Quantum Technology: Computational Models for Quantum Device Design

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1 Introduction

Some of the world's experts on quantum engineering met at the Banff Centre in January 2012 at a workshop hosted by the Banff International Research Station (BIRS) on recent developments and challenges in designing and building functional quantum devices. Until recently quantum physics was predominantly in the domain of physics explaining the workings on the universe at tiny scales and also at the heart of many philosophical discussion about the nature of the universe. Advances not only in physics, but also in manufacturing, computer science and mathematics now promise a wide range of applications of quantum phenomena from communication, to electronics, computing, biology and medicine. Quantum devices would function quite unlike classical devices and enable new functionalities to create faster, smaller and more energy efficient devices for everyday use.

Progress in nano-fabrication enables the realisation of ever smaller and increasingly sophisticated nanoscale devices whose behaviour is no longer classical but strongly influenced by quantum effects such as quantum tunnelling and quantum transport. These effects are unavoidable and are already an issue in conventional semiconductor technologies. Quantum effects such as coherence, interference and entanglement also hold significant potential to enable entirely new devices with novel functionalities. Recent advances in the novel area of coherent control of quantum systems, especially optimal control design, further enable unparalleled levels of control of quantum dynamics, in theory, simulations, and increasingly, laboratory experiments. This creates the real possibility of a new age of quantum engineering utilising quantum effects to devise novel technologies. Emerging applications range from quantum sensors, to spintronics and coherent electronics, to information processing with improvements in communication, imaging, metrology and medical diagnostics along the way.

However, the realisation of such devices is still a challenge. It will require the development of a comprehensive framework for quantum engineering, including new tools for modelling quantum devices, simulations of quantum dynamics, continued improvements to existing models by incorporating experimental data and systematic system identification, control to achieve desired outcomes, and robustness analysis to identify robust device designs. The workshop aimed to advance this goal by bringing together experts in computational modelling, quantum simulations, coherent control, system identification and control engineering to identify key challenges and form new connections. BIRS, with its stimulating environment, excellent facilities and administrational support, provided the ideal location for this.

Device design requires the creation of a physical model of the device for which a control must be found to guide its dynamical behaviour. This in turn requires physically accurate simulation and also identification of

quantum systems to build and verify such models. Hence, a critical task is the development of mathematical models that capture the key properties of the device sufficiently accurately. Modelling even basic properties of complex quantum systems or devices is already non-trivial, but the models required for coherent control of the dynamics of quantum devices are far more demanding. They must describe the dynamical evolution of the system and capture the influence of various possible controls such as voltages, external potentials or coherent control fields on the behaviour of the system. This means we need dynamic control system models of quantum devices.

Accurate models are particularly critical for quantum systems as most control strategies for these systems, even those involving direct or indirect feedback, are model-based. To find the best controls to accomplish various tasks from quantum state engineering to gate implementation to initialization, stabilization and decoherence suppression these strategies rely on a mathematical model of the system and the effect of controls on its behaviour. The computational methods used for simulations, control and identification are thus enabled by the model, but also limited by its restrictions. We also need highly efficient simulation tools to evaluate these models for the computationally very intensive operations required for control and design.

To a certain extent computational models for quantum devices can be derived from basic physical principles. Such models are usually not sufficiently accurate except for very simple systems as they fail to capture many details of the actual device which is subject to effects neglected in the model, imperfections, inhomogeneities, etc. To overcome such limitations, some degree of experimental system identification and model verification is needed to estimate and verify the parameters in the model. For the application of different computational techniques and efficient computation, often different models are required, which means they must be converted into each other. However, often there are no simple relations between different models, even for geometric models and much less for dynamic control models.

2 Overview

The workshop explored models and techniques for designing and controlling quantum devices to establish links between physical (quantum) device modelling, experimental system identification, model verification and quantum control. Having reliable mathematical and computational models and methods is crucial for quantum engineers to design realistic quantum devices. This includes tools that allow not only efficient simulation of complicated quantum devices such as semi-conductor nano-structures, superconducting devices or atom chips, but also device optimisation and dynamic control.

Models with efficient design and control methods are crucial to enable engineering complex quantum devices, whose ultimate importance lies in the applications. Quantum communication and encryption may be the most advanced area on the application side, with significant impact already on secure communication. However, similar high-impact technologies are on the horizon in electronics, metrology, imaging, biology and medicine.

Specifically the workshop evolved around the following questions:

1. What are the most promising applications in nearer future? E.g., semiconductor or superconductor devices for quantum metrology, information processing, or perhaps modelling and understanding quantum effects in biological systems, or medical applications. This further raises questions about what design tools are needed for the most promising applications. An important issue to consider is also the type of models needed for the different operations required for an application such as the relation between a geometric model of the device and the model required for dynamic control.
2. What techniques and models are needed to design, simulate and control the operation of these quantum devices? Dynamic control simulations require control system models, conventionally based on partial differential equations derived from fundamental principles, such as the control dependent Schrödinger or quantum Liouville equation. Efficient simulation algorithms for physically accurate computational models are crucial for this task. Statistical models simply describing the behaviour of an actual device may sometimes be sufficient, or at least be used to augment the differential equation approach to consider specific material properties and the complete behaviour of real devices.
3. What protocols for experimental system identification, parameter estimation and model verification are available? How efficient and reliable are these? What are their experimental requirements and how realistic are these? Do they provide the models we need? E.g. common techniques such as spectroscopy

and quantum process tomography provide information about the system but do not directly provide the type of dynamic control systems models we require. How can techniques be combined, modified or extended to enable construction of the models we need?

4. What are efficient ways to solve the inverse of the modelling and simulation problem? How can we design and control efficient quantum devices, by, e.g., finding optimal device geometries, optimal dynamic voltage profiles applied to control electrodes or optimally shaped control pulses? What should be the main objectives of such optimizations? What are the practical constraints? How well can current algorithms cope with large-scale problems?
5. What computational tools are available and what new tools are required or desirable, especially with a view towards integration of device or system design, dynamic simulations of quantum evolution, experimental data analysis and design and control optimisation. What is the efficiency of simulation algorithms on different hardware platforms? What role could effective visualisation of raw simulation data and automated, though perhaps human-guided, data analysis play? How could it make the process of model analysis and verification more efficient?

These questions were discussed in the context of four areas over four days, details of which are reported below: (a) device modelling, simulation and control of solid state qubits, (b) device modelling, simulation and control of biological and spin systems, (c) quantum system identification, (d) controlling quantum systems.

A diverse range of issues were covered, from computational modelling of physical systems, to high performance and parallel computing, to device design and nano-fabrication, to control and optimisation, to machine learning and pattern analysis, to quantum theory and experimental physics. This was reflected in the list of participants which come from mathematics, computer science, engineering and physics with relevant background in some of these areas. The discussions about identification, simulation and optimisation of quantum devices have shown that there are still many links between physics and control of quantum devices and engineering and computer science to be explored.

During the last day of the workshop the overall findings were drawn together to formulate major challenges to address to devise a roadmap towards computer-aided design systems for quantum devices, listing the required functionalities and various approaches to provide these, ensuring interoperability between the approaches as far as feasible, and dependencies between results and approaches. Furthermore initial plans for future workshops and conferences on quantum technologies were considered to track progress on addressing these issues.

