Probing topological properties of 3D lattice dimer model with neural networks

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Machine learning methods are being actively considered as a new tool of describing many body physics. However, so far, their capabilities has been only demonstrated in previously studied models, such as e.g. Ising model. Here, we consider a simple problem, demonstrating that neural networks can be successfully used to give new insights in statistical physics. Specifically, we consider 3D lattice dimer model, which consists of sites forming a lattice and bonds connecting the neighboring sites, in such a way that every bond can be either empty or filled with a dimer, and the total number of dimers ending at one site is fixed to be one. Dimer configurations can be viewed as equivalent if they are connected through a series of local flips, i.e. simultaneous 'rotation' of a pair of parallel neighboring dimers. It turns out that the whole set of dimer configurations on a given 3D lattice can be split into distinct topological classes, such that dimer configurations belonging to different classes are not equivalent. In this paper we identify these classes by using neural networks.

To address this question, we consider another well-known model of statistical physics - 3D lattice dimer model, which contains sites forming a lattice and edges connecting the sites, so that every edge can be either empty or occupied by a dimer, provided the total number of dimers at each site is equal to one. This simple model has a long history in condensed matter physics. It has been studied since 1960-s, when it was realized that the total number of dimer coverings on a planar lattice can be computed analytically. Soon after, it was realized that dimer model on a so-called Fisher lattice is dual to 2D Ising model on a square lattice, which made it possible to solve the Ising model analytically. Later on, lattice dimer model has been extensively probed as a candidate model for high-temperature superconductivity - it was suggested that dimers may describe electron singlets formed between neighboring sites. More recently, dimer model on a diamond lattice has been interpreted as a dual to spin system on pyrochlore lattice, which, in turn, hosts exotic spin ice state.

A key feature of physics, which distinguishes it from other areas of human knowledge is that it describes the world in terms of exact physical laws. Dynamics of any system can, in principle, be reduced to dynamics of its components and their interactions, and each physical component can be exactly described in terms of its equations of motion. However, this simple paradigm can be difficult to realize in practice, especially when the number of the constituent components becomes too large. Statistical physics deals with systems containing close-to-infinity number of elements, which makes it somewhat similar to various statistical problems, where individual laws are not known, but the only known thing is a small sample of the ensemble and its empirical properties. These properties may be, in principle, uncovered by using statistical learning - a way to extract general patterns within the sample and to use them to predict the properties of the whole system. Statistical learning includes various methods and the most prominent of them are neural networks. From this perspective, it seems interesting to use them to get knowledge about statistical physics. Indeed, in the recent years, neural networks were proven to be successful in describing various physical properties, such as magnetic phases and critical temperature of the Ising model, as well as other similar lattice models (such as e.g. Hubbard model, topological phases in various models, many body localization etc). We also remark that neural networks have also been used in condensed matter physics for other various purposes (e.g. representation of quantum states or many-body quantization state tomography). However, the key question is: can neural networks give new insights about many body physics, which were not discovered before?
Kivelson model \[14\]. The later is known to host a spin liquid phase \[24\], whose excitations spectrum depends on the type of the underlying lattice: on a bipartite lattice gapless $U(1)$ phase is realized, whereas on a non-bipartite lattice, a gapped $Z_2$ phase appears. The difference between bipartite and non-bipartite lattices persists on a classical level: on a bipartite lattice, dimer configurations can be described using effective magnetic field (which in 2D case gets reduced to ‘weights representation’) \[25\], whereas a similar representation is not known on a non-bipartite lattice.

Despite its simplicity, theoretical properties of the classical lattice dimer model are not yet fully explored. For example, one important question about it is: can we use a sequence of local flips in order to transform one given configuration of dimers to another given configuration? This question was in part addressed in the Ref. \[23\] - it was pointed out that configurations in lattice dimer model can be characterized by an invariant, which does not change under local flips, a pfaffian of so-called Kasteleyn matrix. It was found that in the case of a planar lattice (e.g. 2D plane), such invariant is always equal to +1, whereas in the case of a non-planar (e.g. 3D) lattice, there exist both configurations, where this invariant is equal to +1 (such as trivial maximally flippable state, see Fig. 2c), and −1 (a ‘hopfion’ - the name was introduced from a continuum limit of a cubic lattice \[26\], see Fig. 2b).

