

Classical to quantum in large-number limit

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We construct a quantumness witness following the work of Alicki & van Ryn (AvR). We reformulate the AvR test by defining it for quantum states rather than for observables. This allows us to identify the necessary quantities and resources to detect quantumness for any given system. The first quantity turns out to be the purity of the system. When applying the witness to a system with even moderate mixedness, the protocol is unable to reveal any quantumness. We then show that having many copies of the system leads the witness to reveal quantumness. This seems contrary to the Bohr correspondence, which asserts that, in the large-number limit, quantum systems become classical, whereas the witness shows quantumness when several non-quantum systems, as determined by the witness, are considered together. However, the resources required to detect the quantumness increase dramatically with the number of systems. We apply the quantumness witness for systems that are highly mixed but in the large-number limit that resembles nuclear magnetic resonance (NMR) systems. We make several conclusions about detecting quantumness in NMR-like systems.

Keywords: quantumness witness; purity; large-number limit

1. Introduction

A fundamental quest of modern physics is to characterize the crossover between the quantum world and the classical world. There are many different approaches to answer this question; yet no single approach captures the whole breadth of physics. It is clear that, for some systems, classical physics arises from quantum physics in the large-number limit. This is the Bohr correspondence principle.

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Yet, it is not fully understood how the many-particle limit gives rise to classical physics, and how much of quantum physics still remains. Simply put, there are many operational tasks that give sufficient conditions for quantumness of a system. Yet, no single system may satisfy all of these conditions. Therefore, it is desirable to have a broad notion of quantumness that encompasses all (or many) other notions of quantumness.

One answer in this quest that compels many is given by the violation of Bell's inequalities. Bell's theorem gives a recipe to test for strictly quantum features of two spatially separated systems, namely entanglement and non-locality. More often than not, we deal with systems composed of many subsystems that are not spatially distributed, and therefore non-locality may not be the essential quantum feature of the system of interest. Defining quantumness of isolated systems remains a challenge.

The papers of Alicki & van Ryn (AvR) [1] and later with Piani [2] give a test for quantumness of a single system. This test does not necessarily encompass all aspects of quantumness of a system [3,4]; nevertheless, it offers a glimpse at the classical–quantum divide. On the other hand, it should be noted that all entanglement witnesses are also quantumness witnesses, and an important class of entanglement witnesses are actually quantumness witnesses of the AvR type [5]. In this study, we propose a quantumness witness based on the AvR test. Our witness allows for resource accounting, in terms of qubits and controlled-SHIFT gates, to detect quantumness.

2. Quantumness test

The quantumness test due to AvR is based on a mathematical theorem. AvR give a set of simple criteria for classicality; when these criteria are violated by a system, the system is said to be quantum. The criteria are based on observables of the system. The test presented in this study is based on the same mathematical principles, but we work with the states of the system rather than with the observables of the system. We show that working with states gives a new insight into this notion of quantumness. Namely, Alicki and co-workers [1,2] show that, for any quantum state, there exists a quantumness witness as defined by AvR. This is also true in the state approach, but we are able to quantify the resources, number states needed, to witness quantumness. We begin by reviewing the quantumness test due to AvR and then derive our witness.

(a) Observable approach

To test the quantumness of a single system, consisting of many particles, AvR note the following mathematical theorem.

Theorem 2.1. *Given a C^* -algebra \mathcal{A} , the following three statements are equivalent:*

- (i) \mathcal{A} is commutative, i.e. for any pair $X, Z \in \mathcal{A}$, $[X, Z] = XZ - ZX = 0$.
- (ii) For any pair $X, Z \in \mathcal{A}$ with $0 \leq X \leq Z$, then this implies $X^2 \leq Z^2$.

- (iii) For any pair $X, Z \in \mathcal{A}$ with $X \geq 0$ and $Z \geq 0$, then this implies that the operator corresponding to the anticommutator is also positive:

$$\{X, Z\} = XZ + ZX \geq 0. \quad (2.1)$$

The proof is given in Alicki and co-workers [1,2] and the references [6–8]. Above, A is non-negative if it can be written in the form $A = B^\dagger B$ for some B , and $C \geq D$ means that $C - D$ is non-negative.

