

Spanning Trees on a Lattice

Report by

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December 2023 - January 2024

Acknowledgement

I would like to express my sincere gratitude to Prof. Sourendu Gupta for agreeing to supervise this project and his invaluable guidance and supervision throughout this project. His expertise and insights have been instrumental in shaping this research work. His support has been crucial in making this project possible and contributing to my academic growth.

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Part I

Report

I-1 Introduction

Lattice field theories are a powerful computational framework for studying quantum field theories in a non-perturbative regime. In this approach, continuous spacetime is discretized into a lattice of points, allowing for numerical simulations of complex quantum systems. This discretization provides a natural ultraviolet cutoff, regularizing the theory and making it amenable to computational methods. Lattice field theories have been particularly successful in the study of quantum chromodynamics (QCD), the theory of strong interactions, where they have provided insights into phenomena such as quark confinement and chiral symmetry breaking. The lattice formulation also serves as a bridge between the continuum theory and its discrete counterpart, offering a systematic way to approach the continuum limit and extract physical observables.

In this work, we consider the spanning tree gauge fixing on the lattice. Specifically, we show that fixing a spanning tree fixes the gauge, and then we proceed to provide algorithms to count and enumerate all the spanning trees on a hypercubic lattice with periodic boundary conditions, and also to find the local gauge transformation that transforms one spanning tree to another.

I-2 Gauge Fixing on the Lattice

On the lattice, the matter fields live on the lattice sites, and the gauge fields play the role of comparator owing to the local gauge symmetry and therefore live on the links connecting the lattice sites.

Local gauge invariance on the lattice means we have the freedom to assign any group element (that leads to the local gauge transformation) $G(n_i)$ to each lattice site. But such an assignment would also affect the link variables, transforming them according to eq (1).

$$U(n_i, n_j) \rightarrow G(n_i)U(n_i, n_j)G(n_j)^{-1} \quad (1)$$

Therefore in the path integral, one would be overcounting the different configurations by considering their gauge-transformed configurations too.

In the continuum case with continuous groups, this is a huge problem since the relevant fields are lie-algebra valued. The lie algebra is non-compact which implies that the path integral counts infinitely many copies. In the lattice version of the same, the link variables that are group-valued

are relevant, and since the groups are compact, the volume is finite, and we are simply getting a normalization factor equal to the (finite)volume of the gauge group, $\mathcal{N} = V^N$ (where N is the total number of lattice sites).

The gauge fixing procedure is not a necessity for the observables which are gauge invariant, since the finite volume factor gets absorbed into the normalization. On the other hand for gauge variant observables, a class to which many important observables belong, to compare values in different configurations, it becomes necessary to implement some gauge fixing procedure that fixes the gauge and allows us to compare the different configurations even in the presence of local gauge transformations.

I-3 Spanning Trees

Let us start with a random configuration of U on the lattice. Initially, we assume all $G(n)$ to be set to \mathbb{I} . We start with a link $U_{\mu_0}(n_0)$ and set it to \mathbb{I} . This can be done by setting $G(n_0 + \mu_0) = U_{\mu_0}(n_0)$ keeping all other gauge elements at \mathbb{I} . This transforms the link $U_{\mu_0}(n_0)$ as $U_{\mu_0}(n_0) \rightarrow U_{\mu_0}(n_0)G(n_0 + \mu_0)^{-1} = \mathbb{I}$. Now we can fix another link starting from $n_0 + \mu_0$ to \mathbb{I} by fixing the group element at the other end of the link and so on. The whole procedure can be repeated until we reach a link whose other end-point is already fixed and can't be modified.

This procedure generates a cluster of links that are set to \mathbb{I} which does not contain closed loops. Such a cluster is called as a spanning tree on the lattice. This fixes the values of group elements on all the sites, at the same time, since it does not contain closed loops, preserves the values of gauge invariant observables.

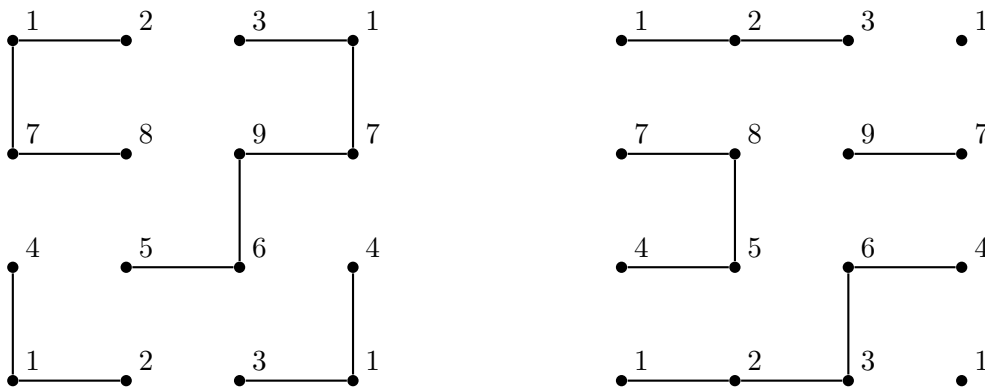


Figure 1: Examples of two spanning trees on a 3×3 lattice with periodic boundary conditions

Deciding a spanning tree for a lattice is equivalent to fixing the gauge for the lattice since for each configuration we are choosing one single gauge transformation that transforms the links to the spanning tree. We prove this statement in the following subsection.

