Tensor networks for complex quantum systems

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Abstract | Originally developed in the context of condensed-matter physics and based on renormalization group ideas, tensor networks have been revived thanks to quantum information theory and the progress in understanding the role of entanglement in quantum many-body systems. Moreover, tensor network states have turned out to play a key role in other scientific disciplines. In this context, here I provide an overview of the basic concepts and key developments in the field. I briefly discuss the most important tensor network structures and algorithms, together with an outline of advances related to global and gauge symmetries, fermions, topological order, classification of phases, entanglement Hamiltonians, holografic duality, artificial intelligence, the 2D Hubbard model, 2D quantum antiferromagnets, conformal field theory, quantum chemistry, disordered systems and many-body localization.

Renormalization
The process of removing degrees of freedom that are not relevant to describe a complex system at different scales of some physical variable (energy, length…).

Anti-de Sitter
(AdS). A geometric space with negative curvature.

Conformal field theory
(CFT). A quantum field theory with conformal symmetry, which includes scale invariance. Low-energy field theories of quantum critical systems are usually CFTs.

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https://doi.org/10.1038/s42254-019-0086-7

Tensor network (TN) states[1] are the building blocks of the mathematical representation of quantum states. The individual tensors encode the key properties of the overall wavefunction, providing a powerful framework that has enabled insights into the theoretical properties of complex quantum systems and the development of new and more powerful numerical simulation algorithms. TNs are now an active interdisciplinary area. This Review aims to provide a brief overview of the key concepts and to outline recent developments in different areas of application.

Background

Some history

TNs have evolved progressively over the years. The field started with a variational approximation for the 2D classical Ising model[2] that is considered to be a precursor of TN variational methods. Similar ideas were later used for classical partition functions[3]. But it was not until the 1990s that researchers started to investigate more seriously how the TN structures arising from classical partition functions were intimately linked to the wavefunctions of quantum lattice systems. A key development was the introduction of the density matrix renormalization group (DMRG)[4,5]. DMRG was constructed as a technique to keep the relevant degrees of freedom in a renormalization procedure targeting low-energy eigenstates of 1D Hamiltonians. These relevant degrees of freedom turned out to be entanglement degrees of freedom of the wavefunction. Later, it was proven that the state produced by DMRG is a 'finitely correlated state', essentially what we call today matrix product states (MPS)[6–8], or equivalently, what some mathematicians call a tensor train[9]. Moreover, it was understood that DMRG was a variational optimization algorithm over MPS[10]. DMRG was extremely successful, and it quickly became the tool of reference for 1D quantum lattice systems at low energies.

In the 2000s, physicists working on quantum information theory started to explore entanglement in the low-energy eigenstates of Hamiltonians, and its behaviour in quantum phase transitions. Developments such as the entanglement entropy of a block for 1D quantum critical systems[11] contributed to the understanding that entanglement has an inner structure that can be described by TNs. Moreover, it was also discovered that MPS are particularly well suited for describing gapped 1D quantum lattice systems with local interactions[12] because of their entanglement structure. Subsequent developments generalized this observation to other scenarios: higher-dimensional systems with projected entangled pair states (PEPSs)[13], critical systems with the multiscale entanglement renormalization ansatz (MERA)[14] and more.

From there on, developments in TN methods continued mostly at the crossover between condensed matter physics and quantum information. But it came as a pleasant surprise that TNs are also relevant to other scientific areas such as quantum gravity, in which the MERA has been proposed to be linked to geometry of space, for example, through the anti-de Sitter/conformal field theory correspondence (AdS/CFT)[15], or artificial intelligence, in which it has been proven that neural networks have a TN structure[16]. More applications are being discovered, sometimes in the most unexpected places. Essentially, anywhere there is a structure of correlations, there is also

Key points

- Tensor networks are mathematical representations of quantum many-body states based on their entanglement structure.
- Different tensor network structures describe different physical situations, such as low-energy states of gapped 1D systems, 2D systems and scale-invariant systems.
- Variational methods over families of tensor networks enable the approximation of the low-energy properties of complex quantum Hamiltonians. Other methods also allow the simulation of time evolution, the calculation of low-energy excitations and much more.
- Symmetric tensor network states enable more efficient simulation methods and the description of fermionic systems, lattice gauge theories, topological order and the classification of phases of quantum matter.
- Tensor networks, such as the multiscale entanglement renormalization ansatz, have been linked to a possible lattice realization of the holographic principle in quantum gravity.
- Tensor networks also provide a natural framework for understanding machine learning and probabilistic language models.

a TN, meaning that there is room to apply our knowledge of quantum many-body entanglement.

Some maths

TNs are representations of quantum many-body states based on their local entanglement structure. They arise naturally whenever one has a tensor product structure (more generally, a tensor category or a braided fusion category). Take, for instance, a quantum many-body system of N spins-1/2 such as a quantum spin chain, or any other spin system modelling the magnetic properties of a material. Once an individual basis for spins is chosen, any wavefunction of the system can be described, in a computationally inefficient way, in terms of $O(2^N)$ coefficients. These coefficients can be understood as a tensor with N indices, where each index can have two possible values (spin up or down). In this case, a tensor will be simply a multidimensional array of complex numbers. The reason for using TNs is that this tensor can be replaced by a network of interconnected tensors with fewer coefficients; see FIG. 1a for a generic case and FIG. 1b–i for useful examples. This construction defines a TN, and it depends on $O(\text{poly}(N))$ parameters only, assuming that the rank of the interconnecting indices is upper-bounded by a constant χ (sometimes also called D). This constant is called the bond dimension. Similarly, interconnecting indices in the network are called bond indices. Depending on the situation, one may use χ, or D, or both. For instance, χ is used for the bond dimension of MPS and MERA. However, when dealing with 2D TNs such as PEPS, one uses D for the PEPS bond dimension and reserves χ for the bond dimension of the environment tensors of 2D numerical algorithms.

In practice, the bond indices provide the structure of the many-body entanglement in the quantum state, and parameter χ turns out to be a quantitative measure of the entanglement present in the quantum state. For example, $\chi = 1$ corresponds to a separable product state, whereas any $\chi > 1$ provides non-trivial entanglement properties. In addition, it is possible to see that TN states satisfy the so-called area-law for the entanglement entropy[17] and characterize the relevant corner of the Hilbert space for a quantum many-body system at low energies.

A key mathematical ingredient in numerical algorithms dealing with TNs is the singular value decomposition (SVD), which is strongly tied to the Schmidt decomposition of quantum states (see Supplementary Information). The Schmidt decomposition states that it is possible to write a bipartite quantum state in terms of orthonormal correlated basis for the two parties (the Schmidt basis), together with χ real and positive coefficients (the Schmidt coefficients). Parameter χ is called the Schmidt rank. At the level of the coefficients of the wavefunction, if the orthonormal basis for two vector spaces, corresponding to a bipartite state, is considered, then the Schmidt decomposition is equivalent to the SVD of the matrix containing the coefficients, and Schmidt coefficients correspond to the singular values. As we shall see, the SVD is one of the key tools in TN algorithms. The interested reader is referred to REF.[1] for more details.

