Detection of entanglement during pure dephasing evolutions for systems and environments of any size

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We generalize the scheme for detection of qubit-environment entanglement to qudit-environment systems. This is of relevance for many-qubit systems and the quantification of the operation of quantum algorithms under the influence of external noise, since only decoherence that is not entangling in its nature can be effectively described by quantum channels and similar methods in more complicated scenarios. The generalization involves an increase of the class of entangled states which are not detected by the scheme, but the type of entanglement which cannot be detected is also least likely to qualitatively influence decoherence. We exemplify the operation of the scheme on a realistically modelled NV-center spin qutrit interacting with an environment of nuclear spins.

I. INTRODUCTION

Qubits are the simplest quantum systems, since their Hilbert space contains only two states. The result of this is that some complex measures of quantumness or quantum correlations are much easier to study for qubits than for larger quantum systems. One example of this is mixed state entanglement [1, 2] which can be found directly from the density matrix for a system of two qubits [3], but otherwise requires minimization over all possible preparations of a state [2, 4] or the use of measures which do not quantify all types of entanglement [5–8]. Similarly bound entanglement [9, 10], a type of entanglement which is not detected by the Peres-Horodecki criterion [11, 12], does not exist for systems of two qubits.

The number of coherences (off-diagonal elements of the density matrix) grows quadratically with the size of the system (as \(N(N−1)/2\) to be precise; obviously a density matrix is Hermitian, hence only half of the coherences are independent variables), so the single qubit coherence is replaced by three coherences for a qutrit, six coherences for a system of size \(N = 4\), and so on. Furthermore, the dependencies between the different coherences are relevant. An example here is the simple task of checking if a matrix is a density matrix and can therefore describe a physical state. This requires checking three conditions: Hermitianity, unit trace, and positivity. Only the third condition is problematic as it requires diagonalization of the matrix, which can only be done numerically for larger matrices. For a two by two Hermitian matrix only the absolute value of the coherence is relevant for positivity, which is not the case already for a qutrit.

The consequence is that there is a qualitative difference when studying larger systems as opposed to studies restricted to qubits and conclusions drawn for qubits rarely translate seamlessly to larger systems. This is also the case for asymmetric bipartite systems composed of a qudit (\(N\) dimensional system of interest) and its environment. In particular, entanglement formed between a qudit and its environment is much harder to study than in the case of a qubit. This is evident for pure-dephasing interactions, the only type of system-environment couplings for which simple, general formulas for qualification of a state obtained during the evolution as entangled or not exist [13, 14]. Qualifying qubit-environment entanglement (QEE) requires checking a single condition [13] and this allowed an entanglement measure tailored specifically to quantify this type of entanglement to be proposed [15], which yields substantial computational advantage with respect to standard entanglement measures [2, 4, 16]. Qualifying system-environment entanglement (SEE) on the other hand requires checking \(N−1\) conditions which are analogous to the QEE conditions and additionally \((N−1)(N−2)/2\) conditions which are qualitatively different [14]. This rapid growth in complexity with system size \(N\) precludes the possibility of an analogous SEE measure to be proposed.

The creation of entanglement with the environment throughout the evolution is relevant because the behavior of the environment is qualitatively different when entanglement is formed and when the evolution is separable [13, 14, 17]. In many situations QEE can lead to effects which cannot be explained by decoherence modeled classically [18]. This backaction, the situation when entanglement manifests itself in the state of the environment, which in turn influences the evolution of the qubit, is the reason why QEE can be measured with little effort [19, 20].

In the following we will study a qudit for which the interaction with the environment leads to pure dephasing, in order to generalize a scheme for the detection of QEE by operations and measurements only on the qubit [19]. This type of interaction is the dominating decoherence mechanism for many solid state qubits [21–28]. One motivation for the importance of SEE is that most solid state qubits are in fact only approximations of qubits (e. g. where two states are energetically distinct and can therefore be addressed separately). The more relevant one is that ensembles of qubits are of vital importance for any type of quantum data processing and ensembles of qubits interacting with an environment can no longer be treated with the methods for studying QEE.
point of view of entanglement with an environment they are in fact qudits and display the whole range of complexity relating to many coherences and phase relations between them.

