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Computer Physics Communications 175 (2006) 145–166
Computer Physics Communications
www.elsevier.com/locate/cpc

Simulation of n-qubit quantum systems. II. Separability and entanglement ☆

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Received 9 December 2005; received in revised form 17 February 2006; accepted 4 March 2006

Available online 3 May 2006

Abstract

Studies on the entanglement of n-qubit quantum systems have attracted a lot of interest during recent years. Despite the central role of entanglement in quantum information theory, however, there are still a number of open problems in the theoretical characterization of entangled systems that make symbolic and numerical simulation on n-qubit quantum registers indispensable for present-day research.

To facilitate the investigation of the separability and entanglement properties of n-qubit quantum registers, here we present a revised version of the FEYNMAN program in the framework of the computer algebra system MAPLE. In addition to all previous capabilities of this MAPLE code for defining and manipulating quantum registers, the program now provides various tools which are necessary for the qualitative and quantitative analysis of entanglement in n-qubit quantum registers. A simple access, in particular, is given to several algebraic separability criteria as well as a number of entanglement measures and related quantities. As in the previous version, symbolic and numeric computations are equally supported.

Program summary

Title of program: FEYNMAN
Catalogue identifier: ADWE_v2_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADWE_v2_0
Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland
Licensing provisions: None
Computers for which the program is designed: All computers with a license of the computer algebra system MAPLE [Maple is a registered trademark of Waterloo Maple Inc.]
Operating systems under which the program has been tested: Linux, MS Windows XP
Programming language used: MAPLE 10
Typical time and memory requirements: Most commands acting on quantum registers with five or less qubits take $\leqslant 10$ seconds of processor time (on a Pentium 4 with $\geqslant 2$ GHz or equivalent) and 5–20 MB of memory. However, storage and time requirements critically depend on the number of qubits, n, in the quantum registers due to the exponential increase of the associated Hilbert space.
No. of lines in distributed program, including test data, etc.: 3107
No. of bytes in distributed program, including test data, etc.: 13 859
Distribution format: tar.gz
Reasons for new version: The first program version established the data structures and commands which are needed to build and manipulate quantum registers. Since the (evolution of) entanglement is a central aspect in quantum information processing the current version adds the capability to analyze separability and entanglement of quantum registers by implementing algebraic separability criteria and entanglement measures and related quantities.
Does this version supersede the previous version: Yes
Nature of the physical problem: Entanglement has been identified as an essential resource in virtually all aspects of quantum information theory. Therefore, the detection and quantification of entanglement is a necessary prerequisite for many applications, such as quantum computation,

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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0010-4655/$ – see front matter
doi:10.1016/j.cpc.2006.03.006

communications or quantum cryptography. Up to the present, however, the multipartite entanglement of n-qubit systems has remained largely unexplored owing to the exponential growth of complexity with the number of qubits involved.

Method of solution: Using the computer algebra system MAPLE, a set of procedures has been developed which supports the definition and manipulation of n-qubit quantum registers and quantum logic gates [T. Radtke, S. Fritzsche, Comput. Phys. Comm. 173 (2005) 91]. The provided hierarchy of commands can be used interactively in order to simulate the behavior of n-qubit quantum systems (by applying a number of unitary or non-unitary operations) and to analyze their separability and entanglement properties.

Restrictions onto the complexity of the problem: The present version of the program facilitates the setup and the manipulation of quantum registers by means of (predefined) quantum logic gates; it now also provides the tools for performing a symbolic and/or numeric analysis of the entanglement for the quantum states of such registers. Owing to the rapid increase in the computational complexity of multi-qubit systems, however, the time and memory requirements often grow rapidly, especially for symbolic computations. This increase of complexity limits the application of the program to about 6 or 7 qubits on a standard single processor (Pentium 4 with $\geqslant 2$ GHz or equivalent) machine with $\leqslant 1$ GB of memory.

Unusual features of the program: The FEYNMAN program has been designed within the framework of MAPLE for interactive (symbolic or numerical) simulations on n-qubit quantum registers with no other restriction than given by the memory and processor resources of the computer. Whenever possible, both representations of quantum registers in terms of their state vectors and/or density matrices are equally supported by the program. Apart from simulating quantum gates and quantum operations, the program now facilitates also investigations on the separability and the entanglement properties of quantum registers.

PACS: 03.67.-a; 03.67.Lx; 03.65.Ud

Keywords: Quantum register; Qubit; Entanglement; Separability

1. Introduction

Supported by the discovery of several efficient quantum algorithms in the mid-1990s, the field of quantum computation and quantum information [1] has become an active research area during recent years. For example, using modern experimental techniques, it has become possible to prepare and control quasi-isolated quantum systems which are nonclassically correlated, i.e. entangled. Today, in fact, quantum entanglement is recognized as a new physical *resource* which is important not only for quantum computation but also for quantum cryptography [2], superdense coding [3], quantum teleportation [4] and other applications.

However, despite the remarkable efforts in classifying the entanglement of multi-qubit systems, this resource is not yet understood in much detail, especially if more but a very few qubits are considered. Apart from the mathematical difficulties, this 'flaw' in dealing with multiple qubit systems is mainly due to the complexity which arises from the exponential increase of the dimension of the associated Hilbert spaces and which has hampered many systematic investigations in the past. Because of the fragile nature of quantum entanglement, moreover, experimental studies are still difficult to be carried out and, thus, require to perform symbolic and/or numerical simulations of the time evolution and the properties of multi-qubit systems.

To facilitate the simulation of general n-qubit quantum systems, we recently introduced the FEYNMAN program within the framework of MAPLE. In a first version of this program [5], this concerned especially the set-up and the manipulation of n-qubit quantum registers as well as of those operators which are defined in the associated Hilbert spaces. In the present work, we now extend the FEYNMAN program in order to facilitate also the study of separability and entanglement properties in quantum registers. In particular, a number of criteria have been implemented in order to test and *measure* the entanglement status of quantum registers, including the partitioning into bi- and multipartite systems. Using these measures, it becomes possible for instance to analyze the properties of quantum registers in the course of an evolution. We therefore hope that the present extension of FEYNMAN will make the program attractive for further applications in the theory of quantum computations and information.

In the next section, we begin with a brief review of the most important concepts and results from the theory of quantum entanglement. Beside of the definition of separability and the entanglement of pure and mixed states, this includes a short account of the distillation of entanglement as well as a number of criteria for separability. Having this 'background' at hand, Section 3 later describes the *new* commands of the FEYNMAN program, including a few additional modifications of the code which are neither connected to separability nor the entanglement of quantum states but which were found convenient to add into the program. Moreover, there are four examples in Section 4 for illustrating some of new features of the FEYNMAN program. Finally, a brief summary and outlook on future developments of the program are given in Section 5.

2. Theoretical background

To understand the capabilities (and limitations) of the present extension to the FEYNMAN program, let us start from the definition of separability and entanglement and by explaining some basic material on these topics. For the sake of brevity, here we shall restrict ourselves to a rather short account on the theory. As appropriate for later use of the program, however, we shall refer below already to the two main procedures, Feynman_is_separable() and Feynman_measures(), which are discussed later in Section 3.

2.1. Definition: separability vs. entanglement

2.1.1. Pure state separability

Of course, the simplest possible case of quantum entanglement may occur for a bipartite *pure* state $|\psi_{AB}\rangle$ of a composite system AB, to which a product Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ is associated. In general, such a bipartite state is called *separable* if there exist the quantum states $|\psi_A\rangle \in \mathcal{H}_A$ of part A and $|\psi_B\rangle \in \mathcal{H}_B$ (of B) such that $|\psi_{AB}\rangle$ can be written in the form

$$|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle, \tag{1}$$

i.e. in terms of a product representation. Otherwise, the state $|\psi_{AB}\rangle$ is said to be *entangled* and to possess hereby a (nonlocal) property that implies that the outcomes of a measurement on the two—possibly spatially separated—subsystems A and B are no longer independent of each other. This characteristic feature of quantum mechanics has been first discussed by Einstein, Podolsky and Rosen (EPR) [6] in their famous debate with Bohr as well as by Schrödinger [7] about seventy years ago. Perhaps, the best known examples of entangled states are the so-called EPR (or Bell) states. Given the state $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, for instance, the outcome of a local measurement on any subsystem, either A or B, is completely random (either "0" or "1")—if measured first. In dependence of this (prior) result, however, the outcome of a corresponding measurement on the remaining subsystem is fixed *instantaneously*, independent from any separation of the two subsystems in space and time.

As seen from Eq. (1), the definition of entanglement of a bipartite state does not provide any constructive criterion in order to decide whether a given state has a product representation or not. For this decision, in fact, the *Schmidt decomposition* [1] has been found to be a very useful tool, which says that any bipartite pure state with dimensions d_A and d_B of the corresponding subsystems can be written in the form

$$|\psi_{AB}\rangle = \sum_{i=1}^{r} \sqrt{\lambda_i}|a_i\rangle|b_i\rangle, \quad r \leqslant \min(d_A, d_B), \tag{2}$$

where $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$ are orthonormal bases in the subspaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and where $\sqrt{\lambda_i}$ denote the positive Schmidt coefficients with $\sum_{i=1}^{r} \lambda_i = 1$. It can be shown that the Schmidt coefficients $\sqrt{\lambda_i}$ correspond to the square roots of the eigenvalues of any of the reduced density matrices $\rho_A = \mathrm{Tr}_B(\rho_{AB}) = \sum_i \lambda_i |a_i\rangle\langle a_i|$ or $\rho_B = \mathrm{Tr}_A(\rho_{AB}) = \sum_i \lambda_i |b_i\rangle\langle b_i|$ [1]. Moreover, the Schmidt rank (or Schmidt number), r, is given by the number of nonzero eigenvalues of ρ_A or ρ_B. From the definition in Eq. (2), therefore, it becomes clear that the product states (i.e. the separable states) are those with exactly *one* Schmidt coefficient or, equivalently, with Schmidt rank $r = 1$. In other words, both subsystems with the (reduced) density matrices ρ_A or ρ_B have to be in a pure state by themselves. In practice, therefore, the Schmidt decomposition often serves as a necessary and sufficient separability criterion for pure *bipartite* states. In the FEYNMAN program, this decomposition has been implemented in the (new) procedure Feynman_decompose() and can be carried out easily as shown by one of our examples in Section 4.1.

Apart from bipartite systems (AB), the definition of separability in Eq. (1) can be extended quite naturally also to multipartite pure states $|\psi_{ABC\ldots Z}\rangle$. Unfortunately, however, here the concept of the Schmidt decomposition cannot be generalized in a straightforward way to the case of N different subsystems. Up to the present, therefore, we do not know an equally convenient criterion for the multipartite separability.

