Quantum Simulators

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Quantum simulators are controllable quantum systems that can be used to simulate other quantum systems. Being able to tackle problems that are intractable on classical computers, quantum simulators would provide a means of exploring new physical phenomena. We present an overview of how quantum simulators may become a reality in the near future as the required technologies are now within reach. Quantum simulators, relying on the coherent control of neutral atoms, ions, photons, or electrons, would allow studying problems in various fields including condensed-matter physics, high-energy physics, cosmology, atomic physics, and quantum chemistry.

More than a quarter of a century after Richard Feynman envisioned a quantum mechanical device for the efficient simulation of quantum systems (*1*), quantum simulators are now attracting increasing interest in many areas of physics (*2*). The level of coherent control of quantum systems necessary for the physical realization of quantum simulation is now within reach (*3*).

The motivation for building a quantum simulator is twofold: It would be very useful for a vast array of problems in physics, chemistry, and biology, and it is feasible with the current technologies. Without the limitations encountered by classical computers when simulating quantum mechanics, quantum simulators would be able to tackle difficult quantum many-body problems. Quantum simulators would not only provide new results that cannot be otherwise predicted or classically simulated, but they would also allow us to test various models. For instance, controllable versions of magnified lattice structures of "solids" (realized with atoms, ions, or electrons) could be used to study difficult problems in condensed-matter physics, such as correlated electrons or quantum magnetism. Moreover, in general, quantum simulations do not require either explicit quantum gates or error correction, and less accuracy is needed. Thus, quantum simulation is typically less demanding than quantum computation. Even with tens of qubits (*4–6*), one could already perform useful quantum simulations, whereas thousands of qubits would be required for factorizing even modest numbers using of Shor's algorithm.

In this review, we wish to highlight the progress that has been made so far and pinpoint some future directions as well as discuss the challenges and expectations related to quantum simulators.

Simulating Quantum Systems with Computers

The direct simulation of quantum systems on classical computers is very difficult because of the huge amount of memory required to store the explicit state of the quantum system. This is due to the fact that quantum states are described by a number of parameters that grows exponentially with the system size. Furthermore, simulating the system evolution requires a number of operations that also increases exponentially with the size of the system. Take, for instance, N spin-1/2 particles; then 2^N numbers must be stored in memory, and a 2^N by 2^N matrix has to be exponentiated to calculate the time evolution of this system. To avoid this "exponential explosion" (*1*), classic stochastic methods have been developed, but, unfortunately, in many practical situations they fail because of the so-called sign problem (i.e., sampling with nonpositive weight functions). The alternative approach suggested by Feynman is to have "one controllable quantum system simulate another" (*1*). This idea is appealing because it would solve both the problem of storing the quantum state and simulating its evolution without the exponential explosion or other intrinsic limitations.

Controllable Quantum Systems As Simulators

The generic quantum simulation procedure can be stated as follows: After preparing an initial state, obtain the final quantum state after a certain time evolution, and measure some quantity of interest. This is not easy to achieve because all these steps must be realized with polynomial resources. Consider the initial state preparation and final measurement. In most cases, the preparation of the initial state is difficult. However, for particular cases of interest (i.e., most of the commonly used chemical wave functions or arbitrary pure and mixed many-particle states on a lattice) efficient state preparation protocols exist (*7–9*). Because quantum state tomography is costly (*10*), for measurements it would be desirable to directly estimate certain physical quantities like correlation functions or spectra of operators (*8*, *11*). Note that extracting the desired information from the quantum simulator is not always easy. For instance, sometimes the desired information can only be derived indirectly from the measurable quantities of the simulator. Measurement is as crucial as the efficient simulation of the time evolution of the quantum system.

