Characteristics and benchmarks of entanglement of mixed states: The two-qubit case

Shanthanu Bhardwaj[1,3,*] and V. Ravishankar[1,2,†]
[1]Department of Physics, Indian Institute of Technology, Kanpur-208016, India
[2]Raman Research Institute, Sadashivanagar, Bangalore-560080, India
[3]Department of Physics, University of Chicago, Chicago, Illinois 60637, USA
(Received 9 January 2008; published 25 February 2008)

We propose that the entanglement of mixed states is characterized properly in terms of a probability density function $\mathcal{P}_\rho(\mathcal{E})$. There is a need for such a measure since the prevalent measures (such as *concurrence* and *negativity*) for two-qubit systems are rough benchmarks and not monotones of each other. Focusing on the two-qubit states, we provide an explicit construction of $\mathcal{P}_\rho(\mathcal{E})$ and show that it is characterized by a set of parameters of which concurrence is but one particular combination. $\mathcal{P}_\rho(\mathcal{E})$ is manifestly invariant under $SU(2)\times SU(2)$ transformations. It can, in fact, reconstruct the state up to local operations—with the specification of at most four additional parameters. Finally, the measure resolves the controversy regarding the role of entanglement in quantum computation in NMR systems.

DOI: 10.1103/PhysRevA.77.022322 PACS number(s): 03.67.Mn, 03.65.Ud, 03.67.Hk, 76.60.−k

I. INTRODUCTION

Quantum entanglement is a unique resource for novel (nonclassical) applications such as quantum algorithms [1], quantum cryptography [2], and more recently, metrology [3]. Thus, it plays a pivotal role in quantum information theory. It is also central to the study of the foundations of quantum mechanics [4]. It is not surprising that an abiding interest in quantum entanglement persists to this date.

Entanglement of a bipartite system in a pure state is unambiguous and well defined. In contrast, mixed-state entanglement (MSE) is relatively poorly understood mainly because entanglement, as an observable (denoting a property of the state), cannot be represented by a linear operator in Hilbert space. Although many criteria such as entanglement of formation and separability have been proposed, there is a realization [5] that no single quantity can adequately represent the entanglement contained in a mixed state. It may, therefore, be worthwhile to investigate whether a complete description of MSE is possible in a manner such that the current criteria emerge as particular, albeit useful benchmarks.

We propose in this paper a characterization of MSE in terms of a suitably defined probability density for entanglement, $\mathcal{P}_\rho(\mathcal{E})$. The proposal is operational for any bipartite system. In this work, we focus on two-qubit systems (2QSs) for which we fully implement the definition. We find that $\mathcal{P}_\rho(\mathcal{E})$ is characterized by its points of nonanalyticity of various orders which completely capture the information on MSE. This central result is employed to shed light on various aspects and manifestations of MSE.

The plan of the paper is as follows. In the next section we review briefly the existing criteria of MSE and their drawbacks. Section III proposes our definition in terms of a probability density function, which will be constructed fully for the two-qubit case in Sec. IV. Section V discusses several examples illustrating the proposal, and we show how an existing criterion—the concurrence—emerges as but one benchmark. In Sec. VI we discuss an interesting application, viz., to the problem of entanglement in NMR quantum computation (QC). In Sec. VII, we address the question of the reconstructibility of the state given its entanglement density. We show that, unlike in the case of every other definition, our prescription allows for an almost complete reconstruction of the state up to local $SU(2)\times SU(2)$ operations. Section VIII concludes with a summary and outlook.

II. CRITERIA AND BENCHMARKS OF MSE

In this section we review very briefly various criteria and definitions of MSE. It is not our purpose to provide an exhaustive description of all the definitions of MSE. We refer the reader to the literature [6] for details. Our intention is to merely provide a motivation and a proper setting for our definition.

Consider a bipartite spin system in a pure state, $|\psi\rangle = \Sigma_{m_1,m_2} c_{m_1 m_2} |m_1 m_2\rangle$, where the expansion is understood in any separable basis. The entanglement in the state is unambiguously quantified by the entropy carried by the reduced density matrix of either of the subsystems, $S[\rho_r]$. In the particular case of two qubits, equivalent criteria (in the sense of being relative monotones) include the degree of mixedness, $1-\mathrm{Tr}\rho_r^2$, the determinant $|\rho_r|$, and the concurrence $\mathcal{C} = 2|c_{\uparrow\uparrow}c_{\downarrow\downarrow} - c_{\downarrow\uparrow}c_{\uparrow\downarrow}|$, in writing which we employ the equivalent and a convenient notation $\uparrow\ (\downarrow) \leftrightarrow \frac{1}{2}\ (-\frac{1}{2})$. Operationally speaking, it is necessary and sufficient to measure a single quantity, the degree of polarization $P_1 = P_2 \equiv P$ of either of the qubits. We note parenthetically that knowledge of P allows a reconstruction of the parent state up to local $SU(2)\times SU(2)$ operations (LOs). Equivalently, entanglement determines the state up to LOs. Indeed, writing $|\psi\rangle = \cos(\theta/2)|\uparrow\uparrow\rangle + \sin(\theta/2)|\downarrow\downarrow\rangle$ in its canonical basis, we obtain the relation $P = |\sin\theta|$, which demonstrates the claim.

A description of MSE is not that straightforward, even in the two-qubit case. It is not difficult to realize that there

*shanth@uchicago.edu
†vravi@iitk.ac.in; vravi@rri.res.in

exists no single parameter that characterizes MSE [5]. Nevertheless, a number of concepts and associated quantities have been introduced in an attempt to capture the entanglement content in a mixed state, the two prominent of them being separability [7] and entanglement of formation (EOF) [5,8]. In addition, other concepts such as entanglement cost, distillable entanglement, relative entropy of entanglement, and entanglement witnesses have been introduced. It is instructive to look at the extent to which the above-mentioned definitions (i) satisfy the requirements of entanglement, (ii) are quantifiable, and (iii) are equivalent.

(i) *Compatibility with the requirements*. An entanglement measure is expected to satisfy continuity, additivity, subadditivity, convexity, and a nonincreasing nature under LOs, together with classical communication (LOCC) [6]. Much work has been done in checking for the compatibility of the above measures. It is found that (i) distillable entanglement violates convexity [9] and that (ii) the relative entropy of entanglement violates additivity [10]. It has not been established whether the entanglement cost is compatible with continuity and if EOF is compatible with additivity [6]. In short, there seems to be no single measure which is consistent with all of the above constraints.

(ii) *Quantifiability*. The measures listed above are quantifiable, at best, in a limited sense: Concurrence which quantifies EOF is defined only for a 2QS [11], and its generalization to higher-spin systems is not available. Negativity as a measure of nonseparability is a necessary and sufficient condition only for two-qubit and qubit-qutrit systems [12,13]; for higher-spin systems, it is only a necessary condition. Other operational criteria such as majorization [14] and reduction [15] are, again, only necessary (but not sufficient) conditions for separability. Entanglement cost and distillable entanglement have eluded any quantification so far.

(iii) *Mutual equivalence*. All of the above criteria are equivalent only for a pure state. Concurrence and negativity are, for instance, not relative monotones and are hence inequivalent [16]: States with the same concurrence can have differing negativities and vice versa, although for any given state, its negativity is never greater than concurrence.

To summarize, none of the above quantities can, by itself, capture fully the entanglement that is contained in a mixed state. This observation strongly suggests that a complete description of MSE requires more than the specification of a parameter.

To further emphasize the need for a better description of MSE, we note that a pure-state description is almost always an idealization and that any future experimental realization of quantum information processes will be with quantum systems in mixed states. An unsatisfactory understanding of MSE will reflect, in turn, an imprecise appreciation of the nonclassical features that render quantum information processing possible. An explicit example is provided by NMR quantum computers [17,18]. Here, the qubits are prepared experimentally in what is known as a pseudopure state

$$\rho_{ps} = \frac{1}{4}(1-\epsilon)\mathcal{I} + \epsilon|\psi\rangle\langle\psi|,$$

where $|\psi\rangle$ is a Bell state. The concurrence and negativity of ρ_{ps} survive if $\epsilon > \frac{1}{3}$, while experimentally, $\epsilon \approx 10^{-6}$ (see [18]).