2.1.2. Mixed state separability

For statistical mixtures of quantum states, i.e. for states of the form $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, the question about their *separability* is much more involved when compared with the case of pure quantum states. This is because one has to discriminate then between classical (local) and quantum (nonlocal) correlations for a given state of the system. As a first consequence of this distinction between local and nonlocal correlations, the terms *product state* and *separable state* are no longer synonymous. While any product state can still be expressed by means of a Kronecker product of the corresponding states of its subsystems,

$$\rho_{AB} = \rho_A \otimes \rho_B, \tag{3}$$

a *separable state* can be represented in general only as a convex combination (mixture) of such product states [8],

$$\rho_{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B = \sum_i p_i |\psi_i\rangle_A\langle\psi_i| \otimes |\phi_i\rangle_B\langle\phi_i| \tag{4}$$

with the classical probabilities $p_i \geqslant 0$ and $\sum_i p_i = 1$. But although the state ρ_{AB} in Eq. (4) cannot be written as a simple product state, all correlations between the subsystems arise from our incomplete knowledge about the state (since it is a *mixture* of states) and, hence, are classical.

Entangled states, in contrast, cannot be prepared by applying only *local* quantum operations and classical communications (LOCC). To create entanglement in a composite system, the (physical) subsystems must be brought together to interact with each other, a process which requires for its description nonlocal operators of the form $U_{AB} \neq U_A \otimes U_B$, with U_A, U_B being unitary operators acting on $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. In general, therefore, mixed state entanglement is defined—again, in a nonconstructive way—through the fact that a decomposition of the form (4) does simply not exist for these mixtures.

The 'definition of the separability' of a quantum system as given in Eq. (4) can be generalized in quite obvious way from the bipartite to the multipartite case. To this end, let us consider a system of N parties with dimensions d_i (in our context usually qubits, i.e. $d_i = 2$). Then, given a density operator $\rho_{1\ldots N}$ which acts on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$, we call $\rho_{1\ldots N}$ *fully separable* (or N-separable) if and only if

$$\rho_{1\ldots N} = \sum_i p_i |\psi_i\rangle_1\langle\psi_i| \otimes \cdots \otimes |\psi_i\rangle_N\langle\psi_i|. \tag{5}$$

Moreover, the state $\rho_{1\ldots N}$ is called k-separable (with $k \leqslant N$) iff it is separable with respect to every possible k-partite split. For example, we may consider the 2-separable (also known as biseparable or semiseparable) three-qubit state $\tilde{\rho}_{ABC} = \frac{1}{4}(I_8 - \sum_{i=1}^{4} |\psi_i\rangle\langle\psi_i|)$ where the $|\psi_i\rangle$ are given as $|0, 1, +\rangle$, $|1, +, 0\rangle$, $|+, 0, 1\rangle$, and $|-, -, -\rangle$ with $|\pm\rangle = 1/\sqrt{2}(|0\rangle \pm |1\rangle)$ [9]. For this mixed 3-partite state, it can be shown that it is separable with respect to any of the bipartite cuts $A|BC$, $B|CA$ and $C|AB$. Still, it is *not* a mixture of (pure) product states $|\psi_A\rangle|\psi_B\rangle|\psi_C\rangle$, i.e. it is not fully separable. Hence, the state $\tilde{\rho}_{ABC}$ exhibits genuine tripartite entanglement which involves all three qubits (simultaneously). In the FEYNMAN program, this strange behavior of not being fully separable can be easily verified by means of the command Feynman_is_separable() as we will demonstrate below in Section 4.2.

2.1.3. Entanglement distillation and bound entanglement

In addition to the distinction between pure state entanglement and mixed state entanglement discussed above, there is an interesting classification of mixed state entanglement, namely *free* and *bound* entanglement. This distinction is made because (the entanglement of) mixed states can in some cases be converted into maximally entangled *pure* states by using only local (quantum) operations and classical communication, i.e. for the case of free entanglement, while it cannot be brought in such form for bound entangled mixtures.

The distinction between free and bound entanglement often arises from the request that, for many applications in quantum teleportation and elsewhere, a quantum mixture must first be converted into a maximally entangled *pure* state (e.g., into one of the Bell states) in order to benefit from the entanglement of the given state. This 'conversion process' is called entanglement *purification* or *distillation* [10–12]. Using some suitable distillation protocol and by starting from m copies of a partially entangled state, one can produce $n < m$ copies of maximally entangled pure states. Of course, the less entangled the initial states is, the smaller will be the yield n/m. This is consistent with the well-known fact that LOCC cannot produce entanglement (since it is essentially a nonlocal resource). In the limit of having infinitely many input copies available, consequently, the yield of the distillation process gives rise also to a *measure* of entanglement (the so-called distillable entanglement $E_D(\rho)$, cf. Section 2.3). Note, however, that—in contrast to the case of pure states—not all partially entangled mixed states can be distilled into maximally entangled pure states [13]. Therefore, in other words, one distinguishes between the *free entanglement* of mixed states, which can be distilled, and the *bound entanglement* which cannot.

2.2. Separability criteria

Having recalled the basic definitions of separability and entanglement, we are now prepared to discuss briefly some popular criteria in order to 'decide' whether a given quantum state is entangled or not. For a recent review of the entanglement vs. separability problem, we refer the reader to Ref. [14].

As mentioned before, entanglement is often described as a *nonlocal* phenomenon in the sense that, for an entangled state, the measurement on one subsystem *instantaneously* affects the outcome of a measurement of the other (possibly very distant) subsystem. It is therefore tempting to apply Bell inequalities in order to test for nonclassical correlations in quantum states. Unfortunately, it turns out that not all entangled states necessarily violate Bell-type inequalities [15,16] so that some stronger criteria had to be developed. In the following, we shall begin the discussion with recalling a rigorous but computationally infeasible (i.e. nonoperational) approach in order to provide the background for the discussion of several feasible (operational) criteria which are usually weaker in the sense that they cannot detect all entangled states.

2.2.1. The positive maps approach

The approach of using positive maps for a decision about the separability of a quantum state is general and considers so-called superoperators, i.e. the transformation of operators $\rho \in \mathcal{B}(\mathcal{H})$ that act on some state space $\mathcal{H}$. In this approach, a linear, self-adjoint and positive map $\Lambda : \mathcal{B}(\mathcal{H}_B) \to \mathcal{B}(\mathcal{H}_C)$ is defined as a map that takes positive and hermitian operators into positive hermitian operators:

$$\rho \geqslant 0 \quad \Rightarrow \quad \Lambda(\rho) \geqslant 0,\ \Lambda(\rho) = \Lambda^{\dagger}(\rho). \tag{6}$$

Moreover, such a positive map is called *completely positive* (CP) if any extension of $\mathcal{H}$ to a larger Hilbert space with arbitrary dimension is again a positive map:

$$\sigma \geqslant 0 \quad \Rightarrow \quad (\mathcal{I}_A \otimes \Lambda_B)(\sigma) \geqslant 0 \tag{7}$$

with $\mathcal{I}_A$ denoting the identity operation on the extension $\mathcal{H}_A$. A well-known example for a (completely) positive map is the standard Hamiltonian time evolution of a quantum system while the transposition operation on some density operator (i.e. the usual matrix transposition operation in some basis) is an example of a positive (but not CP) map.

The connection between positive maps and the separability problem was given in Refs. [17,18] where it was shown that a quantum state ρ is separable if and only if for *all* positive maps $\Lambda : \mathcal{B}(\mathcal{H}_B) \to \mathcal{B}(\mathcal{H}_C)$ we have

$$(\mathcal{I}_A \otimes \Lambda_B)(\rho) \geqslant 0. \tag{8}$$

As seen from Eq. (8), only those maps are of interest for finding a separability criterion which are positive but not CP, since a CP map fulfills Eq. (8) by definition for any positive operator ρ. In practice, therefore, the approach of positive maps is often of little help for determining an operational criterion for the separability of a quantum state. This lack arises from the fact that a complete characterization (of the set) of all positive maps is unfeasible. In some particular cases, however, the concept of positive maps yield operational separability criteria which we shall discuss below.

2.2.2. *Operational, algebraic separability criteria*

Regardless of its theoretical elegance and validity, the approach of using positive maps (or the closely related concept of entanglement witnesses) is often not very useful if we have to decide whether a particular state is entangled or not. Despite the rather simple definition of separability in Eq. (4), there is on the other hand no efficiently computable, necessary and sufficient separability criterion available up to the present. In this section, therefore, we shall summarize some computationally manageable and *algebraic* criteria for the separability of quantum states, which have been implemented into the program and which can be accessed via the appropriate keywords in the Feynman_is_separable() command. For other computational approaches we may refer the reader to Ref. [19] and references therein.

Although the following criteria for the separability of quantum states can be implemented algebraically, they come at the price to represent necessary but *not sufficient* criteria.

(i) *Schmidt decomposition*

As discussed in Section 2.1.1, the separability of bipartite pure states is well understood. Using the Schmidt decomposition (2), one can determine uniquely if a given quantum state is separable by testing whether the Schmidt rank is $r = 1$ or, equivalently, whether there exists exactly one nonvanishing Schmidt coefficient. From a practical viewpoint, this corresponds to the test if both subsystems are in a pure state for the overall state to be separable, i.e. if $\mathrm{Tr}(\rho_A^2) = \mathrm{Tr}(\rho_B^2) = 1$.

(ii) *Peres–Horodecki criterion*

One of the first feasible separability criterion, which could be utilized also for mixed states, has been given in Ref. [20]. This criterion uses a particular choice of a positive map, the partial transposition operation where the usual matrix transposition operation $T(\rho) = \rho^T$ is applied to only one subsystem of a composite state. As an example, here we might consider the general bipartite density matrix $\rho = \sum_{ikjl} |i\rangle_A \langle j| \otimes |k\rangle_B \langle l| = \sum_{ikjl} \rho_{ikjl} |ik\rangle\langle jl|$. Then, the partial transpose with respect to the first subsystem, A, is given by

$$T_A(\rho) \equiv \rho^{T_A} = \sum_{ikjl} \rho_{ikjl} |jk\rangle\langle il|. \tag{9}$$

For this choice of matrix operation, it can be shown that, although the original density matrix ρ is positive (i.e. has only nonnegative eigenvalues), the matrix ρ^{T_A} is not necessarily positive and, hence, not a valid density matrix for all cases. The latter is true, in particular, for many entangled states. For any *separable* state ρ_{sep}, on the other hand, the partial transposition with respect to one (or several) of the subsystems $A, B, \ldots, Z$ must be always a positive operator again,

$$\rho_{\mathrm{sep}}^{T_{\mathcal{X}}} \geqslant 0 \quad \text{for } \mathcal{X} \subset \{A, B, \ldots, Z\}. \tag{10}$$

This different behavior of entangled and separable states under the partial transpose map is known as the positive partial transposition (PPT) or the Peres–Horodecki criterion. Although, in general, this is only a necessary criterion for separability, it was shown to be sufficient for any bipartite systems with subspace dimensions 2×2 and 2×3, for which the separable states are characterized completely by means of the PPT criterion [21].

Owing to the construction of the PPT map, the Peres–Horodecki criterion allows to detect only those entangled states which have a negative partial transpose (NPT). Although these states certainly refer to a large class of entangled states, there are however, as pointed out in Ref. [22], entangled states that nevertheless satisfy the PPT criterion which demonstrates that this criterion is in general only necessary but not sufficient.

