

Can multipartite entanglement be characterized by two-point connected correlation functions?

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Abstract

We discuss under which conditions multipartite entanglement in mixed quantum states can be characterized only in terms of two-point connected correlation functions, as it is the case for pure states. In turn, the latter correlations are defined via a suitable combination of (disconnected) one- and two-point correlation functions. In contrast to the case of pure states, conditions to be satisfied turn out to be rather severe. However, we were able to identify some interesting cases, as when the point-independence is valid of the one-point correlations in each possible decomposition of the density matrix, or when the operators that enter in the correlations are (semi-)positive/negative defined.

Supplementary material for this article is available [online](#)

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(Some figures may appear in colour only in the online journal)

1. Introduction

Entanglement is a central resource in quantum technology [1–3]. Entanglement quantifiers are especially relevant in quantum information, quantum metrology and estimation theory [4–10], and are recognized as valuable tools to describe quantum phases and phase transitions [6, 11]. Research has largely focused on bipartite entanglement [1, 12, 13], typically via the von Neumann entropy [1, 12–16], entanglement spectrum [17–22], and generally pairwise entanglement [1, 13, 23–25].

More recently, considerable attention has been devoted to the so-called multipartite entanglement (ME) among subsets of a quantum state, a concept based on those of producibility and separability [4]. However, the identification and detection of ME criteria are still a challenging problem. Prominent tools for ME quantification are the quantum Fisher information (QFI), presently known as the ultimate bound for ME [4, 8, 9, 26–28], and Wineland’s spin-squeezing parameter (SSP) [2, 29–32]. Methods to extract them from experiments have been discussed [2, 29, 30, 32–34], and results for ultracold atomic gases have been presented [31, 35]. QFI and SSP also provide efficient tomography [36, 37] for quantum phases and transitions [33, 38–43], and are proposed as benchmarks for quantum simulators [36]. In fact, ME has been investigated e.g. in Bose–Einstein condensates [31, 35], spin systems [33, 38, 39, 43–45], also at criticality [46–49], with long-range interactions [50–54], and in topological models [40, 41, 55–57].

Estimating ME for mixed states via the QFI can be difficult in general, and in strongly-interacting systems it has been performed only in a limited number of cases, mainly at equilibrium [42, 45], also establishing a direct link with dynamical susceptibility [33]. The main reason is that the QFI for a mixed state cannot be fully expressed in terms of (one- and two-point) correlation functions, instead it requires a sum over matrix elements with respect to all the states diagonalizing the full density matrix [42] (see the next section for a precise definition).

In this work, focusing on mixed quantum states, we discuss physical and mathematical conditions that make it possible to bound ME, via one- and two-point correlation functions. The conditions to be satisfied turn out to be rather severe. However, we were able to identify

at least two physically relevant situations, such as when the point-independence is valid of the one-point correlations in each possible decomposition of the density matrix or when the operators that enter in the correlations are (semi-)positive/negative defined.

2. ME

2.1. Separability and producibility

For a d -dimensional discrete system with N components (e.g. sites), c -partite entanglement, with $1 \leq c \leq N$, implies that a partition $\{|\psi_i\rangle\}$ exists, where the maximum number of components in a single $|\psi_i\rangle$ is c . The tensor-product state $|\psi\rangle = \prod_{\otimes_i} |\psi_i\rangle$ is then said to be c -producible [4], or to have entanglement depth c . In addition, a system is said to host c -partite entanglement if it is c -producible but not $(c+1)$ -producible. Instead, the number h , with $\frac{N}{c} \leq h \leq N-c+1$, of disentangled subsets is the degree of separability [6, 27]. The usual separability corresponds to $h=N$ and $c=1$. On a lattice, the subsystems are not necessarily adjacent sites. When $c=N$, $|\psi\rangle$ is said to host *genuine* ME [58].

For mixed states, c -producibility in h subsets holds if ρ can be decomposed (generally not uniquely) as

$$\rho = \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} |\tilde{\lambda}\rangle\langle\tilde{\lambda}|, \quad (1)$$

where $p_{\tilde{\lambda}} > 0$ without any lack of generality, and $|\tilde{\lambda}\rangle$ are c -separable states in h subsets, not necessarily with the same space-partition. If $c=N$, then equation (1) is still valid, trivially with a single partition and in every decomposition. In general, the c -producible decomposition $|\tilde{\lambda}\rangle$ is not orthogonal, thus ρ is not diagonal. Moreover, the producibility of $|\tilde{\lambda}\rangle$ is generally lost in other decompositions.