These states would be essentially classical if we employ concurrence as a criterion for MSE, and no quantum gate operation should be possible with these states since the sole feature that distinguishes a quantum system from its counterpart is entanglement [19]. Yet notwithstanding the vanishing of this measure, nontrivial nonclassical gate operations with up to 8 qubits have been reported [20]. More recently, a 12-qubit pseudopure state has been reported for a weakly coupled NMR system [21]. While one could entertain the possibility of QC without entanglement [22], it is perhaps more fruitful to unravel the sense in which the inherent entanglement—not captured by EOF or nonseparability—is a resource for QC in these systems. Thus, there is a clear need to go beyond the above-mentioned benchmarks and attempt to obtain a more complete description. We address this problem and propose an alternative definition of MSE in the next section.

III. DESCRIPTION OF MSE BY A PROBABILITY DENSITY FUNCTION

A. Motivation for the definition

The definition of MSE which we propose differs from existing criteria in that we describe MSE in terms of a probability density for the entanglement. To motivate the idea, we recall that a mixed-state description is required when the system is an ensemble of quantum systems, each of which is in a pure state [23]. Entanglement has a sharp value for each pure state, and it should be natural that MSE be described properly by a distribution defined over the microstates.

This task is, however, not as straightforward as it might seem. Because of the principle of superposition, the ensemble description of a quantum system in a mixed state, as a weighted distribution over a set of pure states, is *not* unique. Expressed equivalently, there is no way of knowing how a system has been "prepared," unless it is in a pure state, for only a pure state $|\psi\rangle$ belongs to a unique one-dimensional projection $|\psi\rangle\langle\psi|$, with an eigenvalue of 1 [24]. Thus, although MSE may be expected to acquire a statistical character and be characterized by a suitably defined probability density function (PDF), care must be exercised such that the PDF for a given ρ is not an artifact of its resolution in terms of any particular incoherent superposition of pure states. As the first step in finding the way out, we consider the class of special systems whose density operators are projection operators. Note that both the pure states and the fully unpolarized state belong to this class.

B. Definition of the PDF when ρ is a projection

Consider the case $\rho = \frac{1}{M}\Pi_M$, where the projection operator Π_M has rank M. Let $\mathcal{H}(\Pi_M)$ be the subspace projected by Π_M. Observe that for all $|\psi\rangle \in \mathcal{H}(\Pi_M)$, $\langle\psi|\rho|\psi\rangle = \text{const}$, which merely expresses the fact that the probability density in the M-dimensional manifold $\mathcal{H}(\Pi_M)$ is uniform. The density in the complementary subspace is, of course, zero. This statement is exact and does not depend on the eigenbasis (or any other set of states) chosen to expand ρ. The probability density for the entanglement associated with the subspace may be defined as follows.

Definition 1 (PDF when ρ is a projection). Let the state $\rho = \frac{1}{M}\Pi_M$ be an M-dimensional projection operator. The probability density function for entanglement of this state is given by

$$\mathcal{P}_{\Pi_M}(\mathcal{E}) = \frac{\int d\mathcal{H}_{\Pi_M}\delta(\mathcal{E}_\psi - \mathcal{E})}{\int d\mathcal{H}_{\Pi_M}}, \tag{1}$$

where $d\mathcal{H}_{\Pi_M}$ is the volume measure for the manifold $\mathcal{H}_{\Pi_M}$.

To fix the volume measure in (1), we observe that the group of automorphisms G of the subspace $\mathcal{H}(\Pi)$ leaves ρ invariant. The measure should naturally be invariant under this group action and is, therefore, intimately related to the Haar measure of G. Indeed, let $\mathcal{H}(\Pi)$ be generated by the group action on any reference state $|\psi_0\rangle$. Any state $|\psi\rangle \in \mathcal{H}(\Pi)$ can be obtained by the action of some $g \in G$: $|\psi\rangle = g|\psi_0\rangle$. Let H be the stabilizer group of the ray associated with the reference state. The measure $d\mathcal{H}_\Pi$ is simply obtained by the Haar measure for G after factoring out the Haar measure for H [25]. Since the Haar measure is invariant under the group action and pure-state entanglement is invariant under LOs, it follows that the PDF is invariant under LOs.

The extension of the pure-state entanglement (one-dimensional projections) to states which are higher-dimensional projections has thus turned out to be straightforward and unambiguous. As we shall see in the explicit case of 2QSs which we study in detail, they have a rich structure which can nevertheless be captured by specifying a few parameters which are invariant under LOs. It remains to further extend the definition to mixed states which are not projections. We take that up in the next subsection.

C. PDF for any mixed state

To extend the above definition to mixed states without any restriction, we adopt the guiding principle that two states which are close to each other should possess "similar" entanglement densities. For example, the entanglement of a state with distinct but nearly equal eigenvalues should not differ from the entanglement of a completely unpolarized system. To accomplish this, we write ρ as a weighted sum of projection operators Π_M which satisfy the following property. Let $\mathcal{H}(\Pi_M)$ be the subspace (of dim M) projected by Π_M. We then require that $\mathcal{H}(\Pi_M) \subset \mathcal{H}(\Pi_{M+1})$, $M=1,\ldots,N-1$, where N is the dimension of ρ. In terms of these nested projections Π_M, we define the following.

Definition 2 (PDF for a mixed state). Let a state ρ be resolved in terms of nested projection operators as $\rho = \sum_{M=1}^{N}\omega_M\Pi_M$, with Π_M satisfying the normalization $\sum_M \omega_M = 1$. The PDF for the entanglement of ρ is given by

$$\mathcal{P}_\rho(\mathcal{E}) = \sum_{M=1}^{N} \omega_M \mathcal{P}_{\Pi_M}(\mathcal{E}), \tag{2}$$

where the PDF for a projection is defined in (1).

The definition given above is unambiguous since the weights can be easily determined in terms of the eigenvalues of ρ. Let $\lambda_i^{\downarrow}$ be the eigenvalues of ρ, arranged in a nonincreasing order, belonging to the respective eigenstates $|\psi_i\rangle$. The eigenstates are not unique if the eigenvalues are degenerate, but they are of no consequence to us here. We first write the trivial identity

$$\begin{aligned}\rho &= (\lambda_1 - \lambda_2)\Pi_1 + (\lambda_2 - \lambda_3)\Pi_2 + \cdots \\ &\quad + (\lambda_{N-1} - \lambda_N)\Pi_{N-1} + \lambda_N\Pi_N \\ &\equiv \sum_{M=1}^{N} \Lambda_M \Pi_M,\end{aligned} \tag{3}$$

where the projections $\Pi_M = \sum_{j=1}^{M}|\psi_j\rangle\langle\psi_j|$, $M=1,\ldots,N$, satisfy the nestedness condition stated above. The weights ω_M in (2) are easily read off as $\omega_M = \Lambda_M/\lambda_1$.

With this identification, we see that the non-negative vectors Ω and Λ, defined by $\Omega = (\omega_1,\ldots,\omega_N) \equiv \Lambda/\lambda_1$, have natural but rather different interpretations. The norm of Λ is a measure of the purity of the state and lies in the range $[1, 1/N]$, the limiting cases corresponding to the pure and completely mixed states, respectively. The norm of Ω represents, on the other hand, the degree of projection onto a subspace. Thus, $\|\Omega\|$ takes its maximum value of 1 when ρ is a pure projection. In any case, the form of ρ in (3) demonstrates the assertion made above—viz., that if the members of a set of eigenvalues are close to each other, the state is then predominantly in the subspace spanned by their respective eigenstates, with only a small spillover to the individual states. In the other case when an eigenvalue is much larger than the other, the spillover to the projection to higher-dimensional subspaces is small. These observations establish the physical viability of the definition.

We remark that the definition of MSE is valid for any bipartite system and is operational in the sense that it can, in principle, always be evaluated. The entanglement distribution is governed by the invariant Haar measure associated with the group of automorphisms of each subspace, as also the entanglements of the pure states belonging to it. Since they are invariant under LOs, their structure cannot be arbitrary. Thus, e.g., the PDF for an $(N-1)$-dimensional projection will be characterized by a single parameter—the entanglement of the pure state orthogonal to the subspace. Postponing an investigation to higher spins to a future work, we now implement the above definition to the most important case in quantum information theory—viz., the two-qubit system.

IV. PDF FOR A TWO-QUBIT SPIN SYSTEM

Two-qubit systems are the most important from the viewpoint of applications, and also because of the extensive theoretical analyses that they have received. We focus our attention exclusively on 2QSs in the rest of the paper. We (a) analyze entanglement in states which are pure projections and (b) their extension to general states, (c) illustrate the distribution in a number of examples, and (d) discuss the role of concurrence, (e) the problem of reconstructing the state given the PDF for entanglement, and (f) the reconciliation of NMR QC with entanglement. As our pure-state measure, we choose concurrence defined in the Introduction. As pointed out, this choice does not amount to any loss of generality since all the measures of pure-state entanglement are monotones of each other.