(iii) *Majorization criterion*

In our discussion of the Schmidt decomposition, we saw already that the reduced density operators of a *pure* entangled state might refer to a *mixed* state of the corresponding subsystem. This somehow surprising result is an example of the more general feature of quantum entanglement that the individual subsystems of an entangled state may exhibit more disorder or ‘mixedness’ (in

the sense of the von Neumann entropy, cf. Section 2.3.2) than the composite systems. Using this fact, it was shown in Ref. [23] that for any *separable* $m \times n$ state ρ_{AB} of a bipartite system, we have

$$\lambda^{\downarrow}_{\rho_{AB}} \prec \lambda^{\downarrow}_{\rho_A} \quad \text{and} \quad \lambda^{\downarrow}_{\rho_{AB}} \prec \lambda^{\downarrow}_{\rho_B}, \tag{11}$$

where $\lambda^{\downarrow}_{\rho_{AB}}$ is the vector of the eigenvalues of ρ_{AB} in decreasing order (i.e. with $\lambda^{\downarrow}_1 \geqslant \lambda^{\downarrow}_2 \geqslant \cdots \geqslant \lambda^{\downarrow}_n$), and with a similar definition of $\lambda^{\downarrow}_{\rho_A}$ and $\lambda^{\downarrow}_{\rho_B}$, respectively. For these two relations in (11), extra zeros have to be appended to the vectors, if necessary, in order to equalize their dimensions. The relation $x \prec y$ ("x is majorized by y") means that $\sum_{i=1}^{k} x_i^{\downarrow} \leqslant \sum_{i=1}^{k} y_i^{\downarrow}$ holds for $1 \leqslant k \leqslant n-1$ and the equality holds for $k = n$. The majorization criterion provides a simple separability criterion which is based only on the spectral properties of the global density operator and the reduced density operators. As stated in [24], moreover, the majorization criterion provides a sufficient condition for the distillability of bipartite states in the sense that all states which violate the majorization criterion are also distillable.

(iv) *Reduction criterion*

According to this criterion [25,26], the two inequalities

$$I_m \otimes \rho_B - \rho_{AB} \geqslant 0 \quad \text{and} \quad \rho_A \otimes I_n - \rho_{AB} \geqslant 0 \tag{12}$$

must hold simultaneously for any separable $m \times n$ state ρ_{AB} of a bipartite system, where $\rho_{A,B}$ denote the reduced density matrices of subsystems A and B, and I_m (I_n) is the m- (n-)dimensional identity matrix. Similar to the PPT criterion, the reduction criterion represents another particular choice of a positive (but not completely positive) map. It is equivalent to the PPT criterion for $2 \times n$ (and, hence, a sufficient criterion for 2×2 and 2×3 quantum states), in general however weaker than PPT in the sense that those states which violate the reduction criterion also violate the PPT criterion (but not vice versa). Furthermore, the reduction criterion implies the majorization criterion [24] and all states that violate the reduction criterion are distillable. For generalized versions of the reduction criterion see, for instance, Refs. [27,28].

(v) *Realignment criterion*

The separability criteria (i)–(iv) discussed so far are typically not sensitive to bound entanglement or they do not generalize straightforwardly to multipartite systems. In an alternative approach, which addresses these two drawbacks explicitly, a particular permutation of the matrix elements of the density operator is therefore considered [29]. For an $m \times n$ bipartite state $\rho = \sum_{ik,jl} \rho_{ik,jl} |ik\rangle\langle jl|$, for instance, this (so-called) realignment operation $\mathcal{R}$ is defined by

$$\mathcal{R}(\rho) = \sum_{ik,jl} \rho_{ik,jl} |ij\rangle\langle kl|, \tag{13}$$

where $|i\rangle$, $|j\rangle$ are the standard m-dimensional real(!) basis vectors of the first subspace, and $|k\rangle$, $|l\rangle$ are n-dimensional real basis vectors of the second subspace, respectively. Note that, similar to the partial transpose operation, the matrix obtained is generally not a valid density matrix and usually not even a square one.

Using the positive map $\mathcal{R}$ in Eq. (13), the realignment criterion is defined similarly to the PPT criterion for any separable bipartite system

$$\big\| \mathcal{R}(\rho_{\text{sep}}) \big\|_{\text{Tr}} \leqslant 1. \tag{14}$$

Here, the trace norm $\| \cdot \|_{\text{Tr}}$ is defined here as $\|A\|_{\text{Tr}} = \text{Tr}\sqrt{A^{\dagger}A}$. In order to generalize this criterion also for multipartite systems, the realignment criterion on the separability of quantum states uses the fact, that any (fully) separable n-partite state ρ with the dimensions $d_1 \times d_2 \times \cdots \times d_n$ of the individual subsystems will satisfy the inequalities

$$\big\| (\mathcal{R}_{(k)} \otimes I_{(n-k)})\rho \big\|_{\text{Tr}} \leqslant 1, \quad k = 2, 3, \ldots, n, \tag{15}$$

where $\mathcal{R}_{(k)}$ means that for each possible selection of $2 \leqslant k \leqslant n$ subsystems, the realignment operation, Eq. (13), is applied to every possible bipartite split within that particular subset of k subsystems. For each selection of k subsystems, the other $n-k$ subsystems are then left unchanged. For example, given a tripartite state ρ_{ABC}, we have to check the condition equation (14) for the bipartite cuts $A|B$, $A|C$, $B|C$ (representing all subsets with $k = 2$) and $A|BC$, $B|CA$, $C|AB$ (for $k = 3$).

The realignment criterion has been found powerful enough to detect many of the bound entangled states, which are known in the literature. An example, that was mentioned at the end of Section 2.1.2, is the biseparable three-qubit state $\tilde{\rho}_{ABC}$. In Ref. [30], in addition, it was shown that the realignment criterion is equivalent also to the (so-called) *computable cross norm criterion* (CCN).

(vi) *Generalized partial transposition criterion (GPT)*

Owing to the ability of the realignment criterion to detect bound and multipartite entanglement, there was a natural interest in generalizing this approach. A first step in this direction is given by the generalized partial transposition criterion (GPT) [31], which now unifies the PPT and the realignment criterion.

To formulate the GPT criterion, one needs the so-called generalized partial transposition operations which have been defined in Ref. [31]. These operations are based on the fact that any n-partite density matrix can be written as

$$\rho = \sum_{ij,kl,\ldots} \rho_{ij,kl,\ldots} |i\rangle\langle j| \otimes |k\rangle\langle l| \otimes \cdots \tag{16}$$

$$= \sum_{ij,kl,\ldots} \rho_{ij,kl,\ldots} \langle j| \otimes |i\rangle \otimes \langle l| \otimes |k\rangle \otimes \cdots . \tag{17}$$

Using the real(!) standard basis for the subspace of every subsystem, then, the row transposition operation is defined by $\mathcal{T}_r : \langle j| \otimes |i\rangle \to \langle j| \otimes \langle i|$, while the column transposition operation is given by $\mathcal{T}_c : \langle j| \otimes |i\rangle \to |j\rangle \otimes |i\rangle$. With these definitions, the GPT criterion says that any *separable* n-partite state ρ with the dimensions $d_1 \times d_2 \times \cdots \times d_n$ of the individual subsystems satisfies

$$\|\rho^{\mathcal{T}_\mathcal{Y}}\|_{\mathrm{Tr}} \leqslant 1 \quad \text{for } \mathcal{Y} \subset \{r_A, c_A, r_B, c_B, \ldots, r_Z, c_Z\}, \tag{18}$$

where $\mathcal{T}_\mathcal{Y}$ means that, for every subsystem $A, B, C, \ldots, Z$, one can leave it unchanged, apply a row transposition or a column transposition or both. In other words, $\mathcal{Y}$ represents some subset of the row and column transposition operations $\{r_A, c_A, r_B, c_B, \ldots, r_Z, c_Z\}$, where, for each of these subsets, the operation $\mathcal{T}_{\{r_k, c_k, \ldots\}}$ is defined as the successive operation $\mathcal{T}_{r_k}\mathcal{T}_{c_k}\ldots$ which acts on one or several of the subsystems, while the remaining subsystems are left untouched. The notation $\mathcal{Y} = \{r_A, c_A\}$, for example, leads to $\mathcal{T}_{r_A}\mathcal{T}_{c_A}$ which is equivalent to the partial transposition operation $T_A : \langle j| \otimes |i\rangle \to |j\rangle \otimes \langle i|$, acting on the subsystem A. Similarly, the realignment operation $\mathcal{R}$ is found equivalent to the subset $\mathcal{Y} = \{c_A, r_B\}$. In this way, the GPT criterion includes both, the realignment criterion and the PPT criterion. For a more detailed discussion on various permutation separability criteria and their dependencies see Ref. [32] and references therein.

Like all the previously discussed separability criteria, in the FEYNMAN program, the GPT criterion can be used to test the separability of any n-qubit qregister() structure by means of the Feynman_is_separable() command. It should be noted, however, that the rapid increase in the number of transposition operations, which have to be performed internally, makes the evaluation of the GPT criterion quite expensive, especially when working with symbolic expressions. Since the realignment criterion is closely related to the GPT criterion, a similar restriction applies also for the realignment criterion.

2.3. Entanglement measures

For many problems in quantum information theory, it is not only necessary to know, whether a state of a quantum system is separable or not, but also how much entanglement is involved and how this entanglement develops in time. Although, the question about the 'amount' of entanglement is often a very essential one, progress in its quantification—especially for mixed states—has been made so far primarily in the domain of bipartite systems. Of course, the main difference in dealing with bi- and multipartite systems arises from the fact that multipartite states may exhibit rather different entanglement properties for different possible splits of the composite systems into parts. In practice, therefore, it is considerably more difficult to define (and even more so to compute!) a meaningful measure of entanglement for multipartite settings. For an introduction to entanglement measures, we refer the reader to the work of Horodecki [33] and references therein.

The first approaches for quantifying entanglement were motivated by physical arguments in the sense that one was looking for those measures which helped to understand, how well a certain operation can be performed on the state of a bipartite system when compared with the maximally entangled Bell states $|\Phi^+\rangle$. Nowadays, instead, these measures are often built on rather formal requirements. Therefore, before we shall discuss the most frequently applied measures of entanglement, let us start with a short summary about the axiomatic requirements which any meaningful entanglement measure has to fulfill. For a more detailed account on different formulations and modifications of these desirable requirements see, for instance, Refs. [36,37].

2.3.1. Formal requirements for entanglement measures

To represent a meaningful entanglement measure, a nonnegative and real-valued functional $E(\rho)$ should satisfy, in addition to these two obvious requests, the following conditions:

C1 If ρ is separable, then $E(\rho) = 0$.

C2 (Normalization) For any maximally entangled (two-qubit) state $|\Phi^+\rangle = \sum_{i=1}^{d} \frac{1}{\sqrt{d}} |ii\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, the entanglement is given by

$$E\big(|\Phi^+\rangle\big) = \log_2 d, \quad d = 2, 3, \ldots . \tag{19}$$

For the common case of two qubits ($d = 2$), this simplifies to $E(|\Phi^+\rangle) = 1$.