I-3.1 Spanning Tree Fixes the Gauge

Consider a spanning tree gauge fixing done on a lattice with n sites, each site labeled by a natural number $m \in \{1, \dots, n\}$ (the order of labeling, along with the labeling convention of adjacent neighbours is irrelevant to the discussion and is not considered). Consider a gauge fixing being done by a spanning tree \mathfrak{T} starting from $G(1) = \mathbb{I}$.

On such a gauge fixing, the gauge elements on sites m_1 and m_2 , $G(m_1)$ and $G(m_2)$ are related by the ordered product of links in the subtree $\mathcal{S}_{m_1 m_2} \subset \mathfrak{T}$ connecting m_1 to m_2 .

In other words

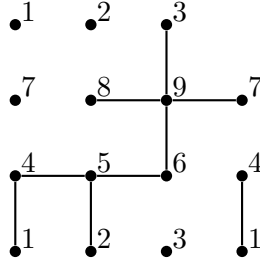
$$G(m_2) = G(m_1)U(m_1, i)U(i, j) \dots U(k, l)U(l, m_2), \quad U \in \mathcal{S}_{m_1, m_2} \quad (2)$$

In particular, since $G(1) = \mathbb{I}$, $G(m) = U(1, \cdot) \dots U(\cdot, m)$, $U \in \mathcal{S}_{1, m}$.

Therefore, when a local gauge transformation $\Omega(n) = g_n$ is applied on the lattice, to preserve the spanning tree, the gauge fixing group elements on each site will transform as (since the intermediate site gauge transformations cancel out in the product of connected links)

$$G(m) \rightarrow G'(m) = g_1 G(m) g_m^{-1} \quad (3)$$

For example, in the lattice below



we start with $G(1) = \mathbb{I}$.

To fix the link $U(1, 4)$, we set $G(4) = U(1, 4) \implies U(1, 4) \rightarrow \mathbb{I} \cdot U(1, 4) \cdot U(1, 4)^{-1} = \mathbb{I}$.

Now, to fix $U(4, 5)$, we set $G(5) = U(1, 4) \cdot U(4, 5) \implies U(4, 5) \rightarrow U(1, 4) \cdot U(4, 5) \cdot (U(1, 4) \cdot U(4, 5))^{-1} = \mathbb{I}$, and so on

Therefore, one can easily see that $G(m) = U(1, \cdot) \dots U(\cdot, m)$.

As an example, under a local gauge transformation $G(5)$ transforms as $G(5) \rightarrow G'(5) = g_1 G(5) g_5^{-1}$.

Now consider an unfixed link $U(m_1, m_2)$ in the spanning tree. The value of the link before gauge transformation (with spanning tree gauge fixing) is

$$U(m_1, m_2) \rightarrow G(m_1)U_{uf}(m_1, m_2)G(m_2)^{-1} \quad (4)$$

Using eq (3), we see that in the locally gauge transformed lattice, the value of the unfixed link would become

$$\begin{aligned}
 U'(m_1, m_2) &= G'(m_1)U'_{uf}(m_1, m_2)G'(m_2) = g_1G(m_1)g_{m_1}^{-1} g_{m_1}U_{uf}(m_1, m_2)g_{m_2}^{-1} g_{m_2}G(m_2)^{-1}g_1^{-1} \\
 &= g_1G(m_1)U_{uf}(m_1, m_2)G(m_2)g_1^{-1}
 \end{aligned}
 \tag{5}$$

Therefore, under a local gauge transformation, all unfixed links on the lattice will transform as

$$U(m_1, m_2) \rightarrow g_1U(m_1, m_2)g_1^{-1}
 \tag{6}$$

Therefore, under spanning tree gauge fixing, a local gauge-transformed lattice becomes a global gauge-transformed configuration. In other words, the spanning tree gauge fixing maps local gauge copies of a configuration to global gauge transformed copies of the same configuration.

I-4 Enumerating the Spanning Trees

The Matrix Tree Theorem of Kirchhoff states that given a connected graph (of which the lattice we consider is also an example), the number of spanning trees of the graph is given by any cofactor of the Laplacian matrix for the graph.

The Laplacian Matrix of a graph is given as

$$Q = D - A
 \tag{7}$$

where D is the degree matrix, which is a diagonal matrix stating how many connections start or end at the i^{th} node, and $A = \{a_{ij}\}$ is the adjacency matrix, which is valued $a_{ij} = 1$ if i^{th} and j^{th} nodes have a connection between them, and 0 otherwise.

For the lattice in consideration, we decide to number the nodes as follows:

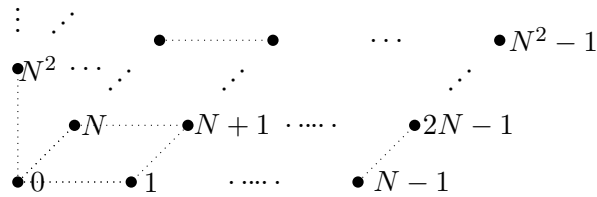


Figure 2: Lattice node numbering

In this lattice, every node is adjacent to 2 nodes in each dimension.

