

## **What Minimal Structure Enables Quantum Computation?**

I investigate the structural conditions under which a physical quantum system supports meaningful computation. By isolating and refining candidate minimal ingredients, I develop unified frameworks linking quantum circuits, Hamiltonian models, and variational algorithms. These frameworks identify what is computationally universal, physically realizable, and practically achievable on quantum hardware.

I pursue this question as a structural decomposition: Model (universality in physical systems), Language (computation from composition), Training (capability and limits), and Hardware (resource-conscious algorithmic constraints)—developing tensor-network languages for computation [1, 2, 3, 4, 5], establishing the universality and trainability limits of variational computation [6, 7, 8, 9, 10, 11], and deriving hardware-constrained algorithms that connect complexity bounds to realistic architectures [12].

A central goal is to identify which physical models of computation are universal and which constraints fundamentally limit them. In 2007, this work proved a physically realizable universal model of quantum computation within the Feynman–Kitaev Hamiltonian–circuit equivalence [13]. These constructions set limits on cost-Hamiltonian optimization in several settings and continue to serve as experimental targets in adiabatic and ground-state quantum computing. This line of work also established the computational universality of feed-forward variational quantum computation [6, 7] and led to the discovery of several non-barren training limitations [8, 9, 10, 11, 14].

Another challenge is representation: how is computational structure logically expressed, manipulated, and composed? A major thread of this research is tensor network theory. Results on efficiently contractible tensor networks and #SAT representations [1], categorical and circuit-level tensor structures [2, 3], and diagrammatic invariant theory for entanglement classification [4] built bridges connecting tensor networks, quantum circuits, and computational complexity. Work on graphical calculus for open quantum systems [5] extended these ideas to noisy dynamics. Tensor networks now form a core analytical toolset in quantum simulation, variational quantum algorithms, entanglement theory, and quantum machine learning. I presented this body of work in the Shapiro Lecture Series in the Department of Mathematics at Pennsylvania State.

These frameworks connect directly to algorithms and physical systems. I co-authored the complexity analysis of quantum algorithms for electronic-structure simulations [12], which received the 2012 Longuet-Higgins Paper Prize. Collaborative work introduced concepts such as chiral quantum walks [15] and developed analytical methods integrating complex network theory into quantum dynamics [16, 17, 18], contributing to the development of quantum complex networks. In collaboration with John C. Baez, we developed a framework for systematically comparing quantum and stochastic processes [2], influencing subsequent work with Manlio De Domenico that provided quantum-information-based complexity measures for classical networks [18].

This work informed both theoretical analyses and experimental implementations. Several publications appear in the Web of Science’s top 0.1% most highly cited papers in physics, with additional recognition in the World’s Top 2% Scientists Ranking (Elsevier–Stanford). I have delivered over 100 invited lectures globally and mentored eight doctoral students and nine postdoctoral researchers. Recent work includes identifying reachability deficits [8], abrupt training transitions [9], parameter concentrations [10], and training saturations [11]—each clarifying fundamental limits of variational training.

## Six Contributions That Have Shaped Quantum Computing

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### 1. Hamiltonian Models of Quantum Computation

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Hamiltonian models of quantum and classical computation utilize the ground state of a physical system as a computational resource. Cost function (non-commutative cost Hamiltonian) optimization is regarded as the task where contemporary quantum computing holds the most potential [19, 20]. More generally, the computational difficulty of Hamiltonian optimization also provides a framework that organizes quantum algorithms into (cost) Hamiltonian complexity classes [21, 22, 13, 23] and was used to prove universality of adiabatic quantum computation [22]. A long standing theme in my research has been developing techniques to map a given quantum circuit to cost Hamiltonians optimized by the given quantum circuit [13, 24, 25, 7].

In 2007, this work proved a physically realizable universal model of quantum computation in sparse 2-local systems: proving QMA-completeness for tunable  $ZZ$  and  $XX$  couplings set fundamental limits on cost-Hamiltonian optimization [13]. The work extended the early results on the the Feynman–Kitaev Hamiltonian–circuit equivalence [26, 22]. Using perturbative gadgets to engineer effective  $ZX$  interactions from  $ZZ$  and  $XX$  terms enabled a universal gate set; these constructions are used in the field and continue to inform experimental targets in adiabatic and ground-state quantum computing. Extending methods from digital circuits, this work introduced new classical [24, 25] and quantum [27] *Hamiltonian-gadgets* [26] that enable one to approximate a target Hamiltonian by engineering the low-energy subspace of a static Hamiltonian. In particular, this work developed a language that enables one to compose logic gates in the lowest energy space of Ising operators [24].

