Entanglement of Formation of Mixed Many-Body Quantum States via Tree Tensor Operators

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We present a numerical strategy to efficiently estimate bipartite entanglement measures, and in particular the entanglement of formation, for many-body quantum systems on a lattice. Our approach exploits the *tree tensor operator* tensor network Ansatz, a positive loopless representation for density matrices which, as we demonstrate, efficiently encodes information on bipartite entanglement, enabling the upscaling of entanglement estimation. Employing this technique, we observe a finite-size scaling law for the entanglement of formation in 1D critical lattice models at finite temperature for up to 128 spins, extending to mixed states the scaling law for the entanglement entropy.

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Quantum entanglement, correlations uniquely present in quantum systems [1], lies at the heart of the second quantum revolution. It is a fundamental resource in the development of present and future quantum technologies [2], and it drives the collective physics of many-body quantum systems at low temperatures [3,4]. The ability to characterize and quantify entanglement in a quantum state is thus crucial. However, even the simplest entanglement characterization, *bipartite* entanglement—quantifying the mutual quantum correlations between two subsystems—is well understood only when the state of the joint subsystems is a *pure* quantum state. This is mostly due to the fact that the estimation strategies for entanglement of mixed states call for minimizations in spaces that scales exponentially with the number of constituents of the system, and thus are effectively limited to small-sized systems [5,6]. In this Letter, we show how tensor network (TN) techniques can tackle this challenge, and efficiently estimate the entanglement of formation (EOF) [7]—the convex-roof extension of the von Neumann entropy—of many-body quantum states. As first application of this approach, we show that for critical one-dimensional systems the EOF obeys a (logarithmic) finite-size conformal scaling law, for temperatures commensurate with the energy gap.

For pure states, the connection between bipartite entanglement and the effective entropy of either subsystem has been largely established, and is typically expressed in terms of von Neumann ($\mathcal{S}$) or Rényi entropies [7–10]. While challenging to measure in an experiment [11], these estimators are often accessible in numerical simulations of many-body quantum systems, and especially in loopless tensor network Ansatz states, where the calculation complexity scales polynomially with the system size [12–16]. Conversely, for *mixed* global quantum states, the problem of characterizing and quantifying bipartite entanglement is much more involved, both conceptually and technically. It is nevertheless a fundamental goal, since any realistic quantum platform faces imperfections, statistical errors, and/or imperfect isolation leading to finite temperatures. From a conceptual standpoint, a major focus is to assess which of the entanglement monotones proposed over the years satisfy the desired properties of entanglement measures [8]. At a technical level, the core problem is to efficiently estimate these entanglement quantifiers. Even those that can be evaluated by linear algebra operations, such as negativity [17] and quantitative witnesses [18,19], are exponentially expensive in the system size. Additionally, many important monotones with a clear physical significance, in terms of resource and information theory, are *convex-roof* extensions of pure-state entanglement measures [7]. Estimating these monotones is a hard nonlinear minimization problem over pure-state decompositions of the global density matrix [20–26], severely limited to small system sizes.

The key point of our strategy is to exploit TN compressing capabilities and the exploitation of the tree tensor operator (TTO) structure to represent a density matrix ρ (Fig. 1) [12–16,27,28]. This TN Ansatz guarantees positivity of ρ, and being loopless it is efficiently contractible. Moreover, it is a natural TN geometry for estimating bipartite entanglement measures: as discussed below, the information about bipartite entanglement is compressed into a single tensor, ultimately simplifying the complexity of the minimization problem. We demonstrate this method

