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Quantum Computing: From Basic Science to Applications

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Quantum mechanics was developed a century ago, and has laid the foundations for many technological breakthroughs like the transistor or the laser. During the past four decades, it has become increasingly clear how the novel resources that are unique to the quantum world, superposition and entanglement, can be harnessed for radically new applications in communication, computing and sensing. In parallel, experimental methods and fabrication capabilities have progressed to a degree where individual quantum systems can be prepared, controlled and kept coherent with outstanding quality, such that ever more complex systems can be realized.

This convergence fuels the belief shared by many academic, governmental and industrial parties that we are currently at the dawn of a second quantum revolution. New quantum technology programs are being ramped up on a national level (Australia, Austria, Canada, China, Denmark, Germany, Japan, Netherlands, UK, USA). Moreover, the Quantum Technology Flagship initiative is gathering momentum as a European platform [1]. Large enterprises in the IT industry (Google, IBM, Intel, Microsoft) as well as a rapidly increasing number of startups are investing heavily in the development of novel quantum products that are expected to become available in the next few years.

Quantum communication, quantum sensing/metrology and quantum computing/simulation have been identified as the central pillars for this new wave of quantum technologies. In this article, we concentrate on quantum computing and digital quantum simulation which arguably requires the most complex quantum systems but also holds promise to solve computing problems that will remain intractable with any classical super-computer.

Computations with Qubits

Whereas classical computers work with binary bits that can be either 0 or 1 and gates that define logic operations on these bits, the resources for quantum computers are controllable two-level systems or qubits and corresponding quantum gates. Key to the power of the quantum computer is that qubits can be in a superposition of 0 and 1 “at the same time”, i.e., the state of a qubit is defined in a quasi-analog way as vector on the Bloch sphere. Therefore, an N -qubit quantum computer in principle operates on a 2^N dimensional complex state space (Hilbert space) with state vectors that already for $N = 100$ could never be accurately stored on any classical computer. However, unavoidable coupling to the environment gives rise to uncontrolled, undesirable state changes. What makes things even more challenging, these cannot be corrected easily because also just measuring the state “collapses” it to either 0 or 1. Hence, decoherence and probabilistic readout of the result require clever quantum algorithms to fully exploit the promises of this so-called quantum parallelism.

The complexity of the algorithms that can be run on a quantum computer not only depends on the number of qubits but more importantly also on the effective error rate, which determines the number of operations that can be performed sequentially before errors mask the output of the calculation [2]. The current state-of-the-art is 10 - 20 qubits with effective gate error rates on the order of 10^{-2} . To further reduce the error rate of a quantum computer, both the coherence of the qubits and their fault-tolerant encoding will have to be improved in the future. Eventually this development is expected to lead to fault-tolerant universal quantum computing. It is expected that a 50+ qubit machine can be built in the next few years that could for the first time demonstrate a “quantum advantage” for a special purpose application that is incomputable using classical systems (see Figure 1). The

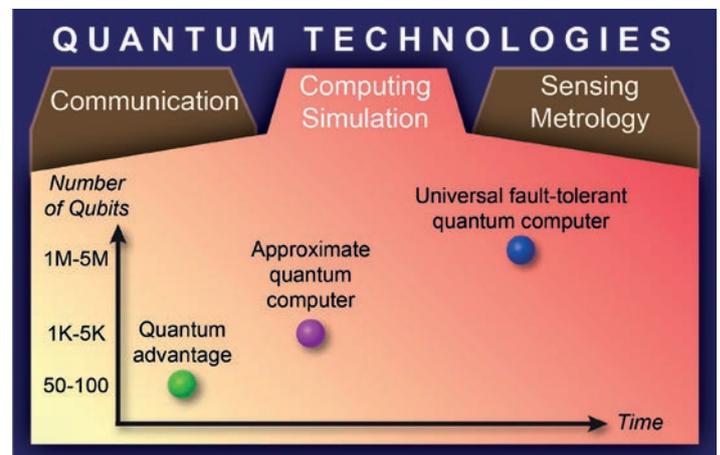


Figure 1: Quantum technology pillars and the expected scaling path towards a universal quantum computer.

