Contextuality Test of the Nonclassicality of Variational Quantum Eigensolvers

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Contextuality Test of the Nonclassicality of Variational Quantum Eigensolvers

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Contextuality is an indicator of non-classicality, and a resource for various quantum procedures. In this paper, we use contextuality to evaluate the variational quantum eigensolver (VQE), one of the most promising tools for near-term quantum simulation. We present an efficiently computable test to determine whether or not the objective function for a VQE procedure is contextual. We apply this test to evaluate the contextuality of experimental implementations of VQE, and determine that several, but not all, fail this test of quantumness.

I. INTRODUCTION

Quantum computing hardware is entering the era of noisy intermediate scale quantum (NISQ) computers [1]. These are machines that are too large to simulate with classical computers, but too small to allow fault tolerant quantum computation. A crucial question is whether NISQ machines can perform useful tasks beyond the capabilities of classical computers [2].

In the last decade much attention has been focused on algorithms for quantum simulation of chemical systems [3–21]. One such algorithm, the variational quantum eigensolver (VQE, first proposed in [11]), has emerged as an important potential application of NISQ computers. Experimental realizations of VQE have been performed on a number of platforms [9–23].

VQE is based on mapping a Hamiltonian H to a weighted sum $\sum_i h_i \mathcal{P}_i$, where the terms $\mathcal{S} \equiv \{\mathcal{P}_i\}$ are Pauli operators and the h_i are (real) coefficients. A short quantum circuit prepares an ansatz state, and the expectation value of each Hamiltonian term is estimated by repeated prepare-and-measure experiments. The ansatz parameters are optimized classically, producing a variational upper bound to the ground state energy.

VQE is advantageous for NISQ computers because of the short coherence times required compared to phase estimation [13]. Theoretical improvements of VQE to date have proposed methods to reduce the number of qubits and measurements required [24–37], and to improve the ansatz states [31, 38, 39], computation of gradients [40–42], and classical optimization techniques [43]. In the present paper we consider a separate issue: how quantum mechanical is this hybrid quantum-classical algorithm, for a given Hamiltonian? We use contextuality as our measure of quantumness.

The study of contextuality began with the Bell-Kochen-Specker theorem [44–46]. Contextuality of preparation, transformation and measurement were defined in 2008, and the relationship of contextuality to negativity of quasi-probability representations was established [47–51]. Contextuality has been extensively studied in the last decade [52–76].

The Bell-Kochen-Specker theorem states that there exist quantum systems for which it is impossible to reproduce the outcome probabilities of every possible measurement as marginals of single joint probability distribution [44–46]. However, if we restrict to some smaller set of measurements corresponding to a set of observables $\mathcal{S}$, properties of the set determine whether a joint distribution may exist for only those measurements. Measurement contextuality refers to various types of contradictions that can appear in attempts to describe sets of measurements by joint probability distributions. We examine "strong contextuality" [77], which is contextuality in the same vein as the Peres-Mermin square [78–80] (see Mermin's outline of a "plausible" hidden-variable theory in [80, §II].) Colloquially, a set of measurements is strongly contextual if it is impossible to consistently assign outcomes to every measurement in the set. In "weak" versions of contextuality such as Bell inequality violations, joint outcomes may be consistently assignable, but statistical predictions based on the existence of joint probability distributions are violated.

Since VQE is an important near-term application of NISQ machines, it is natural to consider how the contextuality of VQE procedures is related to any quantum advantage that they may obtain. In this paper, we present a method to analyze the contextuality of VQE procedures. As applied to VQE, strong contextuality is a property of the target Hamiltonian. It is independent of the ansatz states, and provides a stringent test of the quantumness of the problem being addressed. The set of Hamiltonians that are noncontextual by our definition includes diagonal Hamiltonians that encode a classical objective function. Such problems are addressed by the Quantum Approximate Optimization Algorithm (QAOA), which is closely related to VQE [81]. As we shall see, the set of noncontextual Hamiltonians contains the set of commuting Pauli Hamiltonians, and therefore represents a broader definition of classicality.