We first consider the special class of states, $\rho=\frac{1}{M}\Pi_M$, $M=1,\ldots,4$. The spectrum consists of only two eigenvalues, zero and $1/M$, with respective degeneracies $4-M$ and M. The two limiting cases $d=1,4$ correspond to the completely polarized (pure states) and the completely unpolarized (mixed states), respectively. Each of the above cases will be analyzed in detail. First the simplest of them all—viz., a pure state.

A. One-dimensional projections: The pure states

The Haar measure for the case $\rho=|\phi\rangle\langle\phi|$ is trivial since the group of automorphisms is given by the subgroup consisting only of the identity element. Thus, the PDF has the form

$$\mathcal{P}_1(\mathcal{E})=\delta(\mathcal{E}-\mathcal{E}_\phi),$$

in terms of the entanglement of $|\phi\rangle$. The PDF has a support only at $\mathcal{E}_\phi$, and the entanglement is characterized by a single number. Note that any other choice of pure-state entanglement simply rescales $\mathcal{E}_\phi\to\mathcal{E}'_\phi$ in a monotonic manner. The form of the PDF is unaffected. It may also be noted that the PDF determines the one-dimensional projection up to LOs.

B. Two-dimensional projection $\rho=\frac{1}{2}\Pi_2$

This particular class of states has the richest and most interesting entanglement distribution. Since the definition of PDF in (2) takes care of the normalization through the group volume factor, we pay no attention to the trace factor $\frac{1}{M}$ henceforth. The form of the PDF crucially depends on the nature of the subspace $\mathcal{H}(\Pi_2)$. Suppose that $\mathcal{H}(\Pi_2)$ is spanned by the basis $\{|m_1m_2\rangle,|m_1m_2'\rangle\}$. Without any further computation, we see that every state $\psi\in\mathcal{H}(\Pi_2)$ is separable, giving a PDF which vanishes everywhere, except at $\mathcal{E}=0$. It is not difficult to see that the above statement holds for all subspaces related to the specified subspace by local operations—i.e., $SU(2)\times SU(2)$ transformations. Such an equivalence under LOs is valid for other PDFs as well. It is, therefore, necessary and sufficient to study the PDFs for $\mathcal{H}(\Pi_2)$ which belong to inequivalent classes under LOs. To that end, we construct a canonical basis in $\mathcal{H}(\Pi_2)$ by freely employing LOs.

Canonical basis in $\mathcal{H}(\Pi_2)$. Let $|\psi\rangle\in\mathcal{H}(\Pi_2)$. Let $|\chi_1\rangle,|\chi_2\rangle$ be orthonormal and span $\mathcal{H}(\Pi_2)$. We have

$$|\psi\rangle=\cos\frac{\theta}{2}e^{i\phi/2}|\chi_1\rangle+\sin\frac{\theta}{2}e^{-i\phi/2}|\chi_2\rangle, \tag{4}$$

where $0\le\theta\le\pi$ and $0\le\phi\le2\pi$. The Haar measure is simply read off as $d\mathcal{H}=\sin\theta\,d\theta\,d\phi$.

We assert that in any $\mathcal{H}(\Pi_2)$, there is a state which is separable.

Proof. The demonstration is straightforward. Let $|\chi_1\rangle,|\chi_2\rangle$ be an orthonormal basis in $\mathcal{H}(\Pi_2)$. Let the entanglement of $|\chi_1\rangle$, $\mathcal{E}_{\chi_1}=|\sin\alpha|$. Its canonical form is then given by

$$|\chi_1\rangle=\cos\frac{\alpha}{2}|\uparrow\uparrow\rangle+\sin\frac{\alpha}{2}|\uparrow\downarrow\rangle,$$

from which

$$|\chi_2\rangle=a\left(-\sin\frac{\alpha}{2}|\uparrow\uparrow\rangle+\cos\frac{\alpha}{2}|\downarrow\downarrow\rangle\right)+b|\uparrow\downarrow\rangle+c|\downarrow\uparrow\rangle, \tag{5}$$

with the condition $|a|^2+|b|^2+|c|^2=1$. Let us expand $|\psi\rangle$ in the above basis employing (4). The condition that $\mathcal{E}_\psi=0$ yields the quadratic equation in $z=\tan(\frac{\theta}{2})\exp(i\phi)$,

$$\left(a^2\frac{\sin\alpha}{2}-bc\right)z^2-az+\frac{\sin\alpha}{2}=0,$$

whose solutions are always physical, by virtue of the bijective mapping between the points on a sphere and the complex plane.

Let the separable state be chosen as a basis state and be brought to its canonical form $|\eta_1\rangle=(1,0,0,0)$ in writing which we have ordered the basis states as $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$. Employing the residual LO (which leaves $|\eta_1\rangle$ invariant), we may write the orthogonal basis vector as $|\eta_2\rangle=(0,x,y,z=\sqrt{1-x^2-y^2})$, where $x,y,z\ge0$. The subspace $\mathcal{H}(\Pi_2)$ is, therefore, characterized by two nonnegative parameters—say, x,y. The PDF would also be characterized by the two parameters and gets implicitly determined by (1).

1. Determination of the PDF

The determination of the distribution function is rather involved, and we give the details in the Appendix. Here, we present the results and discuss the salient features.

The generic form of the PDF for Π_2 is shown in Fig. 1 (solid curve). We observe that it has three markers: (i) $\mathcal{E}_{\text{cusp}}$, the entanglement at which the probability density diverges as a cusp; (ii) $\mathcal{E}_{\max}$, the maximum entanglement allowed; and (iii) $\mathcal{P}_2(\mathcal{E}_{\max})$, the probability density at $\mathcal{E}_{\max}$. In fact, any two of them suffice to characterize the PDF completely. One may specify, e.g., $(\mathcal{E}_{\max},\mathcal{P}_2(\mathcal{E}_{\max}))$ or, equivalently, $(\mathcal{E}_{\text{cusp}},\mathcal{P}_2(\mathcal{E}_{\max}))$ for characterizing the curve. A straightforward computation establishes the relations

$$\mathcal{E}_{\max}=xy+\sqrt{z^2+x^2y^2}, \tag{6}$$

$$\mathcal{E}_{\text{cusp}}=\frac{z^2}{\mathcal{E}_{\max}}=\mathcal{E}_{\max}\cos\mu, \tag{7}$$

$$\mu=\sin^{-1}\left(\frac{1}{\mathcal{E}_{\max}\mathcal{P}_2(\mathcal{E}_{\max})}\right)=\sin^{-1}\left(\frac{2\sqrt{xy(xy\mathcal{E}_{\max}+z^2)}}{\mathcal{E}_{\max}^{3/2}}\right), \tag{8}$$

which allow us to determine the parameters x,y that define Π_2. μ is well defined by virtue of the inequality $\mathcal{P}_2(\mathcal{E}_{\max})\ge1/\mathcal{E}_{\max}$.

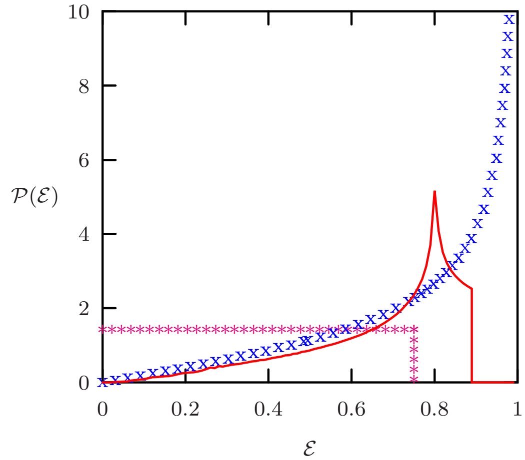

FIG. 1. (Color online) Some typical probability density functions for Π_2. Note the solid curve, which shows all the features of $\mathcal{P}_2(\mathcal{E})$. It has a cusp at $\mathcal{E}_{\mathrm{cusp}}=0.8$ and goes to zero at $\mathcal{E}_{\max}=0.89$. The step function is an extreme example, where $\mathcal{E}_{\mathrm{cusp}}=0$, and the other dotted curve has $\mathcal{E}_{\mathrm{cusp}}=\mathcal{E}_{\max}=1$.

The details of the nature of the PDF are presented in the Appendix, where the above statements are proved. It is also shown that the PDF itself is an incomplete elliptic integral. For our purposes here, it is important that the curve is characterized by the two locally invariant parameters x,y.