AvR make use of statements (i) and (ii) to define a quantumness witness. Theorem 2.1 states that, if \mathcal{A} is non-commutative, there exist two non-commuting positive observables satisfying $X \geq Z$ for all states, but there also exists a state ϕ such that $\langle X^2 \rangle_\phi < \langle Z^2 \rangle_\phi$. This is a violation of the classical principle. In Alicki *et al.* [2], the authors show that, for every quantum state, excluding the maximally mixed state, there exists an observable of statement (iii) type. This quantumness witness was experimentally tested in Brida *et al.* [9,10].

The AvR test can be thought of as a test for complementarity. Observables in classical physics have simultaneous values, but not in quantum mechanics. Any two observables that do not commute do not have simultaneous values and are said to be complementary. For instance, position and momentum are complementary observables in quantum theory and do not have simultaneous values. As Bell's inequalities test for local realism, AvR criteria test for whether two observables have simultaneous values for a given quantum system in a specific state.

Complementary observables in quantum theory are similar to states of a quantum system that cannot be fully discriminated. For instance, if we are given a state, $|0\rangle$ or $|+\rangle$, we will not be able to determine, with full confidence, which state was given. Another way to think about this is that two states that cannot be discriminated are eigenstates of observables that do not commute. On the basis of that intuition, we now construct a quantumness witness using statement (iii) of theorem 2.1 with quantum states rather than the observable approach taken in Alicki *et al.* [1,2]. We will show that this gives us a tool to quantify the necessary resource for witnessing quantumness.

(b) State approach

Let the Hilbert space of the quantum system be $\mathcal{H} \simeq \mathbb{C}^d$. We begin by noting that any Hermitian element $X \in \mathcal{A}$ is a quantum observable. Any Hermitian observable can be expressed as

$$X = x_0 \mathbb{I} + \sum_i x_i \sigma_i, \quad (2.2)$$

where \mathbb{I} is the identity matrix and σ_i are Hermitian basis matrices (traceless generators of the $SU(d)$ group). Hermiticity restricts x_0 and x_i to be real and, if the observable is positive, then $x_0 > 0$ and x_i is a function of x_0 .

If the observable is positive, then it is related to a quantum state in a simple manner. A density operator that represents the state of a d -dimensional quantum system is similarly written as

$$\rho = \frac{1}{d} \left(\mathbb{I} + \sum_i r_i \sigma_i \right), \quad (2.3)$$

where, again, r_i will have some restrictions due to the positivity of ρ [11]. The difference between an observable and a density operator is simply the normalization:

$$\text{tr}[X] = x_0 \quad \text{and} \quad \text{tr}[\rho] = 1. \quad (2.4)$$

There is a clear mapping between density operators and positive observables:

$$X = (x_0 d)\rho_X \iff \rho_X = \frac{1}{d} \left(\mathbb{I} + \sum_i \frac{x_i}{x_0} \sigma_i \right). \quad (2.5)$$

The normalization of a matrix does not alter its positivity. That is, if the operator $XZ + ZX$ is positive, then so is the corresponding density operator $\rho_X \rho_Z + \rho_Z \rho_X$. The duality between states and observables gives us a quantumness witness using statement (iii) of theorem 2.1 for equation (2.1).

Definition 2.2. For every pair of states ρ_X and ρ_Z into which a system can be prepared, let \mathcal{J} be the operator of the anticommutator:

$$\mathcal{J} = \{\rho_X, \rho_Z\} = \rho_X \rho_Z + \rho_Z \rho_X. \quad (2.6)$$

The system is quantum if it can be prepared into two states ρ_X and ρ_Z such that the corresponding anticommutator operator $\mathcal{J} \not\geq 0$.

3. Observing quantumness

Our quantumness witness is experimentally testable. Note that

$$\text{tr}[\mathcal{J}] = \text{tr}[\rho_X \rho_Z + \rho_Z \rho_X] = 2 \text{tr}[\rho_X \rho_Z] = \sum_i \lambda_i, \quad (3.1)$$

where λ_i are the eigenvalues of \mathcal{J} . We are interested in the eigenvalues of \mathcal{J} , not the sum of the eigenvalues. Because there are d eigenvalues and if we know the values of $\text{tr}[\mathcal{J}^l] = \sum_i \lambda_i^l$ for all values of $1 \leq l \leq d$, then we can algebraically solve for $\{\lambda_i\}$. To find the eigenvalues of the \mathcal{J} , we can measure

$$j_l = \text{tr}[(\rho_X \rho_Z)^l]. \quad (3.2)$$

The trace of the product of two density operators is a real positive number: $\text{tr}[\rho_X \rho_Z] = \sum_{xz} r_x r_z |\langle x|z \rangle|^2$, where r_x (r_z) and $|x\rangle$ ($|z\rangle$) are the eigenvalues and eigenvectors of ρ_X (ρ_Z).

