Improving producibility estimation for mixed quantum states

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We introduce a new functional to estimate the producibility of mixed quantum states. When applicable, this functional outperforms the quantum Fisher information, and can be operatively exploited to characterize quantum states and phases by multipartite entanglement. The rationale is that producibility is expressible in terms of one- and two-point correlation functions only. This is especially valuable whenever the experimental measurements and the numerical simulation of other estimators result to be difficult, if not out of reach. We trace the theoretical usability perimeter of the new estimator and provide simulational evidence of paradigmatic spin examples.

Introduction—Entanglement is the queen of quantum behavior, its compelling characterization being central to engineer quantum phases of matter and to develop related quantum technologies [1–3]. Entanglement quantifiers are especially relevant in quantum metrology and estimation theory [4–10], and are recognized to be valuable tools to describe quantum phases and quantum phase transitions [11, 12]. Research has mostly focused on bipartite entanglement [1, 13–14], typically via the Von Neumann entropy [1, 13–17], entanglement spectrum [18–23], and generally pairwise entanglement [1, 14, 24, 25]. Unfortunately, all of these entanglement witnesses are typically challenging to be characterized in experiments [1, 6, 7, 14, 26], if not just unsuited to capture the complexity of certain quantum phases.

Alternative entanglement quantifiers involve the so-called multipartite entanglement (ME) among a number of system subsets [4], a very general property, dense with useful information. The identification of ME criteria is still a challenging problem, especially when their experimental detection is concerned. Prominent tools for ME quantification have been for instance Wineland’s spin-squeezing parameter [2, 27, 28], and the quantum Fisher information (QFI), presently known as the ultimate bound for ME [4, 29]. They are both related to ME via well-stated relations [8, 9, 29–31] and can notably be detected in experiments [32–34]. The spin-squeezing parameter and the QFI provide efficient tomography [35, 36] for quantum phase and relative transitions [32, 37–42], and are proposed as benchmarks for quantum simulators [35]. In fact, ME has been investigated e.g. in spin systems [32, 37, 38, 42–44], also at criticality [45–48], with long-range interactions [49–53], and in topological models [39, 40, 54, 55].

Calculating the QFI in the case of mixed states appears to be difficult, and it has been performed only in a limited number of cases [32, 41, 44]. One reason is that QFI cannot be fully expressed in terms of (one- and two-point) correlation functions [41]. This contrasts with the commonly accepted fact that entanglement can be somehow witnessed entirely by connected correlations [56], and that the QFI has the meaning of a susceptibility [32].

In this work, we therefore propose a new ME quantifier based on the sum of connected correlations. We illustrate the scenarios in which it is favorably used for mixed states, meaning that it either coincides with the QFI, or it shares or even improves the QFI bounds, while remaining easily accessible in measurements and simulations. We identify the usability criteria and trace their relationship with symmetry conditions. After a theoretical classification of examples in which our new estimation tool is valuable, we highlight non-trivial interesting cases by numerical simulations, opening the perspective of its extensions to open quantum systems.

QFI — A central tool in estimation theory [4] is the quantum Fisher information (QFI), defined via the fidelity between a pure quantum state |ψ(θ)⟩, depending on a parameter θ, and its infinitesimal variation |ψ(θ + dθ)⟩: \( F(\theta, d\theta) = ||\psi(\theta)\psi(\theta + d\theta)||^2 \approx 1 - F(\theta)(d\theta)^2/4 \). Among the possible transformations relating |ψ(θ)⟩ and |ψ(θ + dθ)⟩ on discrete systems, like numerable sets of qubits or lattices (in the following labelled by x and y), a relevant choice is the unitary evolution generated by a collective Hermitian operator \( \hat{O} = \sum_{x} \hat{o}(x)|\psi(\theta + d\theta)\rangle = e^{i\hat{O}(\theta)}|\psi(\theta)\rangle \). For d-dimensional N-component systems, the QFI can be cast in terms of two-point connected correlations (the θ dependence being neglected) [57]

\[
\langle \psi|\hat{o}(x)\hat{o}(y)|\psi \rangle_{\text{con}} \equiv \langle \psi|\hat{o}(x)\hat{o}(y)|\psi \rangle - \langle \psi|\hat{o}(x)|\psi \rangle\langle \psi|\hat{o}(y)|\psi \rangle,
\]

(1)
as
\[
F[|\psi\rangle, \hat{O}]_N = 4 \sum_{x, y} \langle \psi | \hat{o}(x) \hat{o}(y) | \psi \rangle_{\text{conn}}. \tag{2}
\]

For general mixed states, described by density matrices \(\rho\) and \(\sigma\), the fidelity is defined as \(\mathcal{F}(\theta, d\theta) = \left( \text{Tr} \sqrt{\rho \sigma \sqrt{\rho}} \right)^2\) [4, 58]. This can be applied to two infinitesimally-separated density matrices \(\rho(\theta)\) and \(\rho(\theta + d\theta) = e^{i d \theta \hat{O}} \rho(\theta) e^{-i d \theta \hat{O}}\), using the same definition for \(\hat{O}\) and the same expansion in \(d\theta\) as for pure states. Thus, in an orthonormal basis \(|\lambda\rangle\), where \(\rho(\theta)\) is diagonal (\(= \rho_D\) in the following), the QFI can be cast in the form:
\[
F[\rho_D, \hat{O}]_N = 2 \sum_{x, y, \lambda, \nu} \left( \frac{p_\lambda - p_\nu}{p_\lambda + p_\nu} \right)^2 \langle \lambda | \hat{o}(x) | \nu \rangle \langle \nu | \hat{o}(y) | \lambda \rangle. \tag{3}
\]

This reduces to (2) when \(p_\lambda = 1\) for just a given state \(|\lambda\rangle\), and is zero otherwise. Given that mixing quantum states cannot increase the entanglement content, as well as the related achievable estimation sensitivity [4], in order to witness entanglement, \(F[\rho_D, \hat{O}]_N\) is strictly required to fulfill the convexity property \(F[\rho_D, \hat{O}]_N \leq \sum_\lambda p_\lambda F[|\lambda\rangle, \hat{O}]_N\), with \(p_\lambda \geq 0\), the bound being saturated by pure states. Relevant properties of the QFI are reported in the Supplementary Material (SM1).

