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Contextuality as a resource for models of quantum computation on qubits

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A central question in quantum computation is to identify the resources that are responsible for quantum speed-up. Quantum contextuality has been recently shown to be a resource for quantum computation with magic states for odd-prime dimensional qudits and two-dimensional systems with real wavefunctions. The phenomenon of state-independent contextuality poses a priori an obstruction to characterizing the case of regular qubits, the fundamental building block of quantum computation. Here, we establish contextuality of magic states as a necessary resource for a large class of quantum computation schemes on qubits. We illustrate our result with a concrete scheme related to measurement-based quantum computation.

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The model of quantum computation by state injection (QCSI) [1] is a leading paradigm of fault-tolerance quantum computation. Therein, quantum gates are restricted to belong to a small set of classically simulable gates, called Clifford gates [2], that admit simple fault-tolerant implementations [3]. Universal quantum computation is achieved via injection of magic states [1], which are the source of quantum computational power of the model.

A central question in QCSI is to characterize the physical properties that magic states need to exhibit in order to serve as universal resources. In this regard, quantum contextuality has recently been established as a necessary resource for QCSI. This was first achieved for quopit systems [4,5], where the local Hilbert space dimension is an odd prime power, and subsequently for local dimension two with the case of rebits [6]. In the latter, the density matrix is constrained to be real at all times.

In this work we ask “Can contextuality be established as a computational resource for QCSI on qubits?” This is not a straightforward extension of the quopit case because the multi-qubit setting is complicated by the presence of state-independent contextuality among Pauli observables [7,8]. Consequently, every quantum state of \( n \geq 2 \) qubits is contextual w.r.t. Pauli measurements, including the completely mixed one [5]. It is thus clear that contextuality of magic states alone cannot be a computational resource for every QCSI scheme on qubits.

Yet, there exist qubit QCSI schemes for which contextuality of magic states is a resource, and we identify them in this work. Specifically, we consider qubit QCSI schemes \( \mathcal{M}_\Omega \) that satisfy the following two constraints:

(C1) Resource character. There exists a quantum state that does not exhibit contextuality with respect to measurements available in \( \mathcal{M}_\Omega \).

(C2) Tomographic completeness. For any state \( \rho \), the expectation value of any Pauli observable can be inferred via the allowed operations of the scheme.

The motivation for these constraints is the following. Condition (C1) constitutes a minimal principle that unifies, simplifies and extends the quopit [5] and rebit [6] settings. While seemingly a weak constraint, it excludes the possibility of Mermin-type state-independent contextuality [7,8] among the available measurements (see Lemma 1 below). A priori, the absence of state-independent contextuality comes at a price. Namely, for any QCSI scheme \( \mathcal{M}_\Omega \) on \( n \geq 2 \) qubits, not all \( n \)-qubit Pauli observables can be measured. Thus, the question arises of whether this limits access to all \( n \) qubits for measurement. As we show in this work, this doesn’t have to be the case.

Addressing this question, we impose tomographic completeness as our technical condition for a true \( n \)-qubit QCSI scheme, cf. (C2). It means that any quantum state can be fully measured given sufficiently many copies. The rebit scheme [6], for example, does not satisfy this.

One of our results is that for any number \( n \) of qubits there exists a QCSI scheme which satisfies both conditions (C1) and (C2).

The reason why both conditions can simultaneously hold lies in a fundamental distinction between observables that can be measured directly in a given qubit QCSI scheme from those that can only be inferred by measurement of other observables. The resulting qubit QCSI schemes resemble their quopit counterparts [4,5] in the absence of state-independent contextuality, yet have full tomographic power for the multi-qubit setting.

The main result of this work is Theorem 1. It says that if the initial (magic) states of a qubit QCSI scheme are describable by a non-contextual hidden variable model (NCHVM) it becomes fundamentally impossible to implement a universal
set of gates. We highlight that Theorem 1 applies generally to any scheme fulfilling the condition [C1] including that of [6].