To measure the product of two operators in an experimental setting, we make use of the controlled-SHIFT operator [12–14]. The SHIFT operator's action is defined as

$$S|\psi_1, \psi_2, \dots, \psi_{l-1}, \psi_l\rangle = |\psi_l, \psi_1, \psi_2, \dots, \psi_{l-1}\rangle. \quad (3.3)$$

The trace of the SHIFT operator's action from one side only yields

$$\text{tr}[S(\rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_l)] = \text{tr}[\rho_1 \rho_2 \dots \rho_l]. \quad (3.4)$$

Notice the tensor product on the l.h.s. and the ordinary matrix product on the r.h.s.

Using a control qubit and implementing the controlled-SHIFT operator, $\mathcal{C}_S = |0\rangle\langle 0| \otimes \mathbb{I} + |1\rangle\langle 1| \otimes S$, we can measure the trace of the product of any number of operators; see figure 1 for a circuit representation. Measuring the control qubit

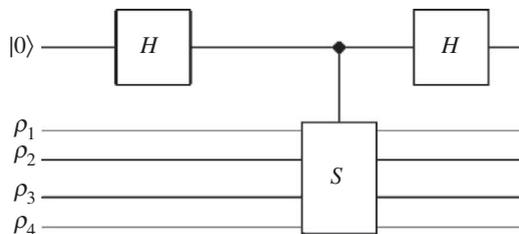


Figure 1. H is the Hadamard gate, and S is the SHIFT gate. The expectation value of the control qubit (top qubit) in z -basis is the trace of the product $\text{tr}[\rho_1\rho_2\rho_3\rho_4]$.

in z -basis will give the product of the density operators. However, to measure the l th power, we will need l copies of the density operator and a suitable SHIFT operation. These resources may not be trivially available and therefore witnessing the quantumness may prove to be difficult.

4. Examples of quantumness witness

Now, we put this quantumness witness to work with a few examples. The examples will illustrate that our witness identifies the crossover between the quantum and classical theories. We consider a system that can be prepared in a set of commuting states, pure states and mixed states. The first example identifies a ‘truly classical’ system, whereas the second gives a ‘truly quantum’ system; in the final example, quantum and classical worlds are blended together.

(a) Commuting states

Suppose a system can be prepared into states that all commute with each other and in this sense are viewed as ‘classical’ by the anticommutator witness in equation (2.6). The density operators of such states then can be simultaneously diagonalized. Therefore, \mathcal{J} is also diagonal in the same basis as the states, and its eigenvalues are twice the products of eigenvalues of ρ_X and ρ_Y , which are positive numbers. It is then clear that $\mathcal{J} \geq 0$ when all states of the system commute, which is in full agreement with theorem 2.1.

(b) Pure states

Pure states show highly quantum behaviour. One can show that an operator of the form

$$\mathcal{J} = \langle \psi | \phi \rangle | \psi \rangle \langle \phi | + \langle \phi | \psi \rangle | \phi \rangle \langle \psi | \geq 0 \iff | \langle \psi | \phi \rangle | = 0, 1. \quad (4.1)$$

That is, \mathcal{J} is a positive operator if and only if $|\psi\rangle$ and $|\phi\rangle$ are orthogonal to each other. Here, $|\psi\rangle$ and $|\phi\rangle$ are vectors in d -dimensional Hilbert space [15].

For concreteness, let us suppose that a two-level system, a qubit, can be prepared into any possible pure state. It is easy to show that states with orthogonal vectors in the Bloch sphere lead to the maximum violation of

classicality. Take, for instance, the anticommutator of states $\rho_X = |+\rangle\langle +|$ with $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ and $\rho_Z = |0\rangle\langle 0|$:

$$\mathcal{J} = \frac{1}{\sqrt{2}}(|+\rangle\langle 0| + |0\rangle\langle +|), \quad (4.2)$$

which has eigenvalues $\lambda_{\pm} = 1 \pm \sqrt{2}$.