We will show that one method for the detection of QEE [19] can in fact be generalized to detect SEE. The complexity of the procedure only grows linearly with the size of the qudit, so it does not reflect the quadratic growth of the number of SEE criteria [14]. The price to pay is the growing number of entangled states that cannot be detected by the procedure. Additionally to the type of entanglement which cannot be detected by the qubit procedure, there is now a second class of entanglement which cannot be witnessed for larger systems. Optimistically, the type of entanglement which is detected by the procedure is the type which is most likely to influence the operation of quantum algorithms [20].

The paper is organized as follows. In Sec. II we introduce the type of system-environment density matrix which can be classified in terms of SEE by the proposed scheme and the conditions on the Hamiltonian and initial state of the system and the environment to guarantee this form throughout the evolution. In Sec. III we restate criteria for separability of such density matrices. We introduce the proposed scheme for the detection of entanglement in Sec. IV and study the limitations of applicability of the scheme in Sec. V. In Sec. VI we study the working of the scheme on an NV-center spin qutrit interacting with a nuclear environment. Sec. VII concludes the paper.

II. CLASS OF PROBLEMS STUDIED

In the following we will present a scheme which allows to detect entanglement between a quantum system of interest (with no limitation on the dimension of its Hilbert space) and its environment. The method can only be used for system-environment density matrices of the form (N is the dimension of the system, the dimension of the environment is unspecified and arbitrary)

$$\tilde{\sigma} = \sum_{k,l=0}^{N-1} c_k c_l^* |k\rangle \langle l| \otimes \hat{R}_{kl}.$$  \hspace{1cm} (1)

Here the states on the left side of the tensor product correspond to some basis \{ |k\rangle \} in the system subspace, while the matrices \hat{R}_{kl} describe the environment. For the full matrix (1) to be a density matrix, the diagonal environmental matrices \hat{R}_{kk} have to be density matrices, but there is no such limitation for off-diagonal matrices, with \( k \neq l \).

Although density matrices of the form (1) are, at certain time-instants, encountered in evolutions governed by different Hamiltonians [29], the prevailing situation when they are encountered is when the system-environment Hamiltonian can only lead to pure-dephasing decoherence of the system. A system-environment Hamiltonian of this class can always be written in the form [14]

$$\hat{H} = \sum_{k=0}^{N-1} \varepsilon_k |k\rangle \langle k| + \hat{H}_E + \sum_{k=0}^{N-1} |k\rangle \langle k| \otimes \hat{V}_k,$$  \hspace{1cm} (2)

where \{ |k\rangle \} is the same system basis as used in eq. (1) and is now specified as the pointer basis of the system [30, 31]. Obviously the first term in the Hamiltonian (2) is the free Hamiltonian of the system, the second term is the (arbitrary) free Hamiltonian of the environment, and the third term describes the evolution. The first and last terms commute, which is the necessary and sufficient condition for the Hamiltonian to lead to pure dephasing for all initial states (such Hamiltonians cannot describe processes which involve energy exchange between the system and the environment).

A Hamiltonian of this type is diagonal in the subspace of the system, and the corresponding evolution operator retains this property,

$$\hat{U}(t) = \sum_{k=0}^{N-1} |k\rangle \langle k| \otimes \hat{W}_k(t).$$  \hspace{1cm} (3)

The environmental operators \( \hat{W}_k(t) \) can be understood as evolution operators of the environment conditional on the pointer state of the system and are given by

$$\hat{W}_k(t) = e^{-\frac{i}{\hbar} \varepsilon_k t} e^{-\frac{i}{\hbar} (\hat{H}_E + \hat{V}_k) t}.$$  \hspace{1cm} (4)

The free evolution of each pointer state is included in the operators (4), but it has no bearing on entanglement and as such is irrelevant for the results presented here.

