Many-body Quantum Mechanics: Too big to fail?

Special purpose quantum computers—realized with current technology—have the potential to revolutionize physics, chemistry, and materials science.

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Quantum computers, devices whose components obey the laws of quantum mechanics, hold promise to solve problems that cannot be tackled with classical computers. As opposed to a classical computer, whose elements are bits that can take on two discrete values, a quantum computer is comprised of quantum bits, or “qubits,” which are quantum mechanical objects with two distinct states. The essential advantage of qubits over bits is they display the quantum mechanical features of “superposition”—a qubit is in a linear combination of its two states—and “entanglement”—the outcome of measurements on one qubit is perfectly correlated with another qubit (see Figure 1), even though measurements on either qubit alone

give random values. Over the past three decades, enormous effort has been put toward the construction of a universal quantum computer with some fantastic successes. Still, at present, realistic quantum computing remains in its early stages. The most fruitful application of quantum computation might turn out to be a more specialized one, which

has the potential to revolutionize research in condensed matter physics, materials science, and chemistry. The prototypes of which have already been realized in labs around the world as the quantum simulator.

The very notion that there are some tasks quantum computers can perform efficiently and classical computers cannot means the computational

complexity, class-bounded error quantum polynomial time (BQP), consisting of problems that are tractable (solvable in polynomial time) on a quantum computer, is assumed to be different than the complexity class P , which contains problems that are tractable on classical computers. Perhaps the most prominent example of a problem that is in BQP but thought not to be in P , is

integer factoring: Given an integer N , what are its prime factors? The best known classical algorithm for solving this problem scales in sub-exponential time, but the now-famous quantum algorithm discovered by Peter Shor solves this same problem in polynomial time [1].

Many widely used cryptographic schemes rely on the fact that it is hard for classical computers to factor large numbers. That a large-scale quantum computer can efficiently break

these schemes has been a powerful impetus driving the field of quantum computing forward. In spite of this, there also exist so-called post-quantum cryptography schemes—tough even for quantum computers to crack [2]. Hence, while integer factoring is a fascinating example of the power of quantum computers, it is likely not the “killer app” of quantum computation. Controllable quantum many-body systems consisting of a few tens or more particles, even while

not capable of universal quantum computation, can efficiently perform tasks that are intractable on classical computers; namely, solving for the dynamics of quantum many-body systems. This seemingly tautological insight, first put forward by Richard Feynman [3], has led to the field of quantum simulation. In which “designer” quantum many-body systems built of well-characterized components—such as ions, atoms, molecules, and superconducting electrodes at very low temperatures—realize the dynamics of some other quantum system of interest—such as a high temperature superconductor, which is much harder to control or probe experimentally.

Before discussing quantum simulation in more detail, it is worth pointing out the enormous conceptual difference between the classical and quantum many-body problems. In classical mechanics, our “microscopic” degrees of freedom are the positions and momenta of N particles, which, in three dimensions, is a set of $6N$ real numbers. Given a set of $6N$ initial conditions for these variables, one then simulates dynamics by solving $6N$ (coupled) differential equations, e.g. Newton’s equations. If our particles interact only pairwise, as is essentially always the case, each one of the differential equations involves N terms, and our total computation scales as $O(N^2)$. Hence, the classical many-body problem can be solved in $\text{poly}(N)$ time on a classical computer, and so is in the complexity class P . This class of prob-

Figure 1. [a] Classical bits are binary, while qubits can be in any superposition state defined by two coefficients that can be represented as the surface of a sphere. [b] The number of coefficients needed to represent N qubits scales exponentially, which makes quantum problems prohibitively hard to solve on classical computers. [c] Two qubits can be in an entangled state.

lems essentially defines what it means for a problem to be tractable.

It should be noted that for a macroscopically large system, say on the order of Avogadro's number of particles ($N \sim 10^{23}$), we still cannot efficiently simulate the dynamics of every single particle efficiently by solving the coupled differential equations as outlined previously. However, for such a large system, the absolute positions and momenta of all particles is completely useless information for obtaining the macroscopic-scale behavior of the system that we usually care about. In addition, macroscopically large systems will also be subject to deterministic chaos, which makes the specification of all 10^{23} initial conditions irrelevant. In such situations, it is more useful to "coarse grain" the system and ask, not about the behavior of its microscopic constituents, but about macroscopic observables. This is in the spirit of defining thermodynamic observables, such as pressure or temperature for a gas, which describe the state of the macroscopic system, but contain no information about the microscopic properties.