Another important concept is that of canonical form. Mathematically, the canonical form of a TN is that in which all the bond indices simultaneously correspond to orthonormal Hilbert spaces. For a TN without loops, this can be achieved by playing with sequential SVDs (see, for instance, REFS[1,18–21] for more details). For TNs with loops, however, this is formally not possible since one cannot define left/right partitions just by 'cutting' one link. On top of providing a useful representation of the TN, the canonical form helps greatly in simplifying tensor contractions and in providing truncation schemes in TN algorithms[18,19].

Main tensor network structures

Some of the most important TN structures are shown diagrammatically in FIG. 1b–i, and a comparison of their properties is provided in TABLE 1. In what follows, I briefly describe them and list their main properties.

TNs without extra dimensions

Matrix product states. MPS[6–8] are 1D arrays of tensors, as in FIG. 1b. Generally speaking, they correspond to low-energy eigenstates of gapped 1D local Hamiltonians[12]. They also satisfy a 1D area-law for the entanglement entropy of a block (TABLE 1). Expectation values of local observables can be efficiently computed and have a finite correlation length (see, for instance, REF.[1]). Hence, MPS cannot formally represent the entanglement structure of a quantum critical system. However, they are extremely efficient to manipulate, and over the years, researchers have used a rich variety of techniques based on finite-size scaling and finite-entanglement scaling[22,23] to extract properties of 1D quantum critical systems (see REF.[24] for a recent example).

Projected entangled pair states. PEPS[13] are 2D arrays of tensors, as in FIG. 1c for the particular case of a square lattice. They are known to capture the correct correlation structure of low-energy eigenstates of 2D local Hamiltonians satisfying the 2D area-law as well as of 2D thermal states[12,25]. Unlike MPS, PEPS can handle critical correlation functions[26], but they cannot be contracted both efficiently and exactly[27]. This is the reason that people developed approximate methods for manipulating them, some of which are sketched later in this Review. They can also handle topological order, both chiral[28] and non-chiral[29,30]. Still, it is not fully

Topological order
A type of order in quantum matter entirely due to global entanglement properties and which does not exist classically. Other characterizations: excitations are anyonic, the topological entanglement entropy is non-zero, ground states are topologically degenerate, and reduced density matrices are locally equivalent.

Area-law
Property by which the entanglement entropy of a region scales proportionally to the size of the boundary of the region.

Tensor contraction
Sum over the common indices of a set of tensors (for example, matrix multiplication).

Correlation length
Non-mathematically, this is the length scale at which correlations are sizeable in a many-body system.

understood whether they can handle chiral topological order with gapped bulk excitations.

TNs with extra dimensions

Tree tensor networks. Tree TNs (TTNs)[31] are tree-like structures as in FIG. 1d. By construction, TTNs have a finite correlation length and an entropy that, on average, satisfies a 1D area law. They are therefore well suited for gapped 1D systems, although they have also been used fairly extensively to deal with 1D critical systems[32] and 2D systems[33]. By construction, they codify a Wilsonian renormalization structure, if the tensors codify a coarse-graining of the Hilbert space and are therefore isometries.

Multiscale entanglement renormalization ansatz. MERA structures[14] are structures such as those in FIG. 1e, which illustrates a 1D MERA. They are essentially like a TTN of isometries, but including the so-called disentanglers, which are unitary operators that account for entanglement between neighbouring sites. Thus, MERAs are made from unitaries and isometries, and have a number of remarkable properties. For instance, they can handle the entanglement entropy of critical 1D systems[34]. Moreover, they are efficiently contractable. They have an extra holographic dimension that encodes a renormalization scale, related to the 'entanglement renormalization'[14]. Finally, MERA is believed to be linked to the AdS/CFT correspondence in quantum gravity[15].

Branching MERA. Branching MERA (bMERA)[35] is illustrated in FIG. 1f. It is similar to the MERA, with the additional fact that at every renormalization scale, the MERA decouples into several copies. In this way, there is an arbitrary scaling of the entanglement entropy of a block, thus allowing the reproduction of the entanglement structure of systems that violate the area-law. Physically speaking, this structure accounts for the decoupling of degrees of freedom at different renormalization scales (for example, spin–charge separation in electronic solid-state systems).

Other important TNs

Operators and mixed states. Linear operators acting on quantum states can be conveniently represented by TNs; for example, by matrix product operators (MPO) in 1D[36] and projected entangled pair operators (PEPO) in 2D[37] (FIG. 1g,h). Mixed states can also be represented by such structures, and also by pure states including environment degrees of freedom over which we trace (the 'purification'), represented as matrix product density operators (MPDO) in 1D[38] (FIG. 1i). The advantage of MPDOs is that they are positive by construction. However, the number of correlations that they can carry for a fixed bond dimension is typically lower than that of a generic MPO with similar bond dimension[39].

Continuous TNs. The structures discussed above allow for a continuum limit, therefore becoming an ansatz for low-energy functionals of states in quantum field theories, as well as for operators acting on such functionals. For instance, one has continuous MPS[40], continuous MERA (cMERA)[41] and continuous PEPS (cPEPS)[42]. Whereas cMPS and cMERA have already been used for various applications, cPEPS are still to be explored.

Main algorithms

In this section, I very briefly outline the main ideas behind some of the most important numerical algorithms using TNs. I focus on the basic idea behind key families of numerical TN methods, leaving out technical