The problem of finding distinct topological classes of dimer configurations can be viewed as a classification problem from machine learning point of view, and therefore, it can be addressed by using the most powerful machine learning method - neural networks. Motivated by this, we study dimer configurations in the following way: first, we train the neural network on a dataset of configurations from two known topological classes, and after it, we test the neural network on a different dataset of configurations from various topological classes. We find that the neural network is able to successfully distinguish dimer configurations from the two topological classes used for training, but more interestingly, the neural network is able to distinguish dimer configurations from other classes, thus answering the question of the full topological classification.

We obtain that on a bipartite (in our case cubic) lattice, hopfions are characterized by an integer topological invariant, whereas on a non-bipartite lattice (we consider an example of stacked triangular lattice), dimer configurations are characterized by $Z_4$ invariant. We remark, that this reasoning gave us a hint that on a bipartite lattice, dimer configurations can be characterized by an exact Hopf number \[27,30\], which we later verified analytically \[37\]. However, on a non-bipartite lattice, the neural network is the only known way to obtain the topological classification of dimer configurations.

This is the main idea of the paper: neural networks can successfully identify new topological phases, not known in advance, and as such, they can be used to give ‘hints’ about unknown properties of physical systems, which can be later verified by other, more rigorous techniques.

This paper is organized as follows. In Sec. \[1\] we introduce 3D lattice dimer model and describe our method in the case of cubic lattice. In Sec. \[III\] we repeat our study in the case of stacked triangular lattice. In Sec. \[IV\] we summarize our findings. In the appendix, we briefly present analytical construction of the Hopf invariant (Sec. \[B\]). For a more detailed discussion about Hopf invariant in 3D lattice dimer model, we refer to the Ref. \[37\].

II. DIMER MODEL ON A CUBIC LATTICE

We start from revising the basic properties of lattice dimer model. Let us consider a lattice, i.e. a chain of periodically aligned sites, and assume that each pair of the nearest neighboring sites is connected with a bond. We place dimers on some of the bonds, i.e. assume that every bond is either empty, or occupied with a dimer. We also assume that the dimers are placed on a lattice in such a way, that they satisfy a constraint: every site is attached to exactly one dimer. A few possible examples of dimer configurations on a lattice with $4 \times 4 \times 4$ sites are shown on the Fig. 2. Indeed, on the Fig. 2 one can see the bonds filled with dimers, and check that every lattice site is attached to exactly one dimer.

We allow dimer configurations to change by applying random local flips. A local flip is a transformation, which simultaneously changes orientation of two parallel dimers within one plaquette (see Fig. 2a). We refer to a pair of configurations as equivalent, if they can be transformed into each other by a series of local flips. For example, on the Fig. 2c all dimers are parallel to each other, and therefore it is possible to apply a local flip to any of its plaquettes. Afterwards, one can repeat applying local flips to to any of the plaquettes, whose dimers are parallel, thus generating various equivalent configurations. On the Figs. 2a 2b not all dimers are parallel to each other, and therefore one can apply local flips to those plaquettes, whose dimers are parallel. Thus from every dimer configuration, it is possible to generate a lot of equivalent configurations by applying local flips.