The condition [C1] plays a pivotal role in our analysis. It is clear that contextuality of the magic states can be a resource only if condition [C1] holds. In this work we establish the converse, namely that contextuality of the magic states is a resource for QCSI if condition [C1] holds. Therefore, condition [C1] is the structural element that unifies the previously discussed quopit [5] and rebit [6] case, and the qubit scenarios discussed here. Together, condition [C1] and Theorem 1 characterize the contextuality types that are needed in quantum computation via state injection, showing that state-dependent contextuality with respect to Pauli observables is a universal resource.

As a final remark, we note that the measurements available in QCSI schemes satisfying [C1] preserve positivity of suitable Wigner functions [9].

Setting. An n-qubit Pauli observable $T_a$ is a hermitian operator with ±1 eigenvalues of form

$$T_a := \xi(a)Z(a_Z)X(a_X) := \xi(a) \bigotimes_{i=1}^{n} Z_{i}^{a_{Z_i}} \bigotimes_{j=1}^{n} X_{j}^{a_{X_j}}, \quad (1)$$

where $a := (a_Z, a_X)$ is a 2n-bit string and $\xi(a)$ is a phase. Pauli observables define an operator basis that we call $T_n$.

A qubit scheme $M_{O}$ of quantum computation via state injection (QCSI) consists of a resource $\mathcal{M}$ of initial “magic” states and 3 kinds of allowed operations:

1. Measurement of any Pauli observable in a set $\mathcal{O}$.
2. A group $G$ of “free” Clifford gates that preserve $\mathcal{O}$ via conjugation up to a global phase.
3. Classical processing and feedforward.

Adaptive circuits of operations 1-3 may be combined with classical post-processing in order to simulate measurements of Pauli observables that are not in $\mathcal{O}$ (cf. Fig. [1]). We name the latter “inferable” and let $\mathcal{I}$ be the super set of $\mathcal{O}$ defined by them. Analogously, we let $\mathcal{J}$ be the set of sets of compatible Pauli observables that can be inferred jointly, which define the “contexts” of our computational model. As shown in Fig. [1] not every set of compatible Pauli observables is necessarily in $\mathcal{J}$. Yet, $A \in \mathcal{I}$ implies that $\{A\} \in \mathcal{J}$. Furthermore, for any pair of observables $\{A, B\} \in \mathcal{J}$ and $\alpha \in \mathbb{R}$, the observables $AB, \alpha A$ can be inferred jointly by measuring $A, B$, since the eigenvalues of the latter determine those of the former. Hence,

$$\{A, B\} \in \mathcal{J} \Rightarrow \{A, B, AB, \alpha A\} \in \mathcal{J}, \quad \forall \alpha \in \mathbb{R}. \quad (2)$$

Constraint [C2] holds iff $T_n \subset \mathcal{I}$, i.e., iff the outcome distribution of any Pauli observable can be sampled from via measurements in $\mathcal{O}$ and classical post-processing.

Contextuality. Above, imposing [C1] means that there exists a quantum state $\rho$ whose measurement statistics can be reproduced by a non-contextual hidden variable model (NCHVM), which we introduce next.

Definition 1. A NCHVM $(\mathcal{S}, \mathcal{G}, \Lambda)$ for the state $\rho$ with respect to a scheme $M_{O}$ consists of a probability distribution $q_{\nu}$ over a set $\mathcal{S}$ of internal states and a set $\Lambda = \{\lambda_{\nu}\}_{\nu \in \mathcal{S}}$ of value assignment functions $\lambda_{\nu} : \mathcal{I} \rightarrow \{\pm1\}$ that fulfill:

1. For any $\lambda_{\nu} \in \Lambda$ and $M \in \mathcal{J}$ the real numbers $\{\lambda_{\nu}(A)\}_{A \in \mathcal{M}}$ are compatible eigenvalues: i.e. there exists a quantum state $|\psi\rangle$ such that

$$A|\psi\rangle = \lambda_{\nu}(A)|\psi\rangle, \quad \forall A \in \mathcal{M}. \quad (3)$$

2. The distribution $q_{\nu}$ satisfies

$$\langle A \rangle_{\rho} = \text{tr}(A\rho) = \sum_{\nu \in \mathcal{S}} \lambda_{\nu}(A)q_{\nu}(\nu), \quad \forall A \in \mathcal{I} \quad (4)$$

The state $\rho$ is said to be “contextual” or to “exhibit contextuality” if no NCHVM with respect to $M_{O}$ exists.

