A tensor-based entanglement measure for mixed states

Christian Carisch\textsuperscript{1} and Oded Zilberberg\textsuperscript{2}

\textsuperscript{1}Institute for Theoretical Physics, ETH Zürich, CH-8093 Zürich, Switzerland.
\textsuperscript{2}Department of Physics, University of Konstanz, 78464 Konstanz, Germany.
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Entanglement is a key resource for quantum technologies and is at the root of exciting many-body phenomena. Nevertheless, quantifying the amount of entanglement in a real-world quantum system is challenging when it interacts with its environment. Here, we devise an entanglement measure for such realistic open systems. Our measure relies on a tensor-network representation of the system’s density matrix and is readily computed using our presented algorithm. We showcase the virtues of our scheme using a case study of spinless particles moving on a chain in presence of dephasing. Crucially, our approach distinguishes classical from quantum correlations in a broad plethora of systems and motivates efficient experimental entanglement quantification.

The advent of quantum mechanics professed that particles can become far more correlated than classically possible. Such correlations, dubbed entanglement, are a key resource in the present-day quantum revolution. For example, entanglement is harvested in quantum information processing devices \cite{1, 4}, in quantum detectors that break sensitivity limits \cite{5, 7}, or in secure quantum communication protocols \cite{8, 10}. Entanglement can also lead to unique effects such as teleportation \cite{11, 13}, the formation of strong correlations in many-body systems \cite{15, 33}, and the high efficiency of light-harvesting processes \cite{34–36}.

The premise of quantum mechanics relies on having a wavefunction description for particles moving in a closed system. The wavefunction entails probability amplitudes for the state to be in different locations in the Hilbert space of the system. Commonly, the Hilbert space is very large, and entanglement has become a modern tool for compressing the required information needed to properly describe a quantum state \cite{37, 38}. For example, in tensor network representation of quantum states, the Hilbert space is truncated such that only entangled regions are kept based \cite{39, 41}. As such, measures for quantifying entanglement (e.g., entanglement entropy \cite{11, 42}) were developed to assess the potential usefulness of quantum resources, as well as to compress their representation.

In reality, however, all quantum systems are open, i.e., they are coupled to an environment and become correlated with it. The direct result of such coupling is that the state of the system can become mixed, i.e., lose its coherent entanglement features. This is best described by considering the system’s density matrix, which is kin to a covariance matrix of the state’s probability amplitudes. As the density matrix describes both classical and quantum correlations of mixed states, it is challenging to distill the amount of entanglement in the system. Indeed, many mixed-state entanglement measures have been proposed, e.g., (Rényi) negativity \cite{43, 47}, squashed entanglement \cite{48}, or the operator space entanglement entropy (OSEE) \cite{49, 51}. However, so far none of them fulfill all of the following criteria for acting as a useful entanglement measure: (i) not increase under local non-entangling operations (entanglement monotone), (ii) map to a known measure when the system is not mixed with the environment (pure-state limit), and (iii) computed efficiently for realistic many-body systems.

In this work, we devise an entanglement measure based on a tensor decomposition of mixed density matrices. The decomposition generates a so-called operator space entanglement spectrum (OSES). Crucially, we identify that these values describe both classical and quantum correlations. Using this insight, we (1) demonstrate the failure of the OSEE as an entanglement measure, due to the classical contributions that enter it, and (2) propose a filtering of the spectrum that keeps only quantum entanglement information. We thus devise an entanglement measure for realistic open systems that fulfills the criteria (i)-(ii) above by mapping to the negativity in the pure-state limit. Furthermore, we present an efficient algorithm for the computation of our measure, and fulfill criterion (iii).

The entanglement spectrum (ES) of a quantum state $|\psi\rangle$ is defined relative to a bipartition of the system into two parts $A$ and $B$ [see Figs. 1(a) and (b)] as the spectrum of the reduced state $\rho_A = \text{Tr}_B\{|\psi\rangle\langle\psi|\}$. We can also write the Schmidt decomposition of the state relative to this cut

\begin{equation}
|\psi\rangle = \sum_{i=1}^{r} \sqrt{\lambda_i} |i, \mu_i\rangle,
\end{equation}

where $r \geq 1$ is the Schmidt rank, $\sqrt{\lambda_i} \geq 0$ are real-valued Schmidt values, and $|i, \mu_i\rangle = |i\rangle_A \otimes |\mu_i\rangle_B$ with suitable orthonormal sets of states for systems $A$ and $B$. Using the Schmidt basis, we obtain that the ES of Eq. (1) is given by the squares $\lambda_i$ of the Schmidt values \cite{22}. As an entanglement measure for pure states, one often uses the corresponding von Neumann entropy, $S_N \equiv -\text{Tr}\{\rho_A \log \rho_A\} = -\sum_{i} \lambda_i \log \lambda_i$.

