Unsupervised machine learning for the detection of exotic phases in skyrmion phase diagrams

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Undoubtedly, machine learning (ML) techniques are being increasingly applied to a wide range of situations in the field of condensed matter. Amongst these techniques, unsupervised techniques are especially attractive, since they imply the possibility of extracting information from the data without previous labeling. In this work, we resort to the technique known as "anomaly detection" to explore potential exotic phases in skyrmion phase diagrams, using two different algorithms: Principal Component Analysis (PCA) and a Convolutional Autoencoder (CAE). First, we train these algorithms with an artificial dataset of skyrmion lattices constructed from an analytical parametrization, for different magnetizations, skyrmion lattice orientations, and skyrmion radii. We apply the trained algorithms to a set of snapshots obtained from Monte Carlo simulations for three ferromagnetic skyrmion models: two including in-plane Dzyaloshinskii-Moriya interaction (DMI) in the triangular and kagome lattices, and one with an additional out of plane DMI in the kagome lattice. Then, we compare the root mean square error (RMSE) and the binary cross entropy (BCE) between the input and output snapshots as a function of the external magnetic field and temperature. We find that the RMSE error and its variance in the CAE case may be useful to not only detect exotic low temperature phases, but also to differentiate between the characteristic low temperature orderings of a skyrmion phase diagram (helical, skyrmions and ferromagnetic order). Moreover, we apply the skyrmion trained CAE to two antiferromagnetic models in the triangular lattice, one that gives rise to antiferromagnetic skyrmions, and the pure exchange antiferromagnetic case. Despite the predictably larger RMSE, we find that, even in these cases, the RMSE is also an indicator of different orderings and the emergence of particular features, such as the well-known pseudo-plateau in the pure exchange case.

I. INTRODUCTION

Machine Learning (ML) has been increasingly incorporated into a wide variety of technological and scientific research in the last few years. In condensed matter physics, some of the first studies using ML include the representation of quantum states [1], the identification of phases of matter [2], inverse design in photonics [3] and the study of phase transitions [4–6]. In particular, ML has been used to explore different aspects of magnetic skyrmions, which are topological textures [7, 8] with potential technological applications, especially in memory storage devices [9, 10]. Feed forward and convolutional neural network have been used to classify different magnetic phases and predict features in simple skyrmion models using simulations data [11–18]. Moreover, ML algorithms have been applied also to experimental data to explore skyrmion phases [19–21].

In general, ML techniques could be devided in three large types of techniques [22, 23]: supervised, unsupervised and reinforcement learning, the latter one being the case where the algorithm "learns" solely from the data. In supervised ML, a previous labeling and knowledge of the data is needed before applying the algorithms to an unknown dataset, and is widely used in classification and regression tasks. On the other hand, no data labeling is required in unsupervised ML, and some of these techniques may be used for example to group similar instances of the data (clustering) or detect atypical instances (anomaly detection). A variety of this type of unsupervised (or semi-supervised) methods has been used in condensed matter physics, from Principal Component Analysis (PCA) in Ising systems [5] to support vector machines with tensorial kernels applied to models in different types of topology [24–31], the use of autoencoders to study neutron scattering data in spin ice systems [32, 33] and to explore anomaly detection in simple frustrated models [34].

In this work, we resort to anomaly detection to explore possible unusual phases in skyrmion systems. In order to this, we train two techniques (PCA and Convolutional Autoencoders, CAE) to process an analitically generated ("artificial") skyrmion crystal dataset. Then, we use the trained algorithms on spin configurations obtained through Monte Carlo simulations from different ferromagnetic skyrmion models at different temperatures under magnetic fields, and calculate the root mean squared error (RMSE) between the input and output snapshot. We find that both the mean value and the deviation of the RMSE from the data reconstructed with the CAE may be used to distinguish between three typical phases found in skyrmion systems (helices, skyrmion crystals and ferromagnetic), and, most importantly, to

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detect possible exotic orderings, such as bimeron glasses at higher magnetic fields [35]. We also apply the trained CAE to snapshots from two antiferromagnetic models, and explore what information may be obtained from the RMSE.

The manuscript is organised in the following way. In Sec. II we go over relevant characteristics from magnetic skyrmions, and describe the ferromagnetic skyrmion models chosen in this work. The ML scheme and details on the dataset and the algorithms are given in Sec. III. We discuss our results in Sec. IV, where we also consider other antiferromagnetic models, and present conclusions and perspectives in Sec. V.