2.2. Bounds for ME

First, we focus on pure states $|\psi\rangle$. We denote by x, y two sites of the lattices and by $\hat{o}(x), \hat{o}(y)$ local operators based on these sites. In this way, the variance of the Hermitian operator

$$\hat{O} = \sum_x \hat{o}(x) \quad (2)$$

on $|\psi\rangle$ is defined as [4]

$$V[|\psi\rangle, \hat{O}]_N = 4 \sum_{x,y} \langle \psi | \hat{o}(x) \hat{o}(y) | \psi \rangle_c, \quad (3)$$

being

$$\langle \psi | \hat{o}(x) \hat{o}(y) | \psi \rangle_c \equiv \langle \psi | \hat{o}(x) \hat{o}(y) | \psi \rangle - \langle \psi | \hat{o}(x) | \psi \rangle \langle \psi | \hat{o}(y) | \psi \rangle \quad (4)$$

two-point *connected* correlations [59]. $V[|\psi\rangle, \hat{O}]_N$ coincides with the QFI for pure states [4]. In the following, the QFI for pure states will be also denoted as $F[|\psi\rangle, \hat{O}]_N$. Importantly, the same quantity is a witness of ME for these states. This means that, if (c, h) -entanglement, but not $(c+1, h')$ -entanglement (with $h' \geq \frac{N}{c+1}$), is present, then the inequality

$$V[|\psi\rangle, \hat{O}]_N \leq 4k [c(N-h) + N], \quad (5)$$

holds [27]. Indeed, (5) bounds the quantum advantage offered by (c, h) -entanglement in terms of the sensitivity, with respect to the shot-noise (separable) limit, $V[|\psi\rangle, \hat{O}]_N = 4kN$. In (5),

$k = \frac{(m-n)^2}{4}$ if $\hat{o}(x)$ is constrained, with eigenvalues $n \leq q \leq m < \infty$ [59]. More in detail, (5) generates other relevant bounds [27]: for instance, it can be extended choosing $h = \frac{N}{c}$, which yields the bound for c -producibility $V[|\psi\rangle, \hat{O}]_N \leq 4kcN$ [4, 26]. This implies that its violation signals at least $(c+1)$ -partite entanglement [8, 9]. The ultimate limit $V[|\psi\rangle, \hat{O}]_N = 4kN^2$, when $|\psi\rangle$ hosts genuine ME, is called the Heisenberg limit. Another similar estimator for c , generally supposed to be not an integer, was found in [28], see SM 1. Similarly, one can maximize in c the right-hand term of equation (5), setting $c = N - h + 1$ and obtaining the bound for h : $V[|\psi\rangle, \hat{O}]_N \leq 4k[(N-h+1)^2 + h - 1]$ [27, 60].

Finally, we notice that, critically, if two lattice sites x and y belong to different partitions and $|\psi\rangle$ is producible, then $\langle \psi | \hat{o}(x) \hat{o}(y) | \psi \rangle_c = 0$, for every conceivable local operator $\hat{o}$, see e.g. [61, 62]. This property can be exploited to demonstrate the bounds of producibility for pure states recalled above, see SM 2.

Now, we focus on mixed states. We define as

$$\bar{V}[\rho, \hat{O}]_N \equiv 4 \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} \left(\sum_{x,y} \langle \tilde{\lambda} | \hat{o}(x) \hat{o}(y) | \tilde{\lambda} \rangle_c \right), \quad (6)$$

the average variance in a producible decomposition, as in equation (1), while the average variance in a generic decomposition $\{p_{\lambda}, |\lambda\rangle\}$ of ρ (functionally defined as in equation (6)) will be again denoted generically as $V[\rho, \hat{O}]_N$. The corresponding functionals involving the sums of the modula of the connected correlations will be denoted as $|V[\rho, \hat{O}]_N$ and $|\bar{V}[\rho, \hat{O}]_N$.

Starting from equation (1) and exploiting the bound in equation (5), we have that, see [27], the inequality in equation (5) holds also for $\bar{V}[\rho, \hat{O}]_N$ in equation (6), the average variance

$$\bar{V}[\rho, \hat{O}]_N \leq 4k[c(N-h) + N], \quad (7)$$

in the presence of (c, h) -entanglement for the density matrix ρ in equation (1), since $\sum_{\tilde{\lambda}} \tilde{p}_{\tilde{\lambda}} = 1$ [63, 64]. Actually, (c, h) -entanglement is a sufficient but not necessary condition for the validity of equation (7). Moreover, maximizing in h the right-hand term in equation (7), the more common bound [4]

$$\bar{V}[\rho, \hat{O}]_N \leq 4kcN, \quad (8)$$

is obtained. Correspondingly, maximizing in c the right-hand term in equation (7), h is bound as $\bar{V}[\rho, \hat{O}]_N \leq 4k[(N-h+1)^2 + h - 1]$. Equation (7) is obtained by exploiting the producibility of all the states $|\tilde{\lambda}\rangle$, with the same c and h (but not necessarily the same space-partition), so that the bound in equation (5) holds for all of them. Instead, no orthonormality hypothesis of the $|\tilde{\lambda}\rangle$ set is required. Moreover, note that the average variance for mixed states in a producible decomposition is related to the pure state variance equation (3) via

$$\bar{V}[\rho, \hat{O}]_N = \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} V[|\tilde{\lambda}\rangle, \hat{O}]_N. \quad (9)$$

In this way, $\bar{V}[\rho, \hat{O}]_N$ also saturates the corresponding convexity inequality

$$V[\rho, \hat{O}]_N \leq \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} V[|\tilde{\lambda}\rangle, \hat{O}]_N, \quad (10)$$

valid in a generic decomposition [4].