One concept upon which we rely is the *closed subtheory*: a set of measurements in which all measurements whose outcomes are determined with certainty by the outcomes of others in the set are themselves members of the set. We introduce this concept here because it pro-

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vides a distinction between this work and the criteria for strong contextuality studied in [53], which are based on sets of observables that are not necessarily closed subtheories. In [65] it is shown that the efficiency of classical simulation is limited by contextuality for sets of measurements that are closed subtheories. We impose the requirement that sets of operators form closed subtheories, so that the results of [65] apply to our setting.

In [56] the authors obtain criteria for contextuality based on compatibility graphs, as do we. However, [56] focuses on weak contextuality, that is, violation of noncontextual inequalities, whereas our interest is in strong contextuality. We further discuss the distinction between our condition for contextuality and previously studied criteria in Section IV, and in [82].

A natural next step is to develop measures that quantify contextuality based on our criterion. We suggest two simple measures at the end of Section II, and discuss more general measures in [82], as well as their relations with prior measures, which include the contextual fraction [52, 61, 69, 70], relative entropy of contextuality, mutual information of contextuality, contextual cost (all in [59]), and rank of contextuality [64].

In Section II, we develop the notion of contextuality we will study and give our main results. In Section III we evaluate the contextuality of several VQE experiments. We conclude in Section IV with a discussion of our results, and directions for future work.

II. STRONG CONTEXTUALITY

We focus on the analysis of strong contextuality for sets of Pauli operators. We use the following notation: $X \equiv \sigma_x$, $Y \equiv \sigma_y$, $Z \equiv \sigma_z$, and $I \equiv 2 \times 2$ identity ($\mathbb{1}$ will denote a generic identity matrix). We omit the tensor product symbol: IX denotes $I \otimes \sigma_x$. Let $\mathcal{S}$ be the set of measurements that are performed in a quantum procedure: in our case these will be Pauli measurements. As we will discuss below, the (non)contextuality of a quantum procedure is determined by properties of $\mathcal{S}$.

A *joint outcome assignment* is an assignment of one outcome (± 1) to each measurement in $\mathcal{S}$. In an ontological hidden-variable theory, joint outcome assignments correspond to *ontic states* ("real states") of a system, since they may be interpreted as definite ontological values for the observables $\mathcal{S}$. A measurement is then seen as revealing information about the ontic state, which exists independently whether it is measured or not.

A *context* on a finite dimensional Hilbert space is a set of pairwise-commuting observables whose eigenvalues uniquely specify the (shared) basis states. If $\mathcal{S}$ is a context, we will see that it is always possible to consistently assign outcomes to the measurements in $\mathcal{S}$. However, if $\mathcal{S}$ is not a context and has nonempty intersection with multiple incompatible contexts (context compatibility is defined in [82]), it may be impossible to consistently assign joint outcomes. In this case the outcomes thus assigned to any individual measurement are context-dependent: hence the term "contextual."

Given any set of measurements $\mathcal{S}$, let $\overline{\mathcal{S}}$ be the set of measurements whose outcomes are predicted with certainty given an assignment of outcomes to $\mathcal{S}$. In the language of [65], $\overline{\mathcal{S}}$ corresponds to the smallest closed subtheory containing $\mathcal{S}$. The outcomes for $\overline{\mathcal{S}}$ induced by an assignment of outcomes to $\mathcal{S}$ may contain contradictions even if the outcomes for $\mathcal{S}$ alone do not.

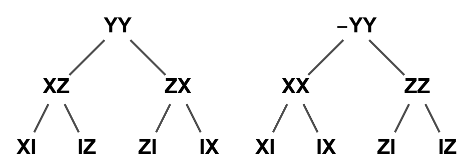
A prediction with certainty occurs when for some observable A' there exists a commuting subset $\mathcal{S}' \subseteq \mathcal{S}$ such that A' is equal to the product of the operators $\mathcal{S}'$. Then since the operators $\mathcal{S}'$ may all be measured simultaneously, in any joint outcome assignment to $\mathcal{S} \cup \{A'\}$ the outcome assigned to A' must be the product of the outcomes assigned to $\mathcal{S}'$: we therefore say that A' is directly determined by $\mathcal{S}$ [78]. A' may now contribute to determining some other operators that are not directly determined by $\mathcal{S}$. Thus in general a measurement A is determined by $\mathcal{S}$ if there is a "determining tree" that leads from $\mathcal{S}$ to A:

Definition 1. A *determining tree* for a Pauli measurement A over a set of Pauli measurements $\mathcal{S}$ is a tree whose nodes are Pauli operators and whose leaves are operators in $\mathcal{S}$, such that...