Now we turn to quantum problems. For concreteness, we will consider quantum problems, which involve some particles arranged in a regular array and each particle has a few discrete quantum states it can occupy. Physicists often call these objects "spins," in analogy to the discrete spin degree of freedom of elementary particles such as electrons. In addition, we will fur-

ther specialize to the case of "spin-1/2," in which each particle has exactly two states, which we will denote $|\uparrow\rangle$ and $|\downarrow\rangle$. Such elemental objects can also be thought of as the qubits defined previously. Here, $|\psi\rangle$ denotes a vector in Hilbert space, the normed linear vector space in which quantum mechanics is formulated. For a single spin, its state $|\psi\rangle$ is completely specified as a linear combination of the two basis states above, $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$, where, e.g., $|a|^2$ can be interpreted as the probability to measure the system to be in the state $|\uparrow\rangle$. The dynamics of this state is de-

scribed by the Schrödinger equation (using units where $\hbar=1$)

$$i \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

where $\hat{H}$ is a matrix acting on Hilbert space, called the Hamiltonian, which represents the total energy of the system. Hence for a single spin, solving the Schrödinger equation amounts to integrating a 2×2 matrix differential equation—this is easy to do.

What happens as we increase the number of spins in our array? It is insightful to first consider the case of two

Figure 2. The set of states that a reasonable quantum system can reach in a reasonable time is an exponentially small fraction of all allowed states.

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spins [1]. Here, the postulates of quantum mechanics specify the Hilbert space of two particles is spanned by the four states: $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, where the left and right objects in $|\bullet\rangle$ denote the quantum state of the two particles in some ordering (say, the left and the right particle in a one-dimensional array). Suppose we are now given the state of the system as: $a|\uparrow\downarrow\rangle + b|\downarrow\uparrow\rangle$ with $a = b = 1/\sqrt{2}$. We are asked what are the states of particle 1 and particle 2? Using our prescription, we find $|a|^2 = 1/2$ of the time we measure particle 1 to be in the state $|\uparrow\rangle$, and $|b|^2 = 1/2$ of the time we measure particle 1 to be in $|\downarrow\rangle$, and similarly for particle 2. However, strikingly, we note whenever we measure particle 1 to be in $|\uparrow\rangle$ we always measure particle 2 to be in $|\downarrow\rangle$, and similarly with $|\uparrow\rangle$ and $|\downarrow\rangle$ reversed. This state illustrates the quantum phenomenon of entanglement mentioned earlier, in which the behavior of two quantum objects are perfectly correlated with each other even though each object displays some randomness. Let's pause to consider how very strange this entangled state is: It is as if we had two double-sided coins that we flipped at the same time. We measure coin 1 to be up half of the time and down half of the time, but we always measure coin 2 to be the opposite of coin 1.

The two particle situation gives us the first inkling of how entanglement produces strange non-classical effects, but something even more profound occurs when we consider larger numbers of spins N . Namely, for N spins the complete realm of quantum possibilities is given by a linear combination of the states $|\sigma_1 \sigma_2 \dots \sigma_N\rangle$, where each of

the σ_i can be $\uparrow$ or $\downarrow$. Counting all these possibilities, we see the size of the Hilbert space for this system, which is the "arena" that quantum mechanics lives in, grows exponentially with the number of spins. Hence, obtaining the dynamics of N particles (or even storing a quantum state of as many particles), is a problem that could be solved with $\text{poly}(N)$ resources in classical mechanics, but requires $\exp(N)$ resources quantum mechanically. Let's again pause to consider how disastrous this is for solving quantum dynamics on a classical computer. For the sake of argument let's say we had at our disposal as many classical bits as we estimate there are particles in the visible universe, $\sim 10^{80}$. With this universe-sized classical computer, we could still only store the quantum state of about 260 spins. Clearly, simulating the behavior of a macroscopically-sized array of quantum particles through this approach is doomed to fail.