We now recast the QFI (3) in a form that explicitly brings forward the connected correlations, that is [41, 59]:
\[
F[\rho_D, \hat{O}]_N = 4 \sum_{x, y, \lambda} p_\lambda \langle \lambda | \hat{o}(x) \hat{o}(y) | \lambda \rangle - 4 M - 4 R, \tag{4}
\]

with \(M = \sum_\lambda p_\lambda \sum_\nu \frac{2 p_\nu}{p_\lambda + p_\nu} \langle \lambda | \hat{O} | \nu \rangle \langle \nu | \hat{O} | \lambda \rangle \geq 0\) and \(R = M - \sum_\lambda p_\lambda \langle \lambda | \hat{O} | \lambda \rangle \langle \lambda | \hat{O} | \lambda \rangle \geq 0\). Before pushing further on the relationship between the QFI and connected correlations, it is useful to introduce the concept of multipartite entanglement.

Multipartite Entanglement (ME)– Part of the recognized importance of the QFI (2) is that it witnesses ME [8, 9, 29], as suggested by the very sum of connected correlations (2). For a discrete system, c-partite entanglement (here meant spatial) implies that a partition \(\{\psi_i\}\) exists, where some states (at least one) contain c components and the others less than c. Thus, \(|\psi\rangle = \bigotimes_i |\psi_i\rangle\) is said c-producible [4], with entanglement depth \(c\) [6, 31]. In a lattice, the subsystems are not necessarily adjacent sites.

Let us begin with the case of pure states. The violation of the inequality for the QFI density \(f[|\psi\rangle, \hat{O}]_N \equiv F[|\psi\rangle, \hat{O}]_N / N\),
\[
\lim_{N \to \infty} f[|\psi\rangle, \hat{O}]_N = f[|\psi\rangle, \hat{O}]_N \leq 4c, \tag{5}
\]
signals at least \((c+1)\)-partite entanglement between the \(N\) components of the considered system, with \(1 \leq c \leq N\) [4, 29]. In (5), \(k = \text{Var} \hat{o}(x) = (m - n)^2\), if \(\hat{o}(x)\) is bounded, with eigenvalues \(n \leq \lambda \leq m < \infty\). Actually, \(c\) can also diverge with \(N, c \sim N^l\). The upper bound \(F[|\psi\rangle, \hat{O}]_N = N\) is called the Heisenberg limit and \(|\psi\rangle\) is then said to have genuine ME. The bound (5) can be modified as [30]
\[
F[\rho_D, \hat{O}]_N \leq 4k [sc^2 + \sum_{\nu} (N - s c^2)], \tag{6}
\]
with \(s = [N/c]\), and generalized to [31]
\[
F[\rho_D, \hat{O}]_N \leq 4k [c(N - p) + N], \tag{7}
\]
accounting for \(p\) disentangled partitions.

The same bounds (5)-(7) apply to mixed states. Quite critically, c-producibility holds here if \(\rho \equiv \rho_P\) can be decomposed (generally not uniquely) as \(\sum_\lambda p_\lambda \prod_i |\lambda_i\rangle\langle \lambda_i|^\otimes\), with \(p_\lambda, i = \sum_{\langle i| i\rangle} |\lambda_i\rangle\langle \lambda_i|\), and equivalently
\[
\rho_P = \sum_\lambda p_\lambda \prod_i |\lambda_i\rangle\langle \lambda_i|^\otimes \prod_k (\lambda, k) = \sum_\lambda p_\lambda |\lambda\rangle\langle \lambda|. \tag{8}
\]

The symbol \(\prod_i |\lambda\rangle\langle \lambda|^\otimes\) labels the Kronecker product, while \((i, j, k)\) label disentangled partitions with fewer than \(c\) components. In general, the states \(|\lambda, i\rangle\), \(\forall i\), and the c-producible \(|\lambda\rangle\) are not an orthogonal basis, thus \(p_\lambda\) is not diagonal in this basis and \(\text{Tr} \rho_P \neq \sum_\lambda p_\lambda\). Eq. (8) means that states of disentangled subsystems are classically correlated, with weights \(\tilde{p}_\lambda\). One example is the set of Boltzmann weights: energy degeneracies can hide producibility, though at least one basis must be producible.

For mixed states, violating (5) is still a sufficient condition for at least \(c+1\)-partite entanglement. However, since entanglement is expected to be encoded in connected correlations, it looks counterintuitive that \(F[\rho_D, \hat{O}]_N\) cannot be expressed entirely in their terms. We now investigate this apparent puzzle.

ME via connected correlations – If c-partite entanglement holds for \(\rho = \rho_P\) along (8), then the bound (5) for pure states works also for the average of connected correlations on \(|\lambda\rangle\), with \(\sum_\lambda \tilde{p}_\lambda = 1\). Indeed [60]:
\[
\hat{F}[\rho_P, \hat{O}]_N \equiv 4 \sum_\lambda p_\lambda \left( \sum_{x, y} \langle \lambda | \hat{o}(x) \hat{o}(y) | \lambda \rangle_{\text{conn}} \right) \leq 4ckN \sum_\lambda \tilde{p}_\lambda = 4ckN. \tag{9}
\]

Thus, \(\hat{F}[\rho_P, \hat{O}]_N\) still witnesses ME, and can similarly be shown to fulfill (6) and (7). Therefore, we propose to exploit \(\hat{F}[\rho_P, \hat{O}]_N\) for producibility estimation. This is possible provided that \(\hat{F}[\rho_P, \hat{O}]_N\) is covariant (it assumes the same form in every basis).