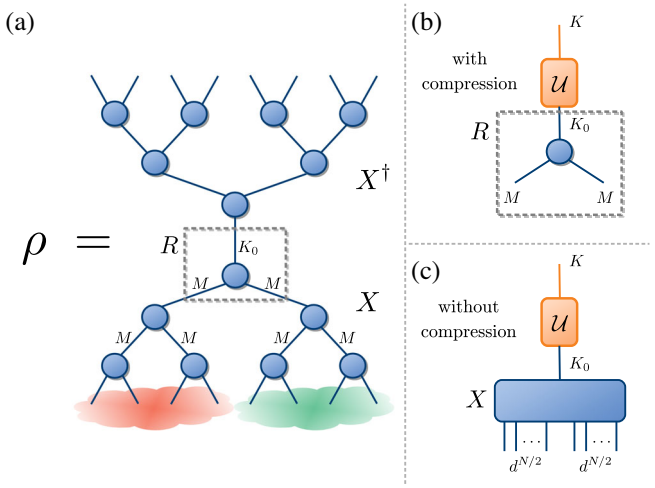

FIG. 1. (a) The tree tensor operator (TTO) representing a density matrix $\rho = XX^\dagger$. K_0 is the number of pure states in the representation used, while M is the maximal dimension for all bonds. The gray dashed square highlights the root tensor R, containing all the information about entanglement between the red and green bipartitions of the physical space. (b) Change of representation for the EOF minimization using R, after having compressed the state with some maximal bond dimension M. (c) Same as (b), but without compression, so that $M = d^{N/2}$. Optimizations are possible for any system size and state that can be efficiently represented as TTOs.

effectiveness computing the EOF of thermal many-body quantum states of the 1D transverse-field Ising and XXZ models.

Tree tensor operator Ansatz.—As positive operators, density matrices $\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ can be written as $\rho = XX^\dagger$, where the rectangular matrix $X = \sum_j \sqrt{p_j}|\psi_j\rangle\langle j|$ has a number of columns equal to the rank of ρ, also known as the Kraus dimension K_0. For many-body quantum states at low temperatures, probabilities p_j decay sufficiently fast that it is possible to approximate ρ using a K_0 that scales at most *polynomially* with the system size N. Therefore, from a numerical viewpoint, it is meaningful to represent X with a tree tensor network as shown in Fig. 1: the lower open links ("leaves," each of dimension d) represent the physical sites, while the upper open link ("root," of dimension K_0) represents the Kraus space of the global purification. As for other tensor network Ansätze, this representation becomes efficient when the connecting links, or "branches," carry an effective dimension M that also scales polynomially with N [16,27,29].

By construction, the TTO Ansatz *guarantees positivity* of ρ, in contrast to the matrix product density operator Ansatz [30,31], whose positivity can be checked only as an NP-hard problem [32]. Locally purified tensor networks [33] also preserve positivity, but the presence of loops in their network geometry leads to numerical limitations when implementing optimization strategies [34,35]. The TTO is instead positive and *loopless* thus encompassing the best of the two words without any drawbacks. When the TTO is properly isometrized to the root tensor, via (efficient) TN gauge transformations [16], all the information about the mixing probabilities p_j ends up stored within that tensor. Thus, also information about global entropies (von Neumann $\mathcal{S} = -\sum p_j \log p_j$ and Rényi $\mathcal{S}_\alpha = (1-\alpha)^{-1}\log\sum_j p_j^\alpha$, including the purity). Moreover, all the information on bipartite entanglement (for a half-half system bipartition) is contained only in the root tensor. Indeed, the action of the isometrized branches is actually an invertible LOCC (operation achievable via local operations and classical communication), and entanglement monotones cannot increase under such transformations [8]. In conclusion, compressing the relevant information into a tensor with polynomially scaling dimension, it is possible to efficiently estimate entanglement monotones by processing only the root tensor, even for complex measures that rely on convex-roof extensions. Below, we specialize this procedure to the specific case of the EOF.