II. BRIEF OVERVIEW ON SKYRMIONS AND SPIN MODELS

Magnetic skyrmions are an arrangement of spins characterised by the topological charge, defined as $Q = \frac{1}{4\pi} \int d^2 r \vec{S} \cdot (\partial_x \vec{S} \times \partial_y \vec{S})$; \vec{S} are the spin unit vectors, with promising technological applications due to their robustness, stability and easy manipulation. A large number of materials and models have been shown to host skyrmions and skyrmion like textures (such as antiferromagnetic skyrmions [36, 37], magnetic bubbles, antiskyrmions [38–40], merons [41], etc). A skyrmion crystal or lattice in a bidimensional system is a periodic arrangement of skyrmions and may simply parametrised as the superposition of three non-coplanar helices [7, 42]; the spin parametrization s_{SkX} at position **r** is given by :

$$s_{SkX}(\mathbf{r}) = \frac{1}{s} \left(\sum_{\mu=1}^{3} \sin\left(\mathbf{q}_{\mu} \cdot \mathbf{r} + \theta_{\mu}\right) \mathbf{e}_{xy,\mu} + \left(1 \right) \\ \left[\sum_{\mu=1}^{3} \cos\left(\mathbf{q}_{\mu} \cdot \mathbf{r} + \theta_{\mu}\right) \mathbf{e}_{z,\mu} + m_0 \right] \right)$$

where s normalizes $|s_{SkX}(\mathbf{r})|$ to 1, m_0 is the homogenous contribution to the magnetization in the z direction, arbitrary unit vectors in the xy plane $\mathbf{e}_{xy,\mu}$ satisfy $\sum \mathbf{e}_{xy,\mu} = 0$, and θ_{μ} are the phase factors that fulfill $\cos\left(\sum_{\mu} \theta_{\mu}\right) = -1$. The \mathbf{q}_{μ} vectors are the three ordering vectors of the helices, that lie in the same plane at 120°, with norm $2\pi/r_0$, r_0 being the skyrmion radius.

The structure factor, which is the Fourier transform of the spin-spin correlations, of this type of arrangement gives six bright peaks, corresponding to the three inequivalent q ordering vectors. Thus, a "triple-q" pattern in reciprocal space is a strong suggestion that a skyrmion lattice is present, as measured first in bulk MnSi [43]. Another parameter that may be calculated in a discrete lattice is the scalar chirality, the sum of the triple product of neighbouring spins (i, j, k) forming a triangle $\chi = \frac{1}{N} \sum_{i}^{N} \vec{S}_{i} \cdot (\vec{S}_{j} \times \vec{S}_{k})$. This quantity is the discrete version of the topological charge, which is

|Q| = 1 for skyrmions [7]. Therefore, for a given arrangement of spins, a non zero value of the chirality may be an indicator of skyrmions, regardless of whether they are organized periodically or not.

As was introduced in [44], a possible simple model to realise these periodic skyrmion arrangements in a bidimensional lattice is one where ferromagnetic nearest neighbors coupling competes with antisymmetric inplane Dzyaloshinskii Moriya (DM) interactions under an external magnetic field:

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \sum_{\langle i,j \rangle} \vec{D} \cdot (\vec{S}_i \times \vec{S}_j) - \vec{B} \sum_i \vec{S}_i \quad (2)$$

here the magnetic moment or spin \vec{S}_i is a three dimensional unit vector (Heisenberg spins) at site i, J = -1is the exchange coupling, \vec{D} the in-plane DMI along the bonds of the chosen lattice $(\vec{D} = \vec{D}^{xy})$, with absolute value D^{xy} , and $\vec{B} = B\vec{z}$ an external magnetic field perpendicular to the lattice plane. At low temperatures and no external field a helical order is found. Under an increasing external magnetic field, a skyrmion crystal is stabilized, and then at higher fields all spins are aligned with the field giving rise to a ferromagnetic or field polarized phase. Intermediate phases are enhanced with temperature: a bimeron phase at lower fields, as helices are distorted into skyrmions, and a skyrmion gas at higher magnetizations, where skyrmions are stabilized in a non-periodic arrangement [44, 45]. The inclusion of additional interactions may imply deviations from this simple scheme. For example, it has been shown that an increasing additional in plane site anistropy may take the skyrmion lattice to an arrangement of merons, which are topological structures with half the skyrmion topological charge [41], and more complex phase diagrams may also be found in models with frustrating exchange interactions and no DMI [46, 47].

Since we aim to explore techniques that may detect exotic phases, we focus on three models. First, we take the Hamiltonian from Eq. (2) in two triangular based lattices: triangular and kagome, which may itself be devided into three triangular lattices formed by the three types of spins in each elementary plaquette. Then, as a third model we take the Hamiltonian from Eq. (2)in the kagome lattice and include an out-of-plane DMI $(\vec{D} = \vec{D}^{xy} + \vec{D}^z)$ at the specific value $D^z = \sqrt{3}$. The combination of this out-of-plane D^z and in plane D^{xy} gives rise to several exotic phenomena, most notably a stabilization of a skyrmion gas at higher temperatures, which preceds the formation of a skyrmion crystal, and a "bimeron glass" phase at higher magnetic fields and lower temperatures, between the skyrmion crystal and the fully polarized phase [35, 49]. Here, we will show that it may be possible to detect these phases using unsupervised machine learning techniques, without inspection of the snapshots.