Analog and Digital Quantum Simulators

How does one quantum system simulate another? One way would be to map the evolution of the system to be simulated onto the controlled evolution of the quantum simulator. Thus, one quantum system would mimic the evolution of another [i.e., a quantum emulator; "...there is to be an exact simulation, that the computer will do exactly the same as nature" (*1*)]. Such a device will be referred to here as an analog quantum simulator (AQS) (*6*, *12–14*). Another approach would be to use qubits to encode the state of the quantum system, "translate" its unitary evolution in terms of elementary quantum gates, and implement them in a circuit-based quantum computer. This can be regarded as a quantum algorithm for the physical model. We will call this circuit-based simulator a digital quantum simulator (DQS) [see, e.g., (*4*, *7*, *8*)].

In analog quantum simulators, the Hamiltonian of the system to be simulated, H_{sys}, is mapped onto the Hamiltonian of the simulator, H_{sim}, which can be controlled to some extent. This can be done when the system and simulator are sufficiently similar, and because of this an AQS would be a dedicated device restricted to simulating a limited class of quantum systems. Moreover, the accuracy of the simulation depends on the degree to which the simulator is able to reproduce the dynamics of the system to be simulated. AQSs are usually emulating an effective many-body theory of the simulated system, so they are limited by the extent to which the theory correctly captures the key physical features of the real system. If the model is incomplete, no matter how good the simulation (i.e., no implementation errors), it will still fail to provide meaningful results about the system being simulated. Two intuitive examples illustrating how analog quantum simulation is achieved are provided in Fig. 1.

In general, the goal of digital quantum simulation is to obtain $|\psi(t)\rangle = e^{-ihH_{sys}t}|\psi(0)\rangle$, the solution of the Schrödinger equation for the time-independent Hamiltonian, H_{sys}, which can be written as a sum of many local interactions. $U = e^{-ihH_{sys}t}$ can be approximated by using several exponentials $e^{-ihH_l t}$, where the H_l term are the Hamiltonians of the local interactions. In other words, a quantum circuit consisting of one- and two-qubit gates (two-body interactions) for the unitary transformation, U, is constructed. Such a circuit can, in principle, efficiently simulate any finite-dimensional local Hamiltonian. The main advantage of the DQS is this universality. However, the generation of many-body interactions using two-body interactions is by no means an easy problem. Several methods have been developed (*15*, *16*), but this still remains a challenge. The precision (i.e., the desired

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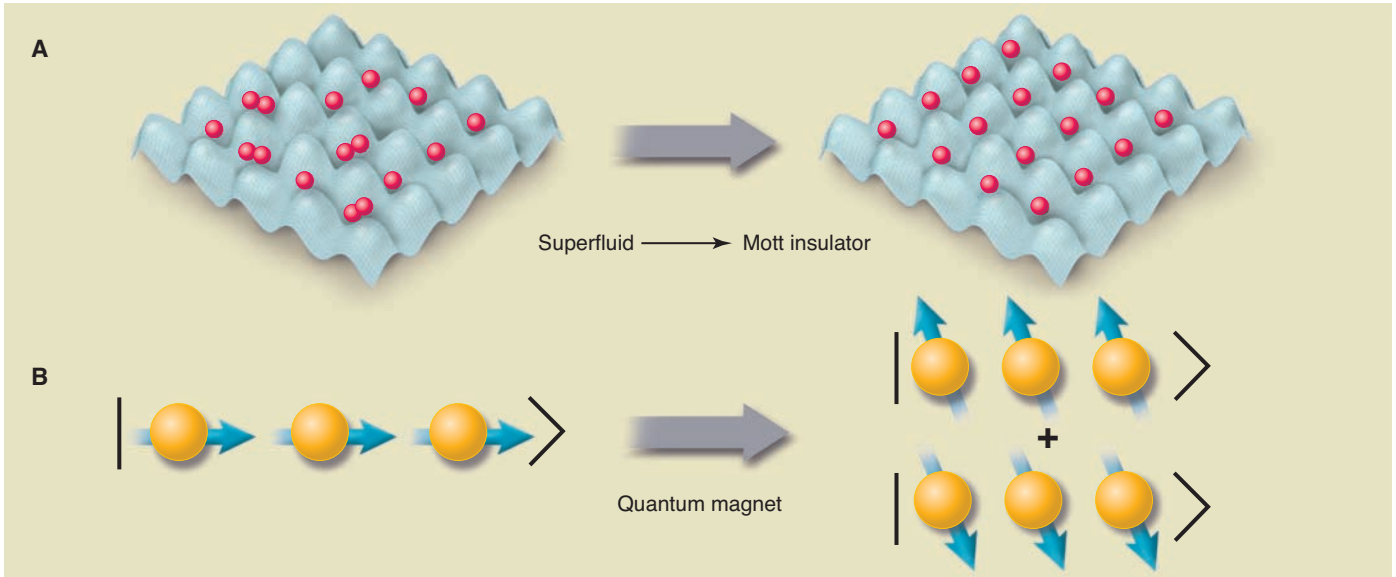
Fig. 1. Examples of analog quantum simulation of quantum phase transitions using ultracold neutral atoms (A) and trapped ions (B). (**A**) The schematics of the quantum phase transition from a superfluid to a Mott insulator phase realized in (*12*) by using rubidium atoms trapped in an optical lattice. The ratio between the tunneling energy and the on-site interaction energy was controlled by adjusting the lattice potential depth such that the quantum phase transition could take place. There are alternative ways of simulating this quantum phase transition with arrays of cavities (*21*) or arrays of Josephson junctions (*27*). (**B**) Magnetic quantum phase transition simulated in (*6*) using trapped calcium ions. The interactions of individual spins were realized by coupling the internal levels (representing the spin-1/2 states) with a resonant RF field, whereas the spin-spin interactions were simulated by using a state-dependent optical dipole force implemented by a walking wave.