(c) Mixed states

For the rest of the study, we will work only with qubits for simplicity. However, all the claims that we will make can be generalized to d -dimensional systems in a straightforward manner.

A mixed state of a qubit can always be written as a mixture of a pure state and a fully mixed state. Consider the two states

$$\rho_X = \frac{1-p}{2}\mathbb{I} + p|+\rangle\langle +| \quad \text{and} \quad \rho_Z = \frac{1-p}{2}\mathbb{I} + p|0\rangle\langle 0|. \quad (4.3)$$

The anticommutator of these two states is not positive-definite only for

$$p > p_c = \frac{1}{\sqrt{2}}, \quad (4.4)$$

where p_c denotes a critical value of the mixedness parameter p . For $p \leq p_c$, we have classicality $\mathcal{J} \geq 0$, and for $p > p_c$, we have quantumness $\mathcal{J} \not\geq 0$.

This implies that single-qubit state with less purity than $\text{tr}[\rho^2] = \frac{3}{4}$ cannot be considered quantum if only the anticommutator of the states in equation (4.3) is considered. This is clearly problematic and has to be dealt with somehow. For instance, NMR systems are highly mixed, yet still retain quantumness to some extent. We will deal with this problem in §5.

5. Highly mixed states of NMR

NMR systems have very stable states that are highly controllable [16]. However, these states are also highly mixed; in the form of equation (4.3), the value of $p_{\text{NMR}} \simeq 10^{-5}$. This is much less than the critical value, i.e. $p_{\text{NMR}} \ll p_c$. Our quantumness witness will not be able to detect quantumness from an NMR system by simply looking at the anticommutator of the states equation (4.3). On the other hand, NMR systems are ensemble systems. That is, there are a lot of qubits available all at once, and we will make use of this fact to regain quantumness. We now explore three approaches to overcome the obstacle at hand.

(a) Purification approach

Suppose we are able to apply some cooling algorithm [17] to our highly mixed ensemble and extract a sub-ensemble of pure states. Suppose we have n qubits, each in state ρ . The entropy of each qubit is $S(\rho)$. The total entropy of the whole ensemble is $nS(\rho)$. Using algorithmic cooling, we can then extract $m = n[1 - S(\rho)]$ pure qubits. For $p_{\text{NMR}} = 10^{-5}$ and $n = 10^{23}$, the value of $m = 10^{12}$. The quantumness of a system with this many qubits should be very high, assuming

that we can simultaneously prepare them all in two complementary directions. In fact, we need to purify only a handful of qubits in order to test our witness. On the one hand, this is a nice solution, but may not be satisfactory, as this method bypasses the central problem, that our anticommutator witness \mathcal{J} in equation (2.6) does not perceive the quantumness of most mixed states. Next, we explore how we can test the witness without applying a purification procedure.

(b) *Quantumness in large numbers*

Note that, if we input more than one copy of the input states, the behaviour (i.e. the positivity) of the witness may change. Consider modifying the witness in equation (2.6) as

$$\mathcal{J}^{(n)} = \{\rho_X^{\otimes n}, \rho_Z^{\otimes n}\} = \rho_X^{\otimes n} \rho_Z^{\otimes n} + \rho_Z^{\otimes n} \rho_X^{\otimes n}. \quad (5.1)$$

Individually, each qubit can be prepared in two possible states ρ_X and ρ_Z as in equation (4.3): in both cases, the states can be considered highly ‘classical’, in the sense that p is well below the critical value given in equation (4.4). Moreover, a single-particle anticommutator witness such as in equation (2.6) would not be able to detect any quantumness. However, the witness in equation (5.1) considers the quantumness of n qubits at the same time. The ensemble of qubits has collective coherence and therefore the ensemble of qubits ought to be considered a single system. After all, it is the ensemble average that is measured in NMR systems.