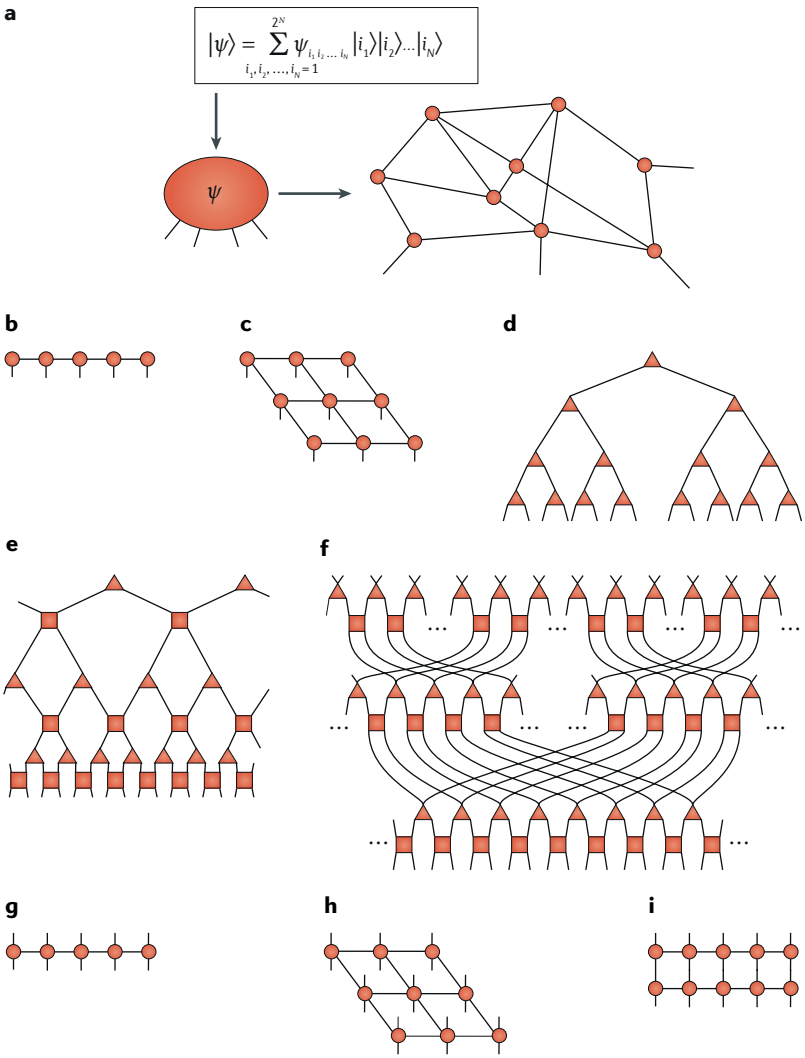

Fig. 1 | **Diagrammatic representation of a tensor network and several examples of tensor networks. a** | The coefficient of the quantum state (...) of a many-body system with *N* sites (for example, *N* spins) can be understood as a tensor with exponentially many coefficients in the system's size. The structure of this tensor is accounted for by a tensor network (TN), which is a network of tensors interconnected by ancillary indices ($i_1, \ldots, i_N$) that take into account the structure and amount of entanglement in the quantum many-body state. This is represented here diagrammatically, in which the (generic) shapes correspond to the tensors, the lines to the indices and the lines connecting the shapes to contracted (summed) common indices. The TN on the right-hand side is intended to be generic. **b**–**i** | Examples of common TNs: matrix product state (panel **b**); projected entangled pair state for a square lattice (panel **c**); tree TN (panel **d**); multiscale entanglement renormalization ansatz (MERA; panel **e**); branching MERA (panel **f**); matrix product operator (panel **g**); projected entangled pair operator (panel **h**); matrix product density operator (panel **i**), in which tensors in the upper row of the diagram are the Hermitian conjugates (with respect to up/down indices) of the tensors in the lower row of the diagram, so that the whole operator is Hermitian and positive.

Table 1 | **Comparison of properties for some of the TNs discussed in the main text**

	MPS	2D PEPS	TTN	1D MERA	1D bMERA
$S(L)$	$O(1)$	$O(L)$	$O(1)$	$O(\log L)$	$O(L)$
$\langle O\rangle$	Exact	Approx.	Exact	Exact	Exact
ξ	$<\infty$	$\leq\infty$	$<\infty$	$\leq\infty$	$\leq\infty$
Tensors	Any	Any	Any	Unit./isom.	Unit./isom.
Canonical form	Obc, ∞	No	Yes	–	–

Multiscale entanglement renormalization ansatz (MERA) and branching MERA (bMERA) are built from unitary (Unit.) and isometric (Isom.) tensors, and we therefore do not consider a canonical form for them. $S(L)$, entanglement entropy of a block of length L (that is, with L sites in 1D and $L\times L$ in 2D); $\langle O\rangle$, calculation of a local expectation value; ξ, correlation length; 'tensors', constraints on tensors; 'canonical form', exact canonical form; MPS, matrix product states; obc, open boundary conditions; PEPS, projected entangled pair states; TTN, tree tensor networks.

details about implementation. Readers interested in more information are referred to the specific papers explaining the details of each technique. Note that numerical TN methods are difficult to classify according to unique criteria. Here I first introduce methods for obtaining 1D states, then methods for contracting 2D TNs, then those for obtaining 2D states and finally mixed methods in which TNs are combined with other techniques.

Methods for obtaining 1D states

Density matrix renormalization group. DMRG[4,5] is by far the most famous TN method. It was originally proposed as a renormalization procedure over the ground-state wavefunction of a 1D quantum lattice system. In the modern formulation, it is a variational optimization algorithm over the family of MPS[43,44]. In particular, one starts from the tensor at the left boundary, optimizes over its parameters and then moves to the next tensor on the right. The optimization is then repeated, sweeping over the tensors towards the right. Once the right boundary is hit, the sweeping goes towards the left, and one repeats the whole process (sweeping left and right) until convergence, with tensor coefficients treated as variational parameters in order to minimize the expectation value of a given Hamiltonian. At every step, the optimization can be written as a quadratic problem for the tensor parameters, which can be solved with standard linear algebra. The method also makes use of other tricks, such as the canonical form for open boundary conditions, to improve stability and performance[43,44]. It can also be adapted to translationally invariant systems in the thermodynamic limit, the 'infinite-DMRG'[45,46]. There are also extensions of the method to deal with periodic boundary conditions[47] and low-energy excitations[48,49]. For open boundary conditions and infinite-size systems, the computational cost is $O(\chi^3)$, with χ the MPS bond dimension. For periodic boundary conditions, if no further approximations are introduced, the computational cost is $O(\chi^5)$.

Time-evolving block decimation. Time-evolving block decimation (TEBD)[18,19] enables the computation of the time evolution of an MPS. If the evolution is in real time, then TEBD allows one to compute dynamics as long as the state remains slightly entangled. If it is in imaginary time, then it allows one to approximate ground states and is a plausible alternative to DMRG. TEBD has also been successfully applied to infinite-size systems[20]. The asymptotic scaling of the computational cost is similar to that of DMRG, that is, $O(\chi^3)$ for an MPS of bond dimension χ with open boundary conditions. TEBD is based on the canonical form of an MPS[21]. In this scheme, the truncation of the MPS bond dimension is done via SVD. In turn, this truncation provides an optimal local approximation between MPS. The optimality of this truncation is formally justified only for TNs without loops. This truncation scheme is similar to the one in the 'two-site DMRG', in which tensors for two sites are optimized by a variational update following an SVD.

TTNs. In addition to MPS, TTNs are a useful tool to study 1D systems. The procedures used in DMRG and TEBD have been extended to TTNs to study 1D gapped and critical systems[31,32]. This is possible given the absence of loops in the TTN. The computational cost depends on the specifics of the tree, but typically it boils down to $O(\chi^4)$, with χ the bond dimension of the TTN[31].

1D MERA. MERA[14] can also be used as a variational ansatz to approximate ground-state properties. For the case of 1D systems, this has been done for both gapped[14] and critical[34] systems. The variational optimization is, however, trickier than for DMRG, for example, because of the constraints on the tensors (they must be unitaries and isometries). Such optimization can be done by using a number of techniques, as explained in detail in REF.[50]. Overall, the computational cost depends on the actual structure of the MERA. For instance, for the 'binary MERA' the cost is $O(\chi^9)$, whereas for the 'ternary MERA' the cost is $O(\chi^8)$, and for the 'modified-binary MERA' it is $O(\chi^7)$[34].

