Quantifying quantumness via commutators: an application to quantum walks

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The question of witnessing or quantifying nonclassicality of quantum systems has been addressed in various ways. For a given system or theory, we propose identifying it with the incompatibility of admissible states. We quantify the nonclassicality of quantum systems using the Hilbert-Schmidt norm of the commutator of two states. As a particular application of this measure, we study the classicalization of a discrete-time quantum walk with a noisy coin.

I. INTRODUCTION

There are a number of ways to characterize the nonclassical nature of quantum phenomena. In connection with the quantum measurement problem, the lack of macroscopic superpositions is the tell-tale sign of nonclassicality [1, 2]. Put differently, the macro-world is classical because the accessible states all commute with each other (being positional eigenstates). We can extend this idea farther to any system S (and even to a theory T), defining it to be classical precisely if all admissible states of S or T are mutually compatible.

What is advantageous in this approach is that references to the dynamics and correlations are removed, which can offer potential simplification and straightforwardness for quantification. As an illustration: maximal entanglement, which is often regarded as quintessential nonclassicality, may be represented as a product state and vice versa, simply by a suitable choice of the degrees of freedom (cf. Ref. [3]). For a 2-qubit system, suppose we define a parity observable by the spectral decomposition \( P = (\Pi_{\Phi^+} + \Pi_{\Phi^-}) - (\Pi_{\Psi^+} + \Pi_{\Psi^-}) \) and the phase observable by \( F = (\Pi_{\Phi^+} + \Pi_{\Phi^*}) - (\Pi_{\Phi^-} + \Pi_{\Phi^-}) \), where \( \Pi_{\Phi^\pm} \) is the projector to the Bell state \( \frac{1}{\sqrt{2}} (|00\rangle \pm |11\rangle) \), and \( \Pi_{\Psi^\pm} \equiv \frac{1}{\sqrt{2}} (|01\rangle \pm |10\rangle) \). In terms of the parity and phase observables, the Bell states have the product form: \( |0\rangle_F |0\rangle_P = |\Phi^+\rangle \), \( |0\rangle_F |1\rangle_P = |\Phi^-\rangle \), \( |1\rangle_F |0\rangle_P = |\Psi^-\rangle \), and \( |1\rangle_F |1\rangle_P = |\Psi^+\rangle \). On the other hand, the separable state \( \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) |0\rangle \equiv \frac{1}{\sqrt{2}} [(|0\rangle_P (|0\rangle + |1\rangle) |0\rangle_F + |1\rangle_P (|0\rangle + |1\rangle) |0\rangle_F] = \frac{1}{\sqrt{2}} (|0\rangle_P |+\rangle_F + |1\rangle_P |0\rangle_F) \).

As one way to overcome this problem, which may be appropriate for systems of the type considered below, we propose basing nonclassicality on the incompatibility of states relative to each other, rather than on correlations. We believe that this approach can be helpful in studying the quantumness of complex processes, such as those encountered in photosynthetic systems, where it may be computationally unfeasible to compute measures of nonclassicality based on correlations. That the experiments in photosynthesis show quantum effects [4], while rivaling classical explanations for exciton transport also exist, suggests that our approach will find fruitful application here. In particular, evidence of long-term coherence [5] and of continuous quantum walks [6], have been reported to play a role in the energy transfer within the Fenna-Mathews-Olson (FMO) complex. Accordingly we have applied our method to quantum walks.

This article is organized as follows. In Section II, we develop the conceptual background for identifying nonclassicality in terms of the incompatibility of states. In Section III, we propose a method for quantifying nonclassicality in quantum systems using the commutator as the basic witness of quantumness. In Section IV, we apply this approach to discrete-time quantum walks. We conclude in Section V.

II. NONCLASSICALITY FROM INCOMPATIBILITY OF STATES

Given a system \( S \), let \( \Sigma \equiv \{\psi_j\} \) be the set of all possible pure states that it can assume in a given situation of interest. Any two pure states \( \psi_m \) and \( \psi_n \) (where \( m, n \) are indices appropriate to the cardinality of \( \Sigma \)) are said to be incompatible if their characteristic properties, \( \Pi(\psi_m) \) and \( \Pi(\psi_n) \) are incompatible. The characteristic property \( \Pi(\psi_m) \) associated with state \( \psi_m \) is a binary (yes/no) property whose measurement asks the question of whether or not \( S \) is in the state \( \psi_m \). The two properties are compatible by any one of the following criteria [7]: (a) in the sequence of measurements \( \Pi(\psi_m)\Pi(\psi_n)\Pi(\psi_m) \), the two instances of \( \Pi(\psi_m) \) yield the same outcome; (b) The sequence \( \Pi(\psi_m) \) followed by \( \Pi(\psi_n) \) produces the same probability distribution over outcomes of \( \Pi(\psi_n) \),

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as a direct measurement of $\Pi(\psi_n)$.