In Table I we list these three different spin models.



TABLE I. Three ferromagnetic spin models used in this work, with nearest neighbor exchange (J) and Dzyaloshinskii Moriya interactions (DMI). The blue arrows indicate the in-plane DMI (with strength D^{xy}) and the circles indicate the direction of the out-of plane DMI (D^z) . The rows show a sketch of the lattice, the value of the exchange interaction (which in this case is always J = -1, ferromagnetic), and of the in-plane and out-of-plane DMI strengths.

We label the one in the triangular with ferromagnetic exchange coupling and in-plane DMI along the bonds TFDM^{xy}. In analogy, the same model but in the kagome lattice is named KFDM^{xy}. Finally, the KFDM^z spin model is as the KFDM^{xy} with additional out of plane DM, D^z . Notice that J is fixed to -1 in all three spin models, but the D^{xy} is larger for the triangular lattice. This is simply so that the radius of the resulting skyrmions be similar to that of the KF spin models.

III. MACHINE LEARNING SCHEME AND DATASET

In this work, we resort to the technique known as anomaly detection to obtain information from skyrmion models, such as if it is possible to distinguish different phases and/or to detect exotic ones. The anomaly detection technique is usually described to detect events such as fraud or spam [50], or new trends in a time series [23]. Simply put, the main idea is that the large amount of "regular" data may have certain general characteristics, that the algorithm must "learn", and that points that deviate from this, "outliers", may be worth looking into. Here, we will consider skyrmion lattices as the "regular" data, and analyze what possible information may be obtained from anomalies or deviations.

In order to do this, we will train two types of algorithms, Principal Component Analysis (PCA) and a Convolutional AutoEntonder (CAE), to reconstruct a set of different skyrmion lattices. Then, we apply the trained algorithm to spin configurations obtained from Monte Carlo simulations of different skyrmion hosting models, and calculate the root mean square error (RMSE) between the reconstructed configuration and the original one. Since the algorithms are trained for skyrmion crystals, a bigger error would imply that the spin arrangement is further from a skyrmion lattice.

The RMSE is calculated as:

$$RMSE = \sqrt{\frac{1}{N} \sum_{i}^{N} \left(S_{i}^{z} - \tilde{S}_{i}^{z}\right)^{2}}$$
(3)

where S_i^z is the component along the magnetic field at site *i* of the input data, and \tilde{S}_i^z is that of the output (or reconstructed) data. Here, as was done before [11, 15], we only consider the S^z projection of the spins (renormalized to take values between 0 and 1), which reduces significantly the volume of data. This may also be interpreted as taking the spin configurations as images, and thus this work may be potentially applied to experimental images obtained with spin-polarized scanning tunneling microscopy techniques [44, 51–53].

For the CAE outputs, we have also calculated de binary cross entropy (BCE) [22], defined as:

$$BCE = -\frac{1}{N} \sum_{i}^{N} \left(S_{i}^{z} \log\left(\tilde{S}_{i}^{z}\right) + (1 - S_{i}^{z}) \log\left(1 - \tilde{S}_{i}^{z}\right) \right)$$

$$\tag{4}$$

The BCE is a quantity usually used as a loss variable to train machine learning algorithms, such as autoencoders. In the results section, we will show that, for the chosen models, in general resorting to the BCE to use the anomaly detection approach does not provide as much information as the use of the RMSE.

In summary, we consider the following scheme:

- 1. We train two types of algorithms, PCA and CAE, with a set of different skyrmion lattices.
- 2. We apply the trained algorithm to spin configurations obtained from Monte Carlo simulations of different skyrmion hosting models, and calculate the root mean square error (RMSE) between the decoded configuration and the original one.
- 3. We study the behaviour of the RMSE and BCE for different parameters and comparing models, to evaluate whether we may obtain information on the physics of each model, and explore the possibility of using this technique to find exotic phases in skyrmion-hosting systems.

Below, we describe in detail the dataset used to train the algorithms, the dataset obtained from the simulations, and give details on the ML models used.

A. Training dataset

We construct "artificial" skyrmions cristals in triangular lattices with 48×48 sites, following the parametrization presented in Eq. (1). We take 7 possible values for the skyrmion radii r_0 and 10 values of the parameter m_0 , which after normalization changes the magnetization of the lattice. Since in our analysis we will be using snapshots from MC simulations as images, in this constructed dataset we do not require periodic boundary conditions, but we must take into account rotations and translations of the parametrization pattern, which we do considering 8 possible rotations and 3 different translations in the position along the 3 directions of the nearest neighbors bonds of the triangular lattice. Therefore, we have a training and validation dataset of $7 \times 10 \times 8 \times 3 \times 3 = 5040$ different skyrmion crystals in triangular lattices.