Using eq. (3) on any initial system-environment state will yield their joint density matrix at time \( t \), but to obtain a density matrix of the form (1), restriction on the initial state is needed. Firstly, the state must be of product form with respect to the environment, and secondly, the initial system state must be pure

$$\hat{\sigma}(0) = |\psi\rangle \langle \psi| \otimes \hat{R}(0),$$  \hspace{1cm} (5)

with \( |\psi\rangle = \sum_{k=0}^{N-1} c_k |k\rangle \). The initial state of the environment \( \hat{R}(0) \) is arbitrary. Acting with the evolution operator (3) on the initial state (5), we obtain a system-environment density matrix of the form (1) for all times \( t \), and the environmental matrices, which are the only time-dependent element, are given by

$$\hat{R}_{kl}(t) = \hat{W}_k(t) \hat{R}(0) \hat{W}_l(t).$$  \hspace{1cm} (6)

III. CRITERIA FOR SYSTEM-ENVIRONMENT SEPARABILITY

In Ref. [14] it has been shown that to qualify a system-environment state of the form (1) as entangled or separable it is enough to check two classes of criteria, which have
been derived from the Peres-Horodecki criterion [11, 12] and the definition of mixed state separability.

The following are criteria of separability, and if any of them is violated then there is entanglement between the system and its environment. The first class of criteria is a generalization of the (single) separability criterion of QEE [13], and states that separability requires that for all $k \neq l$ we have

$$\hat{R}_{kk}(t) = \hat{R}_{ll}(t).$$  \hspace{1cm} (7)

There are $N - 1$ independent criteria of this type [14], where $N$ is the dimension of the system and it is enough to check (7) with $l$ set constantly to a given value e. g. $l = 0$. Physically, if criterion (7) is fulfilled for a given $k$ and $l$, it means that the evolution of the environment is indistinguishable regardless if the system is in pointer state $|k\rangle$ or $|l\rangle$. If all of such criteria are met then the environment evolves in exactly the same way for the system in any of the pointer states. Contrarily to pure initial states of the environment, this does not preclude decoherence of the system which is not initially in a pointer state (or mixture thereof) [13, 14, 32].

The second class of criteria requires commutation between products of different conditional evolution operators of the environment (4), namely for separability we must have

$$\left[ \hat{w}_i(t)\hat{w}_j(t), \hat{w}_k(t)\hat{w}_l(t) \right] = 0 \hspace{1cm} (8)$$

for all $i, j, k,$ and $l$. Only $(N - 1)(N - 2)/2$ of these conditions are independent [14].

The second class of separability criteria lacks the straightforward physical interpretation characteristic for the first class, which correlates SEE with information about the system state that has been transferred into the environment. This correlation allows for the detection of entanglement at least in principle, by measurements performed on the environment. There exist states of the form (1) for which all of the separability criteria of the first type are fulfilled, but not all of the criteria of the second type; such states are entangled [14].

IV. SCHEME FOR DETECTION OF SEE

For a qubit system, there exists only one separability criterion and it is of the first type (7). In this case the distinguishability of entangled and separable states by measurements on the environment alone, can be used to design schemes for entanglement detection which are operated solely on the qubit [19, 20]. This is a result of the back-action of the environment on the evolution of the qubit and the possibility of preparing a state of the environment by allowing it to evolve in the presence of the system in one of its pointer states. If the qubit environment state (1) is entangled in such a way that it violates any of the separability criteria (7) then this type of entanglement can also by detected by operations and measurements restricted to the system.

The procedure for the detection of QEE described in Ref. [19] is particularly straightforward to generalize. To detect if there is entanglement in qudit-environment state given by eq. (1) at time $\tau$ which is obtained using the evolution operator (3) on initial state (5), one must prepare and measure modified qudit-environment states, which involve a preparation of the environment prior to exciting a superposition system state. The idea is as follows. At time $t = 0$ the system is prepared in one of its pointer states $|k\rangle$ and allowed to evolve for time $\tau$. This does not change the state of the system but the environment does evolve, so the system-environment state is given by

$$\hat{\sigma}(\tau) = |k\rangle\langle k| \otimes \hat{R}_{kk}(\tau).$$  \hspace{1cm} (9)

If the system is now (at time $\tau$) prepared in a superposition state $|\psi\rangle = \sum_{k=0}^{N-1} c_k|k\rangle$, then it will evolve according to eq. (1), but with a new initial state, $\hat{R}_{kk}(\tau)$ instead of $\hat{R}(0)$. Further evolution will lead to pure dephasing of the qudit and each of its coherences will evolve according to

$$\rho^{(k)}_{ij}(\tau, t) = c_i c_j^* \text{Tr} \left( \hat{w}_i(t)\hat{w}_j(\tau)\hat{R}(0)\hat{w}_k(\tau)\hat{w}_l^\dagger(t) \right),$$  \hspace{1cm} (10)

where $t$ is the time elapsed from time $\tau$. An ideal test state $|\psi\rangle$ is an equal superposition of all pointer states as it maximizes the chances of determining entanglement.