Thus, these two measurements are incompatible if acquiring knowledge of one disturbs the other and diminishes knowledge of it: $H[\Pi(\psi_m)] \leq H[\Pi(\psi_m)\Pi(\psi_n)]$, where $H(\cdot)$ is Shannon binary entropy and $H(\cdot)$ is binary conditional entropy. Two pure states $\psi_m$ and $\psi_n$ are deemed compatible if and only if the associated measurements $\Pi(\psi_m)$ and $\Pi(\psi_n)$ are compatible. The incompatibility implies an intrinsic randomness, i.e., one not having a deterministic explanation within the theory [8].

We may extend this concept of incompatibility of pure states to mixed states by associating for a state defined by the ensemble $\{p_j, \psi_j\}$ the object $\sum_j p_j \Pi(\psi_j)$. In quantum mechanics, the density operator $\rho$ naturally associates with a quantum state in the role of $\Pi(\{p_j, \psi_j\})$, and the non-vanishing of the commutator of density operators is a ready witness of incompatibility. An interesting approach to exposing this non-classicality by using anti-commutators is studied in detail in Ref. [9]. Here we consider a particular quantification of nonclassicality based on the commutator.

III. NONCLASSICALITY IN QUANTUM MECHANICS

The Hilbert-Schmidt (HS) norm of a (bounded, square) operator $A = \{a_{jk}\}$ is given by

$$||A||_{HS}^2 = \sum_{j,k} |a_{jk}|^2 = \text{Tr}(A^\dagger A),$$  \hspace{1cm} (1)

where $a_{jk} \equiv \langle j | A | k \rangle$ for any basis $\{j\}$. We assume that the dimension is finite (though the arguments here can be generalized to infinite dimension). Given two states $\rho$ and $\sigma$, we propose the measure of their mutual incompatibility to be twice the HS norm of the commutator:

$$\Phi(\rho, \sigma) \equiv 2||[\rho, \sigma]||^2_{HS},$$  \hspace{1cm} (2)

where the pre-factor is required for normalization. $\Phi$ so defined is a convenient measure of state incompatibility. It is symmetric in both arguments, and its interpretation as such is conceptually transparent, while it is computationally facile (e.g., not involving diagonalization). Some of its properties are studied below. That it brings out the intuitively expected features of nonclassicality is shown later.

**Theorem 1** $0 \leq \Phi(\rho, \sigma) \leq 1$.

**Proof.** Since $\Phi(\rho, \sigma)$ is by definition positive, the first inequality in this Theorem follows, with its saturation precisely when $\rho$ and $\sigma$ are compatible. $\Phi$ is a convex function in both arguments, and attains its maximum for pure states. To see this, let $\rho \equiv \sum_j p_j |\psi_j\rangle \langle \psi_j|$ and $\sigma \equiv \sum_k q_k |\phi_k\rangle \langle \phi_k|$, where the $|\psi_j\rangle$’s and $|\phi_k\rangle$’s are not necessarily orthogonal, and $\sum_j p_j = \sum_k q_k = 1$. Let $\alpha_{jk} \equiv \langle \psi_j | \phi_k \rangle$, $r_j \equiv p_j q_k$, with $\sum_j r_j = 1$. We have:

$$\frac{1}{2} \Phi(\rho, \sigma) = \text{Tr} \left[ \left( \sum_{j,k} p_j q_k (\alpha_{jk} |\psi_j\rangle \langle \phi_k| - \alpha^*_{jk} |\phi_j\rangle \langle \psi_k|) \right)^\dagger \left( \sum_{j',k'} p_{j'} q_{k'} (\alpha_{j'k'} |\psi_{j'}\rangle \langle \phi_{k'}| - \alpha^*_{j'k'} |\phi_{j'}\rangle \langle \psi_{k'}|) \right) \right],$$

$$\leq \sum_{m,n} \langle m | \left[ \left( \sum_j r_j M_j^\dagger \right) |n\rangle \langle n| \left( \sum_K r_K M_K \right) \right] |m\rangle,$n}

where we used the fact that $\sum_n |n\rangle \langle n| = 1$, the definition $M_j \equiv M_{jk} = (\alpha_{jk} |\psi_j\rangle \langle \phi_k| - \alpha^*_{jk} |\phi_j\rangle \langle \psi_k|)$ and the convexity of the function $f(x) := |x|^2$.

