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Can one trust quantum simulators?

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Abstract
Various fundamental phenomena of strongly correlated quantum systems such as high-T_c superconductivity, the fractional quantum-Hall effect and quark confinement are still awaiting a universally accepted explanation. The main obstacle is the computational complexity of solving even the most simplified theoretical models which are designed to capture the relevant quantum correlations of the many-body system of interest. In his seminal 1982 paper (Feynman 1982 *Int. J. Theor. Phys.* **21** 467), Richard Feynman suggested that such models might be solved by 'simulation' with a new type of computer whose constituent parts are effectively governed by a desired quantum many-body dynamics. Measurements on this engineered machine, now known as a 'quantum simulator,' would reveal some unknown or difficult to compute properties of a model of interest. We argue that a useful quantum simulator must satisfy four conditions: *relevance*, *controllability*, *reliability* and *efficiency*. We review the current state of the art of *digital* and *analog* quantum simulators. Whereas so far the majority of the focus, both theoretically and experimentally, has been on controllability of relevant models, we emphasize here the need for a careful analysis of reliability and efficiency in the presence of imperfections. We discuss how disorder and noise can impact these conditions, and illustrate our concerns with novel numerical simulations of a paradigmatic example: a disordered quantum spin chain governed by the Ising model in a transverse magnetic field. We find that disorder can decrease the reliability of an analog quantum simulator of this model, although large errors in local observables are introduced only for strong levels of disorder. We conclude that the answer to the question 'Can we trust quantum simulators?' is . . . to some extent.

(Some figures may appear in colour only in the online journal)

Contents

1. Introduction

In his 1982 foundational paper [1], Richard Feynman suggested that the complexities of quantum many-body physics might be computed by 'simulation.' By designing a well-controlled system from the bottom up, one could create a computer whose constituent parts are governed by quantum dynamics generated by a desired Hamiltonian. Measuring the properties of this nano-engineered system thus reveals some unknown or difficult to compute properties of a quantum many-body model, such as the nature of quantum-phase diagrams. Feynman's machine is now known as a 'quantum simulator' (QS).

Fueled by the prospect of solving a broad range of long-standing problems in strongly correlated systems, the tools to design, build, and implement QSs [1–3] have rapidly developed and are now reaching very sophisticated levels [4]. Researchers are making breakthrough advances in quantum control of a variety of systems, including ultracold atoms and molecules [5–17] (for reviews see also [18–20]), ions [21–27] (for recent reviews see [20, 28–30]), photons [31–36] (for a recent review see [37]), circuit quantum electrodynamics (CQED) and polaritons [38–42] (for a recent review see [43]), artificial lattices in solid state [44], nuclear magnetic resonance (NMR) systems [45–50], and superconducting qubits (for reviews see [51–54], for the current state of art [55, 56] and references therein), etc (for a general overview see [57]). At the current pace, it is expected that we will soon acquire the ability to finely control many-body systems whose description is outside the reach of a classical computer. For example, modeling interesting physics associated with a quantum system involving 50 spin-1/2 particles—whose general description requires $2^{50} \approx 10^{15}$ complex numbers—is out of the reach of current classical supercomputers, but perhaps within the grasp of a QS.

In a field brimming with excitement, it is important to critically examine such high expectations. Real-world implementations of a quantum simulation will always face experimental imperfections, such as noise due to finite precision instruments and interactions with the environment. Feynman's QS is often considered as a fundamentally *analog* device, in the sense that all operations are carried out continuously. However, errors in an analog device (also continuous, like temperature in the initial state, or the signal-to-noise ratio of measurement) can propagate and multiply uncontrollably [58]. Indeed, Landauer, a father of the studies of the physics of information, questioned whether quantum coherence was truly a powerful resource for computation because it required a continuum of possible superposition states that were 'analog' in nature [59].

This contrasts with the operation of a universal *digital* quantum computer as envisioned by David Deutsch, in which all operations are digitized into a finite set of logic gates and measurements [60][6]. The invention of quantum-error-correcting codes showed that a quantum computer is in some sense *both* analog and digital. Through a discrete set of unitary transformations, we can get arbitrarily close to any superposition, and imperfections can always be projected on a discrete set and thus can be corrected [61]. When such a digital quantum simulation operates with fault-tolerant quantum error correction [62], we can trust its output to a known finite precision.

Universal digital quantum computers may serve as digital QSs (DQSs) that mimic the dynamics of some such quantum many-body systems of interest. Despite the fact that in such a case error correction and fault tolerance is guaranteed, the question of efficiency of such a device is highly non-trivial. The number of resources needed for precise simulation of continuous-time dynamics of a many-body system by stroboscopic digital applications of local gates might be enormous [63]. One can also consider DQSs which are experimental systems that have at their disposal only a limited, non-universal set of gates. In such a situation, the error correction and fault tolerance are not guaranteed and the question of efficiency is even more pertinent.

This raises the central problem of this key issue paper: can we trust the results obtained with a real-world *analog* or *digital* QS, and under what conditions are they *reliable* to a known degree of uncertainty? Although our main discussion concentrates on analog QSs (AQSs), the article also reports on the state of art of DQSs. The paper is organized as follows. Section 2 develops the general concept of QSs in the spirit of the DiVincenzo criteria for quantum computing [64]. Here we present one of the main results of this paper: a definition of the QS based on four properties that a QS should have—relevance, controllability, reliability and efficiency.

Section 3 is devoted exclusively to DQSs. It contains several subsections in which we review various proposals for DQSs, classify them, and discuss the present state of knowledge concerning their controllability, reliability and efficiency. Section 4 is organized similarly, but focused on AQSs.

Section 5 is perhaps the most important one from the conceptual point of view. Here, we formulate specific proposals to investigate the robustness of AQSs and how to extend standard methods of validation and certification of AQSs. We illustrate these considerations in sections 6–8 with calculations for a paradigmatic model that are not published elsewhere. Section 6 describes the investigated model, and the results concerning statics and dynamics are presented in sections 7 and 8, respectively. We conclude in section 9. The paper also contains an appendix describing technical details of the methods used.

Very recently, *Nature Physics* has published a focus issue with five papers devoted to QSs: a short paper by Cirac and Zoller [65] introducing the subject, and four longer reviews on ultracold atoms [19], ions [30], CQED [66] and photons [37]. Our key issue paper is complementary to these, in the sense that it addresses general and universal problems of the validation of quantum simulations, their robustness, reliability and efficiency—problems that pertain to all kinds of QSs.

[6] Note that we use the notion of digital quantum simulator in this sense, i.e. the digitization of operations, not in the sense of digits of precision. In particular, the outcome of an analog quantum simulator will also yield only a finite digital precision, but its operations are performed continuously.

Table 1. In this table, we characterize the different classes of QSs (digital vs. analog, universal vs. non-universal, Hamiltonian vs. open) focusing especially on the requirements (b) to (d). (Since the relevance (a) depends on the concrete model simulated, we do not list it here.) Note specifically that little is known about the reliability and efficiency of AQSs (question marks). Detailed descriptions are provided in sections 3 and 4.

	Digital			Analog		
	Universal	Non-universal	Open	Universal	Non-universal	Open
Realizations	Trapped ions, ultracold neutral or Rydberg atoms, circuit QED, super-conducting qubits, etc	Same as universal digital	As universal digital (especially trapped ions, ultracold neutral or Rydberg atoms)	?	Many (trapped ions, ultracold atoms, photonic and polariton systems, artificial solid-state lattices, etc)	Same as non-universal analog
Control	Full (long-range inter-actions difficult?)	Partial	Partial	Full	Partial (but long-range interactions 'easy')	Partial
Error correction (EC)	with exponential overhead (Trotterization issues)	Not guaranteed	Not guaranteed	No standard EC	No standard EC	No standard EC
Reliability	Full	Not guaranteed	Not guaranteed	?	? (Partial validation schemes available)	? (Partial validation schemes available)
Efficiency	Efficient without EC (for general class of models); much less efficient with EC (Trotterization issues)	At least as universal digital, but may not be provable	Can be better than universal digital	?	?	?

2. Quantum simulators

Before proceeding, we must establish a clear definition of a QS. We consider here a QS to be a device which, when measured, reveals features of an ideal mathematical model, e.g. the phase diagram for the Bose–Hubbard model on a specified lattice with specified interactions. This contrasts with, and is less demanding than, a full simulation of a real material, since typically a mathematical model attempts to capture only the most relevant properties of the real material. For example, the superconducting properties of a cuprate might be shared, in part, by a Fermi–Hubbard model [67, 68]. A QS may be a special purpose device that simulates a limited class of models, e.g, the Bose–Hubbard model simulated by atom transport in e.g. an optical lattice [69, 70], or a universal machine that is capable, in principle, of simulating any Hamiltonian on a finite-dimensional Hilbert space.

Based on this, we formulate the following 'working' definition of a QS in the spirit of the DiVincenzo criteria for quantum computing [64], providing some more detailed explanations below (see also [3]).

Definition. A QS is an experimental system that mimics a simple model, or a family of simple models of condensed matter (or high-energy physics, quantum chemistry, etc). A QS should fulfil the following four requirements:

(a) *Relevance:* the simulated models should be of some relevance for applications and/or our understanding of challenges in the areas of physics mentioned above.
(b) *Controllability:* a QS should allow for broad control of the parameters of the simulated model, and for control of preparation, initialization, manipulation, evolution and detection of the relevant observables of the system.
(c) *Reliability:* within some prescribed error, one should be ensured that the observed physics of the QS corresponds faithfully to that of the ideal model whose properties we seek to understand.
(d) *Efficiency:* the QS should solve problems more efficiently than is practically possible on a classical computer.

In table 1, we summarize to which extent existing experimental proposals fulfil these requirements. We will characterize the different types of QSs in more detail in the following two sections, but before that, we would like to make some general comments.