1. The root is A.
2. All children of any particular parent pairwise commute (as operators).
3. Every parent node is the operator product of its children (and thus commutes with them).

Fig. 1 shows determining trees for the measurements $\pm YY$ over $\mathcal{S} = \{XI, IX, ZI, IZ\}$. It is easy to check that these trees satisfy the properties of Definition 1. This example is a recasting of the classic Peres-Mermin square [78–80].

FIG. 1. Determining trees for $\pm YY$ over $\{XI, IX, ZI, IZ\}$



Given Definition 1, we say that A is *determined* by $\mathcal{S}$ if and only if there exists a determining tree for A over $\mathcal{S}$. This also provides a formal definition for $\overline{\mathcal{S}}$: it is the set of Pauli measurements for which there exist determining trees over $\mathcal{S}$.

Given a determining tree τ for a Pauli A over a set of Pauli operators $\mathcal{S}$, and a joint outcome assignment to $\mathcal{S}$, we may now find the determined outcome for A. Let $\mathcal{L}$ be the leaves of τ; $\mathcal{L}$ may contain multiple copies of the same operator. By induction on property 3 of a determining tree (see Definition 1), A is the operator product of the elements of $\mathcal{L}$. Therefore, given an assignment of values $\rho_L = \pm 1$ to each $L \in \mathcal{L}$, the value assigned to A must be

$$\rho_A = \prod_{L \in \mathcal{L}} (\rho_L)^{m_L} = \prod_{L \in \mathcal{D}} \rho_L, \tag{1}$$

where the exponent m_L is the multiplicity of the operator L in $\mathcal{L}$. $\mathcal{D}$ is a subset of the leaves that we call the *determining set* of τ, defined as follows:

Definition 2. For a determining tree τ, the *determining set* is defined to be the set containing one copy of each operator with odd multiplicity as a leaf in τ. If for some determining tree with root A, the determining set is empty, then every m_L in the first product in (1) must be even, so the outcome assigned to A is 1.

We may now state our condition for contextuality:

Definition 3. A set $\mathcal{S}$ of Pauli operators is *contextual* if for some Pauli A there exists a determining tree τ for A over $\mathcal{S}$ and a determining tree τ' for $-A$ over $\mathcal{S}$ such that the determining sets for τ and τ' are identical.

By (1), the existence of such trees implies that for any joint outcome assignment, the outcome for A is both $+1$ and -1, which is a contradiction.

How does this apply to the Peres-Mermin square? Fig. 1 gives determining trees for $\pm YY$ over $\mathcal{S} = \{XI, IX, ZI, IZ\}$. In each tree, the set of leaves is $\mathcal{S}$ and each leaf has multiplicity 1, so the determining set for each tree is $\mathcal{S}$. Thus $\mathcal{S}$ satisfies the criteria in Definition 3, and is contextual.

The criterion for strong contextuality in Definition 3 depends on a measurement operator ($A \in \overline{\mathcal{S}}$) that may or may not be an element of $\mathcal{S}$. However, for any $\mathcal{S}$ that is contextual according to Definition 3, we may obtain a contradiction in the assignment(s) to an operator contained in $\mathcal{S}$. This is demonstrated by the following corollary:

Corollary 3.1. *A set $\mathcal{S}$ of Pauli operators is contextual if and only if for some $B \in \mathcal{S}$ there exists a determining tree for $-B$ over $\mathcal{S}$, whose determining set is $\{B\}$.*

The plain language statement of the contradiction in this case is: "the outcome (± 1) assigned to $-B$ must be the outcome assigned to B." A third equivalent definition is also useful:

Corollary 3.2. *A set $\mathcal{S}$ of Pauli operators is contextual if and only if there exists a determining tree for $-\mathbb{1}$ over $\mathcal{S}$, whose determining set is empty.*

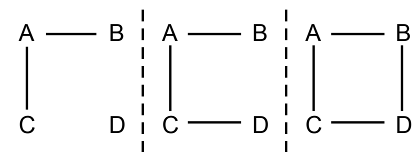
The proofs may be found in [82]. The plain language statement of the contradiction in this case is: "the outcome assigned to $-\mathbb{1}$ (whose eigenvalues are all -1) must be $+1$." Definition 3, Corollary 3.1, and Corollary 3.2 formalize the notion of contradiction in induced joint outcomes for $\overline{\mathcal{S}}$. Since $\overline{\mathcal{S}}$ is the smallest closed subtheory containing $\mathcal{S}$, such a contradiction constitutes strong contextuality of $\mathcal{S}$.