Any two pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ form a 2-dim subspace and we can write without loss of generality $|\psi_2\rangle = \cos \theta |\psi_1\rangle + \sin \theta |\psi_1^\perp\rangle$, where $\langle \psi_1 | \psi_1^\perp \rangle = 0$. Set-
ting $\rho = |\psi_1\rangle\langle\psi_1|$ and $\sigma = |\psi_2\rangle\langle\psi_2|$ in Eq. (2), and maximizing over $\theta$, we find $\theta_{\text{max}} = \frac{\pi}{4}$ and $\Phi_{\text{max}} = 1$. ■

We note that $\Phi$ does not attain its maximum value for two states selected from a pair of mutually unbiased bases (MUBs), even though MUBs are maximally non-commuting in the sense that the entropic uncertainty relation given by $H_P + H_Q \geq -2 \log_2(|\langle p|q \rangle|)$, is the most stringent in this case, the rhs being $\log(d)$. Here $H_P$ ($H_Q$) is the classical binary entropy generated by measuring $P$ ($Q$), while $|\langle p|q \rangle|$ is the largest overlap between the eigenvectors of $P$ and $Q$ [10]. For two states from an MUB pair, without loss of generality, we may take $\Phi (|0\rangle, \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j\rangle) = \frac{4(d-1)}{d^2}$, which falls linearly with dimension $d$. This of course happens because as $d$ increases, these two vectors are increasingly mutually orthogonal, and hence commuting.

Unlike the anti-commutator, which can be measured (possibly by an interactive procedure) using an interferometer [9], determining the value of the commutator experimentally requires a more detailed set-up, ideally a quantum tomography of the state. For sufficiently small systems, this is technologically feasible at the present time. E.g., Ref. [11] reports tomographically determined quantum characteristics of a quantum walk on eight steps.

As an application of $\Phi$, we study below the classicalization of quantum walk, the quantum generalization of classical random walks. Because of quantum interference, the position probability distribution of a QW deviates from the classical linear-spreading Gaussian pattern to a quadratic-spreading twin-peaked pattern. Adding noise gradually imposes classical behavior, returning it to Gaussian behavior, which has been studied by a number of authors (Ref. [12] and references therein). Because $\Phi$ is a relative measure, we require a set $\Sigma$ of states of a system $S$, with $|\Sigma| \geq 2$, to witness or quantify the nonclassicality of $S$. Only if $\Phi(p_j, p_k)$ vanishes (or, is sufficiently low) for all pairs $p_j, p_k \in \Sigma$ ($j \neq k$) can $S$ be called classical. Otherwise, $S$ is nonclassical. Two strategies for choosing $\Sigma$ and quantifying nonclassicality of a noisy time-evolving system are considered below.

\section{IV. APPLICATION TO QUANTUM WALKS}

We model the linear discrete-time (DT) quantum walker (QW) as a qubit (coin) in Hilbert space $\mathcal{H}_C \equiv \text{span}([0], [1])$, that can assume states in position space $\mathcal{H}_P \equiv \text{span}(|\psi_x\rangle)$, where $x$ is an integer. The linear walk may be extended to higher dimensions, as well as assume non-trivial topologies, such as a cycle (Ref. [13] and references therein). The state of the noisy QW after $t$ time steps is obtained iteratively according to:

$$\rho(t) = \sum_{j_1, j_2, \cdots, j_t} A_{j_1} U_{j_1} \cdots A_{j_t} U_{j_t} \rho_0 U_{j_t}^\dagger A_{j_t}^\dagger \cdots U_{j_1}^\dagger A_{j_1}^\dagger$$

$$\equiv \sum_{j_1, j_2, \cdots, j_t} \rho(t; j_1, j_2, \cdots, j_t), \quad (4)$$

through sequential applications of the coin-position unitary operation $U_j$ and the coin-specific noise operation $\mathcal{E}$ determined by the Kraus operators $A_j$. Here the initial state is $\rho_0 \equiv |\Psi_0\rangle\langle\Psi_0|$, where $|\Psi_0\rangle = \frac{([0] + [1])}{\sqrt{2}} \otimes |0\rangle$. At each time $t$, one applies the unitary $U \equiv W(C \otimes I)$, where $C$ is the coin operation $\left(\begin{array}{cc} \cos(\alpha) & \sin(\alpha) \\ \sin(\alpha) & -\cos(\alpha) \end{array}\right)$ that rotates the state of the coin, while $W$ shifts the position conditioned on coin state

$$W \equiv |0\rangle\langle0| \otimes \sum_x |x-1\rangle\langle x | + |1\rangle\langle1| \otimes \sum_x |x+1\rangle\langle x |. \quad (5)$$

The position probability distribution at time $t$ is given by $P(x) = \text{Tr}_{PC} ([\Pi_x \otimes I_C] \rho(t))$, where $\Pi_x \equiv |x\rangle\langle x|$ is the projector to a wave packet localized at position $x$.