B. Monte Carlo simulations dataset

We performed Monte Carlo Metropolis-Hastings simulations, combined with microcanonical updated (overrelaxation) on the three spin models described in the previous section: (1) TFDM^{xy}: a ferromagnetic exchange and in plane DMI model in a 48×48 triangular lattice under a magnetic field, fixing $D^{xy}/|J| = 1$ (2) KFDM^{xy}: a similar model in a $3 \times 48 \times 48$ kagome lattice, for $D^{xy}/|J| = 0.5$ (3) KFDM^z: the model presented in Eq. (2) including an out of plane Dzvaloshinskii-Moriva interaction $D^z = \sqrt{3}$. Simulations were done using periodic boundary conditions, and lowering the temperature from high temperature in 80 steps using the annealing technique. Up to 10 copies with independent seeds were done for each model and magnetic field. To apply the algorithms to the kagome snapshots, we chose one of the three sublattices (each one corresponding to the three types of sites in the kagome lattice, numbered 1, 2, 3 in Table I), so as to work with a 48×48 snapshot.

C. Algorithms

Here we give details on the two algorithms used in this work: Principal Component Analysis (PCA) and Convolutional Auto Encoder (CAE).

1. Principal Component Analysis

Principal Component Analysis [22, 23] is an algorithm usually used for dimensionality reduction. The idea is to find the hyperplane that is closest to the dataset, and project the data onto it. The different principal components are the succesive axes where the variance is preserved, and there are as many as the dimension of the dataset. Dimensionality reduction to n dimensions is done projecting the first n principal components. The number of such components may be chosen as to obtain a large enough accumulated variance, which is the sum of the dataset's variance that lies in each of the ncomponents. We chose to decompose the 5400 snapshot dataset in n = 500 principal components, using a Gaussian kernel, where the 99% of the variance is accumulated. In some studies, the two first principal components are used to explore and analyse the data. Here, we take the PCA with d = 500 components that was trained with the skyrmion lattice dataset and use it to reconstruct snapshots obtained from simulations for different models, temperatures and magnetic field. Then, we calculate the root mean square error between the input snapshot and the output one, as Eq. (3), and explore whether this error may give us information on the physics of the models. Calculations were done using the SciKit Learn Python package [54].

2. Convolutional Autoencoder

Autoencoders (AE) are algorithms where the data is compressed or encoded into a lower dimension space (called latent space) and then it is decompressed or decoded [23]. If the decoded data retains the most relevant features of the input data, which may be measured with some quantity, then the AE has performed satisfactorily. Moreover, the compressed data in the latent space may be used for a certain application instead of the input data, with the advantage that it occupies less memory. Thus, one of the uses of AE is called "data reduction". However, AE has other uses; for example, since spurious features are removed in the process, the output data is "cleaner", and the AE may be used as a "denoiser".

In our work, we will use the "anomaly detection" approach. The idea is to train an AE for a given type of data, and then apply it to a larger dataset, comparing the input and the output with a convenient variable, such as the root mean square error. If the error is small, then the input and output are similar, if it is large, then the input data may not be of the same type as that used in training the AE, so a larger error signals an anomaly. As in the PCA, we will use the artificial skyrmion lattice dataset to train a convolutional autoencoder (CAE - an AE with a convolutional layer), measuring the RMSE. In this case, 80% of the data were used for training and 20% for validation. The RMSE for the trained CAE was 0.00071 in the training set and 0.00073 in the validation set.

The structure of the CAE is the following: the encoder consists of one convolutional layer with activation function 'relu', filter size 3 and padding 'same', followed by a MaxPooling layer with filter size 2 and padding 'same'. The decoder consists of a convolutional layer, with the same carachteristics as the first one, and an UpSampling layer. It finalizes with a convolutional layer with one filter of size 3, a sigmoid activation function and padding 'same'. The CAE was trained and validated with batch size 64, using early stopping for a maximum of 300 epochs with a patience of 10. Implementation of the CAE was done in TensorFlow using Keras [55, 56].

IV. RESULTS AND DISCUSSION

In this section, we present the analysis of the comparison between the input and output data for the MC snapshots obtained when applying the PCA and CAE algorithms that were trained with the artificial set of triple-q skyrmion lattices. We start in Subsec. A focusing on the three ferromagnetic models introduced in Sec. II (Table I). Then, we will explore whether the anomaly detection technique using the same skyrmion-lattice trained CAE is able to provide some insight in two different antiferromagnetic models, which we will describe in Subsec. B.

