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Quantum engineering of superconducting structures: principles, promise and problems

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Quantum technologies went through an explosive development since the beginning of the century. The progress in the field of superconducting quantum structures was especially fast. As the result, the design and characterization of large quantum coherent structures became an engineering problem. We will discuss the current status of the emerging discipline of quantum engineering and possible ways of meeting its main challenge, the fundamental impossibility of an efficient modelling of a quantum system using classical means.

PACS: **85.25.-j** Superconducting devices;
85.25.Am Superconducting device characterization, design, and modeling
85.25.Cp Josephson devices.

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Arguably, the development of Quantum Technologies 2.0 (QT2.0) started in 1999 with the publication of two seminal papers [1,2], which reported the experimental realization of respectively charge and (small-inductance) flux superconducting quantum bits (qubits). Shortly afterwards two other types of superconducting qubits were realized (large-inductance flux qubit [3] and phase qubit [4]), and a steady flow of further improvements followed, such as qutrit [5], transmon [6] and Xmon [7]. As the result of these developments, the qubit's figures of merit, the decoherence rate T_d^{-1} and its ratio to the interlevel spacing of the qubit, ΔE , reduced from respectively $\sim 1 \text{ ns}^{-1}$ and ~ 0.1 to the current values of $\sim 10 \text{ ms}^{-1}$ and $\sim 10^{-5}$.

The initial push was given by Feynman's observation that a quantum system cannot be efficiently simulated by a classical computer [8]. The consequent theoretical work on quantum computing attracting much attention and funding after the discovery of Shor's algorithm [9]; it was soon implemented (factoring the number 15 using 7 qubits) using the NMR techniques [10]. Nevertheless it was understood from the beginning that the NMR approach is intrinsically not scalable. Among the scalable approaches, the superconductor-based one later turned out to be the most successful,

but at the moment the very possibility of observing macroscopic quantum tunnelling or macroscopic quantum superpositions in superconductors was strongly questioned [11]. Therefore the demonstration of coherent quantum operations in superconducting qubits, especially flux qubits, was a real breakthrough*, which spurred the further development of quantum technologies 2.0.

Quantum Technologies 2.0 are produced by the Second Quantum Revolution, which started from the investigation of entanglement in 1960s. Unlike the technologies brought by the First Quantum Revolution of early 20th century by 1960s (e.g., semiconducting electronics, masers, lasers, SQUIDS), QT2.0 essentially use quantum superpositions and entanglement on a meso- or macroscopic scale**. The most celebrated, and admittedly the hardest to achieve, goal of QT2.0 is universal quantum computing (see, e.g., [12]), which requires for its realization a combination of the maximal possible degree of quantum coherence in an essentially macroscopic system and maximal control over its maximally entangled quantum state, maintained over the maximal possible time. Nevertheless the Quantum Manifesto [13] confidently enough predicts that by 2035 such a computer will exceed the power of classical computers, and a num-

* While the stationary states of charge qubits are superpositions of quantum states differing by a single Cooper pair, those of flux qubits differ by at least 10^5 – 10^6 single particle states.

** Quantum effects employed in QT1.0 involve only effectively few-particle quantum superpositions and entanglement. See, e.g., [11].

ber of other applications (like clocks, sensors, quantum internet etc) will be realized before that.

This optimistic view is supported by the developments in the field of superconducting QT2.0, such as the realization of adiabatic quantum annealers by D-Wave Systems, Inc. (see Fig. 1). These devices, now containing about 2000 flux qubits, demonstrate a sufficient degree of coherence and control to perform useful computation, and are the first commercially available quantum computing devices already purchased by the likes of Lockheed–Martin and Google^{*}. Nevertheless, the very success of this programme made clear the fundamental difficulties on the road towards the realization of the full potential of QT2.0, and indicated that the existing theoretical approaches are insufficient.

The difficulties can be illustrated by the discussion around the performance and the principle of operation of D-Wave-produced quantum annealers (see, e.g., [14]).

A quantum annealer, or quantum optimizer, is the simplest realization of a quantum computing device [15] specializing on solving optimization problems. The cost function is identified with the ground state energy of the system, and the solution with the set of qubit states. An adiabatic quantum computer is usually described by the quantum Ising Hamiltonian,

$$\hat{H} = -\sum_j h_j \sigma_j^z - \sum_{j < k} J_{jk} \sigma_j^z \sigma_k^z, \quad (1)$$

where σ_j are the Pauli matrices describing the j -th qubit. It is possible in principle to encode the solution to *any* problem solvable by a universal quantum computer in the ground state of a system of qubits [17], at a price of more complex qubit-qubit interaction. Nevertheless the Ising model is general enough, as it allows to formulate many NPC problems, including all of Karp’s 21 NPC problems [18].