Tangent space methods. An entire family of methods[51,52] is based on the idea that MPS can be understood as a manifold, in the sense of differential geometry. With this in mind, it is possible to obtain a variety of highly efficient and accurate methods using the concept of tangent space of the MPS manifold. A remarkable example is the time-dependent variational principle algorithm[53] for MPS. This algorithm uses concepts of differential geometry to compute the time evolution of a MPS either in real or in imaginary time, without the need of a Trotter decomposition, as in TEBD, and preserving naturally all the spatial symmetries of the physical system. The idea of using the manifold structure of MPS allows the computation of low-energy excitations and energy bands by means of an ansatz with well-defined momentum[54]. The formalism of the tangent space can also be applied to the variational optimization of the expectation value of a Hamiltonian, the 'variational uniform' MPS algorithm[55]. The asymptotic computational cost of this family of methods for 1D systems is similar to that of other MPS approaches, that is, $O(\chi^3)$ for an infinite-size MPS of bond dimension χ.

Other strategies. Other strategies to develop new algorithms focusing on the properties of MPS have been used. Examples include alternative methods of simulating time evolution in 1D[56,57], and of simulating

Wilsonian renormalization
In this context, a renormalization scheme by which different length scales are obtained purely by removing short-distance degrees of freedom, without having previously disentangled them. In many cases, this is done by removing high-energy (and/or high-momenta) degrees of freedom.

Trotter decomposition
Decomposition of the exponential of the sum of two matrices A and B as $e^{(A+B)t}=\lim_{n\to\infty}(e^{At/n}e^{Bt/n})^n$, with t some real parameter.

open quantum dynamics, including non-Markovian processes[58] and effective small reservoirs[59].

Methods for contracting 2D tensor networks

In this section, I overview methods for contracting a TN without open indices, focusing mostly on methods for computing effective environments from 2D PEPS. This is a key step in the simulation of 2D quantum lattice systems. The same methods can be considered for 2D classical partition functions, and with some modifications they can also be used for 3D classical and quantum systems. In fact, many of these methods were originally developed in the context of 2D classical statistical mechanics; see, for instance, REF.[3].

Boundary MPS. Boundary MPS was the first method used to approximate the environment of a site on a 2D PEPS, both for finite[13] and for infinite[60,61] systems. The idea is to contract the full 2D lattice starting from a boundary (either an actual boundary for finite systems, or placing it manually at infinity for systems in the thermodynamic limit), with boundary tensors forming an MPS. The algorithm proceeds by contracting 1D MPOs made of lattice tensors into the MPS, mimicking a non-unitary time evolution that can be treated, with the techniques from REF.[21], for example. For a PEPS of bond dimension D and a boundary MPS of bond dimension χ, the computational cost of this scheme for a 2D square lattice is $O(\chi^3D^6+\chi^2D^8)$ for a horizontal/vertical boundary, and $O(\chi^3D^4+\chi^3D^6)$ for a diagonal boundary[1,60,61].

Corner transfer matrices. The corner transfer matrices (CTM) method is a popular approach nowadays because it is relatively easy to implement and produces good-quality results. Focusing on a 2D square lattice of tensors, the idea is to find renormalized (coarse-grained) approximations to the tensors amounting to the contraction of all the tensors on the corners. Such tensors are the CTMs, which are well-known objects in the context of exactly solvable statistical mechanical models. There are several schemes for dealing with and finding such CTMs[3,62–65]. The computational cost depends on the specifics of the implementation. For example, the method from REFS[63,64] has a cost of $O(\chi^3D^6)$ for a PEPS of bond dimension D and a CTM of bond dimension χ.

Tensor coarse-graining. In tensor coarse-graining, the main idea is to coarse-grain the network by finding new renormalized tensors that amount to a 'zoom-out' (an average description at long distances: like going from individual pixels to an actual picture) and that take into account the main features of the TN at long distances. The approach is similar to a Kadanoff blocking for classical statistical mechanical models (such as the Ising model). Many schemes fall into this category, each with its own advantages and drawbacks: tensor renormalization group[66], second renormalization group[67], higher-order tensor renormalization group, higher-order second renormalization group[68], tensor entanglement-filtering renormalization[69], tensor network renormalization (TNR)[70], loop-TNR[71] and TNR_+ (REF.[72]). The specifics of the implementation for each of these cases are different. However, the idea is that one typically contracts tensors, defining a new lattice in terms of some new tensors that account for the contraction. The new tensors are then renormalized by truncating their bond indices with some isometries. The prescription for finding such isometries is what defines the different schemes. Some schemes (such as TNR) also remove local entanglement before blocking the tensors. The computational cost of each scheme can also be very different, depending on the implementation. For example, for a classical partition function with a TN structure of bond dimension χ on a square lattice, the second renormalization group method has a cost of $O(\chi^{10})$[73].

Nested tensor network. Nested tensor network[74] is not a contraction scheme in itself as in the previous cases, but rather the idea of projecting the tensors of a 3D TN on a 2D plane, so that the resulting 2D TN can be contracted by any of the three strategies discussed above. An example is the TN for the norm of a 2D PEPS with bond dimension D, in which bra and ket tensors are shifted with respect to each other, thus producing a new 2D TN similar to a 2D partition function with bond dimension D. Such a 2D TN can thus be contracted more efficiently than that obtained with a double-layer approach (this is, by dealing simultaneously with the bra and ket bond indices of the TN), which has bond dimension D^2.

Methods for obtaining 2D states

This section focuses on techniques for obtaining TN states for 2D quantum lattice systems. As we shall see, in some cases the techniques previously explained for 1D systems and 2D TN contractions turn out to be fundamental.

2D DMRG. DMRG was also considered for the study of 2D systems[75]. Even though, by construction, DMRG produces an MPS and is therefore a priori better suited to deal with gapped 1D local Hamiltonians, the technique is also successful in 2D because of its efficiency. The idea behind 2D DMRG is to consider a stripe, or wrap the 2D system around a cylinder, and then use MPS as an ansatz for the 2D lattice, following a snake-like pattern. The true 2D properties of the system are recovered by doing careful finite-size scaling with the thickness of the cylinder or the width of the stripe. This approach has been very successful in determining properties of the 2D $t-J$ model[76,77] and the spin liquid nature of the ground state of the kagome Heisenberg antiferromagnet[78–80]. An interesting evolution of 2D DMRG is to combine position and momentum basis for both directions, and this shows better performance in some situations[81]. Still, the computational cost of 2D DMRG is eventually doomed for large 2D systems, owing to an exponential entanglement wall in the transverse direction that cannot be handled by an MPS with finite bond dimension. In other words, the bond dimension of the MPS needs to be exponentially large in the size of the system in order to account for the 2D area-law of entanglement.

2D TTNs. TTNs have also been used to study 2D systems, as their structure can be easily adapted for such geometries[33]. Still, as in the 2D DMRG case, the underlying TN structure has inherently built-in 1D correlations because of the absence of loops in the network, which in turn implies the existence of exponential entanglement walls, and therefore only a relatively good accuracy depending on the system and regime can be achieved. Still, TTNs can be useful since their associated algorithms are fairly efficient (as in 1D). For instance, they have been used to study confinement/deconfinement transitions of 2D $\mathbb{Z}_2$ lattice gauge theories[82].