next, much more important, step would be an “approximate quantum computer” that could solve “useful” problems, e.g., in quantum chemistry or binary constrained optimization but does not require full fault-tolerance. Such a system will require on the order of thousand high fidelity qubits. The ultimate goal is a universal quantum computer that features complete quantum error correction, e.g., by running the surface code [3] and shows exponential speedup over its classical counterparts for a range of important problems [4]. Reasonable current estimates of the rate of progress lead many people to believe that we are still more than a decade away from having such a system available to us.

As the race towards a useful quantum computer intensifies, only two physical systems have currently demonstrated 10+ qubits with long coherence time, high gate fidelity and reasonable connectivity. These are ion traps and superconducting qubits. At IBM, the focus is on the latter because they can be fabricated with standard chip fabrication methods. Furthermore, their manipulation with microwave pulses is relatively straightforward since much of the control hardware is similar to well-established wireless technology. Whereas other qubit architectures such as spin qubits in semiconductor nanostructures may become relevant in the

future, we restrict ourselves here on the superconducting qubit technology and discuss its potential and future challenges in more detail.

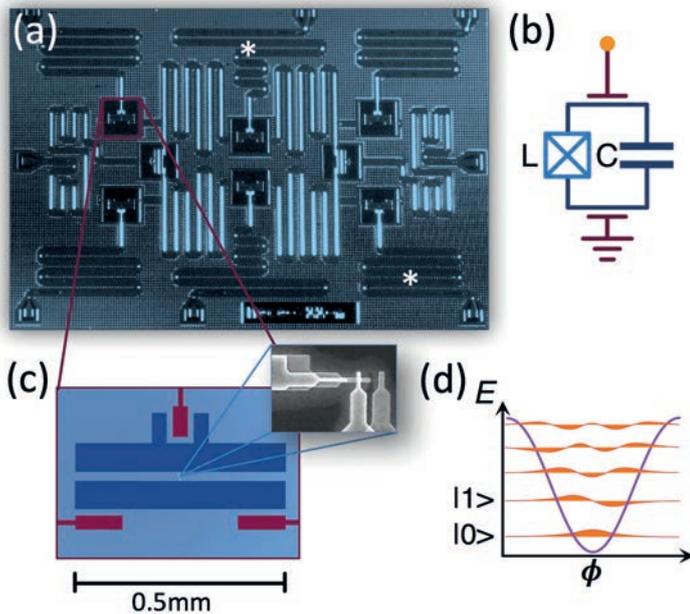


Figure 2: (a) Eight-qubit chip showing qubits (dark square shaped areas) and meandering CPW resonators for coupling and read-out. (b) Equivalent-circuit model of a single qubit. (c) Transmon qubit with the large capacitor pads in blue and the ends of the CPW resonators in red. The inset shows a scanning electron microscopy image of the Josephson junction. (d) Energy spectrum of a transmon qubit.

Superconducting Qubit Architecture

Figure 2(a) shows an eight-qubit chip with the qubits coupled by meandering coplanar waveguide (CPW) resonators. Control of the qubits is achieved by sending microwave pulses to the ports surrounding the chip. Both qubits and CPW resonators can be viewed as LC-resonator circuits [see Fig. 2(b)] that are operated in the quantum regime where zero-point fluctuations are large compared to temperature. In this limit, a resonator circuit can be described by a harmonic oscillator model with photon number states at energies $\hbar\omega_0(n + \frac{1}{2})$. Dissipation (or damping) in these resonators is negligible due to the superconducting materials (niobium and aluminium) that are used, resulting in Q-factors on the order of millions. Figure 2(c) shows a zoom of a transmon qubit with two large blue superconducting capacitor pads. The small Josephson junction between the two pads acts as nonlinear inductance. This is responsible for making the oscillator potential anharmonic and allowing to address the two lowest levels as qubit states $|0\rangle$ and $|1\rangle$ [see Fig. 2(c)+(d)]. The Josephson junction consists of an aluminium oxide tunnel barrier between two superconducting aluminium electrodes and has the unique property of combining nonlinearity with negligible dissipation.