Comments to (a) We should demand that the mimicked models are not purely of academic interest but that they rather describe some interesting physical systems and solve open problems. This also means that the simulated models should be computationally very hard for classical computers (see also requirement (d)).

Comments to (b) and (c) Regarding control over measurable observables, one should stress that very often the amount of output information required from QSs might be significantly smaller than one could demand from a universal quantum computer. QSs should provide information about phase diagrams, correlation functions, order parameters, perhaps even critical exponents or nonlocal hidden order parameters. But a common assumption is that these quantities are more robust than what is required for a universal quantum computer, which typically relies on much higher-order correlation functions than a QS.

Regarding control over model parameters, it is in particular desirable to be able to set the parameters in a regime where the model becomes tractable by classical simulations, because this provides an elementary instance of validating the QS. Furthermore, one of the main results of this paper

is the proposal and analysis of an even more sophisticated manner of validation, namely the checking of the sensitivity of the quantum simulation with respect to the addition of noise and/or disorder. Such a validation is only possible with sufficient control over the system. Note, however, that there are other possibilities of checking the results, as pointed out to us by Hadzibabic [71]. Namely, sometimes it is impossible to simulate the system classically, but it might still be possible by classical means to test the sensibleness of the quantum-simulation results. For instance, the measured ground-state energy should fulfill all known bounds, such as variational ones, and others.

Comments to (d) The notion 'computationally very hard for classical computers' may have several meanings: (i) an efficient (scalable, with polynomial growth in resources as a function of problem size) classical algorithm to simulate the model might not exist, or might not be known; (ii) the efficient scalable algorithm is known, but the required size of the simulated model is too large to be simulated under reasonable time and memory restrictions. The latter situation, in fact, begins to occur with the classical simulations of the Bose– or Fermi–Hubbard models[7], in contrast to their experimental QSs. However, there might be exceptions to the general rules. For instance, it is desirable to realize QSs to simulate and to observe novel phenomena that so far are only theoretically predicted, even though it might be possible to simulate these phenomena efficiently with present computers. Simulating and actually observing in the lab is more than just simulating abstractly on a classical computer.

Comments to (c) and (d) The requirements of reliability and efficiency are interrelated. In fact, we could try to improve the precision of a QS by averaging more experiments, but in hypersensitive regimes (like those close to quantum-phase transitions) the necessary number of repetitions can grow rapidly, bringing the overall efficiency of the QS down to the level of classical computers. A connection between (c) and (d) could also be relevant for the popular cross-validation approach [72]. There, one compares the results of two different physical realizations performing a QS of the same model, and hopes to find universal features which then would be ascribed to the simulated model. It may be, however, that the universal features shared by multiple platforms are robust only because they could have been predicted efficiently with some classical algorithm.

With our working definition at hand, one could ask—What should a QS simulate? An important set of tasks include the following.

(1) Statics of the mimicked system at zero temperature; this implies ground-state simulation and its properties.
(2) Statics at thermal equilibrium, i.e. Hamiltonian dynamics at low energies or thermodynamics at non-zero, typically low, temperatures.
(3) Continuous-time dynamics of the system, in particular Hamiltonian dynamics out of equilibrium.
(4) Dissipative or open-system continuous-time dynamics.

To understand which of these are most relevant, we now discuss briefly which systems can be simulated efficiently classically and which systems are classically computationally hard. Classical simulations of quantum systems are currently performed using one of the following numerical methods [3].

- Quantum Monte Carlo (QMC).
- Systematic perturbation theory.
- Exact diagonalizations.
- Variational methods (mean-field methods, density-functional theory (DFT), dynamical mean-field theory (DMFT), tensor-network states (TNS), density-matrix renormalization group (DMRG), tree tensor-network states (TTN), multiscale entanglement-renormalization ansatz (MERA), projected entangled-pairs states (PEPS), etc)

Each of these methods has its limitations. Let us first focus on points (1) and (2) of the previous list of possible QS tasks. In these cases, QMC works for various large systems, but fails for Fermi or frustrated systems due to the famous sign problem [73]. Perturbation theory works only if there exists a small expansion parameter [74]. Exact diagonalization works only for rather small systems [73]. In the case of 1D systems, DMRG, MERA and TTN techniques scale favorably and can, in principle, treat very large systems [75–77]. In 2D the situation is more complex—similar to exact diagonalization, DMRG and TTN work only for reasonably small systems [78–80], whereas 2D tensor-network methods (PEPS, MERA) in principle work for arbitrarily big systems (bosonic, and even fermionic [81] or frustrated [82]) but are biased toward slightly entangled states. Mean field [83], DFT [84, 85], or DMFT [86], finally, have other limitations, e.g. they are essentially designed for weakly correlated systems.

Which then are the models that are computationally hard for points (1) and (2) in the previous task list? Generally speaking, computationally hard are those 'strongly entangled' models in more than 1D such as

- Fermionic models, with paradigmatic examples being the Fermi–Hubbard or t–J models for spin 1/2 fermions [67].
- Frustrated models, with paradigmatic examples being antiferromagnetic Heisenberg or XY models on a kagomé or anisotropic triangular lattice [87].
- Disordered models, with paradigmatic models being quantum, or even classical spin glasses [88].

When we move to points (3) and (4) of the task list, i.e. studying dynamics, one can safely state that

- Quantum dynamics on a long-time scale is generically computationally hard.

The latter statement implies that while it might be possible to simulate with classical computers short-time dynamics in a restricted class of 1D models, such attempts will nearly always fail at longer time scales. Indeed, this fact is related to correlation and entanglement spreading according to the

[7] In the temperature regimes of current experiments on the Fermi–Hubbard model, the model can be simulated classically by high-temperature expansion, but as soon as experiments achieve lower temperatures, this will cease to work and problems of fermionic simulations (i.e. sign problem in QMC [73]) will become relevant. On the other hand, recent efforts in variational Monte Carlo [201] and fermionic tensor networks [202–206] are rapidly providing ever better variational approximations.

Lieb–Robinson theorem that states that, after a sufficiently large time, states can become strongly entangled [89–94] (see also [95]).

In the following two sections, we will explore in more detail the state of the art concerning the four requirements (a)–(d) of our definition, first for DQSs, then for AQSs.

3. Digital quantum simulators

In this section, we classify DQSs, discuss their general properties and various protocols for implementing such devices, and summarize state-of-art knowledge concerning their controllability, reliability and efficiency.

3.1. Universal digital quantum simulators

While the concept of QSs should be traced back to prophecies of Feynman [1], the ideas were made concrete by Lloyd who showed that any 'local' many-body unitary evolution governed by a 'local' Hamiltonian could be implemented by the control afforded by a universal digital quantum computer [96]. For this reason, in the following we will term Lloyd's DQS a 'universal digital quantum simulator' (UDQS).

Lloyd's UDQS is in fact a universal quantum computer, whose task is to simulate the unitary time-evolution operator of a certain quantum system described by a physical Hamiltonian, which can then be employed to extract quantities such as energy gaps and ground-state properties. This is done by appropriate subsequent stroboscopic applications of various quantum gates that mimic the action of a global unitary continuous time-evolution operator of the system. The mathematical basis for such a digitization is given by the Trotter–Suzuki formula. In order to realize Lloyd's UDQS in a laboratory, the experimentalist has to have at his/her disposal a universal set of unitary quantum gates[8]. Let us list below some possible realizations and properties of UDQSs.

- *Realizations.* While implementation of a fully functioning large-scale digital quantum computer is still in development, there are several physical systems for which the universal sets of quantum gates are available, and for which realization of proof-of-principle UDQSs is possible. These systems include ultracold ions [30], ultracold trapped atoms interacting via cold collisions [19] or the Rydberg-blockade mechanism [97, 98], circuit QED [66], superconducting qubits (for reviews see [51–54], for the current state of the art see [56] and references therein), etc (see also [57]). The first concrete proposals for realization of UDQSs were given in [99, 100], and perhaps the first experiments were performed in NMR systems [45–47, 101]. Using a digital architecture and stroboscopic sequence of gates, the quantum simulation of Ising, XY and XYZ spin models in a transverse field were recently demonstrated in a proof-of-principle experiment with up to six ions [24].
- *Controllability.* In accordance with [96], a UDQS is perfectly controllable, i.e. with the help of a universal set of gates sufficient control of the parameters can be achieved. This control allows for simulation of practically any local Hamiltonian evolution, as well as for the preparation, manipulation, and detection of relevant states and observables of the system in question. Further, Preskill's group has recently proven that the scattering amplitudes in the simple relativistic quantum field theories can be efficiently (in polynomial time) simulated by UDQSs [102, 103]. Note, however, that not much is known about the possibility of quantum simulation of systems with long-range interactions such as Coulomb or dipole–dipole interactions using UDQSs.
- *Error correction.* A UDQS is the only DQS which has guaranteed access to error correction and fault tolerance [104, 105] (for the first proof-of-principle experiments see [56, 106–110]).
- *Efficiency.* So far, the community has mostly focused on developing requirement (b) for suitable relevant models, both theoretically and experimentally. The conditions (c) and (d) have received considerably less attention, especially their interrelation. Most work is focused on efficiency in the absence of errors. Lloyd showed that a Trotter–Suzuki decomposition of a time-evolution operator is efficient in that each logic gate acts on a scalable Hilbert space associated with a small subset of qubits and the total number of gates N scales polynomially, $N \sim t^2/\epsilon$, where t is the time of evolution to be simulated and ϵ is the error in the result [96]. Aharanov and Ta-Shma showed that a UDQS is efficient when the Hamiltonian is 'sparse,' i.e. the number of nonzero entries in any row is at most poly(log(D)), where D is the dimension of the many-body Hilbert space [111]. In the absence of errors, the computational complexity of such a simulation has been well studied [112, 113].
- *Reliability.* In the presence of errors, however, ensuring reliability to a desired precision has profound implications for efficiency even in a digital simulator on a fault-tolerant quantum computer [63, 114]. In the digital approach with a finite universal gate set, one applies error-correction schemes that can make the whole computation fault-tolerant when the error per operation is below a certain threshold—thus digital simulators fulfil the reliability requirement (c). The Trotter expansion, however, can scale poorly when error correction is included, as emphasized by Brown *et al* [63] in studies of an implementation of a quantum algorithm to calculate the low-lying energy gap in pairing Hamiltonians [115]. Because the number of gates in the expansion scales as $1/\epsilon$, in order to achieve $M = -\log_2(\epsilon)$ bits of precision, we must Trotterize the unitary evolution to be simulated into 2^M slices. In the presence of errors, each of the time slices must be implemented with only a finite set of universal gates, according to the Solovay–Kitaev theorem [116]; only then can they be implemented fault tolerantly. The result is that a fault-tolerant implementation of the Trotter expansion requires a number of gates and time