PEPS. Numerical algorithms based on PEPS are well suited to tackling 2D systems because PEPS have inherent 2D correlations and, as such, is a natural ansatz to study a wide variety of 2D systems. It can be applied to both finite-size systems, the 'finite-PEPS'[13,83] and infinite systems, the 'infinite-PEPS'[60,61]. There are different ways of optimizing the tensors of a PEPS to obtain approximations of ground states; for instance, variational updates (both for finite[83] and infinite[84,85] PEPS) and imaginary-time evolution through simple[86], full[60,61] and fast-full[87] updates. Simple updates are very efficient, but not necessarily accurate, whereas full and fast-full updates take into account the effect of the environment on the TN when optimizing a PEPS tensor and are therefore slower, but more accurate. Such tensor environments are usually computed directly from the TN through the renormalization methods for contracting 2D TNs explained in the previous section, for instance, by using boundary MPS, CTMs and tensor coarse-graining. Furthermore, it has also been shown how to compute excited states with PEPS for 2D systems[88], and how to do accurate extrapolations in the bond dimension[89]. The computational cost of PEPS algorithms heavily depends on the type of algorithm chosen. For instance, for a square lattice, simple-update algorithms with a mean-field environment[90] have a cost of $O(D^5)$, whereas full and fast-full updates have a cost of $O(\chi^3 D^6)$ (and with a prefactor that could be large), with χ and D respectively the environment and PEPS bond dimensions.

2D MERA. MERA has also been used as a variational ansatz to approximate ground states of 2D quantum lattice systems (see, for instance, REFS[91–94]) The computational cost of this approach strongly depends on the type of lattice and the specific choice of unitaries and disentanglers. For instance, in REF.[91] for an infinite square lattice the computational cost is $O(\chi^{16})$, where χ is the MERA bond dimension.

Combined methods

In this section, I outline developments in which TNs were combined with other existing methods, or in which TNs proved useful to understand other existing techniques.

Monte Carlo TNs. Monte Carlo methods have been used together with TN techniques in several ways. For instance, Monte Carlo sampling was used to do variational optimizations over TNs, and approximate calculations of effective environments[95]. In the context of string-bond and plaquette-entangled states, Monte Carlo was the sampling technique for optimization and expectation value calculation[96]. The combination of TNs with Monte Carlo in principle allows a higher bond dimension to be reached in the calculations, at the cost of the length of the sampling. For instance, the cost of these methods when combined with MPS for periodic boundary conditions is typically $O(N\chi^3)$, with χ the MPS bond dimension and N the length of the (finite) 1D system, with a prefactor that depends on the number of samples.

TNs for density functional theory. Density functional theory is one of the most popular numerical approaches for performing ab initio calculations of real materials and molecules. In this context, TNs (and especially MPS) have been used to produce systematic approximations to the exchange-correlation potential of electronic systems[97].

TNs for dynamical mean-field theory. TNs have also found important applications in dynamical mean-field theory. In particular, in a series of works[98] it was shown that MPS techniques can be used as a high-accuracy and low-cost impurity solver, including applications to non-equilibrium systems.

TNs and wavelets. A number of connections have also been established between wavelet transformations and TNs. More specifically, in REF.[99] it was shown how Daubechies wavelets could be used to build an analytic approximation to the ground state of the 1D critical Ising model; Daubechies wavelets correspond to instances of the 1D MERA. Additionally, REF.[100] reported how the structure of wavelet transformations adapts to that of a quantum circuit, and REF.[101] showed how the ground state of some fermionic systems could be understood through entanglement renormalization, also using the language of wavelets.

More synergies. In addition to the most relevant combined methods sketched above, there have been further developments in other directions. For instance, the 'entanglement continuous unitary transformations'[102] showed how to mix the idea of continuous unitary transformations and Wegner's flow[103] with TNs, by truncating the flow equation in its operator-entanglement content. Moreover, TNs have been used in combination with perturbation theory; for example, in REF.[104] it was shown how to construct an exact 2D PEPS up to a given order, in perturbation theory. Another fruitful combination has been that of TNs and the randomized SVD[105], which improves the efficiency of numerical algorithms such as TBED, DMRG and TRG[106]. TN states have also been used to develop generalized Lanczos methods[107]. Finally, TN states were useful to understand the mathematical structure of exactly solvable systems, for instance, the algebraic Bethe ansatz[108], the fermionic Fourier transform[109], the XY spin chain[110] and Kitaev's honeycomb model[111].

Daubechies wavelets
Family of orthogonal wavelets defining a discrete wavelet transform and characterized by a maximal number of vanishing moments for some given support.

Wegner's flow
Flow of continuous unitary transformations that diagonalizes a Hamiltonian, as $H_D = \lim_{l\to\infty} U^\dagger(l) H U(l)$ with l the flow parameter and H_D the diagonal Hamiltonian.

Lanczos methods
An adaptation of a power method to find the eigenvalues and eigenvectors of a matrix.

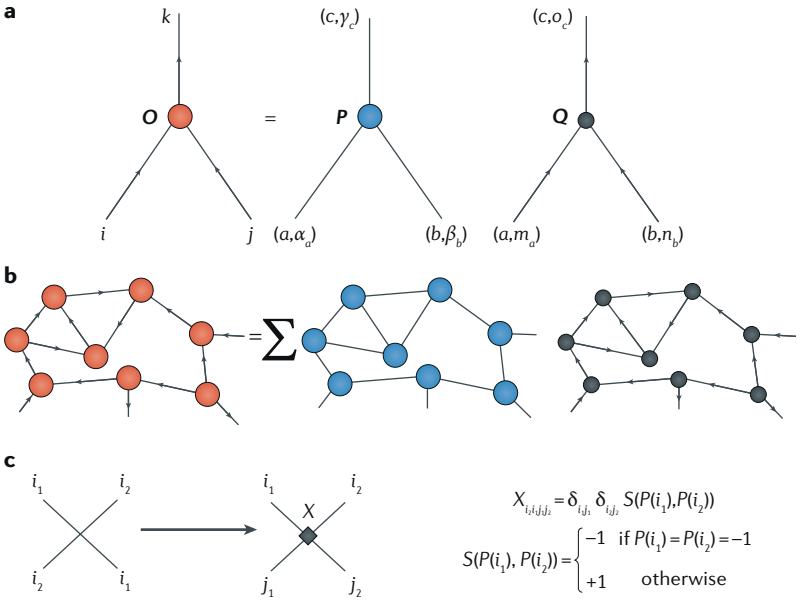

Fig. 2 | **Symmetries in tensors and tensor networks. a** | A three-index symmetric tensor O decomposes into a degeneracy tensor P and an intertwiner of the symmetry group Q (which for SU(2) is a Clebsch–Gordan coefficient). Index k decomposes at a double index γ_c for the degeneracy tensor and o_c for the structural tensor, for a symmetry sector c (and similarly for indices i and j). **b** | A symmetric tensor network (TN) decomposes as the sum of spin networks, with coefficients given by TNs of degeneracy tensors, and the sum being done over the degrees of freedom of internal indices. **c** | In fermionic TNs, crossings between lines in diagrammatic notation are replaced by fermionic SWAP operators X. These operators take into account the anti-commutation relation of fermionic operators in the second quantization. S is the sign that depends on the parities $P(i_1)$ and $P(i_2)$ of indices i_1 and i_2.