As it will be required later on, we introduce the quantity

$$|\bar{V}[\rho, \hat{O}]_N \equiv 4 \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} \left(\sum_{x,y} |\langle \tilde{\lambda} | \hat{o}(x) \hat{o}(y) | \tilde{\lambda} \rangle_c| \right), \quad (11)$$

(notice that $|\bar{V}[\rho, \hat{O}]_N$ is not the modulus of $\bar{V}[\rho, \hat{O}]_N$). The same bounds in equations (7) and (8) also hold, in the presence of (c, h) -entanglement for the density matrix ρ in equation (1), for $|\bar{V}[\rho, \hat{O}]_N$ i.e. $\bar{V}[\rho, \hat{O}]_N \leq |\bar{V}[\rho, \hat{O}]_N$, and $|\bar{V}[\rho, \hat{O}]_N \leq 4kcN$, both for pure states and mixed states. The proof of the latter statement follows from the derivation presented in SM 2, where the bound $\bar{V} \leq 4kcN$ is shown for pure states. Then, the extension to mixed states is done as from equation (7) to equation (6).

2.3. Relation with the QFI

For mixed states, the bounds in equations (7) and (8) are also valid for the QFI [4]. This quantity is defined, in terms of the average variances in every decomposition $\{p_\lambda, |\lambda\rangle\}$, as follows [3, 65–67]:

$$F[\rho, \hat{O}]_N = 4 \text{Tr} [\rho \hat{O}^2] - 4 \sup_{\{p_\lambda, |\lambda\rangle\}} \sum_{\lambda} p_\lambda \langle \lambda | \hat{O} | \lambda \rangle^2. \quad (12)$$

Notice that we are denoting by $\{|\lambda\rangle\}$ a generic decomposition, while $\{|\tilde{\lambda}\rangle\}$ are the c-separable states entering equation (1).

It turns out that $\{\bar{V}[\rho, \hat{O}]_N, V[\rho, \hat{O}]_N\} \geq F[\rho, \hat{O}]_N$, as formalized in the ‘so-called convex roof theorem’ [65, 66]: for chosen ρ and $\hat{O}$, the resulting QFI is the minimum average variance between all the possible decompositions $\{p_\lambda, |\lambda\rangle\}$ of ρ . The same property allows to demonstrate immediately that the bounds in equations (7) and (8) also hold for the QFI, as it is well known in literature [4]. We also stress that the convex inequality in equation (10) is fulfilled also by the QFI, that is saturated for pure states.

In a (spectral) decomposition $|n\rangle$, where ρ is diagonal, the QFI, denoted in the following as $F[\rho, \hat{O}]_N$, is written as [4]

$$F[\rho, \hat{O}]_N = 2 \sum_{x,y} \sum_{n,m} \frac{(p_n - p_m)^2}{p_n + p_m} \langle n | \hat{O} | x \rangle \langle m | \hat{O} | y \rangle \langle n | \hat{O} | y \rangle \langle m | \hat{O} | x \rangle. \quad (13)$$

The described non-trivial relation between the QFI $F[\rho, \hat{O}]_N$ and the average variances $V[\rho, \hat{O}]_N$ calculated in generic decompositions $\{p_\lambda, |\lambda\rangle\}$ can be illustrated considering for instance a one-dimensional array of $N=6$ spin-1/2, described by the XXZ Heisenberg Hamiltonian in a transverse magnetic field,

$$H = - \sum_{i=1}^{N-1} \left[\frac{J_x}{2} (\sigma_i^{(+)} \sigma_{i+1}^{(-)} + \sigma_i^{(-)} \sigma_{i+1}^{(+)}) + J_z \sigma_i^{(z)} \sigma_{i+1}^{(z)} \right] - h_x S_x, \quad (14)$$

where J_x and J_z are exchange interactions, and $S_\beta = \sum_i \frac{\sigma_i^{(\beta)}}{2}$ ($\hbar \equiv 1$), $\beta = \{x, y, z\}$. For $h_x = 0$, the total magnetization, $S_z = \sum_i \frac{\sigma_i^{(z)}}{2}$, is conserved, a fact exploited in [45] to compute the QFI efficiently. Due to this symmetry, the operator $\hat{O} = S_x$ has $\langle \lambda | \hat{O} | \lambda \rangle = 0, \forall |\lambda\rangle$ with definite S_z . To analyze a mixed state scenario, we consider Markovian dissipation, according to a Gorini–Kossakowski–Sudarshan–Lindblad master equation [68–70], with local spin-flip and spin-dephasing noise described by jump operators $L_m = \{\sigma_m^{(x)}, \sigma_m^{(z)}\}$ respectively. Dissipation rates are denoted by γ_{S_x} and γ_{S_z} .