More importantly, we note that unlike with the other measures, the state itself can be reconstructed up to LOs. For, we can reexpress (x,y,z) in terms of the characteristics of the PDF thus:

$$z=\sqrt{\mathcal{E}_{\max}\mathcal{E}_{\mathrm{cusp}}}=\mathcal{E}_{\max}\sqrt{\cos\mu}, \tag{9}$$

$$x=\frac{1}{2}[\sqrt{(1+\mathcal{E}_{\max})(1-\mathcal{E}_{\mathrm{cusp}})}+\sqrt{(1-\mathcal{E}_{\max})(1+\mathcal{E}_{\mathrm{cusp}})}], \tag{10}$$

$$y=\frac{1}{2}[\sqrt{(1+\mathcal{E}_{\max})(1-\mathcal{E}_{\mathrm{cusp}})}-\sqrt{(1-\mathcal{E}_{\max})(1+\mathcal{E}_{\mathrm{cusp}})}], \tag{11}$$

$$xy=\frac{1}{2}(\mathcal{E}_{\max}-\mathcal{E}_{\mathrm{cusp}})=\mathcal{E}_{\max}\sin^2(\mu/2). \tag{12}$$

The above equation expresses the result that the entanglement of a state which is a two-dimensional projection is completely characterized by its $\mathrm{SU}(2)\times\mathrm{SU}(2)$ invariant parameters, which are essentially 2 in number.

2. Relation with concurrence and negativity

We briefly discuss the status of two well-known benchmarks, concurrence and negativity, in this description. It is, in fact, sufficient to consider concurrence since it bounds negativity from above. As a warm-up, it is instructive to look at two extreme cases which occur when $\mathcal{E}_{\mathrm{cusp}}=0$ and $\mathcal{E}_{\mathrm{cusp}}=\mathcal{E}_{\max}$. In the first case, the PDF is a step function, terminating at some $\mathcal{E}_{\max}$. In the second case, the density increases monotonically, diverging at $\mathcal{E}_{\max}$ (see Fig. 1). The relative abundance of the entangled states is more in the latter case. One may *per se* expect that the associated concurrence should also be larger. Interestingly, however, concurrence for a two-dimensional projection is related to the parameters by

$$\mathcal{C}=(\mathcal{E}_{\max}-\mathcal{E}_{\mathrm{cusp}})/2. \tag{13}$$

Thus, contrary to naive expectations, concurrence—as a quantifier of entanglement of formation—vanishes when $\mathcal{E}_{\mathrm{cusp}}=\mathcal{E}_{\max}$. In other words, it is sensitive not to the relative abundance of the microstates at zero (or small entanglements) at all, but to the difference between $\mathcal{E}_{\mathrm{cusp}}$ and $\mathcal{E}_{\max}$. In any case, $\mathcal{C}$ emerges as a particular benchmark of the probability density, describing it only partially.

We note that if $\rho=\Pi_3$ or Π_4, then its concurrence vanishes identically. By virtue of its convexity, we conclude that concurrence of any state $\mathcal{C}_\rho$ obeys the inequality

$$\mathcal{C}_\rho\le(\lambda_1-\lambda_2)\mathcal{C}_{\Pi_1}+(\lambda_2-\lambda_3)\mathcal{C}_{\Pi_2}.$$

Incidentally, the entanglement distribution of a subspace $\mathcal{H}(\Pi_2^c)$ orthogonal to $\mathcal{H}(\Pi_2)$ is the same as that of $\mathcal{H}(\Pi_2)$. The proof of this statement is given in the Appendix.

C. Three-dimensional projection $\rho=\frac{1}{3}\Pi_3$

We now move on to the case $\rho=\Pi_3$, whose PDF has a simpler structure. The simplicity is afforded by the fact that Π_3 is completely characterized by its dual $|\psi_\perp\rangle\perp\Pi_3$. Accordingly, its PDF is characterized by a single parameter $\mathcal{E}_\perp$, which is the entanglement of the orthogonal state $|\psi_\perp\rangle$.

Let $\{|\chi_i\rangle\}$, $i=1,2,3$, be an orthonormal basis spanning the subspace $\mathcal{H}(\Pi_3)$ under consideration. The integrating measure [26] may be conveniently written as $d\mathcal{H}_3=\sin2\beta\sin2\theta\sin^2\theta\,d\alpha\,d\beta\,d\gamma\,d\theta$, with the state expanded as

$$|\psi\rangle=\cos\theta|\chi_1\rangle+e^{i(\alpha+\gamma)}\sin\theta\cos\beta|\chi_2\rangle-e^{i(\alpha-\gamma)}\sin\theta\sin\beta|\chi_3\rangle.$$

The ranges of integration are given by $\theta,\beta\in[0,\frac{\pi}{2}]$ and $\alpha,\gamma\in[0,\pi]$. Using arguments similar to the ones employed for two-dimensional subspaces, one may, conveniently, choose two of the basis states—say, $\chi_{1,2}$—to be separable; by a suitable LO, they can be brought to the form $|\uparrow\uparrow\rangle,|\downarrow\downarrow\rangle$.

In this basis, the state $|\chi_3\rangle=c_1|\uparrow\downarrow\rangle+c_2|\downarrow\uparrow\rangle$ has the same entanglement $\mathcal{E}_\perp$ as the state $|\psi_\perp\rangle=c_2^*|\uparrow\downarrow\rangle-c_1^*|\downarrow\uparrow\rangle$. In this canonical form the state looks like

$$\rho=\begin{pmatrix}\frac{1}{3}&0&0&0\\0&\frac{|c_1|^2}{3}&\frac{c_1c_2^*}{3}&0\\0&\frac{c_1^*c_2}{3}&\frac{|c_2|^2}{3}&0\\0&0&0&\frac{1}{3}\end{pmatrix}.$$

Here, in terms of c_1 and c_2, we have $\mathcal{E}_\perp=2|c_1c_2|$.

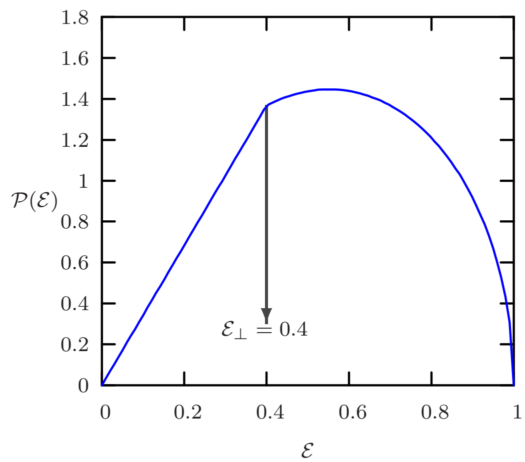

FIG. 2. (Color online) A typical probability density for Π_3. Note the point of discontinuity in the derivative at $\mathcal{E}=\mathcal{E}_\perp$.

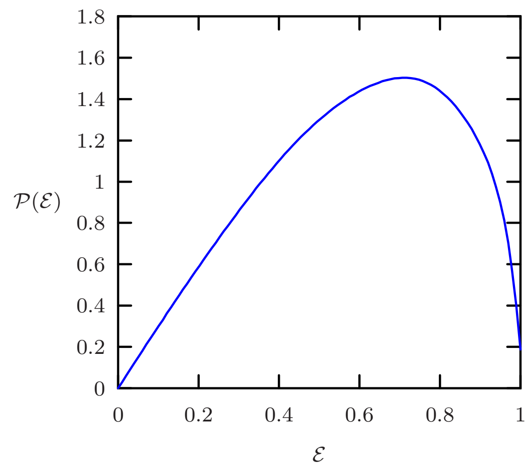

FIG. 3. (Color online) The probability density $\mathcal{P}_4(\mathcal{E})$ for the entire Hilbert space.

We have verified that the resulting probability density can be cast into the simple form

$$\mathcal{P}_3(\mathcal{E}) = \frac{2\mathcal{E}}{\sqrt{1-\mathcal{E}_\perp^2}}\cosh^{-1}\left(\frac{1}{\mathcal{E}_>}\right), \tag{14}$$

where $\mathcal{E}_> = \max(\mathcal{E},\mathcal{E}_\perp)$.

A typical curve for $\mathcal{P}_3(\mathcal{E})$ is shown in Fig. 2, which exhibits the required characteristic. The curve possesses a discontinuity in its derivative at $\mathcal{E}_\perp$. Significantly, concurrence (being identically zero) fails to distinguish different three-dimensional projections—e.g., $\mathcal{E}_\perp=0$ or 1—although their PDFs are vastly different. It simply picks up $\mathcal{E}=0$, at which the probability density, in fact, vanishes.

Since $\mathcal{P}_3(\mathcal{E})$ is characterized entirely by $\mathcal{E}_\perp$, it is clear that the state itself can be reconstructed up to LOs.