[8] Some authors (see [30, 65]) use the term UDQS for DQS that can simulate all possible evolutions governed by arbitrary (or, more precisely, arbitrary 'interesting') Hamiltonians. We put the emphasis here on the universality of the set of gates, rather than the set of simulable Hamiltonians.

to perform the simulation that grows *exponentially* with the degree of precision required, for a fixed number of particles being simulated. Moreover, Brown *et al* showed that for a small number of qubits where one might avoid error correction, analog control errors on the logic gates can lead to faulty results, negating requirement (c), and robust control pulses become essential.

In a similar vein, Clark *et al* [117] performed a careful analysis of the resources necessary to implement the Abrams–Lloyd algorithm [118] to calculate the ground-state energy of the one-dimensional transverse Ising model (TIM) using a state-of-the-art fault tolerant architecture for an ion-trap quantum computer. Again, the overhead in the number of time steps to fault-tolerantly implement the quantum-phase estimation algorithm grows exponentially with the degree of precision required. They found that for 100 spins, in order to achieve $b \geqslant 10$ bits of precision, at least two levels of concatenated error correction are necessary, requiring at least 100 days of run time on the ion-trap quantum computer; for $b \geqslant 18$, three levels are necessary, requiring at least 7.5×10^3 years! These results assume a gate time of $10\,\mu$s. To recover the 100-day limit with only one level of concatenated error-correction coding, a gate time of 300 ns seems necessary (as well as decreasing other parameters such as failure probabilities). On the other hand, for a fixed precision, the number of resources required grows weakly with system size. So, if the error probability per gate can be reduced well below the threshold to achieve the desired precision without many layers of concatenated error-correction encoding, then digital quantum simulation will scale favorably with the number of particles.

Let us finally remark that, to increase their efficiency, digital-quantum-simulation algorithms often compress the number of degrees of freedom that are necessary to describe the many-body system, rather than directly map the Hilbert space of the system to the Hilbert space of the simulator [114], an approach that has been borrowed from classical algorithms such as MPS or PEPS. Currently, there is a new theoretical development toward a 'hybrid' device, where the ground state of many-body Hamiltonians is represented as a PEPS, but implemented on a quantum computer. This is efficiently possible when the gap between the ground and first excited state scales as the inverse of a polynomial in the number of particles. Then, one can use the quantum computer to contract tensor networks and use that to calculate the expectation value of any local variable, such as correlation functions [119]. In a similar spirit, Temme *et al* developed a quantum-algorithmic version of the Metropolis Monte Carlo algorithm that allows one to efficiently sample from a Gibbs thermal state [120]. Such approaches point to efficient DQSs for well-defined classes of problems.

3.2. Non-universal digital quantum simulators

A non-universal digital quantum simulator (nUDQS) is in many aspects similar to a UDQS, except that is it a special-purpose quantum computer. Its task, however, is the same as that of a UDQS: to simulate continuous-time quantum many-body dynamics of a certain quantum system described by a certain physical Hamiltonian. The experimentalist who realizes an nUDQS has to his/her disposal a non-universal set of unitary quantum gates. Let us list below some properties and possible realizations of such an nUDQS.

- *Realizations.* In all systems in which the universal sets of quantum gates are available, one can also restrict the set of gates and realize an nUDSQ. For example, in some of the recent experiments of Blatt and co-workers [24], only a necessary subset of the available set of universal gates was used. All of the systems discussed above (atomic, superconducting, etc) are potentially platforms for implementing nUDQSs. A seminal example of this approach goes back to the so-called 'average Hamiltonian theory' in NMR [121, 122].
- *Controllability.* nUDQSs are typically not perfectly controllable, but in most experimental realizations should allow for a wide control of parameters, which in turn should allow for simulations of evolution for wide families of Hamiltonians of interest.
- *Error correction.* For nUDQSs, it is not guaranteed that error correction and fault-tolerant computing is possible.
- *Efficiency and reliability.* All of the above discussion concerning UDQSs applies also to nUDQSs. But there are many novel, open problems associated specifically with nUDQSs, since, e.g. sometimes giving up on universality can result in substantial efficiency gains. For example, universality could be sacrificed in favor of a highly precise and fast gate [24] (a simple example is an external homogeneous field, which in a UDQS might have to be applied as a sequence of one qubit gates). In particular, it is possible that for some classes of nUDQSs the problems of Trotterization are not as severe as in the case of UDQSs [98].

3.3. Open-system digital quantum simulators

An open-system digital quantum simulator (OSDQS) is a completely new concept, in principle very different from DQSs aimed at Hamiltonian evolutions. OSDQSs are designed to simulate open-system, dissipative dynamics described in the simplest situation by a Markovian Lindblad master equation for the density matrix of a many-body system of interest. OSDQSs can be aimed at a continuous-time simulation of interesting open-system dynamics, or at a designed dissipative dynamics toward a stationary state of interest, in particular a pure, highly entangled state [123–125].

The experimentalist who realizes an OSDQS, in contrast to a UDQS or an nUDQS, needs to have at his/her disposal some non-unitary, dissipative quantum gates, which mathematically correspond to Lindblad superoperators acting on the density matrix in the master equation. This fact opens a plethora of new questions, e.g. what are the universal sets of gates for this type of evolution. Note that in the case of unitary computing, the universal set of gates allows for realization of arbitrary unitary transformations acting on the (pure) state of the system. In the case of open-system dynamics, a universal set of gates should

allow for the realization of an arbitrary completely positive map (CPM) acting on the density matrix of a system. Moreover, for experimental realizations, we require the gates to be local.

While the conditions for controllability of an open quantum system are under exploration [126], the question of a universal set of gates in this context remains open. A non-trivial reduction (see [127, 128]) of this question to the CPMs that correspond to Markovian evolution, is also open. The problem of error correction in this context is unsolved as well. All of these comments imply that in the area of OSDQSs there are more open questions than answers.

- *Realizations.* In systems in which the universal set of quantum gates is available, one way to realize dissipative gates is by tracing out ancillas, thus allowing one to realize an OSDQS. Good testbeds for exploring OSDQSs are provided by Rydberg atoms, atomic ensembles, NMR [129], or trapped ions. In fact, the first concrete proposals for open-system DQSs concerned Rydberg gates [97, 98]. The first experimental realizations of these ideas, however, have been achieved with trapped ions [25].
- *Controllability.* OSDQSs are typically not universal since they are not usually controllable in the sense of realizing an arbitrary quantum map[9]. Nevertheless, many experimental realizations should allow for a wide control of parameters, which in turn should allow for simulations of open-system (Markovian) evolutions for wide families of open systems of interest. As pointed out in [124, 125], due to the purely dissipative nature of the process, this method of quantum information processing exhibits some inherent robustness and defies some of the DiVincenzo criteria for quantum computation. In particular, there is a natural class of problems that can be solved by open-system DQSs or AQSs: the preparation of ground states of frustration-free quantum Hamiltonians.
- *Error correction.* For OSDQSs, it is not guaranteed that error correction and fault-tolerant computing is possible in the sense defined above[10].
- *Efficiency and reliability.* All of the above discussion concerning UDQSs and nUDQSs applies also to OSDQSs. However, due to the purely dissipative nature of the process, this type of simulation has a certain intrinsic robustness and built-in 'error correction'. A clear example is seen in the OSDQS implementation of Kitaev's toric code [25, 98]. However, as discussed in [98], errors in the gates result in effective heating. Also, the problems of Trotterization are not as severe as in the case of QSs of Hamiltonian evolution. Still, most of these general aspects concerning OSDQSs have not yet been investigated systematically. The efficiency of OSDQSs for the case of frustration-free Hamiltonians depends on the size of the gap between the ground state and the excited states, or more precisely on the real part of the first non-zero eigenvalue of the Lindblad equation, which determines the rate of approaching the stationary (ground) state.

Currently, considerable attention has been devoted to the problem of existence and uniqueness of the open-system preparation of ground states of frustration-free Hamiltonians, and in particular, entangled states of interest. These states are annihilated simultaneously by all of the local frustration-free Lindblad superoperators entering the master equation. There is little known in general about the many-body dissipative dynamics with a frustrated set of Lindblad superoperators competing with Hamiltonian dynamics. For the first attempts to understand these kinds of problems in the context of quantum diffusion–exclusion processes competing with Hamiltonian evolution see, e.g. [130].

4. Analog quantum simulators

In this section, we classify general properties of AQSs, discuss various proposals for such devices, and summarize the state-of-the-art knowledge concerning their controllability, reliability and efficiency. AQSs are experimental systems that are designed to mimic the quantum dynamics of interesting quantum many-body models, typically using 'always on' interactions between particles that are augmented by fast local unitary control. While by definition they operate in continuous time and thus the Trotterization problems do not concern them, the standard error-correction methods and fault tolerance cannot be applied.