Indeed, we can easily verify that the critical value of the mixedness parameter decreases simply by introducing extra qubits. For one qubit, the critical value is $p_c = 1/\sqrt{2}$ as given in equation (4.4), for two qubits $p_c^{(2)} = 0.644$, for three qubits $p_c^{(3)} = 0.578$ and so on. We have computed the critical value of the mixedness parameter for $n = 1, \dots, 13$. Computing the eigenvalues of $\mathcal{J}^{(n)}$ for larger n becomes very difficult, because the size of the matrices grows exponentially. However, we have fitted the numerical data to a curve and found that it matches very well with a polynomial function

$$p_c^{(n)} = A_0 + \frac{A_1}{n} + \frac{A_2}{n^2} + \frac{A_3}{n^3}, \quad (5.2)$$

with

$$A_0 = 0.204, \quad A_1 = 1.882, \quad A_2 = -2.660, \quad A_3 = 1.281.$$

(Note that fits with exponential test functions do not yield good results.) Both the numerical results and the fitted curve are plotted in figure 2. Remarkably, as $n \rightarrow \infty$, the mixedness parameter has a finite critical value $p_c^{(n)} \rightarrow A_0 \gg p_{\text{NMR}}$. This implies that, in an NMR system, without any preprocessing, one cannot witness quantumness using the witness in equation (5.1). We have once again failed to detect quantumness in an NMR system. We now allow some preprocessing to see if that helps the emergence of quantumness.

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(c) *Quantumness in large numbers and correlations*

One of the strong points of NMR systems is the unitary gates: they are easy to implement and have high fidelity. We can use the unitary gates to build

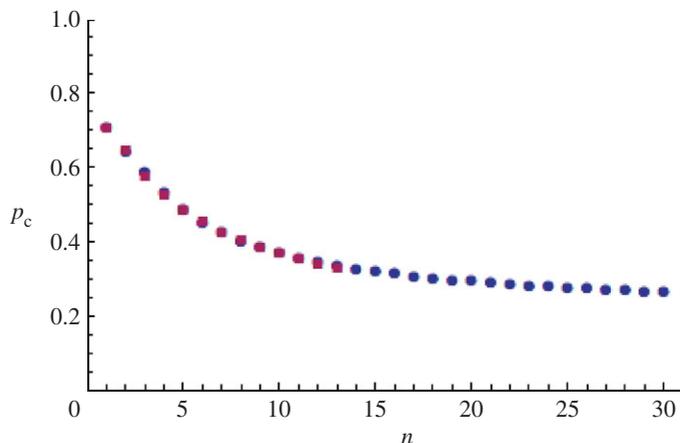


Figure 2. Critical values of mixedness parameter for $\mathcal{J}^{(n)}$. Blue circles are the computed critical values of the mixedness parameter, and red squares are the values of the fitted curve from equation (5.2). The critical value is never less than $p_{\text{NMR}} \simeq 10^{-5}$. (Online version in colour.)

correlations between qubits and perhaps the witness will be sensitive to the correlations. In the light of that, let us once again redefine our witness operators given in equation (5.1) as

$$\mathcal{J}_C^{(n)} = \{U\rho_X^{\otimes n}U^\dagger, V\rho_Z^{\otimes n}V^\dagger\} = U\rho_X^{\otimes n}U^\dagger V\rho_Z^{\otimes n}V^\dagger + V\rho_Z^{\otimes n}V^\dagger U\rho_X^{\otimes n}U^\dagger, \quad (5.3)$$

where U and V are unitary operations that build correlations in ρ_X and ρ_Z , respectively. There is a great deal of freedom in choosing U and V . In fact, optimizing the witness over all possible encodings does not seem trivial and we will leave studies on this problem for a later time.

We have studied one such case: we implement controlled-NOT gates, using the first qubit as control and the rest as target. The controlled-NOT gates are applied in the appropriate basis to achieve maximal correlations in the final state. Specifically, the gates are

$$U = |0\rangle\langle 0| \otimes \mathbb{I}^{\otimes(n-1)} + |1\rangle\langle 1| \otimes \sigma_X^{\otimes(n-1)} \quad (5.4)$$

and

$$V = |+\rangle\langle +| \otimes \mathbb{I}^{\otimes(n-1)} + |-\rangle\langle -| \otimes \sigma_Z^{\otimes(n-1)}, \quad (5.5)$$

where σ_X and σ_Z are Pauli operators. We should note that the correlations in the final state are purely classical. Nevertheless, the correlations enhance the quantumness of the states, as measured by the witness in the last equation.