EOF estimation.—The EOF of a mixed quantum state ρ, defined as [7]

$$E_F(\rho) = \inf_{\{p_j,\psi_j\}}\left\{\sum_j p_j \mathcal{S}(|\psi_j\rangle) : \rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|\right\},$$

quantifies the number of Bell pairs needed to construct a certain number of copies of ρ via LOCC. The minimization runs over all possible decompositions of ρ as a convex mixture of pure states $|\psi_n\rangle$, with probabilities p_n. It is straightforward to recast the previous expression in terms of the matrix X, whose columns $\sqrt{p_j}|\psi_j\rangle$ represent one possible pure-state decomposition of ρ. Via the Schrödinger-HJW theorem [36,37], it is possible to obtain the whole set of X' matrices representing ρ, and thus all possible pure-state decompositions. This is done by multiplying $X' = X\mathcal{U}$, where $\mathcal{U}$ is any right isometry (a semiunitary matrix satisfying $\mathcal{U}\mathcal{U}^\dagger = \mathbb{1}$) of dimension $K_0 \times K$, with $K \geq K_0$. The minimization problem then becomes a minimization over the space of right isometries $\mathcal{U}$, precisely

$$E_F(\rho) = \min_{K\geq K_0}\inf_{\mathcal{U}}\left\{\sum_{j=1}^{K} p_j \mathcal{S}(|\psi'_j\rangle) : X' = X\mathcal{U}\right\}, \quad (1)$$

where the columns of X' represent the new pure-state decomposition of ρ, with wave functions $|\psi'_j\rangle = X'|j\rangle(p'_j)^{-1/2}$ and probabilities $p'_j = \langle j|X'^\dagger X'|j\rangle$.

As depicted in Fig. 1(a), the X matrix composing the isometrized TTO can be written as $X = (\mathcal{V}_L \otimes \mathcal{V}_R)R$, where R is the root tensor, and the branches $\mathcal{V}_\star$ are left isometries ($\mathcal{V}_\star^\dagger\mathcal{V}_\star = \mathbb{1}$). It follows that the columns of R must have the same entanglement entropy $\mathcal{S}$ of the columns of X, and clearly the same probabilities p'_j. Thus, Eq. (1)

can be more efficiently computed by replacing X with the smaller root tensor R.

Numerical simulation.—Hereafter, we estimate the EOF of low-temperature many-body states of 1D quantum lattice models H via TTO. The first step is to approximate the many-body density matrix as a TTO Ansatz. That is, writing $X = (1/\sqrt{Z}) \sum_j^{K_0} e^{-E_j/2T} |\psi_j\rangle\langle j|$ in tensor network format as it appears in Fig. 1, where E_j is the energy of the Hamiltonian eigenstate $|\psi_j\rangle$ and Z ensures normalization $\mathrm{Tr}[XX^\dagger] = 1$. In this work, we achieve this goal with either of the two following methods: (i) Energy eigenstates $|\psi_j\rangle$ are obtained via exact diagonalization (ED). Thus X is calculated exactly, for a given K_0, and then compressed into a TTO as detailed in Supplemental Material (SM) [38]. (ii) $|\psi_j\rangle$ are obtained via a tree-tensor network algorithm capable of targeting each of the K_0 lowest energy eigenstates [40]. Their collected information is then easily formatted into a TTO with standard tensor network operations [16]. The accuracy of this second approximate method is benchmarked against the exact one for thermal states of small size in SM [38]. Beyond these two strategies, we envision the possibility to develop algorithms that directly compute the TTO for finite-temperature quantum states, capture Markovian real-time evolution, or transform other TN states into TTOs [50,51].