4.1. Universal analog quantum simulators

Sometimes known as 'Hamiltonian simulation,' the goal of a UAQS is to transform a given Hamiltonian acting on a fixed Hilbert space into an arbitrary target Hamiltonian through a well-designed control sequence. While not conceived as a practical AQS device, the protocol explores an abstract quantum-information-processing system capable of simulating unitary evolution for all (or at least all local) Hamiltonians.

- *Realizations.* To our knowledge there are no concrete proposals for experimental realizations of UAQSs.
- *Controllability.* While for UDQSs the issue is the access to the universal set of quantum gates, for UAQSs the question is what are the necessary resources (not necessarily quantum gates) that allow for the simulation of all Hamiltonian evolutions of interest. Universal control sets (as opposed to universal digital logic gates) that generate an arbitrary Hamiltonian evolution have been studied [131, 132]. Typically, such an approach using 'always on' interactions is associated with more limited control than is available in a universal digital quantum computer.

[9] Often we do not even know if they are controllable: to our knowledge the problem of what is the universal set of non-unitary 'gates' that allows one to realize an arbitrary, say, completely positive linear map for an N-qubit density matrix has not been directly solved.

[10] The standard schemes for error correction assume that the quantum computer (i.e. DQS) follows a unitary evolution, i.e. dissipation and decoherence are considered there as sources of errors, which the error correction is supposed to remove. To our knowledge, there are no works where these are considered as desired, although not perfect, which error correction is supposed to restore. In this sense, since there are no known methods for error correction under these circumstances, error correction is 'not guaranteed'.

- *Error correction.* UAQSs do not allow for standard error correction and fault tolerance.
- *Efficiency and reliability.* Dür *et al* studied a hybrid construction of always-on interactions with stroboscopic digital control to achieve a universal Hamiltonian simulator via the Trotter construction [133]. They found that decoherence and analog timing errors can make this inefficient for a Hamiltonian simulator. Other issues concerning UAQSs are essentially the same as for non-universal AQSs, so we leave the discussion of them to the next subsection. The only difference is that UAQSs, by definition, are capable of performing tests of robustness of the quantum simulations that we propose in the following section, i.e. tests based on adding disorder or noise in a controlled manner to the simulated Hamiltonian. For non-universal AQSs such an addition requires additional resources.

4.2. Non-universal analog quantum simulators, or simply AQSs

Non-universal AQSs constitute the most popular class of QSs, but despite this fact, there is very little known about their reliability and efficiency. Therefore, we focus on them in the rest of this paper, where, for simplicity, we shall term them AQSs. AQSs are experimental systems that can mimic continuous-time unitary Hamiltonian evolution for a family of models of many-body physics. Their characteristics are as follows.

- *Realizations.* The most advanced experiments with AQSs have been with ultracold atoms in optical lattices [3, 5–15, 19, 70]. The degree of quantum control is even better in ultracold-ion systems, but these are so far limited to a few ions [21–23, 26, 27]. The first step toward large-scale QSs with ions was, however, recently achieved [134]. There has also recently been substantial progress in investigations of other possible candidates for AQSs, such as photonic systems [31, 32, 34–36], photonic and polariton systems [33, 38–42], and artificial lattices in solid-state systems [44].
- *Controllability.* Most, if not all of the proposals for and realizations of AQSs allow for at least partial controllability. The paradigm examples are AQSs employing ultracold atoms in optical lattices (for more details, see chapter 4 of [3]). Here, the typical controls involve optical lattice parameters (laser intensity, wavelength, etc), lattice geometry, lattice dimensionality, temperature and other thermodynamical control parameters, as well as atomic interaction strength and nature (van der Waals interactions are controlled via Feshbach resonances, while dipole interactions by the strength of the dipoles, lattice-site-potential shape, etc). Further, tunneling can be laser-assisted and can mimic artificial Abelian or even non-Abelian gauge fields (see [16, 17]). Dipolar interactions may lead to non-standard terms in Hubbard models, such as occupation-dependent tunneling [135], or various effects involving higher orbitals (see, e.g. [136]).
- *Error correction.* AQSs do not allow for standard error correction and fault tolerance.
- *Efficiency.* The issues of reliability and efficiency are essential for the usefulness of any QSs, and AQSs in particular. In the context of AQSs, however, there has been little analysis of these problems. Firm criteria on computational complexity and efficiency for AQSs are in general difficult to address and have not yet been established. First of all, they require the knowledge of classical computational complexity of the static or dynamical properties of the considered quantum models. Unfortunately, in the realm of classical computation, there are few proofs that a given computational problem is outside the class P, or even if there is a clear delineation between certain complexity classes. In recent years, there has been considerable progress in understanding that the ground states of 1D gapped systems can be efficiently simulated by classical methods [137–139], and that the quantum dynamics is in general computationally hard [94, 95]. If we can set the parameters of our AQS to a regime where efficient classical simulation is possible, we can assess the efficiency and reliability of the AQS in this case by direct comparison with classical simulations (see below). However, there is no guarantee that such a calibration will hold in the truly interesting regimes of parameters, where efficient classical simulations are either impossible, or we do not know how to perform them.
- *Reliability.* So far, there exists no perfect and rigorous way to assess the reliability of AQSs, but there are several complementary approaches. One approach is by cross validation of a variety of different physical systems (e.g. atoms in optical lattices, ions in traps and superconductors) [72]. The hope is that since every platform has its own set of imperfections, they will agree on the universal properties of the ideal quantum many-body model being simulated. While it remains to be seen whether such universal features would emerge, this approach has a number of shortcomings. For example, there may be models that have only one known implementation, or different implementations may suffer in the same way from imperfections, hence consistently exhibiting features associated with noise rather than with the ideal model.

  A more systematic approach is to validate results of a QS against analytical and numerical predictions in the regime of parameters where such comparison is possible. This was recently demonstrated in experiments with ultracold bosonic and fermionic atoms [6–8]; amazingly, in one case numerical simulations helped to correct the expected experimental temperature by up to 30%. Relying solely on validation from classical calculations, however, would restrict QSs to models in regimes where these efficient classical algorithms exist—which means contradicting our relevance and usefulness requirement, point (a) of our definition of a QS. In general, we aim to operate QSs in regimes whose properties are difficult to deduce by classical methods, e.g. near or at the critical point of a QPT, or in genuine *terra incognita*

regimes. In these regimes, however, many relevant models become *hypersensitive* to perturbations [140, 141], and even small levels of noise may completely spoil the results of the quantum simulation. Indeed, the capability of an analog quantum information processor whose dynamics is characterized by quantum chaos (i.e. well described by random matrix theory) can be severely impacted by imperfections [142, 143]. More importantly, this also means that successfully validating a QS in a classically accessible regime does not give certainty about its robustness in regimes which are classically not accessible.

4.3. Open-system analog quantum simulators

Finally, let us mention open-system analog quantum simulators (OSAQSs). Similar to OSDQSs, OSAQSs are supposed to simulate dissipative dynamics described in the simplest situation by a continuous-time Markovian Lindblad master equation for the density matrix of a many-body system of interest. OSAQSs can be aimed at a simulation of interesting open-system dynamics, or at a designed dissipative dynamics toward a stationary state of interest. Many-body Lindblad master equations have been studied in the context of evaporative [144–150], laser [151–162] and sympathetic [163–167] cooling of degenerate atomic gases (see also [168]). Recently, there has been a revival of interest in such systems in the context of possibly using them for the preparation of interesting, pure, highly entangled states [123–125]. Open-system QSs employing superconducting qubits may also give insight into exciton transport in photosynthetic complexes [169].

The experimentalist who realizes an OSAQS, in contrast to an AQS, has to have at his/her disposal some non-unitary, dissipative quantum mechanism: in a sense, all designed cooling or entropy-reduction methods are of this sort.

- *Realizations.* All AQS systems can, in principle, be used as OSAQSs.
- *Controllability.* OSAQSs are typically not universal in the same sense as OSDQSs; they allow neither for simulating arbitrary (local) Markovian dynamics, nor for preparation of arbitrary states. Nevertheless, in most of the proposals [123–125] or experimental realizations they allow for a wide control of parameters, which in turn allows for simulation of open-system (Markovian) evolutions for wide families of open systems.
- *Error correction.* For OSAQSs, it is not guaranteed that error correction and fault-tolerant computing is possible in the sense defined in the subsection on OSDQSs.
- *Efficiency and reliability.* All of the above discussion concerning AQSs applies also to OSAQSs. But again due to the purely dissipative nature of the process, this type of simulation has a certain degree of intrinsic robustness and built-in 'error correction'—this is particularly clear for the OSAQSs of quantum kinetic Ising models or Kitaev's toric code [168]. Still, as in the case of OSDQSs, most of these general aspects concerning OSAQSs have not yet been investigated systematically.

5. Robustness of AQSs

All of the above considerations clearly lead to the fundamental question: can we trust QSs? From what we have said, the rigorous answer to this question is 'no', yet in practice we do tend to trust them, at least to some extent.

In order to gain more trust in the results of quantum simulations, it is thus extremely important to design novel tests and to certify the reliability and validity of QSs. In this section, which constitutes some of the most important results of this paper, we propose such tests, which we call tests of *robustness of QSs*. Our tests consist in checking the robustness of QSs with respect to the addition of imperfections, such as static disorder or dynamical noise. This would then allow us to (i) judge how strong the reaction of the QS is with respect to these perturbations and (ii) might even open possibilities to extrapolate interesting observables to the ideal, zero-disorder limit. Such tests can also be applied to DQSs, but are particularly suited to AQSs. For example, in an implementation with trapped ultracold atoms, disorder can be increased in a controlled manner [170].