C3 (Monotonicity) Since the entanglement in some state ρ always refers to genuine quantum correlations the amount of entanglement cannot be increased further under some protocol Λ which applies only local operations and classical communication

(LOCC):

$$E\big(\Lambda_{\mathrm{LOCC}}(\rho)\big) \leqslant E(\rho). \tag{20}$$

C4 (Continuity) A small perturbation of ρ should lead to only a slight change of $E(\rho)$, i.e. in the limit of vanishing distance between two states ρ and σ, the difference between their entanglement should also vanish,

$$\|\rho - \sigma\| \to 0 \quad \Rightarrow \quad E(\rho) - E(\sigma) \to 0. \tag{21}$$

C5 (Additivity) A number $n \geqslant 1$ of identical copies of a given state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ should contain n times the entanglement of a single copy,

$$E(\rho^{\otimes n}) = nE(\rho). \tag{22}$$

C6 (Subadditivity) The entanglement of the tensor product $\rho \otimes \sigma$ of two states should not exceed the sum of the individual entanglement measures,

$$E(\rho \otimes \sigma) \leqslant E(\rho) + E(\sigma). \tag{23}$$

C7 (Convexity) The entanglement measure should be a convex function, i.e. the mixing of states does not increase the entanglement,

$$E\big(\lambda\rho + (1-\lambda)\sigma\big) \leqslant \lambda E(\rho) + (1-\lambda)E(\sigma) \tag{24}$$

for all $0 \leqslant \lambda \leqslant 1$. Note, however, that convexity is merely a mathematical requirement for entanglement monotones rather than being connected to a physical process which leads to the loss of information about a quantum system [61].

Finally, it should be noted that it is not yet clear if all of the conditions mentioned above are indeed necessary. Moreover, a measure typically fails to fulfill all of these desirable requirements [38].

2.3.2. Physically motivated entanglement measures

In this section, let us start with recalling some of the entanglement measures which are *outstanding* owing to their physical meaning and their importance for the theory of entanglement. Unfortunately, most of these 'physically motivated measures' are not supported in the FEYNMAN program because they appear computationally rather unfeasible. However, since many of the measures implemented below are indeed related to these physically motivated entities, a short review of the latter ones seems to be appropriate.

Entropy of entanglement (reduced von Neumann entropy). From the early days of quantum mechanics it has been known that, for an entangled pure state, the states of the subsystems (as given by the reduced density matrices) are mixed. For a bipartite *pure* state the amount of 'mixedness' in either of the subsystems is therefore a natural measure of entanglement [11,39]. This mixedness can be quantified in terms of the von Neumann entropy S [40] of the reduced density matrices and is known in the literature as the entropy of entanglement:

$$E_E\big(|\psi\rangle\big) = S(\rho_A) = S(\rho_B), \qquad \rho_A = \mathrm{Tr}_B\big(|\psi\rangle\langle\psi|\big), \qquad \rho_B = \mathrm{Tr}_A\big(|\psi\rangle\langle\psi|\big). \tag{25}$$

For a general state ρ, moreover, the von Neumann entropy is defined as

$$S(\rho) = -\,\mathrm{Tr}(\rho \log_2 \rho) = -\sum_i \lambda_i \log_2 \lambda_i, \tag{26}$$

where λ_i are the eigenvalues of ρ. For mixed states, unfortunately, the entropy of entanglement fails to distinguish between classical and quantum mechanical correlations so that there is no unique generalization known for this measure in the case of mixed states. Interestingly, however, the *uniqueness theorem* [37] states that, for pure bipartite states, all entanglement measures should coincide with the entropy of entanglement.

Distillable entanglement. The distillable entanglement $E_D(\rho)$ refers to the possibility of transforming an entangled state of a bipartite system into a maximally entangled pure state by means of LOCC [10,12,41], as mentioned before in Section 2.1.3. This measure quantifies how many maximally entangled states of the type $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ can be extracted ("distilled") from a partially entangled input state ρ. More precisely, it gives the ratio of the number $n^{\mathrm{out}}_{|\Phi^+\rangle}$ of maximally entangled output states $|\Phi^+\rangle$ over the number n^{in}_{ρ} of input states, maximized over all distillation protocols Λ_{LOCC}. For large number n^{in}_{ρ} (of copies) of the input state, this leads to [38]

$$E_D(\rho) = \sup_{\{\Lambda_{\mathrm{LOCC}}\}} \lim_{n^{\mathrm{in}}_{\rho} \to \infty} \frac{n^{\mathrm{out}}_{|\Phi^+\rangle}}{n^{\mathrm{in}}_{\rho}}. \tag{27}$$

Entanglement cost. Complementary to the distillable entanglement, the entanglement cost $E_C(\rho)$ quantifies the amount of pure state entanglement that is needed in order to create an entangled state ρ by using LOCC (which is sometimes also called entanglement "dilution") [12,42]. The entanglement cost is defined as the ratio between the number $n^{\text{in}}_{|\Phi^+\rangle}$ of maximally entangled input states and the number n^{out}_{ρ} of created output states, if minimized over all dilution protocols and if a large number of input states is considered

$$E_C(\rho) = \inf_{\{\Lambda_{\text{LOCC}}\}} \lim_{n^{\text{in}}_{\rho}\to\infty} \frac{n^{\text{in}}_{|\Phi^+\rangle}}{n^{\text{out}}_{\rho}}. \tag{28}$$

Entanglement of formation (EOF). It is known that any mixed state quantum state ρ has infinitely many ensemble realizations [43]. In other words, any state ρ can be decomposed as a convex combination of projectors on pure states (e.g., the eigenstates), $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ with $p_i \geqslant 0$ and $\sum_i p_i = 1$. As discussed above, for each pure (bipartite) state $|\psi_i\rangle$ in the ensemble, the entropy of entanglement provides a good measure of entanglement. The so-called entanglement of formation is therefore defined as the average of the entropy of entanglement (reduced von Neumann entropy), minimized over all possible ensemble decompositions [12],

$$E_F(\rho) = \inf_{\rho=\sum_i p_i |\psi_i\rangle\langle\psi_i|} \sum_i p_i E_E\big(|\psi_i\rangle\big). \tag{29}$$

The ensemble that realizes the infimum is called *optimal*.

This way of generalizing an entanglement measure originally defined for pure states is called *convex roof extension*. By construction, it preserves monotonicity and convexity of the pure state measure. The entanglement of formation E_F is conjectured to be equal to the entanglement cost E_C. In Ref. [42], it was proved that at least the regularized version of the entanglement of formation is equal to the entanglement cost: $E_F^{\infty} = \lim_{n\to\infty}(E_F(\rho^{\otimes n})/n) = E_C(\rho)$.

Relative entropy of entanglement (REE). The relative entropy of entanglement (REE) $E_R(\rho)$ is given as the (quasi-)distance of an entangled state ρ from its closest disentangled (i.e. separable) state $\sigma \in \mathcal{D}$ where $\mathcal{D}$ denotes the set of disentangled states [34,35]. In some more detail, the relative entropy of entanglement is defined as

$$E_R(\rho) = \inf_{\sigma\in\mathcal{D}} S(\rho\|\sigma) = \inf_{\sigma\in\mathcal{D}} \operatorname{Tr}(\rho\log_2\rho - \rho\log_2\sigma), \tag{30}$$

where $S(\rho\|\sigma)$ is the quantum relative entropy [44,45]. It can be roughly interpreted as the 'unlikelihood' for a separable state to yield results in some measurement which are consistent with the results for the given (entangled) state. It should be noted, though, that the quantum relative entropy $S(\rho\|\sigma)$ does not satisfy all properties of a metric. Additionally, although the quantum relative entropy is by far the most used of the distance based measures, other distance functions have been investigated as well [46–48]. Well-known examples of such 'distance measures' for distinguishing between quantum states are the Hilbert–Schmidt distance

$$D_{\text{HS}}(\rho,\sigma) = \|\rho-\sigma\|_{\text{HS}} = \sqrt{\operatorname{Tr}\big[(\rho-\sigma)^{\dagger}(\rho-\sigma)\big]}, \tag{31}$$

the trace distance

$$D_{\text{Tr}}(\rho,\sigma) = \frac{1}{2}\|\rho-\sigma\|_{\text{Tr}} = \frac{1}{2}\operatorname{Tr}\sqrt{(\rho-\sigma)^{\dagger}(\rho-\sigma)}, \tag{32}$$

or the Bures distance, which is related to the fidelity $F(\rho,\sigma)$ of two states,

$$D_{\text{B}}(\rho,\sigma) = \sqrt{2-2\operatorname{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}} = \sqrt{2-2\sqrt{F(\rho,\sigma)}}. \tag{33}$$

In order to support similar investigations, these measures for the distance of two quantum states have been implemented also into the command Feynman_measures(), where they can be called via some appropriate keyword.

2.3.3. Relations between different entanglement measures

Although different measures typically reflect different aspects of entanglement, there exist some relations between these measures which are worth to explain. For example, since we cannot distill more entanglement from any state ρ than the amount which was needed to create it we would expect always

$$E_D(\rho) \leqslant E_C(\rho). \tag{34}$$

For pure states, indeed, it was shown in Ref. [11] that in the asymptotic limit of infinitely many copies, state transformations such as entanglement distillation or entanglement dilution become *reversible* and, hence, that the entanglement cost E_C and the distillable entanglement E_D then coincide with the entropy of entanglement

$$E_D\big(|\psi\rangle\big) = E_C\big(|\psi\rangle\big) = E_E\big(|\psi\rangle\big). \tag{35}$$

For two pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ which have the same entropy of entanglement $E_E(|\psi_1\rangle) = E_E(|\psi_2\rangle)$, this means that they can be interconverted with an efficiency approaching unity in the limit of infinitely many copies. For nonequal values of the entropy of entanglement, in addition, the conversion rate is given by $E_E(|\psi_1\rangle)/E_E(|\psi_2\rangle)$.

The special case of Eq. (35) for pure states is part of a more general theorem about the *uniqueness of entanglement measures* [37,39] which says that the distillable entanglement and the entanglement cost are two extreme measures, providing a lower and an upper bound for *all* other entanglement measures E. More precisely, this theorem states that [37]

$$E_D(\rho) \leqslant E(\rho) \leqslant E_C(\rho) \tag{36}$$

for any entanglement measure E satisfying the requirements C2–C5 from above. In practice, however, these strong conditions are not fulfilled by most entanglement measures. On the other hand, by imposing weaker conditions, a similar statement can be formulated also for the regularized (or asymptotic) version $E^{\infty}(\rho) = \lim_{n\to\infty}(E(\rho^{\otimes n})/n)$ of some entanglement measure E:

$$E_D(\rho) \leqslant E^{\infty}(\rho) \leqslant E_C(\rho). \tag{37}$$

This inequality is satisfied, for example, by the entanglement of formation and the relative entropy of entanglement. The bound entangled states are examples where the difference between E_C and E_D is especially obvious since E_D is (by definition) zero, while E_C is always finite. This example illustrates that, for a given mixed quantum state, one single measure is often not enough to quantify the amount of entanglement, even in the limit of infinitely many copies.