The key question, that we want to answer is: are all dimer configurations on a given lattice are equivalent, i.e. can be obtained from each other by applying local flips, or are there distinct topological classes, such that configurations from different classes cannot be transformed into each other by applying local flips? Previously, in the Ref. \[26\], there was presented an argument that not all configurations in 3D lattice dimer model are equivalent. The idea was the following: the lattice can be characterized by Kasteleyn matrix $M_{ij}$ with the indices $i,j$ enumerating all lattice sites, such that its components take values $\pm i$, and their signs are chosen in such a way, that a product of $M_{ij}$ around each plaquette is equal to $−1$.
(see Figs. [1a][1b] for the precise arrangement). Similarly, each dimer configuration can be characterized by another matrix $n_{ij}$, whose components are equal to 1 if the sites $i, j$ are connected with a dimer, and zero otherwise. It is straightforward to check that the expression $\text{Pf}(M_{ij} n_{ij})$ is invariant under local flips. On the other hand, one can explicitly compute this invariant for specific dimer configurations and see that it may take different values. For example, this invariant is equal to 1 for a trivial dimer configuration, shown on the Fig. (2c). In contrast, a non-trivial configuration, shown on the Figs. (2b) [2d], has $\text{Pf}(M_{ij} n_{ij}) = -1$. Since the invariant $\text{Pf}(M_{ij} n_{ij})$ does not change under local flips, but at the same time it takes different values for two configurations '0' (Fig.2c) and '1' (Fig.2d), these configurations cannot be transformed to each other by applying a series of local flips. We refer the configuration shown on the Fig. (2b) as a hopfion, following the Ref. [26], where it was given such name, because in the continuum limit, it behaves as a field configuration with a non-trivial Hopf number.

The previous argument makes it possible to see that space of all dimer configurations contains different inequivalent classes, but there still remains a question whether a pair of dimer configurations with the same value of $\text{Pf}(M_{ij} n_{ij})$ always belong to the same class. For example, if we 'stack' two hopfions on top of each other (see Fig. 2e, the resulting configuration has $\text{Pf}(M_{ij} n_{ij}) = +1$, i.e. the same as for the trivial dimer configuration (Fig. 2c), but do they belong to the same topological class? To find an answer to this question, we implement one of the most popular machine learning algorithms - a neural network. The main idea is the following: if we train the neural network to distinguish configurations equivalent to the trivial (Fig. 2c) and the hopfion (Fig. 2d), what will it tell us about the unknown configuration containing two hopfions (Fig. 2e)?

We create our training and test datasets by Monte Carlo method. More specifically, we consider a cubic lattice of the size of $4 \times 4 \times 4$ and with open boundary conditions. We start from configurations of each of the classes, shown on the Figs. (2c), and apply a sequence of local flips to each of these two configurations. In particular, to generate the training dataset, we start from two configurations '0' and '1' from each of the classes: the first ('0') has all dimers aligned in $z$ direction (see Fig. 2c), and the second ('1') is a hopfion surrounded by vertically aligned dimers (see Fig. 2d). We apply a sequence of local flips to each of these two configurations, and assign the label '0' or '1' to the outputs by using the fact that local flips preserve the topological class.

We train the neural network to distinguish, whether each configuration belongs to the class '0' or '1'. More specifically, we define the neural network in such a way, that it takes a dimer configuration as input, and outputs its topological class. We use a fully-connected neural network with one hidden and output layer, and repeat the procedure for different number of hidden units. In each hidden unit, we use the activation function $\text{relu}$, but in the output layer, we do not use any activation function: in other words, the output is simply a linear superposition of the results from hidden units with an added bias.

After training, we apply the neural network to a test dataset, which is generated by applying local flips to configurations containing zero, one and two hopfions respectively (see Figs. 2c, 2d). We find, that our neural network can successfully distinguish all of them. It outputs a real number approximately equal to the number of hopfions (which can be either zero, or one, or two), and its accuracy improves with increasing number of units. Thus, if we assume that the trivial configuration (Fig. 2c) has topological number 0, and configuration with one hopfion (Fig. 2d) has topological number 1, then the neural network tells us that the configuration with two hopfions (Fig. 2e) has topological number 2. In other words, the neural network gives us a hint that the dimer configurations (Fig. 2c, 2d) are characterized by an integer topological invariant, as we would expect from its continuum limit. Since, we know that in the continuum limit, field configurations are characterized by a Hopf invariant, we believe that our lattice configurations are characterized by the same integer topological invariant.