The transition frequency between the $|0\rangle$ and $|1\rangle$ states of such a fixed-frequency transmon qubit is designed to lie close to 5 GHz with a fabricated accuracy of about 1%. Its large capacitor pads facilitate strong coupling between CPW resonators and qubits and at the same time reduce the qubits susceptibility to charge noise. Read-out of the qubit state occurs by weakly probing the reflection phase of

the CPW resonators that link the qubits to the outside world (two of them are marked with an asterisk in Fig. 2(a)). Their resonance frequency depends on the qubit state which leads to a measurable change in the reflected microwave signal phase near resonance [5].

It is worth noting that over the past decade improvements in materials and circuit designs have led to a steady increase in qubit coherence, as illustrated in Figure 3.

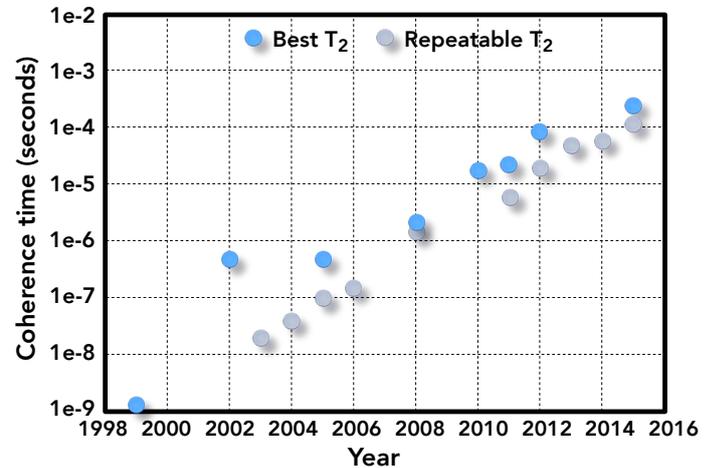


Figure 3: Improvement of superconducting qubit coherence times over the past two decades.

Quantum Circuits

The construction of arbitrary classical logic circuits can be achieved just using NAND gates, which are said to have functional completeness. Similarly, any digital quantum circuit can be built from single qubit rotations and a two-qubit entangling gate, the controlled-not (CNOT) operation, which inverts the state of the target qubit depending on the state of the source qubit. On the hardware level, single qubit rotations are implemented by modulating amplitude and phase of the microwave pulses that are applied to the qubits. The CNOT gate can be realized, e.g., by driving a source qubit at the transition frequency of a neighboring target qubit. This cross-resonance gate [6] in combination with single qubit rotations allows construction of arbitrary quantum circuits on a lattice of superconducting qubits.

The "IBM Q experience" provides a platform to explore basic quantum circuits on real quantum processors based on superconducting qubits. Figure 4 shows the web-interface, which allows simple implementation of basic quantum algorithms and is geared towards education. More functionality can be accessed through the Quantum Information Software Kit (<https://www.qiskit.org>) which provides an open-access programming interface for working with both the real quantum processors and a cloud-based simulator that currently handles up to 20 qubits. It uses OpenQASM [7] as an intermediate representation of quantum circuits and performs some important compilation and optimization tasks on the circuits.

Even though quantum processors such as the ones currently accessible through the "IBM Q experience" can still be simulated with relative ease on classical hardware, it is believed that future more powerful quantum processors could be used in the same way: They would be accessed through



Figure 4: The "IBM Q experience" web interface gives access to experimental quantum processors with 5 and 16 qubits for exploring basic quantum circuits. (see <https://www.ibm-research.com/ibm-qx>)

the cloud and in tandem with classical high performance computing systems for which they would act as accelerators in specific applications.