A. Application to ferromagnetic skyrmion models

First, we compare the RMSE obtained for both algorithms for the $TFDM^{xy}$ snapshots. In order for the method to work, we would expect the RMSE to be lower at the skyrmion lattice phase, which is found at intermediate magnetic fields and lower temperature, and higher in the other phases, such as the low field helical phase at lower magnetic fields, or the high temperature paramagnetic phase. In Fig. 1, we present a series of examples comparing the input Monte Carlo snapshot with the output (decoded) snapshot after applying trained PCA and CAE. The first four rows correspond to the low temperature snapshots, for four phases that arise as the magnetic field B is increased: helical, skyrmion lattice, skyrmion gas and ferromagnetic. At first glance, the low temperature decoded images seem very close to the input ones, both for PCA and CAE, even for the helical and the ferromagnetic cases, which are types of configurations that were not used to train the algorithms. In these examples, the RMSE (indicated in each decoded image) for PCA is even lower in the helical and ferromagnetic cases than in the skyrmion lattice. This is not ideal, since we are proposing to use a larger RMSE as an indicator that the system is further from an ordered skyrmion phase. However, there is a significant difference in the output images at higher temperatures, illustrated in the last row of Fig. 1 for a snapshot in the paramagnetic phase: both the PCA and the CAE have a significantly higher RMSE.

To further explore and quantify whether the RMSE obtained with PCA or CAE is a useful tool to distinguish between the low temperature phases, in Fig. 2 we present these RMSE as a function of the external magnetic field B at the lowest simulated temperature for the TFDM^{xy} model (T = 0.0009). The curves are averaged over 10 independent copies, and the error bars are calculated as the standard deviation. The background color in Fig. 2 are a guide to the eve and indicate three type of phases: a helical phase, a skyrmion phase (which includes skyrmion lattices and skyrmion gas) and a ferromagnetic or field polarized region. We also present the absolute value of the scalar chirality χ (scaled by a factor for better comparison), the MC calculated parameter that distinguishes between the different phases: it is zero at low field in the helical case, goes up significantly where the skyrmion lattices are stabilized, gets lower as these lattices go into a skyrmion gas with increasing magnetic field, and finally is zero when all spins are aligned with the external field. Let us recall that the chirality cannot be "learned" by the algorithms, since in this proposal only the z spin component is used for training.

As for the RMSE calculated from the output images of both algorithms, it can be seen that the RMSE from PCA is in fact lowest for the ferromagnetic phase, highest



FIG. 1. Examples of MC Snapshots and their corresponding decoded counterparts using the trained PCA and CAE for a simple ferromagnetic model in the triangular lattice (TFD M^{xy} in Table I).

for the skyrmion gas, and, within the error, does not significantly distinguish between the helical and skyrmion lattice phases. On the other hand, the RMSE obtained comparing the MC snapshots and the CAE decoded ones



FIG. 2. Different variables as a function of the external magnetic field B at the lowest simulated temperature for simple ferromagnetic skyrmion model in the triangular lattice (TFSM^{xy}): RMSE obtained comparing the MC input and the PCA and CAE outputs, BCE calculated from the CAE outputs and the absolute value of the scalar chirality $|\chi|$ obtained from the MC simulations. BCE and $|\chi|$ are scaled by a factor of 0.2 to for comparison. The errorbars are the standard deviation of the quantities averaged over 10 independent copies. The background colors are a guide to the eye to indicate the three main phases of this model.



FIG. 3. RMSE from CAE, scalar chirality χ and magnetization M from MC simulations as a function of the external magnetic field B at the lowest simulated temperature (T = 0.0002) averaged over 10 copies for two ferromagnetic skyrmion models in the kagome lattice: one with only in-plane DMI (KFDM^{xy}, left panel) and one with an additional out of plane DMI with the specific value $D^z = \sqrt{3}$ (KFDM^z, right panel). The background colors are a guide to the eye to indicate the three main phases of the simple skyrmion models, and the region where an exotic one emerges in panel (b).

shows a more interesting behaviour, clearly distinguishing three regions: a low field one with higher RMSE, corresponding to the helical phase, an intermediate one with the lowest values (the skyrmion phases), and then a third region where the RMSE goes slightly but noticeably up with B and flattens at the ferromagnetic phase. We also present the binary cross entropy curve for the CAE. The BCE (scaled by a factor for better comparison) also seems to distinguish between these three regions, showing an abrupt change as the system enters the skyrmion phases, but it is lowest in the ferromagnetic phase, and not in the skyrmion region, where the CAE was trained. Therefore, we choose the RMSE from the CAE to apply the anomaly detection technique in other models. As a comment, a closer inspection of the RMSE curve also suggests that the RMSE error may also be a useful variable, an idea we will shortly come back to.