3 Solid State Device Modelling

The presentations for the first day centred around the current state of quantum device modelling, particularly in solid-state qubit systems (dots and donors):

- Richard Muller: Development of Few-Electron Si Quantum Dots for Use as Qubits;
- Jim Fonseca: NanoHUB and NEMO5: Science Cyberinfrastructure and Nanoelectronic Modeling Tool;
- Erik Nielsen: The QCAD Framework for Quantum Device Simulation;
- Suzey Gao: Semiclassical Poisson and Poisson-Schroedinger Solvers in QCAD;
- Rajib Rahman: High Precision Quantum Device Simulation with Atomistic Tight-Binding Technique Coupled with Semi-Classical Poisson Solver and Many-Electron Configuration Interaction Method.

The audience broke into four groups to address the following discussion topics on quantum system/device modelling. A summary of the reports is as follows.

3.1 Realism of the Model: Speed vs Accuracy and Comparison with Experiment

The central issue of theoretical modelling of quantum devices is how to describe the essential physics without compromising too much on realism and without the model becoming intractably complex. It was noted that one should first define clearly the purpose of modelling and the level of modelling (micro vs. macro) necessary. The realism required depends on the purpose of the modelling and the degree and precision of experimental knowledge of the system. For some systems, such as quantum dots, it was noted that semi-classical

calculations appear adequate for most experimentalist needs at present, but fully quantum mechanical models may be required for new applications such as quantum information. At the engineering level a proper discretisation scheme or coarse graining level that represents the correct physics of the system is essential. There is always a trade-off between accuracy and complexity when choosing a discretisation or coarse graining of the microphysics involved. In some cases, such as when constructing stochastic models for real-time feedback control, improved model accuracy will come at the expense of increased feedback delay time, possibly favouring simpler models even if less accurate.

Compressed sensing was discussed as a particular tool to extract a minimal set of information pertinent to the behaviour of the system. Compressed sensing has been useful to reconstruct large but low-rank matrices given $n \ln n$ random entries using the Singular Value Threshold Algorithm. However, compressed sensing can be quite sensitive to noise (beyond a threshold) and it is less obvious how to apply this approach to reconstruct generators of the dynamics as opposed to dynamical maps or states.

3.2 Multi-Scale Models: from Microscopic Physics to High Level Device Description

For solid-state based quantum devices such as donor atoms embedded in a substrate or quantum dots one cannot hope to perform an ab-initio calculations up to and including the device scales without some form of coarse graining of the physics. The question therefore arises how to interface large scale ab-initio approaches such as density functional theory, which cover relatively small device volumes, with higher-level effective approaches such as tight-binding and Poisson-Schrödinger equation modelling.

The example of simulating coherent transport (CTAP) through a triple (donor) well structure was given: atomistic tight-binding simulations of a multi-million atom device with a range of gate biases were used to derive a higher-level description in terms of adiabatic control of an effective 3×3 Hamiltonian. Another example was the evolution of models for highly-doped phophorous in silicon nanostructures fabricated by STM, from ab-initio treatments of small supercell regions, to tight-binding to a high-level and computationally simpler self-consistent effective mass model informed by microscopic band-structure calculation.

The importance of understanding the domains of validity of a model or theory, and careful model validation by comparing with data from experiments or verifying predictions made by the model, were stressed, raising also the question of efficient strategies for validating models.

3.3 QCAD Approaches: Optimisation and Time-Dependence

For solid-state devices the focus was on how to optimise the atomistic tight-binding calculations, interfacing with gate-level simulation and going beyond single electron descriptions. For multi-electron device simulations the most expensive computations in the tight binding model are the Coulomb integrals. One approach to make the integrations more tractable that was discussed is the transformation from a plane-wave to a Gaussian basis although it was noted by one participant that this had been tried before (presumably unsuccessfully?). Other approaches such as matrix product states or density matrix renormalisation group may be useful if the system is effectively low-dimensional.

It was also discussed what other systems could be modelled with QCAD and what additional capabilities would be needed to be able to model other physical systems. Superconducting flux qubits appear to be amenable to QCAT modelling, which could be useful to model the effect of imperfect J-junction topography, for example. A comment was made about the problem that de-facto standard simulation tools, mainly finite element analysis, often do not preserve properties of the simulated continuous systems: a moving rigid body may gain or loose momentum or a cavity may exhibit fictitious eigenmodes in an electromagnetism (E-M) simulation. This loss of fidelity follows from discretisation processes which fail to preserve underlying geometric and topological structures on the continuous model. There are excellent results from the calculus of differential forms in E-M and Lagrangian mechanics to avoid such problems.

To incorporate the effect of temporally varying fields, one could compute an effective Hamiltonian in the configuration space imposing piecewise constant classical E-M fields. This was thought to be adequate for many applications. A suggestion was made to look at existing quantum dynamics simulators, e.g., Q-TIP. In this context it was also discussed how to differentiate between coherent and incoherent dynamics and control, considering signatures, e.g., related to quantum transport, external E-M fields, effective spin descriptions.

There was also discussion about what a quantum system is, and it was and agreed that calling QCAD a quantum device simulator may be too broad, since there are types of quantum devices (e.g. biological systems) that it is not designed to simulate.

3.4 Open Quantum System Description

It was discussed when a given open quantum system should be modelled as Markovian, non-Markovian or a combination of the two, when the Lindblad formalism of open quantum systems was sufficient and when a stochastic model or something else was needed, and what effective descriptions of non-Markovian behavior existed in general. In principle, for any system interacting with non-Markovian environment, one may always enlarge the original system so that the interaction of the enlarged system with the environment can be treated as Markovian, where the shell added to enlarge the system is a finite-dimensional subspace of the bath degrees of freedom that encompasses the non-Markovian dynamics. In practice, finding the right shell is not trivial, however, and the resulting enlarged system may be too large to be computationally tractable.

Another approach to derive open-system models employed by some participants is singular value decomposition of the Redfield superoperator to obtain matrix product operators acting on matrix product states, and finally non-Hermitian generators for non-unitary dynamics. However, this approach is likely to work only for 1D models. An alternative used in NMR is to start with a Gaussian theory and move to lower temperatures by adding n-point correlations with increasing n, a sort of Lie closure of a cluster expansion. In biological systems it was suggested that 5-point functions are needed for an effective description.

Time-dependent density matrix renormalisation group (tDMRG) was also discussed, but it was suggested that instead of simulating the dynamics of the entire system as in tDMRG, we should find a renormalisation group approach that yields an effective theory where the effective degrees of freedom are those we actually care about. Information spreads via the system-bath interactions in the Hamiltonian and the Lieb-Robinson bound tells us how this information spreads. A renormalisation program restricting the computation to the cone of this spread could render otherwise intractable problems tractable. Objections to this approach were that general theories often yield prohibitively expensive routes to computation. On the positive side it was noted that Hamiltonian interactions of finite order yield graphs of finite order and often only low-order interactions need to be considered. For example, in NMR, the scale of the coupling and relaxation are both several Hertz, so that we only have to worry about a few concatenations of two-body interactions. It was also noted that in a linear chain or tree, there is a unique traversal of the chain making compression tractable.