Notice that (9) critically exploits c-producibility of all
the states $|\lambda\rangle$, with the same space partition, so that the bound (5) holds for all of them. No orthonormality hypothesis of the $|\lambda\rangle$ set is therefore required. As far as the standard QFI, violating (9) implies at least $c+1$-partite entanglement; accordingly $\tilde{F}[\rho_P,\hat{O}]_N$ correctly fulfills (saturates) the convexity inequality after Eq. (3).

**Requiring covariance** – The producible basis $|\lambda\rangle$ and $p_{\lambda}$ are not generally known a priori. Thus, for $\tilde{F}[\rho_P,\hat{O}]_N$ to be really useful in practical calculations, a covariant form is required.

Even if $\text{Tr}_\rho$ is not expressed as $\sum_\lambda p_{\lambda}$ when the $|\lambda\rangle$ are not orthogonal, the first term $\tilde{F}_1[\rho_P,\hat{O}]_N \equiv 4 \sum_{x,y} \sum_\lambda p_{\lambda} (|\lambda\rangle\langle\lambda|\hat{O}(x)\hat{O}(y)|\lambda\rangle)$ in $\tilde{F}[\rho_P,\hat{O}]_N$ can be recast as

$$\tilde{F}_1[\rho_P,\hat{O}]_N = 4 \sum_{x,y} \text{Tr}_\rho \langle\hat{O}(x)\hat{O}(y)\rangle = 4 \text{Tr}_\rho \tilde{F}^2.$$ (10)

This expression is covariant under a generic local basis change, i.e. $U : |\lambda\rangle \rightarrow |\lambda\rangle$, $\tilde{F}_1[\rho_P,\hat{O}]_N \rightarrow \tilde{F}_1[\rho_P,\hat{O}']_N = \tilde{F}_1[\rho,\hat{O}]_N$, with $\rho = U \rho_P U^{-1}$, and $\hat{O}' = U \hat{O} U^{-1} = \sum_x \hat{O}(x)$. The second term $\tilde{F}_2[\rho_P,\hat{O}]_N \equiv \sum_{x,y} \sum_\lambda p_{\lambda} (|\lambda\rangle\langle\lambda|\hat{O}(x)\hat{O}(y)|\lambda\rangle \langle\lambda|\hat{O}(y)\hat{O}(x)|\lambda\rangle) \geq 0$ instead is not covariant, transforming as

$$\tilde{F}_2[\rho,\hat{O}']_N = 4 \sum_{x,y} \sum_\lambda p_{\lambda} (|\lambda\rangle U \hat{O}(x) U^{-1}|\lambda\rangle \langle\lambda| U \hat{O}(y) U^{-1}\rangle |\lambda\rangle.$$ (11)

Notably, since $p_{\lambda} \neq p_{\lambda}$ in (4) and (11), $\tilde{F}_2[\rho,\hat{O}']_N \neq 4(M-R)$, also if $|\lambda\rangle$ is an orthogonal basis diagonalizing $\rho$, provided that they both differ from zero. Instead, the vanishing of one quantity implies the vanishing of the other quantity, in all the equivalent bases. From now on, $\hat{O}' \equiv \hat{O}$ in any basis.

To summarize, the functional $\tilde{F}[\rho,\hat{O}]_N$ is mathematically well defined in any basis for $\rho$, and is by construction the best possible estimation for $c$-producibility (neglecting high-order correlations). However, it is generally inapplicable in real physical calculations or experiments, since $\tilde{F}_2[\rho,\hat{O}]_N$ is not covariant. In spite of this, there are a number of physically relevant cases where this problem can be avoided:

(i) A lattice whose states fulfill the cluster decomposition condition $|\lambda\rangle\hat{O}(x)\hat{O}(y)|\lambda\rangle = |\lambda\rangle\hat{O}(\lambda)\hat{O}(\lambda)|\lambda\rangle$ while $|x-y| \rightarrow \infty$ [61–63] (see also SM2). In this case, $\tilde{F}[\rho,\hat{O}]_N$ can be cast in an orthonormal basis as

$$\tilde{F}[\rho,\hat{O}]_N = 4 \sum_{x,y} \left[ C(x,y) - C_{\infty}(x,y) \right].$$ (12)

with $C(x,y) \equiv \sum_{n,m} p_{nm} m \langle m|\hat{O}(x)\hat{O}(y)|n\rangle$ and $C_{\infty}(x,y) \equiv \sum_n \lim_{|x-y| \rightarrow \infty} p_{nm} \langle m|\hat{O}(x)\hat{O}(y)|n\rangle$. This expression takes a particularly simple trace form: indeed the sum of connected correlations, in a basis where $p_{nm} = p_{nm} \delta_{nm}$ (see SM3 for details). Cluster decomposition is generally required, but not sufficient, to have $c < N$ in (5). Indeed, its violation by non-degenerate pure states requires that $\langle\psi|\hat{O}(x)\hat{O}(y)|\psi\rangle_{\text{conn}} \sim |x-y|^\beta$ for $|x-y| \rightarrow \infty$, $\beta \geq 0$, implying $c = N$. Instead, the described trouble with $\tilde{F}_2[\rho,\hat{O}]_N$ (which $C_{\infty}(x,y)$ stems from) is directly related to its general violation by mixed states. The limit $|x-y| \rightarrow \infty$ in $C_{\infty}(x,y)$ is a single number under the additional assumption that $|\lambda\rangle\hat{O}(x)|\lambda\rangle$ does not depend on $x$. This might be the case for the stronger condition of translational invariance, or for an emerging order parameter. In the former case, ME immediately holds and $\tilde{F}[\rho,\hat{O}]_N$ can still characterize many-body phases [35, 40, 41], though not strictly required as a producibility estimator.