Once the TTO is built, we proceed to calculate the optimization from Eq. (1) on the top tensor R. To build sets of $\mathcal{U}$ matrices, we fix a value for $K \geq K_0$ and parametrize a Hermitian matrix $A = A^\dagger$ of dimensions $K \times K$. Then, we get the corresponding unitary from $U = \exp\{iA\}$, and finally we take K_0 random rows of U to build $\mathcal{U}$. For every column of $R' = R\mathcal{U}$, its entanglement entropy is calculated via $\mathcal{S} = -\sum_i s_i^2 \log s_i^2$, where the singular values s_i are obtained by a singular value decomposition (SVD). In the results section, entropies are expressed in basis of $\log_2$, so that a Bell pair defines the unit of entanglement. For a given $K \geq K_0$, minimization in the space of the $\mathcal{U}$ is carried out via direct search methods, but other choices are possible. Extensive proofs of the stability of this method, as well as some results on many-body random density matrices, are provided in SM [38]. Convergence of the minima is rapidly reached when increasing $K \geq K_0$. For all practical purposes, choosing $K \approx K_0$ is often sufficient to achieve close convergence (see SM [38]). We stress that, even in case of incomplete or failed convergence, our method still provides an upper bound to the actual EOF of the quantum state. In particular, in every case we could check, the results provided tight bounds. The accuracy and convergence of the EOF estimation is discussed in detail in SM [38]: we (i) benchmark the optimization procedure applied to exact states of small systems, whose EOF is known *a priori*, and (ii) test how state compression into a TTO affects the EOF computation, by comparing optimizations done on the approximate root tensor R and on the exact X, for thermal states of small systems.

Results.—We consider two well-known prototype quantum critical spin-$\frac{1}{2}$ models as benchmarks [52]: specifically, the Ising model

$$\hat{H}_{\mathrm{Ising}} = J \sum_{j=1}^{N} (\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + h\hat{\sigma}_j^z) \tag{2}$$

in a transverse field h, and the XXZ model

$$\hat{H}_{XXZ} = J \sum_{j=1}^{N} (\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + \xi \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z), \tag{3}$$

with anisotropy ξ, both models considered in periodic boundary conditions (PBC) and $\hat{\sigma}_j^\alpha$s ($\alpha = x, y, z$) are the Pauli matrices. The temperature T, defining the thermal state $\rho = (1/Z)e^{-\hat{H}/T}$, is expressed in units of the Hamiltonian energy scale ($J = k_B = 1$). To appropriately choose a suitable number K_0 we start from $K_0 = 2$. We then evaluate the resulting EOF, gradually increasing K_0 until convergence of the estimated EOF is reached. We employ a similar strategy to choose the best M.

Figure 2 shows a typical benchmark comparison of the total computational time required to acquire the EOF,

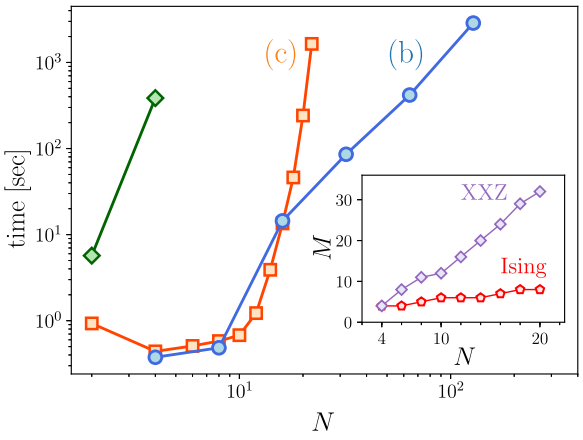

FIG. 2. Computational times of EOF estimation "from scratch" as a function of system size N, for critical $\hat{H}_{\mathrm{Ising}}$ ($h = 1$) at temperature $k_B T = 0.5\Delta$, where $\Delta \sim N^{-z}$ ($z = 1$) is the finite-size gap. Two data sets show EOF estimation without TTO compression: either using the full exact density matrix (green diamonds), or from the exact X matrix at convergence in columns K_0 (orange squares). The last data set shows EOF estimation with TTO method, where the Hamiltonian eigenstates were calculated via tree-tensor network eigensolver algorithm. Inset: bond dimensions M required to achieve convergence of the EOF estimator (approximation less than 1% from its exact value). Red pentagons and purple diamonds refer, respectively, to the critical Ising model at $k_B T = 0.1J$ and to the XXZ model with $\xi = 0.5$ (critical) at $k_B T = 0.5J$.