No matter what approach is employed to model an open quantum system, the resulting model is likely to be high-dimensional and model reduction techniques may still be required to make the model computationally tractable. A compressed description could also help understand dynamic decouplings and the dissipative dynamics in general. While there are a number model reduction techniques out there, it is not obvious which are the most suitable and there was concern that it may be difficult to obtain accuracy criteria.

4 Biological and Spin Systems

The role of quantum effects and technology in biological systems has more recently attracted a lot of attention. This is likely because of the wide range of interesting applications in biology and medicine, including improving understanding of biological processes, light harvesting systems, sensors for biological and medical applications, medical imaging, targeted drug delivery, etc. Some of which have been discussed in the following presentations at the workshop:

- Martin Plenio: Quantum Coherence and Biological Systems;
- Stephan Hoyer: Quantum Control of Light-Harvesting Systems;
- Paul Rees: Mathematical Techniques for Cell Cycle Analysis;
- Jianming Cai: Diamond Based Single Molecule Magnetic Resonance Spectroscopy;
- Ilya Kuprov: Algorithms and Software for Large-Scale Quantum Spin Dynamics Simulations;
- André Bandrauk: Modelling Molecules in Intense Laser Pulses and Attosecond Simulations;
- Lloyd Hollenberg: Quantum Sensing Technology and Modelling.

Naturally there is a lot of overlap with modelling, simulating, system identification and control topics related to other areas. So details on some of the discussions have been combined with topics in other sections

of this report. Nevertheless the different nature of the systems might mean that different techniques might be more effective and of course new ideas and insights from this area can also be useful for other applications areas. This exchange has inspired workshop participants to consider this area more actively, as in particular there is a range of immediate applications on the horizon, especially possibly in the form of bio-molecular systems as devices.

4.1 Simulation Tools for Quantum Biology

On the question of simulating quantum effects and technology in biology, it was mainly discussed how far any of the existing simulation tools would be useful for solid-state device simulation. In particular how far could similar approximations and simplifications used for biological systems also apply to solid state devices. Density matrix renormalisation group (DMRG) techniques were considered to be of practical use only in 1D and mainly of use for questions of ground state, though.

4.2 Structured and Non-Markovian Environments

A particular issue that arises in biological systems is the use structured and/or non-Markovian environments as a tool to design systems/devices. They might well be a resource utilised in biological systems by nature.

There are problems that cannot be solved by coherent control alone such as preparation of a system in a certain state starting with an unknown state or entropy reduction in general. Noise can help here by offering new effective pathways. Recent work on reservoir engineering has shown that environments can be designed to initialise and stabilise systems in a wide range of desired states. Furthermore, reservoir engineering can be achieved by various means including incoherent control, measurements and direct feedback. In the latter cases it is the backaction from the measurement and the feedback that effectively modifies the Lindbladians. Control by backaction is an interesting and promising idea but it was noted that in some cases such as for ensembles of spins backaction effects are very small. The focus of the discussion was mostly on classical baths but the question of nonclassical baths was raised.

4.3 Role of Coherence in Biological Systems and Quantum Biotechnology

It was noted that one can see quantum effects in room temperature NMR processes and that entanglement is pervasive throughout chemistry. Spin dynamics results from processes involving singlet-correlated electrons. Such processes may play a role in biological systems although likely at a different time scale than excitonic dynamics. For example, in radical chemistry the radicals interact as singlet pairs. Whether the pair is singlet or triplet depends on the magnetic field, making these processes magneto-sensitive both to internal and/or external fields. Such magnetic field effects appear to be used by birds to navigate while biological functions in humans appear to be insensitive to even strong magnetic fields as experienced in MRI scanners.

In the application of qubit technology for sensing in biology, quantum coherence of the probe itself needs to be maintained in the complex ambient environment. So far the nitrogen-vacancy defect centre in diamond is proving to be an ideal qubit platform for such quantum sensing (nano-magnetometry) applications in biology with a number of early proof-of-concept experiments already reported. It was noted that for sensing applications the modelling challenge is to understand the biological origins and nature of the magnetic fields being detected.

5 Quantum System Identification

Knowledge about a system's behaviour is required in order to use it to build practical quantum devices. This means that the model must describe the system with sufficient accuracy for the task. If no such model exists a-priori, certain parameters of the model, or even the complete model, must be derived from data about the physical system. While techniques such as spectroscopy and quantum process tomography provide information about a system, they typically do not describe it completely, especially its dynamical evolution and response to external fields. Yet, for effective control, such dynamic models of the system are required.

At the workshop common system identification techniques were discussed with a view to understanding how efficient, reliable and practically realisable these are. To start the discussion various system identification approaches and how these are used for quantum systems were presented in the following talks:

- Frank Langbein: Bayesian Learning;
- Jonathan Quinn: Optimisation;
- Steffen Glaser: Optimal Control of Uncoupled and Coupled Spins;
- Daniel Oi: Maximum Likelihood Hamiltonian and Decoherence Estimation;
- Daniel Burgarth: Quantum System Identification with Limited Resources;
- Clemens Muller: Characterizign Defects in Superconducting Phase Qubits;
- Edmond Jonckheere: Differential Topology of Adiabatic Gap.

These formed the basis for the group discussions on the topics summarised below.

5.1 Bayesian Estimation

Bayesian learning has been discussed in detail as a possible approach to system identification. The main difference to more traditional approaches is that Bayesian models explicitly encode the uncertainty in what is being learned based on the available observations. Bayesian approaches do not start with effectively arbitrary priors or pick a maximum likelihood answer, but provide a probability distribution. While this improves the prediction qualities of the model and avoids over- and underfitting problems, it does not actually provide a definite model and is quite expensive to compute. So approximations and simplifications are required.

Core questions to address are to determine to what accuracy the model actually has to be learned for the problem it is used for, and what we can actually learn about a quantum system purely from (repeatedly) measuring it. Selecting suitable parameters and models appears crucial, but also requires a way to test the appropriateness of the model and the parameters to learn. Likely a hybrid approach between a completely modelled and a completely statistical model is required to achieve a useful, but computationally feasible system identification approach.

Because of the computational costs and the potentially large amount of measurements needed, important questions on the Bayesian approach are how well it will scale to larger systems, with potentially thousands of random variables to be learned, and how robust the approach is to deal with real physical systems under non-ideal conditions, and what priors and approximations should be used (depending on the model). To determine the dynamics of a quantum system it is not at all clear at what times to measure, how to initialise the system and what to measure (repeatedly) to obtain a dynamical model that is sufficient for control. Partly this might be determined from a physical model of the system using utility theory and value of information approaches. Yet this is only as good as the model describes the system and in particular achieving high accuracy might be difficult.

To improve data acquisition it was suggested to use compressed sensing techniques, possibly also for sparse defect identification and to determine biases on the fly. This would largely depend on selecting physically possible compressive sensing bases that reveal sufficient information about the system.

There was also some discussion about whether spectroscopy or Bayesian learning is more suitable. However, it seemed that Bayesian learning might well be used in spectroscopy or spectroscopy could provide data to Bayesian models to learn the system behaviour. Possibly Bayesian techniques may also be used to estimate parameters in a tight-binding model.