(ii) A system with a non-degenerate energy spectrum, e.g. with no Hamiltonian symmetries $\hat{V}$ for $\rho$, such that $[\hat{V},\rho] = 0$ [64]. In this case, $H = \sum_i H_i$, with $H_i$ governing each non-entangled $i$-th subset. This is the case for $\rho$, the spectrum is also producible and $\tilde{F}[\rho,\hat{O}]_N$ can be directly calculated on it. If degeneracies instead occur, mixing producible eigenstates of $H$ generally spoils their producibility. The same reasoning holds for any Hermitian operator $\hat{O}$ commuting with $\rho$, if its eigenvectors are not degenerate.

(iii) $\tilde{F}_2[\rho,\hat{O}]_N = \sum_{\lambda} p_{\lambda} (|\lambda\rangle\langle\lambda|\lambda\rangle^2 = 0 \text{ in (11)}, i.e.}$ $|\lambda\rangle\langle\lambda|\lambda\rangle \neq 0 \forall |\lambda\rangle = U|\lambda\rangle$, since $p_{\lambda} \geq 0$. In this case, $\tilde{F}[\rho,\hat{O}]_N = \tilde{F}_1[\rho,\hat{O}]_N$ in any basis, since the condition is independent of $U$ (indeed, $\hat{O}$ also changes with $U$). Importantly, to estimate producibility via $\tilde{F}[\rho,\hat{O}]_N$, the precise form of $\hat{O}$ is required in the working basis only. $\tilde{F}_2[\rho,\hat{O}]_N = 0$ occurs e.g. whenever $\hat{O}$ changes some quantum number $n$ due to a symmetry $\hat{V}$ of $\rho$. Given a $|\lambda\rangle$ basis, $\hat{O}$ can be chosen with the above criterion. Instead, for a chosen $\hat{O}$, a physically relevant $|\lambda\rangle$ can be often identified, such that $\tilde{F}_2[\rho,\hat{O}]_N = 0$. One very general situation of this kind is an array of qubits or a spin lattice [4, 31, 40, 41], with $\hat{O}(x)$ being e.g. a spin component $\hat{s}_i$, $i = 1-3$. For instance, for $n \geq 2$ spin-1/2, $\hat{O}(x) = \sigma_+^x / \sqrt{2}$ and the basis are eigenstates of $\sigma_+^x$. Thus $\tilde{F}_2[\rho,\hat{O}]_N = 0$, and $\tilde{F}[\rho,\hat{O}]_N = \tilde{F}_1[\rho,\hat{O}]_N$.

**F vs. QFI** – In the light of Eq. (4), it is worthwhile to ask if and how the QFI and $\tilde{F}[\rho,\hat{O}]_N$ are related. Due to (11), this comparison is difficult in generic bases and situations. Instead, we assume that $\rho = \rho_D$ in an orthogonal basis, and $\tilde{F}_1[\rho,\hat{O}]_N = 4(M-R) = 0$. Then, the QFI and the covariant $\tilde{F}[\rho_D,\hat{O}]_N$ differ by $4M = 4R$. This fact also implies that they cannot just differ by a basis change, in general. Strikingly, since $M \geq 0$, $\tilde{F}[\rho_D,\hat{O}] \geq \tilde{F}[\rho_D,\hat{O}]_N$, a better producibility estimation is provided by $\tilde{F}[\rho_D,\hat{O}]_N$ (when covariant), compared to $\tilde{F}[\rho_D,\hat{O}]_N$, via the common bounds (5)–(7). Notably, the condition $M = 0$, such that the QFI reduces to (10), can be much more restrictive and (computationally) demanding than that for the covariant $\tilde{F}[\rho_D,\hat{O}]_N$, $|\lambda\rangle\langle\lambda|\lambda\rangle = 0 \forall \lambda$. Application of the same argument as in (iii) (for $\tilde{F}_2[\rho,\hat{O}]_N$) to $|\langle\lambda|\hat{O}|\nu\rangle|^2$, implies that if $M = 0$
Dissipation rates are denoted by $\gamma_S$ and $\gamma_{S_z}$.

Fig. 1 shows the time evolution of the different functionals, starting from the ground state of $H$, with $S_z = 0$, in the presence of two forms of dissipation. We also plot the variance of $S_x$ (defined in Fig. 1 (a)), which reduces to (10), and also coincides with $\mathcal{F}[\rho, S_x], N$, when $M - R = 0$. In Fig. 1 (a), we include dissipation $L_j = \hat{\sigma}_j^z$. As the $S_z$ symmetry is conserved throughout the evolution, $\langle \lambda \hat{S}_j^z | \nu \rangle = 0$ and $M - R = 0$ at any time, then also the QFI reduces to (10). In contrast, when the dissipation $L_j = \hat{\sigma}_j^z$ does not preserve the magnetization, as in Fig. 1 (b), the QFI quickly differs from the variance. However, $\mathcal{F}[\rho, S_x], N = \mathcal{F}[\rho, S_x], N$ is still an effective estimator, bigger than QFI, even when the symmetry is dissipatively broken. There are naturally also scenarios where $M - R \neq 0$ and $\tilde{F}_2[\rho, S_x], N \neq 0$, e. g. in the case of a non-zero transverse field $h_x \neq 0$, see SM4.