Having chosen our variable, the RMSE between the MC input snapshot and the decoded output from the trained CAE, we now apply the CAE to the other two ferromagnetic skyrmion models, both in the kagome lattice with in-plane interactions (KFDM^{xy}), and one with an additional out of plane DMI (KFDM^z) (see Table I). We plot the RMSE and show the MC chirality [57] and magnetization as a function of magnetic field at the lowest simulated temperature for both models in Fig. 3, where all curves are normalised to 1 to qualitatevely compare the behaviours. For the KFDM^{xy}, left panel, the behavior is very similar to the triangular lattice case. However, for the KFDM^z model, before flattening in the ferromagnetic phase, the RMSE goes clearly up. In the MC variables this is connected to a jump in the magnetization, but no significant differences are seen in the chirality, which is the order parameter connected to the skyrmion phases. Thus, the RMSE suggests that there is a different phase at higher magnetic fields, for $B \sim 0.13 - 0.14$. Inspection of the snapshots reveals this is indeed the case; an example is shown in Fig. 4, top row. It is an unusual high field bimeron + skyrmion phase, with possible glassy behaviour [35]. Regardless of the nature of the ptextures, the RMSE indicates that at higher fields the $KFDM^{z}$ presents a different phase than the other two ferromagnetic models. We compare the mean value and the standard deviation of the RMSE as a function of the external field for the three models in Fig. 5. In the plot, B is scaled for the TFDM^z model, but the RMSE is not. From the comparison, it is clear that the RMSE is quantitavely and qualitatevely very similar in the three models in three regions (corresponding to helices, skyrmions and ferromagnetic), but evidently there is an exotic phase for the KFDM^z case before the system goes into the ferromagnetic phase. The jump of the RMSE for this model in this region is not seen in the other two cases, strongly supporting the idea that in that region of B the system goes into a different type of ordering.

The KFDM^z model has been shown to have several exotic behaviors, due to the competition between skyrmion and chiral spin liquid physics [35, 49]. Besides the



FIG. 4. MC Snapshots and their corresponding CAE decoded counterpart for the skyrmion model in the kagome lattice with an additional out of plane DMI (KFDM^z, see Table I) at two different high field phases: a low temperature "bimeron glass" phase (top row) and an intermediate temperature skyrmion gas (bottom row).



FIG. 5. Mean value (left panel) and standard deviation (right panel) of the CAE RMSE as a function of magnetic field for the three ferromagnetic skyrmion models introduced in Table I (the magnetic field for the triangular lattice case was scaled to facilitate the comparison) at the lowest simulated temperature.

"bimeron glass" above mentioned, for the value of D^{xy} chosen here, it has been shown that, coming from the high temperature paramagnetic phase, the skyrmion lattice is formed by the discrete emergence of skyrmions at intermediate temperatures, forming a skyrmion gas that gets more densely populated as the temperature is lowered. We compare the RMSE and BCE as a function of temperature for the two ferromagnetic kagome skyrmion models, at three different values of the magnetic field B = 0.03, 0.09, 0.13. In panels (a) and (b) it can be seen that for the KFDM^{xy} model both RMSE and CAE go down smoothly with temperature. The BCE is smaller for higher fields, but the RMSE is similar for both B = 0.09, 0.13. This is simply due to the fact that for this model at those magnetic fields the system is in a



FIG. 6. RMSE and BCE as a function of temperature for three magnetic fields B = 0.03, 0.09, 0.13 for the two skyrmion ferromagnetic kagome models, with in-plane DMI, KFDM^{xy} (panels (a,b)) and with in-plane and an additional out of plane DM, KFDM^z (panels (c,d))

skyrmion crystal phase (see Fig. 3, left panel). The variables hint a different physical process for the $KFDM^{z}$ model. At B = 0.13, both the RMSE and BCE abruptly go up at intermediate temperatures, a feature which is much sharper in the BCE curve. As discussed in previous works [35, 49], for this B the KFDM^z model goes through an skyrmion gas phase at intermediate temperatures, with a field polarized chiral spin liquid background. Since this type of phase is better decoded by the CAE than the bimeron glass phase, the BCE and RMSE are smaller. This type of intermediate phase is also present at B = 0.09, which is seen as a small well before the "bump" in the BCE curve. We show an example MC snapshot in this phase and its decoded image in Fig. 4, bottom row. Since the temperature is higher and the background is a polarized chiral spin liquid, it can be seen that it is not completely aligned with the field (i. e. the bakcround is not completely red). On the other hand, this changes when decoding the image with the CAE, where thermal fluctuations are smoothed. This is related to the potential "denoising" use of convolutional autoencoders, showing that these algorithms, if needed, may also be considered as tools to "erase" fluctuations and better define structures such as skyrmions.