Selecting a specific model, e.g. for a maximum likelihood approach, usually requires an optimisation or search method which may struggle with the complicated "landscape" of the probability distribution. Various approaches toward approximating the probability distributions to enable identifying the peaks without computing the whole distribution may be used, also for the evaluation of the distribution over all possible outcomes. Gibbs sampling or swarm intelligence approaches could also be employed for evaluation and optimisation.

5.2 Role of Control in System Identification

One central issue raised was whether (open loop and feedback) control could help to estimate parameters. In particular feedback control and system identification seem to address related issues. Linear classical systems

are often secretly subject to feedback, which often suppresses the impact of the actual parameters on the system's behaviour. This might work similarly for using feedback to control quantum systems and avoid that the actual parameters need to be determined, but only their impact on the system dynamics must be suppressed. Specifically to deal with idiosyncrasies of a specific system, feedback might then be better than complete identification.

However, unlike classical systems, a quantum feedback mechanism becomes part of the system that is intended to be controlled. Hence, feedback might make the system non-Markovian. While this can be avoided by considering the control and system variables together, one must be cautious, particularly if the feedback mechanism may in fact amount to a measurement. Effectively the results from an observation is fed back into some parametrised family of controls. When the measurements are weak measurements, as in some examples of quantum optics, then, to some degree, it is understood how to treat such systems. Extending and improving the understanding of such approaches and identifying realisable classes weak feedback systems might lead to bootstrapping methods for quantum devices.

These discussions further raised questions on how far a system with feedback is or remains controllable and how to deal with non-Markovian systems; including discussing examples of non-Markovian systems and how to determine that a system is Markovian. Typically we apply control to a system, make an observation and throw the system away, hoping that we can learn the dynamics from these measurements. Instead, is it possible to learn more about the system if we do not throw it away? At least for understanding the "Markovianity" of the bath, the answer seems to be positive. The control process and the partial measurement in the first iteration could push information into the environment, and the subsequent iteration could perhaps detect that the environment has remembered this information.

Another issue considered was if feedback models from control can be combined with with Lie Algebraic approaches into an overall framework as either side misses something: the interface between quantum and classical models, semi-classical modelling; Heisenberg vs. Schrödinger picture. Are the feedback approach and Lie algebra approach compatible?

5.3 Modelling for System Identification

Models provide prior knowledge for system identification, usually as a hard constraint and not a probabilistic prior. Models may nevertheless be used to provide priors to Bayesian estimates. It is critical to choose the model such that the relevant parameters can be estimated efficiently, while it also captures the essential physics and is suitable for control. While system identification without any model (or rather a very generic model) may be possible, it might be advantageous to use models more specific to the problem that encode existing knowledge about the system for faster and more accurate identification. This may in certain cases even reduce very complicated systems to low-dimensional models (in terms of identification complexity).

Currently the focus seems to be too strongly on single devices performing a simple operation and not a complete mechanism. This includes models to deal with open quantum systems robustly, especially considering environmental noise. To model more complex mechanism, hierarchical models may also be required. This hierarchy might be on a multi-scale level, but also on other aspects, such as function or physics. Certainly one will have to use different models as they are needed and relations, as far as relevant, between the different models must be clear.

Certainly not everything needs to be modelled, but it remains unclear how much we actually need to know about a system to control it effectively. However, if the observables relevant to a calculation we care about cannot separate two potential implementations, we likely do not have to care either. This, however, means system identification is not just about finding parameters for a model, but includes the at least equally important issue of determining whether a particular model describes the system sufficiently well for the control task. Furthermore, if the model is determined to be insufficient, approaches to expand it are needed.

Another question considered was the issue of how far the environment can be characterised with system identification approaches, and consequently also how it could be used as part of the function of the device instead of considering it to be a defect. This would require identifiable properties of the environment that can be included in the model. Restrictions in the model, prior knowledge and incomplete knowledge about the environment might affect the environment's characterisability.

6 Quantum Control

For most applications of quantum physics in engineering, control takes a central role. Modelling, simulation, system identification, etc. seem to be largely in the service of dynamic control. The only exception there is the actual device design, which forms the static companion of dynamic control. Both are crucial to obtain effective devices and a large part of the task can be automated, meaning that in particular dynamic control algorithms, alongside the actual design of a device and how it can be controlled, are central to many quantum technologies.

Consequently at the workshop many different approaches toward controlling quantum systems have been discussed based on the following talks:

- Sophie Schirmer: Closing the Modelling-Simulation-Control-Identification Loop;
- Matthew James: Quantum Feedback Networks;
- Ian Petersen: Robust Stability of Uncertain Quantum Systems;
- Giulia Gualdi: Appoximating Open Quantum System Dynamics in a Controlled and Efficient Way: A Microscopic Approach to Decoherence;
- Tomasso Calarco: Quantum Technology Taken to its (Speed) Limit;
- Barry Sanders: Efficient Quantum Algorithms for Simulating Hamiltonian Evolution on a Quantum Computer / Optimal Phase Estimation Using Particle Swarm Optimisation;
- Thomas Schulte-Herbruggen: Symmetry Principles in Quantum Systems Theory.

These lead to many group discussions on a variety of topics as summarised below.

6.1 Adiabatic Transport and Adiabatic Computing

The discussion on adiabatic transport and computing focused on clarifying the different terms.

Adiabatic passage or transport refers to adiabatic following of the system state under a perturbation of the Hamiltonian. It is an old technique that has been used for laser control of atomic and molecular systems, e.g., in the form of STIRAP for a long time and has recently found new applications in solid-state quantum devices. Adiabatic transport can be optimised in a non-adiabatic way when the target state is known.

Adiabatic computing is related to the idea of adiabatic passage. It can be used for computation is by encoding the result of a computation in the ground state of a target Hamiltonian. As a given Hamiltonian is adiabatically transformed into the target Hamiltonian, the ground state of the starting Hamiltonian evolves into the ground state of the target Hamiltonian, which is the desired solution. Control may be important for adiabatic computing to change the path in Hamiltonian space. D-wave was mentioned as an example of a commercially available prototype quantum computer constructed from superconducting elements based on the principle of adiabatic computation (using Hamiltonian homotopy of classical Ising models), but doubts were expressed whether it is indeed an adiabatic *quantum* computer or simply an adiabatic classical computer.

6.2 Validity of Rotating Wave Approximation

The validity of the rotating wave approximation (RWA) depends on the relative time scales in the problem at hand. In particular, the Rabi frequency must be much smaller than transition frequency. The RWA may therefore break down when control fields with high amplitudes are applied, which could invalidate solutions obtained by unconstrained optimisation based on RWA Hamiltonians. It was also suggested there may be a connection between this problem and the Markovian assumption in that the neglected dynamics in the environment may interact with the dynamics neglected in the rotating wave approximation.

6.3 Necessity of Measurement for Quantum Control

Open-loop coherent control does not require measurements while the control is acting on the system. However, state preparation or gate implementation using open-loop coherent control relies on knowledge of the initial state of the system. Initialisation can be accomplished either by measurement, collapsing the state of the system to an eigenstate of the observable (in the simplest case), or by relaxation dynamics that drive the system to a definite steady state. Coherent control assisted by relaxation dynamics can also be used to drive

the system to a desired target state but coherent control alone cannot do this as entropy is conserved under unitary evolution. The latter process could be interpreted as measurement by the environment. Beyond this, it was agreed that measurement can be useful in certain quantum control problems depending on the control objective. Measurement, for example, enables stabilization of states, the possibility of environment-driven control and reservoir engineering.