Qubit QCSI for which all possible inputs exhibit contextuality are forbidden by [C1]. Specifically, in this work, $\mathcal{O}$ must be a strict subset of $T_n$ [7,8].

Main Result. We now establish contextuality as a resource for quantum computational universality for all qubit QCSI schemes that fulfill [C1]. Below, we call a scheme $M_{O}$ universal if for any integer $n \geq 1$ and $V \in U(2^n)$ there exists a finite-size circuit of $M_{O}$ operations that prepares the $n$-qubit state $V|0\rangle$ up to any positive trace-norm error.

Theorem 1. A qubit QCSI scheme $M_{O}$ satisfying [C1] is universal for $n \geq 3$ qubits only if its magic states exhibit contextuality.

Theorem 1 applies even in the setting where the computation happens in an encoded subspace, reproducing the rebit.
Lemma 2. qubit QCSIs on non-contextual inputs. namely, a method to construct NCHVMs that can simulate With these tools, we arrive at a powerful intermediate result, \( \text{Lemma 1.} \) that contextuality cannot be freely

\[ \lambda_\nu(AB) = \lambda_\nu(A)\lambda_\nu(B), \quad \lambda_\nu(\alpha A) = \alpha \lambda_\nu(A), \]  
that any \( \lambda_\nu \in \Lambda \) must fulfill for any pair \( A, B \in \mathcal{J}, \alpha \in \mathbb{R} \).

Second, we prove the following lemma.

**Lemma 1.** For any QCSI scheme \( \mathcal{M}_\Theta \) fulfilling [C1] the phase \( \xi(a) \) in [7] can be chosen w.l.o.g. so that

\[ T_{a+b} = T_{a+b} \quad \text{for any triple \( \{T_a, T_b, T_{a+b}\} \in \mathcal{J}. \} \]

**Proof.** Let \( \xi \) be given and let \( \lambda_\nu \) be a consistent value assignment for the scheme \( \mathcal{M}_\Theta \). W.l.o.g., we can redefine \( T'_{a+b} := \lambda_\nu(T_a)T_b(T_{a+b}) = \lambda_\nu(a)\lambda_\nu(b)T_{a+b} \) 

\[ (\pm 1)^2 \lambda(T_a)T_b \lambda(T_{a+b})T_{a+b} = T_{a+b} \]

Last, we observe that for any \( M \in \mathcal{J}, |\psi\rangle \) as in (3) and \( T_b \in T_n \), the state \( T_b|\psi\rangle \) is a joint eigenstate of \( M \):

\[ \langle \gamma T_b | T_b |\psi\rangle \left( \frac{\lambda_\nu(T_b)}{(\pm 1)|T_a T_b \rangle \langle T_{a+b}| \pm (\pm 1)|T_a T_b \rangle \langle T_{a+b}| \right), \quad \forall \gamma T_b \in \mathcal{J} \]  
where \( [a, b] := a_X \cdot b_Z + a_Z \cdot b_Y \mod 2 \); combined with (5), this induces a group action of \( \mathbb{Z}_2^n \) on value assignments

\[ \nu \stackrel{u}{\rightarrow} \nu + u(T_a) := \lambda_\nu(T_a)(-1)^{[u,a]}, \forall u \in V. \]

With these tools, we arrive at a powerful intermediate result, namely, a method to construct NCHVMs that can simulate qubit QCSIs on non-contextual inputs.

**Lemma 2.** For any qubit scheme \( \mathcal{M}_\Theta \) fulfilling [C1] and any quantum circuit \( C \) of \( \mathcal{M}_\Theta \) operations, if there exists a NCHVM \( \langle S, q_\rho, \Lambda \rangle \) for some given input state \( \rho_\alpha \), then there exists a NCHVM \( \langle S, q_\rho, \Lambda \rangle \) for the output \( \rho_{\alpha+\lambda} \) of \( C(\rho_\alpha) \).

