Research Statement

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Despite the recent surge in interest in quantum computation and the potential of useful quantum devices in the near future, the field rests on surprisingly shaky foundations. That is, although there are clear tasks on which quantum computation is known to outperform classical computation, the source of this quantum advantage is unclear. My research delves into that critical question at the heart of quantum computation: what is the essential quantum resource that provides this advantage over classical computation? By focusing on a particular model of quantum computation, known as quantum computation with magic states, we can make progress on this problem, and we can relate the possibility of quantum computational advantage to physical and mathematical properties of quantum systems. Similar ideas can then be applied to other models of quantum computation, and potentially to other tasks exhibiting a quantum advantage. This marriage of two fields—quantum information and quantum foundations—provides fruitful grounds for a deeper understanding of both.

Introduction

The field of quantum computation has seen a huge surge in interest in recent years. In addition to academic interest, these days big tech companies (e.g. Google, IBM, Microsoft) and tech startups (e.g. Xanadu, PsiQuantum, IonQ) are also involved in the effort to realize useful quantum technologies. A number of governments have even published official strategies for the development of quantum science and technology [1–5]. This surge is not so surprising as quantum computers promise to be able to solve some computational problems that are intractable for any classical computer, even the largest modern supercomputers. Although it was originally conceived in the early 1980s as a means of simulating quantum systems [6, 7], the fire has been fueled by the more recent development of quantum algorithms for useful tasks with broader appeal [8–10]. As a result, it is now widely believed that the era of quantum advantage is upon us and that we are entering the realm of so-called Noisy Intermediate-Scale Quantum (NISQ) computation [11, 12].

But in spite of the age of the field and the recent surge in interest, a crucial question at the foundation of quantum computation remains unresolved, namely, *what is the essential quantum resource that provides the quantum computational advantage over classical computation?* This is clearly an important question as its resolution could inform the design of quantum computer architectures and the development of new quantum algorithms.

Classical simulation of quantum computations A common way to approach this question is to try to determine families of quantum circuits which can be efficiently simulated by a classical computer [13–15]. Once an efficient classical simulation algorithm is established for a certain family of circuits, it can be concluded that some quantum resource beyond the scope of that family is required for the possibility of a quantum computational advantage. As a simple example of this approach, consider quantum circuits on n qubits consisting of only local operations and local measurements performed on an unentangled initial state. Although you may have access to many qubits resulting in a large Hilbert space dimension (exponential in n), if the initial state is unentangled and the operations do not allow for the creation of entanglement, you are confined to a very small subspace of the full Hilbert space (dimension linear in n). This results in these circuits being efficiently simulable classically. Therefore, we can conclude that entanglement is necessary for a quantum computational advantage. The form of this entanglement can be different depending on the model of quantum computation: in the measurement-based model [16] it is all contained in the preparation of the initial state whereas in the circuit model the initial state is unentangled and the entanglement is generated by the unitary gates of the circuit, but the fact remains entanglement in some form is necessary [13].

As another example, consider quantum circuits consisting of only Toffoli gates. These gates are universal for classical computation, but they cannot perform arbitrary quantum computations because they cannot generate quantum superpositions of computational basis states. This limitation also results in an efficient classical simulation of these circuits. Supplementing the Toffoli gates by Hadamard gates, which do generate superposition states, we obtain a universal gate set for quantum computation [17]. Thus, we can conclude that superposition in some form is also necessary for a quantum computational advantage. In addition to entanglement and superposition, many other candidates for essential quantum properties have been proposed, such as large Hilbert space dimension, contextuality, and Wigner function negativity. Many of these result in similar necessary conditions for quantum advantage.

Magic states and Wigner functions The question posed above can be approached in a more systematic way by focusing on the model of quantum computation with magic states (QCM) [18, 19]—a universal model of quantum computation closely related to the circuit model, and one of the leading candidates for scalable fault-tolerant quantum computation [20]. In QCM, the allowed operations are restricted to a subset of unitary gates forming the so-called Clifford group, as well as Pauli measurements. These operations alone are not sufficient for a quantum computational advantage, and in fact, any quantum circuit consisting of only these operations can be simulated efficiently on a classical computer [21, 22]. Quantum computational universality is restored in QCM through the inclusion of additional "magic" quantum states at the input of the circuit. Therefore, this model allows us to refine the question posed above. Instead of asking broadly "which non-classical resources are required for a quantum computational advantage?", we can focus on the quantum states and ask "which states could be useful for QCM?"