If we believe, that a hopfion is actually described by a Hopf number, then its mirror image has to be described by Hopf number of the opposite sign. We are interested in checking it using our neural network. If we reflect the configurations within our test dataset, and substitute them into the neural network, it outputs negative number, which, for a small training dataset, does not as closely approach $-1$ or $-2$, as it approaches the positive integers describing hopfions without reflection. However, its accuracy increases with increasing number of samples in the training dataset. Thus we believe that at sufficiently large number of samples, the neural network
FIG. 2: A lattice dimer model consists of a dimer lattice lattice, and dimers placed on its bonds, in such a way that every site is attached to exactly one dimer. (a) Two dimer configurations are considered equivalent if they can be connected to each other by a series of local flips. The simplest dimer configuration, which is not equivalent to trivially aligned dimers is a hopfion. To perform our study we used (c) a 4 × 4 × 4 lattice with trivially aligned dimers, (d) a hopfion placed on a lattice of the same size and surrounded by trivially aligned dimers, and (e) two hopfions stacked on the same lattice, and also surrounded by trivially aligned dimers.

We note that recognizing samples with negative Hopf numbers can be improved by incorporating them into the training algorithm. Particularly, we can repeat our training procedure and to include three kinds of configurations in the training sample: trivial configurations with Hopf number 0, configurations obtained from one hopfion with assigned Hopf number +1, and their mirror images with assigned Hopf number −1. In this case, the neural network can equally well recognize all configurations with Hopf numbers between −2 and 2 (see Fig. 3). We believe that this result is consistent with an idea, that neural network can be successfully applied to samples within the space, where it was trained, but, generally, it poorly extrapolates.

A. Cubic lattice with periodic boundary conditions

We are also interested, whether the fact that configurations in lattice dimer model can be characterized by Hopf number, depends on the kind of boundary conditions imposed on the lattice. To find it out, we repeat our procedure in the case, when the lattice obeys periodic boundary conditions, and we obtain similar results: if a neural network were trained on configurations with zero or one hopfion, it can successfully distinguish configurations obtained from zero, one, or two hopfions, but it has slightly lower accuracy when distinguishing their mirror reflected images, i.e. configurations with Hopf numbers −1 and −2. The fact that Hopf number can be defined either on a lattice with open, or periodic boundary conditions is a non-trivial result, because a-priori, one might expect that topological properties of a model depend on topological properties of the manifold, where it is placed. Furthermore, we mention that in the work [37] we develop a method of computing Hopf number analytically, but the idea presented there works only in the case of open boundary conditions. Thus, neural networks provide us with a qualitatively new result: dimer configura-
tions on a lattice with periodic boundary conditions are characterized by Hopf number in the same way, as on a lattice with open boundary conditions.

FIG. 4: Outputs of the neural network trained on configurations "0" and "1" for a $4 \times 4 \times 4$ lattice with periodic boundary conditions. ($\sim 6 \times 10^5$ samples, 500 epochs).

III. DIMER MODEL ON A STACKED TRIANGULAR LATTICE

In the previous section we demonstrated that neural network can successfully distinguish topological sectors of lattice dimer model on a cubic lattice. However, from previous studies of the lattice dimer model (e.g. [24]), it is known that it has qualitatively different properties on a bipartite and non-bipartite lattices. For instance, the notion of effective magnetic field exists only if the lattice is bipartite, and furthermore, quantum dimer model has different strongly coupled phases: on a bipartite lattice, it has a gapless $U(1)$ phase, but on a non-bipartite lattice a gapped $\mathbb{Z}_2$ phase is realized. Motivated by this, we would like to apply our method to study hopfions on a non-bipartite lattice. We consider the most straightforward generalization of cubic lattice - stacked triangular lattice. It has the same sites and bonds as the cubic, but in addition, it has bonds aligned diagonally. Thus, on a stacked triangular lattice, we can create initial configurations with zero, one or two hopfions in exactly the same way, as we did for a cubic lattice, but when we transform them, we apply more kinds of local flips: six kinds in total (see Fig. 5).