6.4 Coherent Control, Feedback and Quantum Error Correction

Quantum error correction relies on encoding quantum information in a physical quantum system in such a way that errors that take the system state outside a code space can be detected and subsequently corrected. Typically error detection is done by performing so-called syndrome measurements, which identify the error that has occurred (amongst a discrete set of codeword errors) but leave the code space invariant. Subsequent correction is usually achieved by applying unitary gates. Error correction in encoded logic gates can also be accomplished using coherent or measurement-based feedback.

Quantum error correction can be thought of as a form of discrete-time feedback control in the sense that the syndrome measurements identify the error that has occurred (amongst a discrete set of possible errors) and the subsequent unitary operations applied are conditional on the outcome of the error syndrome measurement. However, it is different from the continuous real-time feedback control schemes commonly found in classical engineering applications, and some participants considered that error correction was only superficially like feedback control. There was consensus, however, that the implementation of the dynamical maps required to correct the errors can be posed as a coherent control problem and that control could lower the overhead due to error correction by lowering the error rate and improving gate fidelities.

On the question of quantum feedback network modelling, the question was raised about constructing a Lie algebra description of a quantum network connected by quantum wires and allowing swap operations based on the Lie algebra description of the subsystems. The argument was made in the 90s by Lidar, Zanardi et al that decoherence free subspaces constituted some sort of error correction, but, when viewed this way, it is a mode of error correction which requires exponential resources. It was thought that an analogy with classical error correction was not useful and that a feedback control formulation may be useful in the quantum case because of the inherent dynamics of quantum systems.

6.5 Deleterious Backaction Effects vs Control by Backaction

Unlike in the familiar classical case, measurements of a quantum system disturb the system and can change its state and dynamics. Similarly, even direct Hamiltonian feedback conditioned on a measurement results in additional terms that disturb the system. One explanation for this so-called backaction effect is that the system and controller become entangled. The strength of the measurement backaction is related to the measurement strength; generally the more information about the system we acquire the more the measurement will disturb the system. Similarly, the strength of the feedback backaction depends on the feedback control strength. It was suggested that this implies a trade-off between the quality of the control and the quality of knowledge about the system, and perhaps that entanglement between the controller and the system could be the quantifiable measure of the backaction.

Backaction effects are usually considered a nuisance especially from the point of view of control. However, recent work on reservoir engineering has shown that backaction effects can be a resource for control especially quantum state engineering and stabilization provided we have precise knowledge of the backaction. It was therefore suggested that perhaps it is our ignorance of the specific nature of this back action that is deleterious. It was also suggested that measurement-based quantum computation could be regarded as an example of control by backaction. It was noted that there remains considerable confusion regarding the terminology.

6.6 Relevance of Robustness and Stability

The meaning of the terms robustness and stability were debated. Stability is a concept that derives from dynamical systems. A steady state of a dynamical system is stable if the state remains close to the steady steady when subjected to small perturbations. A stronger concept is that of asymptotic stability or attractivity

which provides that the system returns to the steady state after a small perturbation. For quantum systems subject to Markovian dynamics, asymptotic stability is equivalent to the existence of a unique steady state and implies global attractivity, i.e., convergence to a known equilibrium state. It was thought that this could be useful for system initialisation which could then be followed by open loop control.

Robustness can be regarded as a measure of feature persistence in a system subject to perturbations. For a system subject to control such perturbations can arise due to environmental effects or systematic errors or noise in the controls. Minimising the sensitivity of the systems to such perturbations was generally thought to be important. Robustness with respect to model uncertainty, especially uncertainties in Linblad terms, was considered to be an important issue and the question was raised whether coherent or measurement-based control can compensate for uncertainties in the Linblad terms. It was thought that this might not be possible in general, but may be possible for physically relevant problems.

A related issue of stabilisation to an identity operator was raised. It was thought that this might be possible only on a certain subspace of the whole space. It was thought that this might relate to the concept of rank-k numerical range. This also led to a discussion of dynamic decoupling for a given subspace and raised issues of error avoidance versus error correction.

6.7 Quantum Device Networks

Assuming we succeed in building individual quantum elements such as qubits, the next step is to connect them and create networks of interacting quantum systems. In this context, it was thought to be important to understand the connectivity of the interaction graph, conditions for approximate locality, the velocity of information propagation and the topology of graph.

7 Outcomes and Challenges

The final day's discussion focused on outcomes and directions. On the general issue of modelling, capturing essential physics in a simple way and scalability of the models were seen as the most important issues for systems from silicon-based solid-state devices to quantum biology. In particular, capturing the influence of the environment on the system was considered to be very important and identifying the best approaches (Lindblad, QSDE, etc) for modelling different types of open systems. Among the challenges are complexity and uncertainty. Beyond basic system identification, how can we quantify our confidence in model and how can we validate models? How much uncertainty can be tolerated before control becomes ineffective? The latter issue is closely related to robustness and stability of controlled systems, which were thought to be important issues that require further study. It was also noted that some powerful tools (Bayesian learning, finite element analysis, etc.) have not yet been fully exploited for quantum modelling. Another suggestion made was to focus on Heisenberg picture as this formalism is more natural for quantum stochastic differential equations and understanding the dynamics of quantum observables. Finally, it was thought to be important to progress from study of single devices to quantum networks and to develop a better, and especially more integrated, mathematical framework for quantum control.

The workshop also improved the mutual understanding of the various problems and issues involved and enabled participants to network, across different fields. This was instrumental in promoting collaborations and the formation of the EU-funded network QUAINT, and a Welsh network for Quantum Technologies (QYMRU). Some of the participants met again a the the Kavli Institute for Theoretical Physics in Santa Barbara as part of the special program on Control of Complex Quantum Systems during the first quarter of 2013. Other follow-up meetings include a Hereaus Seminar (2013) and a workshop at the Newton Institute in 2014. There are also efforts on the way to create a conference series on quantum technologies and engineering linked with a journal as a regular platform to discuss and disseminate results.

Acknowledgements

We thank the participants of the workshop for their active engagement, interesting talks and discussions, and notes from the discussions which formed the basis for this report, and BIRS for the financial support and excellent organization.

Appendix: Talk Abstracts

Modelling Molecules in Intense Laser Pulses and Attosecond Simulations

Bandrauk, André D
Université de Sherbrooke

The description and simulation of the nonlinear nonperturbative interaction of molecules with intense laser pulses requires the numerical solution of multidimensional partial differential equations, pde's such as the time-dependent Schroedinger equation, TDSE for fs-asec electron-nuclear movement beyond traditional Born-Oppenheimer approximations and for the zps time scale, TimeDependent Dirac Equations, TDDE's for relativistic effects such as the increase of spin-orbit coupling with increasing nuclear charge and pulse intensity. The complete description of the nonlinear nonperturbative response of intense molecule-laser interactions requires finally the coupling of Maxwell's (laser, photon) equations to include collective effects via propagation in a medium. The main goal of the FAZSST large scale computation project is to use advanced numerical algorithms on large memory machines to advance the development of the new Attosecond Science via numerical solutions of multidimensional TDSE and TDDE's coupled to appropriate Maxwell equations.