In the following of this key issue paper, we use the example of the quantum Ising chain to substantiate our discussion of the reliability of AQSs and the relationship to the complexity/efficiency of the simulation. We study how imperfections affect the results of an AQS simulating that model, where, for simplicity, we assume quenched disorder as the only possible imperfection. In the future, it will be particularly interesting to also investigate the effects of dynamical noise, and the decoherence and relaxation that occurs due to coupling with an environment (see also [171]).

The quantum Ising model, which we describe in detail in section 6, is exactly solvable, which allows us to explore regions with universal behavior such as second-order QPTs. In section 7, we show that the ground-state expectation values of certain local observables appear fairly robust under disorder, while this need not be true for the global many-body state of the simulator. In particular, disorder can have a significant effect on relevant quantities that one could hope to extract from the simulator, such as critical points and exponents, or—if the system is described by a conformal field theory (CFT)—its central charge [172]. Finally, we briefly address the relationship between robustness and complexity by studying the dynamics of different thermal states after a quench of the Hamiltonian (section 8). We show evidence that QSs appear to work better in regimes that are classically easier to solve or simulate (high-temperature states), thus hinting at a connection between the amount of quantum correlations and the robustness of a QS.

6. The model

To illustrate the influence of disorder on an AQS, we study the TIM

$$H = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i^x\sigma_j^x - \sum_i h_i\sigma_i^z, \qquad (1)$$

where $\sigma_i^{x,z}$ are the usual Pauli spin matrices and $\sum_{\langle i,j\rangle}$ is the sum over nearest neighbors. The system is subject to quenched

disorder in both the interaction and field terms. We denote the nearest-neighbor spin coupling and the transverse field by $J_{ij} = J(1 + r\delta_{ij})$ and $h_i = h(1 + r\eta_i)$, respectively, where δ_{ij} and η_i are independent random variables with a Gaussian distribution of mean zero and variance r. All details of our calculations are presented in the appendix.

The TIM, even under the presence of disorder, is efficiently solvable—by which we mean that the eigenstates and eigenenergies of the system can be found using a classical computer, and that the cost of the algorithms (in time and hardware) is polynomial with the size (number of particles) of the system. The TIM, in particular, can be solved using a Jordan–Wigner transformation to a system of non-interacting fermions—and the cost of solving the non-interacting fermion system is the cost of diagonalizing a matrix with rank equal to twice the number of spins in the chain [173]. This model is well studied (see for instance [174]): for low fields, the ground state is a ferromagnet, while for large fields it is a paramagnet. At zero temperature and disorder, the system undergoes a QPT when the dimensionless control parameter $\lambda = h/J$ approaches the critical value, $\lambda_c = 1$, i.e. when the field intensity equals the interaction strength. The influence of disorder can have dramatic effects on this phase diagram: imperfections can create new phases, or even destroy the ones we want to investigate. Indeed, in the TIM when the disorder strength is comparable with the interactions, the critical point disappears and is replaced by a so-called Griffiths phase [175], extending across a region of size proportional to the disorder strength. Furthermore, in this Griffiths phase observables become non-self-averaging, i.e. fluctuations increase with system size, and hence dominate the thermodynamic limit. In this study, we consider small disorder strengths, which allows us to ignore the Griffiths phase, especially in finite-size systems. Moreover, a state-of-the-art AQS can achieve very low levels of disorder, whence this is the experimentally relevant regime. Note that, while the TIM has been studied extensively in the limit of very large disorder [176], there are few studies directly addressing the influence of small disorder on the universal properties near quantum-phase transitions. However, it is well known that even small disorder can lead to novel quantum phases such as Bose [177] or Fermi [178] glasses (see also the section on disorder in [179] and references therein). In the following, we analyze the robustness of relevant observables to disorder in static and dynamic situations.

7. Results—statics

First, we investigate the static properties of the AQS and their robustness to disorder (summarized in figure 1). We average all the analyzed static quantities over many realizations of disorder.

One can evaluate the response of the AQS to disorder using the *simulator fidelity*, which we define for pure states as the overlap between the state obtained with a perturbed simulator, $|\Psi_r(\lambda)\rangle$, and the ideal state $|\Psi_0(\lambda)\rangle$,

$$F(r, \lambda) = |\langle\Psi_0(\lambda)|\Psi_r(\lambda)\rangle|. \quad (2)$$

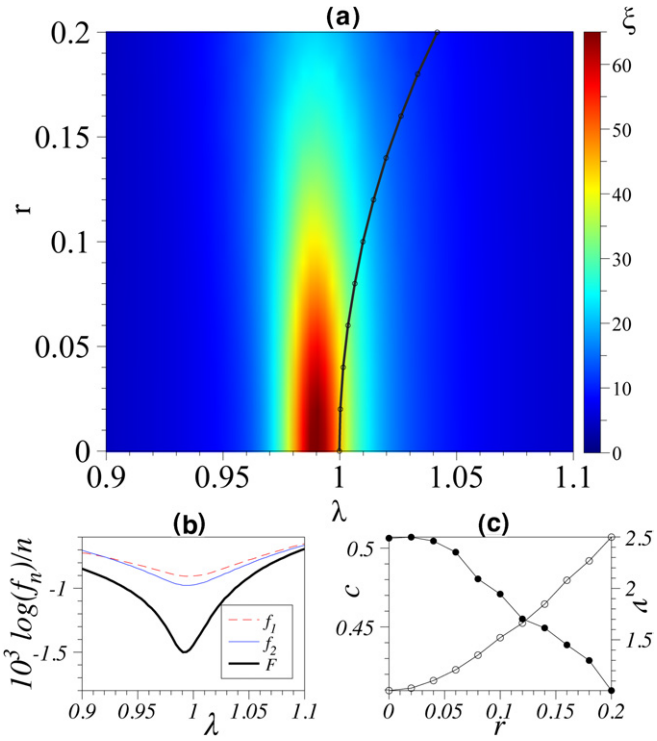

Figure 1. (*a*) The correlation length ξ decreases with disorder r and its peak broadens (shown for a chain of 400 spins). The critical point (as extracted from a finite-size scaling of the energy gap Δ) moves to larger λ with increasing disorder (black line). (*b*) For a chain of 400 spins, we show the mean single- and two-site reduced simulator fidelities (f_1 and f_2), and the total simulator fidelity (F) for a fixed disorder level $r = 0.1$. Local fidelities are more robust, which gives hope that local quantities can be reliable even if disorder deteriorates the overall ground state. As expected, disorder has more severe effects close to the QPT. (*c*) The central charge c (full circles, left axis), extracted from a fit to the part-chain entropy, and the critical exponent ν (open circles, right axis), extracted from a collapse of the correlations in different chain lengths. Both change with disorder, which can lead to erroneously assigning the QPT to an incorrect universality class. However, the change begins relatively smoothly at low levels of disorder.

Although we define the simulator fidelity for any possible target state, we focus on the ground state. As figure 1(*b*) shows, this overlap is considerably suppressed near the QPT, reaching values as low as 55% (for $r = 0.1$ in a chain of $L = 400$ sites). When scaling to larger systems, $F(r, \lambda)$ will typically vanish exponentially fast, simply due to the exponential growth of the dimension of the Hilbert space (a kind of 'orthogonality catastrophe'). In a universal quantum computation, the fidelity would have to be very close to 1 for the quantum computer to work fault tolerantly. However, QSs have the advantage that we do not necessarily demand of the entire state to be robust. Often, it is enough if we can distinguish the relevant phases by measuring faithfully *local* observables (local in the quantum information sense that few sites are involved, although they may be physically far apart). Obviously, this is less demanding, yet very useful.

To quantify the robustness of local observables, we investigate the single-site and (nearest-neighbors) two-site simulator fidelity $f_1(r, \lambda)$ and $f_2(r, \lambda)$, respectively. As the one- and two-particle density matrices will generally be mixed

when the overall pure many-body state is entangled, these are defined as the Uhlmann fidelity [180] between the single- or two-site reduced density matrices of the ideal state and the one at disorder strength r, $f \equiv \mathrm{Tr}\sqrt{\sqrt{\rho_0}\rho_r\sqrt{\rho_0}}$. It can be assumed that fidelities of the reduced system decrease more or less monotonically with the number of sites involved. As seen in figure 1(*b*), the reduced simulator fidelities are much more robust to disorder than the global one—near the phase transition, $f_2(r, \lambda)$ decreases to approximately 0.998, and $f_1(r, \lambda)$ remains above 0.999. This gives optimism that local quantities are robust enough to allow a faithful distinction between different quantum phases.

One step beyond local properties of the ground state are the *correlation lengths* dictating the exponential decay of long-distance correlation functions. We investigate the correlation length ξ extracted from the correlation function

$$C(i, j) = \langle\Psi_r|\sigma_z^{(i)}\sigma_z^{(j)}|\Psi_r\rangle - \langle\Psi_r|\sigma_z^{(i)}|\Psi_r\rangle\langle\Psi_r|\sigma_z^{(j)}|\Psi_r\rangle\,, \tag{3}$$

where away from criticality $C(i, j) \propto \exp(-|i - j|/\xi)$. Without disorder and for infinite systems, ξ diverges at the critical point, because criticality is the emergence of collective phenomena involving infinite degrees of freedom at all length scales. In practice, we can only deal with finite systems so that we cannot observe real criticality but only smoothed out signatures of it, a phenomenon which one normally calls 'pseudo-criticality'. For example, the correlation length ξ is bounded by the system size. Still, its peak gives a reliable signature for the location of the critical point. As figure 1(*a*) shows, however, disorder suppresses correlations and broadens the peak of ξ, thus making an extraction of the critical point much less reliable.

