Topology in quantum states.  
PEPS formalism and beyond

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Abstract. Topology has been proposed as a tool to protect quantum information encoding and processes. Work concerning the meaning of topology in quantum states as well as its characterisation in the projected entangled pair state (PEPS) formalism and related schemes is reviewed.

1. Introduction

1.1. Quantum computation and its difficulties
Quantum information theory was born with the proposal to use quantum mechanical computers to simulate quantum systems [1]. Indeed, the number of parameters needed to describe many-body quantum states grows exponentially with the number of components of the system. This makes simulation a hopeless problem for conventional computers. However, due to the parallelism the superposition principle implies, quantum systems may be intrinsically more powerful than classical ones.

Computation based on quantum physics is able to tackle computationally hard problems more efficiently than classical computers [2]. In particular, Shor’s quantum algorithm for the factorisation of integers [3] achieves its goal in polynomial time, while the best classical algorithms to date are exponential in the length of the number to be factored. The validity of the Church-Turing conjecture is thus challenged by a model of computation based on new physical principles.

Several ways to implement quantum computation have been proposed, e.g., nuclear magnetic resonance [4], solid state devices (see [5]), ion traps [7]. The requirements for a good experimental proposal have been summarised by DiVincenzo [8].

One of the problems facing the construction of quantum computers is the phenomenon of decoherence: interaction with the environment typically destroys the quantum correlations needed to perform quantum information processing. Methods to protect a quantum memory and quantum gates from decoherence are needed to ensure feasibility of a computer of reasonable size to perform nontrivial tasks. Of course, extreme laboratory conditions can be used to minimise interaction with the environment, although the scalability of these conditions for . The discovery of quantum error correcting codes [6], based on (the quantum analogue of) redundancy in the encoding of information, triggered a lot of activity.
An alternative way towards decoherence-immune quantum information processing dwells on the application of topology, a branch of mathematics dealing with those properties of objects invariant under continuous maps. The key idea is to encode information in topological invariants (global properties) of the manifold underlying the quantum memory, so that the effect of local errors is suppressed. Degenerate ground levels of topological phases of matter (see [9]) are good candidates for this architecture of quantum computers. Quantum gates are typically implemented by manipulating (non-Abelian) anyonic excitations of the system.

1.2. The TQFT model of quantum computation

The abstract setting for topological quantum computation was established in [10], providing an alternative to the standard quantum circuit model. The physical picture is a two-dimensional gas of non-Abelian anyonic particles, whose dynamics is governed by a topological quantum field theory (TQFT): the state of the system is invariant under topologically trivial evolution of the anyon configuration, and only nontrivial braiding and exchange of these particles gives rise to nontrivial transformations of the state.

Formally, anyons are represented by labelled punctures, or holes with labelled boundaries, where labels (topological charges) form a finite set with well defined fusion and braiding rules. Different TQFTs provide different sets of labels and different braiding and fusion rules.

The category of surfaces with labelled boundaries, where morphisms are topological equivalence classes of homeomorphisms, is mapped into the category of finite-dimensional Hilbert spaces (with unitary gates as morphisms) by a topological functor defined by the TQFT.

Though based on quantum field theory, and therefore on an extension of quantum mechanics, this model of quantum computation was shown in [11] to be equivalent to the quantum circuit model. However, it provides a natural language to describe systems with anyonic excitations, such as (as widely believed) the fractional quantum Hall effect at filling fractions \( \nu = 5/2, 12/5 \), where quantum computing based on an effective description in terms of TQFT is thought to be possible.

1.3. Kitaev’s toric code

Historically, the first proposal of topological quantum computation was put forward by Kitaev [12], who considered a square lattice on the surface of a two-torus (square with periodic boundary conditions), with qubits at the edges. Kitaev’s topological error-correcting code can be described in physical language as the ground level of a Hamiltonian made of mutually commuting constraints,

\[
H = - \sum_{\square} B_{\square} - \sum_{+} A_{+},
\]  

(1)

where each plaquette (\(\square\)) or vertex (+) constraint operator acts on all four qubits around it by

\[
B_{\square} = \prod_{j \in \square} Z_j, \quad A_{+} = \prod_{j \in +} X_j,
\]  

(2)

where \(Z\) and \(X\) are Pauli operators.