which include both calculation of the thermal state and entanglement measure estimation. Three data sets show, respectively, EOF estimation using the full exact density matrix (green), the exact X matrix at convergence in K_0 (red), and the TTO method with tree-tensor network eigensolver (blue). Complexity of the exact methods increases exponentially, basically as $\mathcal{O}(\dim\{\mathcal{H}\}^{3/2})$, since the bottleneck of our algorithm is the SVD to calculate $\mathcal{S}$ for each of the K pure states. By contrast, this runtime scales like $\mathcal{O}(M^3)$ for a TTO representation, with $M \ll \sqrt{\dim\{\mathcal{H}\}}$. At size 20 and beyond, the TTO algorithm clearly outperforms exact methods, displaying a visibly polynomial scaling. Typical bond dimensions M required to have a good approximate estimation (99% of the exact EOF value) are displayed in the inset, and show a roughly linear scaling with the system size.

Equipped with our diagnostic tool, we quantified the bipartite entanglement properties of two quantum systems at finite T. The two panels in Fig. 3 focus on critical phases of the two models, the quantum phase transition point of the Ising model ($h = 1$, top), and the Luttinger liquid phase of the XXZ model ($\xi = 0.5$, bottom) respectively. While the system is strongly correlated at zero temperature, entanglement seems to survive roughly unaltered up to T of the order of $0.2\Delta(N)$, with $\Delta(N)$ the finite-size energy gap, and smoothly drop at higher T. This phenomenon is to be contrasted with the von Neumann entropy $\mathcal{S}$ (global, or of either subsystem), which instead *grows* with T, and cannot capture alone the entanglement decrease [53,54]. More importantly, we observe an emergent scaling behavior when plotting $E_F(T, N)$. In fact, the EOF appears to follow the logarithm of a conformal scaling function, in proximity of the quantum critical point (i.e., for small temperatures $T \sim \Delta$). For PBC, this behavior can be expressed as $E_F = \log[N^{c/3} f(TN^z)]$, or

$$E_F(T, N) = \frac{c}{3}\log N + g(TN^z) \tag{4}$$

in analogy to Ref. [55], where c is the critical exponent that connects length scales to entanglement, while z is the critical exponent that connects length scales to energy scales ($\Delta \propto N^{-z}$). The functions $f(\cdot)$ and $g(\cdot) = \log f(\cdot)$ are nonuniversal and depend on the microscopical details of the model. This behavior actually extends, to finite T, the known scaling law for the entanglement entropy with size, valid for critical ground states [53,54]. We validate this argument in the inset of Fig. 3, where the $E_F(T, N)$ data sets are appropriately rescaled, according to N. As we expect, the curves collapse when the appropriate critical exponents of the corresponding model are used ($c = \frac{1}{2}$, $z = 1$ for critical Ising; $c = 1$, $z = 1$ for Luttinger liquid XXZ). In the former case, we pushed the numerics to very large system sizes and fully exploited the TTO approach. Larger system analysis of the XXZ model is feasible but numerically challenging: we thus limited our analysis to ED methods as it already clearly confirms the scaling behavior of critical systems.