2.3.4. Computable measures of entanglement

Most of the measures discussed above are motivated by physical operations which can be performed on the state of some quantum system, such as the 'distillation' of entanglement. From a mathematical point of view, in contrast, the formal evaluation of these measures typically involves an optimization problem over a state space which grows exponentially with the number of constituent particles. The lack of a simple operational procedure for calculating these measures of entanglement is therefore ultimately related to the complexity of distinguishing entangled from separable states, a problem which was shown to be NP-hard [49]. As a consequence of this complexity, the direct evaluation of these measures is exceedingly difficult and, hence, a great deal of effort has been dedicated to finding more *feasible* numerical methods, bounds and approximations (mostly in the bipartite setting). For a more detailed discussion on computational aspects, we refer the reader to Refs. [50–54].

With regard to these difficulties, there has been a great interest in developing computationally manageable monotones for the entanglement of quantum states, even if these (auxiliary) measures often lack an intuitive physical interpretation. Although some success was achieved, e.g., in the case of two-qubit states [55] or by exploiting the symmetry properties of certain quantum states [56–58], closed expressions for entanglement measures are still not unavailable in general. In the design of the FEYNMAN program, therefore, we restrict ourselves to the implementation of those measures and bounds which have been defined in the literature in an algebraic form. In the next subsection, we first summarize the definition and basic information about those quantities which are implemented into the program. Similar to the separability criteria, the computation of these quantities are invoked via the single command Feynman_measures() by using appropriate keywords. Whenever possible, moreover, the program supports both, symbolic and numerical computations [cf. Table 3].

2.3.5. Measures for bipartite entanglement

(i) *Negativity and logarithmic negativity*

As discussed above in the context of the Peres–Horodecki criterion [cf. Section 2.2.2], the positivity of the partial transpose of a density operator is a *necessary* condition for separability. Therefore the (amount of) 'negativity' in the spectrum of the partial transpose gives rise also to an entanglement measure. For the density matrix ρ of a bipartite system, for example, the negativity is defined as [59]

$$\mathcal{N}(\rho) = \frac{\|\rho^{T_A}\|_{\mathrm{Tr}} - 1}{d-1}, \tag{38}$$

where ρ^{T_A} denotes the partial transpose with respect to the subsystem A and where $d = \min(d_A, d_B)$ is the dimension of the smaller of the two subspaces and $\|A\|_{\mathrm{Tr}} = \mathrm{Tr}\sqrt{A^{\dagger}A}$ the trace norm. While there is no direct physical interpretation for the negativity, there is an operational interpretation of a closely related quantity, the logarithmic negativity

$$E_{\mathcal{N}}(\rho) = \log_2 \|\rho^{T_A}\|_{\mathrm{Tr}}, \tag{39}$$

as a special type of entanglement cost under PPT preserving operations [60]. This logarithmic negativity is known also for providing an upper bound to the distillable entanglement.

Although, in contrast to the negativity (38), the logarithmic negativity is *not* convex, it can be shown that both measures are indeed entanglement monotones [61]. It should be noted, however, that $E_{\mathcal{N}}$ does not reduce to the entropy of entanglement for all pure states. Because of their close relation to the PPT criterion, moreover, both measures, $\mathcal{N}$ and $E_{\mathcal{N}}$, fail to detect bound

entanglement for bipartite systems with dimensions higher than 2×2 or 2×3, respectively. An extension of the negativity concept, which addresses this problem, has been given recently in Ref. [62].

(ii) *Concurrence*

Another successful concept for defining an entanglement measure is the so-called concurrence, which is closely related to the entanglement of formation and which has been defined originally for a system of two qubits [55]. For a general two-qubit state ρ, this measure is based on the 'spin-flipped' (time-reversed) density matrix

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y), \tag{40}$$

where σ_y denotes the Pauli matrices and ρ^* the complex conjugate of ρ (in the usual computational basis). With this definition, the concurrence is then defined as

$$\mathcal{C}(\rho_{AB}) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{41}$$

where λ_i are the square roots of the eigenvalues of $\rho\tilde{\rho}$ given in decreasing order $\lambda_1 \geqslant \lambda_2 \geqslant \cdots$. In order to extend this measure also for multipartite systems, moreover, there exists the notion of the so-called tangle τ_{AB}

$$\tau_{AB}(\rho_{AB}) = \mathcal{C}^2(\rho_{AB}) = \big[\max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}\big]^2. \tag{42}$$

Although the concurrence is used very frequently in the literature, it was introduced rather as an auxiliary quantity for calculating the entanglement of formation for a pair of qubits. For a general two-qubit state, namely, these two measures are connected to each other via the relation

$$E_f(\rho) = h\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - \mathcal{C}^2(\rho)}\right), \tag{43}$$

where $h(x) = -x \log_2 x - (1-x)\log_2(1-x)$ is the binary entropy function. There have been several attempts to generalize the concept of concurrence some of which are discussed below (see also Refs. [63,64]).

(iii) *I-concurrence*

A generalization of the concurrence to a pair of quantum systems A, B of arbitrary dimension is the I-concurrence [65], whose name comes from the fact that it generalizes the concept of the spin-flip operator in Eq. (40) to the so-called universal inverter superoperator. For a pure state $|\psi_{AB}\rangle$ of a bipartite system, the I-concurrence is related to the purities of the reduced density operators ρ_A or ρ_B,

$$IC(\psi_{AB}) = \sqrt{2\big[1 - \mathrm{Tr}\big(\rho_A^2\big)\big]} = \sqrt{2\big[1 - \mathrm{Tr}\big(\rho_B^2\big)\big]}, \tag{44}$$

and has become quite a standard in the literature. Unfortunately, there is no closed expression of the I-concurrence known for the case of mixed states. However, there is a purely analytical lower bound for the concurrence of bipartite mixed states of arbitrary dimensions [52]. This approximation is related to the quite powerful realignment criterion for separability (cf. Section 2.2.2) and, hence, can be computed straightforwardly. In the command Feynman_measures(), this bound is accessible via the keyword (string) "concurrence bound". An alternative (but more complicated) lower bound and an approximation for the case of quasi-pure states was given in Refs. [53] and [54], respectively.

2.3.6. *Measures for multipartite entanglement*

In contrast to the reasonably well understood bipartite setting, multipartite quantum states exhibit a richer structure in the sense that there exist several inequivalent types of multipartite entanglement [66]. For multipartite systems, therefore, the (multipartite) entanglement is more difficult to quantify, even in the case of pure states. In fact, if the number of subsystems is increased, an exponentially growing amount of different measures is needed in order to fully characterize the entanglement in a given multipartite state. For this reason also, the measures below can cover only a few different aspects of multipartite entanglement, leaving its full quantification as an open problem.

(iv) *Global entanglement*

One attempt to provide a computationally feasible and scalable quantification of entanglement in multipartite systems was made in Refs. [67,68]. For a pure n-qubit state $|\psi\rangle$, the so-called global entanglement is defined as

$$Q\big(|\psi\rangle\big) = 2\left[1 - 1/n \sum_{i=1}^{n} \mathrm{Tr}\big(\rho_i^2\big)\right], \tag{45}$$

where ρ_i represents the density matrix of ith qubit after tracing out all other qubits. As seen from this definition, the global entanglement can be interpreted as the average over the (bipartite) entanglements of each qubit with the rest of the system.

Apart from being defined only for *pure* states, a major drawback of the global entanglement is, that it only extracts the bipartite correlation between each subsystem (qubit) and the remainder of the system. For this reason, the global entanglement cannot really account for multipartite entanglement nor can it distinguish global from sub-global entanglement. For example, the two states $|\Phi\rangle = 1/\sqrt{2}(|00\rangle + |11\rangle) \otimes 1/\sqrt{2}(|00\rangle + |11\rangle)$ and the GHZ-type state $|\Psi\rangle = 1/\sqrt{2}(|0000\rangle + |1111\rangle)$ both yield the same value $Q(|\Phi\rangle) = Q(|\Psi\rangle) = 1$.

(v) *N-concurrence*

Another generalization of the bipartite I-concurrence in Eq. (44) to N-partite states was given in Refs. [64,69]. For a pure and normalized N-partite state $|\psi\rangle$, the N-concurrence measure is defined as

$$C_N\big(|\psi\rangle\big) = 2^{1-(N/2)} \sqrt{2^N - 2 - \sum_i \mathrm{Tr}\big(\rho_i^2\big)}, \tag{46}$$

where i runs over all $\sum_{n=1}^{N-1} \binom{N}{n} = 2^N - 2$ different reduced density matrices which are obtained by tracing out n different subsystems (i.e. not only the single qubits but also all possible groups of $n = 1, 2, \ldots, N-1$ qubits!). The measure C_N has the property to vanish for fully N-separable states and to reach its maximum for GHZ states. In contrast to the before-mentioned global entanglement Q, the N-concurrence accounts also for real multipartite entanglement. Moreover, C_N allows for a meaningful comparison of multipartite states with different numbers of constituents since, for a product state $|\Psi_N\rangle = |\Psi_{N-1}\rangle \otimes |\Phi\rangle$, the N-partite concurrence simply reduces to the $(N-1)$-partite concurrence $C_{N-1}(|\Psi_{N-1}\rangle)$. Note, however, that the C_N measure is not normalized to unity.

(vi) *3-tangle*

Based on the two-qubit, mixed-state concurrence $\mathcal{C}$, the (so-called) 3-tangle, τ_{ABC}, has been constructed as an entanglement monotone for quantifying the amount of genuine three-way entanglement in a pure three-qubit state $|\psi\rangle_{ABC}$ [70], known also as 'residual entanglement'. This entanglement measure is defined as

$$\tau_{ABC}\big(|\psi\rangle_{ABC}\big) = \mathcal{C}^2_{A(BC)} - \mathcal{C}^2_{AB} - \mathcal{C}^2_{AC}, \tag{47}$$

where $\mathcal{C}_{AB} = \mathcal{C}(\rho_{AB})$ and $\mathcal{C}_{AC} = \mathcal{C}(\rho_{AC})$ are the concurrences of the corresponding two-qubit subsystems and where $\mathcal{C}_{A(BC)} = 2\sqrt{\det \rho_A}$ describes the bipartite entanglement between the subsystem A and BC, respectively.

The prototype of the three-partite entangled states is the Greenberger–Horne–Zeilinger (GHZ) state $|\mathrm{GHZ}\rangle = 1/\sqrt{2}(|000\rangle + |111\rangle)$ [73] which also yields the maximum value $\tau_{ABC}(|\mathrm{GHZ}\rangle) = 1$. Since there exist no bipartite correlations in $|\mathrm{GHZ}\rangle$, tracing out one of the qubits destroys all entanglement in the state.