The idea of adiabatic quantum computing (AQC) [17] is based on (1) the possibility of such a “ground state encoding”, and (2) the adiabatic theorem of quantum mechanics stating that a slowly perturbed quantum system will generally remain in its ground state^{*}. Therefore an isolated system with the Hamiltonian

$$\hat{H}_\lambda(t) = \lambda(t)\hat{H} + (1-\lambda(t))\hat{H}_0, \quad (2)$$

where $\hat{H}_0 = -h_0 \sum_j \sigma_j^x$, will evolve from the ground state of \hat{H}_0 (which is presumably easy to reach) to that of \hat{H} , which provides the solution, as λ changes from 0 to 1, if only $\dot{\lambda}$ is small enough. The approach is immediately attractive, since it disposes of the fast and precise time-domain manipulation of qubit states, required in the stand-

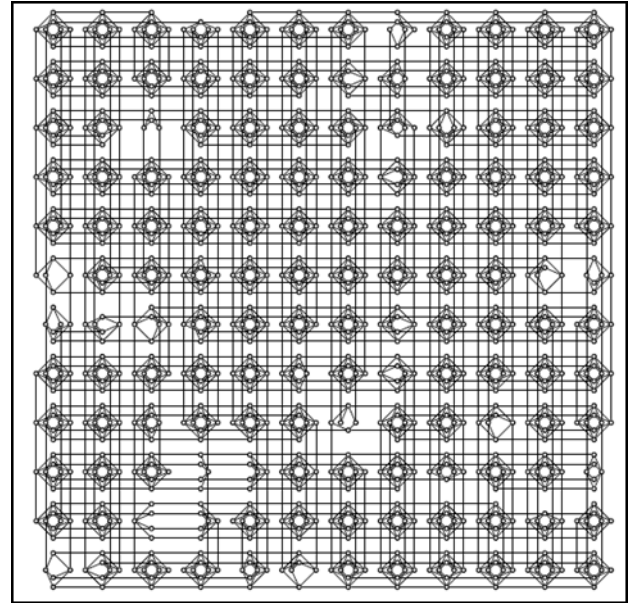


Fig. 1. Schematics of D-Wave 2X quantum annealer (dots represent qubits, lines connections) [16]. Each of 144 registers nominally contains 8 flux qubits (not all qubits and connections are operational).

ard “gate-based” quantum computing, replacing it with the fixed qubit-qubit couplings (something readily realizable with superconducting hardware [20]) and a slow application (or rather, lifting) of a simple perturbation acting uniformly on all qubits. This “swap of time for space” greatly reduces the complexity and sheer size of the structure and thus eliminates additional sources of decoherence.

Strictly speaking, the AQC approach “in narrow sense” only works if the system in question (i.e., the *relevant* degrees of freedom of the constituent qubits) is effectively isolated from the environment (including other degrees of freedom in the qubits themselves and their control wiring) while λ changes from zero to one. This condition is not satisfied in D-Wave devices; their typical evolution time ($\sim 5\text{--}15 \mu\text{s}$) greatly exceeds the decoherence time of a single qubit ($\sim 100 \text{ ns}$) used in these devices. This gave rise to questions whether and to what extent these devices operate in quantum regime (see [14] and references therein).

The difficulty with answering this question is the same fundamental impossibility of an efficient modelling a quantum system with classical means that gave rise to the idea of quantum computing in the first place. While for an 8-qubit register one could definitely establish quantum evolution [21], modelling fully quantum evolution of a hundred or more qubits with classical computers is beyond

* It gives me a great pleasure to highlight the significant role played by A.N. Omelyanchouk, as a consultant and collaborator, on critical early stages of D-Wave’s operations, 2000–2004.

** See [19] for the most general formulation.

any realistic possibilities^{*}. This forced the researchers to develop indirect methods (e.g., comparing the statistics of the performance of an AQC device on a large set of optimization problems with known solutions to that of different types of optimization algorithms [22,23]), which do not allow an unequivocal interpretation [24] and are not scalable beyond several hundred qubits^{**}. Anyway, these methods are of a very limited use in application to engineering (design, characterization and optimization) of large quantum coherent structures. What is worse, currently there is no accepted general criterion of “quantumness”, which could be efficiently accessed on experiment and theoretically evaluated. It seems likely that such criteria are not universal and depend on the specifics of the structure and the tasks it is designed to perform.

It is therefore necessary to find means of bridging the gap between our current ability to simulate large quantum systems and the capacities of the smallest workable quantum computers, which hopefully will be able to effectively do this job. This requires developing specific quantum engineering approaches — a task, which can be illustrated on the example of quantum engineering of superconducting devices.

