Phase transition is a general phenomenon which can occur in different physical systems. It is characterized by a singular behavior of a state function under certain conditions. The standard example is the liquid-gas transition in fluids where a discontinuity in the density happens when the system reaches a critical temperature. Analogous situations can happen in quantum systems, a phenomenon called Quantum Phase Transitions. It has been widely discussed that entanglement - exclusively quantum correlations - plays a major role in quantum phase transitions. A great effort has been devoted to understand the relations between entanglement and critical phenomena in several systems. In fact, it is natural to associate these concepts once correlations are behind both of them. By sharing this point of view, i.e. that entanglement can be treated as a singular state function and thus as an order parameter, we obtain interesting novelties such as the appearance of a new kind of phase transition, that we term “geometric phase transition”, concerning a singular behavior of entanglement solely due to geometric consequences of quantum correlations. It happens whenever the set of quantum states presents a singular shape. We also show how this phenomenon allows a more accurate study regarding the geometry of the set of entangled states. Moreover it is also shown how this study can be made experimentally by implementing entanglement-witness operators. But what means a state to be entangled? This question, although very clear in the bipartite context, becomes vague in the multipartite case. When several parts are involved, we have to specify the kind of entanglement we are interested in. Let us be more specific. For two systems A and B, a state is said to be separable if it can be written as ρ = ∑ᵢ pᵢ ρᵢ ⊗ ρᵢ (pᵢ is a probability distribution), if not, it is said entangled. However, if a system has n parts, A, B, C, ..., N, one can talk about entanglement with respect to any specific partition; moreover, one can also talk about entanglement with respect to a certain number of parts. For example, take n = 3. If one consider AB as a single object, one can define separability with respect to the partition AB|C exactly as is done for bipartite systems. Of course, the same can be done with respect to other bipartitions (only 3 bipartitions are possible for n = 3). Explicitly, a tripartite state is (AB|C)-separable if it can be written as ρₐᵦᵢ = ∑ᵢ pᵢ ρᵢᵦᵢ ⊗ ρᵢᵪ. In opposition, any (AB|C)-non-separable state has (AB|C)-entanglement. If a state can be written as a convex combination of (AB|C)-separable, (BC|A)-separable and (CA|B)-separable states, then it is said 2-separable. By this example, it should become clear the existence of a multitude of kinds of entanglements for (large n) multipartite systems.

An important progress in the quantum information field was to note that entanglement can be treated as a useful resource in various tasks such as cryptography, quantum computation, and teleportation. Thus, like any physical resource, it would be interesting to properly quantify it. However this goal was not achieved yet, in spite of the large number of interesting quantifiers already proposed. A nice example is the robustness of entanglement, which relies on an interesting geometric interpretation. We should start by defining the robustness of a state ρ with respect to another state π as...
the completely random state
\[ \sigma = \frac{\rho + s\pi}{1 + s} \]  

is separable. We will be interested in two special situations. The first of them, called random robustness of \( \rho \), and denoted \( R_r(\rho) \), is obtained when \( \pi \) is fixed to be the completely random state \( \frac{I}{d} \), where \( I \) is the identity \( d \times d \) matrix. The random state is an interior point in the set of separable states\(^{[16]} \), which ensures a finite value to \( R_r(\rho) \). In the second case, we consider the generalized robustness, denoted \( R_g(\rho) \), which is obtained by the minimization of the relative robustness over all states \( \pi \).\(^{[17]} \)

It follows \( R_g(\rho) \leq R_r(\rho) \). As we shall see, robustness has another advantage as an entanglement quantifier: it is generalizable to multipartite entanglement. The geometrical aspects of those robustnesses are explained in Figure 1.