Lemma 2 establishes that contextuality cannot be freely generated in qubit QCSI. A surprising aspect of this fact is that it holds for circuits that contain intermediate measurements. Intuitively, unitary gates in \( \Phi \) must induce an action on the set of non-contextual states since they preserve the set \( \mathcal{O} \). However, the evolution of non-contextual states under measurement is far from intuitive since the latter can often prepare states that are inaccessible to gates [11].

Lemma 2 leads to a simple classical random-walk algorithm for sampling from the output distribution of all measurements in \( C \), which is further efficient if oracles for sampling from \( q_\rho, \Lambda \) are given. The random walk first samples a state \( \nu_0 \in S \) from \( q_\rho, \Lambda \) and, upon measurement of \( T_{a_1} \in \mathcal{O} \) at time \( t \), outputs \( \lambda_\nu(T_{a_1}) \) given \( \nu_t \) and updates \( \nu_t \rightarrow \nu_t + a \) with \( 1/2 \) probability. The correctness of this algorithm follows from Eq. (9) below and is analyzed in detail in [9].

**Proof.** We fix a phase convention for \( T_a \) so that Eq. (6) in Lemma 1 holds and introduce a simplified notation

\[ \lambda_\nu(a) := \lambda_\nu(T_a), \quad \text{where } T_a \in \mathcal{A}, a \in \mathbb{Z}_2^n. \]

Because free unitaries preserve \( \mathcal{O} \) they can be propagated out of \( C \) via conjugation. Hence, we can w.l.o.g. assume that \( C \) consists only of measurements. Our proof is by induction. At time \( t = 1 \), \( \rho_1 = \rho_m \) has an NCHVM by assumption. At any other time \( t + 1 \), given an NCHVM \( \langle S, q_{\rho_t}, \Lambda \rangle \) for the state \( \rho_t \), we construct an NCHVM \( \langle S, q_{\rho_{t+1}}, \Lambda \rangle \) for \( \rho_{t+1} \). Specifically, let \( T_{a_1} \in \mathcal{O} \) be the observable measured at time \( t \) with corresponding outcome \( s_t \in \{\pm 1\} \), \( s_{t+1} := (s_1, \ldots, s_t) \) be the string of prior measurement records, and \( p(s_t|s_{t-1}) \) the conditional probability of measuring \( s_t \); we will now show that \( \rho_{t+1} \) admits the hidden-variable representation

\[ q_{\rho_{t+1}}(\nu) := \frac{\delta_{s_t, \lambda_\nu(a)} q_{\rho_t}(\nu) + q_{\rho_t}(\nu + a)}{2}, \]

where \( p(s_t|s_{t-1}) \) can be predicted by the HVM, since

\[ 2p(s_t|s_{t-1}) = (1 + s_t T_{a_1}) \rho_t = (T_{a_1} + s_t T_{a_1}) \rho_t - \text{which are known by the induction promise. Our goal is to show that} \]

\[ \langle S, q_{\rho_{t+1}}, \Lambda \rangle \text{ predicts the expected value of any } T_a \in \mathcal{A} \text{ measured at time } t + 1. \text{ For this, we derive a useful expression,} \]

\[ \langle T_a \rangle_{\rho_{t+1}} = \sum_{\nu \in S} q_{\rho_{t+1}}(\nu) \lambda_\nu(a) \]

\[ \sum_{\nu \in S} \frac{\delta_{s_t, \lambda_\nu(a)} q_{\rho_t}(\nu)}{2p(s_t|s_{t-1})} \lambda_\nu(a) + \sum_{\nu \in S} \frac{\delta_{s_t, \lambda_\nu(a)} q_{\rho_t}(\nu + a)}{2p(s_t|s_{t-1})} \lambda_\nu(a), \]

\[ \sum_{\nu \in S} \frac{\delta_{s_t, \lambda_\nu(a)} q_{\rho_t}(\nu)}{2p(s_t|s_{t-1})} \lambda_\nu(a) + \frac{\delta_{s_t, \lambda_\nu(a)} q_{\rho_t}(\nu + a)}{2p(s_t|s_{t-1})} \lambda_\nu(a)(-1)^{[a,a]}, \]

which we evaluate on two cases:

(A) \( T_a, T_{a-1} \) anticommute, hence, \( [a, a] = 1 \). We get

\[ \langle T_a \rangle_{\rho_{t+1}} = \sum_{\nu \in S} 1 + s_t \lambda_\nu(a) + s_t \sum_{\nu \in S} q_{\rho_t}(\nu) \lambda_\nu(a + a_1) \]

(B) \( T_a, T_{a-1} \) commute. In this case \( [a, a] = 0 \). Using the identity \( \delta_{s, \lambda} = (1 + s\lambda)/2, \lambda \in \{\pm 1\} \), we obtain
Finally, by induction hypothesis, we arrive at
\[
\langle T_{a} \rangle_{\rho_{t+1}} = \langle T_{a} \rangle_{\rho_{t}} + s_{t} \langle T_{a+\sigma_{t}} \rangle_{\rho_{t}} \cdot \left( \frac{\rho_{t+1}^{I+\sigma_{t}} \rho_{t+1}}{2p(s_{t}|s_{-t})} T_{a} \right) = \text{tr} \left( \frac{1+\sigma_{t}}{2} \rho_{t+1} T_{a} \right) = \text{tr} (\rho_{t+1} T_{a})
\]
which is again the quantum mechanical prediction. □

Finally, we prove our main result.

**Proof of theorem**[1] We derive a contradiction by assuming (A1) that \( M_{O} \) is universal and (A2) that all magic states in \( M \) are non-contextual. We first consider the computation to be error-free and drop this assumption at the end.

Recall that, by assumption (*), two complementary Pauli observables, denoted \( Z_{i}, X_{i} \in O \) w.l.o.g., can be measured on any qubit. By (A1), the scheme \( M_{O} \) can prepare the encoded GHZ state \( |\psi\rangle \) that is uniquely stabilized by \( X_{1}X_{2}X_{1}, -X_{1}Z_{2}Z_{3}, -Z_{1}X_{2}Z_{3}, -Z_{1}Z_{2}X_{3} \). Furthermore, \( M_{O} \) can also infer the value of any correlator of form \( A_{1}A_{2}A_{3} \) with \( A_{1} \in \{ X_{i}, Z_{i} \} \) (in particular, \( |\psi\rangle \)'s stabilizers) by measuring \( A_{1}, A_{2}, A_{3} \) individually. Quantum mechanics predicts
\[
\langle X_{1}X_{2}X_{3} - X_{1}Z_{2}Z_{3} - Z_{1}X_{2}Z_{3} - Z_{1}Z_{2}X_{3} \rangle_{|\psi\rangle}^{QM} = 4.
\]

On the other hand, by (A2) and Lemma 2, there exists an NCHVM for \( |\psi\rangle \) with respect to all quadruples of form \( \{ A_{1}, A_{2}, A_{3}, A_{1}A_{2}A_{3}, A_{1} \in X_{i}, Z_{i} \} \). Using constraint 5 for non-contextual value assignments, we derive an inequality for the NCHVM's prediction
\[
\langle X_{1}X_{2}X_{3} - X_{1}Z_{2}Z_{3} - Z_{1}X_{2}Z_{3} - Z_{1}Z_{2}X_{3} \rangle_{|\psi\rangle}^{HVM} \leq 2,
\]
originally due to Mermin[12], which contradicts quantum mechanics. Hence, either (A1) or (A2) must be false.

Last, our argument holds if arbitrarily small errors are present because the HVM’s prediction deviates from the quantum mechanical one by a finite amount (larger than 2). □

A qubit QCSI scheme powered by contextuality. Here we prove that for any number \( n \) of qubits there exists a universal qubit QCSI scheme \( M_{O} \) that fulfills the conditions [C1] and [C2]. The \( O \) measurements available in this scheme are all single-qubit Pauli measurements, the group \( G \) contains all single-qubit Clifford gates, and the magic state is locally unitarily equivalent to a 2D cluster state. This family of examples demonstrates that the classification provided by our main result (Theorem 1) is not empty.