We now present three theorems that give necessary and sufficient conditions for measurement contextuality in the sense of Definition 3. We will make use of the following concept:

Definition 4. For a set $\mathcal{S}$ of Pauli operators, the *compatibility graph* of $\mathcal{S}$ is an undirected graph whose nodes are the operators in $\mathcal{S}$, and in which a pair of operators is adjacent if and only if they commute.

Theorem 1. *A set of four Pauli operators $\{A, B, C, D\}$ is contextual if and only if its compatibility graph has one of the forms given in Fig. 2 (up to permutations of the operators).*

FIG. 2. Compatibility graphs for contextual sets of four Pauli operators.



Theorem 2. *A set of n Pauli operators is contextual if and only if it contains a subset consisting of four operators whose compatibility graph has one of the forms given in Fig. 2 (up to permutations of the operators).*

The proofs of Theorems 1 and 2 are given in [82]. Theorem 2 provides an efficient algorithm for determining whether an arbitrary set $\mathcal{S}$ of Pauli measurements is contextual. First remove any operators from $\mathcal{S}$ that commute with all others (searching for these takes $O(|\mathcal{S}|^2)$ steps): let $\mathcal{T}$ be the remaining set. Then over $\mathcal{T}$, search for a set of three operators A, B, C such that A commutes with B and C, but B and C anticommute. If such a set exists, then since there is some $D \in \mathcal{T}$ that anticommutes with A, the compatibility graph of A, B, C, D has one of the forms Fig. 2 (up to exchange of B and C): thus $\mathcal{S}$ is contextual. If no such set exists, then $\mathcal{S}$ is noncontextual. There are $O(|\mathcal{S}|^3)$ subsets of size three in $\mathcal{S}$, so this is the runtime for the search. In many VQE procedures some structure on the set $\mathcal{S}$ is known, which may improve the efficiency of determining whether it is contextual.

Although we ultimately only need to search for triples of operators in the algorithm, the contextual compatibility graphs in Fig. 2 have four nodes instead of three because we must first remove universally-commuting operators. Note that after this is done (to obtain $\mathcal{T}$), we search for a subset $\{A, B, C\}$ in which commutation is not transitive. Each such subset represents an obstacle to commutation being an equivalence relation on $\mathcal{T}$. This is formalized in the following theorem:

Theorem 3. *For a set $\mathcal{S}$ of Pauli operators, let $\mathcal{T}$ be the set obtained by removing any operator that commutes with all others in $\mathcal{S}$. Then $\mathcal{S}$ is noncontextual if and only if commutation is an equivalence relation on $\mathcal{T}$.*

The proof of Theorem 3 is given in [82]. That commutation is not transitive in general is a non-classical property. Operators that commute with all others in the set cannot contribute to contextuality (see Lemma 2.1, in [82]), so it is satisfying that after removing these non-transitivity of commutation is equivalent to contextuality.

Can we extend our evaluation procedure to a measure of the amount of contextuality present in a contextual set $\mathcal{S}$? One natural measure of the contextuality of H is obtained by evaluating the distance from H to any noncontextual Hermitian operator, as suggested in [69]. Any choice of metric on observables will induce such a measure. Let a *decontextualizing set* $\mathcal{S}'$ be any subset of $\mathcal{S}$ such that $\mathcal{S} \setminus \mathcal{S}'$ is noncontextual. Then we may define another measure of contextuality as the minimum of $\sum_j |h'_j|$ over all subsets $\{h'_j\}$ of the coefficients that are associated to decontextualizing sets. This measure provides an upper bound on the error in the energy estimate induced by "decontextualizing" the Hamiltonian. We discuss generalizations of these measures, and their relations with previously studied measures in [82].