Further estimators – We finally turn to provide additional producibility estimators, starting from (9), i.e:

$$\mathcal{F}[\rho, S_x], N = 4 \sum_{x,y} \sum_{\lambda} \left| \langle \lambda | \hat{o}(x) \hat{o}(y) | \lambda \rangle \right| \left| \lambda \rangle \right| \left| \lambda \rangle \langle \lambda \right| \con (14)$$

$$\mathcal{F}[\rho, S_x], N = 4 \sum_{x,y} \sum_{\lambda} \left| \langle \lambda | \hat{o}(x) \hat{o}(y) | \lambda \rangle \right| \left| \lambda \rangle \right| \left| \lambda \rangle \langle \lambda \right| \con (15)$$

Notably, also $| \hat{F}[\rho, S_x], N$ can be covariant, similarly as $\mathcal{F}[\rho, S_x], N$. Exploiting the triangular inequality on $\mathcal{F}[\rho, S_x], N$ in (9), it can be shown that (14) and (15) both bound $\mathcal{F}[\rho, S_x], N$ from above, and still fulfill the bound (9), under the hypothesis of c-producibility:

$$\mathcal{F}[\rho, S_x], N \leq | \hat{F}[\rho, S_x], N \leq \mathcal{F}[\rho, S_x], N \leq 4 c k N. \ (16)$$

Moreover, $| \hat{F}[\rho, S_x], N$ and $\mathcal{F}[\rho, S_x], N$ also fulfill the convexity inequality after Eq. (3). Therefore, they are both efficient estimators for c-producibility, even better than the QFI and $\mathcal{F}[\rho, S_x], N$. In particular, $\mathcal{F}[\rho, S_x], N$ is the best possible estimator for mixed states, at least when the dominance of higher-order correlations can be ruled out. This requirement is customary in physical systems; however, the general lack of covariance for $\mathcal{F}[\rho, S_x], N$ can limit its applicability (as in the cases (iii)) for not pure states. Finally, (16) can be also generalized as in (6) and (7).

Conclusions – We have provided the producibility estimator $\mathcal{F}[\rho, S_x], N$ in (9), in terms of one- and two-point correlations, and its applicability perimeter. This quantity, when exploitable, resulted to be more efficient than the QFI, and likely more accessible in simulations and measurements. Our analysis holds for discrete systems, however it can be extended to continuous systems [68, 69], though in general one does not know to which degree. Future efforts are also worth to extend the present approach to open and out-of-equilibrium systems [44, 70, 71], under conditions
of progressive symmetry breaking, as due to dissipative processes and external fields, and to neural networks.

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Improving producibility estimation for mixed quantum states:
Supplementary Material

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In this Section, we recall some elements of the general theory of QFI for mixed states [1]. For two mixed states, described by density matrices ρ and σ, the fidelity, similar to that for pure states, is defined as:

$$F(\theta, d\theta) = \left( \text{Tr} \sqrt{\rho \sigma} \sqrt{\rho} \right)^2.$$  \hspace{1cm} (1)

The last expression is considered applied to two infinitesimally-separated density matrices

$$\rho(\theta) = \sum_{\lambda} p_{\lambda} \rho_{\lambda}(\theta), \quad \rho_{\lambda}(\theta) = |\lambda(\theta)\rangle \langle \lambda(\theta)|,$$  \hspace{1cm} (2)

and $\rho(\theta + d\theta) = e^{-i d\theta \hat{O}} \rho(\theta) e^{i d\theta \hat{O}}$, $\hat{O}$ labelling a generic Hermitian operator. There, $0 \leq p_{\lambda} \leq 1$, and the basis $|\lambda\rangle$ is chosen orthonormal, then $\rho(\theta) = \rho_D$ is in its diagonal form. The resulting QFI, $-2 \frac{d^2 F(\theta, d\theta)}{d\theta^2}$, reads:

$$F[\rho_D, \hat{O}]_N = 2 \sum_{x,y, \lambda, \nu} \frac{(p_{\lambda} - p_{\nu})^2}{p_{\lambda} + p_{\nu}} \langle \lambda|\hat{o}(x)|\nu\rangle \langle \nu|\hat{o}(y)|\lambda\rangle,$$  \hspace{1cm} (3)

that clearly reduces to the QFI for a pure state in Eq. (1) of the main text, since in that case $p_{\lambda} = 1$ just for a certain state $|\lambda\rangle$, vanishing for the other ones. The QFI in Eq. (3) fulfills the inequality [1]

$$F[\rho_D, \hat{O}] \leq \sum_{\lambda} p_{\lambda} F[|\lambda\rangle, \hat{O}]_N,$$  \hspace{1cm} (4)

the bound being saturated by pure states. This convexity inequality is strictly required by a entanglement witness, since physically this property reflects the fact that mixing quantum states cannot increase the entanglement content, as well as the related achievable estimation sensitivity [1].

The QFI cannot be expressed entirely in terms of two-point connected correlation functions, indeed the following relation holds [2, 3]

$$F[\rho_D, \hat{O}]_N = 4 \sum_{x,y} \left( \sum_{\lambda} p_{\lambda} \langle \lambda|\hat{o}(x)|\hat{o}(y)|\lambda\rangle_{\text{conn}} - 2 \sum_{\lambda, \nu} \frac{p_{\lambda} p_{\nu}}{p_{\lambda} + p_{\nu}} \langle \lambda|\hat{o}(x)|\nu\rangle \langle \nu|\hat{o}(y)|\lambda\rangle \right).$$  \hspace{1cm} (5)

The second term of this equation is the difference between the QFI and $\tilde{F}[\rho_D, \hat{O}]_N$ in the main text.

**SM 2: ON THE CLUSTER-DECOMPOSITION THEOREM FOR PURE STATES**

In this Section, we provide additional details on the role of the so-called cluster decomposition theorem for correlation functions on pure states on lattices. In this way, cluster decomposition encodes the locality principle [4–6] for...
Hamiltonian systems, and it is valid at least for all the physical systems where the area law for the entanglement entropy is not massively violated, like in systems with volume-law.