We now show that single-qubit Pauli measurements satisfy [C1] and [C2]. First, note that the value of any Pauli observable can be inferred by measuring its single-qubit tensor components, hence, local QCSI fulfills [C2]. Second, we show [C1] is also met by giving a NCHVM for the mixed state \( \rho = 1/2^{n} \) with respect to single-qubit operations. The most general joint measurement in \( J \) that we can implement with the latter is to measure \( n \) single-qubit Paulis \( \sigma_{1}, \ldots, \sigma_{n} \) on distinct qubits, which lets us infer the value of any observable \( \gamma \otimes_{i=1}^{n} \sigma_{i}^{a_{i}} \) with \( a_{i} \in \{ I, X, Y, Z \} \). Hence, the function \( \lambda_{0}(\otimes_{i=1}^{n} \sigma_{i}^{a_{i}}) := 1 \) is a joint eigenvalue of \( \{ \otimes_{i=1}^{n} \sigma_{i}^{a_{i}} \mid a_{i} \in \{ I, X, Y, Z \} \} \), extends linearly to a value assignment fulfilling Def. 1. Picking \( T_{n} = \{ I, X, Y, Z \}^{\otimes n} \), we obtain an NCHVM via 5 with value assignments \( \lambda_{0}(T_{n}) := (-1)^{|a_{i}}, b_{i} \in \{ I, X, Y, Z \}^{\otimes n} \) wherein \( \rho \) corresponds to a probability distribution \( q_{\rho}(b) := 1/2^{n} \); indeed, our HVM predicts \( \langle \gamma T_{n} \rangle_{\rho} = \gamma \) for \( T_{n} = T_{0} = I \) and 0 otherwise, matching the quantum mechanical prediction—this can be checked by computing the average of \( \lambda_{0}(T_{n}) \) over \( b \) in each case.

Last, we present a family of magic states that promote our local QCSI scheme to universality. Unlike in standard magic state distillation[11], which relies on product magic states, our scheme has no entangling operations and requires entanglement to be present in the input to be universal. We show that a possibility is to use a modified cluster state \( |\Psi\rangle \) that contains cells as in Fig. 2 with “red-site” qubits that are locally rotated by a \( T \)-gate \( e^{-i\pi/4}Z \). Our approach is to use such state to simulate a universal scheme of measurement based quantum computation based on adaptive local measurements \( \{ Z, X, Y, X \pm Y / \sqrt{2} \} \) on a regular 2D cluster state[13]. Local Pauli measurements are available by assumption. Now, an on-site measurement of \( X \) or \( Y \) on one of the red-qubits of \( |\Psi\rangle \) has the same effect as measuring \( (X \pm Y) / \sqrt{2} \) on a cluster state. To complete the simulation, it is enough to re-route the measurement-based computation through a red-site (this can be done with the available \( X \) measurements[13]) whenever a measurement of \( (X \pm Y) / \sqrt{2} \) is needed. (See Fig. 2 for illustration.)

**Conclusion.** In this work we investigated the role of contextuality in qubit QCSI and proved that it is a necessary resource for all such schemes that meet a simple minimal condition: namely, that the allowed measurements do not exhibit state-independent contextuality. Our result applies if and only if contextuality emerges as a physical property possessed by quantum states (with respect to the measurements available in the computational model). We extended earlier results on odd-
prime dimensional qudits [4, 5] and rebits [6], and thereby completed establishing contextuality as a resource in QCSI in arbitrary prime dimensions. We conjecture that this result generalizes to all composite dimensions [14] (the composite odd case was recently covered after completion of this work [15]) and to algebraic extensions of QCSI models based on normalizer gates [11, 16–19]. Further, we demonstrated the applicability of our result to a concrete qubit QCSI scheme that does not exhibit state independent contextuality while retaining tomographic completeness.

Finally, we refer to a companion paper [9] where we investigate the role of Wigner functions in qubit QCSI. There, we use Wigner functions to motivate the near-classical sector of the free operations in qubit QCSI, and relate their Wigner-function negativity to contextuality and hardness of classical simulation. In comparison, in this work, constraint (C1) completely removes the need to introduce Wigner functions, and leads us to the simplest and most general proof that contextuality can be a resource in qubit QCSI that we are aware of. For this reason, we regard the establishing of condition (C1) as a fundamental structural insight of our work.

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