Along the first dimension, which is taken to be the one where node numbering increases by one as

we traverse, the neighbours of n^{th} node are $n + 1$ and $n - 1$. If the node belongs to the *forward boundary* ($N - 1, 2N - 1, \dots, N^d - 1$) then the neighbours of n are $n - (N - 1)$ and $n + 1$. Similarly for node belonging the *backward boundary*, ($0, N, 2N, \dots, N^{d-1}(N - 1)$), the neighbours are $n + 1$ and $n + (N - 1)$.

Along the second dimension, where the increment takes place by N , the nodes (not in boundary) have two neighbours $n + N$ and $n - N$. For nodes on *forward boundary* ($N^2 - 1, N^2 - 2, \dots, N^2 - N, 2N^2 - 1, 2N^2 - 2, \dots, 2N^2 - N, \dots, N^D - 1, N^D - 2, \dots, N^D - N$) in the second dimension, the neighbours are $n - N(N - 1)$ and $n - N$, while for those in the *backward boundary* the neighbours are $n + N$ and $n + N(N - 1)$.

Similar analysis holds for the other dimensions too.

The Mathematica code for obtaining the boundaries, and the neighbours, given the number of lattice sites in each dimension and the number of dimensions is discussed in Section II-1.

As an example, in a 3×3 lattice, each node is adjacent to 4 other nodes, with them being

$$\begin{aligned} 0 &\rightarrow \{1, 2, 3, 6\}, 1 \rightarrow \{2, 0, 4, 7\}, 2 \rightarrow \{0, 1, 5, 8\}, \\ 3 &\rightarrow \{4, 5, 6, 0\}, 4 \rightarrow \{5, 3, 7, 1\}, 5 \rightarrow \{3, 4, 8, 2\}, \\ 6 &\rightarrow \{7, 8, 0, 3\}, 7 \rightarrow \{8, 6, 1, 4\}, 8 \rightarrow \{6, 7, 2, 5\} \end{aligned}$$

Therefore, for the lattice in consideration, the degree matrix, which gives the number of nodes adjacent to the said node, is simply $2 \times d \times \mathbb{I}_{N^d}$ where d is the number of dimensions and N is the number of lattice sites in each dimension.

The adjacency matrix can be constructed with the knowledge of the neighbours of a given site, and therefore, one can calculate how many spanning trees exist in a given lattice.

As an example, for a 3×3 lattice, with the above given neighbours, the adjacency matrix and degree matrix are given as

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix}, D = 2 \times 2 \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (8)$$

The $(1, 1)$ cofactor of $D - A$ is 11664, which gives the number of spanning trees on the 3×3 lattice.

The Mathematica code for counting the number of spanning trees on a hypercubic lattice with periodic boundary conditions is discussed in Section II-2.

We calculate the number of trees for different lattices. From the calculations, we see that the number of spanning trees grows exponentially with the number of lattice sites available,

- A 3×3 lattice has 11,664 spanning trees
- A 4×4 lattice has 4,24,67,328 spanning trees
- A $3 \times 3 \times 3$ lattice has 25,29,99,02,31,17,90,46,912 spanning trees

The case of a 2×2 lattice is special since a 2×2 lattice with periodic boundary conditions becomes a doubly connected *multigraph* with 4 nodes, 0 connected doubly to 1 and 2, 1 connected doubly to 0 and 3, 2 connected doubly to 0 and 3, 3 connected doubly to 1 and 2.

In this case the adjacency matrix modifies as $A = \{a_{ij}\}$, $a_{ij} = 2$ iff i and j are adjacent., while the degree matrix remains the same, i.e. $2 \times 2 \times \mathbb{I}_4$. Therefore the number of spanning trees on 2×2 lattice with PBC is given by the cofactor of

$$Q = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} - \begin{pmatrix} 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \\ 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \end{pmatrix} \quad (9)$$

and the number of spanning trees is equal to

$$\det \begin{pmatrix} 4 & 0 & -2 \\ 0 & 4 & -2 \\ -2 & -2 & 4 \end{pmatrix} = 32 \quad (10)$$

I-4.1 Generating all spanning trees

A spanning tree is characterized by the property that it visits all the sites of a given lattice and contains no loops. Using this property, we can write down a general algorithm to generate all possible spanning trees as follows:

```

1 trees = collection of the spanning tree, visited sites, checked sites, along with the
   information if the spanning tree is completed or not
2 while there is at least one incomplete tree do
3   for each tree in the set of trees do
4     for all sites in tree do
5       if site is not already checked then
6         | Add the neighbours that are not in the tree to the possible neighbours set
7       end
8       for each combination of the possible neighbours do
9         | Create a copy of the current tree and add the new links to the tree
10        | Add the said neighbours to the visited set of the tree
11        if all the sites in the lattice belong to the visited set then
12          | Mark the tree as completed
13        end
14        | Append the new tree to the set of new trees
15      end
16    end
17  end
18  Delete duplicates from the set trees and replace the current set of trees with the set of
   new trees
19 end

```

The above-described algorithm is a brute force enumeration algorithm.

The Mathematica code for enumerating all the spanning trees on a given hypercubic lattice with periodic boundary conditions is discussed in Section II-3.