Another criterion to locate the QPT is provided by the *energy gap* Δ between ground state and first excited state. At criticality, the low-energy spectrum of the Hamiltonian is gapless in the thermodynamic limit. In finite systems, it presents non-vanishing gaps that decrease in a systematic way with increasing system size. Due to this characteristic scaling of physical observables as a function of system size in pseudo-critical systems, criticality can be detected by studying a sequence of finite but increasingly large systems, a technique called *finite-size scaling* [181]. We describe this technique for the energy gap in the appendix (see figure A1), and show in figure 1(*a*) (black line) the location of the critical point extrapolated in this way. As can be seen, if one does not correct for disorder effects, one would locate the critical point at values of λ that are larger than the ideal value.

Perhaps of more fundamental interest than the exact location of a critical point is its *universality class*. All models within a given universality class give rise to the same collective behavior at large distances (typically large with respect to the lattice spacing), irrespective of their microscopic details [172]. Therefore, all relevant thermodynamic quantities for all models within a class are characterized by the same small set of *critical exponents* which describe the power-law decay of the correlation functions of local observables in the large-distance regime, a property that allows differentiation among different emerging collective behaviors. To investigate how robust the universal behavior is, we compute the critical exponent for the correlation length, ν, from a collapse of the correlations (as explained in the appendix, see equation (A10) and figure A1). As shown in figure 1(*c*), already for a few percent of disorder, ν increases strongly from its ideal value 1. Therefore, if one simply neglects the influence of disorder, the extraction of critical exponents yields incorrect results.

If the QPT is described by a CFT (a specific subclass of one-dimensional critical systems), it is characterized by a *central charge* c. The central charge appears ubiquitously [182]. For example, it governs the temperature dependence of the free energy (Stefan–Boltzmann law) and the Casimir effect in finite geometries, but also the scaling of the entanglement entropy of sub-regions of the ground state of the corresponding quantum models. Models with different central charge have different emerging collective behavior. For example, models whose collective behavior is that of a free Majorana fermion (as in the disorder-free TIM) have central charge $= 1/2$, while models whose collective behavior is that of a free boson have central charge $= 1$. Strictly speaking, the TIM has an underlying CFT only in the disorder-free case, but there have been efforts to extract an effective central charge also for the disordered model [176], for example, from the von Neumann entropy S of the reduced density matrix of a part of the chain of size l. At criticality, this entropy scales as $c/6\log(L/\pi\sin(l\pi/L)) + A$ [183–185]. Figure 1(*c*) shows that disorder decreases the effective central charge. Hence, ignoring the effects of disorder would give completely erroneous results, since even a small deviation of the central charge indicates a completely different universality class. Note also that the decrease of c with disorder indicates the destruction of correlations by disorder.

Fortunately, for all the extracted quantities (except the global simulator fidelity), the levels of disorder for appreciable changes to occur are at least a few percent. If the AQS can be operated below such a value, its results seem to be robust, at least in this simple model system. State-of-the-art experiments are good enough to fulfil this requirement. In fact, in many experimental situations one hopes to reach levels of disorder or noise that are below a few percent, ensuring the robustness of the AQS. Frequently, however, changing parameters from the regime where validation via classical simulation is possible to the regime of *terra incognita* might lead to uncontrolled disorder or noise. This is why checking sensitivity to disorder and noise in those regimes where it can be checked is of great importance.

8. Results—dynamics

Efficient classical algorithms for computing static properties of quantum systems are more developed than for computing dynamics (the difficulty arises mainly because entropy and correlations grow rapidly with simulated time). Therefore, one can assume that in the absence of disorder, a quantum simulation of dynamics can much more easily outperform classical computers. Indeed, in a recent experiment based on ultracold bosonic atoms, the controlled dynamics ran for longer than present classical algorithms based on matrix product states

could efficiently track [14]. We thus turn to the issue of how disorder affects the reliability of quantum simulations of dynamics. As with statics, we investigate the behavior of the simulator fidelity, but now also as a function of time, initial state, and external driving.

Typically, we expect that the simulator fidelity will decay with time, and eventually reach an asymptotic finite value. The effect of disorder in both the decay rate and the asymptotic saturation value can, in general, be understood from established techniques such as Fermi Golden's rule, and random matrices [186]. On the other hand, the effect of the initial state and the external driving is known to be nontrivial and of particular interest for our purposes. For example, it is known that numerical techniques such as the time-dependent density matrix renormalization group (tDMRG) can efficiently simulate the dynamics after a sudden quench of the field h, as long as the quench is restricted to a few sites on the chain. However, if the quench is global, it has been shown that the computational resources needed to keep a fixed amount of error grow exponentially with time [187, 188]. Generically, solving for the dynamics of a quantum many-body system is a hard problem for classical algorithms. Our model is special because it can be solved exactly for all cases, although it remains hard for the tDMRG algorithm. We use this to our advantage to study how this class of classical algorithms behaves when solving for quantum dynamics.

We studied the behavior of the full simulator fidelity under the following driving. As the initial state we prepare the ground state of the Hamiltonian for a given value of the external field. At time zero, the field is quenched instantaneously to a larger strength, and the system is allowed to evolve. In panels (b) and (c) of figure 2, we compare the short- and long-time behavior of fidelity for the case of a global and a local (single-site) quench. The AQS keeps a high fidelity in the case of a local quench, while it performs poorly for the global quench, with fidelities reaching lows of 0.8 even for small systems of 50 spins. We also observe that the AQS performs worse when the quench crosses the critical point, as shown in figure 2(c), where we fix the strength of the quench and vary the initial field value.

The initial state can also have an effect on the efficiency of classical algorithms. Using the same setup with a global quench, but starting from a thermal initial state, tDMRG becomes efficient for high temperatures [187] where the state and its correlations are almost classical. However, it becomes exponentially inefficient with time for low-temperature initial states. For initial thermal states, we can still compute the dynamics exactly, although computationally it becomes too expensive to calculate the full many-body fidelity between the evolved states. In this case, therefore, we focus on the reduced simulator fidelity. For the regimes of disorder that we studied, we observe that the time-dependent fidelity decays with a rate roughly proportional to the strength of the disorder squared (typical of a Fermi golden rule [186]). For this reason, we show in figure 2(a) a rescaled form of the fidelity, $(1 - f_1)/r^2$, that exemplifies the typical behavior for all disorder strengths, as a function of time and temperature of the initial state.

As with the classical algorithms [187], the AQS remains faithful when the state is almost classical (high temperatures).

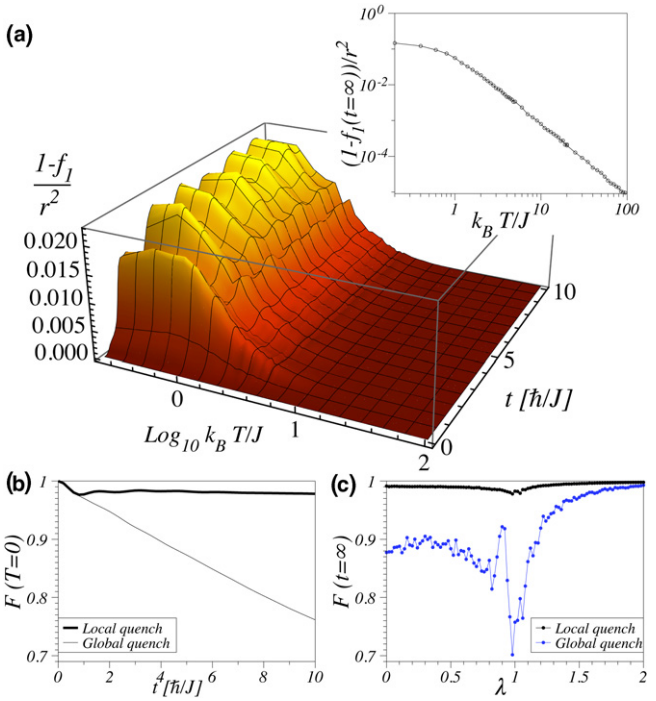

Figure 2. (a) Evolution of the average reduced simulator fidelity as a function of the temperature of the initial state. The system is an Ising spin chain of length 50, the initial state is a thermal state at criticality ($\lambda = 1$), and at time zero the field is suddenly quenched to $\lambda = 2$. In the vertical axis we show the infidelity (one minus fidelity) normalized by the disorder strength r squared. For larger temperatures (where there are less correlations) the state is more robust. In the inset, we show the average asymptotic infidelity as a function of temperature. For large temperatures it decays as $1/T^2$. (b) Evolution of the full simulator fidelity for an initial state equal to the ground state (zero temperature) at $\lambda = 0.75$ after a sudden quench to $\lambda = 1.25$. For a local quench in a single site, fidelity saturates rapidly at large values, but decreases strongly for a global quench. (c) Asymptotic value of the total simulator fidelity as a function of the initial value of the field λ, with a fixed quench strength of $\delta\lambda = 0.25$. The system is much less robust for global quenches and near criticality ($\lambda = 1$).

The simulator fidelity decreases rapidly for low temperatures, although it saturates at a fairly high value. In terms of distinguishability, the values we find imply that a fair observer would have only a 4% chance of distinguishing the 1-spin reduced state of the AQS from the ideal state. In the inset of figure 2(a) we show the average asymptotic fidelity as a function of temperature of the initial state. Again, for low temperatures fidelity worsens, but saturates to a few percent. For high temperatures, an expansion of the fidelity can be simply performed which shows that $f_1 \simeq 1 - T^{-2}$.

9. Discussion and outlook

A key issue for future investigation is the relationship between the robustness of an analog quantum simulator and its computational power. For the models we have considered here, the physically relevant correlation functions are robust for a reasonable degree of disorder. This suggests that such an AQS could perform well in a laboratory demonstration. However, the TIM that we considered here is simulatable on a

classical computer. Is this connection between robustness and classical simulatability coincidental, or does it reflect a deeper relationship?