For the noise model, we choose the amplitude damping channel [14], which describes a qubit interacting with a vacuum bath:

$$A_0 \equiv \left(\begin{array}{cc} \sqrt{1-\mu} & 0 \\ 0 & 1 \end{array}\right); \ A_1 \equiv \left(\begin{array}{cc} 0 & 0 \\ 0 & \sqrt{\mu} \end{array}\right), \quad (6)$$

where $\mu \in [0, 1)$ describes the strength of the noise. Other possible models include dephasing noise or more general amplitude damping noise on the coin, such as squeezed generalized amplitude damping [15], or dephasing in the position degree of freedom. The above simple noise model suffices for our present purpose.

Two approaches may be considered to apply the $\Phi$ formalism. In one case, $\Sigma(t)$ may be defined as the ensemble of states obtained along different trajectories during the time interval $[0, t]$ starting from $|\Psi_0\rangle$. For the discrete-time evolution given by Eq. (4), one considers
the ensemble-dependent average quantumness

$$\Phi_{av}(t) \equiv \sum_{j_m,j_n} \Phi[\rho(t; j_1, \ldots, j_l), \rho(t; j'_1, \ldots, j'_l)],$$

(7)

where the unnormalized density operators $\rho(t; j_1, \ldots, j_l)$ are already factored by their statistical weight.

Another method, which is used here, would be to consider $\Sigma(t) \equiv \{\rho(t), \rho(t+\Delta)\}$, where $\rho(t)$ is the time-evolved mixed state density operator of the system, and $\Delta$ is a time step that may be optimized to maximize $\Phi$. Thus:

$$\Phi_{\Delta}(t) \equiv \Phi(\rho(t), \rho(t-\Delta)),$$

(8)

where $\rho(t)$ is given by Eq. (6). Keeping $t$ fixed, we varied $\Delta$ to numerically determine the $\Delta$ that maximizes $\Phi_{\Delta}$. We find that $\Delta = 2$ is optimal for this system. The data for $t = 100$ is depicted in Figure 1. For $\Delta = 0$, we find trivially that $\Phi_{\Delta} = 0$. As $\Delta$ increases, so does $\Phi_{\Delta}$ as the state of the QW is rotated away from $|\Psi_0\rangle$. Eventually, a fall with $\Delta$ is expected because the dominant support for two QW states will move apart quadratically with time, so that they will nearly commute even in the unitary case.

Figure 2 depicts $\Phi_{\Delta}(t)$ with $\Delta = 2$ and the time being varied till 100 for a QW described by Eqs. (3) and (6) for various levels of noise $\mu$. We find that at any given time, quantumness is larger when the evolution is unitary (topmost plot), and is successively smaller as the noise level increases. For any fixed noise level, quantumness is seen to reduce with time (the bottom three plots), whereas it remains roughly the same when the walk is unitary. These observations give evidence that $\Phi$ is a reasonable measure of the quantumness.

In practice, $\Phi$ may be normalized by a suitable constant depending on the system $S$ at hand. As one example, we plot in Fig. 3 a time-normalized version of the data in Fig. 2, where the noisy values of $\Phi_2$ are divided by the noiseless value at that time $t$. This removes an artefact of our method whereby a low $\Phi$ results not from noise but from the fact that the compared pair of states are not highly non-commuting even in the unitary case.

V. CONCLUDING REMARKS

The quantumness of noisy quantum walks has been studied by means of $\Phi$, applied here to quantify the non-commutativity of temporally near-by states. Applying this measure to the case of DT linear QW to which an amplitude-damping noise is applied to the coin degree of freedom, we show that it brings out the expected classicalization of the walk, thereby illustrating the quantitative usefulness of this intuitive measure of quantumness. It can be implemented experimentally using quantum state tomography in NMR systems, and potentially apply to study the quantumness of photosynthetic systems.

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