Supplemental Material for
"Quantum states with a positive partial transpose are useful for metrology"

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The supplemental material contains some additional results helping to characterize the bound entangled states found numerically, as well as results of the maximization of the quantum Fisher information for a constrained negativity. We also provide a list of quantum states that are available from the electronic supplement as text files.

Maximum of the quantum Fisher information for separable states.—For any of the single qudit operators $a^{(n)}$ we have

$$\begin{aligned}(\Delta a^{(n)})^2 &= \min_{\mu}\langle(a^{(n)}-\mu\mathbb{1})^2\rangle\\ &\le \min_{\mu}\lambda_{\max}[(a^{(n)}-\mu\mathbb{1})^2]\\ &= [\lambda_{\max}(a^{(n)})-\lambda_{\min}(a^{(n)})]^2/4. \end{aligned} \quad \text{(S1)}$$

The first equality in Eq. (S1) is a well known identity for the variance. The inequality is based on the idea that an expectation value of an operator is never larger than its largest eigenvalue. In the second line, the μ leading to the minimum is $\mu=[\lambda_{\max}(a^{(n)})+\lambda_{\min}(a^{(n)})]/2$. A state maximizing the variance, and hence saturating the inequality, is the equal superposition of the eigenstates corresponding to the minimal and maximal eigenvalues, respectively. Then, for a pure product state $|\Psi\rangle_{\rm prod}=|\psi\rangle^{(1)}\otimes|\psi\rangle^{(2)}\otimes...\otimes|\psi\rangle^{(N)}$ we have

$$\begin{aligned}\mathcal{F}_{\rm Q}[|\Psi\rangle_{\rm prod},\sum_n a^{(n)}] &= 4\sum_n(\Delta a^{(n)})^2\\ &\le \sum_n[\lambda_{\max}(a^{(n)})-\lambda_{\min}(a^{(n)})]^2,\end{aligned} \quad \text{(S2)}$$

where the inequality can be saturated. Equation (S2) is valid for separable states due to the convexity of the quantum Fisher information.

Comments on scaling.—We examine the scaling of the metrological performance of PPT states with the number of particles. If we construct a tensor product of metrologically useful states, the quantum Fisher information scales as

$$\mathcal{F}_{\rm Q}\left[\varrho^{\otimes M},\sum_{m=1}^{M}A^{[m]}\right]=\left(\mathcal{F}_{\rm Q}[\varrho,A]\right)^M, \quad \text{(S3)}$$

where $A^{[m]}$ acts on the $m^{\rm th}$ copy of the state. Using the four-qubit state mentioned above we obtain for $A=J_z$

$$\mathcal{F}_{\rm Q}=1.0022N, \quad \text{(S4)}$$

where N is divisible by 4. Hence, we have a constant factor compared to the shot-noise limit given in Eq. (3). Using the state above as an initial state, one could start a numerical maximization of $\mathcal{F}_{\rm Q}$ for PPT states. It is expected that a higher level of metrological usefulness can be achieved, since we allow PPT entanglement between the four-qubit units.

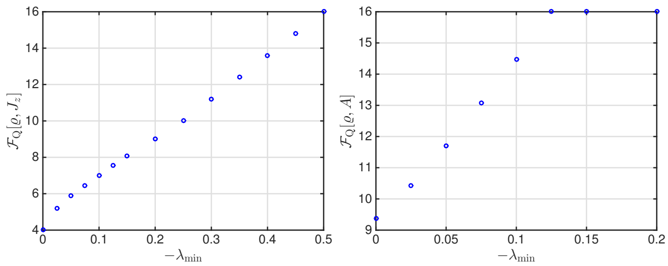
Description of the SDP algorithm to compute a lower bound to $p_{\rm noise}$.—Let us consider a $d\times d$ system, and denote the maximal quantum Fisher information achievable by separable states in this system by $\mathcal{F}_{\rm Q}^{(\rm sep)}$. Let ϱ be a quantum state for which $\mathcal{F}_{\rm Q}[\varrho,A]$ is higher than $\mathcal{F}_{\rm Q}^{(\rm sep)}$. We define the robustness of the metrological usefulness of a state as follows. It is the minimal amount of separable noise that has to be mixed with ϱ in order to have $\mathcal{F}_{\rm Q}\le\mathcal{F}_{\rm Q}^{(\rm sep)}$. This definition is analogous to that of the robustness of entanglement in Ref. [39]. Mathematically, we ask for the minimal amount of p, denoted by $p_{\rm noise}$, such that $\mathcal{F}_{\rm Q}[\varrho(p),A]\le\mathcal{F}_{\rm Q}^{(\rm sep)}$, where $\varrho(p)=(1-p)\varrho+p\varrho_{\rm sep}$, and $\varrho_{\rm sep}$ belongs to the set of separable states.