D. Full Hilbert space

Last, we consider the full space $\mathcal{H}(\Pi_4)$, whose PDF is universal. This curve is obtained by using the Haar measure on SU(4) [27]. Note that the curve is smooth everywhere, as shown in Fig. 3.

E. General mixed state

The generalization of the pure-state entanglement to higher-dimensional projections has been accomplished so far. It remains to merely illustrate the nature of the PDF for entanglement when we have a superposition of nested projections, as given in (3). The entanglement density, as defined in (2), does retain information on the contribution from the constituent nested projections, with appropriate weights ω_M. Indeed, each dimension produces a PDF with its indelible characteristic. The PDF for Π_1 is highly singular, being a Dirac δ distribution. The PDF for Π_2 is less singular, but has a cusp as well as a step function discontinuity at $\mathcal{E}_{\max}$. The PDF for Π_3 is smoother, possessing only a discontinuous derivative at $\mathcal{E}_\perp$. Finally, the PDF for the fully unpolarized state Π_4 is entirely smooth everywhere. Thus, the definition of mixed-state entanglement given in (2) captures all the features and stands vindicated. Recall that the weights have been so chosen that the continuity requirement is maintained naturally.

Before going on to discuss more interesting examples, we pause to illustrate explicitly how $\mathcal{P}_3(\mathcal{E})$ may be determined for a rather arbitrarily chosen state. Consider the density matrix ρ with eigenvalues $\{\lambda_i\}=\{0.385, 0.288, 0.231, 0.096\}$ and the respective eigenvectors given by

$$|\psi_1\rangle = (0.998, 0.000, 0.031, 0.050),$$

$$|\psi_2\rangle = (0.059, -0.009, -0.528, -0.847),$$

$$|\psi_3\rangle = (0.000, 0.924, 0.325, -0.202),$$

$$|\psi_4\rangle = (0.000, 0.383, -0.784, 0.489).$$

Now, for the one-dimensional (1D) subspace, we simply have $\mathcal{E}_1 \approx 0.1$ and the weight associated with this δ-function PDF is $(\lambda_1-\lambda_4)/\lambda_1 \approx 0.25$. Similarly, for the 2D subspace spanned by $|\psi_1\rangle, |\psi_2\rangle$ it is easy to verify that the canonical basis in Π_2 can be chosen to be $|\chi_1\rangle=(1,0,0,0)$, $|\chi_2\rangle=(0,x,y,z)=(0,0.00945,0.5290,0.8485)$. From this it follows that $\mathcal{E}_{\max}\approx 0.9$ and $\mathcal{E}_{\text{cusp}}\approx 0.8$ using (6)–(8). Also, we can easily see that $\mathcal{E}_\perp \approx 0.6$ directly from $|\psi_4\rangle$.

Figure 4 illustrates the PDF for this general case. Note how all the essential features stand out in the graph.

V. EXAMPLES

We proceed to study $\mathcal{P}(\mathcal{E})$ for states which are often encountered and also those which have a natural geometric structure. The exercise serves to highlight the richness of the definition.

A. Strongly separable states

As the first example we consider states which are strongly separable, $\rho=\rho_1\times\rho_2$. Conventional definitions attribute no

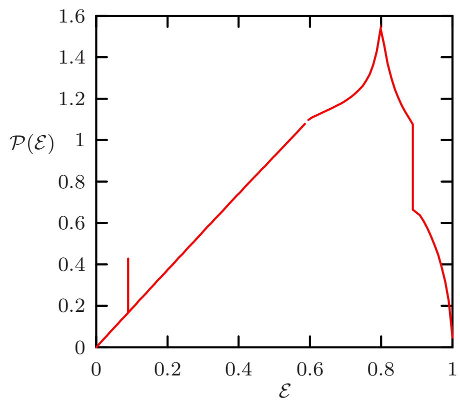

FIG. 4. (Color online) The overall probability density $\mathcal{P}_4(\mathcal{E})$ for a typical mixed state, ρ, with eigenvalues {0.385,0.288,0.231, 0.096}. The features of the individual subspaces are vividly preserved. Note that the delta function is represented as a vertical line of height equal to its weight at the abscissa of its support

entanglement to this class of states. We can very readily look at what form the PDF will take by making simple local rotations so that ρ_1 and ρ_2 are both written as $\frac{1}{2}(\mathbf{1}+k_i\sigma_z^{(i)})$ (where $i=1,2$, respectively), with $k_1,k_2\geq 0$. Thus ρ acquires the form

$$\frac{1}{4}\mathrm{diag}(1+k_1+k_2+k_1k_2, 1-k_1+k_2-k_1k_2, 1+k_1-k_2 - k_1k_2, 1-k_1-k_2+k_1k_2).$$

The eigenvector corresponding to the largest eigenvalue, in this case, is clearly $|\uparrow\uparrow\rangle$; therefore, the 1D part of the PDF has no entanglement. The 2D subspace is also separable since the eigenvector with the next largest eigenvalue is either $|\downarrow\uparrow\rangle$ or $|\uparrow\downarrow\rangle$, both of which form a separable subspace with $|\uparrow\uparrow\rangle$. In other words, the PDF in Π_2 vanishes everywhere, except at $\mathcal{E}=0$. Therefore the first nonzero contribution to the PDF comes from the 3D subspace. In this case too, it is the least possible contribution that is possible from a 3D subspace because $\mathcal{E}_\perp=0$. Thus, our measure of entanglement, the PDF, gives the minimum possible PDF to separable states. Thus the PDF is a simple superposition of Figs. 2 and 3. The entanglement vanishes of course if the state is pure.

B. Purely vector polarized states

In the previous example, we had a nonvanishing tensor polarization which was not independent of its vector polarization. We now consider states which are purely vector polarized. These states are not factorizable. Further, they are never in a pure state. Writing $\rho=\frac{1}{4}(\mathbf{1}+\vec{p}_1\cdot\vec{\sigma}_1+\vec{p}_2\cdot\vec{\sigma}_2)$, we can bring it to the canonical form $\rho=\frac{1}{4}(\mathbf{1}+p_1\sigma_1^z+p_2\sigma_2^z)$. An easy adaptation of the previous case shows again that the nonvanishing contribution comes from Π_3.

C. Purely tensor polarized states

These states come in three classes, each of which we study below.

1. Pseudopure states

An important but an easily analyzable state is a pseudopure state which is an incoherent superposition of a one-dimensional projection and the projection operator for the full space. These states are employed in NMR QC, and unraveling their entanglement is not without interest. Pseudopure states have the form $\rho=\frac{1}{4}(\mathbf{1}+k\vec{\sigma}_1\cdot\vec{\sigma}_2)$. Unlike in the previous cases, the sign of k cannot be altered by a local transformation and it lies in the range $-1\leq k\leq 1/3$. The eigenvalue decomposition of ρ is given by

$$\rho=\frac{1+k}{4}\{\Pi_{\uparrow\uparrow}+\Pi_{\downarrow\downarrow}+\Pi_B\}+\frac{1-3k}{4}\Pi_B'\equiv\frac{1-\epsilon}{4}\mathbf{1}+\epsilon\Pi_B', \tag{15}$$

where $\epsilon=-k$ and $\Pi_{\uparrow\uparrow}$ and $\Pi_{\downarrow\downarrow}$ are the projection operators for the states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$; Π_B and Π_B' are the projection operators for the respective Bell states

$$|\psi_B\rangle=\frac{1}{\sqrt{2}}\{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle\},$$

$$|\psi_B'\rangle=\frac{1}{\sqrt{2}}\{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle\}.$$

The state is pure at the extremal value $k=-1$ and is the completely entangled singlet state. It is completely unpolarized at $k=0$; at the other extremal value $k=1/3$, it is a three-dimensional projection, orthogonal to the singlet state. Thus, for $k<0$, $\mathcal{E}_\rho$ gets a contribution from the Bell state (the Dirac δ has its support at $\mathcal{E}=1$) with a weight $\omega_1=\frac{-4k}{1-3k}$ and the full space with a weight $\omega_4=\frac{1+k}{1-3k}$. Similarly, when $k>0$, its entanglement gets a contribution from the full space with a weight $\frac{1-3k}{1+k}$ and the three-dimensional subspace (orthogonal to the singlet) with a weight $\frac{4k}{1+k}$. The curve corresponding to Π_3 is a straight line since $\mathcal{E}_\perp=1$. There is no contribution from the two-dimensional projection in either case. We take up a discussion of the import of this example to NMR QC in the next section.