I-5 Gauge Transformations Between Two Spanning Trees

As a simple example behind the idea, consider two spanning trees, as given in Figure 3.

Assume the convention $(i, j) \equiv U(i, j)$ for the gauge fixed lattices, and denote by $(i, j)'$ the value of the link in the original lattice, i.e., before performing any gauge fixing.

To find the gauge transformation that takes us from tree A to tree B, we first see that the unaltered links should have the same group elements on the sites, meaning we have the constraints $G_1 = G_2 = G_3, G_6 = G_5 = G_4 = G_7 = G_8 = G_9$

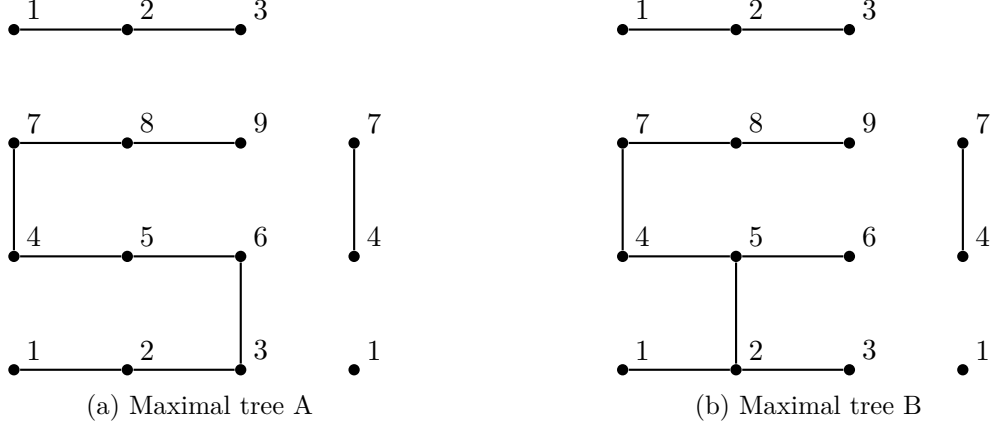


Figure 3: Two spanning trees on a 3×3 lattice

To do the gauge transformation, we use the requirement $(2, 5) \rightarrow G_2(2, 5)G_5^{-1} = \mathbb{I}$ to set $G_2 = (2, 5)^{-1}$ and $G_5 = \mathbb{I}$.

Setting $G_2 = (2, 5)^{-1}$, we get $G_1 = (2, 5)^{-1}$ & $G_3 = (2, 5)^{-1}$, from which the link $(3, 6) \rightarrow (2, 5)^{-1}$. Therefore we can go from tree A to B with the local gauge transformation

$$G_n = \mathbb{I}, \forall n \neq 1, 2, 3; \quad G_1 = G_2 = G_3 = (2, 5)^{-1} \quad (11)$$

In this example, the local gauge transformation is small. But there are trees between which the gauge transformation can become arbitrarily large. As an example, the trees in Figure 1 are related by gauge transformation that involves a product of 28 group elements.

In terms of the link variables of the original unfixed lattice,

$$\begin{aligned} (2, 5) &= (1, 2)' \cdot (2, 5)' \cdot ((1, 2)'(2, 3)'(3, 6)'(6, 5)')^{-1} \\ &= (1, 2)'(2, 5)'(5, 6)'(6, 3)'(3, 2)'(2, 1)' \end{aligned} \quad (12)$$

the trace of which, gives the information about the loop $2 \rightarrow 5 \rightarrow 6 \rightarrow 3 \rightarrow 2$.

Therefore, the gauge transformation between the spanning trees involves the product of loops on the lattice. To see why this is the case, notice that on a lattice, all the gauge invariant observables are constructed out of traces of loops on the lattice. While the individual links can take on any values, the values of the traces of loops in two physically equivalent copies should be the same, in other words, a local gauge transformation should preserve the values of the traces of all loops on the lattice. A spanning tree gauge fixing transfers the information about the loops to the unfixed links while setting the other links to identity. Therefore, transforming from one spanning tree to another involves gauge elements that are products of multiple loops in order to transfer the loop information from the previously unfixed links to the new unfixed links.

Following is a general procedure to find the gauge transformation between two trees:

```

1 modifiedLinks = the links of the gauge transformed lattice, set according to the first tree
2 toAdd = tree2 - tree1; i.e. the set of links in tree2 and not in tree1, and therefore to be
   added to tree1
3 gaugeTransformation =  $\mathbb{I}(n_i)$ ; initialise the gauge transformation to the identity.
4 equalityConstraints = for a given site, gives the list of sites to be modified to preserve the
   unchanged links in the tree.
5 for every link in toAdd do
6   | Set the second site of the link (i.e., if the link is  $(n_i, n_j)$ , then  $n_j$ ) to be equal to
   |    $U(n_i, n_j)$  (from the modified links) and the first site to be equal to  $\mathbb{I}$  to add the link.
7   | for every site in equalityConstraints[ $n_j$ ] do
8   |   | multiply the existing gauge element at the site by  $U(n_i, n_j)$  to preserve the
   |   |   unchanged links
9   |   end
10 end

```

To transform the first tree into the second, we recognize the links that have to be added to the first tree, and the constraints obtained by ensuring that the common links are unchanged. Implementing the gauge transformations that add the said links along with the constraints will transfer the information from the now-fixed link to another link that is fixed in the first tree but not fixed in the second, transforming the first tree into the second.