Quantum System Identification with Limited Resources

Burgarth, Daniel
Imperial College

The aim of quantum system identification is to estimate the ingredients inside a black box, in which some quantum-mechanical unitary process takes place, by just looking at its input-output behavior. Here we establish a basic and general framework for quantum system identification, that allows us to classify how much knowledge about the quantum system is attainable, in principle, from a given experimental setup. Unlike usual quantum metrology, our theory applies to cases where the set of observables are not topographically complete, and where knowledge about the system can only be retrieved indirectly. When the topology of the system is known, the framework enables us to establish a general criterion for the estimability of the coupling constants in its Hamiltonian.

Diamond Based Single Molecule Magnetic Resonance Spectroscopy

Cai, Jianming
University of Ulm

We demonstrate that a single nitrogen-vacancy (NV) center in diamond can be used to construct a nano-scale single molecule spectrometer. The proposed device may find applications in single molecule spectroscopy in chemistry and biology, such as in determining protein structure or monitoring macromolecular motions and can thus provide a tool to help unravelling the microscopic mechanisms underlying bio-molecular function.

Quantum Technology Taken to its (Speed) Limit

Calarco, Tomasso
University of Ulm

Quantum effects form the basis of most present-day information technologies. However, the full power of quantum coherence has not yet been tapped for everyday technological applications. The exquisite level of control of current atomic physics experiments may enable this, for instance in the field of quantum communication and quantum computing - but scalable quantum information processing requires extremely precise operations. Quantum optimal control theory allows to design the evolution of realistic systems in order to attain the best possible performance that is allowed by the laws of quantum mechanics. I will present a range of its applications to a variety of quantum technologies, and discuss its use in probing the ultimate limits to the speed of the corresponding quantum processes.

NanoHUB and NEMO5: a Science Cyberinfrastructure and a Nanoelectronic Modeling Tool

Fonseca, Jim
Purdue University

The NanoHUB is a cyberinfrastructure for the development, deployment, and use of scientific software. Students, teachers, developers, and researchers are able to collaborate in an online environment. A web browser provides the user with access to available tools that are run on high performance parallel computers. One tool that is under construction for nanoelectronic modeling is NEMO5. The core capabilities of NEMO5

lie in the atomic-resolution calculation of nanostructure properties: a multimillion-atom strain calculation, bulk electron and phonon band structures, a 1-D Schrödinger-Poisson simulation, a multiphysics simulation of a resonant tunneling diode, and quantum transport through a nanowire transistor.

Semiclassical Poisson and Poisson-Schrodinger Solvers in QCAD

Gao, Suzey
Sandia National Laboratories

We discuss the technical details of the semiclassical Poisson and the self-consistent quantum Poisson-Schrödinger solvers in the Quantum Computer Aided Design (QCAD) LDRD project at Sandia. We have developed as a first step a nonlinear Poisson solver, including Boltzmann or Fermi-Dirac statistics and incomplete ionization of dopants, which provides a good first-order description of the electrostatics in quantum devices. We have also developed a self-consistent Poisson-Schrodinger (P-S) solver to capture the unique quantum effects. This description includes the exchange-correlation potential within the local density approximation. Efficient convergence of the self-consistent solution is achieved using a predictor-corrector iteration scheme. Applications of the QCAD framework to 1-, 2-, and 3-D quantum systems demonstrate high accuracy and robustness of the solvers.

Optimal Control of Uncoupled and Coupled Spins

Glaser, Steffen
Technical University Munich

Based on principles of optimal control theory, the physical limits of quantum control can be explored and time-optimal and relaxation-optimized pulse sequences can be designed to control the dynamics of spin systems. Furthermore, robust pulse sequences, compensating experimental imperfections and taking into account experimental limitations can be optimized. Recent advances include time-optimal pulses for saturation and for maximizing contrast in magnetic resonance imaging (MRI), robust pulses that effect point-to-point transfers and/or desired unitary transformations that tolerate a large range of rf scaling, e.g. a factor of six in toroid NMR probes. As demonstrated experimentally, these pulses make it possible to perform sophisticated 2D NMR experiments on this hardware platform. The design of cooperative pulses opens new avenues for improved performance of multi-pulse experiments. Finally, the application of optimal control methods to the problem of spin decoupling yields not only significantly improved performance but also unprecedented flexibility in the design of tailored decoupling sequences.

Approximating Open Quantum System Dynamics in a Controlled and Efficient Way: A Microscopic Approach to Decoherence

Gualdi, Giulia
University of Kassel

We demonstrate that the dynamics of an open quantum system can be calculated efficiently and with predefined error, provided that a basis exists in which the system-environment interactions are local and hence obey the Lieb-Robinson bound. We show that this assumption can generally be made. Defining a dynamical renormalization group transformation, an effective Hamiltonian for the full system plus environment is obtained that comprises only those environmental degrees of freedom that are within the effective light cone of the system. The reduced system dynamics can therefore be simulated with a computational effort that scales at most polynomially in the interaction time and the size of the effective light cone. Our results hold for generic environments consisting of either discrete or continuous degrees of freedom.

Quantum technology: qubits in quantum computing to sensing in biology

Hollenberg, Lloyd
Centre for quantum Computation and Communication Technology, University of Melbourne, Australia

The fundamental building blocks of a quantum computer are qubits - individually controlled two-level quantum systems. As the march towards quantum computing continues apace, the quantum control of qubit systems has been achieved in a range of physical platforms - electronic, photonic and atomic - together with a deep understanding of their environmental interactions. In this talk we will discuss the use of a qubit system as a nanoscale probe, where the qubit is deliberately exposed to the worst possible, but most interesting, environment - room temperature biology. The nitrogen-vacancy (NV) defect centre in diamond represents an

ideal single spin qubit for use in biology as a nanoscale magnetometer probe. It possesses a broad absorption band from 512-560 nm, sustained fluorescence from 630-750 nm, is chemically inert and bio-compatible and most importantly has relatively long quantum coherence at room temperature. These defect centres have been used as highly stable fluorescence beacons to track the position and diffusion of diamond nanocrystals in vitro and in vivo. Recent experimental demonstrations of nanomagnetometry using these single spin systems create opportunities for new applications in biology. We explore the viability of diamond-based nanomagnetometry bio-applications by performing the full suite of quantum control and measurement protocols on NV-nanodiamonds in a living human HeLa cell, and demonstrate the enhancements that the quantum properties of the NV qubit enable for orientation tracking in the intra-cellular context.

Quantum Control of Light-Harvesting Systems

Hoyer, Stephan
University of California, Berkeley

I will review the evidence for the relevance of quantum coherence to photosynthetic energy transfer, and discuss our theoretical progress towards controlling these dynamics using shaped ultra-fast laser pulses. I will also present a scheme for experimental validation in a pump-probe spectroscopy setup.

Quantum Feedback Networks

James, Matthew
Australian National University

Background: Systems and control theory is concerned with ensuring that systems behave in a desired way. At the most basic level, the system should operate in a stable manner, and beyond this, systems and control theory endeavours to assess, and where possible, optimise, performance. For example, in the 18th century James Watt designed a governor system to ensure that his steam engines maintained a constant speed, (and as is well known, the steam engine powered the industrial revolution). The steam engine governor is a classic example of a feedback control system. A feedback system is a network: an interconnection of the system being controlled (e.g. steam engine or atom) and the system facilitating the control (e.g. governor or another atom). Networks are ubiquitous in science and technology, e.g. electronic circuits, the internet, etc, etc.