The role of symmetries

In this section, I briefly overview the effect of symmetries in TNs. I outline why having a symmetry implies a tensor factorization, and its important consequences. I also comment on some basic aspects of fermionic TNs as a special case, and on gauge symmetries, topological order and the classification of quantum phases of matter.

Global symmetries

The implementation of global symmetries in TN algorithms has been considered (at least) since the early years of DMRG, and it is well-known that it can lead to important computational advantages. This fact was exploited especially in DMRG[112], the 1D MERA[113] and 2D PEPS[114,115], both for Abelian symmetries such as U(1) particle-conservation, but also for non-Abelian symmetries such as SU(2) rotation-invariance. For further details, see REFS[113,116,117], which provide in-depth overviews. In addition to numerical advantages, an important theoretical consequence is that the 'spin networks' appear naturally from TN states with symmetries. Spin networks are used in loop quantum gravity to describe quantum states of space at a certain point in time[118]. In this sense, TNs with symmetries turn out to offer not only efficient numerical methods for complex quantum systems, but also an intriguing connection between quantum entanglement and gravity.

When dealing with local symmetries in TN states, Schur's lemma[119] ultimately implies that symmetric tensors can be decomposed into two parts: one completely determined by the symmetry thatacts on the subspaces of irreducible representations, and another that contains the actual degrees of freedom of the tensor and acts on a degeneracy subspace. For example, for a symmetric tensor O_{ijk} with three indices (i,j,k), the Wigner–Eckart theorem implies that it can be decomposed as $O_{ijk} = (P^{abc})_{\alpha_a\beta_b\gamma_c} Q^{abc} m_a n_b o_c$, where index i decomposes as $i \equiv (a, \alpha_a, m_a)$ (and similarly for the rest), P^{abc} is a degeneracy tensor that contains all the degrees of freedom of O_{ijk}, and the structural tensor Q^{abc} is completely fixed by the symmetry group. This is represented in the TN of FIG. 2a. In practice, this means that the symmetry constraint heavily reduces the degrees of freedom of the tensor. As a consequence, the whole TN also factorizes into two parts: a TN of degeneracy tensors, and a TN of structural tensors. The latter is a spin network (FIG. 2b). Thus, a symmetric TN for a quantum state $|\psi\rangle$ of N sites is a superposition of exponentially many spin networks with N open indices, with coefficients determined by TNs of degeneracy tensors, whose indices amount for the degeneracy of the different irreducible representations labelled by the indices of the structural tensors.

There are many reasons why it is a good idea to implement symmetries in TN algorithms whenever this is possible. For instance, they allow systems with specific quantum numbers to be simulated. But most importantly, symmetries also allow a compact description and manipulation of the TN, thus leading to more efficient algorithms that can reach a larger bond dimension.

Fermionic systems

TN methods can also be used to simulate fermionic systems in any dimension, and directly in the language of the second quantization. Fermionic statistics can be implemented in TN algorithms in different but equivalent ways[93,94,120–124]. The graphical implementation from REF.[120] is perhaps the simplest to describe. This is based on two fermionization rules: first, use parity-symmetric tensors, and second, replace crossings in the planar representation of the TN by fermionic SWAP gates. The first rule is justified because fermionic parity (whether the total number of fermions is even or odd) is a good $\mathbb{Z}_2$ symmetry for fermionic systems. The second rule is also justified because fermionic SWAP gates, defined as in FIG. 2c, correctly take into account the anticommutation of fermionic operators in the second quantization. Finally, fermionic TN algorithms can be programmed in the same way as their bosonic counterparts, but taking into account these two simple rules, which only imply a sub-leading increase in the computational cost of the algorithm.

Gauge symmetries

Gauge symmetries can also be naturally implemented in the framework of TNs, leading to a similar TN decomposition as for global symmetries, but slightly different owing to the local (gauge) nature of the symmetry[125,126]. Many works have implemented the formalism of gauge-invariant TNs, focusing mostly on 1D, and sometimes 2D, systems. In particular, $\mathbb{Z}_2$ lattice gauge theories in $(1+1)$ dimensions have been considered with DMRG[127].

Clebsch–Gordan coefficient
Coefficient of the change of basis in angular momentum, from a tensor product basis to a coupled basis (for instance, from spins $1/2 \otimes 1/2$ to spins $0 \oplus 1$.

SWAP gate
Unitary gate that swaps the quantum states of two physical systems.

For the Schwinger model (quantum electrodynamics in (1 + 1) dimensions), DMRG (without the MPS formulation) was considered in several works[128], whereas MPS simulations were used to compute the chiral condensate[129] and thermal properties[130], the mass spectrum[131], the Schwinger effect[132], the effect of truncation in the gauge variable[133], the case of several fermionic flavours[134], and the thermodynamic limit of DMRG and its possible extrapolation to (2 + 1) dimensions[135]. The consequences of gauge symmetry in the MPS description of the Schwinger model was first elaborated in REF.[126]. A gauge-invariant MPS ansatz was also used to compute the confining potential[136] and the scattering of two quasiparticles[137]. TN simulations have also been implemented for non-Abelian lattice gauge theories in (1 + 1)D[138,139]. For higher-dimensional systems, gauge-invariant TN ansatzes have also been proposed analytically[125,140,141], which can be used as variational wavefunctions to study lattice gauge theories in (2 + 1) dimensions.

Phases of quantum matter

TN states are the natural language for topologically ordered systems, which can in turn be understood using gauge symmetries. There are several developments along this direction, both from the analytical and numerical perspective. From the analytical point of view, it has been proven that eigenstates of string-net models[142] admit an exact TN description[29,30,143], in which tensors have specific gauge symmetries. This means that all non-chiral topologically ordered 2D phases on a lattice admit a TN description. Moreover, it has been shown that certain PEPS for fermionic systems as well as for spin systems can handle chiral topological order, although the corresponding parent Hamiltonians (which can be obtained directly from the PEPS tensors) have either gapless bulk excitations or long-range interactions[28]. It is therefore a theoretical challenge to understand the correct TN framework to describe chiral topological states with gapped bulk and short-range parent Hamiltonians. From the numerical perspective, TN algorithms have been used to compute phase diagrams of topological systems under perturbations, for example, using TTNs[82] and 2D PEPS[144] and DMRG on cylinders[145]. In addition to these developments, TNs have also proven to be an extremely useful tool in computing symmetry-protected topological order in 1D[146], representing fractional quantum Hall states[147], simulating anyonic systems[148], and describing theoretically topological quantum computation[149] and symmetry-enriched topological order[150]. A separate set of results, related to the developments on topological order, has concerned the theoretical classification of quantum phases of matter[151], for which TNs have also been useful. For instance, MPS and PEPS were used to classify phases of 1D and 2D quantum spin systems[152–154]. The classification of fermionic topological phases has also been studied using fermionic MPOs and fermionic PEPS[155–157].