Similarly to the pure case, we can define the OSES of a density matrix $\rho$ relative to a bipartition of the system into two parts $A$ and $B$. The density matrix can be written...
relative to the bipartition of the system as

$$\rho = \sum_{i,j \in A, \mu, \nu \in B} \rho_{i,\mu;j,\nu}[i,\mu]⟨j,\nu|,$$

where |i,μ⟩ = |i⟩_A ⊗ |μ⟩_B, and |i⟩_A and |μ⟩_B are basis states of the two parts of the system A and B, respectively. The density matrix is Hermitian, and hence the prefactors in Eq. (2) follow the relation $p_{i,\mu;j,\nu} = p_{j,\nu;i,\mu}^*$. We define the vectorized density matrix as

$$|\rho⟩⟩ = \sum_{i,j \in A, \mu, \nu \in B} \rho_{i,\mu;j,\nu}[i,\mu]⟨j,\nu|,$$

which is obtained by stacking the columns of the density matrix [2] into a column vector. The inner product over such column vectors in terms of their respective density operators is defined as $⟨⟨|ρ⟩|ρ⟩⟩ = Tr|ρ⟩σ$. The OSES of ρ consists of the eigenvalues of the matrix [37]

$$C = \frac{1}{C} Tr_B|\rho⟩⟨|ρ⟩⟩ = \sum_{i,j,k,l \in A, \mu, \nu, p \in B} \rho_{i,\mu;j,\nu}^*[k,\mu,\nu]⟨l,\nu,j,l⟩,$$

where $Tr_B|O⟩ = \sum_{\mu, \nu \in B} ⟨⟨|\mu,\nu⟩|O⟩|\mu,\nu⟩$ is the partial trace over subsystem B. Note that the matrix [1] is a positive operator with trace equal to the purity of the system, i.e., $TrC = Tr(|ρ⟩⟨|ρ⟩⟩ = Tr|ρ⟩$ $2 = P(ρ)$. It involves correlations up to fourth order in the state’s probability amplitudes, and we dub it the kurtosis matrix. Interestingly, the OSES of ρ contains numerous values encoding both cross-boundary classical correlations as well as quantum entanglement contributions. Yet, the sum of all of these values adds up to the purity of the system.

Ostensibly, we would like to employ the OSEE, $S \equiv -Tr(C log C)$, as an entanglement measure [39, 40]. However, for mixed states, doubts on the validity of this approach arose [41, 42]. Using our construction [1], we can readily show why entanglement in open systems cannot be captured by this entropy. We use a counterexample: consider a pure state with a single excitation residing solely within subsystem A, e.g., subsystem A is composed of states |1⟩ and |2⟩, whereas subsystem B of state |3⟩, see Fig. 1(b). We take the quantum state to be in an equal superposition, $|ψ⟩ = (|1⟩ + |2⟩)/\sqrt{2}$. The corresponding OSES has a single nonvanishing value $Λ_A$ [cf. Eq. (3) and discussion below]. Hence, for our pure system $C = Tr(C) = P(ρ) = 1$. Correspondingly, $S = -Λ_A log Λ_A = 0$ as expected for a pure product state. We now couple subsystem A to a dephasing environment, i.e., no particles leak out, but the system decoheres into a mixed state $ρ'$ after some time. As the particle remains in subsystem A, we still have a single eigenvalue $Λ_A'$ that corresponds to a reduced purity $P(ρ') < 1$ of the system. We, thus, obtain that the resulting entanglement entropy increases to $S' = -Λ_A' log Λ_A' > 0$ even though the local operation on subsystem A cannot generate entanglement between subsystems A and B. This is the first main result of this work.

In Fig. 1(c), we show the outcome of our counterexample with increasing dephasing. The latter is obtained by mixing the pure state with the classical mixture of the particle being either in state |1⟩ or |2⟩, namely

$$ρ_p = (1 - p)|ψ⟩⟨ψ| + pσ,$$

with $σ = (|1⟩|1⟩ + |2⟩|2⟩)/2$, see Fig. 1(b). The entanglement entropy increases with increasing weight p of the non-entangled classical mixture. As a result, the density matrix entanglement entropy is not an entanglement monotone and cannot serve as a good measure for bipartite entanglement in an open system. Furthermore, we identify that some of the OSES bear no bipartite information, e.g., $Λ_A$ in our example. Hence, any entanglement measure of the system should exclude such values from the spectrum. Such a filtering of spectral values may be challenging for a many-body system on a large Hilbert space.