Hamiltonian (1) is gapped and frustration free for all 2d lattices. Its ground level satisfies all constraints, i.e.,

\[
B_{\square} = 1, \quad \forall \square, \quad A_{+} = 1 \quad \forall +,
\]  

(3)

and its degeneracy depends on the topology of the manifold \(\mathcal{M}\) underlying the lattice: it is easy to check that the product (\(\mathbb{Z}_2\) holonomy)

\[
h_{\gamma} = \prod_{j \in \gamma} Z_j
\]  

(4)
along any closed edge path $\gamma$ in the lattice commutes with all constraints (2). Two such paths $\gamma, \gamma'$ belonging to the same class in the first homology group $H_1(M)$ carry the same values of $h$ due to the plaquette constraints. Moreover, states in the ground level are characterised by the $\mathbb{Z}_2$ holonomies associated with a set of generators of $H_1(M)$; in the case $M = T^2$, e.g., with $h_\alpha$ and $h_\beta$, with $\alpha$ and $\beta$ two inequivalent nontrivial loops around the torus. More precisely, all computational basis kets compatible with an assignment $(h_\alpha, h_\beta) \in \mathbb{Z}_2 \times \mathbb{Z}_2$ appear in state $|h_\alpha, h_\beta\rangle$ with the same weight due to the vertex constraints. Hence, two logical qubits (four Kitaev states) are encoded in the generators of the first homology group.

If the dynamics of the system is restricted to the ground level (this would correspond to low temperatures compared with the gap,) this topological information is protected against local errors, since only operators with support on a non-contractible region of $T^2$ can connect different Kitaev states.

Beyond its value as a topological quantum memory, Kitaev’s system allows processing of information via manipulation of its excitations. Elementary excitations consist of pairs of magnetic or electric defects, defined respectively by the action of a product of spin flips $X$s along a dual lattice path, or by a product of $Z$s along a lattice path. In each case, only two constraints of the Hamiltonian are broken, and the gap is 2 in the units of (1).

Now nontrivial gates within the subspace of Kitaev states are performed by creating a pair of magnetic defects, winding one of them around a nontrivial loop on the torus, and annihilating the pair again. The overall effect is the application of the product

$$\prod_{j \in \tilde{\gamma}} X_j$$

of spin-flip operators along a nontrivial dual loop $\tilde{\gamma}$ of the toric lattice, which flips the logical qubit associated with the direct lattice loop in the other nontrivial direction (logical $X$.) Logical $Z$ along direction $\alpha$ is obtained by creating a pair of electric defects and winding one of them along the $\alpha$ direction before annihilating them.

To end this cursory introduction to the toric code, let us remark that it can be seen as a reinterpretation of Wegner’s $\mathbb{Z}_2$ gauge theory [13].

In the following sections, the toric code and related states will be studied in the context of several ansätze for many-body quantum systems.

1.4. Topological entropy and Levin-Wen state

One very important question is whether topology is a property of a certain Hamiltonian, or rather of the states themselves. The criterion of topology-dependent degeneracy of the ground level, for instance, clearly refers to a given Hamiltonian. However, the idea has gained ground that states carry topological properties irrespective of any Hamiltonian they might be related to.

The most important criterion to discover topological properties in 2d quantum states is the so-called topological entropy, discussed in [14] and [15]. This is defined in terms of a region of perimeter $L$: The entropy of the reduced density matrix for this region scales as

$$S^d_L(\rho) = - \text{Tr}_{N-L}(\rho \log 2\rho) \sim \alpha L - \gamma + \ldots ,$$

where $\alpha$ is a non-universal constant, dependent on the microscopic model, but $\gamma$ only depends on the topological order.