As a summary, we present a comparison of the B-T phase diagrams of the (third nearest neighbor) chirality, RMSE and BCE from CAE for the two kagome models, in Fig. 7. For both models, we first see that the RMSE and BCE are higher at higher temperature, as expected. Then, for BCE, at the lower temperatures it goes down



FIG. 7. Phase diagrams for the chirality obtained from simulations, RMSE and BCE from CAE, for the two skyrmion ferromagnetic kagome models, with in-plane DMI, KFDM^{xy} (top row) and with in-plane and an additional out of plane DMI, KFDM^z (bottom row)

with magnetic field and is lowest when the system is in the field polarized phase, and it does not seem to easily distinguish the lower field phases. However, at intermediate temperatures we see a particular behaviour for the $KFDM^z$ case: a drop in the BCE, which matches the chiral spin liquid region [35, 49]. As for the RMSE, in the $KFDM^{xy}$ model at lower temperatures it distinguishes between three regions, with a higher value at lower magnetic field (corresponding to helices and bimerons), lowest values at intermediate magnetic fields (skyrmions phase) and then goes a bit up at higher fields, in the field polarized region. An important difference is observed for $KFDM^z$: a small region at higher field where the RMSE goes up again, between the skyrmion lattice phase and the field polarized one. This is another exotic feature of this model, a higher field bimeron phase with potentially glassy characteristics [35], which is not evident inspecting the chirality. Thus, we see that the RMSE, and also BCE, are powerful tools to pinpoint regions in parameter space where a system may deviate from the "typical" skyrmion phase diagram. Given that we only analyse snapshots, this technique may be applied to real-space images, and provide helpful insight of a skyrmion system without resorting to designing a model and permorfing simulations.

B. Application to antiferromagnetic models

Although the CAE was trained on ferromagnetic tripleg skyrmion lattices, in this subsection we aim to explore whether this CAE may give some insight in two wellknown antiferromagnetic models in the triangular lattice, presented in Table II. For these models, the exchange interaction is antiferromagnetic (J = 1), which implies a frustrated system due to the lattice geometry. In the first model, $TAFDM^{xy}$, there are in-plane DMI $(D = D^{xy} \neq 0)$. It has been shown that under a magnetic field, at finite temperature an antiferromagnetic skyrmion lattice formed by three interpenetrated sublattices is stabilized [36], a texture that has been shown to be stabilized in other frustrated models [40, 58, 59], and connected to the fractional antiferromagnetic skyrmions in $MnSc_2S_4$ [37, 60]. As a second model we consider the pure exchange antiferromagnetic model (J = 1, D = 0), where the Hamiltonian may be rewritten as a sum of the total spin of triangular plaquettes. Under a magnetic field B , a notable feature of this model is that at $B \sim 3$ at finite temperature order-by-disorder (entropic selection) induces a pseudo-plateau at magnetization M = 1/3, where in each plaquette two spins are parallel to the external field ("up", u) and one is antiparallel ("down", d), and is thus known as a uud pseudo-plateau [61–63]. For lower fields, there is a coplanar "Y" state, and for higher fields a coplanar "V" state [61].

Clearly, the emergent antiferromagnetic low-temperature textures from these models are quite



TABLE II. Two well known antiferromagnetic (AF) models in the triangular lattice. Both have antiferromagnetic exchange interactions J = 1, one has in-plane DMI (TAFDM^{xy}) and the other one is the pure exchage model (TAF)

different from the triple-q ferromagnetic skyrmion lattices, and thus a significantly larger RMSE is expected. To explore whether some information on these models may nonetheless be extracted with the skyrmion-trained CAE, we proceed as before: we apply the CAE to low temperature snapshots obtained from MC simulations of both models, and calculate the RMSE and the BCE.



FIG. 8. RMSE and BCE calculated after applying the CAE and chirality from MC simulations as a function of the external magnetic field B at the lowest simulated temperature (T = 0.0009) for TAFDM^{xy} (panel (a)) and the TAF (panel (b)) models. In both panels, the shaded background colors are guides to the eye to indicate the different phases. Comparison of the CAE (panel (c)) and BCE (panel (d)) as a function of B for the three models in the triangular lattice: the ferromagnetic skyrmion model TFDM^{xy}, the antiferromagnetic skyrmion model TAFDM^{xy} and the pure exchange antiferromagnetic case TAF. B^* indicates that for a better comparison, the magnetic field in the x-axis was scaled for the TFDM^{xy} curves.