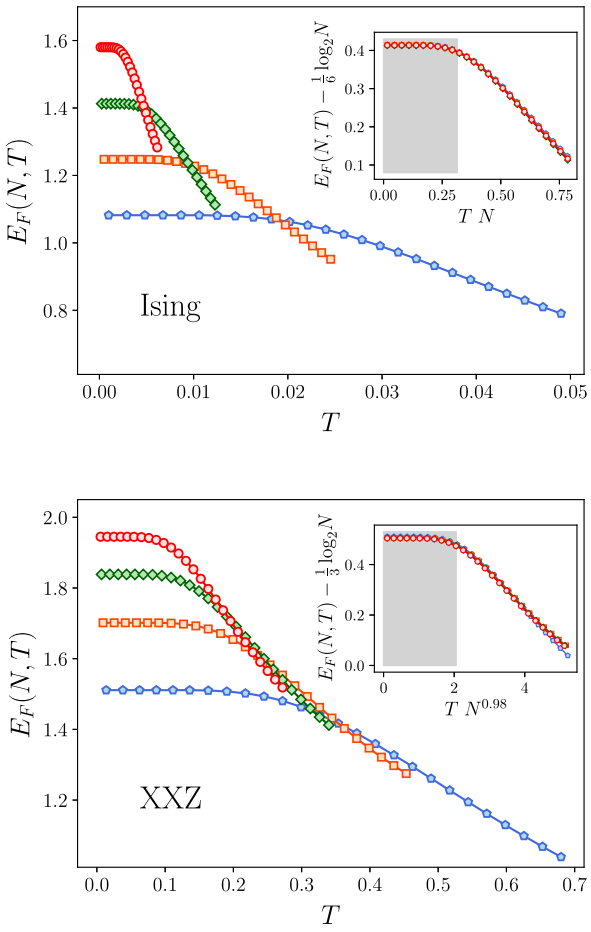

FIG. 3. Scale invariance of the EOF at temperatures T (in units of J/k_B) in the range $k_B T \leq 0.5\Delta$, where $\Delta \propto N^{-z}$, for the critical Ising model in Eq. (2) (top panel) and the XXZ model in Eq. (3) in the critical phase at $\xi = 0.5$ (bottom panel). Data for $N = 16$, 32, 64, 128 (top, approximate method for TTO computation) and $N = 8$, 12, 16, 20 (bottom, exact TTO from ED), from the flattest to the steepest curve. Inset: curves in the main figures after rescaling according to Eq. (4). The agreement is stunning, using $c = 1/2$ and $z = 1.00 \pm 0.01$ (top) and $c = 1$ and $z = 0.98 \pm 0.02$ (bottom). The gray area highlights the temperature range $T \leq 0.2\Delta(N)$.

As a final remark, we stress that the EOF analysis enabled by the TTO method is not limited to low-temperature many-body states of lattice models. We have employed the same diagnostic tool on other classes of mixed many-body states, including on sets where the EOF is known to further benchmark our approach, as reported in SM [38].

Conclusions.—In this Letter, we have presented a new tensor network approach that enables the numerical analysis of bipartite entanglement for many-body quantum systems, even for those entanglement monotones that are

considered *hard* since they require convex-roof optimization. We employed a tree tensor operator (TTO) to well approximate the global density matrix at low temperatures. Such a tensor network architecture compresses information of the bipartite entanglement into a single tensor, whose dimensions in many cases scale polynomially with the system size. As a result, evaluating entanglement monotones is numerically efficient, as illustrated for 1D interacting lattice models. Our analysis observed a scaling law for the entanglement of formation, compatible with a logarithmic conformal scaling law. We successfully tested this argument for a free fermion (Ising) and an interacting fermion (XXZ) critical models, where it is satisfied in a temperature range commensurate with the finite-size energy gap ($T \sim \Delta$).

While we built TTOs by collecting information on low-lying energy eigenstates, we envision the possibility of developing algorithms capable of directly targeting finite-temperature states on a TTO architecture. Similarly, we envision the possibility of replacing the tree tensor network branches of the Ansatz with matrix product state branches: an alternative TN design that is still efficient toward EOF estimation. Finally, we expect that TTO may be capable to accurately capture some features of open-system quantum dynamics. This will actually extend the bipartite-entanglement analysis, presented here, from finite-temperature states to a larger set of open-system physically relevant states, i.e., the stationary states of a Lindblad master equation [56–58]. The time-dependent variational principle [59,60] is surely a good candidate strategy toward this goal. This will likely be the focus of our research in the near future.

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