For pure states $|ψ⟩$, however, such filtering is relatively straightforward: we can write the C-matrix [4] of a density matrix $|ψ⟩⟨ψ|$ using the state’s Schmidt basis [cf. Eq. (1)]

$$C = \sum_i λ_i^2|i,i⟩⟨i,i| + \sum_{j \neq i} λ_iλ_j⟨i,j⟩⟨j,i⟩.$$

In this basis, the C-matrix is diagonal and its spectrum consists of r eigenvalues of type $λ_i^2$ and $r(r-1)/2$ two-fold degenerate eigenvalues of type $λ_iλ_j$. Thus, we see that in this pure limit, the OSES of the density matrix is
equivalent to the outer product of the ES of the state \[^{37}\]. We can also readily verify using Eq. (6) that only a single nonvanishing value appears in the pure limit of the example of Fig. 1(b), stemming from a single \(\lambda_i^2\) value.

Now, recall that a pure state \(^{1}\) is entangled if and only if its Schmidt rank is \(r > 1\). As the second sum in Eq. (6) also vanishes for \(r = 1\) and is finite and positive for \(r > 1\), we propose the sum over these eigenvalues as our entanglement measure,

\[
\mathcal{M} := \sum_{j \neq i} \lambda_i \lambda_j .
\] (7)

In other words, we define our entanglement measure for pure states as the sum over eigenvalues of the matrix \(\mathbf{C}\) that are inherently degenerate and filter out the \(\lambda_i^2\) values.

Crucially, our measure (7) is closely related to the negativity of the state, which is defined as the absolute value of the sum over all negative eigenvalues of the partial transpose \(\rho^{12}\) of the density matrix \[^{13}\]. Using the Schmidt basis \(^{3}\) the negativity reads

\[
\mathcal{N} = \frac{1}{2} \sum_{j \neq i} \sqrt{\lambda_i \lambda_j} .
\] (8)

Thus, our Eq. (7) inherits the desirable properties of the negativity as an entanglement measure for pure states, which is a second main result of this work. Furthermore, the definition of the measure (7) via the matrix \(\mathbf{C}\) lends a natural extension to open systems. The challenge of this block diagonal form is shown in Fig. 1(d).

We can also readily verify using Eq. (6) that only a singlet form of this block diagonal form is shown in Fig. 1(d).

FIG. 2. (a) Examples of configurations of two particles on four sites with respect to a bipartition in the middle. Yellow shadings mark entanglement. (b) and (c) OSES corresponding to the configurations in (a) along a mixing interpolation [cf. Eq. (5)]. (1) marks an avoided crossing between spectral values of a classically correlated and those of an entangled \(AB\) configuration. (d) MPO representation of a density matrix on 4 sites. (e) Negativity \(\mathcal{N}\) [cf. Eq. (5)], purity \(P\), and entanglement measures \(M_1\) and \(M_2\) for the spectrum in (b) and (c).

In the following, we compare the eigenvalues of the blocks \(\mathcal{C}_{n,n'}\) with the pure case limit (6), and thus arrive to the definition of an entanglement measure for mixed states. We accompany our general discussion with an example of a chain with \(N = 2\) spinless particles residing on 4 sites, see Fig. 2. We begin with the blocks \(\mathcal{C}_{0,0}\) and \(\mathcal{C}_{N,N}\), which are rank 1 and have eigenvalues \(\Lambda_{0,0} = \sum_{\mu,\nu} |\rho_{0,\mu;0,\nu}|^2\) and \(\Lambda_{N,N} = \sum_{\mu,\nu} |\rho_{N,\mu;N,\nu}|^2\), corresponding respectively to the scenario where all \(N\) particles reside solely in subsystem \(B\) or \(A\), see Fig. 2(a).

Therefore, these eigenvalues do not contain any information about cross-boundary coherence and should not contribute to our entanglement measure. Indeed, these values are generally non-degenerate, and we identify that they reduce to eigenvalues of type \(\lambda_i^2\) in the pure case limit, cf. Eq. (7). Furthermore, such values do not vanish for a fully mixed state [see Fig. 2(b)], justifying our original choice to not include them in our entanglement measure (7).