Figure 1 shows the time evolution of the different functionals $F[\rho, \hat{O}]_N$ and $V[\rho, \hat{O}]_N$ (here both calculated in the diagonal decomposition), starting from the ground state of H , with $S_z = 0$, in the presence of two forms of dissipation. In figure 1(a), we include dissipation, as $L_i = \sigma_i^{(z)}$. As the S_z symmetry is conserved throughout the evolution, $\langle \lambda | \sigma_i^{(x)} | \nu \rangle = 0$ at any time,

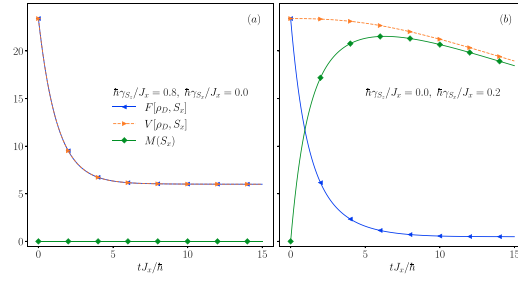


Figure 1. Dissipative evolution of a XXZ chain of $N = 6$ site, using exact diagonalization, with a time-step of $J_x dt/\hbar = 0.01$, chosen to ensure numerical convergence. We begin the evolution from the ground state of H , with $S_z = 0$, in the gapless phase for $J_z/J_x = 0.8$, and study the evolution with (a) symmetry-respecting $\sigma_i^{(z)}$ dissipation, and (b) symmetry-breaking $\sigma_i^{(x)}$ dissipation. The observables for all panels are shown in the legend of (a). We also defined $M(S_x) \equiv V[\rho, S_x] - F[\rho, S_x]$, with both $V[\rho, S_x]$ and $F[\rho, S_x]$ calculated in a diagonal decomposition.

then both $F[\rho, \hat{O}]_N$ and $V[\rho, \hat{O}]_N$ reduce to the first term in equation (12), $4 \text{Tr}[\rho \hat{O}^2]$. In contrast, when the dissipation $L_i = \sigma_i^{(x)}$ does not preserve the magnetization, as shown in figure 1(b), then the QFI quickly differs from $V[\rho, \hat{O}]_N$, the last quantity being higher in value, as expected from the convex roof theorem.

3. Discussion of conditions to estimate ME by correlation functions

3.1. The general problem

The producible decompositions $|\tilde{\lambda}\rangle$ and $p_{\tilde{\lambda}}$, where $\bar{V}[\rho, \hat{O}]_N$ is defined as in (6), are not generally known *a priori*. Thus, in order to be a useful witness of ME, $\bar{V}[\rho, \hat{O}]_N$ is required to be calculable without the knowledge of $|\tilde{\lambda}\rangle$. To focus on this central problem, it is useful to decompose $\bar{V}[\rho, \hat{O}]_N$ into two terms: $\bar{V}[\rho, \hat{O}]_N \equiv \bar{V}_1[\rho, \hat{O}]_N - \bar{V}_2[\rho, \hat{O}]_N$. The first term, $\bar{V}_1[\rho, \hat{O}]_N \equiv 4 \sum_{x,y} \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} \langle \tilde{\lambda} | \hat{o}(x) \hat{o}(y) | \tilde{\lambda} \rangle$, can be recast as

$$\bar{V}_1[\rho, \hat{O}]_N = 4 \sum_{x,y} \text{Tr}[\rho \hat{o}(x) \hat{o}(y)] = 4 \text{Tr}[\rho \hat{O}^2] \quad (15)$$

(the first term in equation (12)), where ρ and $\hat{o}(x)$ are meant to be expressed in a generic basis $|\alpha\rangle$ of the Hilbert space, possibly orthonormal, as $|\tilde{\lambda}\rangle = \sum_{\alpha} c_{\tilde{\lambda}\alpha} |\alpha\rangle$. This expression does not depend explicitly on $|\tilde{\lambda}\rangle$, thus it is covariant, and invariant in value, under changes of decomposition. This transformation is realized via a unitary operator U , acting as (see SM 3):

$$\sqrt{p_{\tilde{\lambda}}} |\tilde{\lambda}\rangle = U_{\tilde{\lambda}\lambda} \sqrt{p_{\lambda}} |\lambda\rangle. \quad (16)$$