Near-Term Quantum Applications

On the long journey towards a large, fault-tolerant quantum computer, useful applications of approximate quantum computers will become available much earlier. On these intermediate systems, the limited number of sequential gates restricts the depth of meaningful quantum circuits that can be run, and algorithms will have to be tailored to cope with noise and errors [8]. Still, even a relatively small-scale quantum computer with hundred qubits can already process quantum states that could not even be stored in any classical memory.

One concrete example to make use of this quantum advantage is via a hybrid quantum-classical architecture: A quantum co-processor is used to prepare multi-qubit quantum states $|\Psi(\theta)\rangle$, parametrized by control parameters θ . The subsequent measurement of a cost function $E(\theta) = \langle \Psi(\theta) | H_q | \Psi(\theta) \rangle$, typically the energy expectation

value of a problem Hamiltonian H_q , serves as an input for a classical computer to find new values θ in order to minimize $E(\theta)$ and converge towards the ground-state energy $E(\theta^*) = \min(\langle \Psi(\theta) | H_q | \Psi(\theta) \rangle)$.

This variational quantum eigensolver approach, which is outlined in Fig. 5, has recently been applied in various contexts in proof-of-concept experiments [9-11]. In fact, the Hamiltonian H_q can take many forms, the only requirement being that it can be mapped to a system of interacting qubits with a non-exponentially increasing number of terms. Here we distinguish two relevant cases: Hamiltonians that describe fermionic condensed-matter or molecular systems and Hamiltonians that describe the cost function of a classical optimization problem. For the latter, the mapping of the problem Hamiltonian to qubits is simple and yields an Ising spin Hamiltonian. For fermionic systems, the mapping from fermions to qubits is not straightforward and requires one of several schemes that exist to keep track of parity [8].

For both types of problems, one can either focus the effort on creating a sophisticated trial state that is known to be close to the expected solution with ideally few parameters θ [9], or use a hardware-centric heuristic approach with gates that can be implemented efficiently on a given platform. The latter technique was recently used to calculate the ground-state energy of H_2 , LiH, BeH_2 as a function of the atomic separation of the corresponding nuclei [11].

Hence, even though errors from decoherence and imperfect gates in near-term quantum processors limit the depth of useful quantum circuits, the exponential capacity of such devices may still be used for preparing trial states that cannot be stored on any classical system. The challenge for this approach will be to find good parametrizations of trial states that are both hardware efficient and span the relevant solution space.

Building a Quantum Computing Ecosystem

The construction of a useful quantum computer comprises tremendous cross-disciplinary challenges within the next years, ranging from the design of hardware-efficient quantum algorithms, over building large qubit arrays and quantum gates that are sufficiently immune to decoherence, cross-talk and fabrication variations, to developing highly integrated specialized electronics and tools for control, driving and readout of the system. It is unlikely that a single enterprise or institution can succeed with all of this alone, and hence, a whole ecosystem needs to grow (Figure 6). Some of the effort here in Switzerland is already bundled in the National Center of Competence in Research (NCCR) "QSIT" [12]. There are many opportunities for academia, SMEs and startups to get involved and take part in this global race by developing and engineering the tools for the required hardware and software ecosystem. There is a clear sense in the community that we should not wait for a fully fault-tolerant quantum computer, but should leverage quantum advantages in near-term approximate quantum computers now, as we build up a quantum computing ecosystem. In other words, the exciting journey from basic science to applications is already fully on its way.