number of bits in the final answer) of DQS can be arbitrarily high; however, this is costly because the required number of quantum gates scales exponentially with the precision of the answer (*17*).

A DQS is not restricted to recreating the unitary evolution of the system, but it also includes efficient quantum algorithms [e.g., phase estimation for computing eigenvalues (*18*) or algorithms for computing partition functions (*19*)]. In some instances, this approach may prove more efficient than directly trying to simulate the unitary time evolution.

Although in the long run the goal would be to build a universal, all-mighty quantum simulator (i.e., a DQS), in terms of practical implementation in the near future, AQS has the advantage. For this reason, most research groups studying quantum simulators are currently investigating AQS, and therefore this trend is reflected in our review.

Applications

Quantum simulators would be able to emulate far larger quantum systems than classical computers. Moreover, being quantum systems themselves, quantum simulators would be able to provide insight on quantum phenomena. Therefore, they are best suited for problems that are intractable on classical computers and those for which more direct experimental studies are very difficult or impossible. Quantum simulators could help tackling difficult problems in condensed-matter physics, most notably quantum phase transitions (Fig. 1), quantum magnetism,

or high-temperature superconductivity. Quantum simulators would also have applications in high-energy physics, the simulation of analog cosmological models, as well as in chemistry. As practical quantum simulators become available, more disciplines might add quantum simulation to their toolbox. Table S1 summarizes some of the proposed applications, as well as the physical systems in which they could be implemented.

Building a Quantum Simulator

Building an AQS requires a controllable quantum mechanical system that can mimic (emulate) the evolution of other quantum systems. However, to reproduce the dynamics of any quantum system, one would need a DQS, which is the yet-to-be-built quantum computer. As experience has shown, such a device is rather difficult to make. However, designing an AQS for a specific problem or a certain class of problems is a much simpler task.

As an example, the study of many-body problems in condensed-matter physics could be achieved with an AQS consisting of an array of qubits together with control fields. A simulator of this kind could be realized with atoms in optical lattices (*2*, *20*), atoms in arrays of cavities (*21*, *22*), arrays of trapped ions (*23*–*25*), quantum dots (*13*, *26*), superconducting circuits (*27*, *28*), or electrons trapped on the surface of liquid helium (*29*, *30*) (Fig. 2). The controls of the quantum simulator vary from system to system. They could be laser pulses, radio frequency (RF) pulses, or electric or mag-

netic fields. Next, let us look at some potential quantum simulators.