The broadly stated goal of engineering is “to build reliable structures out of unreliable unit elements” (Fig. 2). *Quantum unit engineering* is mature. The quantitative theory of various types of superconducting qubits is well developed^{***} and is in an excellent agreement with the experiment, building on fifty years of science and technology of the Josephson effect. The evidence of this is the fast development of a number of improved qubit types and the above mentioned spectacular increase in their decoherence time. As long as a direct numerical simulation is possible, design, characterization and optimization of a superconducting quantum register is a routine task. The difficulties start at the structural level^{****}.

The goal of conventional structural engineering is to determine the properties of a complex structure based on the properties of its constituent elements, to evaluate and optimize the overall design ensuring that its performance will

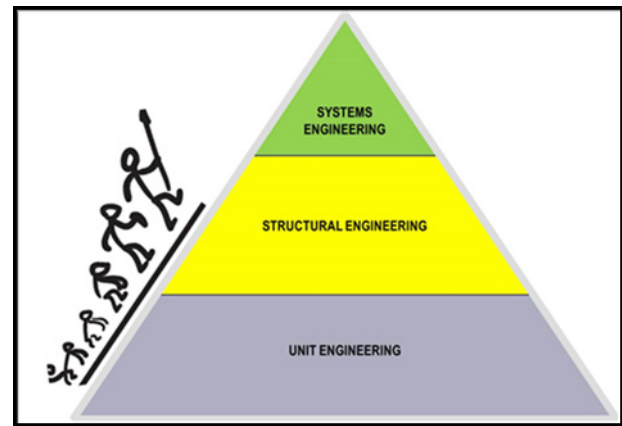


Fig. 2. Levels of engineering.

satisfy the set requirements. *Quantum structural engineering* pursues the same goal, with the fundamental complication that a direct simulation is impossible. This should not be apriori considered as an insurmountable obstacle: such simulations were impossible in conventional structural engineering as well until the arrival of high-performance computers, and it did not stop the development of complex structures, e.g., aircraft and first modern computers. In our case the solution could be based on the identification of efficient “quantumness” criteria, which would provide a probabilistic estimate of the system’s performance, the development and application of generalized approximate methods of nonequilibrium, nonstationary many-body theory tailored to compute these criteria and taking into account essential quantum correlations. This can be only done in a close collaboration with experiment, the theory both providing guidance and obtaining important insights and feedback.

We concede that it is impossible to simulate an individual “instance” of a large quantum device (e.g., a quantum annealer with a given set of interqubit couplings). But it is plausible that the essential properties of an ensemble of such systems will be reflected in certain higher-level, global characteristics (“figures-of-merit”), which are insensitive to details of a particular instance, computable by classical tools and accessible to experimental investigation. Draw-

* This seems to contradict the well-known successes of quantum theory of many-body systems. But there the number of degrees of freedom being actually considered is small. For example, the “macroscopic wave function” of a BCS superconductor is characterized by just one complex-number field (superconducting order parameter) The Josephson effect per se involves quantum superpositions of macroscopic states differing by two single-electron states only [11]. The drastic reduction of the effective Hilbert space to be dealt with to a manageable size. It is also worth noting that establishing quantum evolution even in a single qubit is not a trivial task [25,26].

** One can consider less restrictive operation modes of a quantum annealer, such as “proper” quantum annealing [27–29] (where quantum fluctuations assist the open system’s evolution towards its ground state) or approximate AQC [30,31] (when the goal is to find a good enough approximation, i.e. ending up in a low-lying excited state). Nevertheless their evaluation meets the same fundamental difficulty.

*** For a review see, e.g., [30], Ch. 2.4.

**** Development of quantum *systems* engineering, aiming to ensure a smooth and reliable interaction of different types of QT2.0 devices, other technology, and their human operators, is at the moment not an urgent task.

ing on the analogy with aero/hydrodynamics, such “quantum Reynolds numbers” could then be used to characterize and optimize a complex quantum coherent structure. What is lacking is the “quantum scaling theory”, which would identify such criteria and allow extending the data from small-scale experiments to larger-scale devices.

There is no clear candidate for such a theory at the moment. Several approaches seem possible.

One can try to generalize the methods of nonequilibrium, nonstationary theory of quantum many-body systems, such as the Keldysh formalism (see, e.g., [32, Ch. 10]). It is necessary to hold on the essential multipoint phase relations while keeping the number of variables low enough to be classically computable. What relations are “essential” will be dictated by the system. An example of a QT2.0 device system where such approach may succeed is provided by quantum metamaterials [33,34]. Quantum metamaterials are the artificial optical (in the broad sense) media (Fig. 3), which have the following properties:

- They are comprised of quantum coherent unit elements with desired (“engineered”) parameters;
- Quantum states of all or some of these elements can be controlled;
- The whole structure can maintain global coherence for the duration of time, exceeding the traversal time of a relevant electromagnetic signal.