Disorder reduces the correlation length of the spin chain. Because less-correlated quantum states can be described with fewer parameters, there is reason to suspect that certain aspects of weakly disordered quantum many-body systems could actually be *easier* to simulate on classical computers than their clean idealized versions. This happens, for example, in the realm of digital quantum computation, where a quantum circuit becomes classically simulatable for noise above a certain level when quantum gates lose their entangling power [189–191]. In the context of many-body physics, the success of DMRG in, e.g. 1D spin chains, is rigorously related to the existence of efficient matrix-product-state representations [192]. These take advantage of the small amount of quantum correlations in such systems, thus compressing the $O(\exp(n))$ parameters needed to describe a general n-particle state to $O(n)$ finite-dimensional matrices. In higher-dimensional lattices, states which obey the so-called 'area law' [95], where quantum correlations are smaller than in generic states, may still be amenable to a classical simulation using state-of-the-art techniques such as tensor networks [75, 79, 80, 193, 194], density functional theories [84], or quantum Monte Carlo [73].

We thus arrive at the fundamental question: *Do the finite imperfections of an analog quantum simulator reduce the correlations, and thus the number of parameters needed to describe the system, so as to render the device simulatable by classical means*? We know that for noise above certain levels a digital quantum circuit is classically simulatable and for levels below a certain threshold it can be rendered fault tolerant. Is there an *intermediate regime* for which noise is too great to allow fault-tolerant universal quantum computation, but small enough that an AQS accesses physics beyond classical simulation? The existence of an intermediate regime would imply that a whole class of problems exists outside P that we can access in the near future, even without a fully functioning quantum computer.

The results we present here, in particular those for dynamics, are an initial attempt—albeit in a trivial model—at understanding the above problem. We can see how an analog quantum simulator works well when a classical solution is efficient, and worsens (but only in a limited way) when the problem becomes classically hard to simulate. Even though the underlying model is actually solvable, this may be positive evidence for the existence of an intermediate regime of noise, and the efficiency of AQSs in more complex situations.

Our main discussion focused on AQSs, but similar issues pertain to DQSs. Since to date there exists no known way to fault-tolerantly error-correct AQSs, there is a natural tendency to explore the advantages of DQSs, where error correction is possible. The above discussion shows, however, that a digital implementation of a quantum simulation does not, in itself, guarantee an efficient and more powerful simulation than one that is carried out classically. As in any quantum algorithm, initialization, evolution of the state, and measurement must be performed efficiently, i.e. with a polynomial use of physical resources (space and time). Digital quantum simulation is no exception. Indeed, as discussed above, a fault-tolerant implementation of the standard approach based on the Trotter expansion [96] comes at the cost of an overhead in the number of gates and time required that grows exponentially with the degree of precision required [63, 117]. If we can guarantee the reliability of analog quantum simulators while avoiding such exponential costs, many open problems from all areas of physics could suddenly come within reach of being solved.

Finally, we can turn the problem of quantum simulation on its head and ask, what does Nature do? For any real material, like a high-T_c cuprate, has imperfections. Does Nature access highly correlated states that cannot be efficiently simulated on a classical computer? Certainly, in some cases we believe it does, as for example in high-T_c superconductors [68] or in certain ground states of frustrated quantum antiferromagnets which are believed to carry topological order [87]. If noise is low enough, does Nature protect quantum correlations to a degree that classical methods cannot efficiently represent the physically interesting quantities? And can we exploit this capability with a quantum simulator? If Nature does it, we should take advantage of it!

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Appendix

Quadratic fermionic systems. The transverse field Ising model, equation (1) of the main text, even with disorder, can be solved by casting it into the form of non-interacting fermionic particles using the Jordan–Wigner transformation,

$$\sigma_j^+ = c_j^\dagger \prod_{m=1}^{j-1} \mathrm{e}^{-\mathrm{i}\pi c_m^\dagger c_m}, \tag{A1a}$$

$$\sigma_j^- = \prod_{m=1}^{j-1} \mathrm{e}^{\mathrm{i}\pi c_m^\dagger c_m} c_j, \tag{A1b}$$

$$\sigma_j^z = 2c_j^\dagger c_j - 1. \tag{A1c}$$

The $c_j, c_j^\dagger$ obey on commutation relations. This transformation leads to

$$\hat{H} = \sum_{i,j} \left[c_i^\dagger A_{ij} c_j + \left(c_i^\dagger B_{ij} c_j^\dagger + h.c. \right) \right] - \frac{1}{2} \sum_j A_{jj}, \tag{A2}$$

where

$$A_{ij} = -J_{ij} \left(\delta_{j,i+1} + \delta_{j,i-1} \right) - 2h_i \delta_{j,i}, \tag{A3a}$$

$$B_{ij} = -J_{ij}\gamma\left(\delta_{j,i+1} - \delta_{j,i-1}\right). \tag{A3b}$$

Hamiltonian equation (A2) can be diagonalized to

$$\hat{H} = \sum_{k=1}^{N} \Lambda_k \eta_k^\dagger \eta_k + E_0, \tag{A4}$$

where $\Lambda = \Phi\,(A-B)\,\Psi^\intercal$ is diagonal. Λ, Φ and Ψ can be obtained from the singular-value decomposition of $Z \equiv A-B$. The normal modes are $\eta_k = \sum_{j=1}^{N}\left(g_{k,j}c_j + h_{k,j}c_j^\dagger\right)$, where $g = (\Phi+\Psi)/2$, and $h = (\Phi-\Psi)/2$. From this, we can compute the relevant ground-state properties.

Ground-state fidelity and correlations. From the normal modes obtained in the diagonalization of the previous section, we can compute the observables we are interested in: the simulator fidelity F (the overlap to the disorder-free ground state), reduced simulator fidelities, the energy gap, and the ZZ-correlations.

In general, the overlap between the ground states of two realizations Z and $\widetilde{Z}$ is [195]

$$F\left(Z,\widetilde{Z}\right) = \sqrt{\det\frac{1+T^{-1}\widetilde{T}}{2}}, \tag{A5}$$

with $T = \left(\Phi^{-1}\Lambda\Phi\right)^{-1} Z$. We define the simulator fidelity F as the overlap at fixed λ between the ideal, disorder-free state and the state at disorder strength r,

$$F(r,\lambda) \equiv F\left(Z(\lambda)_r, Z(\lambda)_0\right). \tag{A6}$$

This is a global quantity, but one can expect that local observables are less affected by disorder. A measure for the change of local quantities is the *single-site simulator fidelity*

$$f_1(r,\lambda) = \sum_{i=1}^{L} \mathrm{tr}\sqrt{\sqrt{\rho_0^{(i)}(\lambda)}\rho_r^{(i)}(\lambda)\sqrt{\rho_0^{(i)}(\lambda)}}, \tag{A7}$$

where $\rho_r^{(i)} = \mathrm{tr}_{j\neq i}\rho$ is the reduced density matrix of site i under disorder r, and $\rho_0^{(i)}$ is the equivalent in the disorder-free case. The single-site reduced density matrix is completely determined by the expectation values of σ_i^μ, $\mu = x, y, z$, since one can expand $\rho^{(i)} = \frac{1}{2}\sum_\mu \langle\sigma_i^\mu\rangle\sigma^\mu$. Here, the sum runs over σ^μ, $\mu = x, y, z$ and $\sigma^{(0)} = \mathbb{I}$. We also analyse the *two-site simulator fidelity*

$$f_2 = \sum_{i=1}^{L} \mathrm{tr}\sqrt{\sqrt{\rho_0^{(i,i+1)}(\lambda)}\rho_r^{(i,i+1)}(\lambda)\sqrt{\rho_0^{(i,i+1)}(\lambda)}}, \tag{A8}$$

for nearest neighbors. Here, $\rho_r^{(i,i+1)} = \mathrm{tr}_{j\neq i,i+1}\rho$ is the reduced density matrix of sites $(i, i+1)$ under disorder r, and $\rho_0^{(i,i+1)}$ is the equivalent in the disorder-free case. We compute all considered static quantities as the mean over a large number of disorder realizations; for the fidelities F, f_1 and f_2 displayed in figure 1(*b*) of the main text, we used 5000 realizations at chain length $L = 400$.

The correlations can finally be computed using the fact that the ground state $|\Psi\rangle$ of equation (A4) is the vacuum of the normal modes (i.e. $\eta_k|\Psi\rangle = 0, \forall k$). For example, for the ZZ-correlations this yields

$$\begin{aligned} C(i,j) &\equiv \langle\Psi_r|\sigma_z^{(i)}\sigma_z^{(j)}|\Psi_r\rangle - \langle\Psi_r|\sigma_z^{(i)}|\Psi_r\rangle\langle\Psi_r|\sigma_z^{(j)}|\Psi_r\rangle \\ &= 4\langle\Psi_r|c_i^\dagger c_i c_j^\dagger c_j|\Psi_r\rangle - 4\langle\Psi_r|c_i^\dagger c_i|\Psi_r\rangle\langle\Psi_r|c_j^\dagger c_j|\Psi_r\rangle \\ &= 4\,(h^\intercal h)_{ij}\,(g^\intercal g)_{ij} - 4\,(h^\intercal g)_{ij}\,(g^\intercal h)_{ij}\,. \end{aligned} \tag{A9}$$

Away from criticality, the correlations decay as $C(i,j) \propto \exp(-|i-j|/\xi)$ with *correlation length* ξ. In figure 1(*a*) of the main text, we display ξ extracted from fits to part of the wings of $C(i,j)$ (for $L = 400$ and 10 000 disorder realizations).