As previously, we start from two initial configurations: the first with all dimers aligned in the vertical direction, and the second with one hopfion surrounded by vertically aligned dimers, and apply a series of local flips to both of them. In this way, we obtain a large number of configurations, which we use as a training dataset for the neural networks.

FIG. 5: An example of stacked triangular lattice forming a trivial dimer configuration and a hopfion. (a) six possible local flips on a stacked triangular lattice that preserve signPf($M_{ij}n_{ij}$).

After it, we create our test dataset by applying local flips to the dimer configurations '0' and '1' (trivial and a hopfion), as well as configurations with two hopfions and mirror reflected images of the configurations with one or two hopfions. We note, that in this setting, the neural network with only one hidden layer cannot be trained successfully, and therefore we have to increase the number of hidden layers, while keeping the number of units
in each layer fixed. We obtain that the neural network with three or more layers can successfully distinguish configurations obtained from one or two hopfions, it outputs a real number very close to the parity of the number of hopfions. Thus, the neural network tells us that on a stacked triangular lattice, hopfion is a topological defect characterized by $Z_2$ invariant, equal to the parity of the number of hopfions. Equivalently, we can conclude that on a non-bipartite lattice, the invariant sign $\text{Pf}(M_{ij}n_{ij})$ (discussed in the beginning of the Sec. II) is a physical topological invariant.

IV. DISCUSSION

In this work, we have demonstrated that neural network can be used to distinguish topological phases of lattice dimer model. Using it, we verified that topological defects in the dimer model on a cubic lattice can be characterized by integer Hopf invariant, whereas on a stacked triangular lattice, the same defects are characterized by $Z_2$ invariant. In addition, in the case of the cubic lattice, we have explicitly checked that topological defects are characterized by Hopf invariant both in the case of open and periodic boundary conditions (strictly speaking, in the latter case, we limited our study to the subsector with trivial winding number). In fact, the neural network gave us a hint to the whole idea, that Hopf number can be defined on a lattice dimer model, which we verified analytically afterwards (see [37]). Thus, our paper can be viewed as the first work, where neural networks were successfully used to identify new topological phases. This is in contrast to the previous works, where machine learning algorithms were only able to identify previously known topological phases.

We remark, that we found a qualitative difference between the optimal neural networks used in the cases of cubic and stacked triangular lattices. More specifically, we found that, in the case of cubic lattice, the neural network with just one hidden layer gives reasonably good predictions, whose accuracy increases with increasing number of hidden units. In contrast, in the case of stacked triangular lattice, one hidden layer is insufficient to train the neural network: the minimal required number of layers is three, and the accuracy improves if we take larger number of hidden layers. We suggest, that this difference may be related to complexity of the function, which the neural network approximates. Indeed, on a cubic lattice, configurations are characterized by Hopf number, which can be expressed as a quadratic function of the effective magnetic field, or equivalently, dimer occupation number. However, on a stacked triangular lattice, the physical topological invariant is $\text{signPf}(M_{ij}n_{ij})$, which is a high power function of the dimer occupation number. Thus, probing 3D lattice dimer model with neural networks leads us to conjecture, that the optimal number of hidden layers in a neural network is related to complexity of the function, which the neural network approximates. Moreover, we believe that, in the future, it might be of interest to apply machine learning algorithms to simple physical systems in order to better understand the properties of machine learning algorithms themselves.