Atoms and Photons

Neutral atoms in optical lattices. Atoms in optical lattices are very well suited for mimicking condensed-matter physics, as discussed in detail in two recent reviews (*2*, *20*).

Optical lattices can be used for implementing both DQS and AQS. The dimensionality of the lattice can be changed, and various lattice geometries can be obtained by manipulating the optical potential. Moreover, optical lattices are flexible and provide several controllable parameters such as tunneling, on-site interactions, next-neighbor, long-range and multiparticle interactions, external potentials, and Rabi transitions. Spin models can be simulated in a very similar manner as in ion traps. For instance, for optical lattices the interaction between two atoms could be achieved by selectively displacing the optical lattices, whereas in the case of trapped ions the interaction could be realized by pushing the ions with a state-dependent force. In the experiment realizing the quantum phase transition from a superfluid to a Mott insulator (*12*) (Fig. 1A), the ratio between the tunneling and on-site interaction energies was controlled by adjusting the depth of the optical lattice, but it should also be possible to control the atom-atom interactions via Feshbach resonances (*31*). So far, addressing individual atoms in optical lattices has been difficult because the separation between neighboring trapping sites is smaller than the best achievable focusing width of the laser beams,

but very recent results show that this technical issue can be solved (*32*).

Arrays of cavities. Atoms in arrays of cavities could be an alternative to optical lattices (*21*, *22*). In this approach an array of cavities in an arbitrary geometry (Fig. 2), where each cavity interacts with an ensemble of atoms driven by an external laser, is used. The atoms trapped in the cavity together with the photons form polaritons. This system provides a way of simulating the Bose-Hubbard model and quantum phase transitions and allows for the manipulation and measurement of the properties of individual constituent particles. Proposals also suggest measurements and feedback control as tools for realizing quantum simulations (*33*).

Ions

Trapped ions are another good candidate for implementing a practical quantum simulator. An early experiment investigated nonlinear interferometers (*34*), and, recently, the transition from paramagnetic to ferromagnetic order has been realized experimentally (*6*) (Fig. 1B). Trapped ions could be used to study some problems in condensed-matter

physics and to realize even more exotic simulations, such as high-energy physics or cosmology.

Ion trap quantum simulators are quite flexible and allow the implementation of both DQS and AQS. Moreover, one can exploit both the internal energy levels and the vibrational modes of the trapped ions. Coherent control can be realized with high fidelity (*3*), so the scalability to many ions is the major challenge for ion trap quantum simulators. Several solutions may be available: using long strings of ions, planar Coulomb crystals (*23*), or arrays of microtraps (*24*) or it could also be possible to trap ions in optical lattices as suggested in (*25*). The two-qubit interactions are usually realized with optical forces, but a method for laserless simulation (avoiding the scattering problem) with ions in arrays of microtraps has been proposed (*24*). A substantial advantage of trapped ions is the ease of measuring and manipulating individual ions. Such a feature is not available in typical condensed-matter systems.

Electrons

Quantum dots. Arrays of semiconducting quantum dots can be realized in two-dimensional

electron gas with superposed two-dimensional mesh gates (*13*, *26*). The material of choice is usually GaAs. By adjusting the mesh gate design and voltage, various lattice geometries can be realized. Other types of quantum dots can be introduced in the semiconductor during growth (i.e., small islands of InGaAs within a GaAs matrix). In these quantum dots, one can make use of optical transitions. In quantum dot arrays, the Fermi-Hubbard model (*26*) or the CuO plane in high-temperature superconductors (*13*) could be simulated. Using quantum dots may provide an advantage over atoms in optical lattices because of the very low temperatures relative to the Fermi temperature that can be reached and the natural long-range Coulomb interaction (*26*). An interesting feature of quantum dots is that they behave like "artificial atoms," and coupled quantum dots can be seen as "artificial molecules" so they can be used for the analog simulation of chemical reactions (*14*).