The Mathematica code implementing this procedure is discussed in Section II-4.

I-6 Conclusion

We have discussed the spanning tree method for fixing the gauge on a given lattice. This method provides a systematic approach to eliminate gauge redundancy while preserving the physical content of the theory. We have shown that enforcing a spanning tree on the lattice maps all the local gauge rotations of configurations to global gauge rotated configurations. Further, we have discussed procedures to count the number of spanning trees on a lattice, to generate all the spanning trees, and also to find the gauge transformation that transforms one tree to another.

Additionally, (in part II) we have touched upon the computational aspects of these methods, including their implementation in Mathematica. Future work could focus on optimizing these algorithms for larger lattices and exploring their applications in more complex gauge theories.

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Part II

Mathematica Implementation

II-1 Neighbours and Boundaries on a Lattice

The Mathematica code for obtaining the neighbours and boundaries of a hypercubic lattice in `nDim` dimensions with `nSites` sites in each dimension is given below.

```
In[1]:= (*In each dimension, there are two bounding surfaces.
Here we determine the elements of the two surfaces for all the dimensions.
The boundaries are in the format
{{x axis boundary points}, {y axis boundary points} ... } *)
getBoundaries[nSites_, nDim_] :=
Module[{ForwardBoundary, BackwardBoundary, d, n, n1},
ForwardBoundary = {};
For[d = 1, d <= nDim, d = d + 1,
AppendTo[ForwardBoundary, {}];
For[n = 1, n <= nSites^(nDim - d), n = n + 1,
For[n1 = 0, n1 < nSites^(d - 1), n1 = n1 + 1,
AppendTo[ForwardBoundary[[d]], n*nSites^d - n1 - 1]
]
]
];
BackwardBoundary = {};
For[d = 1, d <= nDim, d = d + 1,
AppendTo[BackwardBoundary, {}];
Do[AppendTo[BackwardBoundary[[d]] ,
elem - (nSites^(d - 1)) (nSites - 1)],
{elem, ForwardBoundary[[d]]}
]
];
{ForwardBoundary, BackwardBoundary}
];


In[2]:= (* Each site element will have 2*nDim neighbours, i.e. 2 in each
dimension. Here we determine the 2 neighbours of each element in each
of the dimensions *)
getNeighbours[nSites_, nDim_] :=
```

```

Module[{boundaries, ForwardBoundary, BackwardBoundary, neighbour,
nTot, n, d, nNeigh},
boundaries = getBoundaries[nSites, nDim];
ForwardBoundary = boundaries[[1]];
BackwardBoundary = boundaries[[2]];
nTot = nSites^nDim;
neighbour = <||>;
For[n = 0, n < nTot, n = n + 1,
nNeigh = {}];
For[d = 0, d < nDim, d = d + 1,
(* Forward *)
If[Not[MemberQ[ForwardBoundary[[d + 1]], n]],
AppendTo[nNeigh, n + nSites^d],
AppendTo[nNeigh, n - (nSites^(d)) (nSites - 1)]];
(* Backward *)
If[Not[MemberQ[BackwardBoundary[[d + 1]], n]],
AppendTo[nNeigh, n - nSites^d],
AppendTo[nNeigh, n + (nSites^(d)) (nSites - 1)]]
]
AppendTo[neighbour, n -> nNeigh];
];
neighbour
];

```

II-2 Counting the Number of Spanning Trees

Get it on 

The following Mathematica module calculates the number of spanning trees on a given lattice.

```

In[3]:= numberOfSpanningTrees[nSites_, nDim_] := Module[
{adj, neighbour, nTot, deg, Q},
adj = {};
neighbour = getNeighbours[nSites, nDim];
nTot = nSites^nDim;
Do[
AppendTo[adj, {}];
Do[
AppendTo[adj[[i + 1]], If[MemberQ[neighbour[i], j], 1, 0]],


```

```

        {j, Range[0, nTot - 1]}
    ],
    {i, Range[0, nTot - 1]}}];
deg = 2*nDim*IdentityMatrix[nSites^nDim];
Q = adj - deg;
Det[Drop[Q, {1}, {1}]]
];

```

II-3 Generating the Spanning Trees

Get it on 

The following Mathematica module generates all the spanning trees on a given lattice.

```

In[4]:= treeEqualQ[Tree1_, Tree2_] :=
    (Tree1[[1]] === Tree2[[1]] && Tree1[[3]] === Tree2[[3]]);

In[5]:= getTrees[nSites_, nDim_] :=
Module[
    {neighbour, Trees, tree, change, count, generatedTrees,
    newTrees, visited, completed, checked, neighbours,
    unvisitedNeighbours, possibleCombinations, newTree,},

    neighbour = getNeighbours[nSites, nDim];

    Trees = {{{}, {0}, {}, False}}; (*links in the tree ,visited sites,
    checked sites, complete or incomplete*)
    change = True;
    SetSharedVariable[change];
    While[change,
    change = False; (* while there is atleast one incomplete tree *)
    generatedTrees = WaitAll[
    ParallelTable[(*For each tree*)
        newTrees = {};
        visited = tree[[2]];
        checked = tree[[3]];
        completed = tree[[4]];
        If[completed, AppendTo[newTrees, tree],
        change = True;