We presented lower bounds on the noise tolerance denoted by $p_{\rm noise}^{\rm LB}$ in Table II. The calculation was carried out using the following SDP

$$\begin{aligned} p_M(X) = &\min_{\sigma} p,\\ &\text{s.t. } p={\rm Tr}(\sigma), \sigma\ge 0, \sigma^{\rm T1}\ge 0,\\ &\varrho(p)=(1-p)\varrho+\sigma,\\ &{\rm Tr}\{\varrho(p)i[A,M]\}=X,\\ &\frac{1}{(\Delta\theta)^2_{\varrho(p)}}=\frac{X^2}{{\rm Tr}[M^2\varrho(p)]}\le\mathcal{F}_{\rm Q}^{(\rm sep)}. \end{aligned} \quad \text{(S5)}$$

Here, ϱ is the state for which we would like to obtain a bound on the robustness. The operator M is obtained according to formula (8). Note that the last condition can be written as ${\rm Tr}[M^2\varrho(p)]\ge(X^2/\mathcal{F}_{\rm Q}^{(\rm sep)})$ to make it suitable for an SDP formulation. Then, the robustness of the quantum Fisher information is computed as

$$p_{\rm noise}^{\rm LB}=\min_{X\in[X_{\min},X_{\max}]}p_M(X), \quad \text{(S6)}$$



(a) (b)

FIG. S1. The maximal quantum Fisher information as the function of the smallest eigenvalue of the partial transpose. (a) four-qubit systems and (b) 4×4 systems with A given in Eq. (4).

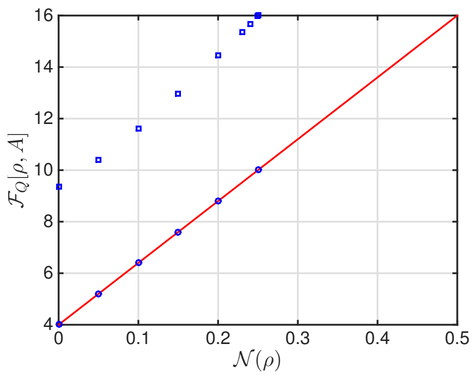


FIG. S2. The maximal quantum Fisher information as the function of the smallest bipartite negativity for (circles) four-qubit systems with $A = J_z$. (squares) 4×4 systems with A given in Eq. (4). (solid) Line corresponding to $\mathcal{F}_Q = 24\mathcal{N}+4$.

where $X_{\min}$ and $X_{\max}$ are the minimum and maximum eigenvalues of the expression $i[A, M]$, respectively.

In order to see that the SDP (S5) gives indeed a lower bound we note that (i) the state $\tilde{\sigma} = \sigma/p$ approximates the set of separable states ϱ_{sep} from the outside. (ii) $\mathcal{F}_Q[\varrho(p), A] \geq 1/(\Delta\theta)^2_{\varrho(p)}$. Both (i) and (ii) potentially increase the feasible p values defined by the condition appearing in the last line of the optimization (S5), which entails a lower bound to p_{noise}.