One could reasonably ask the question: "Why is the arena of many-body quantum mechanics so vast?" The answer is entanglement; a state pulled at random from Hilbert space is generally very highly entangled, displaying non-local correlations between measurement outcomes for all of its constituent particles. Again using our coin toss analogy, a "typical" many-body quantum state in Hilbert space would correspond to finding random outcomes for each coin when a million coins are tossed, but these random outcomes are near-perfectly correlated when all coins are considered collectively. Such very highly entangled states are quite fragile in the sense that their correlations are destroyed when placed in a noisy classical environment.

A natural question, then, is whether an experiment with a quantum many-body system utilizes the full Hilbert space?

The physical answer to this question is no! This can be made precise by asking how far in Hilbert space can a given quantum state travel after a reasonable evolution by the Schrödinger equation with a reasonable Hamiltonian operator $\hat{H}$. Here, a reasonable evolution means we only allow the evolution to occur for a time that scales polynomially with the number

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of particles, and a reasonable Hamiltonian is one in which interactions occur between a fixed number of particles at a time (as occurs for all “natural” interactions like electromagnetic forces). In fact, the “volume” of Hilbert space that can be accessed with such a reasonable experiment is exponentially tiny (see Figure 2)[4]. Hence, the Hilbert space really is too big to fail. In order for quantum mechanics to be complete mathematically, we must include all of the highly entangled states that occupy the vast volume of a many-body Hilbert space. But most of these states simply have no meaning physically, meaning that it is difficult even for a physical quantum computer to prepare them.

While the previously stated result seems to preclude useful computation with quantum many-body systems, it also points out one specific problem that reasonable quantum systems can solve efficiently in a reasonable time, which is generating the dynamics of reasonable quantum many-body systems over reasonable times. This statement is not vacuous, as we do not know how to simulate generic, yet reasonable, quantum many-body systems with classical computers.

Over the last decades physicists have vastly improved their abilities to cool atoms to temperatures near absolute zero, to suppress any interaction with their (classical) environment, and to control and tune the interactions between them. These developments enabled them, using various different physical set-ups, to get remarkably close to the realization of quantum simulators with near-perfect isolation and exquisite control over all degrees of freedom. Milestone examples range from atoms and molecules trapped in lattices formed by laser beams, charged atomic ions in self-assembled structures, and arrays of superconducting electrodes coupled through Josephson junctions [5]. Among the most exciting implementations are fermionic alkali atoms, such as lithium, cooled to millionths of a degree above absolute zero and trapped in crystals of light mimicking a solid-state ionic lattice. Their interactions can be tuned so they behave like electrons in an unconven-

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tional superconductor, potentially providing insights into problems from condensed matter physics that are prohibitively hard to solve using a classical computer. Solving quantum many-body problems is not only of interest to basic research in physics, such problems are also central to chemistry and materials physics. Enormous amounts of supercomputer time are spent studying quantum many-body phenomena. Hence, the development of a non-universal quantum computer that could efficiently solve for chemical or material structures would completely revolutionize the development of new technologies.

So, what is left for current theorists, who at present only have access to classical computers, to do? For one, emerging quantum simulators must be verified to perform as we think they should in benchmark experiments. While this is a very difficult problem, there are certain places in which physicists have developed well-controlled approximations that can be used to compare with quantum simulators. For example, in one spatial dimension, our understanding of the entanglement structure of the exponentially tiny fraction of Hilbert space that we can access has led to a framework known as matrix product states, which enable efficient computations over moderate times. For certain systems in two and higher dimensions, we can estimate equilibrium properties of certain quantum many-body systems by treating them as classical systems in one higher dimension and sampling their trajectories with probabilistic Monte Carlo schemes. The direct comparison of such advanced numerical techniques

with quantum simulation experiments not only gives experimentalists faith that the simulator is performing as it should, but also gives theorists a unique opportunity to test and hone new methods. This positive feedback between theory and experiment has become a hallmark of the burgeoning quantum simulation field.

In conclusion, we argue perhaps the most useful enterprise a quantum computer can do is to forget about being a computer and just behave as a quantum many-body system. Even though such a many-body system can only explore a tiny fraction of the realm of mathematical possibilities afforded to it by the framework of quantum mechanics, this tiny fraction encompasses essentially all systems of interest from physics, chemistry, and materials science. Using designer quantum systems to simulate many-body physics holds great promise for teaching us about the structure of our quantum world, and has the potential to transform computation as we know it.

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Biographies

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