```



```

Do[(*For each visited site*)

If[Not[MemberQ[checked,
    visitedSite]],(*If site is not already checked *)
neighbours = neighbour[visitedSite];
unvisitedNeighbours = Complement[neighbours, visited];

If[unvisitedNeighbours == {}, ,
    possibleCombinations =
    Subsets[unvisitedNeighbours, {1,
    Length[unvisitedNeighbours]}];

Do[(*For each possible combination of links that can be
added*)
newTree = tree;

Do[(*Add the links to the tree,and the sites to visited*)
AppendTo[newTree[[1]], {visitedSite, site}];
newTree[[1]] = Sort[newTree[[1]]];
AppendTo[newTree[[2]], site];
AppendTo[newTree[[3]], visitedSite];
newTree[[3]] = Sort[newTree[[3]]];
, {site, combination}];
(*Check if the newTree created has visited all elements*)
If[Sort[newTree[[2]]] == Range[0, nSites^nDim - 1],
newTree[[4]] = True, ,];
(* Append the new tree to the net of newtrees *)
AppendTo[newTrees, newTree];
, {combination, possibleCombinations}
]
]]
, {visitedSite, visited}
]; newTrees
, {tree, Trees}
]];
Trees =

```

```

DeleteDuplicates[Flatten[generatedTrees, 1], treeEqualQ]; (*
delete duplicates and replace the current set of trees by the new
set *)
];
Trees];

```

On Mathematica, a single tree with all the details in a 3×3 lattice takes up 1368 bytes of memory. Attempting to generate the possible spanning trees of even a 4×4 lattice requires storing of 58095304704 bytes (or equivalently 58.09 Gigabytes) in the RAM, rendering the task impossible on a regular computer. A possible alternative is the use of SSD storage instead of RAM for calculations, but it has not been explored.

One can generate a smaller subset of spanning trees on larger lattices by restricting the choices of links in each step to a smaller subset of the set of all possible ones. A random tree can be generated by selecting one of the possibilities in random rather than considering all of them.

We also draw the spanning trees by using the following code.

```

In[6]:= getVertexCoords[nSites_, nDim_] := Module[ (*Only for 2D lattices*)
  {nTot, n, x, y},
  vertexPos = {};
  nTot = nSites^nDim;
  x = 0;
  y = 0;
  For[n = 0, n < nTot, n = n + 1,
    AppendTo[vertexPos, n -> {x, y}];
    If[Mod[n, nSites] == nSites - 1, x = 0; y = y + 1, x = x + 1];
  ];
  vertexPos
];

```

```

In[7]:= showTree[nSites_, nDim_, tree_] := Module[
  {links, neighbour, n, nTot, treeLinks},
  links = {};
  nTot = nSites^nDim;
  neighbour = getNeighbours[nSites, nDim];
  For[n = 0, n < nTot, n = n + 1,
    Do[
      AppendTo[links,

```

```

UndirectedEdge[Sort[{n, i}][[1]], Sort[{n, i}][[2]]], {i,
neighbour[n]}
]
];
treeLinks =
Table[UndirectedEdge[link[[1]], link[[2]]], {link, tree}];
HighlightGraph[
Graph[DeleteDuplicates[links], VertexLabels -> "Name",
VertexCoordinates -> getVertexCoords[nSites, nDim],
EdgeShapeFunction -> "CurvedEdge", EdgeStyle -> {Gray}],
Style[treeLinks, {Black, Thick}], ImageSize -> Small]
];

```

A few of the generated trees are drawn using the module above in the following figures.