This cost Hamiltonian research program [13, 24, 25, 27] includes the derivation of a gadget for  $YY$ -interactions, the Bravyi-Kitaev transform [28] immediately implied that electronic structure Hamiltonians can be embedded [27] and hence optimized using quantum computing architectures implementing the cost Hamiltonians derived in [13]. This work has also used cost-Hamiltonian engineering techniques to prove computational universality of feed-forward variational quantum computation [7]—selected as an Editors’ Selection (*Physical Review A*, Letters Section, Biamonte, 2021).

The work appearing in [13] was also patented by D-Wave Systems (US-11816536-B2). U.S. government programs, including IARPA and NRL, have supported the experimental development of these physically realizable universal ground state models predicted in [13]. This includes William Oliver’s MIT lab which realized instances of the predicted 3-qubit interactions, key components in future universal cost Hamiltonian based quantum computing architectures.

### 2. Quantum Algorithms Simulating Quantum Chemistry

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Richard Feynman proposed that, unlike classical computers—which would presumably experience an exponential slowdown when simulating quantum phenomena—a quantum simulator would not [29, 30]. This early insight gave rise to a vibrant field focused on the use of quantum computers to simulate quantum systems. Quantum simulation is now widely regarded as the leading future application domain of quantum processors, particularly for problems in electronic structure, materials science, and chemical dynamics.

A contribution in this area was the derivation of complexity-theoretic gate counts for quantum algorithms simulating electronic structure. In collaboration with James Whitfield and Al'an Aspuru-Guzik, we analyzed the scaling behavior and resource requirements of algorithms for optimizing cost Hamiltonians arising in electronic structure instances [12]. The paper appears in the *Web of Science Top 1% Highly Cited Paper Index for Physics* and received the 2012 Longuet-Higgins Paper Prize from Taylor & Francis.

Beyond complexity analysis, my research has contributed to unifying quantum simulation with variational and learning-based approaches. Working with Alexey Uvarov, we proposed a merger of quantum simulation and quantum machine learning, resulting in quantum classifiers capable of detecting phases of matter directly from quantum data [31]. In related work, we demonstrated how variational quantum algorithms can be used to simulate dynamical and ground-state properties of many-body systems, including solutions of the Heisenberg model on realistic hardware [32].

### 3. Quantum Tensor Networks

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Tensor networks form a modern framework for representing, analyzing, and numerically simulating quantum states. Tensor networks trace their origin to Penrose's 1971 graphical calculus [33] and, in certain special cases, even to Cayley's 19th-century invariant theory [34]. Since then they have developed into a unifying formalism spanning mathematical physics [33], category theory [35, 36], computer science, algebraic logic, and related areas [35]. In modern quantum theory, tensor networks emerged as a principled approach to approximating quantum states [37]. Independently, tensor networks arose as diagrammatic representations of quantum circuits [38], digital circuits [39], and a variety of compositional systems [36, 40, 33].

My doctoral thesis introduced the early algebraic normal forms showing that any qubit state can be expressed using XOR, COPY, and AND tensors together with scalar weights, giving an explicit tensor-language characterization of qubit states in graphical form. It also showed that  $|-\rangle$  states combined with AND generate Hadamard gates, while AND with COPY yields Toffoli gates, resulting in a computationally universal quantum gate set [41] found from three generating tensors. This body of work was done in collaboration with Ville Bergholm, Stephen Clark, and Dieter Jaksch. It was recognized with a 2010 Doctoral Thesis Prize from the University of Oxford's Mathematical, Physical and Life Sciences Division. We also adapted these tools in several ways. In particular, we used them to efficiently describe finite Abelian lattice gauge theories [42], identifying a class of efficiently contractible tensor networks [1].

