Focus on quantum simulation

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\textbf{Abstract.} The endeavour to control increasingly larger systems of particles at the quantum level is a natural goal, and will be a driving force for the physical sciences in the coming decades. The control of a many-body system at the highest level possible can indeed be regarded as the ultimate form of engineering. Within this general research avenue, building quantum simulators and performing experimental quantum simulations will play a key role. A quantum simulator is a promising candidate to become the first application of quantum information science reaching beyond classical limitations \cite{1}, since the requirements on the number of quantum particles and fidelities of operations are predicted to be substantially relaxed compared to that envisioned for a universal quantum computer. This issue forms an extensive open-access resource spanning the various areas of experimental quantum simulation, from its relation to quantum information processing to its potential use for different applications.
1. Introduction

What is a quantum simulator? One possible definition is an experimental system that reproduces the physics of a precisely defined Hamiltonian. One class of applications deals with problems that are efficiently solvable on classical computers. However, the quantum simulator might provide an analogue that allows us to experimentally address intriguing questions that are not directly tractable in the laboratory, such as effects in the vicinity of black holes. A second class of simulators deals with objectives that are not accessible via classical computation, for example the complex quantum ground states and dynamics in solid state systems, and may be employed to better understand and enable the design of exotic materials.

What is necessary to build a quantum simulator? A system of quantum particles is required, where (i) the initial state and its dynamics can be precisely controlled, (ii) as many relevant parameters as possible manipulated and (iii) the readout of the important characteristics of the final state performed in an efficient way.

What will a quantum simulator do? This may be the trickiest part: the ultimate goal is to provide an answer to an open and relevant question. The challenges are both conceptual and technical. Can one identify well-defined and relevant problems that cannot be answered by classical computational techniques? And, can one engineer a system which displays the physics of the corresponding Hamiltonian at a sufficiently high level of accuracy? In this context, even though considering that a quantum simulator might be robust against many disturbances, how can we assure that the result of a quantum simulation is trustworthy? One approach is to realize several quantum simulations based on different physical systems to simulate the identical models (Hamiltonians) to allow cross-checking the validity of the results [2]. Another is to persistently `calibrate' the simulator with problems that are tractable, even as the system gets bigger.

The research field of quantum simulation is in its infancy and many divergent approaches are being proposed, studied and tested. Different systems offer different advantages to address the specific physics of interest. Some examples are quantum dots, superconducting circuits and neutral atoms within optical lattices [3–6]. Another promising candidate is based on trapped atomic ions [7, 8], receiving extensive coverage within this focus issue. (We note that the research presented in this issue neither reflects the proportion of groups working in the field nor the importance of the different contributions.)

This issue covers a range of research that emphasizes that these various approaches compliment one another, perhaps shedding light on the question of what relevant problems are best addressed by quantum simulations in a sufficiently reliable and efficient way [1, 9].
The goal of this focus issue is to provide an overview of the state-of-the-art and new ideas from different disciplines of physics. This issue combines 21 contributions from the leading groups in the field, with these including the theoretical identification of interesting and challenging problems in physics that may be amenable to quantum simulation. Furthermore, the issue also covers early experiments that hold great promise for solving vexing problems in quantum physics.

The contributions can be broadly aligned with three research fields within the topic of quantum simulation: (i) complex many-body physics, such as quantum spin systems in condensed matter physics, (ii) transport phenomena and (iii) relativistic physics. In the following, we will shortly introduce the scientific objectives pursued within this issue.

1.1. Complex many-body physics—quantum spin models

The strategy of quantum simulations here is to experimentally initialize the quantum spin system in a state that can still be accurately prepared and to subsequently evolve the system adiabatically by changing its parameters to reach a new state, for example, via a quantum phase transition—a state that is fundamentally or, at least, currently impossible to create otherwise. The aim here is not to simulate the effects including all disturbances and peculiarities, because the simulator would than become as complex as the system itself. Instead, it is to investigate whether the implemented simplifying model still yields the (puzzling) effects observable in nature and therefore helps to explain and further explore the related physics of interest. Thereby, we might gain a concise deeper understanding of the essential ingredients in an idealized model system, isolated from disturbances [7].

In [13], the authors exploit laser fields for implementing an effective spin–spin (typically 1/2) interaction between trapped ions. However, they substantially extend the common scheme by an appropriate design of the laser fields to provide arbitrary, multidimensional spin–spin interaction graphs even for the case of a linear spatial array of ions within a common trapping potential. Later in the issue [19], several of the same authors describe their recent developments and status in experimentally simulating quantum spin systems using the paradigmatic transverse Ising model as a showcase.

- The approach described in [17] is based on the same system of a linear chain of ions, however, mediating the interactions by oscillating magnetic fields. A considerable extension in comparison to existing schemes is proposed by embedding different species of atomic ions and therefore enlarging the basis of spin states beyond the two-level system of spin 1/2. In [29], a different additional tool is introduced by considering Rydberg states of trapped ions and exploiting their huge atomic dipole moments for increasing interactions strength and therefore shortening operational durations.