Relation between the negativity and the metrological usefulness.—We consider the constraint that the eigenvalues of $\varrho^{\text{T}k}$ are larger than $\lambda_{\min}$ for all k. We present the maximal quantum Fisher information for various values of $\lambda_{\min}$ in Fig. S1.

We now put a constraint on the negativity of the quantum state [40]. In the multipartite case, we limit the minimum of the bipartite negativities. We use the following

Bipartite state	Entanglement
3×3	0.0003
4×4	0.0147
5×5	0.0239
6×6	0.0359
7×7	0.0785
UPB 3×3	0.0652
Breuer 4×4	0.1150

TABLE S1. Lower bound on the linear entanglement for some of the bipartite states considered in Table II. For a comparison, the entanglement is also shown for the 3×3 state based on unextendible product bases (UPB) [23] and for the Breuer state with a parameter $\lambda = 1/6$ [24].

semidefinite program [40]

$$\begin{aligned} f_M^{\mathcal{N}}(X, Y) = \min_{\varrho} & \operatorname{Tr}(M^2\varrho), \\ \text{s.t. } & \varrho = \varrho_+ - \varrho_-, \\ & \varrho \geq 0, \operatorname{Tr}(\varrho) = 1, \\ & \operatorname{Tr}(\varrho_-) = \mathcal{N}, \\ & \varrho_+^{\text{T}k}, \varrho_-^{\text{T}k} \geq 0 \text{ for all } k, \\ & \langle i[M, J_z] \rangle = X \text{ and } \langle M \rangle = Y, \end{aligned} \quad \text{(S7)}$$

where the minimal bipartite negativity is not larger than $\mathcal{N}$. We changed the original iterative algorithm by replacing $f_M(X, Y)$ defined in Eq. (6) by $f_M^{\mathcal{N}}(X, Y)$ defined in Eq. (S7). The results are shown in Fig. S2. In the four-qubit case, the line connects our bound entangled state with the four-qubit Greenberger-Horne-Zeilinger (GHZ) state, which has a negativity of 0.5 and $\mathcal{F}_Q[\varrho_{\text{GHZ}}, J_z] = 16$ (see, e.g., Ref. [6]).

Entanglement of the PPT entangled states.—Next, we calculate a very good lower bound on the the entanglement measure based on the convex roof of the linear entropy of entanglement, called linear entanglement, for some of the bound entangled states presented in this paper [25]. This measure has already been used to characterize bound entangled states [26]. The results can be seen in Table S1. Two programs to calculate the entanglement measure are given in Ref. [27].

Cluster states.—Cluster states attracted a large attention since they can be used as a resource in measurement-based quantum computing [30]. They arise naturally in Ising spin chains and have been realized with photons and cold atoms on an optical lattice [15, 16, 31]. Cluster states are fully entangled pure states, hence they are not PPT with respect to any partition. They violate a Bell inequality [32–34]. Linear cluster states of three qubits are equivalent to GHZ states under local unitaries, hence they are metrologically useful. Linear cluster states with $N \geq 4$ particles are also useful metrologically. On the other hand, for $N \geq 5$ particles, ring cluster states as well as cluster states in more than one dimension are metrologically not useful (see Proposition 3 in Ref. [10]). In Fig. 1, such cluster states are in the set $\mathcal{M}\backslash\mathcal{P}\backslash\mathcal{L}$.