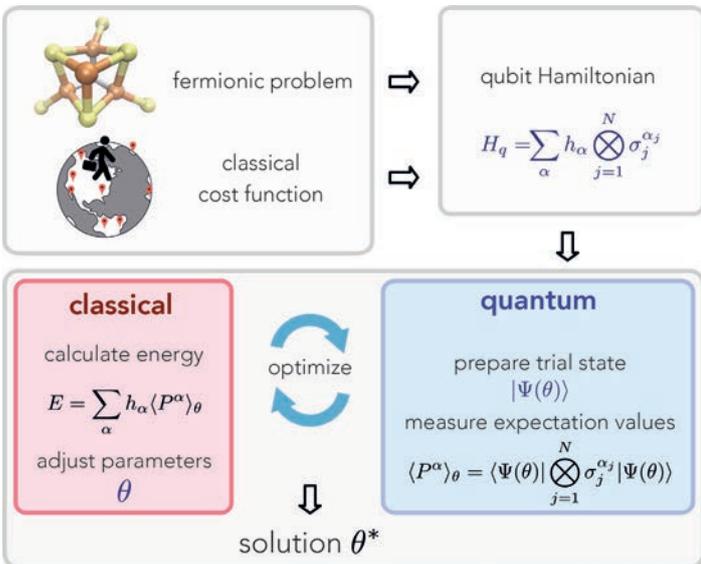


Figure 5: Process flow for the variational quantum eigensolver method. A trial state $|\Psi(\theta^*)\rangle$ is parametrically generated on the quantum processor. Expectation values of the Hamiltonian terms are measured and used on a classical optimizer to find the optimal parameters θ^* defining the solution $|\Psi(\theta^*)\rangle$.

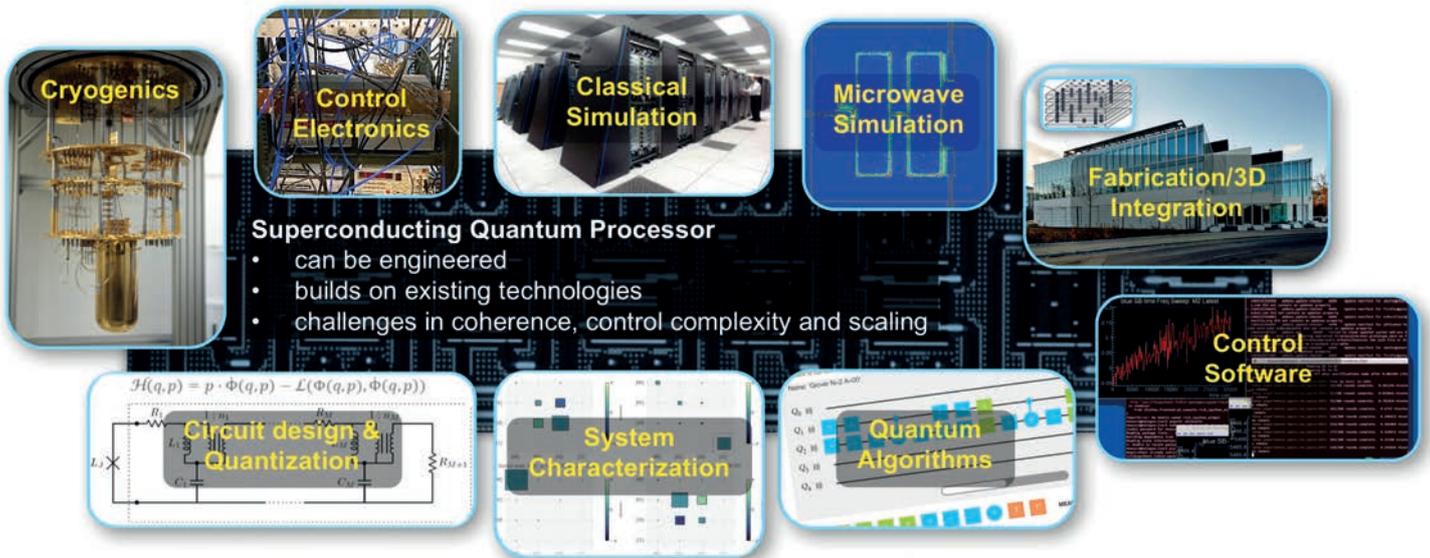


Figure 6: Ecosystem of hardware and software that is required to build a superconducting quantum processor.

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