3. Extensions to the FEYNMAN program

3.1. Overview

As described previously [5], our intention in developing the FEYNMAN program refers to the simulation of n-qubit quantum systems (quantum registers) within the framework of the MAPLE computer algebra system. For this purpose, the FEYNMAN program has been organized as a *module* for MAPLE, containing a hierarchy of currently about 40 procedures at quite different level of complexity. Apart from a number of basic subprocedures, which remain *hidden* to the user, the main commands can be used either for interactive work or simply as language elements in order to build-up new commands at some higher level of the hierarchy. Unlike several other, purely numerical implementations, however, the FEYNMAN program has been designed to enable the user to perform either symbolic or numerical computations. Moreover, by using MAPLE's large number of built-in mathematical functions, a minimum of programming effort is usually required in order to support various user-specific extensions.

To summarize our previous work, our first version [5] established the basic data structures for the simulation of n-qubit quantum systems, such as qbit(), qregister(), qoperator(), etc. This version also introduced several commands in order to 'act' on these data structures, e.g., in order to apply some pre- or user-defined quantum gates and/or to perform some other operations like the tensor product of quantum registers or the computation of reduced density operators. Additionally, simple state visualization tools for quantum registers are provided such as probability plots or the Bloch vector representation.

3.2. Current changes in the program

With the present update of the FEYNMAN program, our main motivation now is to provide also tools concerning the analysis of the separability and the entanglement properties of quantum registers. Therefore, the new commands Feynman_is_separable() and Feynman_measures() have been developed. Since one of MAPLE's advantages is its ability to evaluate symbolic expressions, rather than performing large-scale numerical optimizations, here we restricted ourselves to algebraic separability criteria and to several entanglement measures which are defined analytically in the literature. In particular, the Feynman_is_separable() procedure implements all the separability criteria from Section 2.2.2 which are briefly summarized again in Table 2. In addition, the Feyn-

Table 1
Additional *main* commands of the FEYNMAN program which are accessible by the user. A detailed description of all commands is given in the manual `Feynman-commands.pdf` which is distributed together with the program

Command	Short explanation
Feynman_decompose()	Calculates the Schmidt as well as several matrix decompositions.
Feynman_is_separable()	Tests for the separability of a qregister() or some general density matrix.
Feynman_measures()	Evaluates several (entanglement) measures for the quantum state as given in a qregister().

Table 2
List of the separability criteria which are supported by the command Feynman_is_separable(). These criteria were discussed in Section 2.2.2. A more detailed description of all argument options of this command is provided in the manual `Feynman-commands.pdf`

Argument option	Explanation
("Schmidt", ...)	Utilizes the Schmidt decomposition Eq. (2), i.e. the purity of subsystem states, in order to determine the bipartite separability of a pure-state qregister().
("PPT", ...)	Utilizes the Peres–Horodecki or positive partial transposition (PPT) criterion Eq. (10) to determine the separability of a given qregister() or density matrix.
("majorization", ...)	Utilizes the majorization criterion (11) to determine the bipartite separability of a given qregister() or density matrix.
("reduction", ...)	Utilizes the reduction criterion (12) to determine the bipartite separability of a given qregister() or density matrix separability.
("realignment", ...)	Utilizes the matrix realignment criterion (15) to determine the separability of a given qregister() or density matrix.
("GPT", ...)	Utilizes the generalized partial transposition (GPT) criterion (18) to determine the separability of a given qregister() or density matrix.

man_measures() command implements the entanglement measures discussed in Section 2.3.4 as well as a few related quantities [cf. Table 3]. Both of the new commands use a similar syntax where the first argument is a keystring for specifying the desired separability criterion or measure, typically followed by some qregister() structure and two (or more) integer lists in order to specify the considered splitting of the qregister, i.e. the qubit numbers which belong to the according groups. Typical examples for examining the entanglement properties of the split $A|BC$ in some arbitrary three-qubit qregister() structure, $\texttt{qregister}_{ABC}$, could be:

```
Feynman_measures("negativity", qregister_ABC, [1],[2,3])   or
Feynman_is_separable("PPT", qregister_ABC, [[1],[2,3]]).
```

It should be noted, however, that the entanglement vs. separability problem or the quantification of entanglement is in general a computationally hard problem, especially in the multipartite setting. Moreover, a sufficient understanding of the different aspects of (multipartite) entanglement is still not reached. Therefore, the intention of the new FEYNMAN commands is mainly to provide simple access to those criteria and measures which are widely known in the literature. As a consequence, the program does not implement new efficient schemes for the quantification of (multipartite) entanglement. Instead, the main advantage of the FEYNMAN program lies rather in its great flexibility, the ease of use and extendibility which may significantly simplify the investigation of the entanglement properties in small to medium-sized systems.

Apart from the two new main commands, which are dedicated especially to the separability and entanglement quantification, another new command is Feynman_decompose(). Besides several useful matrix decompositions, such as the spectral decomposition or the singular value decomposition, the main purpose of this command is to provide the Schmidt decomposition for pure bipartite states (as demonstrated in Section 4.1).

In addition to the new procedures in Table 1, some changes have been made also to the code in order to facilitate the development of user-defined procedures based on the FEYNMAN commands. As a first step into this direction, we now introduced several types of *objects* which can be used with MAPLE's internal `type()` command in the form `type(a, keyword)` where `true` is returned if the variable or expression `a` is of the `keyword`-type and `false` otherwise. Up to the present, however, most of these types refer to the FEYNMAN data structures as introduced in Ref. [5]. A short list of the new object types can be found in Table 4.

3.3. Program distribution

As with the previous version, the FEYNMAN program is distributed via the CPC program library as an compressed archive file containing the FEYNMAN library files and the source code as well as the manual `Feynman-commands.pdf`, example worksheets (see next section) and a `Read.me` file which explains the installation of the program package. After proper installation, the package can be loaded at the MAPLE prompt using the command `with(Feynman)`.

Table 3
Measures and quantities from Section 2.3.4 which are currently supported by the command Feynman_measures(). A more detailed description of all argument options of this command is provided in the manual `Feynman-commands.pdf`

Argument option	Explanation
(i) *Fidelity and distance measures*	
("fidelity", ...)	fidelity $F(\rho,\sigma) = [\mathrm{Tr}(\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}})]^2$
("trace distance", ...)	trace distance $D_{\mathrm{Tr}}(\rho,\sigma) = \frac{1}{2}\|\rho-\sigma\|_{\mathrm{Tr}} = \frac{1}{2}\,\mathrm{Tr}\sqrt{(\rho-\sigma)^\dagger(\rho-\sigma)}$
("Hilbert–Schmidt distance", ...)	Hilbert–Schmidt distance $D_{\mathrm{HS}}(\rho,\sigma) = \|\rho-\sigma\|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}[(\rho-\sigma)^\dagger(\rho-\sigma)]}$
("Bures distance", ...)	Bures distance $D_{\mathrm{B}}(\rho,\sigma) = \sqrt{2-2\,\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}}$
(ii) *Entropy measures and related quantities*	
("entropy", ...)	von Neumann entropy $S(\rho) = -\mathrm{Tr}(\rho\log_2\rho)$
("linear entropy", ...)	linearized version of the von Neumann entropy, $S_l(\rho) = \frac{d}{d-1}(1-\mathrm{Tr}(\rho^2))$
("participation ratio", ...)	participation ratio $R(\rho) = 1/\mathrm{Tr}(\rho^2)$ of a given state. It can be interpreted as the effective number of pure states that enter the mixture
("relative entropy", ...)	relative entropy $S(\rho\|\sigma) = -S(\rho) - \mathrm{Tr}(\rho\log_2\sigma)$
("conditional entropy", ...)	(von Neumann) conditional entropy $S(A\|B) = S(\rho_{AB}) - S(\rho_B)$
("mutual information", ...)	mutual information $S(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$
(iii) *Bipartite entanglement*	
("entropy of entanglement", ...)	entropy of entanglement $E_E(\|\psi_{AB}\rangle) = S(\rho_A) = S(\rho_B)$
("negativity", ...)	negativity $\mathcal{N}(\rho) = (\|\rho^{T_A}\|_{\mathrm{Tr}} - 1)/(d-1)$
("logarithmic negativity", ...)	logarithmic negativity $E_{\mathcal{N}}(\rho) = \log_2\|\rho^{T_A}\|_{\mathrm{Tr}}$
("concurrence", ...)	concurrence for two qubits, $\mathcal{C}(\rho_{AB}) = \max\{0,\lambda_1-\lambda_2-\lambda_3-\lambda_4\}$
("entanglement of formation", ...)	entanglement of formation for two qubits, $E_F(\rho_{AB}) = h(\frac{1}{2}+\frac{1}{2}\sqrt{1-\mathcal{C}_{AB}^2})$, where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$
("I-concurrence", ...)	I-concurrence $IC(\psi_{AB}) = \sqrt{2[1-\mathrm{Tr}(\rho_A^2)]} = \sqrt{2[1-\mathrm{Tr}(\rho_B^2)]}$
("concurrence bound", ...)	lower bound of the bipartite mixed-state concurrence $\mathcal{C}(\rho) \geqslant \frac{1}{m-1}(\max(\|\rho^{T_A}\|, \|\mathcal{R}(\rho)\|) - 1)$ where ρ^{T_A} and $\mathcal{R}(\rho)$ are the partially transposed and realigned density matrices
(iv) *Multipartite entanglement*	
("global entanglement", ...)	global entanglement $Q(\|\psi\rangle) = 2[1-1/n\sum_{i=1}^n \mathrm{Tr}(\rho_i^2)]$
("n-concurrence", ...)	n-qubit concurrence $C_N(\|\psi\rangle) = 2^{1-(N/2)}\sqrt{2^N-2-\sum_\alpha \mathrm{Tr}(\rho_\alpha^2)}$
("3-tangle", ...)	three-qubit residual entanglement $\tau_{ABC} = \mathcal{C}_{A(BC)}^2 - \mathcal{C}_{AB}^2 - \mathcal{C}_{AC}^2$ with $\mathcal{C}_{A(BC)} = 2\sqrt{\det\rho_A}$

Table 4
New `type` definitions for the FEYNMAN program. A detailed description of the underlying data structures can be found in the manual `Feynman-commands.pdf` which is distributed together with the code

`type(a,...)`	Returns `true` if `a` is a ...
`type(a, cbs)`	cbs() structure (computational basis state)
`type(a, qbit)`	qbit() structure
`type(a, qregister)`	qregister() structure (either a pure or mixed state)
`type(a, qregister_pure)`	qregister() structure containing a (state) vector as third operand
`type(a, qregister_mixed)`	qregister() structure containing a (density) matrix as third operand
`type(a, qoperator)`	qoperator() structure
`type(a, qoperation)`	qoperation() structure

4. Interactive work using the FEYNMAN procedures: Examples

To illustrate the interactive use of the FEYNMAN procedures, four small examples will be displayed below. Apart from these test cases, of course, the same procedures can be utilized also for dealing with more complex tasks. In the following examples it is assumed that the FEYNMAN module has been loaded by means of the command `with(Feynman)`. Moreover, since some of the procedures result in a rather large MAPLE output, a colon (instead of a semicolon) is used at the end of several input lines in order to suppress the corresponding printout to screen.