Let us consider a pure state $|\lambda\rangle$, which is not degenerate in energy. For this state, the theorem claims that, when $|x - y|$ diverges ($x$ and $y$ still labelling lattice sites), then $\langle\lambda|\hat{o}(x)\hat{o}(y)|\lambda\rangle$ tends to $\langle\lambda|\hat{o}(x)|\lambda\rangle\langle\lambda|\hat{o}(y)|\lambda\rangle$: this is the subtracted second part in Eq. (12) of the main text. In order to justify the theorem in these conditions, $x$ and $y$ must be supposed belonging to different unconnected sets: the infinite $|x - y|$ limit assures this condition, even if genuine multipartite entanglement, $c = \infty$, is hosted on the analyzed system. Indeed, the theorem can be someway justified starting from the following decomposition of the two-points connected correlations:

$$
(\lambda|\hat{o}(x)\hat{o}(y)|\lambda)_{\text{conn}} = \sum_{\lambda'} (\lambda|\hat{o}(x)|\lambda')(\lambda'|\hat{o}(y)|\lambda) - (\lambda|\hat{o}(x)|\lambda)(\lambda|\hat{o}(y)|\lambda) = \sum_{\lambda' \neq \lambda} (\lambda|\hat{o}(x)|\lambda')(\lambda'|\hat{o}(y)|\lambda),
$$

where $|\lambda\rangle$ and $|\lambda'\rangle$ form again an orthonormal basis. In fact, in Eq. (6) we assume that the whole system has an orthonormal producible basis, to be inserted in $\langle\lambda|\hat{o}(x)\hat{o}(y)|\lambda\rangle_{\text{conn}}$. In Eq. (6), we notice that (for instance) $\langle\lambda'|\hat{o}(x)|\lambda\rangle \to 0$ if $\lambda \neq \lambda'$, then $\langle\lambda|\lambda'\rangle = 0$, if they are separate in energy, and if $x$ (or $y$ or both) is (are) located on the (infinite) boundary of the system. More in general, the cluster decomposition theorem implies that

$$
\sum_{\lambda' \neq \lambda} a_{\lambda,\lambda'} \langle\lambda|\hat{o}(x)|\lambda'\rangle\langle\lambda'|\hat{o}(y)|\lambda\rangle \to 0 \quad \text{if} \quad |x - y| \to \infty,
$$

at least if $|a_{\lambda,\lambda'}| < \infty$, a generally fulfilled condition in physical systems.

The latter argument suggests that the cluster-decomposition theorem, often referred to the ground-state(s) of local Hamiltonians, if valid for a non-degenerate ground state, must hold also for excited states, although more entangled in general, for instance fulfilling a volume law for the Von Neumann entropy, see e.g. [7–9]. Indeed, Eq. (7) means that a local operator $\hat{o}$ applied on (one point of) the infinite boundary of the state $|\lambda\rangle$ or $|\lambda'\rangle$ (no matter their energies), cannot change the same state in a way to induce a nonvanishing overlap with other states of the orthogonal basis.

Expressed in a alternative manner, the cluster decomposition theorem must be valid for all the states of the considered systems at least if $c < \infty$, and therefore if some producibility holds. Otherwise, the entanglement between the infinite boundary and a point in the bulk, or between two points of the boundary, would immediately set $c \to \infty$. More in detail, if $N \sim L^D$ in that case, then $c \sim L^\delta$, with $\delta \geq D - 1$, $D - 1$ being the dimension of the boundary, then also $N^\gamma$, $\gamma \geq D - 1/D$. The bound for $\delta$ can be further improved by noticing that if cluster decomposition fails and translational invariance is assumed, then:

$$
\langle\psi|\hat{o}(x)\hat{o}(y)|\psi\rangle_{\text{conn}} \sim |x - y|^\beta \quad \text{for} \quad |x - y| \to \infty, \quad \beta \geq 0.
$$

Merging Eq. (8) and the scaling property $f[\|\psi\|,\hat{O}]_N \sim N^{1-2\beta/D}$ (see [10] for critical lattice systems and [11] for one-dimensional lattices), we obtain $\delta = D + 2\beta \geq D$. Therefore, failure of the cluster decomposition condition implies the reach of genuine multipartite entanglement. Thus, no producibility of any kind is allowed.

For the same reason, we point out that cluster decomposition turns out to be strictly required to prove the bound in Eq. (5) of the main text, even though in those proofs no explicit mention to it is made [12]. Finally, the validity of the cluster decomposition theorem does not require translational invariance, avoiding any prescription on the limit operations in Eqs. (7) and (8).

Above, we claimed that cluster decomposition holds if the ground state is unique. Instead, if the ground state is degenerate, the theorem can not hold in a generic basis. However, at least in the presence of a finite number of degenerate states, the theorem can be recovered, provided to choose properly the combination of them. This fact can be illustrated via a paradigmatic example, i.e. the ferromagnetic quantum Ising model in a transverse field, governed by the Hamiltonian

$$
\hat{H}_{\text{IS}} = \hbar \sum_{i=1}^N \hat{\sigma}_i^{(x)} + J \sum_{i=1}^N \hat{\sigma}_i^{(z)}\hat{\sigma}_{i+1}^{(z)}, \quad J < 0.
$$

It is known that, if $J < \hbar$, the ground state in the thermodynamic limit is doubly degenerate, in the states $|\uparrow, \ldots, \uparrow\rangle \equiv |\uparrow\rangle$ and $|\downarrow, \ldots, \downarrow\rangle \equiv |\downarrow\rangle$, orthonormal to each other. However, at finite volume, these states are mixed, forming the almost degenerate states $|\pm\rangle = |\uparrow\rangle \pm i|\downarrow\rangle \sqrt{2}$, exactly degenerate in the thermodynamic limit only. For the latter states,
the cluster decomposition theorem is not fulfilled, exactly since they result from the mixing of $|\uparrow\rangle$ and $|\downarrow\rangle$. Indeed:

$$\lim_{x-y \to \infty} \langle \pm | \hat{\sigma}^{(z)}(x) \hat{\sigma}^{(z)}(y) | \pm \rangle \to \frac{1}{2}$$

but

$$\langle \pm | \hat{\sigma}^{(z)}(x) | \pm \rangle \langle \pm | \hat{\sigma}^{(z)}(y) | \pm \rangle = 0.$$ (10)

