbf{S} \simeq \mathrm{e}^{A_1} \mathrm{e}^{A_2} \cdots \mathrm{e}^{A_\ell} \end{aligned} \tag{12}$$

with $A_1, A_2, \ldots, A_\ell \in \mathfrak{w}$ and where usually few factors suffice to give a good estimate.

3 Applications

Building upon [Khaneja et al., 2005; Schulte-Herbrüggen et al., 2005], recently we have lined up all the principle numerical algorithms into a unified programming framework DYNAMO [Machnes et al., 2011]. Their respective control problems follow a general line: subject to the equation of motion (1) a target function $f(X_{\mathrm{target}}, X_0) := \mathrm{Re}\,\mathrm{tr}\{X_t^\dagger X_0\}$ is to be maximised over all admissible (piece-wise constant) control vectors $u_j(t) := (u_j(0), u_j(\tau), u_j(2\tau), \ldots, u_j(M\tau = T))$. this turns a control vector (pulse sequence) from an initial guess

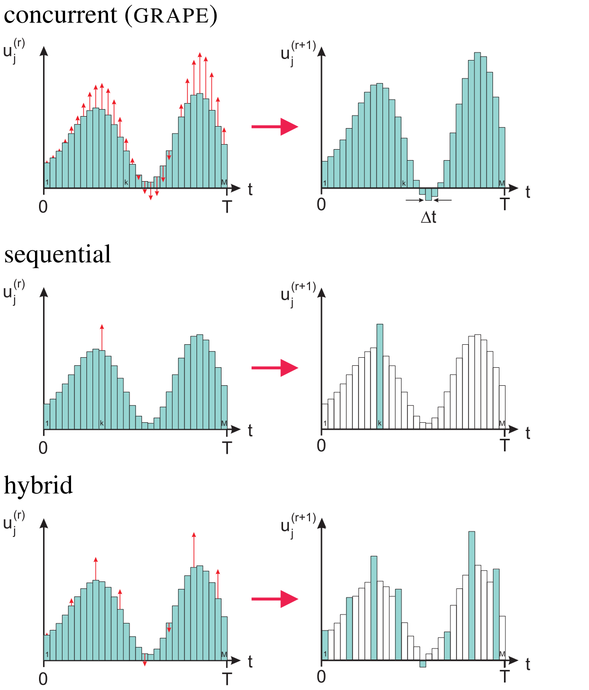

Figure 3. Numerical optimal control schemes turn an initial guess of a contrl vector (left panels) into optimised control vectors by gradient-based first or second-order updates, which may be done concurrently, in a hybrid fashion, or sequentially. Our new DYNAMO programme package [Machnes et al., 2011] offers all these options in a unified modular way.

into an optimised shape by following first-order gradients (or second-order increments) to all the time slices of the control vector as shown in Fig. 3, which may be done sequentially [Krotov and Feldman, 1983; Krotov, 1996; Sklarz and Tannor, 2006; Singer et al., 2010], or concurrently [Khaneja et al., 2005; Schulte-Herbrüggen et al., 2005] or in the newly unified version DYNAMO allowing hybrids as well as switches on-the-fly from one scheme to another one [Machnes et al., 2011].

These numerical schemes have been put to good use for steering quantum systems (in the explicit experimental parameter setting) such as to optimise

(1) the transfer between quantum states (pure or non-pure) [Khaneja et al., 2005],
(2) the fidelity of a unitary quantum gate to be synthesised in closed systems [Schulte-Herbrüggen et al., 2005; Spörl et al., 2007],
(3) the gate fidelity in the presence of Markovian relaxation [Schulte-Herbrüggen et al., 2011], and also
(4) the gate fidelity in the presence of non-Markovian relaxation [Rebentrost et al., 2009]

In the lecture, examples for spin systems [Schulte-Herbrüggen et al., 2005; Spörl et al., 2007] as well as Josephson elements [Spörl et al., 2007] have been illustrated in all detail. For optimising quantum maps in open systems, time-optimal controls have been compared to relaxation-optimised controls [Schulte-Herbrüggen et al., 2011] in the light of an algebraic interpretation [Dirr et al., 2009].

4 Conclusion

We have put some of our recent results into the context of engineering and steering quantum dynamical systems with high precision. In doing so, we have shown how a quantum systems theory emerges, which immediately links to many applications in quantum simulation and control without sacrificing mathematical rigour. We have pointed out how to optimise the explicit steerings (control amplitudes) for manipulating closed and open (Markovian and non-Markovian) systems in finite dimensions. In particular during the talk a plethora of such examples was presented.

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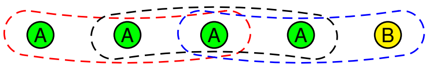
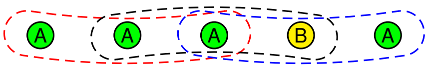
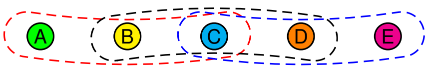
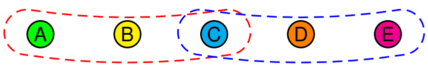
Table 1. Heisenberg-xx spin chains with a single control on one end (or both) can simulate either fermionic or bosonic systems depending on the chain length as summarised in [Zeier and Schulte-Herbrüggen, 2011]. Local control over two adjacent qubits is required to make the system fully controllable (last row).

system type n-spins-$\frac{1}{2}$	number of levels	fermionic (order of coupling)	bosonic (order of coupling)	system Lie algebra
(A) —XX— ○ —XX— ○ ⋯⋯ ○	n	quadratic (i.e. 2)	–	$\mathfrak{so}(2n+1)$
(A) —XX— ○ —XX— ○ ⋯⋯ (B)	$n+1$	quadratic (i.e. 2)	–	$\mathfrak{so}(2n+2)$
○ —XX— (A) —XX— ○ ⋯⋯ ○				
for $n \bmod 4 \in \{0,1\}$	n	up to n	–	$\mathfrak{so}(2^n)$
for $n \bmod 4 \in \{2,3\}$	n	–	up to n	$\mathfrak{sp}(2^{n-1})$
(A) —XX— (B) —XX— ○ ⋯⋯ ○	n	up to n	up to n	$\mathfrak{su}(2^n)$

Table 2. Ising-zz spin chains with joint controls on all the qubits locally can simulate bosonic systems provided the coupling constants of the right and left branches leaving the cetral qubit have opposite signs as is also summarised in [Zeier and Schulte-Herbrüggen, 2011]. Note that even physically unavailable three-body interactions can be simulated by such systems. The system algebras given on the right specify that for a given chain length all systems are dynamically equivalent, which otherwise would be extremely difficult to analyse.

system type $n=2k+1$ spins-$\frac{1}{2}$	number of levels	bosonic coupling order	system Lie algebra $\mathfrak{sp}(2^{n-1})$
(A) —+ZZ— (A) —−ZZ— (A)	$n=3$	up to $n=3$	$\mathfrak{sp}(8/2)$
(A) —+ZZ— (B) —−ZZ— (A)	—”—	—”—	—”—
(A) —+ZZ— (A) —+ZZ— (A) —−ZZ— (A) —−ZZ— (A)	$n=5$	up to $n=5$	$\mathfrak{sp}(32/2)$
(A) —+ZZ— (A) —+ZZ— (B) —−ZZ— (A) —−ZZ— (A)	—”—	—”—	—”—
(A) —+ZZ— (B) —+ZZ— (C) —−ZZ— (B) —−ZZ— (A)	—”—	—”—	—”—
	—”—	—”—	—”—
	—”—	—”—	—”—
	—”—	—”—	—”—
	—”—	—”—	—”—