4.1. Entanglement of a pure two-qubit state

In our first example, let us employ the ubiquitous Schmidt decomposition for exploring the entanglement properties of a pure two-qubit state. As explained in Section 2.1.1, any pure bipartite n-qubit system AB, which is described by a state vector $|\psi_{AB}\rangle$,

can be brought into the form

$$|\psi_{AB}\rangle = \sum_{i=1}^{r} \sqrt{\lambda_i}|a_i\rangle|b_i\rangle, \tag{48}$$

where $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$ are two orthonormal bases of the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively, and where $\sqrt{\lambda_i}$ denotes the positive Schmidt coefficients with $\sum_{i=1}^{r} \lambda_i = 1$. Here, we wish to use the FEYNMAN program for showing such a decomposition explicitly for a test state for which the result is by far not obvious and where a rather tedious although straightforward calculation would be needed. As example, let us take the two-qubit state

$$|\psi_{AB}\rangle = \frac{1+\sqrt{6}}{2\sqrt{6}}|00\rangle + \frac{1-\sqrt{6}}{2\sqrt{6}}|01\rangle + \frac{\sqrt{2}-\sqrt{3}}{2\sqrt{6}}|10\rangle + \frac{\sqrt{2}+\sqrt{3}}{2\sqrt{6}}|11\rangle \tag{49}$$

which can be 'entered' into the FEYNMAN environment as the state vector of a qregister() by using a linear combination of computational basis states (cbs()):

```
> psi_AB := Feynman_set_qregister((1 + sqrt(6))/(2*sqrt(6))*cbs("00")
            + (1 - sqrt(6))/(2*sqrt(6))*cbs("01") + (sqrt(2) - sqrt(3))/(2*sqrt(6))*cbs("10")
            + (sqrt(2) + sqrt(3))/(2*sqrt(6))*cbs("11")):
```

Having defined the state in this way, the decomposition can be carried out simply by typing:

```
> Feynman_decompose("Schmidt", psi_AB);

                [  1/2 ]  [  1/2 ]          [ 1/2]  [ 1/2]
                [ 6    ]  [ 2    ]          [3   ]  [2   ]
           1/2  [ ---- ]  [ ---- ]          [----]  [----]
          3     [  3   ]  [  2   ]          [ 3  ]  [ 2  ]
       [[----, [      ], [      ]], [1/2, [    ], [    ]]]
          2     [   1/2]  [   1/2]          [ 1/2]  [ 1/2]
                [  3   ]  [  2   ]          [6   ]  [2   ]
                [ ---- ]  [ ---- ]          [----]  [----]
                [    3 ]  [    2 ]          [ 3  ]  [ 2  ]
```

Here, the output is given in the form $[[\sqrt{\lambda_1}, [|a_1\rangle, |b_1\rangle]], [\sqrt{\lambda_2}, [|a_2\rangle, |b_2\rangle]]]$, so that each of the two list elements represents one term in the sum of Eq. (48). From the fact that there is more than just a single term in the summation (i.e. that the Schmidt rank is greater than one) we already see that the original state $|\psi_{AB}\rangle$ was entangled, although not maximally entangled. The same result could be obtained also by tracing out either qubit A or B and by analyzing the reduced density matrix of the remaining qubit. In MAPLE's graphic mode, for instance, the state of the second qubit, B, can be visualized conveniently in the well-known Bloch sphere, by using the command Feynman_plot_Bloch_vector() which internally traces out all remaining qubits which are not shown.

Here, we do not display the individual steps explicitly for obtaining the reduced density matrix of one of the qubits which has been demonstrated in a similar way in Section 4.3 in [5]. Fig. 1 shows the corresponding output graphic for the second qubit; as seen from this figure, the Bloch vector of the reduced density operator ρ^A has a length less than unity, indicating that the subsystem A is in a mixed but not maximally mixed state as expected for a subsystem of an entangled state. In addition, we can easily determine the entropy of entanglement $E_E(|\psi_{AB}\rangle)$ between the two qubits by typing:

```
> evalf(Feynman_measures("entropy of entanglement", psi_AB, [1],[2]));
    0.8112781242
```

which is found close to one in good agreement with our qualitative discussion of $|\psi_{AB}\rangle$ above.

4.2. Separability as a consequence of mixing

From the literature, a variety of experiments are known which focused on a controlled preparation and evolution of entangled states [71,72]. For any initially prepared state ρ of an n-qubit quantum system, in fact, the interaction of this system with some environmental degrees of freedom typically leads to mixing which can often by modeled by:

$$\rho' = (1-p)\rho + p\, I/d, \tag{50}$$

where I is the corresponding $d \times d$ identity matrix and $0 \leqslant p \leqslant 1$ the mixing parameter.

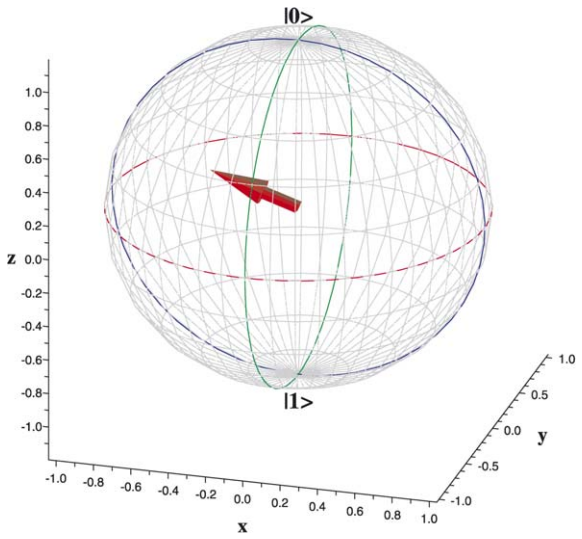

Fig. 1. Bloch sphere visualization of qubit A in Eq. (49), as returned by the MAPLE command line `Feynman_plot_Bloch_vector(psi_AB, 1);`. It can be seen that the Bloch vector (polarization vector) has a length less than unity which indicates that the state is mixed.

Of course, any degree of mixing with the maximally mixed (and separable) state I/d decreases the quantum correlations for the state of the qubit system and, eventually, leads to their complete destruction. An interesting question in this context therefore refers to the 'amount of mixing', which is allowed before the state becomes separable and how the destruction proceeds. Using the FEYNMAN program, we can answer such questions by comparing the susceptibility to mixing of different states and, in particular, for states with different types of entanglement. For example, let us consider the following three states:

(a) the three-qubit GHZ state

$$|\psi_{\mathrm{GHZ}}\rangle = \frac{1}{\sqrt{2}}\big(|000\rangle + |111\rangle\big), \tag{51}$$

(b) the W-state

$$|\psi_{\mathrm{W}}\rangle = \frac{1}{\sqrt{3}}\big(|010\rangle + |100\rangle + |100\rangle\big), \tag{52}$$

(c) some biseparable mixed three-qubit state with genuine tripartite (bound) entanglement (cf. Section 2.1.2)

$$\tilde{\rho}_{ABC} = \frac{1}{4}\left(I_8 - \sum_{i=1}^{4} |\psi_i\rangle\langle\psi_i|\right), \tag{53}$$

where the $|\psi_i\rangle$ are given as $|0,1,+\rangle$, $|1,+,0\rangle$, $|+,0,1\rangle$ and $|-,-,-\rangle$, respectively, and with $|\pm\rangle = 1/\sqrt{2}(|0\rangle \pm |1\rangle)$.

Within the FEYNMAN program, the three states above can be defined in the form of Eq. (50) as follows:

```
> GHZ     := Feynman_set_qregister((1-p)*Feynman_set_qregister("GHZ") +
                                   p*Feynman_set_qregister("maximally mixed",3)):

> W       := Feynman_set_qregister((1-p)*Feynman_set_qregister("W") +
                                   p*Feynman_set_qregister("maximally mixed",3)):

> rho_ABC := Feynman_set_qregister((1-p)*Feynman_set_qregister("biseparable") +
                                   p*Feynman_set_qregister("maximally mixed",3)):
```

Moreover, we may convince ourselves that all three states are initially not fully separable, i.e. for $p = 0$. To this end, let us apply the command Feynman_is_separable() and specify that we wish to use the "realignment" criterion from Section 2.2.2 in order to decide about the separability of the states:

```
> Feynman_is_separable("realignment", eval(GHZ, p=0), [[1],[2],[3]]);
     false
```

```
> Feynman_is_separable("realignment", eval(W, p=0), [[1],[2],[3]]);
     false

> Feynman_is_separable("realignment", eval(rho_ABC, p=0), [[1],[2],[3]]);
     false
```

Here, the last argument `[[1],[2],[3]]` is used to indicate that each qubit is regarded as an individual subsystem. Apart from this *boolean* test on the separability, of course, the command Feynman_is_separable() can be used also to establish a small procedure which increases the mixing parameter, p, successively and which simply stops when the state becomes fully separable according to either the realignment criterion or any other implemented criterion.

```
> max_mixing := proc(qreg)
local i;
for i by 0.001 from 0 to 1 do
   if Feynman_is_separable("realignment", eval(qreg, p=i), [[1],[2],[3]]) then
      printf(`The state becomes separable for p >= %a`, i);
         break;
      end if;
   end do;
   end proc:
```

Using this simple procedure, we now obtain the following estimates:

```
> max_mixing(GHZ);
The state becomes separable for p >=.800

> max_mixing(W);
The state becomes separable for p >=.791

> max_mixing(rho_ABC);
The state becomes separable for p >=.127
```

Note that the command Feynman_is_separable() also supports the use of general density matrices instead of a qregister(). With this feature in mind, we could examine also the separability of general multi-qudit states. Using, in addition, the Feynman_apply() command together with some properly defined data structure of a quantum operation (qoperation()), more realistic decoherence scenarios can be studied as well.

4.3. Distance measures in a noisy circuit

In our third example, finally, we shall investigate the distinguishability of two quantum states. For this purpose, let us apply the trace distance $D_{\mathrm{Tr}}(\rho, \rho')$ and the Hilbert–Schmidt distance $D_{\mathrm{HS}}(\rho, \rho')$ in order to compare the output from an ideal quantum gate with those from a noisy implementation. In particular, let us utilize the fact that the controlled-not gate is equivalent to a simple circuit of Hadamard gates and a controlled-z gate, see Fig. 2. As a simple noise model, here we apply the so-called amplitude damping channel $\rho' = \mathcal{E}_{\mathrm{AD}}(\rho) = \sum_i E_i \rho E_i^\dagger$ which acts on a single qubit [1]. Using the operator-sum (or Kraus) representation, the corresponding operation elements (Kraus operators) E_i are then given as follows:

$$E_0 = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{bmatrix}, \qquad E_1 = \begin{bmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{bmatrix}, \tag{54}$$

where $0 \leqslant p \leqslant 1$ can be interpreted as the probability of a decay process $|1\rangle \to |0\rangle$ of the referring qubit (i.e., No. 2 in our example above).