If the procedure is repeated for a different initial system pointer state $|l\rangle$ and any of the coherences (10) show a different evolution at any point after time $\tau$, $\rho^{(k)}_{ij}(\tau, t) \neq \rho^{(l)}_{ij}(\tau, t)$, this signifies that at time $\tau$ the criterion (7) is not fulfilled for states $|k\rangle$ and $|l\rangle$. This further means that if the system was initialized in any superposition which contains pointer states $|k\rangle$ and $|l\rangle$ and the environment was initialized in the state $\hat{R}(0)$, then at time $\tau$ the joint system-environment state would be entangled.

Otherwise the procedure has to be repeated for a different choice of system pointer state $|k\rangle$ and again compared with the evolution for $|l\rangle$. Only when all possible values of $k \neq l$ are exhausted can one be sure that no entanglement can be witnessed by the procedure. The procedure is schematically represented in Fig. 1.

V. LIMITATIONS OF APPLICABILITY

The method described above is an entanglement witness [33–36], so a negative result does not signify separability. There are two situations when entanglement is present, but cannot be witnessed here. The first is the same as in the case when the system is a qubit [14], namely the will not detect entanglement if all of the conditional evolution operators of the environment, $\hat{w}_k(t)$, commute. In this case the preparation of the environment for time $\tau$ does not change the resulting evolution of the system coherences, which are now always
if and only if the state \( |k\rangle \) for a given set of indices \( k \) will be entangled with its environment at time \( \tau \) of undisturbed evolution.

This type of entanglement could still be detected by measurements on the environment since we still have

\[
\hat{R}_{kk}(t) \neq \hat{R}_{ll}(t)
\]

if and only if the state \( |1\rangle \) is entangled, but there is no effect on the evolution of the qudit.

Note that if only some of the conditional evolution operators of the environment mutually commute then entanglement for some initial states of the system can still be detected, and in many cases even for all system states.

This is because the number of independent criteria (7) is \( N - 1 \) [14] as opposed to the \( N(N - 1)/2 \) nontrivial combinations of indices \( k \) and \( l \). If criterion (7) is broken for a given \( k \) and \( l \) this means that a superposition with \( c_k \neq 0 \) and \( c_l \neq 0 \) will be entangled with its environment at time \( \tau \). This works analogously with indices \( k \) and \( l' \), but if the criterion is shown to be broken (using the scheme described in the previous section) for both sets of indices, the consequence is that a superposition with \( c_l \neq 0 \) and \( c_{l'} \neq 0 \) will also be entangled with its environment at time \( \tau \). Hence even if \( \hat{w}_l(t) \) and \( \hat{w}_{l'}(t) \) commute, it is possible to check entanglement for an initial state with \( c_l \neq 0 \) and \( c_{l'} \neq 0 \) using the proposed scheme.

The other situation is when no entanglement of the type witnessed by criterion (7) is generated during the evolution. If only separability criteria of the second type (8) are violated, this type of entanglement does not manifest itself in the conditional evolution of the environment and cannot be detected using this simple scheme. In fact, detecting such entanglement would most likely require tomography of the system-environment state.

\[
\rho_{ij}^{(k)}(\tau, t) = c_i c_j^* \text{Tr} \left( \hat{w}_i(t) \hat{R}(0) \hat{w}_j^\dagger(t) \right). \tag{11}
\]