In contrast, the second term

$$\bar{V}_2[\rho, \hat{O}]_N \equiv 4 \sum_{x,y} \sum_{\tilde{\lambda}} p_{\tilde{\lambda}} \langle \tilde{\lambda} | \hat{o}(x) | \tilde{\lambda} \rangle \langle \tilde{\lambda} | \hat{o}(y) | \tilde{\lambda} \rangle \geq 0 \quad (17)$$

is neither invariant nor covariant under the transformation U in general, hence to evaluate it requires the explicit knowledge of $|\tilde{\lambda}\rangle$. In turn, the non-covariance of $\bar{V}_2[\rho, \hat{O}]_N$ makes it difficult to calculate $\bar{V}[\rho, \hat{O}]_N$ in a generic decomposition, and to use it as an efficient ME estimator. The same problem occurs in calculating the QFI, via $[\sup_{\{p_{\lambda}, |\lambda\rangle\}} \sum_{\lambda} p_{\lambda} \langle \lambda | \hat{O} | \lambda \rangle^2]$

in equation (12). This is the main reason why the cumbersome expression in equation (13) must be used, in general.

3.2. Two conditions for the calculability of equation (6)

In the present subsection, we discuss two situations when the quantity

$$\sum_{\lambda} p_{\lambda} \langle \lambda | \hat{O} | \lambda \rangle^2 = \sum_{\lambda} p_{\lambda} \sum_{x,y} \langle \lambda | \hat{o}(x) | \lambda \rangle \langle \lambda | \hat{o}(y) | \lambda \rangle \quad (18)$$

in equation (12) can be calculated, in a generic decomposition $|\lambda\rangle$, in spite of the difficulties mentioned above.

- (a) Let first consider $\hat{O}$ as a semipositive or seminegative defined operator in the considered Hilbert space. We recall that an operator $\hat{o}$ is called positive definite on a given Hilbert state if, for any vector $|v\rangle$ on this space, $\langle v | \hat{o} | v \rangle > 0$. Similarly, it is called semi-positive definite if $\langle v | \hat{o} | v \rangle \geq 0$. We mention for instance collective spin operators $(S^{(x,y,z)})^2 = \sum_i (s_i^{(x,y,z)})^2$ for $s > \frac{1}{2}$ or $\tilde{S}^{(x,y,z)} = \sum_i (\pm s \mathbf{I} + s_i^{(x,y,z)})$ for $s \geq \frac{1}{2}$ (notice that $F[\rho, a \mathbf{I} + \hat{O}]_N = F[\rho, \hat{O}]_N$). In this condition, if $\langle \lambda | \hat{O} | \lambda \rangle = 0$, for any state $|\lambda\rangle$ in a chosen decomposition, then the quantity in equation (18) vanishes in any other decomposition, since also $\sum_{\lambda} \langle \lambda | \hat{O} | \lambda \rangle = \text{Tr}[\rho \hat{O}] = 0$ and $\text{Tr}[\rho \hat{O}]$ is invariant under changes of decompositions.
- (b) Second, let us consider states with the property that

$$\langle \lambda | \hat{o}(x) | \lambda \rangle \equiv o_{\lambda} \quad (19)$$

is independent of x , for the chosen local operator $\hat{o}(x)$ and for every $|\lambda\rangle$ of a certain decomposition. Translationally invariant states can be included, see more details below. In this condition, the quantity in equation (18) is evaluated as follows. Defining $\text{Tr}[\rho \hat{o}(x) \hat{o}(y)] \equiv c(x, y)$ (appearing in $\bar{V}_1[\rho, \hat{O}]_N$, equation (15), and always depending on x and y), if

$$\sum_{\lambda} p_{\lambda} \langle \lambda | \hat{O} | \lambda \rangle^2 = N^2 \lim_{|x-y| \rightarrow \infty} c(x, y) \equiv N^2 c_{\infty}, \quad (20)$$

then it is possible to recast the average variance $V[\rho, \hat{O}]_N$, in the present decomposition $\{p_{\lambda}, |\lambda\rangle\}$, as

$$V[\rho, \hat{O}]_N = 4 \left[\sum_{x,y} c(x, y) - N^2 c_{\infty} \right]. \quad (21)$$

The conditions for the validity of equation (20) will be discussed in the next subsection.

Although evaluated in a specific decomposition, this functional will be used to determine conditions under which it is possible to bound ME for the mixed state described by ρ . This result will be shown in the next section, as well as the relation of the same functional with $\bar{V}[\rho, \hat{O}]_N$ in equation (6) and with the QFI, $F[\rho, \hat{O}]_N$.