Levin and Wen consider a loop model on a honeycomb lattice (figure 1): edges can be either marked (qubit at $|1\rangle$) or not (qubit at $|0\rangle$), and the loop constraint imposes that the number of marked edges incoming to any given vertex is even. Since the statistical weight of all allowed configurations is imposed to be the same, it is easy to compute the topological entropy $\gamma = 2$,
which is the same as for Kitaev’s code. As we will see, there is a close relation between these models.

2. MPS, PEPS, and topology
2.1. Matrix product states

Since the number of parameters needed to pinpoint a state in the Hilbert space of a many-body system scales exponentially with the number of components, it is important to devise approximate descriptions involving fewer parameters but capturing the essential properties of interesting states, e.g., ground states of spin systems.

One such description, the matrix product state (MPS) ansatz for 1d systems, has been shown [16][17] to underlie the effectiveness of White’s density matrix renormalisation group (DMRG) [18]. This realisation has even led to new algorithms beyond DMRG (see [19] for a discussion.)

The prototype of MPS construction, the valence bond solid, was first introduced in [20]. The general ansatz is as follows: Pairs $i_L, i_R$ of auxiliary systems (left and right ancillae, with Hilbert spaces $h_{i_L}, h_{i_R}$) are associated with physical sites $i$ (with $d_i$-dimensional Hilbert spaces $\mathcal{H}_i$ spanned by orthonormal bases $\{|I\rangle\}$) along the 1d chain. The dimensions of ancilla Hilbert spaces $i_R$ and $(i+1)_L$ match (say, they equal $D_i$), and ancilla dimensions are upper bounded. Ancillae are ‘prepared’ in a pairwise completely entangled state

$$\bigotimes_i |\phi^+_{i, i+1}\rangle$$

with

$$|\phi^+_{i, i+1}\rangle = \sum_{\alpha=1}^{D_i} |\alpha,\alpha\rangle \in h_{i_R} \otimes h_{(i+1)_L}$$

in terms of orthonormal bases $\{|\alpha\rangle\}$. The physical state is recovered by means of projections

$$P_i: \quad h_{i_L} \otimes h_{i_R} \longrightarrow \mathcal{H}_i,$$

$$|\alpha,\beta\rangle \longrightarrow \sum_{I=1}^{d_i} A^I_{i,\alpha\beta} |I\rangle,$$

so that

$$|\text{MPS}\rangle = \left( \bigotimes_i P_i \right) \left( \bigotimes_j |\phi_{j, j+1}\rangle \right)$$

This construction is depicted in figure 2.
Due to the $\phi^+$ ancilla bonds, the resulting structure of the MPS can be written (for periodic boundary conditions) as

$$|\text{MPS}\rangle = \sum_{I_1, I_2, \ldots, I_N} \text{Tr} (A_{I_1}^{I_1} A_{I_2}^{I_2} \cdots A_{I_N}^{I_N}) |I_1, I_2, \ldots, I_N\rangle,$$

with matrices $A_I = \langle A_{I, \alpha\beta} \rangle$ defined in (9). Translation invariant systems have, of course, site-independent matrices $A_I$. Structure (11) is also valid for open boundary conditions when the leftmost and rightmost ancillae are chosen one-dimensional.

One can also derive (11) by a sequence of Schmidt decompositions, showing that every state of the system can be written as an MPS. The deep physical observation is that typical ground states of relevant systems are well described by MPS of low ancilla dimension (which is a measure of entanglement.) Properties of MPS are discussed in depth in [21].

DMRG algorithms are variational procedures over sets of MPS states. This has shed light on the success of DMRG for noncritical systems, and its failure in tackling critical systems. In intuitive terms, critical systems contain too much entanglement for any MPS states of bounded ancilla dimension.

2.2. PEPS and the toric code
Projected entangled-pair states (PEPS) are a powerful generalisation of the MPS structure to higher-dimensional systems [22][23]. Their construction proceeds along the same lines: physical sites in, say, a two-dimensional lattice are endowed with as many ancillae as nearest neighbours, and pairs of neighbouring ancillae are entangled in $\phi^+$ states (8). Projectors from the whole ancilla space onto physical space yield a PEPS. Instead of matrices, tensors with one physical index and as many ancilla indices as nearest neighbours are contracted according to the lattice structure, as shown in figure 3.