Once again we have numerically computed the critical value of the mixedness parameter for the preprocessed states. We numerically computed the critical values of the mixedness parameter for $n = 1, \dots, 12$ and plotted the numerical data, along with the fitted curve, in figure 3. The fitted curve is once again a polynomial of the form

$$p_c^{(n)} = B_0 + \frac{B_1}{n} + \frac{B_2}{n^2} + \frac{B_3}{n^3}, \quad (5.6)$$

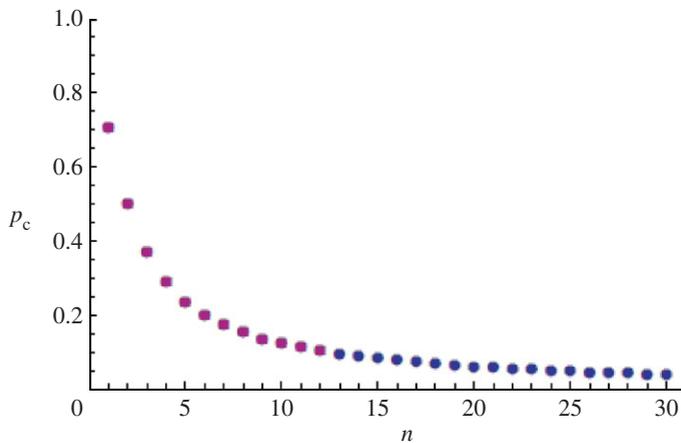


Figure 3. Critical values of mixedness parameter for $\mathcal{J}_C^{(n)}$. Dots are the computed values of the critical mixing point, and squares are the values of the fitted curve equation (5.6). For $n \simeq 140\,000$ the critical value is expected to be less than $p_{\text{NMR}} \simeq 10^{-5}$. (Online version in colour.)

with

$$B_0 = -0.006, \quad B_1 = 1.350, \quad B_2 = -0.711, \quad B_3 = 0.075.$$

(We stress that the fits with exponential test functions do not yield good results and that adding more terms does not yield better results, in that B_3 is noticeably smaller than the other coefficients.) Note that the leading coefficient is compatible with zero, implying that as $n \rightarrow \infty$ the critical value of the mixedness parameter $p_c^{(n)} \rightarrow 0$. We can therefore set $B_0 = 0$ and compute the number of qubits needed to achieve $p_c^{(n)} < p_{\text{NMR}}$. This turns out to be around $n_{\text{NMR}} \simeq 1.35 \times 10^5$.

An analogue to the witnesses in equations (5.1) and (5.3) using the observable approach of AvR is difficult. For the observable approach, it would simply mean that you would define some observable in the space of n qubits and look for states of the system that would lead to quantumness. Here, we have to be able to keep the state of the system fixed, but simply change the number of systems that lead to quantumness. This gives an operational meaning to mixed state ensembles. It is worth noting that quantumness arises in the large-number limit. For the example mentioned earlier, we would need $\simeq 1.35 \times 10^5$ qubits to witness it. This is contrary to the popular notion that quantumness goes to classicality in the large-number limit.

On the other hand, witnessing this quantumness is not trivial. For the experimental prescription that we laid out in §3, we would need 1.35×10^5 sets of 1.35×10^5 qubits. Then, we would have to implement a SHIFT operator among all of these qubits. That is, we would need over 10 billion qubits and be able to interact them all. This is far from what is achievable with the current technology. We would need to reduce the number of qubits necessary somehow in order to witness this sort of quantumness in NMR, perhaps using some different preprocessing techniques.

6. Conclusion

We have extended the work of Alicki *et al.* [1,2] and have given a quantumness witness in terms of states of the system. Our witness works in the same spirit as the work of AvR, but we find some surprising results; namely, that the witness does not detect quantumness for even moderately mixed states of the system. We overcame this obstacle by noting that the witness sees more quantumness as the number of system states grows. This gives us an operational interpretation of quantumness for ensemble size. Further, our quantumness witness allows us to deal with correlations in a natural way.

Although quantumness grows with the number of systems, detecting the witness remains difficult. This is because, when working with n qubits, we need n sets of n qubits. If n were a marginally large number, we would need to work with a reasonable number of qubits. Otherwise, this test is not possible with current technology. Perhaps a different correlation class of states will lower this number significantly and allow for observation quantumness in NMR-like systems.

Lastly, we note that our witness is related to quantum discord [15] using the necessary and sufficient criteria for classicality of correlations given in Chen *et al.* [18]. This is interesting because, when classically correlated states are put together, a quantum correlated state emerges within the discord framework of quantumness of correlations. This begs the question: should we consider quantum mechanics to be the basis for classical physics? Perhaps the universe is a bit more complicated than that.

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