A partial answer to this question is provided by quasi-probability representations like the Wigner function [23]. The Wigner function is the closest quantum mechanical counterpart to the classical notion of a probability distribution over a phase space, but unlike a probability distribution it can take negative values (making it a *quasi*-probability function). Accordingly, negativity in the Wigner function has traditionally been considered an indicator distinguishing classically behaving quantum states from those that exhibit genuinely quantum features [24, 25]. When adapted to finite-dimensional quantum mechanics, the setting relevant for quantum computation, quantum states are represented by a discrete Wigner function [26–32]—a quasi-probability function over a finite set (a generalized phase space) usually satisfying certain constraints [33, 34].

Veitch et al. [14] applied this idea to QCM and showed that a necessary condition for a quantum computational speedup on odd-prime-dimensional qudits (quantum systems with odd prime Hilbert space dimension) is that the Wigner function of the input state of the quantum circuit must take negative values (this result is easily extended to QCM on qudits with any odd dimension [35]). In particular, the amount of negativity in the Wigner function quantifies the cost of classical simulation of a quantum computation [36] with simulation being efficient if the Wigner function is non-negative everywhere. At a technical level, establishing this connection between Wigner function negativity and the possibility of a quantum advantage rests on two facts about the Wigner function [30–32], namely (a) that it is covariant with respect to all Clifford transformations, and (b) that its positivity is preserved under all Pauli measurements.

It turns out, non-negativity of the discrete Wigner function also implies the existence of a non-contextual (read classical) hidden variable model (HVM) describing the computation [15, 37, 38]. Thus, two traditional notions of non-classicality for quantum systems—Wigner function negativity and failure of a classical HVM description—herald a quantum computational advantage over classical computation. This aligns with work that shows contextuality is required for quantum advantage in other settings [39, 40].

Previous research

No-go theorems for discrete Wigner functions in even-dimensions This is a satisfying result, but as mentioned above it applies only to qudits with odd Hilbert space dimension. The case of even dimensions (including systems of multiple qubits) is much trickier [29, 41–47]. Do these results on Wigner function negativity and contextuality carry over to even dimensions?—The Peres-Mermin square proof of contextuality [48] prevents the latter. Regarding the former, until recently an answer was known only in certain special cases [44].

In Ref. [34], we resolved this question for the general case. Therein, we provided two main technical contributions: first, we formalized the obstructions to the existence of Wigner functions with the properties needed for describing quantum computation mentioned previously. Second, we applied these general results to the case of even dimension. The result is, in all even dimensions, Wigner functions constructed from operator bases cannot be Clifford covariant and cannot represent Pauli measurement positively. We found that the source of the difference between even and odd dimensions is a question of cohomology.

This appearance of cohomology may seem surprising, but in fact, homology and cohomology have a long history in physics [49]. Cohomological phenomena have also recently found widespread use in the field of quantum computation, for example: (i) quantum error correction with the Kitaev surface code [50, 51], and its measurement-based counterpart with 3D cluster states [52], (ii) proofs of contextuality of quantum mechanics [53–55], and (iii) the contextuality of measurement-based quantum computation (MBQC) [39, 56]. Cohomology emerges as a language to navigate this web of fundamental facts about quantum computation, and to explain those facts in a unified fashion.

Alternative quasi-probability representations of quantum computation The idea of negativity as a precondition for quantum advantage can be salvaged for the case of even dimensions *if* one admits more general quasi-probability functions, specifically, quasi-probability functions that do not stem from an operator basis, and hence are not uniquely defined for each state [57]. One example of this is obtained by defining a quasi-probability function over stabilizer states [45], bypassing

Wigner functions entirely. It has the advantage of efficiently simulating all QCM circuits on all probabilistic mixtures of stabilizer states.

In Ref. [43], we provided the previously missing phase space picture for QCM on multi-qubit systems. Therein, we define a new quasi-probability function for all Hilbert space dimensions, with a phase space of increased size in accordance with Ref. [57]. In all dimensions, the function is Clifford covariant and the positivity of the representation is preserved under all Pauli measurements. When applied to odd dimensions, it reproduces and extends the existing Wigner function arguments [14], and for multiple qubits, this simulation contains the efficient classical simulation of stabilizer mixtures [45] as a special case. We thus reproduce the essential features of the odd-dimensional scenario in all dimensions.

A hidden variable model for universal quantum computation As noted, obtaining the unified phase space picture of QCM above required relaxing some of the assumptions that traditionally go into the definition of the Wigner function. This relaxation is required in order for the representation to effectively describe quantum computation in all dimensions [34, 57], but it leads to some interesting consequences.