The general form of a PEPS in a region $R$ is thus

$$|\text{PEPS}\rangle = \sum_{I_R} C_R(\{A^{I_R}\}) |I_R\rangle,$$

Figure 2. MPS construction. Lozenges stand for ancillas, pairwise connected by completely entangled states. Arrows stand for projectors onto physical space.

Figure 3. PEPS ansatz. Lozenges stand for ancillae. The contraction pattern follows the nearest neighbour structure.
where $I$ stands for all physical indices within this region and $C_R$ represents the contraction of ancilla indices following the nearest neighbour structure. In other words, projectors onto physical space at sites $i$ are

$$P_i: \quad h_{iL}^\dagger \otimes h_{iR} \mapsto \mathcal{H}_i,$$

with obvious notation for upper, lower, left and right ancilla systems, and the contraction for a $2 \times 2$ region is

$$C_{R_{2\times2}}(\{A^f_{R_{2\times2}}\})_{\alpha\beta\gamma\delta\epsilon\zeta\theta} = \sum_{\lambda\mu\eta\kappa} \varepsilon_{\lambda\delta\kappa} \lambda_{\gamma\delta} \mu_{\alpha\beta} \eta_{\epsilon\zeta}.$$

(14)

For general properties of PEPS, see [24]. They are the basis for new, efficient algorithms for computing ground state energies and correlations in more than one dimension.

This ansatz is also adequate to describe topological states such as Kitaev’s toric code. The projectors in this case were given in [24]. For qubits in vertical bonds, they read

$$P_i = |0\rangle \langle 0| + |1\rangle \langle 1|,$$

and the projectors for qubits in horizontal bonds are a $\pi/2$ rotation of (15). Here, maximally entangled states of pairs of same-qubit ancillae are shown as $\ldots = |\phi^+\rangle = |00\rangle + |11\rangle$, $\ldots = |\phi^+\rangle = |00\rangle - |11\rangle$. Actually, the PEPS corresponding to these projectors is the equal weight superposition of all four Kitaev states on the torus. A nonlocal measurement is needed to tell each one apart.

The PEPS picture allows us to understand the toric code in ancilla space. Projectors (15) impose the parity constraints $B_{\square} = 1$ of (3) at each plaquette, because ancilla index loops (figure 4) contribute a trace of Pauli matrix $Z$ to the power of the number of $|1\rangle$-qubits surrounding the plaquette. Considering a region with boundary, enclosed ancilla loops enforce plaquette constraints, and the remaining ancilla strings (cut by the boundary) define a tensor in ancilla space. The topological entropy $\gamma = 2$ (section 1.4) can be computed by studying the interplay of this tensor and of physical configurations.

Projectors (15) can also be used to construct a toric code in an arbitrary (two-dimensional) toric lattice [27]. The count of configurations and entropies goes along the same lines. As an example, if this PEPS is imposed on a triangular lattice, its dual (exchanging plaquettes and vertices, and rotating $\pi/2$ all edges) turns out to be exactly Levin and Wen’s loop model. These projectors can also be put to work to devise topological codes in more than two dimensions.

2.3. Beyond PEPS

The toric code can be written in an alternative way, no longer a PEPS but easily generalisable to include many interesting models [27]. Consider an equal weight superposition of all states of the computational basis, i.e., a Hadamard transform of the $|0\rangle^\otimes N$ state. Then, a simultaneous projection of all plaquettes onto GHZ states of the form

$$|\text{GHZ}\rangle \propto \left| + \right\rangle \left| + \right\rangle \left| + \right\rangle + \left| - \right\rangle \left| - \right\rangle \left| - \right\rangle$$

(16)
yields the equal weight superposition of the four Kitaev states on the torus.