2. States of the form $\rho=\frac{1}{4}[\mathbf{1}+\vec{p}\cdot(\boldsymbol{\sigma}_1\times\boldsymbol{\sigma}_2)]$

We can easily utilize local rotations to align $\vec{p}$ along the z axis, thus converting the density matrix to the form

$$\rho=\frac{1}{4}\mathbf{1}+p(\sigma_1^x\otimes\sigma_2^y-\sigma_1^y\otimes\sigma_2^x),$$

$$\rho=\begin{pmatrix}\frac{1}{4} & 0 & 0 & 0\\ 0 & \frac{1}{4} & 2ip & 0\\ 0 & -2ip & \frac{1}{4} & 0\\ 0 & 0 & 0 & \frac{1}{4}\end{pmatrix}.$$

Thus, we have the eigenvalues $\{\frac{1}{4}+2p,\frac{1}{4},\frac{1}{4},\frac{1}{4}-2p\}$, with the respective eigenvectors $\{\frac{|\uparrow\downarrow\rangle-i|\downarrow\uparrow\rangle}{\sqrt{2}},|\uparrow\uparrow\rangle,|\downarrow\downarrow\rangle,\frac{|\uparrow\downarrow\rangle+i|\downarrow\uparrow\rangle}{\sqrt{2}}\}$.

From the above structure, the PDFs for various subspaces and the associated weights may be easily obtained. For the one-dimensional projection, we have the PDF and its associated weight given by

$$P_1(\mathcal{E}) = \delta(\mathcal{E}-1), \quad \omega_1 = \frac{2p}{\left(\frac{1}{4}+2p\right)}.$$

There is no contribution from the 2D subspace, since $\omega_2 = \lambda_2 - \lambda_3 = 0$. Considering the 3D subspace, since $\mathcal{E}_\perp = 1$, the probability density and the weights are read off as

$$P_3(\mathcal{E}) = 2\mathcal{E}, \quad \omega_3 = \frac{2p}{\left(\frac{1}{4}+2p\right)}.$$

Interestingly, $\omega_1 = \omega_3$.

Thus the states belonging to the above class simply have PDFs that are linear with a slope varying from 0 to 1, with a weighted δ-function at $\mathcal{E}=1$.

3. States with traceless symmetric tensor polarization

Finally, we consider tensor-polarized states in their most familiar—the quadrupolar—form $\rho = \frac{1}{4}\{1 + A_{ij}\cdot(\sigma_1^i \otimes \sigma_2^j)\}$, where A_{ij} is a traceless symmetric matrix. This matrix is diagonalizable by a local $SU(2)\times SU(2)$ transformation. We bring the matrix to the form $A = \mathrm{diag}(A_{xx}, A_{yy}, -A_{xx}-A_{yy})$, where $A_{xx} \geq A_{yy} \geq 0$. In this basis, ρ acquires the form

$$\rho = \begin{pmatrix} \frac{1}{4}-\lambda & 0 & 0 & \mu \\ 0 & \frac{1}{4}+\lambda & \lambda & 0 \\ 0 & \lambda & \frac{1}{4}+\lambda & 0 \\ \mu & 0 & 0 & \frac{1}{4}-\lambda \end{pmatrix},$$

where $\lambda = A_{xx}+A_{yy}$ and $\mu = A_{xx}-A_{yy}$. This gives us the eigenvalues

$$(\lambda_1,\lambda_2,\lambda_3,\lambda_4) = \left(\frac{1}{4}+2\lambda, \frac{1}{4}, \frac{1}{4}-\lambda+\mu, \frac{1}{4}-\lambda-\mu\right),$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$, and the corresponding eigenvectors are the Bell states

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle),$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$

$$|\psi_3\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle),$$

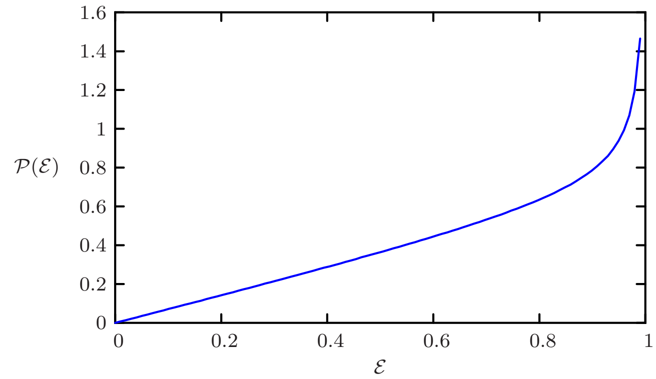

FIG. 5. (Color online) A typical quadrupolar state, with the values $\lambda=0.15$ and $\mu=0.08$. Note that the weighted δ function at $\mathcal{E}=1$ is not shown in the plot since the PDF goes to ∞ at this point.

$$|\psi_4\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle).$$

The rest of the analysis is straightforward. The probability density function and the associated weight for the Bell state $|\psi_1\rangle$ are simply read off as

$$\mathcal{P}_1(\mathcal{E}) = \delta(\mathcal{E}-1), \quad \omega_1 = \frac{2\lambda}{\frac{1}{4}+2\lambda}.$$

The PDF for the two-dimensional projection spanned by $|\psi_{1,2}\rangle$ also has a simple expression and the weight given by

$$\mathcal{P}_2(\mathcal{E}) = \frac{\mathcal{E}}{\sqrt{1-\mathcal{E}^2}}, \quad \omega_2 = \frac{\lambda-\mu}{\frac{1}{4}+2\lambda}.$$

Since $|\psi_4\rangle$ is a Bell state, we obtain for the three-dimensional subspace

$$\mathcal{P}_3(\mathcal{E}) = 2\mathcal{E}, \quad \omega_3 = \frac{2\mu}{\frac{1}{4}+2\lambda}.$$

Finally the weight for the full space is given by $\frac{1/4-\lambda-\mu}{1/4+2\lambda}$. It is remarkable that for this class of states, the details of the state manifest only in the weights. The density function for each dimension is itself universal. Furthermore, we have constraints on the coefficients $\lambda+\mu \leq \frac{1}{4}$ and $\lambda \geq \mu \geq 0$.

Figure 5 illustrates the PDF for a typical state of this class.

Before we conclude this section, we wish to add the cautionary remark that although the above analysis reveals entanglement in a host of states which are otherwise considered to be classical, it does not imply that all of them may be harnessed with equal facility. For instance, the entanglement of the uniform distribution cannot be accessed by standard gate operations which are unitary and the corresponding PDF (Fig. 3) has to be treated as a background. While more study is needed to discern the role of the entanglement density in various quantum information processes, there is one application of topical interest which we take up below.

VI. ENTANGLEMENT IN NMR QUANTUM COMPUTATION

As an application of our description, we address the issue of the role played by entanglement in QC with NMR. NMR QC employs the so-called pseudopure states which have the form $\frac{1-\epsilon}{4}\mathbf{1}+\epsilon\Pi_B'$, Eq. (15). It has been experimentally demonstrated that the quantum logic operations used in QC are implementable with NMR, and we know that no quantum logic operation is possible with classical states. Interestingly, concurrence and negativity vanish when $\epsilon<\frac{1}{3}$, while in experiments, $\epsilon\sim 10^{-6}$.

This has led to a debate on the role of entanglement in NMR QC [22] although, as we saw, experiments clearly show that such states cannot be completely classical.

The PDF constructed for the pseudopure states in the previous section resolves this problem naturally. First of all, its $\mathcal{P}_\rho(\mathcal{E})$ is given by a weighted Dirac δ which is nonvanishing for all $\epsilon>0$, superposed on the background contribution from the uniform distribution. We know that the NMR signal is sensitive only to the pure component, the so-called deviation density matrix. Thus, although the uniform background is invariant under unitary operations, the one-dimensional fluctuation is not, allowing for nontrivial gate operations. In other words, NMR QC exploits the excess of entangled states over the unpolarized background as a resource and this feature is correctly captured by the PDF of the state. Incidentally, this analysis also raises the interesting possibility of QC with more general pseudoprojection states.