We emphasize that, from our perspective, the main role of machine learning in physics is to provide insights about physical systems rather than rigorous results. In fact, like many other numerical methods, our approach has limitations due to fixed lattice size, finite number of samples in the datasets etc. For example, if one tries to draw conclusions based only on the neural networks, they may face such questions as e.g.: can it be that hopfions belong to a separate topological class on a $4 \times 4 \times 4$ lattice, but to the same topological class on a larger lattice? Or, can it be that a hopfion does not belong to a separate topological class from a trivial configuration, but lies in a different part of the same topological class? The answers to these questions have to be found by using other techniques, than machine learning. Indeed, we claim that a hopfion is topologically distinct from a trivial dimer configuration (in both cases of cubic and stacked triangular lattices), because they have different values of a topological invariant $\text{signPf}(M_{ij}n_{ij})$. Furthermore, in Ref. [37], we claim that, in the case of cubic lattice, hopfions are characterized by an integer topological invariant based on its analytical derivation. On the other hand, our new result that on a stacked triangular lattice, $\text{signPf}(M_{ij}n_{ij})$ is a physical topological invariant, is suggestive - it has to be checked by other means.

We mention that topological defects in lattice dimer model are interesting from physical point of view. In fact, lattice dimer models are known to be dual to various spin systems, many of which indeed have been realized experimentally. For example dimer model on a 3D diamond lattice (which, similarly to cubic, is also bipartite) is dual to spin ice on a pyrochlore lattice. The latter has been widely studied in the context of frustrated magnetism (see [17]) for review), and have been proven to exist in various materials, such as e.g. $\text{Dy}_2\text{Ti}_2\text{O}_7$ and $\text{Ho}_2\text{Ti}_2\text{O}_7$. We believe that in these systems, it would be interesting to explore the effects resulting from the presence of distinct topological classes and consequently non-ergodicity.

We also suggest that hopfions can be experimentally realized in ‘artificial spin ice’, where lattice dimer model is simulated by nanomagnets (see e.g. [19]). The simplest scenario of two-dimensional artificial spin ice has been extensively studied, and it has been found to share unique properties of lattice dimer model, such as magnetic monopoles and even Coulomb phase [20, 21]. However, in the last years, there have been ongoing efforts to realize three-dimensional artificial spin ice [22, 23, 59]. Since, the existence of hopfions requires only two stacked
ACKNOWLEDGMENTS

We would like to thank Roger Melko for proposing this problem and having multiple discussions about it. We would also like to thank L. Sierens, B. Kulchitski, S. Wetzel, J. Rau, C. Nisoli, R. Moessner, L. Balents, L. Wang, A. Smith for the discussions about this problem. Calculations were performed using the supercomputing facilities of Sharcnet. Financial support was provided by NSERC of Canada.

Appendix A: Methods

As we mentioned in the Sec. 1, we generate our training and testing datasets by applying local flips to configurations with fixed number of hopfions, shown on the Figs. 2c, 2d and Figs. 2c, 2d, 2e respectively. We apply a thousand of random local flips between each pair of recorded configurations to make samples in the dataset more diverse. Samples with negative Hopf numbers are obtained by my mirror reflecting (over 100 plane in the case of cubic lattice, and 001 plane in the case of stacked triangular lattice) the samples with the positive Hopf numbers.

After generating the datasets, we train the neural networks. In the case of cubic lattice, we consider neural networks with one hidden and one outputs layers and vary the number of units in the hidden layer. In the case of triangular lattice, we vary the number of layers, but fix the number of units in the hidden layer. In the case of cubic lattice, we vary the number of layers, but fix the number of units in each of them to be 128. In both cases, we use relu as activation function in the hidden layers, and do not use any activation in the outputs layers. We perform our computations using Keras-2.1.5 library, use SGD optimizer and minimize mean square error between the outputs and the Hopf numbers 0 and 1. This choice is natural assuming that the topological number can take any integer value. We perform a few hundreds of epochs and ensure that the loss decreases during training.

Finally we test the neural network on \( \sim 10^4 \) configurations with each value of Hopf number. We compute the output of a fixed neural network for each configuration, and then compute its average and standard deviation. We present these results on the graphs 3, 4, 6.