Now, by projecting plaquettes onto different (cyclic) permutation classes of $|±⟩^⊗4$ states, a wealth of systems is obtained, which can be classified in general terms as dimer/string/loop models, with different properties as regards density or possibility of self-intersection. Some of them degenerate into purely one-dimensional dynamics in a way reminiscent of holography. Work is in progress to understand their possible topological properties and characterise them in terms of the projection ansatz.

3. The MERA ansatz and the toric code.

A novel ansatz for many-body quantum states, devised to overcome difficulties posed by critical systems, goes under the name of MERA (multi-scale entanglement renormalisation ansatz) [25][26].

The underlying idea behind this ansatz is an improvement of real space renormalisation group, introducing extra operation between blocking steps. The intuition is that a critical system contains correlations at all scales (larger than the lattice spacing.) If unitary transformations (called disentanglers) affecting the interfaces of blocks are applied, prior to the coarse-graining procedure, so that short range correlations between pairs of blocks are minimised (in other words, entanglement is redistributed and concentrated within blocks or in higher range correlations,) it is easier to find isometries taking the system to a coarse-grained (‘blocked’) version similar to the starting point. The properties of the system, in finite volume, are encoded in a tensor network of disentanglers and isometries, in number exponentially decreasing with ‘renormalisation group time.’ The difficult problem of simulating quantum critical many-body systems, which make DMRG fail, can be tackled with this ansatz, as has been shown for the Ising model in two dimensions [25].

This ansatz, whose initial aim was to provide a basis for numerical procedures adequate for critical systems, has turned out to be a natural language to describe topological states. The toric code has a simple MERA form [28] which also exhibits the close relation of Kitaev’s code with Levin and Wen’s state.

The building blocks of this construction are elementary deformations of the toric code on a general lattice by introduction of new qubits, creating either new plaquettes or new vertices [29], as depicted in figures 6 and 7.

Only a qualitative discussion of the full form of the MERA ansatz for the toric code will be given here, details forthcoming in [28]. A complete MERA step takes the code to a $\pi/4$ rotation

Figure 4. Cell structure of the toric code PEPS on the square lattice.
Figure 5. MERA ansatz. Disentanglers $U$ (dashed circles) are applied to minimise interblock correlations prior to coarse-graining isometries $V$ (arrows.)

Figure 6. Addition of a qubit to a toric code with creation of a new plaquette. The qubit is introduced in state $|0\rangle$ and is acted upon with CNOTs with control qubits in one of the new plaquettes.

Figure 7. Addition of a qubit to a toric code with creation of a new vertex. The qubit is introduced in state $|+\rangle$ and acts as control qubit of CNOTs with target qubits incoming at one of the new vertices.

thereof, where half of the qubits are eliminated (decoupled in $|0\rangle$ or $|+\rangle$ states.) Each step consists of two substeps, the first of which ends in a triangular lattice, the dual of Levin and Wen’s model (hence, the toric code MERA is also a MERA for the loop model.) The evolution of defects (excitations) can be traced along the RG flow, and one can see that the ground states are fixed points (in infinite volume, where the ground states are self-similar.) Some pairs of defects eventually annihilate along the flow, decreasing the energy.

Interestingly, this ansatz, read backwards in time, constitutes a recipe to grow the toric code sequentially.

4. Conclusions and outlook
Summing up, several ansätze proposed to deal with typical many-body quantum states have proven useful to describe states of the kind proposed as topological quantum memories. These ‘topological states’ describe topological phases of matter, whose interest for condensed matter physics goes beyond quantum information theory.

Different ansätze provide different handles on the properties of these states. The PEPS ansatz
gives a direct way to visualise the ‘loop condition’ and the origin of the topological entropy of Kitaev’s and related codes, like Levin and Wen’s, and exhibits the identity of the topological order in seemingly different states. A generalisation of the PEPS ansatz allows us to study several kinds of states, of relevance in many areas of condensed matter, some of which may have different topological orders. With the MERA formulation, a recipe for the sequential growth of the code is obtained, and insight into the renormalisation group behaviour is gained.

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