VII. RECONSTRUCTIBILITY OF ρ FROM THE PDF

Last, we return to the issue of the reconstructibility of the state (up to LOs). We have seen that when ρ is a projection, the reconstructibility is assured by construction. When ρ is more general, the reconstruction is somewhat partial; we are not permitted to perform independent LOs on various subspaces if the reconstruction is desired. Indeed, the action of $SU(2)\times SU(2)$ on ρ produces an orbit of dimension 6, characterized by nine invariants. The parameters which characterize the entanglement are 7 in number, which may be chosen, for example, to be $\{\mu_1,\mu_2,\mu_3,\mathcal{E}_1,\mathcal{E}_{\rm cusp},\mathcal{E}_{\max},\mathcal{E}_\perp\}$. Thus we need two additional parameters which would determine ρ. To understand their role, we note that, geometrically, $\mathcal{P}_\rho(\mathcal{E})$ is invariant under independent local operations L_i acting on the subspaces Π_i, where $\Pi_i\subset\Pi_{i+1}$. If ρ is to be unique up to a global LO, one needs the additional constraint $L_i=UL_i^{(0)}$, where $L_i^{(0)}$ may be chosen freely. Let us choose $L_2^{(0)}=\mathbf{1}$ (where $\mathbf{1}$ is the identity operator). The nestedness condition—viz., that $|\psi_1\rangle\in\Pi_2$ and $|\psi_4\rangle\in\Pi_2^c$—entails that $L_1^{(0)}$ and $L_3^{(0)}$ get specified by two[1] parameters each.

We make the above argument more explicit. If we have Π_2 in its canonical form, it is spanned by $|\chi_1\rangle$ and $|\chi_2\rangle$ given, respectively, as (1, 0, 0, 0) and $(0,x,y,z)$. Therefore, we can specify $|\psi_1\rangle=|\chi_1\rangle\cos\frac{\theta}{2}e^{i\phi/2}+|\chi_2\rangle\sin\frac{\theta}{2}e^{-i\phi/2}$ by giving the values of (θ,ϕ). Similarly, $|\psi_\perp\rangle$ can be specified by $(\theta_\perp,\phi_\perp)$ when it is expanded in the canonical basis of $\Pi_2^c=(\mathbf{1}-\Pi_2)$, given by $|\chi_1^c\rangle=(0,0,c/\sqrt{c^2+b^2},-b/\sqrt{c^2+b^2})$ and $|\chi_2^c\rangle=(0,\sqrt{c^2+b^2},ab/\sqrt{c^2+b^2},ac/\sqrt{c^2+b^2})$. The above construction completes the argument. It is noteworthy that the question of reconstructibility cannot even be raised with other criteria.

VIII. CONCLUSION

In conclusion, we have shown that mixed-state entanglement has a rich structure and is properly described via a suitably defined probability density. We have explicitly implemented the definition to the most important case—the two-qubit systems—and shown how criteria such as concurrence emerge as specific benchmarks. Their precise role in describing the entanglement is also clarified. The role of entanglement in NMR QC is resolved and the issue of the reconstructibility of the state discussed. Nevertheless, the study is incomplete since possible applications to teleportation, quantum algorithms, and error-correcting codes still need to be explored. The generalization to higher-spin systems would also provide a deeper and a better appreciation of quantum information processes.

APPENDIX

The properties of the entanglement density $\mathcal{P}_\rho(\mathcal{E})$ for a two-dimensional projection Π_2 will be worked out in detail here.

Consider Π_2 first. Recall that we are considering the subspace spanned by $|\alpha\rangle=(1,0,0,0)$ and $|\beta\rangle=(0,x,y,z)$. A general state $|\psi\rangle=\cos\frac{\theta}{2}e^{i\phi/2}|\alpha\rangle+\sin\frac{\theta}{2}|\beta\rangle$ has its entanglement given by

$$\mathcal{E}^2=|2[z\sin(\theta/2)\cos(\theta/2)e^{i\phi/2}+xy\sin^2(\theta/2)]|^2. \quad \text{(A1)}$$

It follows from the above expression that the maximum entanglement allowed is given by

$$\mathcal{E}_{\max}=xy+\sqrt{z^2+x^2y^2}. \quad \text{(A2)}$$

It is further convenient to introduce the variable μ defined by $z=\mathcal{E}_{\max}\sqrt{\cos\mu}$ and $xy=\mathcal{E}_{\max}\sin^2(\mu/2)$. It follows that the entanglement of *every* state in the subspace scales linearly in $\mathcal{E}_{\max}$. Therefore, we can write

[1] In fact, we need only one parameter each to fix the states up to discrete ambiguities. This is because from the $\mathcal{P}_i(\mathcal{E})$ we already know the entanglement of the states, which fixes one parameter. However, there remains a discrete ambiguity if only one of θ or ϕ is specified.

$$\mathcal{P}(E)|_{(\mathcal{E}_{\max},\mu)} = \frac{1}{\mathcal{E}_{\max}} \mathcal{P}'(\mathcal{E}/\mathcal{E}_{\max})|_{(\mathcal{E}'_{\max}=1,\mu)}$$

if $\mathcal{E}<\mathcal{E}_{\max}$ and $\mathcal{P}(E)|_{(\mathcal{E}_{\max},\mu)}=0$ if $\mathcal{E}>\mathcal{E}_{\max}$. We shall now utilize this scaling and concentrate on studying the distribution for $\mathcal{E}_{\max}=1$. At $\mathcal{E}_{\max}$, $xy=(1-z^2)/2$ and

$$\mathcal{E}^2(\theta,\phi) = z^2 \sin^2 \theta + \left(\frac{1-z^2}{2}\right)^2 (1-\cos\theta)^2 + 2z\left(\frac{1-z^2}{2}\right)\sin\theta(1-\cos\theta)\cos\phi$$

and

$$\mathcal{P}(E) = \frac{1}{4\pi}\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\ \delta(\mathcal{E}-\mathcal{E}(\theta,\phi)) = \frac{\mathcal{E}}{2\pi}\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\ \delta(\mathcal{E}^2-\mathcal{E}^2(\theta,\phi)).$$

Now we can do the ϕ integral fairly easily, and it leaves us with

$$\mathcal{P}(E) = \frac{\mathcal{E}}{2\pi}\int_0^\pi 2\left(\frac{\sin\theta\, d\theta}{2z\left(\frac{1-z^2}{2}\right)\sin\theta(1-\cos\theta)|\sin\phi_0|}\right),$$

where

$$\cos\phi_0 = \frac{\mathcal{E}^2 - z^2\sin^2\theta - \left(\frac{1-z^2}{2}\right)^2(1-\cos\theta)^2}{2z\left(\frac{1-z^2}{2}\right)\sin\theta(1-\cos\theta)}.$$

However, we need this solution for $\cos\phi_0$ to lie in $[-1,1]$. Therefore,

$$\mathcal{E} < \left| z\sin\theta + \left(\frac{1-z^2}{2}\right)(1-\cos\theta)\right| = U(\theta) \Rightarrow \mathcal{E} < \left(\frac{1-z^2}{2}\right) - \left(\frac{1+z^2}{2}\right)\cos(\theta+\theta_0) \tag{A3}$$

and

$$\mathcal{E} > \left| z\sin\theta - \left(\frac{1-z^2}{2}\right)(1-\cos\theta)\right| = L(\theta) \Rightarrow \mathcal{E} > \begin{cases} \left(\frac{1+z^2}{2}\right)\cos(\theta-\theta_0) - \left(\frac{1-z^2}{2}\right), & \theta<2\theta_0, \\ \left(\frac{1-z^2}{2}\right) - \left(\frac{1+z^2}{2}\right)\cos(\theta-\theta_0), & \theta>2\theta_0, \end{cases} \tag{A4}$$

where $\theta_0=2\tan^{-1} z$.

The integral for $\mathcal{P}(E)$ now becomes:

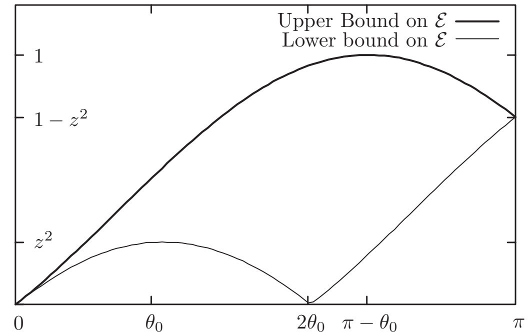

FIG. 6. The upper and lower bounds on $\mathcal{E}$ (y axis) from inequalities (A3) and (A4) are plotted above as a function of θ (x axis).

$$\frac{\mathcal{E}}{\pi}\int \frac{\sin\theta\, d\theta}{\sqrt{[\mathcal{E}^2-L^2(\theta)][U^2(\theta)-\mathcal{E}^2]}},$$

where the integration is carried out over the region where inequalities (A3) and (A4) are satisfied (see Fig. 6). The denominator of the integrand goes to zero only at the boundaries, and both $U(\theta)$ and $L(\theta)$ have nonzero slopes almost everywhere [except $L(\theta)$ at θ_0]. Therefore, if we look near such a point, θ_b, we see that

$$L^2(\theta_b+\epsilon) - \mathcal{E}^2 = [\mathcal{E} + L'(\theta_b)\epsilon + O(\epsilon^2)]^2 - \mathcal{E}^2 = 2\mathcal{E}L'(\theta_b)\epsilon + O(\epsilon^2).$$