### VI. EXAMPLE: NV CENTER SPIN QUTRIT

To exemplify the operation of the scheme described above, we will use it to detect entanglement between an NV center spin interacting with an environment of partially polarized nuclear spins of the spinful carbon isotope \(^{13}\text{C}\) in the diamond lattice [37–40]. The dominant carbon isotope \(^{12}\text{C}\) is spinless and does not contribute to NV center spin decoherence, so that the environment is sparse. The lowest energy level of the NV center is effectively a spin qutrit, with \( S = 1 \), so the dimension of the system is \( N = 3 \) and only two entanglement criteria of the first type (7) need to be checked to show that entanglement would be present for any initial superposition.
we plot the difference of the evolution which shows the difference in coherence between the NV center. The zero-field splitting, $\Delta$, the gyromagnetic ratio for $^{13}$C nuclei and the hyperfine interaction between the qutrit and the NV center. The term is responsible for the asymmetry of the NV center. The hyperfine interaction describes the coupling of a nuclear spin to the magnetic moment of the electron. The zero-field splitting, $\Delta$, is a displacement vector between the nucleus and the qutrit, while $\hat{I}_j$ is an operator of the $j$-th component of the nuclear spins.

The hyperfine interaction between the qutrit and the NV center is given by $\hat{H}_E = \sum_j \gamma_j B_z \hat{I}_j$, where $\gamma_j$ is the gyromagnetic ratio for $^{13}$C nuclei and $\hat{I}_j$ is an operator of the $j$-th component of the nuclear spins. For convenience we will consider a dynamically polarized nuclear environment 

$$\hat{V}_0 = 0 \text{ and } \hat{V}_{\pm} = \pm \hat{V},$$

with $\hat{V} = \sum_j \left( \hat{A}^{z,x}_{j} \hat{I}^{x}_{j} + \hat{A}^{z,y}_{j} \hat{I}^{y}_{j} + \hat{A}^{z,z}_{j} \hat{I}^{z}_{j} \right).$ (12)

Here the coupling constants for each direction are of the form

$$A^{z,i}_{j} = \frac{\mu_0 \gamma_j}{4 \pi r_j^3} \left( 1 - \frac{3(r_j \cdot \hat{z})(r_j \cdot \hat{z})}{r_j^2} \right),$$

where $r_j$ is a displacement vector between the $j$-th nucleus and the qutrit, while $\hat{x}, \hat{y}, \hat{z}$ are unit vectors in three distinct directions. $\mu_0$ is the magnetic permeability of the vacuum.

The conditional evolution operators of the environment (4) which enter the full system-environment evolution operator (3) are now straightforward to compute (see Ref. [16] for details) and are given by

$$\hat{w}_{\pm 1}(t) = \bigotimes_j \left[ \cos(M^j_{\pm} t) \hat{I}_{j} \pm i \frac{\sin(M^j_{\pm} t)}{M^j_{\pm}} \left( \pm \hat{A}^{z,pl}_{j} \hat{I}^{x}_{j} + (\gamma_c B_z \pm \hat{A}^{z,z}_{j} \hat{I}^{z}_{j}) \right) \right],$$

$$\hat{w}_0(t) = \bigotimes_j \left[ \cos(\gamma_c B_z t) \hat{I}_{j} - i \sin(\gamma_c B_z t) \hat{I}^{z}_{j} \right],$$

with $M^j_{\pm} = \sqrt{A^2_{j} + (\gamma_c B_z \pm A_z)^2}$ and $\hat{A}^{z,pl}_{j} = \sqrt{(\hat{A}^{z,y}_{j})^2 + (\hat{A}^{z,y}_{j})^2}$.

The initial state of the environment, we can find the evolution of the coherences which are needed to detect QEE, namely eq. (10). The thermal-equilibrium state of this environment (with respect to its free Hamiltonian) is effectively proportional to unity due to the small value of the gyromagnetic ratio for $^{13}$C nuclei. As such a state will not lead to entanglement, we will consider a dynamically polarized nuclear environment [41–43], so that

$$\hat{R}(0) = \bigotimes_j \frac{1}{2} (\hat{I}_{j} + p_{j} \hat{I}^{+}_{j}),$$

where $p_{j} \in [-1,1]$ is the polarization of the $j$-th nucleus. In Figs 2 and 3 we plot the difference of the evolution of a single chosen coherence of the qutrit (as a function of time $t$) for different pointer states in the preparation part of the procedure (up to time $\tau$). $\rho_{ij}^{(k)}(\tau, t) - \rho_{ij}^{(q)}(\tau, t)$.