However, it is fulfilled for the states $|\uparrow\rangle$ and $|\downarrow\rangle$. This means that, adopting the basis formed by $|\uparrow\rangle$, $|\downarrow\rangle$, and by the excited states above them, cluster decomposition can be recovered, and locality made explicit. In a sense, in the presence of a finite degenerate ground state, cluster decomposition still holds, up to global unitary transformations, as that linking the states $|\pm\rangle$ and $|\uparrow\rangle$ in the example above. In Eq. (7), they transform the states $|\lambda\rangle$ and $|\lambda'\rangle$ but, critically, not the operators $\hat{\sigma}(x)$ and $\hat{\sigma}(y)$ set at the beginning acting on them. Therefore, the value of the sums in the same equation can change. Clearly, the bounds after Eq. (8) still hold; in particular the absence of cluster decomposition in any basis implies the simultaneous absence of any sort of producibility. In real experiments, the states corresponding to $|\uparrow\rangle$ and $|\downarrow\rangle$ are generically selected by the fluctuations (also classical) or by perturbations suitably added, as well as in simulations: for instance, in the example above, by an additional term $h' \sum_{i=1}^{N} \hat{a}_{i}^{(z)}$, $h' \to 0$, customary e.g. in DMRG calculations.

The discussion above does not cover the important cases of continuous degeneracies, as for spontaneously broken continuous symmetries and for genuine topologically ordered matter [13]. Moreover, it is not clear whether a volume-law dependence for the von Neumann entropy is enough to guarantee the violation of cluster decomposition. These issues are beyond the scope of the present work.

**SM 3: DERIVATION OF EQ. (12) OF THE MAIN TEXT**

Starting from Eq. (9) of the main text,

$$\hat{F}[\rho_{p}, \hat{O}]_{N} \equiv 4 \sum_{\lambda} p_{\lambda} \left( \sum_{x,y} \langle \hat{\lambda} | \hat{\sigma}(x) \hat{\sigma}(y) | \hat{\lambda} \rangle_{\text{conn}} \right),$$

in this Section we obtain Eq. (12) of the main text, expressed in a generic basis, possibly orthonormal. This step is strictly required to operatively evaluate $\hat{F}[\rho_{p}, \hat{O}]_{N}$, since in general the producible basis $|\hat{\lambda}\rangle$, fulfilling Eq. (8) of the main text, is not known. For this purpose, it is useful to consider how Eq. (11) evolves under a transformation to an orthonormal, and generally entangled, basis, i.e. via the Gram-Schmidt procedure corresponding to a *not unitary* transformation. Setting this transformation as

$$|\hat{\lambda}\rangle = \sum_{n} a_{\hat{\lambda},n} |n\rangle, \quad \sum_{n} |a_{\hat{\lambda},n}|^{2} \neq 1,$$ (12)

where $|n\rangle$ are all orthonormal each others, and forgetting for the moment the asymptotic therm involved in the connected correlations, we can write:

$$\sum_{\lambda} p_{\lambda} \sum_{x,y} \langle \hat{\lambda} | \hat{\sigma}(x) \hat{\sigma}(y) | \hat{\lambda} \rangle \to \sum_{x,y} \sum_{\lambda} p_{\lambda} \sum_{n,m} a_{\hat{\lambda},n}^{*} a_{\hat{\lambda},m} \langle m | \hat{\sigma}(x) \hat{\sigma}(y) | n \rangle \equiv \sum_{x,y} \sum_{n,m} p_{n,m} \langle m | \hat{\sigma}(x) \hat{\sigma}(y) | n \rangle.$$ (13)

Exploiting again the orthonormality of the $|n\rangle$ basis, it is now easy to convince ourselves that the latter expression is equal to

$$\sum_{x,y} \text{Tr}[\rho \hat{\sigma}(x) \hat{\sigma}(y)],$$ (14)

where

$$\rho = \sum_{\lambda} p_{\lambda} \sum_{n,m} a_{\hat{\lambda},n}^{*} a_{\hat{\lambda},m} |n\rangle \langle m| \equiv \sum_{n,m} p_{n,m} |n\rangle \langle m|$$ (15)

is now expressed in a orthonormal basis. We also have

$$\text{Tr} \rho = \text{Tr} \rho_{p} = \sum_{\lambda} p_{\lambda} \sum_{n} |a_{\hat{\lambda},n}|^{2} = 1.$$ (16)
Importantly, the quantity in Eq. (14) is a trace invariant in the space of the conceivable unitary transformations from the orthonormal basis \(|n\rangle\). Notice also that Eq. (16) is explicit if a change of basis is unitary, \(\sum_n |a_{\lambda,n}|^2 = 1\) as referred to Eq. (12), since, by hypothesis, \(\sum \lambda p_{\lambda} = 1\).