Thus near the points where the integrand blows up the behavior is $\sim 1/\sqrt{\epsilon}$, which is convergent. A special point to check is when $\mathcal{E}=1-z^2$; then, near $\theta=\pi$, both terms in the denominator of the integral behave as $\sim 1/\sqrt{\epsilon}$, which is a $\sim 1/\epsilon$ behavior. However, the $\sin\theta$ in the numerator also goes as $\sim\epsilon$; therefore, the integral is convergent for this value as well. Therefore, we are left to consider the case when $\mathcal{E}=z^2$. In this case near θ_0, the slope of $L(\theta)$ vanishes. Therefore, for $\theta=\theta_0+\epsilon$, $\mathcal{E}^2-L^2(\theta)\sim\epsilon^2$. Thus the integrand behaves as $\sim 1/\epsilon$ and we have a logarithmic divergence at $\mathcal{E}=z^2=\cos\mu$. This is the cusp in the PDF. This will also scale as $\mathcal{E}_{\max}$ for values of $\mathcal{E}_{\max}\neq 1$. Thus $\mathcal{E}_{\text{cusp}}=\mathcal{E}_{\max}\cos\mu$ as mentioned earlier.

It may be noted that the integral for the PDF can be recast into the form

$$\mathcal{P}(E) = \begin{cases} \displaystyle\int_{t_1}^{t_2} \frac{dt}{\sqrt{R(t)}} & \text{if } \mathcal{E}>z^2, \\ \displaystyle\int_{t'_1}^{t'_2} \frac{dt}{\sqrt{R(t)}} + \int_{t'_3}^{t'_4} \frac{dt}{\sqrt{R(t)}} & \text{if } \mathcal{E}<z^2, \end{cases} \tag{A5}$$

where $R(t)$ is a polynomial of degree 4 in t, if we make the substitution $t=\cos\theta$. This is basically an incomplete elliptic integral [the limits $t_1,t_2,\ldots$ are obtained from the inequalities (A3) and (A4)].

We last prove the result that the PDFs for two complementary two-dimensional projections are identical. This follows from the fact that there is a bijective mapping from $\mathcal{H}(\Pi_2)$ to $\mathcal{H}(\Pi_2^c)$ which preserves the Haar volume [in fact, this map is an $SU(2)\times SU(2)$ transformation]. To demonstrate this we will once again choose our basis as $|\chi_1\rangle$ and $|\chi_2\rangle$ defined above. Now, $\mathcal{H}(\Pi_2^c)$ consists of all states orthogonal to $|\chi_1\rangle$ and $|\chi_2\rangle$. We now construct a basis for $\mathcal{H}(\Pi_2^c)$, as $|\chi_1'\rangle=(0,z/\sqrt{z^2+x^2},0,-x/\sqrt{z^2+x^2})$ and $|\chi_2'\rangle=(0,xy/\sqrt{z^2+x^2},-\sqrt{z^2+x^2},zy/\sqrt{z^2+x^2})$. It is easy to see that $|\chi_1'\rangle$ is separable and $\mathcal{E}_{\chi_2'}=\mathcal{E}_{\chi_2}$. Furthermore, the entanglement of a general state, $|\psi\rangle=\alpha|\chi_1'\rangle+\beta|\chi_2'\rangle$, in the subspace is given by $\mathcal{E}(\alpha,\beta)=2|-\alpha\beta z-\beta^2 xy|$. This is identical to the entanglement of $\alpha|\chi_1\rangle+\beta|\chi_2\rangle$. Since the entanglement of each state in the subspace is identical to that in $\mathcal{H}(\Pi_2)$ and the SU(2) measure is the same, we will have the same PDFs in both these cases. In fact, the $\mathrm{SU}(2)\times\mathrm{SU}(2)$ transformation that takes from $|\chi_1'\rangle$ to $|\chi_1\rangle$ and from $|\chi_2'\rangle$ to $|\chi_2\rangle$ connects these two subspaces.

[1] P. W. Shor, SIAM J. Sci. Comput. (USA) **26**, 1484 (1997); L. K. Grover, in *Proceedings of the 28th Annual Symposium on the Theory of Computing, Philadelphia, 1996*, (ACM Press, New York, 1996), pp. 212–219.

[2] C. H. Bennett and G. Brassard, in *Proceedings of IEEE International Conference on Computers, Systems and Signal Processing, Bangalore, India*, (IEEE, New York, 1984), p. 175; C. H. Bennett, F. Bessette, G. Brassard, L. Salvail, and J. Smolin, J. Cryptology **5**, 3 (1992).

[3] C. F. Roos, M. Chwalla, K. Kim, M. Riebe, and R. Blatt, Nature (London) **443**, 316 (2006).

[4] J. S. Bell, Physics (Long Island City, N.Y.) **1**, 195 (1964); J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt, Phys. Rev. Lett. **23**, 880 (1969).

[5] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **54**, 3824 (1996).

[6] For a very interesting discussion of the measures and criteria for entanglement, see Dagmar Bruß, J. Math. Phys. **43**, 4237 (2002).

[7] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).

[8] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).

[9] P. W. Shor, J. A. Smolin, and B. M. Terhal, Phys. Rev. Lett. **86**, 2681 (2001).

[10] K. G. H. Vollbrecht and R. F. Werner, Phys. Rev. A **64**, 062307 (2001).

[11] S. Hill and W. K. Wootters, Phys. Rev. Lett. **78**, 5022 (1997).

[12] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).

[13] P. Horodecki, Phys. Lett. A **232**, 333 (1997).

[14] M. A. Nielsen, Phys. Rev. Lett. **83**, 436 (1999).

[15] M. Horodecki and P. Horodecki, Phys. Rev. A **59**, 4206 (1999).

[16] A. Miranowicz and A. Grudka, J. Opt. B: Quantum Semiclassical Opt. **6**, 542 (2004).

[17] D. G. Cory, A. F. Fahmy, and T. F. Havel, Proc. Natl. Acad. Sci. U.S.A. **94**, 1634 (1997).

[18] N. Gershenfeld and I. L. Chuang, Science **275**, 350 (1997).

[19] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935); E. Schrödinger, Naturwissenschaften **23**, 807 (1935); Proc. Cambridge Philos. Soc. **31**, 555 (1935); **32**, 446 (1936).

[20] K. Dorai Arvind and A. Kumar, Phys. Rev. A **61**, 042306 (2000).

[21] C. Negrevergne, T. S. Mahesh, C. A. Ryan, M. Ditty, F. Cyr-Racine, W. Power, N. Boulant, T. Havel, D. G. Cory, and R. Laflamme, Phys. Rev. Lett. **96**, 170501 (2006).

[22] S. L. Braunstein, C. M. Caves, R. Jozsa, N. Linden, S. Popescu, and R. Schack, Phys. Rev. Lett. **83**, 1054 (1999); L. Gurvits and H. Barnum, Phys. Rev. A **68**, 042312 (2003); R. Rahimi, K. Takeda, M. Ozawa, and M. Kitagawa, e-print arXiv:quant-ph/0405175.

[23] The system behaves classically only when the measuring apparatus fails to see the quantum features in the microstates. Thus, a completely unpolarized spin-half state is to be distinguished from an ensemble of unbiased coins. In other words, classicality emerges when coherent superposition in the microstates is not detectible.

[24] See, e.g., L. D. Landau and E. M. Lifschitz, *Quantum Mechanics* (Pergamon, New York, 1958), pp. 35–36.

[25] The relevant measure is, strictly speaking, the volume element of the coset space G/H, where H is the stabilizer group of the reference state, $\mathcal{H}(\Pi_M)$. Put more simply, the volume element corresponding to the stabilizer group gets dropped. This is illustrated for a two-dimensional projection, where the SU(2) measure $\sin\theta\, d\theta\, d\phi\, d\psi \rightarrow \sin\theta\, d\theta\, d\phi$, since the stabilizer U(1) has the Haar measure $d\psi$.

[26] M. S. Byrd and E. C. G. Sudarshan, J. Phys. A **31**, 9255 (1998); M. Byrd, e-print arXiv:physics/9708015.

[27] T. E. Tilma, M. Byrd, and G. Sudarshan, J. Phys. A **35**, 10445 (2002); for a similar computation, see O. Giraud, e-print arXiv:quant-ph/0611285, who, however, does not employ the Haar measure.