3.3. Derivation of equation (19)

In this section, we derive and motivate equation (21). In order to perform this task, we have to discuss first the conditions for the validity of equation (20). For this purpose, beyond equation (19), the second property that we assume at first is:

$$\langle \lambda | \hat{\rho}(x) \hat{\rho}(y) | \lambda \rangle \rightarrow \langle \lambda | \hat{\rho}(x) | \lambda \rangle \langle \lambda | \hat{\rho}(y) | \lambda \rangle, \quad (22)$$

if $|x - y| \rightarrow \infty$ [71–73]. However, this property will be relaxed in the following subsections, since eventually it will not be strictly required to justify equation (21) as an entanglement witness.

Notice that the simultaneous validity of equations (19) and (22) requires strictly that $\langle \lambda | \hat{\rho}(x) \hat{\rho}(y) | \lambda \rangle$ does not depend on the unit vector of $x - y$, nor on x and y themselves, at least if $|x - y| \rightarrow \infty$. Sufficient, but not necessary, conditions for this scenario are rotational invariance and again translational invariance.

We also stress that, in order to guarantee that the one-point correlations are not point-dependent, here translational invariance must be understood for every translation a_i , connecting two sites of the lattice and for every state $|\lambda\rangle$. For regular lattices, these translations decompose into sums of translations inside a unit cell and primary lattice vectors, see e.g. [74]. Finally, if the condition in equation (22) holds for every local operator $\hat{\rho}(x)$, this is called ‘cluster decomposition’ in the literature.

Importantly, equation (22) does not imply at all that $\text{Tr}[\rho \hat{\rho}(x) \hat{\rho}(y)]$ tends, even for large space separations, to the product $\text{Tr}[\rho \hat{\rho}(x)] \text{Tr}[\rho \hat{\rho}(y)]$: this can be seen also as an effect of the classical weights p_λ , not encoding entanglement. Moreover, the fact that ρ_λ is not x -dependent implies the same fact for $\text{Tr}[\rho \hat{\rho}(x)] = \sum_\lambda p_\lambda \rho_\lambda$. The opposite implication does not hold in general, requiring further assumptions, as translational invariance.

We also comment that the latter property sets a tight limitation to the degree of producibility c , even for a single pure state $|\psi\rangle$: indeed, consider two adjacent points x and y : as argued in section 2.2, if they belong to the same entangled subset $|\psi_i\rangle$, then $\langle \lambda | \hat{\rho}(x) \hat{\rho}(y) | \lambda \rangle_c$ is nonzero in general, otherwise the same quantity is forced to vanish. Translational invariance, for every translation a_i , connecting two sites of the lattice, implies

$$\langle \lambda | \hat{\rho}(x + a_i) \hat{\rho}(y + a_i) | \lambda \rangle_c = \langle \lambda | \hat{\rho}(x) \hat{\rho}(y) | \lambda \rangle_c. \quad (23)$$

From the discussion in section 2.2, the latter equality implies immediately that $c = 1$ or $c = N$. More involved scenarios would be possible instead if translational invariance was allowed only for a subset of the entire set of lattice-translation $\{a_i\}$.

Under the two conditions in equations (19) and (22), the quantity in equation (18) can be evaluated straightforwardly, leading to equations (20) and (21) (see more details in SM 5). We stress that the same derivation exploits that all the states of the decomposition $|\lambda\rangle$ fulfill equation (22). However, the same property ceases to hold in general, as the decomposition is changed along equation (16). Consequently, one can verify that equation (21) is not equal to $\bar{V}[\rho, \hat{O}]_N$ nor to $F[\rho, \hat{O}]_N$, in general. Nevertheless, the same functional (21) will reveal still useful to bound ME in any decomposition.

3.4. Comments on the space independence of the one-point correlations

Here, having in mind the point (b) of section 3.2, we discuss under which conditions the independence of the one-point correlations on the point itself can hold in every decomposition.

At first, we consider, in a given decomposition $|\lambda\rangle$, the matrix elements $\langle \lambda | \hat{\rho}(x) | \lambda \rangle$ and $\langle \lambda | \hat{\rho}(y) | \lambda \rangle$, $y \neq x$, and we assume the stronger condition of translational invariance. Note that we do not *a priori* require that these conditions hold in every decomposition. We can interpolate between the two matrix elements above, writing:

$$\langle \lambda | \hat{\rho}(y) | \lambda \rangle = \langle \lambda | \hat{T}_{y-x} \hat{\rho}(x) \hat{T}_{y-x}^{-1} | \lambda \rangle, \quad (24)$$

where $\hat{T}_{y-x} = e^{i\hat{P}(y-x)}$ is a unitary translation operator, generated by the momentum operator $\hat{P}$. Here $y-x$ is a multiple number of the lattice steps, possibly even in different primary directions for regular lattices. If $|\lambda\rangle$ is translationally invariant, then $\hat{T}_{y-x}|\lambda\rangle = e^{ik(y-x)}|\lambda\rangle$, k being the momentum quantum number. The space-dependent phases cancel out in the matrix element $\langle\lambda|\hat{o}(y)|\lambda\rangle$, so that, in the end:

$$\langle\lambda|\hat{o}(y)|\lambda\rangle = \langle\lambda|\hat{o}(x)|\lambda\rangle, \quad (25)$$

as expected. Notice that, critically, the same cancellation does not occur in general for the off-diagonal matrix elements $\langle\lambda'|\hat{o}(y)|\lambda\rangle$, $|\lambda'\rangle \neq |\lambda\rangle$.