With Jacob Turner and Jason Morton, we proved that read-once Boolean formulae reduce to tree tensor networks and are therefore efficiently solvable by graphical contraction [1]. More generally, we showed that counting problems formulated as tensor contractions are efficiently solvable whenever their normal form contains only logarithmically many COPY tensors. As such, we proved that #P-hard counting problems and 3-SAT decision problems on  $n$  bits become efficiently solvable when their tensor-network representation contains at most  $\mathcal{O}(\ln n)$  COPY tensors and has polynomially bounded fan-out [1]. This result linked read-once formulae to tensor contractions and produced the early graphical rewrites establishing satisfiability through tensor-network structure.

Additionally, working with Ville Bergholm and Marco Lanzagorta, we developed a diagrammatic theory of algebraic invariants for entanglement classification using matrix product states (MPS) [4]. I presented this work as a Shapiro Lecture Series at the Department of Mathematics at Pennsylvania State University. Later, in collaboration with Alexey Uvarov, we used related tensor-network structures to evaluate Haar-random integrals in our study of barren plateaus in variational quantum algorithms [43], drawing directly on contraction patterns first introduced in [4].

Tensor-network tools remain integral to my research. For example, working with Chris Wood and David Cory, we introduced a graphical-tensor formalism that interrelates different representations of

open quantum systems via graphical rewrites [5]. We applied projected-entangled-pair-state (PEPS) techniques to bound bipartite entanglement in low-depth circuits on realistic quantum-processor topologies [44, 7]. With Andrey Kardashin and Alexey Uvarov, we introduced a quantum-machine-learning approach to contracting tensor networks on quantum computers [45]. Several of these developments were surveyed in my earlier overview [46].

## 4. Walks and Quantum Transport on Complex Networks

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Complex networks encode dynamical behavior through connectivity and spectral structure. In classical systems, degree distributions, modularity, and Laplacian spectra predict diffusion, synchronization, epidemics, and mass-action kinetics [47, 48, 49]. When quantum correlations and measurement enter, however, classical network descriptors often fail to predict behavior relevant to quantum information processing [50]. Why do they fail?

This research develops a transport-centered framework enabling graph-theoretic reasoning about quantum systems [51, 52, 50, 18, 15, 16, 17]. The central object is the Hamiltonian generator defined by a graph (adjacency or Laplacian), and the question is which structural features control coherence, interference, directionality, and quantum information flow.

To address this, we studied continuous-time quantum walks and quantum transport on complex networks [18, 15, 16, 17]. In particular, [16] developed the low-energy theory of continuous quantum walks and determined when quantum transport inherits scale-free behavior from underlying network topology, and when interference fundamentally alters classical scaling laws. This work provided a systematic comparison between quantum and stochastic processes [18, 15, 16, 17], identifying both formal parallels and sharp dynamical differences. Building on this transport-centric viewpoint, we translated various classical network-science tasks into quantum settings. For example, we introduced a quantum analogue of community detection [17], defining modular structure through quantum dynamical signatures rather than purely combinatorial measures [49]. This body of work was published in a series of papers in *Physical Review X* [16, 17, 18] and contributed to the development of applications of quantum information tools to complex networks [18, 50].

As part of this program, I co-introduced chiral quantum walks [15], demonstrating that controlled breaking of time-reversal symmetry can serve as a resource for directional quantum transport. This effect was subsequently emulated experimentally in collaboration with researchers at the Institute for Quantum Computing at the University of Waterloo [53], linking symmetry breaking directly to operational control of transport. The controlled directionality enabled by time-reversal symmetry breaking has since been realized in multiple experimental platforms and underpins what is now termed *chiral quantum routing* [54].

Finally, with John C. Baez, we coauthored *Quantum Techniques in Stochastic Mechanics* [2], proposing a mathematical framework placing stochastic and quantum dynamics within a unified formal structure. With the publisher's consent, the book was made publicly available on arXiv to broaden accessibility [48]. This line of research has contributed to the interface between quantum information and network science, stimulating funding programs, workshops, and special issues. A comprehensive survey of the area was published with Manlio De Domenico and Mauro Faccin in [50], appearing in the 2019 Anniversary Collection: Editors' Selection.

## 5. Quantum Machine Learning & Variational Algorithms \_\_\_\_\_

Quantum computer programs are described by quantum circuits. Modern quantum processors facilitate the execution of fixed quantum circuits with gates tuned by classical outer-loop optimization. This yields two main classes of algorithms to optimize cost functions (Hamiltonians):

- (1) The Variational Quantum Eigensolver (VQE) [55].
- (2) The Quantum Approximate Optimization Algorithm (QAOA) [56].