Over many years, many methods have been developed for modeling and design. Models and design techniques have been developed for particular purposes, at different levels of abstraction and detail. For example, detailed transport equations could be used to describe the flow of electrons and holes in a transistor within a standard operational amplifier chip, or a simple model could be used when the opamp is included in a negative feedback circuit. Widely used abstractions include Gaussian and white noise models (e.g. for the movement of particles in a fluid, or to describe sensor noise) and Boolean algebra (used to describe classical logic). Methodologies that have been developed at these levels of abstraction include probability and stochastic processes, information theory, and computational complexity.

At the present time, quantum technology is developing rapidly, spurred on by the significant potential of key application areas, notably, quantum computation, information, and metrology. The qbit is now omnipresent, and fundamental to the conceptual and experimental developments in quantum technology in recent decades. The qbit, of course, is a quantum generalization of the classical bit from classical logic, and indeed quantum generalizations of information theory and computation have been developed. Gaussian states are very common, particularly in quantum optics, and a theory of quantum stochastic processes has been available now for several decades. However, this later theory has yet to be fully exploited in quantum technology.

This talk will discuss ideas concerning quantum feedback networks (QFN). These ideas go back to Yurke-Denker in the 1980's, Wiseman-Milburn, Gardiner and Carmichael in the 1990's, and Yanagisawa and others in the 2000's. QFNs consist of components modeled as open quantum systems, interconnected by free fields and/or by direct physical couplings (it is worth thinking about how electronic amplifiers are cascaded together, and how a steam engine is connected to a governor). An important feature of the developing theory of QFNs are the simple symbolic rules for describing interconnections, based on underlying quantum stochastic models. The talk will discuss this theory, as well as some recent applications in quantum optics and quantum information.

Differential Topology of Adiabatic Gap

Jonckheere, Edmond
USC

In this talk, we provide a new interpretation of the adiabatic theorem in quantum computation with special attention to the gap problem and the crossing avoidance of the various energy levels. It is indeed argued that the mere plotting of the various energy levels versus the time spent in the adiabatic process hides some deeper issues as to how the energy levels are intertwined. Central in this new interpretation is the numerical range of a matrix constructed with the initial and terminal Hamiltonians. The fundamental fact is that the various energy levels encountered along the time through the adiabatic process are the various critical value curves of the numerical range viewed at an angle that parameterizes the time spent in the process. The boundary of the numerical range represents the ground state, while that curve closest to the boundary is the first excitation level. Generically, the boundary curve is smooth, but all other energy level curves are highly singular with cusps. With this interpretation, the known scaling of the gap is easily recovered and new results are derived from topological consideration on the numerical range. But probably most importantly, this approach explains how the various energy levels are intertwined by a two-stage unraveling process: (i) by going from the classical energy level plots to the highly singular critical value curves in the numerical range, and (ii) by lifting the critical value curves to (smooth) Legendrian knots in a contact space. The smooth curves in the contact space are possibly knotted, possibly linked, which provides the ultimate explanation of the non-crossing phenomena observed "down" at the most elementary level of the classical energy level plots.

Algorithms and Software for Large-Scale Quantum Spin Dynamics Simulations

Hogben, HJ[1], Edwards, LJ[2], Krzystyniak, M[2], Charnock, GTP[2], Hore1, PJ[1], Kuprov, Ilya[2]
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[2] Oxford e-Research Centre, University of Oxford, 7 Keble Road, Oxford, UK.

We introduce a software library incorporating our recent research into efficient time-domain simulation algorithms for large spin systems. Liouville space simulations (including symmetry, relaxation and chemical kinetics) of most liquid state NMR experiments on 40+ spin systems can now be performed without effort on a desktop workstation. Much progress has also been made with improving the efficiency of ESR, solid state NMR and Spin Chemistry simulations. The functionality available at the time of writing includes:

- Low-dimensional matrix representations for spin operators in large spin systems that enable the simulation of magnetic resonance experiments on systems previously considered too big for any practical simulations.
- Generalized symmetry module (any number of groups of equivalent spins of any quantum number).
- Krylov subspace based time propagation routines that avoid matrix exponentiation.
- Generalized rotation module and a Lebedev powder integrator.
- Generalized relaxation theory module, supporting all types of magnetic resonance spectroscopy (NMR, ESR, DNP, Spin Chemistry, etc.). Anisotropic rotational diffusion tensors are supported in full generality.
- Optimal Control waveform design module using BFGS-GRAPE algorithm with exact gradients. Optimization of broadband pulses, selective pulses and universal rotations is implemented in both Cartesian and phase-amplitude coordinates.
- Functions for multi-grid parallel soft pulses and (algebraic) decoupling.
- Functions for the simulation of magnetochemical experiments.
- Functions for the simulation of common NMR experiments (COSY, DQF-COSY, NOESY, HSQC, HMQC, HETCOR, etc.), basic ESR experiments (ESEEM, ENDOR, etc.) as well as building blocks for the writing of user-specified experiment simulations.

Spinach is an open-source Matlab library available at http://spindynamics.org.

Bayesian Learning and Optimisation

Langbein, Frank C, Quinn, Jonathan A
Cardiff University

Machine learning aims to construct a model for an unknown or only partially known environment. This is directly related to identifying quantum systems. We give an overview of various machine learning techniques, the underlying models and efficient algorithmic techniques, especially focused on Bayesian learning techniques. In the second part we overview core search and optimisation methods, useful for model fitting, parameter identification and control.

Development of Few-Electron Si Quantum Dots for Use as Qubits

Muller, Richard P, Bielejec, ES, Bishop, N, Ezra Bussman, E, Carroll, MS, Gao, S, Landahl, A, Lilly, MP, Lu, TM, Nielsen, E, Pluym, T, Rahman, R, Shirkhorshidian, A, Stalford, HL, Tracy, LA, Witzel, WM, Young, RW

Sandia National Laboratories, Albuquerque, NM

This talk will describe a modeler's perspective on existing experimental efforts to create a Si qubit, the challenges to overcome, and the opportunities for modeling to have an impact on the experimental direction. The talk will review options we?ve considered for the materials stack and the gate layout, and will discuss how issues like spin- and charge disorder, valley splitting, and gate design impact the development of few-electron quantum dots. I will conclude with observations on how computer simulation can help accelerate this development. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories.

Characterizing Defects in Superconducting Phase Qubits

Müller, Clemens

Université de Sherbrooke

Spectroscopy of superconducting phase qubits often shows characteristic anti-crossings, indicating the presence of additional coherent and strongly coupled quantum systems. The origin of these two-level defects is not yet fully understood, although a variety of models have been proposed. I will show a summary of our joint theory-experiment efforts to determine the parameters of possible microscopic models of the defects in order to determine their physical nature. I will also talk about the possibility of applying Hamiltonian tomography on this system and present the specific challenges we face there.