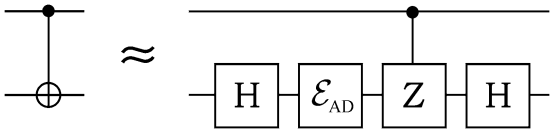

Fig. 2. Schematic noisy circuit implementation of the controlled-not gate. The one qubit amplitude damping channel $\mathcal{E}_{\mathrm{AD}}(\rho)$ determines the deviation of the noisy circuit from the ideal controlled-not gate.

We start by creating a two-qubit input register in the state $|+\rangle|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle$.

```
> input := Feynman_set_qregister("+0"):
```

Next, we calculate the two different output states for the ideal gate and for the noisy circuit implementation, respectively. While, in the former case, we only have to apply a single quantum operator (qoperator()), which describes the ideal controlled-not gate,

```
> out1 := Feynman_apply(qoperator("cnot"), input):
```

there are several of such quantum operators in the latter case. To simulate the noisy channel, in particular, we can define the quantum operation from the operation elements E_0, E_1 above by:

```
> assume(p<=1, p>=0);
> E0 := Matrix([[1,0],[0,sqrt(1-p)]]):
> E1 := Matrix([[0,sqrt(p)],[0,0]]):
> noise := qoperation(2, [E0, E1], [2]):
```

and can use it to apply it in line with the quantum circuit from Fig. 2:

```
> out2 := Feynman_apply(qoperator("IH"), input):
> out2 := Feynman_apply(noise, out2):
> out2 := Feynman_apply(qoperator("cz"), out2):
> out2 := Feynman_apply(qoperator("IH"), out2):
```

Finally, we can compare the two output states conveniently by computing their trace distance $D_{\mathrm{Tr}}(\rho, \rho') = \frac{1}{2}\,\mathrm{Tr}\sqrt{(\rho-\rho')^\dagger(\rho-\rho')}$ and the Hilbert–Schmidt distance $D_{\mathrm{HS}}(\rho, \rho') = \|\rho - \rho'\|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}[(\rho-\rho')^\dagger(\rho-\rho')]}$

```
> TD := Feynman_measures("trace distance", out1, out2);

                          1/2           2 1/2
            (2 - 2 (1 - p~)     - p~ + p~ )
     TD := ---------------------------------
                            2

> HS := Feynman_measures("HS distance", out1, out2);
             1/2                1/2                 2 1/4
            2   (4 - 4 (1 - p~)       - 2 p~ + 2 p~ )
     HS := ------------------------------------------
                             2
```

The resulting curves of the trace distance and the Hilbert–Schmidt distance as a function of the noise parameter p are shown in Fig. 3.

4.4. Finite-time disentanglement via spontaneous decay

In the last example, we investigate the entanglement dynamics of a simple model system. More precisely, we demonstrate that under the influence of spontaneous emission two entangled two-level atoms (i.e. qubits) can become completely disentangled in *finite* time [74]—in contrast to the purely exponential decay of the individual atoms. In order to show this, an initial two-qubit state of the general form

$$\rho = \frac{1}{3}\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & z & 0 \\ 0 & z^* & c & 0 \\ 0 & 0 & 0 & d \end{pmatrix} \tag{55}$$

with the choice $0 \leqslant a \leqslant 1$, $d = 1 - a$ and $b = c = z = 1$ is assumed. By varying the input state parameter a, the initial entanglement can be changed between $1/3$ and $2/3$. Within the FEYNMAN package, a corresponding qregister() structure may be created by typing

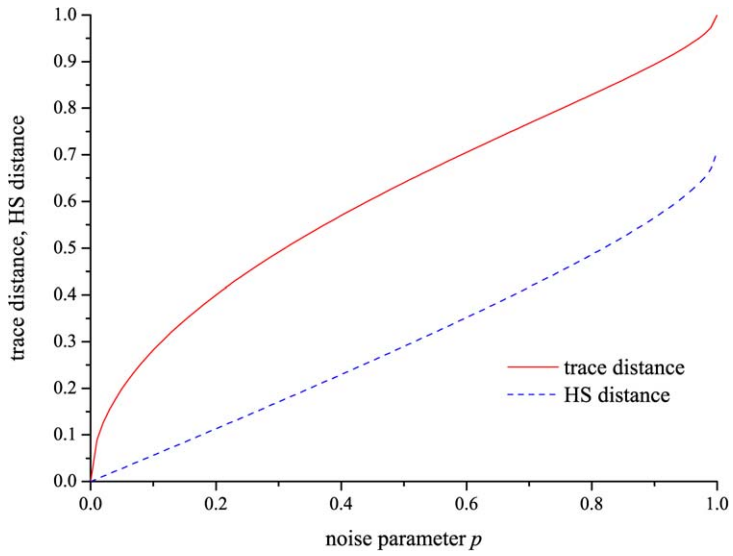

Fig. 3. Trace distance and Hilbert–Schmidt distance between the output of the ideal circuit and the noisy circuit from Fig. 2 as a function of the noise parameter p.

```
> rho := 1/3*Matrix([[a,0,0,0],[0,1,1,0],[0,1,1,0],[0,0,0,1-a]]):

> input := qregister(id, 2, rho);

                                [a/3     0      0          0    ]
                                [                              ]
                                [ 0     1/3    1/3         0    ]
     input := qregister(id, 2, [                              ])
                                [ 0     1/3    1/3         0    ]
                                [                              ]
                                [ 0      0      0     1/3 - a/3]
```

As shown in [74], using the interaction picture, the spontaneous decay of the two atoms (qubits) can be described within the operator-sum or Kraus representation in the form

$$\rho' = \sum_{i=1}^{4} E_i \rho E_i^{\dagger} \tag{56}$$

with the Kraus operators

$$E_1 = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix}, \tag{57}$$

$$E_2 = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix}, \tag{58}$$

$$E_3 = \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix} \otimes \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix}, \tag{59}$$

$$E_4 = \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ \omega & 0 \end{pmatrix}, \tag{60}$$

where $\omega = \sqrt{1-\gamma^2}$ and $\gamma = e^{-\Gamma t/2}$. For simplicity, we take $g = 1-\gamma$ as the decoherence strength parameter ranging from 0 to 1 (which corresponds to the time evolution from $t = 0$ to $t = \infty$). Using the qoperation() structure, this evolution may be easily simulated and the resulting output state ρ' is obtained as follows

```
> E1 := Feynman_product("Kronecker", Matrix([[gamma,0],[0,1]]), Matrix([[gamma,0],[0,1]])):
> E2 := Feynman_product("Kronecker", Matrix([[gamma,0],[0,1]]), Matrix([[0,0],[omega,0]])):
> E3 := Feynman_product("Kronecker", Matrix([[0,0],[omega,0]]), Matrix([[gamma,0],[0,1]])):
> E4 := Feynman_product("Kronecker", Matrix([[0,0],[omega,0]]), Matrix([[0,0],[omega,0]])):
```

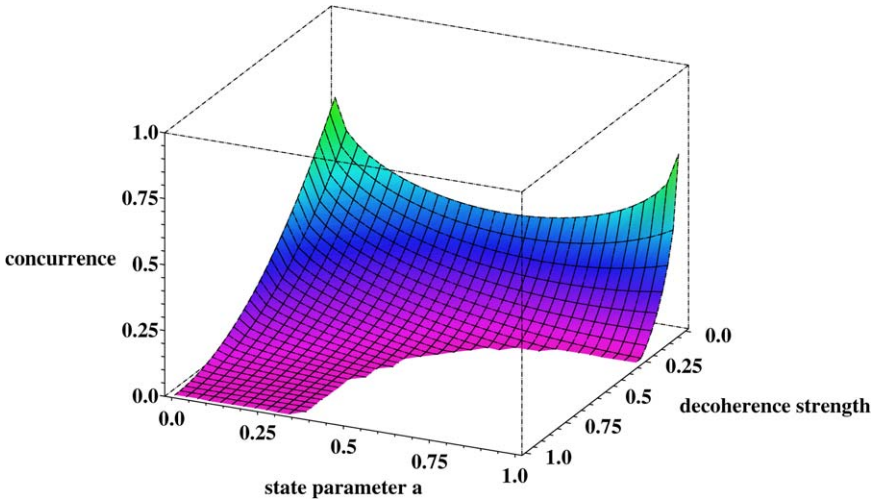

Fig. 4. Entanglement decay via spontaneous emission with an initially entangled state of the form of Eq. (55) with $0 \leqslant a \leqslant 1$, $d = 1 - a$ and $b = c = z = 1$. Complete disentanglement in finite time takes place for $a > 1/3$, while for $a \leqslant 1/3$ the disentanglement is completed only asymptotically.

```
> assume(g>=0, g<=1):
> Kraus_ops := subs(omega=sqrt(1-gamma^2), [E1, E2, E3, E4]):
> Kraus_ops := simplify(subs(gamma=1-g, Kraus_ops)):

> output := simplify(Feynman_apply(qoperation(Kraus_ops), input)):
```

Finally, in order to visualize the decay of the system's two-qubit entanglement (in terms of the concurrence measure $\mathcal{C}(\rho')$) as a function of the initial state parameter a and the decoherence strength parameter g, we generate a set of data points which yield a plot similar to Fig. 4.

```
> k := 20;
> temp := [seq([seq([i/k, j/k, evalf(Feynman_measures("concurrence", eval(output,
              {g=i/k, a=j/k})))], i=0..20)], j=0..20)]:

> plots[surfdata](temp, view=1E-15..1, axes=boxed, labels=["decoherence strength",
                  "state parameter a", "concurrence"]);
```

5. Summary and outlook

In a recent version of the FEYNMAN program [5], we provided all the tools necessary in order to define and manipulate n-qubit quantum registers within the framework of MAPLE. Based on this interactive and flexible environment, here we developed an extension to this code which helps investigate the separability and entanglement properties of such quantum registers. Several algebraic separability criteria as well as a variety of entanglement measures and other related quantities have been implemented and can now be accessed conveniently through the new main commands Feynman_is_separable() and Feynman_measures(). Following moreover the design and philosophy of our first version, the new FEYNMAN commands support both, symbolic and numerical computations and seamlessly integrate into the existing hierarchy of procedures.

With these new features of the FEYNMAN code, its range of applications is greatly extended. For instance, it now becomes possible to monitor the evolution of entanglement in quantum circuits. This might be useful also for studying the performance of various quantum algorithms for which the speed-up and the efficiency is known to be connected to the entanglement of the quantum register used.

A further possible application concerns the investigation of the decay of entanglement due to 'decoherence effects' of various kinds which is of central interest in all realistic scenarios. For example, one might look for a detailed comparison of the noise susceptibilities for different quantum states with the same amount of initial entanglement. A better understanding of the decay process (of entanglement) will help to optimize the lifetime of entanglement in quantum memories. Having such applications in mind, we remark that the FEYNMAN program performs not only unitary transformations but was designed from the very beginning to facilitate also the nonunitary evolution of a quantum register in terms of quantum operations. Obviously, however, further design and program developments are needed in order to provide a powerful tool for studying different decoherence models for quantum registers that interact with their environment. In particular, it would be highly desirable to have implemented a time-dependent

Hamiltonian-driven dynamics for the states of some quantum register as well as several simplified models for an open-system evolution.

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