Holography

Several notions related to holography also play a key role in TN states. In this section, I briefly describe how TNs provide a natural bulk–boundary correspondence through the 'entanglement Hamiltonians'. I also comment on the connection to the geometry of space-time in quantum gravity and the idea that space-time may emerge from quantum many-body entanglement.

Parent Hamiltonian
Hamiltonian that has a given PEPS or MPS as unique ground state.

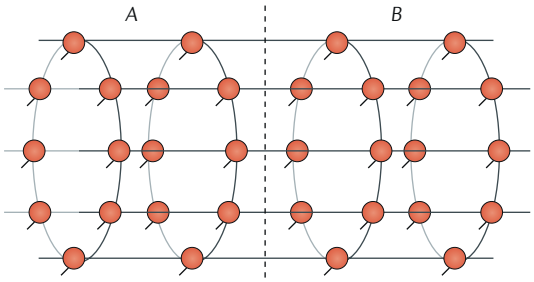

Fig. 3 | **2D projected entangled pair state (PEPS) on a cylinder.** To compute the entanglement Hamiltonian H_E, a bipartition of the system (*A* versus *B*) is made, and the reduced density matrix ρ of one of the subsystems is computed using standard contraction techniques for PEPS (for example, boundary-matrix product state with periodic boundary conditions). The eigenvalues of ρ then define the eigenvalues of H_E, which can be grouped according to quantum numbers such as the vertical momentum (since there is translation invariance if the cylinder is rotated around its axis).

Entanglement Hamiltonians

The eigenvalues of the reduced density matrix of a bipartition encode important information about the boundaries of the system[158]. Such a reduced density matrix can be written as $\rho \propto e^{-H_E}$, with H_E the entanglement Hamiltonian. H_E describes the fundamental degrees of freedom of the projection of the quantum state on a boundary. TNs turn out to lend themselves naturally to the investigation of such entanglement Hamiltonians for various systems, and especially for 2D PEPS[159]. The main idea in such derivations is to wrap the 2D PEPS around a cylinder, and then study the entanglement spectra (the eigenvalues of H_E) of half of the cylinder versus the other half (FIG. 3). Such eigenvalues can be grouped in terms of their momentum quantum number, and encode very useful information about the PEPS, such as possible gapless edge states and chiral topological order[28].

An interesting correspondence emerged from the studies done so far. Consider PEPS that are ground states of 2D Hamiltonians with local interactions. It seems that, if the 2D system is gapped and not topologically ordered, H_E is usually a 1D Hamiltonian with short-range interactions. However, for 2D critical systems, H_E is a 1D Hamiltonian with long-range interactions. In addition, if the 2D system is gapped and topologically ordered, then H_E is essentially a projector. This is very interesting, because it justifies the numerical observation that environment calculations in infinite 2D PEPS, for example, converge quickly with very few iterations of a boundary MPS[12]. Therefore, it appears that 2D PEPS foreground states of gapped 2D systems with no topological order can be contracted efficiently with good accuracy, even if this is not the case for a generic PEPS[27] or even on average[160]. Some steps towards turning this observation into a mathematical theorem have already been taken[161].

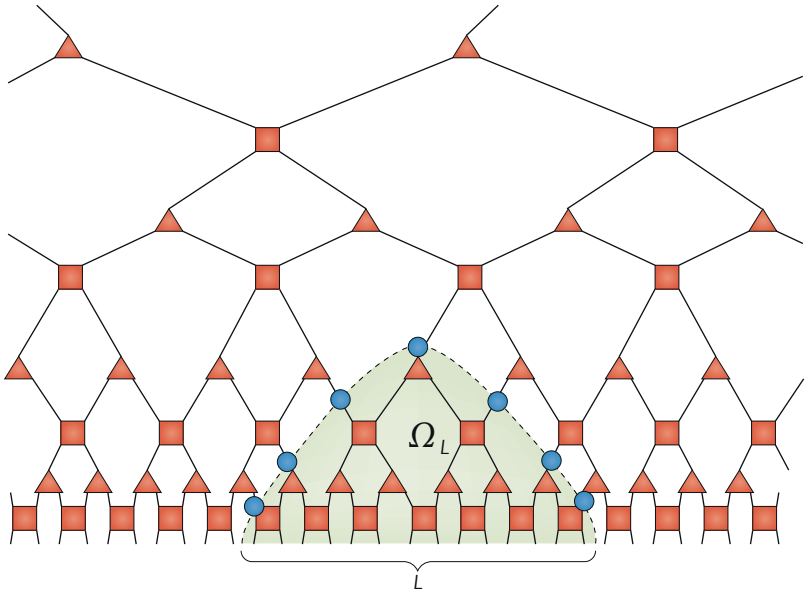

Fig. 4 | **1D MERA.** The entanglement entropy of a block of length L for a multiscale entanglement renormalization ansatz (MERA) is upper-bounded as $S_L \leq \log\chi \times \partial\Omega_L$, with $\partial\Omega_L$ the boundary of region Ω_L in the tensor network (that is, the number of links crossed by the blue dashed line) and χ the bond dimension. It is easy to realize that $\partial\Omega_L = O(\log L)$, and therefore one has that $S_L = O(\log L)$ for the 1D MERA. This calculation matches the behaviour from conformal field theories (CFTs) in (1 + 1)D, and corresponds, precisely, to the lattice version of the Ryu–Takatanagi prescription to compute the entanglement entropy in anti-de Sitter (AdS)/CFT[196]. Entanglement is thus the area in holographic space of the minimal surface separating the two regions. This is one of the key observations that motivates the analogy between MERA and AdS/CFT.

Emergent geometry

In the framework of holography, there is a very suggestive connection between entanglement, TNs and quantum gravity: it looks like the MERA is a lattice realization of a space with some geometry, in which the curvature is somehow linked to entanglement. The observation implies that space-time geometry may emerge from the underlying structure of entanglement in complex quantum states. An instance that has been studied in some detail is the possible relation between MERA and the AdS/CFT or gauge/gravity duality[162]. This connection between TNs and quantum gravity was originally noticed in REF.[15], and later investigated in other studies[163–166]. More specifically, for a scale-invariant MERA, the tensors in the bulk can be understood as a discretized AdS geometry, whereas the indices at the boundary correspond to the local Hilbert spaces obtained after a discretization of a CFT (FIG. 4). The connection can be made more formal by taking the continuum MERA[41] and evaluating the metric of the resulting smooth space in the bulk, with the curvature of the geometry being linked to the density of disentanglers[164,165]. Currently, the connection is intriguing and has motivated a lot of research, especially from the string theory community. In particular, there have also been claims that MERA does not correspond to an AdS geometry, but rather to a de Sitter geometry[167]. In recent work, however, it was shown that MERA is neither AdS nor de Sitter, but rather a lightcone geometry[168]. Although this connection is certainly suggestive and remarkable, the role played by TNs in the quantization of gravity remains unclear.