Superconducting circuits. Superconducting circuits can also behave like "artificial atoms," so they can be used to test quantum mechanics at macroscopic scales and conduct atomic phys-
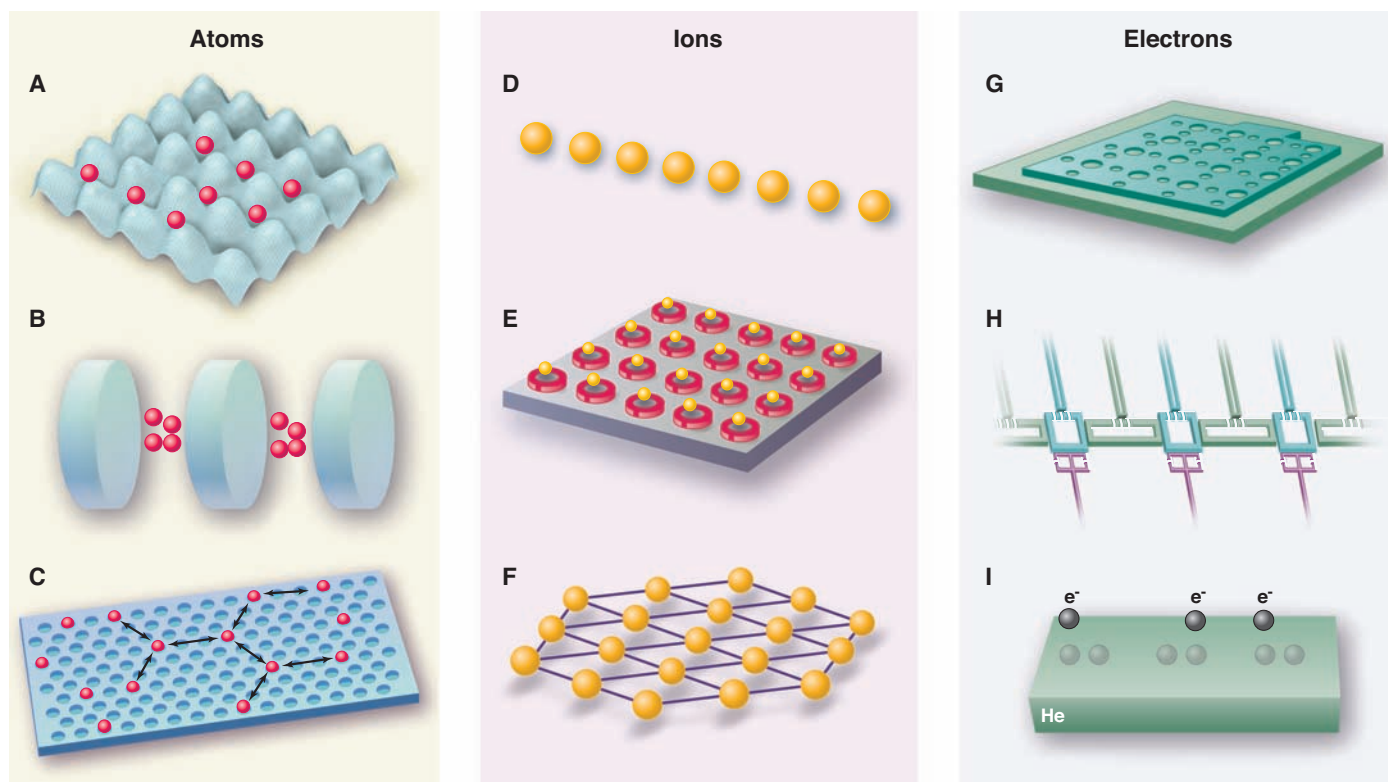
Fig. 2. One-dimensional or 2D arrays of qubits plus controls could be used to simulate various models in condensed-matter physics. Examples of physical systems that could implement such analog quantum simulators include the following: atoms in optical lattices (*20*) (**A**) or in 1D (**B**) or 2D (**C**) arrays of cavities (*21*, *22*); ions in linear ion chains (**D**), 2D arrays of planar traps (*24*) (**E**), or 2D Coulomb crystals (*23*) (**F**); or electrons in quantum dot arrays created by a 2D mesh (*13*, *26*) (**G**), or arrays of superconducting circuits (*28*) (**H**), or trapped on the surface of liquid helium (*30*) (**I**). The average distance between the atoms is, in the case of optical lattices, less than 1 μm; in 2D arrays of cavities, it would scale as the ratio between the wavelength and the refractive index. As for the interior distances in ion trap arrays, they should be about 10 to 50 μm and about the same for 2D Coulomb crystals. In arrays of quantum dots, the spacing between dots is about 0.1 μm. In superconducting circuits, the distance between junctions can be less than a micrometer. In the case of electrons on helium the distance between neighboring sites would be about 1 μm. These interqubit distances (from 0.1 to 10 μm) should be compared with the far smaller average interatomic distances in solids, which are ≤1 nm. The systems shown above realize a 1- or 2D array of qubits, which can be manipulated in different manners. The larger distances between qubits make quantum simulators more controllable and easier to measure. Therefore, they can be thought of as toy models of the magnified lattice structure of a "solid," with a magnification factor of three orders of magnitude.