III. EVALUATION OF CONTEXTUALITY IN VQE EXPERIMENTS TO DATE

We now use the methods in Section II to assess contextuality in VQE experiments performed to date. The results are summarized in Table I, in which we also give CD_0, a measure of contextuality given by the minimum size of any decontextualizing set as a fraction of the total number of terms. For the larger Hamiltonians, we use a heuristic approximation for CD_0: see [82] for details about this method and about the experiments. Note that each simulation of H_2 in the STO-3G minimal basis is noncontextual. This is not surprising if one considers these simulations as encoding a two-dimensional Hilbert space spanned by a bonding and antibonding state, i.e., a single qubit, for which Bell gave a noncontextual hidden-variable theory [83].

Citation:	System:	Contextual?	CD_0	$\lvert\mathcal{S}\rvert$
Dumitrescu *et al.* [22]	Deuteron	No	0	—
Kandala *et al.* [17]	H_2	No	0	4
O'Malley *et al.* [13]	H_2	No	0	5
Hempel *et al.* [18]	H_2 (BK)	No	0	5
Hempel *et al.* [18]	H_2 (JW)	No	0	14
Colless *et al.* [19]	H_2	No	0	5
Kokail *et al.* [23]	Schwinger Model	Yes	∼0.16	231
Nam *et al.* [20]	H_2O	Yes	0.27	22
Hempel *et al.* [18]	LiH	Yes	0.33	12
Peruzzo *et al.* [11]	HeH^+	Yes	0.38	8
Kandala *et al.* [17]	BeH	Yes	∼0.74	164
Kandala *et al.* [17, 21]	LiH	Yes	∼0.77	99

TABLE I. Evaluation of contextuality in VQE experiments. CD_0 is the minimum number of terms we must remove from the Hamiltonian to reach a noncontextual set, as a fraction of the total number of terms ($|\mathcal{S}|$). In [22], $|\mathcal{S}|$ varies.

IV. DISCUSSION

All VQE procedures that have been implemented to date, whether noncontextual or contextual, have been small enough to simulate classically. The purpose of such experiments is not to demonstrate quantum advantage, but to apply current hardware to small examples of real-world applications. Such efforts have been instrumental in developing both experimental and theoretical capabilities; indeed, VQE itself was developed in this context [11].

For these reasons, we should be clear that our classification of these experiments as contextual or noncontextual is not a judgement of the value of the experiments, but rather a constructive categorization whose purpose is to inform future experiments and theoretical work. Contextuality of a Hamiltonian according to our definition is connected to inefficiency of classical simulation [65]. Furthermore, as noted above, we may regard a noncontextual Hamiltonian as an instance of an essentially classical problem, akin to quantum algorithms for explicitly classical problems as in QAOA [81] (note that QAOA's diagonal Hamiltonians are always noncontextual.)

In spite of this last point, however, a noncontextual VQE procedure may still be hard to simulate classically, since classical problems can be classically hard. However, contextuality in a VQE procedure provides a strict separation between it and any classical algorithm, by ruling out the existence of a description of the problem in terms of joint probability distributions over a classical phase space, and thus precluding any classical approach either explicitly or implicitly based on such distributions. We suggest therefore that future VQE implementations, even at small scales, should focus on contextual Hamiltonians, according to the criteria we have developed.

Our criterion for contextuality of a set of Pauli operators $\mathcal{S}$ is that joint outcome assignments to $\overline{\mathcal{S}}$ are necessarily self-contradictory. In other words, we analyze contextuality for the minimal closed subtheory containing $\mathcal{S}$; this allows us to invoke the results of [65], which show that efficient simulation by sampling from the discrete Wigner function is only possible in the absence of contextuality. This is not the only choice: for example, [52, 53, 66] do not require the measurements to form a closed subtheory. The relationship of our criterion to that of [52, 53, 66] is discussed further in [82].

The set of noncontextual Hamiltonians contains the set of commuting Pauli Hamiltonians, but is distinct from the set of frustration-free Hamiltonians, as may be seen by taking A, B, C, and D in Fig. 2 to be four consecutive projectors in the AKLT model (e.g., [84]). We leave further consideration of the set of noncontextual Hamiltonians to future work.

Subsequent to the appearance of our work, the result given in our Theorem 2 was independently discovered in [76, §IV], which presents a Wigner function treatment of qubit systems using a phase space constructed from noncontextual closed subtheories.

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