Whenever one chooses a kind of entanglement, the set of states which do not have such entanglement is convex (as a consequence of the definition of separability). Just to fix ideas, let us talk about \( k \)-separability, i.e. the states which can be written as convex combination of states which are product of \( k \) tensor factors. The reader should note that any state is 1-separable, and that, for a system of \( n \) parts, \( n \)-separability is separability itself. Let us denote by \( S_k \) the set of \( k \)-separable states, and by \( D = S_1 \) the set of all states. Let us also define the random \( k \)-robustness of the state \( \rho \), \( R^k_r(\rho) \), in the same way as before, as the minimum \( s \) such that the state of Eq. 1, with \( \pi = \frac{I}{d} \), is \( k \)-separable, and also the generalized \( k \)-robustness, \( R^k_g(\rho) \), as the minimum over all \( \pi \) state of the relative \( k \)-robustness.

Now the scenario is set and we can present the geometric phase transitions. The low dimensionality of our figures hides some facts. The border of convex sets can be, locally, of two kinds: curved or flat. To avoid details, let us use three-dimensional examples: a ball and a polyhedron. In one of them, the boundary is smooth, and there are no singular points; in the other we have edges and vertices, which are singularities. The general picture is neither of them. For a low dimensional example, one can think of a cylinder, in which there are some (not too) singular points. If one take a smooth one parameter family of states, \( \rho(q) \), i.e., a curve on \( D \), and calculate \( R^k_r \) and \( R^k_g \), they will usually be smooth functions of \( q \). However, singularities may appear in these functions whenever singularities happen on the boundaries of \( S_k \) (in \( R^k_r \)) and of both \( D \) and \( S_k \) (in \( R^k_g \)) - see Figure 2. This is a phase transition due to the geometry of the set of states, and it is what we call a geometric phase transition. One should note that this abstract picture of a curve on \( D \) is just to keep things general. Important examples are given by the time evolution of states under the effect of a Hamiltonian (for closed systems), a master equation (open systems), or the thermal equilibrium state as a function of temperature, or even the ground state of a multipartite system as a function of some coupling parameter of the Hamiltonian.

Until now we have claimed that a singularity in \( R^k_g(q) \) or in \( R^k_g(q) \) is a sufficient condition to attest singularity in \( D \) or \( S_k \). In fact it was possible to confirm the geometric phase transition in some examples, two of them are displayed in Figure 3.

As seen before the entanglement quantifiers \( R^k_g(q) \) and \( R^k_g(q) \) provide information about the geometry of the (entangled) states set. Interestingly, these functions can be evaluated experimentally, since they are directly related to the expected value of a physical observable. To shed light in this point let us present the notion of entanglement witnesses\(^{[18]} \): for every \( k \)-entangled state \( \rho \) there exists a Hermitian operator \( W^k \) (called an entan-
FIG. 2: Above: The dot line represents the path $\rho(q)$ followed by $\rho$ when some parameter $q$ is changed. It is possible to see that both $D$ and $S_k$ present singular points in its shapes. Below-left: In a schematic picture, the pentagon represents $D$ and the triangle $S_k$, and we can draw a phase diagram for random $k$-robustness. In addition to the separable phase, there are two other separated by the line which starts in the random state and passes through a vertex of the triangle. Below-right: Analogously, the phase diagram for generalized $k$-robustness, where we can recognize three entangled phases, separated by lines starting at a vertex of the pentagon and passing through a vertex of the triangle.

Analogous to the geometric phase transitions in photons [22], we can recognize three entangled phases, separated by lines starting at a vertex of the pentagon and passing through a vertex of the triangle.

A related concept is the idea of the optimal entanglement witness [18], that is a witness operator $W_{\text{opt}}^k$ which maximizes the value of $|\text{Tr}(W^k \rho)|$ when restricted by some additional condition. It was shown [21] that if the optimal witness satisfy the constraint $W_{\text{opt}}^k < I$, then

$$R_g^k(\rho) = -\text{Tr}(W_{\text{opt}}^k \rho) = -\langle W_{\text{opt}}^k \rangle,$$  

(3)

while if it is imposed $\text{Tr}(W_{\text{opt}}^k) = d$, with $d$ the dimension of the total state space, then

$$R_r^k(\rho) = -\text{Tr}(W_{\text{opt}}^k \rho) = -\langle W_{\text{opt}}^k \rangle.$$  

(4)