- The authors of [18] study how to explore quantum spin-Hamiltonians realized in a two-dimensional (2D) array of individually trapped ions, hovering above a proposed surface-electrode ion trap. After deriving the optimized form of the required surface-electrodes, they propose the implementation of the hexagonal Kitaev model with the perspective to provide the required interactions via ac-currents conducted by a realistic wire structure incorporated into their design for a micro-fabricated surface trap, suitable to implement also a huge variety of other interactions and spin-models.

- In [26], the authors propose a quantum simulator within a triangular and a square lattice. Exploiting Heisenberg interactions and the spatial anisotropy of the system/lattice they
reveal how to study the phases of a \( s = 1/2 \) quantum anti-ferromagnet with up to next–next-nearest-neighbour couplings taking full advantage of the long-range interaction featured by the Coulomb potential.

One of the most demanding challenges for the bottom up approach in the system of trapped ions is to find the right strategy as well as technology to scale the system in size and dimension.

- In [13], as well as in other contributions, a scheme relying on currently available technology featuring linear strings of ions is described that is already scalable to levels where the classical methods of simulation are intractable. The methods presented in [17, 29] are also proposed to ease scalability by incorporating additional ionic species or Rydberg ions in already available systems.

- Siverns et al [14] and Moehring et al [25] describe how further optimization of surface ion trap technology will propel this field of research, where the implementations of the proposals of [18, 26] already rely on this development. In [25], the authors from Sandia National Laboratories demonstrate their design, fabrication and experimental implementation of micro-fabricated radio-frequency (rf) surface electrode traps, as depicted in figure 1. Their scheme is suitable to advance the multiplex architecture of interconnected linear traps, featuring a scheme of many memory and processor traps, housing sub-ensembles of ions and spanning the architecture for a universal quantum computer. For this purpose, their contributed experimental show case already incorporates a junction of three linear traps (see left part of figure 1). Their related experiment already demonstrates ion shuttling, position swapping and splitting of ion chains with near unit fidelity. However, benefiting from the identical fabrication techniques, arrays of individually trapped ions will allow to span a (direct) 2D quantum simulation (see right part of figure 1). In [14], the authors present an optimization process to potentially reduce the technological efforts based on a single rf-electrode, however, providing an optimal lattice geometry for maximizing the ratio of coupling strength between the ions and the motional heating rates causing decoherence.

### 1.2. Transport phenomena

Transport processes are widespread and fundamental in many fields of physics, chemistry and biology (see e.g. [10], and references therein). Quantum simulations allow to address classical and quantum aspects of transport and diffusion to elucidate the related processes in nature.

In [28], the quantum analogue to heat propagation within a classical (discretized) bar with its two ends kept at different temperatures is investigated numerically. A linear chain of ions is locally coupled to different thermal baths leading to an equilibration within this dissipative quantum many-body system leading to a temperature distribution along the chain that strongly depends on the coupling strength to the baths, the location of the driven ions and the dissipation rates of the rest of the ions in the chain. Several scenarios for chains of less than ten ions are discussed and experimental implementations proposed to lead to counter intuitive results, such as, the absence of a temperature gradient between the two ions coupled to the different baths.

The authors of [31] propose to superimpose the regular potential of an optical lattice on a chain of ions trapped in the harmonic potential of a conventional rf trap. Exploiting this approach, they describe how they aim to investigate the emergence of phenomena of dry friction and, most important, to study energy transport along the chain.
Figure 1. Micro-fabricated ion trap arrays imaged by a scanning electron microscope (bird’s eye views). 2D trapping structures could allow for a great variety of configurations and interactions in ion-trap quantum computing and quantum simulations. (left) Surface-electrode ion trap junction for transport and reordering of multiple ions, a key feature of scalable ion-based quantum information processing units. In surface-electrode ion traps, the ions are typically held by rf and dc electric fields in potential wells 30–100 µm above the electrodes (taken from Moehring et al [25]). (right) Cut through an otherwise fully functional triangular array of individual surface-electrode ion traps, providing additional insight into construction details, for example buried electrode interconnects and electrode overhang for the shielding of the ions from insulating surfaces and a loading hole for loading from the back-side mitigating electrode contamination. This architecture could be scalable to provide quantum simulations of coupled spins in arbitrary 2D lattices (see the article by Schmied, Wesenberg and Leibfried [18] in this issue. Image courtesy of M G Blain, Sandia National Laboratories).

Quantum simulations of complex open system dynamics with a precisely engineered environment are proposed by the authors in [12]. They aim at experimentally simulating energy transfer pathways as well as non-Markovian noise-correlation effects in analogy to a controllable single-molecule photosynthesis complex. The system chosen to further test the applicability of this proposal is based on superconducting circuits.