The limited character of the necessary quantum coherence and control required allows a simplified description. For example, such effects as controlled signal propagation [33], lasing [36,37] or superradiance [38] can be described by approximating the quantum state of the qubit system by a factorized two-component wave function $\hat{\Psi} = \otimes_j \hat{\psi}(\mathbf{r}_j, t) = \otimes_j (u(\mathbf{r}_j, t), v(\mathbf{r}_j, t))^T$, where the product is taken over all constituent qubits. In the continuum limit, when the period of the structure is much less than the signal wavelength, it reduces to a set of equations for $\hat{\psi}(\mathbf{r}, t)$ reminiscent of Bogoliubov–de Gennes equations*. Together with the equations for the electromagnetic field they yield the equations for the electromagnetic wave propagating in a medium with an effective refractive index dependent on the qubit quantum state (which in turn is affected by the electromagnetic field). This approach becomes inadequate when the entanglement between qubits is essential, but quantum metamaterials due to their relative simplicity are a good testing bed for developing more powerful theoretical tools. For example, nonlinear response functions of a quantum medium provide information about multiqubit entanglement [39].

Another possibility is to use the Pechukas–Yukawa formalism [40]. It turns out that in a quantum system describ-

* Unlike the case of a superconductor, the phase coherence between the components in a quantum metamaterial are not supported dynamically and only survive as long as the decoherence time.

** It is rather surprising that, given all the attention paid to quantum adiabatic computation, there seems to be no systematic investigation of adiabatic invariants in these systems.

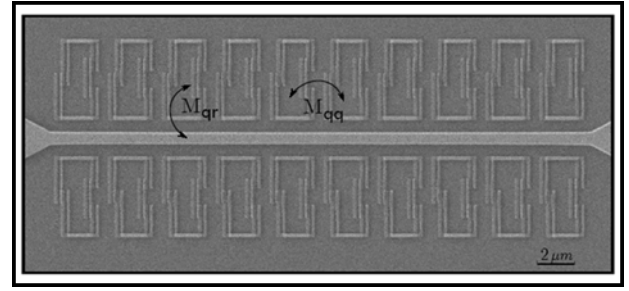


Fig. 3. Quantum metamaterial prototype based on superconducting flux qubits [35].

ed by the Hamiltonian Eq.(2) the energy levels, $E_j(\lambda)$, satisfy a set of equations analogous to the Calogero–Sutherland model for one-dimensional *classical* gas of particles with cubic repulsion. The parameter λ plays the role of time, the diagonal matrix elements of the full Hamiltonian $x_j(\lambda) \equiv \langle j | \hat{H}_\lambda | j \rangle$, that of positions, and of the perturbation, $v_j(\lambda) \equiv \langle j | (\hat{H} - \hat{H}_0) | j \rangle$, the role of velocities. (Here $\{|j\rangle\}^N$ is the set of “instantaneous” eigenstates of the full Hamiltonian at a given λ .) While the original Calogero–Sutherland model is exactly solvable, this is not case here, because the cubic repulsion between “particles”, $|l_{jk}|^2 / (x_j - x_k)^3$, depends on the “momenta” l_{jk} , which are expressed through off-diagonal matrix elements of the Hamiltonian and depend on x, v ’s. Nevertheless this approach provides useful insights in the level dynamics and when supplemented by equations describing interlevel transitions — about the evolution of the quantum state of the system [41]. The approach is general, but is especially convenient in an application to adiabatic quantum annealers. Recently we have derived the BBGKY chain for this system, which will serve as the basis for the “kinetic theory of energy levels” [42]. The supplementing equations for the density matrix elements will allow to present the solution as a systematic expansion in powers of λ , thus building an hierarchy of adiabatic invariants of the system. Such invariants are good candidates for the “Reynolds numbers” characterizing a quantum annealer**.

One more approach would directly address the influence of decoherence on the structure of the Hilbert space. Decoherence tends to factorize the (generally entangled) quantum state of a multiqubit system:

$$\Psi(1, \dots, n) \rightarrow \bigotimes_{\{Z_j\}} |\psi_{Z_j}^j\rangle \quad (3)$$

where Z_j denotes the j th cluster of mutually entangled qubits. The Hilbert space of the system accordingly reduces to a direct sum of smaller-dimension subspaces, making the simulation of the system manageable. A direct numeri-

cal modelling of decoherence by random factorizations (3) after certain number of steps can be realized for a larger-scale partially coherent quantum systems (like a D-Wave processor).

In conclusion: The essence of quantum technologies 2.0 is in the utilization of multiparticle quantum superpositions and entanglement. This makes impossible a straightforward quantitative modelling, characterization and optimization of devices, which can be fabricated and have already been fabricated using the existing experimental techniques. New theoretical tools must be developed to answer this need, and an “engineering” combination of theory, heuristics, “rule-of-thumb” estimates, and extrapolation from model experiments may provide the solution.

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