Thus both $R_g^k$ and $R_r^k$ are given by the mean value of some Hermitian operator $W_{\text{opt}}^k$, which, by the other hand, can be linked with physical observables [19, 21] (different observables for different quantifiers, despite of our notation). The experimental detection of $\langle W_{\text{opt}}^k \rangle$ was confirmed through an optical setting to attest entanglement in photons [22]. A more detailed discussion on how to experimentally follow such geometric phase transition is given in the appendix. Furthermore an optimal entanglement witness $W_{\text{opt}}^k$, can be viewed as a tangent hyperplane separating $\rho$ from the set $S_k$ [18]. It is possible to see that both robustnesses $R_g^k$ and $R_r^k$ are not only linear functions of $\rho$ itself, but also of $W_{\text{opt}}^k$. Thus a discontinuity in $W_{\text{opt}}^k(q)$, which means a discontinuity in the family of hyperplanes tangent to $S_k$, will cause a singularity in the corresponding entanglement of $\rho$. As this discontinuity must be caused by a sharp shape of $S_k$, singularities in functions [20] or [21] are also necessary conditions to attest singularities in $D$ or $S_k$.

Other entanglement quantifiers were also shown to exhibit singularities when calculated for smooth curves $\rho(q)$ in $D$. That is the case of the Asymptotic Relative Entropy of Entanglement [23] and the Entanglement of Formation [24]. Although a geometric interpretation of these quantifiers is not clear, these results can be considered as predecessors of geometric phase transitions, which suggests more research on the theme.

We finish this Letter highlighting the surprising fact...
that a purely mathematical abstraction, the shape of the set of quantum states, can be directly tested by real experiments. Despite it being a philosophical question that deserves further investigation, a better comprehension of the geometry behind entanglement can help on understanding several physical phenomena. In fact, the understanding of quantum correlations is one of the greatest challenges to the contemporary physics, with a wide range of applications.

It is a pleasure to thank R. Dickman, F. Brochero, M. B. Plenio, and V. Vedral for enlightening discussions, and F. Tenuta for helping us with the figures. The authors also thank T.G. Mattos and R. Falcão for useful comments on a previous version of this manuscript. Financial support from Brazilian agency CNPq is also acknowledged.

Appendix- It was argued in the main text that optimal entanglement witnesses (OEW’s) can be experimentally implemented and, thus, used to study the geometry behind entanglement. However, in order to do that, one must firstly have a feasible way of determining an OEW to general states and, in a second moment, one must know how to implement this OEW in a real experimental setting. In this appendix we aim to show some methods to reach this end.

First of all let us discuss how to find an OEW with the prior knowledge of the state ρ. If ρ is a pure state, i.e., ρ = |ψ⟩⟨ψ|, then an analytical method can be used. An OEW, Woptk, of ρ is given by [19, 22, 25]

\[ W_{opt}^k = \lambda I - |ψ⟩⟨ψ| , \]

(5)

with

\[ \lambda = \max_{|σ⟩ ∈ S_k} |⟨ψ|σ⟩|^2 , \]

and I being the identity matrix. A way to compute λ is already known [22]. For mixed states (with the exceptions of two qubits and qubit-qutrit cases, where the Peres partial transposition criterion is decisive and can be interpreted in the entanglement witness context), there is no analytical way of finding it. However, there exist efficient numerical algorithms to approximate it [20, 21, 22].

In this way, we envisage to follow experimentally such geometric phase transition begins with a procedure to prepare states depending on one parameter q, ρ(q). For each fixed q value, the experimentalist proceeds a tomographic experiment. Then, one of the numerical algorithms should be executed to find an OEW for this state, Wopt(q). The next step involves to measure ⟨Wopt(q)⟩. This must be repeated for other values of q and, in this way, graphics like the ones showed in the text can be generated experimentally.

This can be criticized as being a very indirect way of measuring something. But one must remember that any physical experiment is guided by a theory that one wants to put in check. On the other hand, this is just a general procedure that can be much easier in specific cases. In many situations, the same EW is optimal for some range of value of q, and if one experimentally believes in the state that is being generated, the comparison of two specific entanglement witnesses can be enough to show a geometric phase transition.
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