In Refs. [47, 58] we showed that, if sufficiently general quasi-probability representations are admitted, we can define a fully *probabilistic* representation of QCM. That is, a hidden variable model can be defined which represents all quantum states, operations, and measurements relevant for QCM using only (non-negative) probabilities. This model is structurally similar to previously defined quasi-probability representations (modulo absence of negativity) and it leads to a classical simulation method for universal quantum computation based on sampling from the defining probability distributions. The model is based on the so-called Λ polytopes—polytopes in the space of Hermitian operators on the multi-qudit Hilbert space which contain the space of physical quantum states (see e.g. Ref. [58] for their definition). We identify the generalized phase space points of the model with the vertices of these polytopes.

This model appears classical and this gives us an interesting puzzle. Namely, if any quantum computation can be simulated by sampling from a finite family of probability distributions, then where is the quantumness that provides the advantage for quantum computation hiding?

Trading negativity for complexity The absence of negativity in the HVM of Refs. [47, 58] comes at a cost. We can no longer guarantee that the generalized phase space points over which the model is defined (i.e. the vertices of the Λ polytopes) have efficiently computable state update rules under Clifford gates and Pauli measurements. Therefore, although the model can classically simulate any universal quantum computation (magic state quantum computations on any input state), the simulation is not guaranteed to be efficient in general.

There are, however, some special cases in which the simulation is efficient. For example, for odd-dimensional qudits, the phase space point operators which define the odd-dimensional Wigner function are vertices of the Λ polytopes [58]. Similarly, in the multi-qubit case, the phase space point operators of described in the unified phase space picture [43] above are also vertices of Λ [47, 59], these are the so-called CNC vertices. The update of these vertices under Clifford gates and Pauli measurements will be efficiently computable classically, and so the simulation algorithm is efficient whenever the support of the probability distribution representing the input state of the circuit is restricted to vertices of this type. In other words, these subsets of Λ vertices define sub-polytopes inside the full Λ-polytopes, wherein the simulation remains efficient.

Future work

The observation above leaves us with a clear path forward, which proceeds in steps.

1. First, some sub-polytope models inside Λ provide efficient classical simulation of quantum computations, but if a quantum computational advantage is possible as is commonly believed then this efficiency must breakdown somewhere in between the CNC sub-polytope model and the full Λ polytope. Now we can probe this phenomenon by characterizing more vertices of Λ. The more vertices we can efficiently characterize, the more quantum computations we can efficiently simulate classically, thus effectively pushing back the boundary between classical and quantum. Some progress has been made in this regard. In Ref. [60], some new vertices were characterized, and in Ref. [61] we found new infinite families of vertices for all numbers of qubits. That said, the vertices characterized so far remain a small fraction of the total number of vertices for $n \geq 3$ qubits, and so there is still much work to be done here and much to be gained from it.
2. Second, since negativity in a quasi-probability function is no longer the source of inefficiency of classical simulation, inefficiency must come another source. One early suggestion was that it came from a blowup in the size of the generalized phase space of the model. Although seemingly a reasonable suggestion, we recently ruled this out as the source of inefficiency as well [62]. The only possibility remaining is that it lies somewhere in the sampling from the probability distributions that represent states and measurements in the model. We would like to be able to better describe this source of the inefficiency in the classical simulation algorithm.

3. Finally, in the past sources of inefficiency in the classical simulation of quantum computation were linked to traditional indicators of non-classicality in quantum theory, such as contextuality [15, 38]. We would like to determine how the inefficiency in the classical simulation based on the Λ polytopes relates to other notions of non-classicality like generalized contextuality. Alternatively, here we could reverse this process, and derive an indicator of non-classicality from the source of inefficiency found in the first two steps above. This indicator could then be applied to other quantum information processing tasks, and possibly to the foundations of quantum computation and quantum theory.

Solutions to the problems proposed here would allow us to better characterize the foundation on which the phenomenon of quantum computational advantage rests. As a result, they also have the potential to significantly influence design of quantum computers and new quantum algorithms both in the NISQ era and beyond.

The research proposed here is, in part, a continuation of work that began during the course of my PhD. There are many reasons for continuing this line of research. As demonstrated above, although significant progress has been made, there is still much work to be done and much to be gained from pursuing this line of research further. In addition, the Λ polytopes are still relatively new objects [47, 58]. As a result, some information is known about them [58, 60–62], but there is much still to be discovered. In particular, they have so far only been used for the problem of characterizing quantum computational advantages in the magic state model. Some progress has been made in extending their applicability beyond this model [62], but we believe there could yet be more applications.

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