My work helped understand the computational capacity of both approaches to cost Hamiltonian optimization. Assuming quantum fault tolerance, an idealized version of VQE's feed-forward structure was shown to be a universal quantum computation model [7, 6], appearing as an Editors' Selection in the letters section of *Physical Review A*. With Zoltán Zimborás and building on results from Seth Lloyd, we considered how QAOA's simple split-operator sequences can simulate general quantum circuits [57].

Analyzing the quantum computing architectures with classical outer-loop optimization for training variational quantum algorithms has proven challenging. In 2019 we found that increasing the constraint to variable ratio in random  $k$  satisfiability instances induces under-parameterization, causing QAOA to fail [8]. This phenomenon, termed reachability deficits [8], has since been extensively studied. We further analyzed the presence of reachability deficits in Google's experimental data [58], concluding that Google's processor [59] approaches a performance fall-off, implying circuit depth requirements beyond current experimental capabilities.

This work also studied abrupt training transitions [9], where the penalty functions become unlearnable below a certain circuit depth and perfectly learnable with just an additional layer [9]. Prior to our work, this effect, while noted in some numerical data, does not appear to have been predicted analytically.

Our collaboration also established parameter concentrations [11]. We specified how solving a problem instance on  $k$  qubits gives a good approximation for  $k + m$  qubits. We also observed that single-layer training halts at critical values but can be revived under certain noise types [10], sparking interest in noise-assisted training. In collaboration with Alexey Uvarov, we proved several results concerning barren plateaus in quantum circuit training [43]. More recent work has examined robustness to noise [60, 61] and, more constructively, exploits noise structure via gauge transformations of the penalty Hamiltonian so that the dissipative dynamics is steered toward the current best candidate solution [62].

Finally, we wrote a *Perspective* appearing in *Nature* [63]. This paper appears in the *Web of Science Top 0.1% Highly Cited Paper Index for Physics*. I also contributed to the European Physical Society Grand Challenges volume outlining long-term trajectories in quantum computing and machine learning for secure societies [64].

## 6. Contributions to the Experimental Development of the Field \_\_\_\_\_

Much of my research has focused on what makes quantum information processing structurally different. Being aware of experimental constraints helped me refine the minimal ingredients required for quantum computation, and develop hardware-aware and resource-conscious tools for electronic structure simulation, optimization, and quantum machine learning, connecting algorithmic models to realistic processor architectures. This program has supported a range of experimental qubit modalities, including trapped ions, trapped atoms, superconducting qubits, nitrogen vacancy-centers in diamond, quantum optics and wave-guides [65, 66, 67, 68, 53, 69, 70].

Collaborating to support experimental quantum information processing research began by support-

ing the numerical simulations of the first *in situ* tunable coupler for flux qubits [65]. This program contributed to the theory [12] supporting the first experimental demonstration of quantum algorithms for electronic structure problems using quantum optics [66], a paper listed in the *Web of Science Top 0.1% Highly Cited Paper Index for Physics*.

In collaboration with Jörg Wrachtrup, we developed theory and software for early experimental demonstrations of optimal control using NV-centers in diamond [68]. This paper appears in the *Web of Science Top 0.1% Highly Cited Paper Index for Physics*. We then used that same NV-platform to demonstrate a quantum algorithm calculating the ground energy of helium hydride cation [67]. Later, this work contributed the theory for the first experiment connected to neural network based tomography to correct SPAM errors in wave-guide data [69]. This work achieved improvements over existing methods.

This research also influenced experimental developments in adjacent fields of computing. My work on embedding Boolean functions into Hamiltonians [24, 25] bridged the gap between problem embedding and techniques appearing in digital circuit theory. The language itself turned out to describe how to program stochastic magnetic tunnel junctions [71], a key element in the emerging field of experimental probabilistic  $p$ -bits.

I approach the question of *What Minimal Structure Enables Quantum Computation?* identifying features that distinguish quantum information processing from other models of computation. By incorporating experimental constraints, I continue to refine the minimal ingredients required for quantum computation. This led to the development of mathematical frameworks for analyzing and programming quantum systems that connect quantum circuits, Hamiltonian models, and variational quantum algorithms. These methods are routinely used in quantum information research.

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