In [15], the prospects of quantum walks are examined, relevant for quantum computation but also to examine quantum diffusion. The authors discuss in detail the limitations related to the currently applied protocols based on trapped ions as quantum walkers, confined in a rf-trap and performing conditional step operations realized by optical dipole forces being state dependent. To reach towards scalability in the amount of applicable quantum steps, the authors propose a new scheme using short laser pulses, derived from a protocol from the field of quantum computation. It is proposed to allow for 100 s of steps and should be extendable to higher dimensional quantum walks.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
The numerical study of the dynamics presented in [20] covers the transfer properties observed in experiments on cold atoms in a 2D, optical lattice, realized by an anisotropic speckle potential. The authors show that the density profile is strongly peaked and not Gaussian. They further propose to exploit their approach to help in the interpretation of future experiments searching for a deviation from classical diffusion and traces of Anderson localization.

1.3. Relativistic physics

Quantum simulations addressing quantum relativistic systems are promising candidates to advance the field out of two perspectives (see e.g. [11], and references therein). Firstly, even though computationally still tractable, the physics lacks of observation. Secondly, generalizing the description of the problem also challenges classical computational resources.

In [27], quantum simulations are proposed for addressing the long lasting problem of causality for Fermi’s two-atom system. In contrast to Einstein causality and final signal velocity, the excitation probability of a ground-state atom in close vicinity of an excited one is predicted to be non-zero immediately after its decay. Although the question could, in principle, get tested experimentally, the smallness of the expected violations of causality in quantum electrodynamics have prevented the observation of this effect as well as related further studies of its modifications. However, the authors show that the problem can be reformulated in discrete systems and propose to experimentally simulate it within the framework of trapped atoms in optical lattices and trapped ions.

The authors of [16] describe their proposal for a quantum simulation addressing relativistic fermionic field theories and topological insulators, to get implemented within atoms trapped in spin-independent optical lattices. The combination of bi-chromatic lattices with Raman transitions will allow engineering a spin-dependent tunnelling to be interpreted as an assisted-hopping process of atoms between lattice sites required to experimentally simulate relativistic fermionic theories ranging in between non-interacting up to topological insulators.

To step beyond the state-of-the art of quantum simulation of relativistic quantum mechanics based on trapped ions and to implement and analyse novel features of dynamics related to the Klein paradoxon, the authors in [23] describe puzzling effects of several Dirac particles coupled by a common confining potential. This model can be interpreted as a version of the Massachusetts Institute of Technology bag model of nuclear physics, permitting to investigate effects in quantum chromo-dynamics, such as, asymptotic freedom, in a table top experiment controlled by laser fields.

This issue also reports work on a variety of other topics, including the proposal of [21], where the authors study the minimal circuit quantum electrodynamics system in which breaking of time-reversal symmetry is observable, a three site James–Cummings ring of superconducting qubits coupled to microwaves, simulating a synthetic gauge field which induces nontrivial phase-factors in the photon hopping terms. This quantum simulation will allow studying photon-based many-body physics based on effective interactions between photons. In their proposal, the authors report the generalization of vacuum Rabi splittings and identify fingerprints of interactions beyond the regime of linear response. Exploiting well-established fabrication techniques for coupled, on-chip microwave resonators and superconducting qubits renders this bottom-up approach scalable in size and dimension.

In [24], the authors present the implementation of an experimental tool to increase the information exploitable from local fluctuations and their correlations in weakly and
strongly interacting 2D Bose gases. Investigating and removing systematics due to imaging 
imperfections allows better identifying a phase transition of the many-body system. The authors of [30] show how to map a bosonic lattice model onto a self-consistent solution of a bosonic impurity model with coupling to a reservoir of normal and condensed bosons. As a prove of principle, they present their solution of phase diagrams for the bosonic Hubbard model describing atoms in 2D and three-dimensional lattices via a continuous-time Monte Carlo algorithm.

This issue also includes contributions, envisioning already how to perform quantum simulations on a potential universal quantum computer.

In faster quantum chemistry on fault tolerant quantum computers by Jones et al [32], the authors investigate how quantum simulations addressing quantum chemistry could be implemented within a device that already incorporates quantum error correction and therefore provides fault-tolerance, that is, already requires the main ingredients for universal quantum computation. They examine how to improve the efficiency in general and analyse, as a specific example, the ground-state energy calculation for lithium hydride.

On a comparably powerful device, the authors of [22] describe their method for simulating the time evolution of the Bardeen–Cooper–Schrieffer Hamiltonian on a so called qubus quantum computer, such that a continuous variable ancilla generates the interactions between qubits. They show that deriving the energy gap could be improved significantly.

2. In summary

This focus issue of New Journal of Physics presents complementary approaches identifying intriguing and challenging problems in physics as well as early experiments that hold great promise for solving problems in quantum physics. Currently the field is driven by rapid development and active research. Therefore, the larger picture is in no way complete and we envision the most exciting developments and, most importantly, the related results providing deeper insight into complex quantum behaviour, in the (near) future.

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