The QCAD Framework for Quantum Device Simulation

Nielsen, Erik

Sandia National Laboratories

The Quantum Computer Aided Design (QCAD) LDRD project at Sandia National Labs is developing an integrated tool designed for the simulation of few-electron quantum devices. We discuss the software framework and capabilities of this tool, and compare these with existing tools. We emphasize the close relationship with our experimental effort, and discuss how QCAD has been utilized for rapid design guidance. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories.

Maximum Likelihood Hamiltonian and Decoherence Estimation

Oi, Daniel

Strathclyde University

Advances in quantum systems engineering and control are leading to the ability to fabricate and manipulate large scale devices operating in the coherent regime. However, precision operation requires knowledge of the behaviour of the system, both in response to control fields and to environmental noise and decoherence. The traditional approach to system behaviour, process tomography, presupposes the ability to prepare complete sets of initial states and to be able to measure in many different bases, abilities which may not be initially present without control. A method is required to bootstrap the characterisation process utilising a more restricted set of preparation and measurement primitives. Even for small systems, signal complexity can overwhelm conventional analysis. We have applied maximum likelihood methods to extract model parameters and invert system dynamics. Scaling up and increasing efficiency remain as challenges, these may be possible using adaptive experiment design and compressive sensing methods.

Robust Stability of Uncertain Quantum Systems

Petersen, Ian

UNSW

This talk considers the problem of robust stability for a class of uncertain quantum systems subject to unknown perturbations in the system Hamiltonian. Some general stability results are given for different classes of perturbations to the system Hamiltonian. Then, the special case of a nominal linear quantum system is considered with either quadratic or non-quadratic perturbations to the system Hamiltonian. In this case, robust stability conditions are given in terms of strict bounded real conditions.

Quantum Coherence and Biological Systems

Plenio, Martin
University of Ulm

The interplay between coherence and the vibrational environment is of key interest for the quantum dynamics of bio-molecular systems. In this talk I will present some fundamental ideas in this regard, then I will discuss briefly methods to simulate the dynamics in the relevant regime of intermediate strength coupling between system and environment. Finally, if time allows I may discuss some aspects concerning measurement techniques in these systems.

High Precision Quantum Device Simulation with Atomistic Tight-Binding Technique Coupled with Semi-Classical Poisson Solver and Many-Electron Configuration Interaction Method

Rahman, Rajib
Sandia National Laboratories

Due to the rapidly shrinking dimensions of semiconductor devices, modeling techniques need to incorporate the underlying atomistic nature of the materials the devices are built from. Widely used continuum models very often fail to capture the subtle quantum properties that govern the operations of modern devices. The semi-empirical tight-binding method offers a promising way to simulate these devices as it treats interactions on an atomic scale and is also scalable to realistic device sizes of millions of atoms. In general, the tight-binding approach captures various features of materials and devices such as hetero-structure properties, inhomogeneous strain distributions, lattice miscuts, surface roughness, full bandstructure, interfaces, electro-magnetic fields - all under a unified framework.

However, tight-binding being essentially a single electron theory misses out important many electron interactions that some quantum devices rely on. Here, we describe two methods to augment the tight-binding method with many electron interactions. The first is based on coupling the tight-binding Hamiltonian with a semi-classical Poisson solution of the device with realistic gate geometries and voltages to describe mean field interactions in terms of the electron density. The second is based on coupling tight-binding to an exact many-electron configuration interaction method, which captures Coulomb, exchange, and correlation effects with accurately. The complete suite of these tools constitutes a powerful package for high precision device simulation.

As applications of these techniques, we show simulations of two important quantum information processing systems in silicon. Simulations of a single donor spin qubit in silicon in a field effect transistor show the subtle electric field tuning of the donor spin and explain experimental measurements. Computations of the many electron levels of a double quantum dot in silicon along with nearby defects reveal complex interplay of valley physics and many electron effects, which are manifested in the nature of the voltage tuned exchange curve of the double quantum dot.

Mathematical Techniques for Cell Cycle Analysis

Rees, Paul
Swansea University

The aim of systems biology is to understand the complex interactions which occur between the components of a biological system. By identifying the relevant components within the complex system a host mathematical tools can be used to attempt to identify the nature of the mechanisms between them. Here we take inspiration from a traditional systems engineering approach which relates the output of a system to the input by a transfer function. This requires a significant simplification of the complex biological system however we will demonstrate that appropriately designed experiments couple with simple mathematic models of the transfer function can accurately elucidate biological function. In casting the problem in this manner we are able to use systems engineering theory to describe and analyze the biological system. We outline this technique by giving examples for the assessment of drug treatments on cancer cell populations and the study of uptake of nanoparticles and the toxic effect on cells.

Efficient Quantum Algorithms for Simulating Hamiltonian Evolution on a Quantum Computer / Optimal Phase Estimation Using Particle Swarm Optimisation

Sanders, Barry

I present efficient quantum algorithms for simulating Hamiltonian evolution on a quantum computer both for an oracle setting for the Hamiltonian and also without the oracle model for the specific case that Hamiltonians are sums of non-commuting tensor products of Pauli operators. For the time-dependent Hamiltonian case, we establish sufficient smoothness criteria to deliver bounded-error quantum simulations of state evolution efficiently. Technically we employ Lie-Trotter-Suzuki approximations for ordered-operator exponentials with strict error bounds for these expansions. For the specific case of Hamiltonians that are sums of non-commuting tensor products of Pauli operators, our efficient classical algorithm delivers circuit designs for efficient quantum simulation, and I show applications to Kitaev's toric-code and honeycomb Hamiltonian systems.

Closing the Modelling-Simulation-Control-Identification Loop

Schirmer, Sophie
Swansea University

When we talk about quantum devices there is an implied assumption of functionality, i.e., the device is supposed to perform certain tasks as required by an application. Achieving such functionality requires careful device design as well as control to manipulate the behaviour of the system. Effective device and control design is a non-trivial task that requires understanding the intrinsic dynamics of the system as well as its interaction with the control apparatus, sensors and actuators, as well as the effect of the environment. Generally, this means that we require a model not only of an isolated system but its interaction with a controller and environment. In simple cases such models can be constructed directly from first principles, e.g., for a simple quantum system we may be able to write down a Hamiltonian for the intrinsic dynamics of the system and maybe the effect of certain types of coherent control fields. For more complex systems from nano-electronics to biomolecules, however, this approach usually does not suffice, and it is crucial to incorporate data from observations of the actual behaviour of the system to construct effective models. In this talk we will discuss some general requirements for control system models as well as some techniques for constructing and adaptively refining such models.

Symmetry Principles in Quantum Systems Theory

Schulte-Herbruggen, Thomas
Technical University Munich

Elucidating quantum optimal control in terms of symmetry principles has triggered us in a number of recent advances to be elucidated in survey:

(i) it leads to a new and handy controllability criterion,
(ii) it guides the design of universal quantum hardware,
(iii) it governs which quantum system can simulate another one given,
(iv) with little modification it specifies the limit between time-optimal control and relaxation-optimised control of open systems, and
(v) it provides a pattern that may help to understand new coherent pathways in noise-assisted energy transfer in light-harvesting biomolecules.

How principles turn into practice is illustrated in a plethora of examples showing practical applications in solid-state devices and circuit-qed. The algorithmic tools are presented in a unified programming framework.