The blocks \(\mathcal{C}_{n,n'}\) for \(n \neq n'\) describe a scenario where at least one of the particles is in a coherent cross-boundary state and clearly encode entanglement information. Note that in this case the blocks \(\mathcal{C}_{n,n'}\) and \(\mathcal{C}_{n',n}\) generate the same eigenvalues as they are related via a unitary transformation, \(\mathcal{C}_{n,n'} = \mathcal{U}\mathcal{C}_{n',n}\mathcal{U}^{-1}\), with the permutation \(U[i,j'] = |j',i\rangle\). Hence, such “coherent” eigenvalues of \(\mathbf{C}\) are inherently degenerate, and must map to the eigenvalues of type \(\lambda_i\lambda_j\), in the pure case limit (6). Therefore, we will include these eigenvalues in our extension of the entanglement measure to the mixed case, i.e., by sum-
purity

P

keep the (blue) spectral values that vanish for \( p \) using interpolation of the state to a fully decohered state. We bipartition at the middle bond. (b) OSES at the bipartition.

A function of space along time. Dashed white line denotes subject to dephasing [cf. Eq. (11)]. (a) Particle density as follows algorithm that is readily realized using a (tensor) matrix-product operator (MPO) decomposition of \( \rho \) [cf. Fig. 2(d)]: (i) obtain the OSES of \( \rho \) using the MPO, (ii) interpolate the given distribution to a pure-state limit [cf. Eq. (3)] and sum over the values that smoothly end up degenerate under this homotopy \( M_1 \), and (iii) similarly interpolate [also using Eq. (3)] to the fully mixed limit and sum over the values that vanish under this second homotopy \( M_2 \). Importantly, such an interpolation is conveniently performed in the MPO representation, as additions of MPOs is efficient. Note, however, that due to the avoided crossings in the eigenvalues of blocks with \( n = n' \notin [0, n] \) [cf. Fig. 2(c)], the two homotopies do not necessarily identify the same values, \( M_1 \neq M_2 \), see Fig. 2(e): Using (ii) we find the correct entanglement measure value in the pure limit, but overestimate the entanglement in the fully mixed limit, whereas using (iii) we correctly identify zero entanglement in the fully mixed limit, but underestimate the entanglement of the pure state. To better identify the correct values, our algorithm can be augmented to identify points where avoided crossing occur, e.g., by comparing the overlaps between the eigenstates before and after such crossings. The algorithm is the fourth main result of this work.

We turn now to demonstrate our algorithm by measuring the entanglement of a realistic open system scenario. We consider a system of \( N = 2 \) spinless particles moving on a 1D chain with 12 sites in the presence of dephasing. The time evolution follows a Lindblad master equation

\[
\frac{\partial \rho}{\partial t} = -i[H, \rho] + \gamma \sum_i (2n_i \rho n_i - \{n_i, \rho\}) ,
\]

where \( H = J \sum_i c_i^\dagger c_{i+1} + h.c. \) and local density operators \( n_i = c_i^\dagger c_i \). The parameters \( J \) and \( \gamma \) are the hopping amplitude and the dephasing coupling rate to local baths, respectively.

We initialise the system in a product state of one particle on site 1 and the other on site 11, and evolve Eq. (11) using time evolving block decimation (TEBD) with the JULIA ITensors package [54]. In Fig. 3(a), we present the resulting particle density of the quantum random walk of the two particles. The OSES associated with a bipartition at the middle bond is directly obtained from the MPO representation throughout the time evolution [11], see Fig. 3(b). Note that the MPO description relies on a singular value decomposition with singular values that are square-roots of the OSES values. As expected for a product state, the OSES at \( t = 0 \) consists of a single value only, describing one particle in each of the subsystems to the left and right of the cut. Along the time evolution, the particles may delocalize across the cut, thus leading to bipartite entanglement, whereas the Lindblad terms decrease the purity of their distribution, see Fig. 3(c). Importantly, we can extract our entanglement measure from the OSES at any point along the time evolution,
see Fig. 3(c). This is performed using our filtering algorithm at different time steps, see inset of Fig. 3(b). Note that by repeated entanglement analysis during the time evolution, we avoid large discrepancies between \( \mathcal{M}_1 \) and \( \mathcal{M}_2 \) [see minor jumps in the entanglement measure in Fig. 3], and for simplicity do not include cross-gap homotopy tracking.

Our OSES filtering approach is readily generalized to mixed particle number cases, where we expect avoided crossings between the OSES of the different Fock blocks that our homotopy-based algorithm will identify. Experimentally, our measure can be obtained by estimating the purity of the mixed state \([56, 57]\) and subtracting the values encoding classical correlations, which are constructed out of local density measurements. Our study provides an important step towards the understanding of entanglement in open many-body systems with potential impact in a plethora of contemporary activities, including noisy intermediate-scale quantum era systems \([58, 59]\) and error-correction schemes \([60, 63]\).

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