Each figure contains curves corresponding to the all three combinations of pointer states in the preparation stage, $k, q = -1, 0, 1$ (any two would suffice to determine if entanglement would be present for any initial system superposition state after time $\tau$). Fig. 2 shows the difference in evolution for the coherence between the $|0\rangle$ and $|1\rangle$ qutrit states, while Fig. 3 for the coherence between the $|0\rangle$ and $|1\rangle$ states. The evolution of the third coherence is not shown as it would be superfluous. Furthermore, we only show the imaginary part of the difference of the evolution, because the results are more striking in this case, and the real part would not bring anything relevant to the discussion (since the scheme has already witnessed entanglement).

The preparation time $\tau = 3\mu s$ was chosen long so that the presence of the qutrit in a pointer state has the strongest possible effect on the new (post-preparation) state of the environment and consequently the states differ most notably for different pointer states. This in turn enhances the differences observed in qutrit evolution. The magnetic field is $B_z = 0.02$ T. Each plot contains four panels corresponding to four different initial

### Table I: Table of calculated coupling constants for fourteen environmental spins at randomly generated locations around the NV center.

| $k$ | $r_k$ [nm] | $A^{z,x}_{k}$ [1/µs] | $A^{z,y}_{k}$ [1/µs] | $A^{z,z}_{k}$ [1/µs] |
|-----|------------|---------------------|---------------------|---------------------|
| 1   | 0.504422   | 1.37617             | 0                   | 0.973096            |
| 2   | 0.539611   | 0.196941            | 0.682223            | -0.417743           |
| 3   | 0.539611   | -0.689293           | 0.170656            | -0.417743           |
| 4   | 0.539611   | 0.492352            | -0.511667           | -0.417743           |
| 5   | 0.61788    | 0.49393             | 0                   | -0.353124           |
| 6   | 0.63081    | 0.49395             | -0.487809           | -0.018964           |
| 7   | 0.63081    | 0.0134113           | -0.116145           | -0.47416            |
| 8   | 0.667287   | -0.297224           | 0.220631            | -0.300241           |
| 9   | 0.667287   | -0.169842           | 0.58835             | 0.060483            |
| 10  | 0.667287   | 0.282145            | 0.220631            | 0.660531            |
| 11  | 0.667287   | 0                   | 0                   | -0.420338           |
| 12  | 0.684925   | 0.326087            | 0.212057            | -0.223993           |
| 13  | 0.684925   | 0.255553            | -0.048414           | -0.329308           |
| 14  | 0.684925   | -0.327671           | 0.161371            | -0.223993           |
states of the environment, characterized by different polarizations. As in the NV-center spin qubit case [19], an unpolarized environment does not entangle with the qutrit and the magnitude of the observed effect grows with higher initial polarization. The results are given for an environment consisting of fourteen nuclear spins placed at randomly generated locations. Table I contains the distances between each nuclear spin and the NV center, as well as of the coupling constants used, which were calculated using eq. (13).

VII. CONCLUSION

We have proposed a scheme for the indirect detection of entanglement between a system of any dimensionality with an environment interacting via a Hamiltonian which leads to pure dephasing of the qudit. This is a generalization of a scheme proposed for a system composed of a single qubit [19], but even though the number of separability criteria grows quadratically with the size of the system [14], the complexity of the scheme only grows linearly. The price to pay is that the set of states for which entanglement cannot be detected using the scheme is also larger, and entanglement connected with breaking separability criteria based on commutation between products of conditional evolution operators of the environment (which does not exist for a qubit system) cannot be detected.

On the other hand, the scheme only requires straightforward operations and measurements on the system of interest and allows for detection of entanglement in systems too large for any type of state tomography to be feasible. It detects entanglement which manifests itself in the evolution of the environment, and as such is most likely to have an effect on the evolution of the system. The mechanism of the scheme directly relies on the influence of SEE on the evolution of the system, so it will detect the type of entanglement which is bound to be most detrimental to the system (or description of system evolution which assumes separability, such as using quantum channels [1]).

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