Description of a 4 × 4 bound entangled PPT state.—Let us define the following six states $|\Psi_1\rangle = (|0,1\rangle + |2,3\rangle)/\sqrt{2}$, $|\Psi_2\rangle = (|1,0\rangle + |3,2\rangle)/\sqrt{2}$, $|\Psi_3\rangle = (|1,1\rangle + |2,2\rangle)/\sqrt{2}$, $|\Psi_4\rangle = (|0,0\rangle - |3,3\rangle)/\sqrt{2}$, and $|\Psi_5\rangle = (1/2)(|0,3\rangle + |1,2\rangle) + |2,1\rangle/\sqrt{2}, |\Psi_6\rangle = (1/2)(-|0,3\rangle + |1,2\rangle) + |3,0\rangle/\sqrt{2}$. Then our 4×4 state in question is a convex mixture of the following states $\varrho_{4\times4} = p\sum_{n=1}^{4}|\Psi_n\rangle\langle\Psi_n| + q\sum_{n=5}^{6}|\Psi_n\rangle\langle\Psi_n|$, where $q = (\sqrt{2}-1)/2$ and $p = (1-2q)/4$. The state is invariant under the partial transposition, which ensures that the state is PPT. We next show that $\rho_{4\times4}$ is in fact a metrologically useful bound entangled state. We consider the operator $A = H \otimes \mathbb{1} + \mathbb{1} \otimes H$, where $H = \mathrm{diag}(1, 1, -1, -1)$. For the $\varrho_{4\times4}$ state, $\langle\Psi_k|A|\Psi_l\rangle = 0$ for all $k, l = 1, 2, \ldots, 6$. Straightforward calculations show that this property implies the equality $\mathcal{F}_\mathrm{Q}[\varrho, A] = 4(\Delta A)^2$. Then, we obtain $\mathcal{F}_\mathrm{Q}[\varrho, A] = 4(\Delta A)^2 = 32 - 16\sqrt{2} \simeq 9.3726$. Since for separable states $\mathcal{F}_\mathrm{Q}[\varrho_\mathrm{sep}, A] \leq 8$ holds, we find that the state $\varrho_{4\times4}$ is indeed bound entangled.

Wigner-Yanase skew information.—There are alternatives of the quantum Fisher information, that, apart from a constant factor, coincide with it for pure states and are convex [19, 28]. The Wigner-Yanase skew information $I(\varrho, A) = \mathrm{Tr}(A^2\varrho - A\sqrt{\varrho}A\sqrt{\varrho})$ is such a quantity [29]. The limit for separability for $I(\varrho, A)$ is the same as for $\mathcal{F}_\mathrm{Q}[\varrho, A]/4$, since in general $I(\varrho, A) \leq \mathcal{F}_\mathrm{Q}[\varrho, A]/4$. We find that even for the skew information, there are PPT entangled states that violate the separable limit. For the 4×4 bound entangled state presented in the previous paragraph, $|\Psi_k\rangle$ for $k, l = 1, 2, \ldots, 6$ have been used to denote the eigenvectors of the density matrix corresponding to nonzero eigenvalues. For these, as has already been mentioned, the property $\langle\Psi_k|A|\Psi_l\rangle = 0$ holds. Straightforward algebra shows that due to this, $I(\varrho, A) = \mathcal{F}_\mathrm{Q}[\varrho, A]/4 = 9.3726/4 = 2.3431$, where A is given in Eq. (4) and $\mathcal{F}_\mathrm{Q}[\varrho, A]$ is shown in Table II. The skew information signals entanglement since the bound for separability is 2.

Quantum states obtained numerically.—The list of quantum states submitted with the supplement are given in Table S2.

System	File name
four qubits	`rho_fourqubits_r.txt` `rho_fourqubits_i.txt`
three qubits	`rho_threequbits_r.txt` `rho_threequbits_i.txt`
2×4	`rho_2x4_r.txt` `rho_2x4_i.txt`
3×3	`rho3x3.txt`
4×4	`rho4x4.txt`
5×5	`rho5x5.txt`
6×6	`rho6x6.txt`
7×7	`rho7x7.txt`
8×8	`rho8x8.txt`
9×9	`rho9x9.txt`
10×10	`rho10x10.txt`
11×11	`rho11x11.txt`
12×12	`rho12x12.txt`

TABLE S2. Quantum states submitted with this work, which have appeared in Tables I and II. The elements of the density matrices are given in text files. For the first three states, the real and imaginary parts are given in two separate files, while for the rest the imaginary part is zero.