Boltzmann machine
A specific type of neural network in which the target is to reproduce some Gibbs thermal probabilities.

MERGE
Linguistic operation introduced by Noam Chomsky, which picks up two entities (for example, noun and adjective) and produces a new one from the two (for instance, noun phrase).

Artificial intelligence

In this section, I will comment on the recent observation that neural networks (such as those used in deep learning) are in fact particular cases of TNs, and on the use of MPS to improve some methods of artificial intelligence. Additionally, I will outline the result that syntactic relations in language have a TN structure that is inherited by probabilistic language models.

Machine learning

Several promising connections between TNs and machine learning have been put forward. In REF.[16], it was shown that deep learning architectures can be understood using the language of quantum entanglement. To name a couple of examples, convolutional networks correspond to specific cases of TTNs, and recurrent neural networks correspond to MPS. More generically, the whole machinery of quantum information and entanglement theory can be applied to understand neural networks in new ways. One must, however, be careful, since in general neural networks are characterized by nonlinear functions, whereas TNs are linear and therefore obey the superposition principle. In REF.[169], it was shown that there is an equivalence between restricted Boltzmann machines (a simple type of neural network) and TN states. Boltzmann machines were also shown to be connected to some classes of TN states in arbitrary dimensions[170]. In REFS[171–174], MPS and TTNs were used for supervised and unsupervised learning tasks of classifying images. Finally, in REF.[175], it was discussed how quantum circuits based on MPS and TTNs could be used to implement machine-learning tasks in near-term quantum devices, and REF.[176] explored how probabilistic graphical models motivate the concept of generalized TNs, in which information from a tensor can be copied and reused in other parts of the network, thus allowing for new types of variational wavefunctions.

Language models

From the perspective of computational linguistics, probabilistic language models used for speech and text recognition were found to have a TN structure. This is a consequence of the fact that Chomsky's MERGE operation can be understood as a physical coarse-graining of information[177]. Such probabilistic models usually have the form of a TTN or even an MPS, for example, loop-free TNs. In turn, this matches the empirical observation that convolutional neural networks are quite good at language processing. In connection with the results mentioned in the previous section, it is clear that this is indeed so because such neural networks are TTNs, which encode the renormalization group structure of language found in REF.[177], and are therefore naturally well-suited for the task.

Further topics

There are many other interesting results related to TN states and methods, and I cannot attempt to summarize all of them here. Nevertheless, here I outline a few that I believe are particularly relevant.

Many-body localization (MBL). Property of interacting quantum many-body systems with disorder leading to a phase of matter that does not self-thermalize.

2D Hubbard model

The Hubbard model tries to capture the dynamics of electrons hopping on a lattice. In 2D, it is believed to be related to high-temperature superconductivity, but unfortunately its phase diagram has not been conclusively determined, even in the single-band approximation. In this context, it is worth mentioning that the best variational ground-state energies computed so far for this model in the strongly correlated regime have been with TNs, specifically with the iPEPS algorithm for fermions[89]. Other related simpler fermionic models, such as the $t-J$ model, have also been simulated successfully using various TN techniques, including 2D DMRG and iPEPS[76,77,178].

2D quantum antiferromagnetism

The antiferromagetic Heisenberg model on the kagome lattice is the archetypical example of a frustrated magnet. Its ground state remained elusive until not long ago, when 2D DMRG simulations revealed that it is a quantum spin liquid[78–80]. Other TN methods have also tackled this problem, including 2D MERA with a specific disentangling structure[92], projected entangled simplex states[179] and iPEPS on coarse-grained lattices[180]. Some of these simulations are compatible with a gapless quantum spin liquid ground state, but so far have not been able to produce better energies than those obtained with 2D DMRG. Other models of quantum antiferromagnetism have also been studied with TNs. For example, iPEPS have been used extensively in the study of SU(N) magnets[180,181].

Conformal field theory

The role of the MERA TN in the AdS/CFT correspondence has already been discussed. However, there are several results in which TNs directly target properties of CFTs, not necessarily with the holographic duality in mind. In the context of (1 + 1) dimensions CFTs, it was shown[182] how to determine the quotient of a MERA representation of the vacuum, taking it to a thermal state. The way to describe and coarse-grain the partition function of the 2D critical Ising model in the presence of topological conformal defects was demonstrated in REF.[183]. Moreover, REF.[184] studied how space-time symmetries are reflected in the cMERA of a free boson CFT, REF.[185] explored the TN description of conformal transformations and REF.[186] proposed the interpretation of such TNs as path integrals on curved spacetime. In addition to these, and in connection to topological order, REF.[187] investigated the mapping of topological quantum field theories to CFTs using 2D TNs. This family of results establishes a valuable dictionary between TNs and CFTs.

Quantum chemistry

TN numerical methods have also found important applications in quantum chemistry. For instance, DMRG has long been used in this context[188]. The reordering of the fermionic orbitals has also been considered with MPS simulations[189]. For a discussion of recent TN approaches to quantum chemistry, see REF.[190].

Disorder and many-body localization

Several TN methods have been proposed to deal with disordered systems[191]. Moreover, many-body localization (MBL) phases have been studied using tailored numerical TN methods. For instance, in REF.[192], a spectral TN was explored to represent the whole spectrum of energy eigenstates. In REF.[193], a variational method over unitary MPOs was proposed to diagonalize MBL Hamiltonians. An alternative TN encoding of all eigenstates of MBL systems in 1D was suggested in REF.[194]. Finally, TNs were used to prove the robustness of MBL phases with symmetry-protected topological order[195].

Outlook

This Review is a brief overview of developments around TN states and methods along different directions. I have tried to collate valuable information, including basic notions and bits of the overall current perspective. It is of course impossible to cover all the developments, but this Review does, I hope, summarize some of the key ones. The applications go well beyond quantum science. It is thus worth keeping in mind that, in such crossover applications (for example, to artificial intelligence), the typical properties of quantum mechanics, such as unitarity, are lost. In such situations, the TNs no longer encode an entanglement structure of a complex system, but rather the structure of its generalized correlations, quantum or not.

TNs are likely to continue finding numerical and theoretical applications, both along established research directions and along new ones. The lesson we have learned over the years is that wherever one finds correlations, there may be a TN behind it. And sometimes this leads to unexpected connections and pleasant surprises, pushing forward the boundaries of science.

Published online 5 August 2019

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Acknowledgements
The author acknowledged financial support from Ikerbasque, Donostia International Physics Center (DIPC) and Deutsche Forschungsgemeinschaft (DFG), as well as discussions over the years with many people on topics presented here. The author also acknowledges M. Rizzi and P. Schmoll for critical reading.

Competing interests
The author declares no competing interests.

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Supplementary information
Supplementary information is available for this paper at https://doi.org/10.1038/s42254-019-0086-7.