Consider now a second decomposition $|\eta\rangle$: this is obtained from $|\lambda\rangle$ as in equation (16), so that:

$$\langle\eta|\hat{o}(y)|\eta\rangle = \sum_{\lambda, \lambda'} \frac{\sqrt{p_\lambda p_{\lambda'}}}{p_\eta} [U^*]_{\lambda', \eta} U_{\eta, \lambda} \langle\lambda'|\hat{o}(y)|\lambda\rangle. \quad (26)$$

Importantly, the involved unitary matrix $U_{\eta, \lambda}$ is not space dependent, as well as the numerical factors $\sqrt{p_\eta}$ and $\sqrt{p_\lambda}$. Therefore, the only difference between the elements $\langle\eta|\hat{o}(y)|\eta\rangle$ and $\langle\eta|\hat{o}(x)|\eta\rangle$ can come from the phases $e^{ik(y-x)}$, $e^{ik'(y-x)}$, not canceling out in the off-diagonal matrix elements $\langle\lambda'|\hat{o}(y)|\lambda\rangle$, $|\lambda'\rangle \neq |\lambda\rangle$.

We conclude that, if the states of the decomposition $|\lambda\rangle$ are such that $\langle\lambda|\hat{o}(x)|\lambda\rangle$ does not depend on x , the same property holds for another related decomposition $|\eta\rangle$ (at least) if $\langle\lambda'|\hat{o}(x)|\lambda\rangle = 0$ when $|\lambda'\rangle \neq |\lambda\rangle$ and $\forall x$. A required, but not sufficient, condition, is clearly that, in the same condition, also $\langle\lambda'|\hat{O}|\lambda\rangle = 0$. Due to equation (26), the same conclusion is reached in the more general case when the independence of $\langle\lambda|\hat{o}(x)|\lambda\rangle$ is realized without the strongest assumption of translational invariance (still provided the vanishing of the off-diagonal matrix elements, assumed x -dependent).

Various examples are plausible with the feature described above. Consider for instance a density matrix with an orthogonal decomposition (as a spectral one) $|\lambda\rangle$, such that its elements are eigenstates of $\hat{O} = S_z = \sum_i \sigma_i^{(z)}$ (i labelling the sites, now), as in the example of section 2.3, with periodic boundary conditions. However, now all these states are characterized by different eigenvalues of $\hat{O}$. Since clearly $[S_z, \sigma_i^{(z)}] = 0$, then $\sigma_i^{(z)}|\lambda\rangle = \sum_{\lambda''} a_{\lambda, \lambda''} |\lambda''\rangle$, where $|\lambda''\rangle$ are eigenstates of S_z with the same eigenvalue of $|\lambda\rangle$. In the subspace spanned by the set $|\lambda''\rangle$, the same states $|\lambda''\rangle$ can be always assumed to be arranged orthogonal to $|\lambda'\rangle \neq |\lambda\rangle$. Therefore $\langle\lambda'|\sigma_i^{(z)}|\lambda\rangle = 0$.

3.5. Further comments on the property in equation (22)

In the following, we analyze some consequences of equation (22), relevant for our purposes. In particular, the same equation immediately implies, and is implied by, that, for a certain pure state $|\psi\rangle$, the scaling of $V[|\psi\rangle, \hat{O}]_N$ with N is below the Heisenberg one. Similarly, if the average variance $V[\rho, \hat{O}]_N$ in a certain decomposition $\{p_\lambda, |\lambda\rangle\}$ can be written in the invariant form (21) (then it is possible to set $\sum_\lambda p_\lambda \sigma_\lambda^2 = c_\infty$), its scaling with N is below the Heisenberg one, and vice versa.