ics experiments on a silicon chip (*3*, *35*). There is a deep analogy between natural atoms and the artificial atoms composed of electrons confined in small superconducting islands. Whereas natural atoms are driven by using visible or microwave photons, the artificial atoms in the circuits are driven by currents, voltages, and microwave photons. The effects of electric and magnetic fields on the circuits are the analogs of the Stark and Zeeman effects in atoms. Superconducting circuits as artificial atoms can be used to simulate atomic physics and quantum optics (*35*). Furthermore, early experiments have observed a one-dimensional (1D) Mott insulator formed by quantum vortices in arrays of Josephson junctions (*27*). Other applications are summarized in table S1.

A limitation of microfabricated solid state qubits is the difficulty of producing them with high uniformity. This can yet turn into an advantage when modeling condensed-matter systems, where defects and disorder are often crucially important. Furthermore, the uniformity of solid state qubits has been increasing in time and should be less of a problem in the future.

We also mention that electrons trapped on the surface of liquid helium could be used for simulating spin models (*29*, *30*).

Others

The quantum simulators discussed so far are 1D or 2D arrays of qubits plus controls as illustrated in Fig. 2. Nuclear spins in organic molecules manipulated with nuclear magnetic resonance (NMR) techniques have been used for quantum simulation (especially DQS). In one of the first quantum simulation experiments, the dynamics of truncated quantum harmonic and anharmonic oscillators have been simulated (*36*). More recently, the pairing Hamiltonian has been simulated by using NMR (*17*). Solid-state NMR has been proposed for simulating the phase transition from a paramagnetic to antiferromagnetic phase (*37*). Although liquid-state NMR is not scalable, experiments on spin diffusion in solid state systems can be thought as large-scale AQS, and, therefore, NMR may be used for quantum simulation.

Linear optics has been used to implement some quantum simulations (table S1).

Decoherence and Limitations

Although quantum simulators are affected by the interactions with the environment in the same way as quantum computers, decoherence is not such a big problem because in quantum simulations only limited precision is required. Moreover, it was suggested that the decoherence of the simulator might be useful (*4*) because it could serve as a rough way of modeling the decoherence of the simulated system. In (*38*), it was demonstrated through calculations and an NMR experiment that it is indeed possible to exploit the natural decoherence of the simulator, and with an appropriate choice of the mapping

between the system and simulator, one may take advantage of the natural symmetries in order to modify the effective decoherence of the simulator. However, there are certain limitations. The simulated system does not necessarily decohere in a similar way as the simulator (*39*), and, therefore, one should be cautious when trying to include decoherence in the simulation. To what extent one can make use of decoherence in the simulations depends on the type of decoherence, the simulated system, and the specific way the system is mapped onto the simulator. Note that the simulation of quantum open systems does not necessarily require the inclusion of the decoherence of the simulator (*40*).