Without disorder,

$$C(i,j)L^{2\nu} \propto f(|i-j|/L) \tag{A10}$$

for some universal function f [172]. Hence, one can extract the critical exponent for the correlation length ν from a data collapse of the correlations. In figure 1(*c*) of the main text, we show the erroneous values for ν, extracted from equation (A10) if one naively neglects that this relationship is no longer true in the presence of disorder. Figure A1 shows the best collapse achieved with equation (A10) for disorder levels $r = 0$ and 0.2. The value of ν for the best collapse increases with disorder. Hence, using equation (A10) on a disordered AQS yields a very large critical exponent, compared with the ideal model. Moreover, the quality of the collapse worsens with increasing disorder, demonstrating that a naive application of equation (A10) is unjustified if disorder is large. For this analysis, we used $L = 100$ to 190 in steps of 10 with 10^6 disorder realizations, $L = 200$, 250 and 300 with 5×10^5 realizations, and $L = 350$ and 400 with 10^5 realizations.

The correlations are intrinsically connected to the energy gap $\Delta(L)$, since a gapped system necessarily has exponentially decaying correlations [196]. Via a finite-size scaling, the gaps at finite systems also allows us to extract the location of the QPT in the infinite system, as seen in figure A1. There, we plot curves $1/(L^\zeta\Delta(L))$ for closeby chain lengths L, where ζ is the dynamical critical exponent, which for the disorder-free case equals 1. These cross at a series of pseudo-critical points which with increasing L tends rapidly to the critical point of the thermodynamic limit [197]. Assuming that it does not change much for small disorder, we identify as an approximation the critical point with the mean of the crossing points curves $1/(L\Delta(L))$ for $L = 100, 150, 200, 300, 350, 400$ with 10 000 realizations of disorder each. As displayed in figure A1, the crossing point moves to larger values of λ with increasing disorder (see also figure 1(*a*) of the main text). This means that applying this analysis to a real-world AQS without correcting for disorder can yield erroneous results (compared with the ideal model) for the location of the QPT. Moreover, the crossing point becomes less well defined with increasing disorder showing that this analysis should be corrected for the presence of disorder. Finally, at large disorder, a second crossing point appears at lower λ. The two crossing points open up to a V-like structure with increasing disorder. This could be interpreted as an indication of the Griffiths phase (the

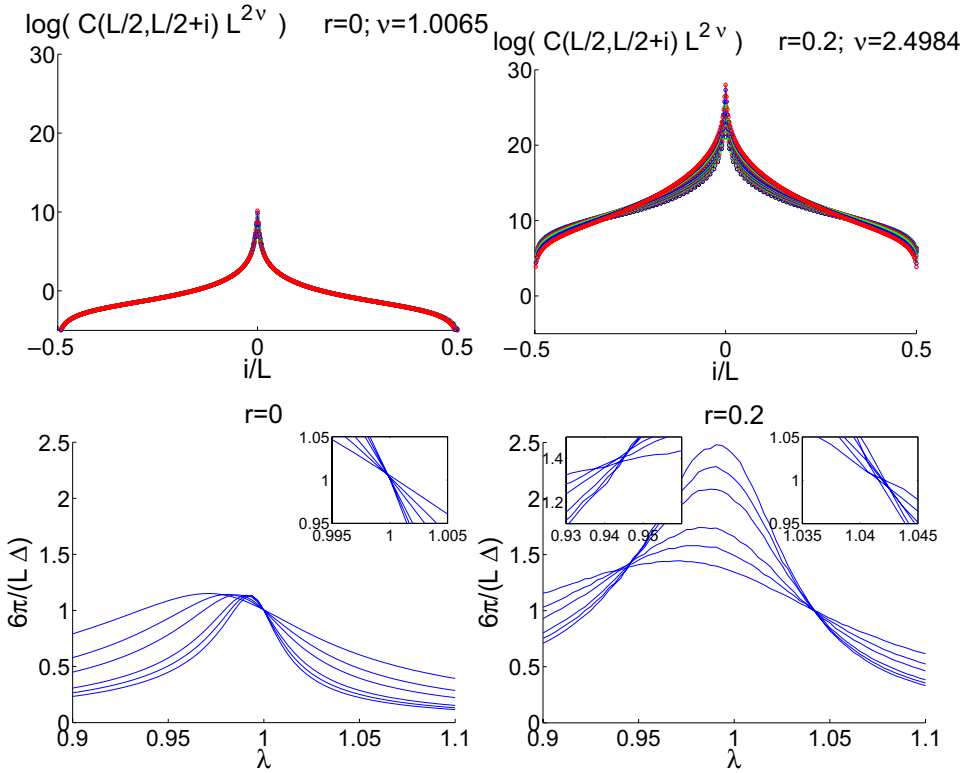

Figure A1. Top row. For low disorder ($r = 0$, left), the curves $C(i, j)L^{2\nu}$ for different L plotted as functions of $|i - j|/L$ collapse perfectly for the physically correct value of the critical exponent $\nu = 1$ (dots of different color correspond to different L). For increasing disorder ($r = 0.2$, right), the collapse worsens, and the best collapse is obtained for some $\nu > 1$. Bottom row. For low disorder ($r = 0$, left), the curves $1/(L\Delta(L))$ cross perfectly at the location of the critical point, $\lambda = 1$. With increasing disorder ($r = 0.2$, right), the crossing point moves to larger values of λ and becomes less well defined. Also, at large disorder a second crossing point appears below $\lambda = 1$. The insets show zooms on the crossing points. The findings of both rows of figures mean that, ignoring the effects of disorder in an imperfect AQS yields, compared with the ideal model, too large values for the critical exponent as well as the location of the critical point.

crossing points are qualitatively consistent with the extent of the Griffiths phase found in [198]). For a more quantitative analysis, however, one would need to account for a change of ζ with increasing disorder.

If a given model can be described by a CFT, its universal critical behavior (including all critical exponents) is completely defined by a single number, the central charge c. To extract it, we compute the von Neumann entropy S of the reduced density matrix of a part of the chain of size l for $L = 300$ with 10 000 disorder realizations. For systems with open boundary conditions, a fit to $c/6 \log(L/\pi \sin(l\pi/L)) + A$ (excluding small values of l) yields the effective central charge c [183–185]. The disorder-free value is $c = 0.5$. Increasing disorder suppresses this, indicating the decrease of entanglement in the system (see figure 1(c) of the main text). Again, applying the analysis that is correct in the disorder-free case (where the system is indeed described by a CFT) without adjustments to the disordered system, yields results which deviate from the desired ideal case.

Time-dependent fidelities. For time evolution, we distinguish between the zero and finite temperature fidelities, although the underlying technique is the same. We start by rewriting the fermionic Hamiltonian above as

$$\hat{H} = \frac{1}{2}\vec{\Psi}^\dagger \cdot \mathrm{H} \cdot \vec{\Psi}, \tag{A11}$$

where $\vec{\Psi}^\dagger = (c_1^\dagger, ..., c_N^\dagger, c_1, ..., c_N)$ is a $2N$ length vector composed of all creation and annihilation operators present in $\hat{H}$, and $\mathrm{H} = A \otimes \sigma_z + \mathrm{i}B \otimes \sigma_y$ is a $2N \times 2N$ matrix with complex coefficients.

For computing fidelities, we use the convenient Levitov's formula [199, 200], which relates traces of operators in the Hilbert space of the fermions to determinants of much smaller matrices (like H). For example, let $\hat{P} = \vec{\Psi}^\dagger \cdot \mathrm{P} \cdot \vec{\Psi}$ and $\hat{Q} = \vec{\Psi}^\dagger \cdot \mathrm{Q} \cdot \vec{\Psi}$ be two operators in the space of fermions, with P and Q complex valued $2N \times 2N$ matrices. Then,

$$\mathrm{Tr}\left(e^{\hat{P}} e^{\hat{Q}}\right) = \det\left(1 + e^{\mathrm{P}} e^{\mathrm{Q}}\right). \tag{A12}$$

Similar formulae hold for more or less operators.

In the zero-temperature case, when the initial state remains pure after evolution, the fidelity takes the form of an overlap

$$F = |\langle\psi_0(t)|\psi_r(t)\rangle|, \tag{A13}$$

where $|\psi_0(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}_0 t}|\psi_0\rangle$ is the initial state evolved with the target Hamiltonian of the simulation, $\hat{H}_0$, and $|\psi_r(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}_r t}|\psi_0\rangle$ is the same state evolved with an imperfect Hamiltonian $\hat{H}_r = \hat{H}_0 + r\hat{V}$. Rewriting the fidelity,

$$F = \mathrm{Tr}\ \rho_0 \mathrm{e}^{\mathrm{i}\hat{H}_r t} \mathrm{e}^{-\mathrm{i}\hat{H}_0 t}, \tag{A14}$$

with $\rho_0 = |\psi_0\rangle\langle\psi_0|$, we can use Levitov's formula and obtain

$$F = \det\left(1 - G_0 + G_0 e^{\mathrm{i}H_r t} \mathrm{e}^{-\mathrm{i}H_0 t}\right), \qquad \text{(A15)}$$

with $G_0 = \langle\psi_0|G|\psi_0\rangle$, and G the correlation matrix of the original fermionic operators, $G_{i,j} = \Psi_i^\dagger \Psi_j$.

If the initial state is not pure, but a thermal state, the state remains mixed even if the evolution is unitary. In this case, we cannot compute the fidelity for the full many-body state, but only the fidelity of the reduced density matrix for a few spins. For this we must evaluate the correlation functions of the Pauli operators at different sites of the chain. For the case of a single spin, the symmetry of the system ensures that at all times the reduced density matrix can be written as $\rho = (1 + \langle\sigma_x^i\rangle\sigma_x^i)/2$. Since $\langle\sigma_x^i\rangle = c_i^\dagger c_i$, we only need to compute the evolution of the diagonal terms in the G correlation matrix.

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