These facts hold because, if

$$|\langle\psi|\hat{o}(x)\hat{o}(y)|\psi\rangle_c| \sim |x-y|^{-2\alpha} \quad \text{when } |x-y| \rightarrow \infty, \quad (27)$$

then $|V[|\psi\rangle, \hat{O}]_N$, scales with $N \rightarrow \infty$ as [33, 41, 75]:

$$|V[|\psi\rangle, \hat{O}]_N \sim N^{2-2\frac{\alpha}{d}}. \quad (28)$$

Notice that, as required by the simultaneous validity of equations (19) and (22) (see section 3.5), in equation (27) we still assumed that $\langle \lambda | \hat{\rho}(x) \hat{\rho}(y) | \lambda \rangle$ does not depend on the unit vector of $x - y$, nor on x and y themselves, at least if $|x - y| \rightarrow \infty$. Conversely, equation (27) implies the scaling $|\langle \psi | \hat{\rho}(x) \hat{\rho}(y) | \psi \rangle_c| \sim |x - y|^{-2\alpha}$. Moreover, equation (28) completes the previously known result (see e.g. [33, 41]) that $|V[[\psi], \hat{O}]|$ increases extensively with N if $|\langle \psi | \hat{\rho}(x) \hat{\rho}(y) | \psi \rangle_c|$ decays exponentially with $|x - y|$, as for short-range gapped systems.

It is immediate to check, by direct analogy, that the same proof of equation (28) [75] holds for the link between $|V[[\rho], \hat{O}]_N$ and the argument

$$\sum_{\lambda} p_{\lambda} |\langle \lambda | \hat{\rho}(x) \hat{\rho}(y) | \lambda \rangle_c| \quad (29)$$

of the sum in x and y in its definition, as in equation (11).

From equation (28), it results that the ‘clustering’ property in equation (22) ($\alpha \geq 0$ in equation (27)) is generally required, but not sufficient (since another operator $\hat{\rho}(x)$ could evade it), to have $c < N$, c bounded as in equation (5). Instead, its violation, $\alpha \leq 0$, implies $c = N$. Actually, even when the point-independence holds of the one-point correlations in equation (19), the described difficulty to evaluate $\bar{V}_2[\rho, \hat{O}]_N$ in equation (17) (and c_{∞} in a generic decomposition $\{p_{\lambda}, |\lambda\rangle\}$) is directly related with the general violation of equation (22).

Finally, we notice that a lower bound for the scaling of c can be obtained further from the failure of equation (22) and without exploiting the scaling of $|V[[\psi], \hat{O}]_N|$: $c \sim N^{\gamma}$, $\gamma \geq (d-1)/d$, see SM 4. This bound reflects the entanglement between a bulk point and the boundary of the lattice implied by the failure of equation (22). Moreover, it demonstrates $c \sim N$ in the mean-field limit $d \rightarrow \infty$.

4. Use of the functional in equation (21) to bound ME

We are not able to provide constraints on a density matrix ρ , sufficient to assure that the property in equation (22) holds in any decomposition. However, this task will turn out not to be strictly required for our purposes.

Indeed, in the present section, we show how the functional in equation (21) can be exploited to bound ME, provided that the property in equation (19) holds for each decomposition—even without invoking the cluster decomposition property (22).

Two main situations can occur:

- $c < N$: in this case, the property in equation (22) holds for the decomposition $\{p_{\tilde{\lambda}}, |\tilde{\lambda}\rangle\}$ in equation (1), from the discussion of the previous subsection. Therefore, the average variance $\bar{V}[\rho, \hat{O}]_N$ can be expressed in the form of equation (21). The same expression is covariant and invariant under changes of decomposition (therefore, it can be equivalently evaluated in $\{p_{\tilde{\lambda}}, |\tilde{\lambda}\rangle\}$ or in any other decomposition), and it is also equal to the QFI in the present conditions:

$$\bar{V}[\rho, \hat{O}]_N = V[\rho, \hat{O}]_N = F[\rho, \hat{O}]_N. \quad (30)$$

Indeed, referring to equation (12):

$$\sup_{\{p_{\lambda}, |\lambda\rangle\}} \sum_{\lambda} p_{\lambda} \langle \lambda | \hat{O} | \lambda \rangle^2 = \inf_{\{p_{\lambda}, |\lambda\rangle\}} \sum_{\lambda} p_{\lambda} \langle \lambda | \hat{O} | \lambda \rangle^2 = c_{\infty}. \quad (31)$$

Therefore, equation (21) can be exploited to bound, via the bounds in the section 2.2, the actual value of c . Clearly, this value must be lower than N , as implied also by the construction of equation (21)).

– $c = N$: in this case, if the property in equation (22) holds, everything works as in the previous case, apart from the fact that now the estimated value of c by the functional $V[\rho, \hat{O}]_N$ in equation (21) can saturate to N .

Instead, if equation (22) does not hold, the same functional (not sharing any clear general relation with $F[\rho, \hat{O}]_N$, at the best of our understanding), still calculated in a chosen working decomposition, can yield a lower value $c < N$ (again by construction of equation (21)). Therefore, a lower bound for c is still established.

5. Conclusions

We discussed some physical and mathematical conditions that make it possible to bound ME for mixed quantum states, via one- and two-point correlation functions.

Our analysis holds for discrete systems, but it could be extended—although not straightforwardly—to continuous systems [28, 76]. Further investigation is required to identify other physically interesting cases, where our approach can be useful.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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