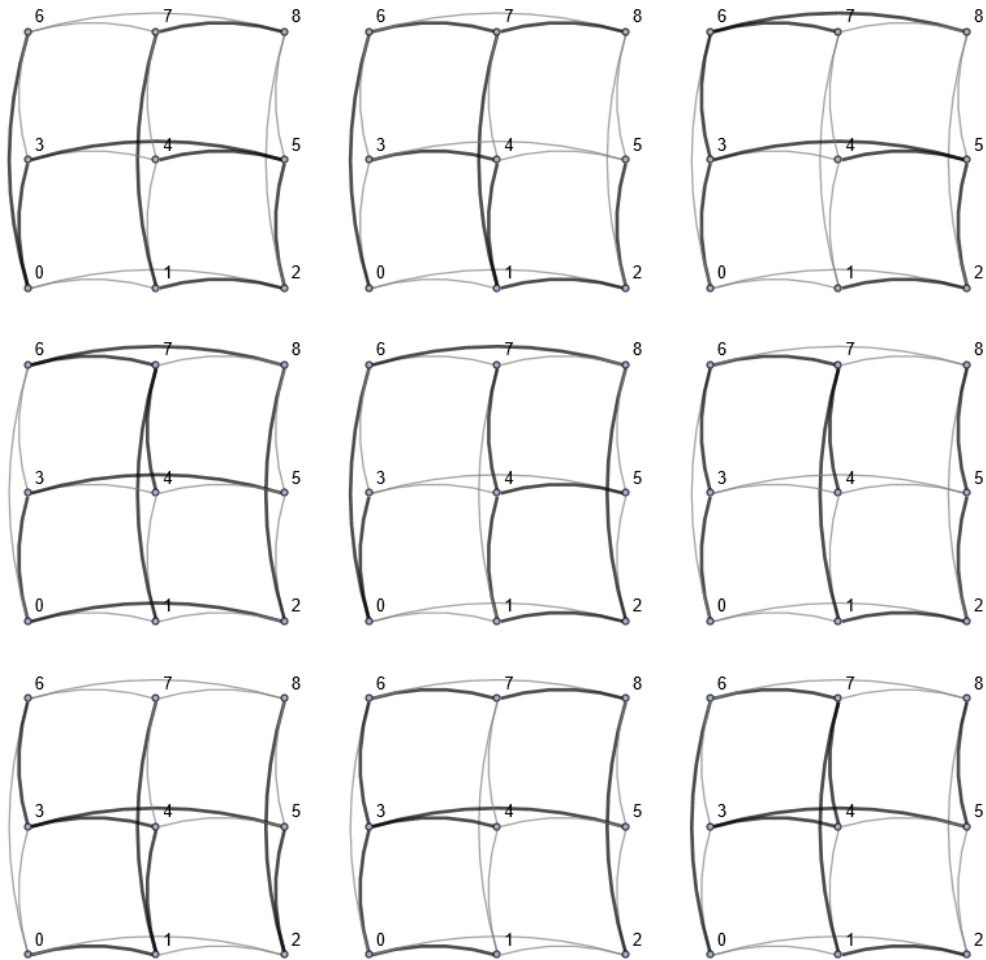



Figure 4: Few spanning trees on a 3×3 lattice generated using the brute-force algorithm

II-4 Gauge Transformation between Spanning Trees

Get it on 

The following modules calculate the gauge transformation between two spanning trees.

```
In[8]:= (* In the modules below, we have considered the notation that
{11, 12} = {12, 11}^{-1} *)

(* Returns all the links (unidirectional) for a given lattice *)
getLinks [nSites_, nDim_, neighbour_] := Module[{sites, links},
  sites = Range[0, nSites^nDim - 1];
  links = <||>; (* Association of all links -> values.
Please mind the abuse of notations. I am using (11,
12) for denoting both the connection between 11 and 12,
and also the value of the link element between 11 and 12*)
  Do[
    Do[
      If [Not[KeyExistsQ[links, Sort[{site, siteNeighbour}]]]
        , AppendTo[
          links, {site, siteNeighbour} -> {site, siteNeighbour} ]
        ]
      , {siteNeighbour, neighbour[site]}
      , {site, sites}];
    links];

In[9]:= (*List which site is connected to which other sites via the spanning tree*)
getConnections[nSites_, nDim_, tree_] :=
Module[{treeConnections, sites},
  treeConnections = <||>;
  sites = Range[0, nSites^nDim - 1];
  Do[
    AppendTo[treeConnections, site -> {}];
    Do[
      If[ IntersectingQ[{Sort[{site, site1}]}, tree],
        AppendTo[treeConnections[site], site1]
        ]
      , {site1, sites}
      , {site, sites}];
```

```

treeConnections];

In[10]:= (* We follow the norm that the 0th site is set to I. Starting from
this, we traverse the tree and obtain the gauge elements on each site
that gives rise to the said spanning tree *)
getGaugeTransformation[nSites_, nDim_, tree_] := Module[
  {GaugeTransformation, sites, treeConnections, fixedSites,
   newFixedSites},
  sites = Range[0, nSites^nDim - 1];
  GaugeTransformation = <|sites[[1]] -> {}|>; (*
Group elements on each site, site -> element*)
  treeConnections = getConnections[ nSites, nDim, tree];
  fixedSites = {{sites[[1]]}};(*Starting from 0*)
  While[Not[Equal[Sort[Flatten[fixedSites]], sites]],(*
While all sites are not fixed*)
    newFixedSites = {};
    (*Start from 0,
and fix all the other end points of links starting from 0. These
new end points that are fixed go to the newFixedSites,
on which the next loop will run *)
    Do[
    Do[
    If[
    Not[KeyExistsQ[GaugeTransformation,
connectedSite]], (*If site is not already fixed*)
    AppendTo[GaugeTransformation,
connectedSite ->
Join[GaugeTransformation[
site], {{site, connectedSite}}] ]; (*on the left,
the gauge transformation on 'site' will be acting.
To set the link to I,
we need to set the gauge transformation on the 'connectedSite'
to 'GaugeTransformation[site] x link' *)
    AppendTo[newFixedSites, connectedSite]
, {connectedSite, treeConnections[site]}
],
{site, Last[fixedSites]}}];
    AppendTo[fixedSites, newFixedSites];
  ];