Let us now consider the product of matrix elements \(\langle \lambda | \hat{\varnothing} (x) | \lambda' \rangle \langle \lambda' | \hat{\varnothing} (y) | \lambda \rangle\), with \(\lambda' \neq \lambda\), like those appearing in Eq. (6). It is immediately clear that this product can be nonvanishing only if \(\langle \lambda_j | \lambda'_j \rangle = 0\) for just a single domain \(D_j\), and only if \(x\) and \(y\) belong exactly to \(D_j\), so that they are entangled. Therefore, exploiting further the cluster decomposition theorem described in SM3, as well as translational invariance, it turns out that the sum in Eq. (11) can be expressed again as
\[
\tilde{F}[\rho, \hat{O}]_N = 4 \sum_{x,y} \sum_{\lambda} p_\lambda \langle \lambda | \hat{\varnothing} (x) \hat{\varnothing} (y) | \lambda \rangle_{\text{conn}} = 4 \sum_{x,y} p_\lambda \left( \langle \lambda | \hat{\varnothing} (x) \hat{\varnothing} (y) | \lambda \rangle - \lim_{|x-y| \to \infty} \langle \lambda | \hat{\varnothing} (x) \hat{\varnothing} (y) | \lambda \rangle \right). \tag{17}
\]
Consequently, this can be cast in a covariant-trace form:
\[
\tilde{F}[\rho, \hat{O}]_N = 4 \sum_{x,y} p_\lambda \langle \lambda | \hat{\varnothing} (x) \hat{\varnothing} (y) | \lambda \rangle_{\text{conn}} = 4 \sum_{x,y} \left( \text{Tr} [\rho \hat{\varnothing} (x) \hat{\varnothing} (y)] - \lim_{|x-y| \to \infty} \text{Tr} [\rho \hat{\varnothing} (x) \hat{\varnothing} (y)] \right). \tag{18}
\]
As a result, in a generic orthonormal basis where in general the density matrix is not diagonal, i.e.
\[
\rho = \sum_{n,m} p_{n,m} |n\rangle \langle m|, \tag{19}
\]
it can finally be written as:
\[
\tilde{F}[\rho, \hat{O}]_N = 4 \sum_{x,y} p_{n,m} \left( \langle m | \hat{\varnothing} (x) \hat{\varnothing} (y) | n \rangle - \lim_{|x-y| \to \infty} \langle m | \hat{\varnothing} (x) \hat{\varnothing} (y) | n \rangle \right). \tag{20}
\]
So, apparently, we end up in the "strange correlators" \(\langle m | \hat{\varnothing} (x) \hat{\varnothing} (y) | n \rangle\), known to be relevant for topology probing [14].

Thanks to the cluster-decomposition theorem, described in the SM 3, the second addendum in Eq. (17) is physically equivalent to the term from the transformation of the product \(\langle \lambda | \hat{\varnothing} (x) | \lambda \rangle \langle \lambda | \hat{\varnothing} (y) | \lambda \rangle\) in Eq. (11), via the Gram-Schmidt change of basis. In this way, and oppositely to the product of one-point correlations, both the terms in Eq. (17) are still expressed as a trace and are covariant under changes of basis. Therefore, the cluster-decomposition theorem allows to obtain the covariant expression in Eq. (18) from Eq. (11), a not possible task otherwise.

In order to be valid for all the ground and excited states of the considered system, cluster decomposition is strictly required to guarantee some sort of producibility: \(c \sim N^\delta\), \(0 \leq \delta < 1\), when \(N \to \infty\). Therefore, the validity of Eqs. (8) and (12) of the main text implies in itself that cluster decomposition is fulfilled for all the states \(|\lambda\rangle\) in the same equation. Finally, if the ground state is degenerate in the thermodynamic limit, we recall that the orthogonal basis \(|n\rangle\) must be properly chosen to make cluster decomposition explicit, as discussed in SM 2.

Since \(\langle m | k \rangle = \delta_{m,n}\) and transformations of basis preserve the scalar products between the states, Eq. (20) can be simplified further. Indeed, if \(m \neq n\), then \(\lim_{|x-y| \to \infty} \langle m | \hat{\varnothing} (x) \hat{\varnothing} (y) | n \rangle = 0\). This fact can be somehow justified after inserting in the last expression a complete set \(|\lambda\rangle\) of states, and noticing that (for instance) \(\langle m | \hat{\varnothing} (x) | \lambda \rangle \to 0\) if \(\lambda \neq m\) (then \(\langle m | k \rangle = 0\)) and if \(x\) is located on the (infinite) boundary of the system. In this manner, Eq. (20) can be recast as follows:
\[
\tilde{F}[\rho, \hat{O}]_N = 4 \sum_{x,y} \sum_{n,m} p_{n,m} \langle m | \hat{\varnothing} (x) \hat{\varnothing} (y) | n \rangle - \sum_{n} p_{n,n} \lim_{|x-y| \to \infty} \langle m | \hat{\varnothing} (x) \hat{\varnothing} (y) | n \rangle \right]. \tag{21}
\]
Notably, Eqs. (20) and (21) become particularly manageable in the orthonormal basis \(|\alpha\rangle\) where \(\rho\) is diagonal. Indeed:
\[
\tilde{F}[\rho, \hat{O}]_N = 4 \sum_{x,y} \sum_{\alpha} p_{\alpha,\alpha} \langle \alpha | \hat{\varnothing} (x) \hat{\varnothing} (y) | \alpha \rangle - \sum_{\alpha} p_{\alpha,\alpha} \lim_{|x-y| \to \infty} \langle \alpha | \hat{\varnothing} (x) \hat{\varnothing} (y) | \alpha \rangle \right]. \tag{22}
\]
The limits in Eqs. (20), (21), and (22) can be evaluated in a number of physically interesting cases, making these expressions manageable even at an operative level.
Fig. 1 shows an additional example of the time evolution of the different functionals described in the main text, starting from the ground state, having $S_z = 0$, of the Hamiltonian $H$, in the presence of a symmetry breaking transverse field $h_x/J_x = 0.05$. Here, we break the global $S_z$ symmetry at the Hamiltonian level, leading the QFI to differ from the variance of the operator, $\text{Var}(S_x)$ (defined in Fig. 1 (a) of the main text). Moreover, the instantaneous state $\rho(t)$ no longer has a well defined magnetization, and thus the diagonal terms $\langle \lambda | \hat{O} | \lambda \rangle$ become finite, despite the dissipator respecting the $S_z$ symmetry in this case ($L_j = \hat{s}_j^z$). This leads to the interesting and complex situation where all our estimators differ from one another and are non-zero. Finally, note that, since $M - R \neq 0$, the functional $\tilde{F}[\rho, O]_N = F_1[\rho, O]_N + F_2[\rho, O]_N$ is no longer covariant.
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