As we mention in the main text, we use neural networks with one hidden layer in the case of the cubic lattice, and many hidden layers in the case of stacked triangular lattice. It is interesting to note, that in the case of cubic lattice, the neural network can distinguish Hopf numbers not used in training (i.e. ”2”, ”-1”, ”-2”) only if it has just one hidden layer. If we increase the number of layers, and test the neural network on configurations with Hopf number 2, its output becomes closer to 1, but if we test it on configurations with Hopf numbers −1 or −2, its output becomes close to 0. We attribute this to overfitting, which naturally occurs if the number of training parameters is too large. We hypothesize that since Hopf number is a quadratic function of effective magnetic field, which is in turn proportional to a filling number, two layers are optimal for a neural network to distinguish it. In addition, we note that the accuracy of the neural networks decreases if we replace its activation functions with e.g. tanh or sigmoid. We think that it happens, because the magnitudes of such activation functions are constrained below one, and thus it is ‘harder’ to create a neural network configuration, which outputs a number close to an integer with a magnitude larger than one.

Appendix B: A brief construction of the Hopf number

In this section we briefly describe analytical derivation of the Hopf invariant in 3D lattice dimer model. As we mentioned previously, Hopf invariant can be defined on a bipartite lattice, i.e. whose sites can be labeled by \( \sigma = \pm 1 \) in such a way that any bond connects sites with opposite values of \( \sigma \). A particular example of a bipartite lattice is cubic lattice, whereas an example of a non-bipartite lattice is stacked triangular lattice. The main idea is that on a bipartite lattice, dimer filling can be described in terms of effective magnetic field

\[
B_i(\vec{r}) = \sigma(n_{r,r+e_i} - w_{r,r+e_i}).
\]

Here \( w_{r,r+e_i} \) is a fixed number characterizing each bond of the lattice. Conventionally, \( w_{r,r+e_i} \) is chosen to be equal to inverse coordination number of the lattice, but in Ref. 37, we develop a more general approach, which makes it possible to account for finite size of the lattice. As one can see, \( B_i(\vec{r}) \) characterizes filling of each bond connecting the sites at positions \( \vec{r} \) and \( \vec{r} + e_i \). It is called an effective magnetic field, because it satisfies the constraint of zero divergence:

\[
\begin{align*}
B_x(x,y,z) - B_z(x-1,y,z) \\
+ B_y(x,y,z) - B_y(x,y-1,z) \\
+ B_z(x,y,z) - B_z(x,y,z-1) &= 0,
\end{align*}
\]

(B1)

which in turn follows from the constraint of exactly one dimer attached to each site.

The condition of zero divergence (B1) makes it possible to introduce effective vector potential - a vector defined at each plaquette, such that its discrete rotor gives the
effective magnetic field

\[ B_x(x, y, z) = A_x(x, y, z) - A_x(x, y - 1, z) \]
\[ - A_y(x, y, z) + A_y(x, y, z - 1), \]

\[ B_{y,z} \] are defined through cyclic permutations.

Once we defined the effective magnetic field and vector potential, we can write Hopf number as a sum of their products

\[ \chi = \sum_{x,y,z} \frac{A_x(x, y, z)}{8} \times (B_x(x, y, z) + B_x(x, y + 1, z) + B_x(x, y + 1, z + 1) + B_x(x, z - 1, y + 1, z) + B_x(x - 1, y, z + 1) + B_x(x - 1, y, z + 1) + B_x(x - 1, y + 1, z + 1)) + \text{(cyclic permutations)}. \] (B2)

\[ \chi \]

Here we took vector potentials at each plaquette and multiplied it by average magnetic field along the bonds adjacent and perpendicular to the plaquette.

Through explicit calculations, (see Ref. [37]) one may check that the Hopf number \( B_2 \) is

- gauge-invariant
- invariant under local dimer flips
- is equal to 0, 1, 2 for the dimer configurations shown on the Figs. [29] [28] [26] (correspondingly and changes sign through mirror reflection).

Thus, the result about about existence of Hopf number in 3D lattice dimer model, which was first obtained by using neural networks, can be verified analytically.
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