```

```
GaugeTransformation];
```

```
In[11]:= (* Given two trees, equalityConstraints[site] gives the neighbouring sites to be modified in order to preserve the unchanged links while setting the value of the lattice site 'site' *)
```

```
getEqualSites[ nSites_, nDim_, tree1_, tree2_] :=
```

```
Module[{sites, unchanged, equalityConstraints},
```

```
  sites = Range[0, nSites^nDim - 1];
```

```
  unchanged = Intersection[tree1, tree2];
```

```
  equalityConstraints = <||>;
```

```
  Do[
```

```
    AppendTo[equalityConstraints, site -> {}];
```

```
  Do[
```

```
    If[ IntersectingQ[{Sort[{site, site1}], unchanged},
```

```
      AppendTo[equalityConstraints[site], site1
```

```
    ]
```

```
    , {site1, sites}]
```

```
  , {site, sites}];
```

```
  equalityConstraints];
```

```
In[12]:= (* Given a spanning tree, obtain the gauge transformation using getGaugeTransformation, and act upon the links by the gauge transformation*)
```

```
getModifiedLinks[nSites_, nDim_, links_, tree_] :=
```

```
Module[{modifiedLinks, gaugeTransformation},
```

```
  modifiedLinks = <||>;
```

```
  gaugeTransformation = getGaugeTransformation[ nSites, nDim, tree];
```

```
  Do[
```

```
    AppendTo[modifiedLinks,
```

```
      link -> Join[gaugeTransformation[link[[1]]], {link},
```

```
      Reverse[gaugeTransformation[link[[2]]], {1,
```

```
        2}]] ] (*The inverse of a product of gauge elements reverses
```

```
the order of multiplication.
```

```
At the same time we also reverse the order in the links since
```

```
{11, 12}^{-1} = {12, 11}*)
```

```
  , {link, links}];
```

```
  modifiedLinks];
```

```
In[13]:= (* Given two spanning trees, this obtains the gauge transformation relating one to another *)
```

```

gaugeTransformationBetweenTwoTrees[nSites_, nDim_, tree1_, tree2_,
neighbour_] :=
Module[{links, modifiedLinks, toAdd, gaugeTransformation1to2,
equalityConstraints, addedSites, added, newAdded, equalSites},
links = getLinks[nSites, nDim, neighbour];
modifiedLinks = getModifiedLinks[ nSites, nDim, links, tree1];
toAdd =
Complement[tree2,
tree1]; (*The links that are to be added to the first tree*)
gaugeTransformation1to2 = <||>;
Do[AppendTo[gaugeTransformation1to2, site -> {}], {site,
Range[0, nSites^nDim - 1]};
(* We start off with an identity element, i.e.
for each site there is no gauge element *)
equalityConstraints = getEqualSites[ nSites, nDim, tree1, tree2];
Do[(*For each link to be added*)

(* for a link {l1, l2}, we set G[l1] = I and G[l2] = {l1,
l2} to enforce the gauge transformation *)

(* here we obtain first,
all the sites that should be set equal to G[l2] according
to the equality constraints *)
addedSites = {{link[[2]}}];
added = True;
While[added,
added = False;
newAdded = {};
Do[
Do[
If[Not@MemberQ[Flatten@addedSites, connected], added = True;
AppendTo[newAdded, connected]]
, {connected, equalityConstraints[site]}]
, {site, Last[addedSites]};
AppendTo[addedSites, newAdded];
]; (* The above while loop, for every site added,
checks the equality constraints and adds the other
required sites also *)

```

```

equalSites = Flatten@addedSites;
Do[(* For each site to be set for the given link, i.e.
    for each site in equalSites*)
    gaugeTransformation1to2[site] =
    Join[gaugeTransformation1to2[site], modifiedLinks[link] ];
    , {site, equalSites}];

, {link, toAdd}];
gaugeTransformation1to2
];

```

We can now use the above declared functions to generate the spanning trees on a 3×3 lattice and obtain the gauge transformation between two spanning trees.

```

In[14]:= nSites = 3;
         nDim = 2;
         neighbour = getNeighbours[nSites, nDim];
         Trees = getTrees[nSites, nDim];
         tree1 = Map[Sort, Trees[[1, 1]]]
         tree2 = Map[Sort, Trees[[11664, 1]]]

Out[14]= {{0, 1}, {1, 2}, {2, 5}, {3, 4}, {3, 6}, {3, 5}, {6, 7}, {6, 8}}
         {{0, 1}, {0, 2}, {0, 3}, {0, 6}, {4, 5}, {6, 7}, {6, 8}, {5, 8}}

In[15]:= gaugeTransformationBetweenTwoTrees[nSites, nDim, tree1, tree2,
         neighbour]

Out[15]= <|0 -> {},
         1 -> {},
         2 -> {{0, 2}, {2, 1}, {1, 0}},
         3 -> {{0, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}},
         4 -> {},
         5 -> {{0, 1}, {1, 2}, {2, 5}, {5, 3}, {3, 4}, {4, 5}, {5, 2},
         {2, 1}, {1, 0}},
         6 -> {{0, 6}, {6, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}, {0, 1}, {1, 2},
         {2, 5}, {5, 8}, {8, 6}, {6, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}},
         7 -> {{0, 6}, {6, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}, {0, 1}, {1, 2},
         {2, 5}, {5, 8}, {8, 6}, {6, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}},
         8 -> {{0, 6}, {6, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}, {0, 1}, {1, 2},
         {2, 5}, {5, 8}, {8, 6}, {6, 3}, {3, 5}, {5, 2}, {2, 1}, {1, 0}},|>

```