The errors in quantum simulation are usually taken too lightly. Indeed, the required level of precision and control is much lower than for quantum computation; however, errors still need to be minimized. Recently, the effect of noise in two-body interactions and local control operations used for the simulation of many-body interaction Hamiltonians has been investigated in detail (*16*). However, this problem clearly needs more attention.

Challenges and Prospects

Recent theoretical and experimental results on quantum simulation are quite encouraging, and it seems that in the near future practical quantum simulators might be built. However, there still are some problems to be overcome. From the experimental point of view, improved controllability and scalability should be realized. Besides optical lattices, other systems cannot yet handle large arrays of qubits. However, even with a relatively small quantum simulator, various interesting physical regimes could be explored.

Further theoretical studies of decoherence and control would be useful. For each physical system, the minimum requirements for realizing useful quantum simulations and the potential limitations have to be investigated further. Moreover, new applications of quantum simulation should be explored.

Finally, two interesting directions closely related to quantum simulation should be mentioned: One is the study of entanglement in many-body systems and its relation with quantum phase transitions; the other is the development of classical numerical algorithms, inspired by the methods in quantum information and computation, for the simulation of quantum many-body systems.

Conclusions

Considerable progress toward building a quantum simulator has been achieved in the past decade, and in the near future we might witness the first practical applications. Surely, Feynman (*1*) would be very pleased by these results and promising perspectives, especially the first experimental demonstration of benchmark quantum simulations with tens of qubits. Quantum simulators would have tremendous impact in

many fields, providing a means of exploring new physical phenomena.

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Supporting Online Material for

Quantum Simulators

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Table 1: Potential applications of quantum simulators and the physical systems in which they could be implemented. This is not an exhaustive list. By DQS we mean any physical system that can implement a Digital Quantum Simulator. Asterisks denote actual experimental realizations.

Application		Proposed implementation
Condensed matter physics:		
	Quantum phase transitions	atoms (*1*) *, ions (*2*), (*3*) *, NMR (*4*), cavities (*5*), supercond. circuits (*6*) *
	Hubbard models	atoms (*7*), ions (*8*), quantum dots (*9, 10*), cavities (*5, 11*)
	Spin models	atoms (*12, 13*), ions (*12, 14–16*), NMR (*4*), cavities (*17, 18*), supercond. circuits (*19, 20*), electrons on helium (*21, 22*)
	Spin glasses	DQS (*23*), supercond. circuits (*24*), atoms (*25*)
	High Tc superconductivity	DQS (*26*), quantum dots (*27*)
	BCS pairing	NMR (*28–30*) *
	BCS-BEC crossover	atoms (*31*) *
	Metamaterials	supercond. circuits (*32*)
	Disordered systems	atoms (*33–36*) *, supercond. circuits (*37*), NMR (*38*) *
	Frustrated systems	ions (*39*)
	Tonks-Girardeau gas	atoms (*40*) *
	Anyons	optical lattices (*41*), photons (*42*) *, supercond. circuits (*43*) , (*44, 45*)
High-energy physics:		
	Lattice gauge theories	DQS (*46*), atoms (*47*)
	Dirac particles	ions (*48, 49*)
Cosmology:		
	Hawking radiation	ions (*50*), supercond. circuits (*51*) photons (*52*)
	Unruh effect	ions (*53*)
	Universe expansion	atoms (*54*)
Atomic physics:		
	Cavity QED	supercond. circuits (*55, 56*)
	Cooling	supercond. circuits (*57–59*)
Open systems:		
		NMR (*60*) *, ions (*61*),
Chemistry:		
	Thermal rate calculations	DQS (*62*)
	Molecular energies	DQS (*63*)
	Chemical reactions	DQS (*64*), quantum dots (*65*), (*66*)
Quantum chaos:		
		NMR (*67*) *, photons (*68*)
Other:		
	Schrödinger equation	DQS (*69, 70*)
	Quantum thermodynamics	(*71*)
	Nonlinear interferometers	ions (*72, 73*) *

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