In Fig. 8 (a) and (b) we show the RMSE, BCE and chirality χ as a function of the external field *B* for the TAFDM^{xy} and TAF models, respectively, at the lowest

simulated temperature T = 0.001). In the TAFDM^{xy} case (panel (a)), the RMSE and the BCE are relatively flat at lower B and present a sharp decrease at $B \sim 2$, which matches the jump in the chirality χ associated with the stabilization of the AF skyrmion lattice. Then as B is increased both quantities go down, and the curves get steeper when χ drops to zero. Although the behaviour of the RMSE and the BCE is similar, the features in the RMSE are sharper than for BCE, particularly the steep drop at lower field. So, in this case, the RMSE shows that there is a first type of phase up to $B \sim 4$, where the RMSE starts to drop until it flattens at its minimum value at higher fields, associated to the ferromagnetic phase, with all spins aligned with B.



FIG. 9. Example of MC Snapshots and their corresponding CAE decoded counterparts for the skyrmion model in the antiferromagnetic triangular lattice at low temperature (TAFDM^{xy}, top row) and the pure exchange antiferromagnetic model in the triangular lattice (TAF, bottom row).

The BCE and RMSE curves are quite different for the TAF case (panel (b)): the BCE goes down with increasing magnetic field, presenting a small kink at $B \sim 3$, the pseudo-plateau magnetic field. On the other hand, the RMSE curve has two clearly distinct regions, separated at $B \sim 3$: a low magnetic field region where the RMSE goes up, and a higher field region where it goes down, presenting thus a peak at $B \sim 3$. Therefore, even if, as expected since the CAE was trained for skyrmion lattices, the obtained RMSE values are quite large, the RMSE calculated after applying this CAE to the MC snapshots indicates that there are two types of phases at lower and higher field, and that there is a particular feature in the TAF model at $B \sim 3$.

Panels (c) and (d) show the RMSE and BCE curves, respectively, for these two AF models and the simple ferromagnetic skyrmion model (TFDM^{xy}; here the magnetic field *B* has been rescaled for a better comparison of the magnitude and characteristics of the curve). As expected, the magnitude of both quantities, particularly RMSE, is significantly larger for the antiferromagnetic models. The three RMSE curves, contrary to the BCE ones, have different characteristics, showing that the three models have different types of phases. The kinks and jumps in the three curves are also indicators of the different phases within each model.

Finally, in Fig. 9 we show the input and output of a low temperature snapshot in each AF model. The first row corresponds to a three-sublattice antiferromagnetic skyrmion crystal (TAFDM^{xy}) and the second one to the pseudo-plateau at M = 1/3 in the pure exchange model (TAF). Clearly, in both cases the decoded image is quite different from the input one. This is due to the fact that the CAE was trained with perfect ferromagnetic skyrmion sizes, where the textures are smoothly modulated, and here it is applied to two snapshots where there is an abrupt change in the texture at nearest neighbor distances, given the antiferromagnetic nature of the models. The RMSE is largest at the *uud* pseudo-plateau, which is completly washed away by the CAE, trained for more "coarse-grained" textures.

V. CONCLUSIONS

In this work we propose the use of the anomaly detection technique to explore skyrmion phase diagrams. We trained two types of algorithms, Principal Component Analysis and Convolutional Autoencoder, with a data set of analytically generated skyrmion lattices. Our main idea was to compare input configurations, obtained with Monte Carlo simulations from a given model, with the decoded (output) snapshot generated when applying these algorithms to the input data. A large deviation from the original MC data would imply that the chosen configuration is "further" from a skyrmion lattice. To quantify the difference between the input and output snapshots, we calculated the Root Mean Square Error for both PCA and CAE, and the Binary Cross Entropy for CAE.

First, we chose a simple and well known skyrmion model in the triangular lattice, one that combines ferromagnetic exchange and in-plane Dzvaloshinskii-Moriva interactions under an external magnetic field. At low temperature and low magnetic field, helices are stabilised. As the field increases, a skyrmion lattice is formed, which then gives place to a skyrmion gas until the spins are completely polarized. Comparing the RMSE from PCA and CAE, we found that for PCA the lowest RMSE was found for the ferromagnetic phase, and that, within the errorbars, it was not possible to distinguish between the helical and the skyrmion phases. On the other hand, the CAE RMSE showed a clear distinction between these three main phases, and was lowest in the skyrmion region, which is essential for out proposal. Surprisingly, the RMSE is not very large for helical and ferromagnetic phases, and the decoded snapshots are quite close to the input ones. We also compared the behaviour of the RMSE and the BCE. Although the BCE may be able to separate between the low temperature regions of this model, it monotonically goes down with the magnetic field, and thus is minimum for the ferromagnetic snapshots.

Secondly, we applied the CAE to two models in the kagome lattice, the well known skyrmion model we had simulated in the triangular lattice, and one where an additional out-of-plane DMI is included. As expected, the behaviour of the RMSE in the first case (only planar DMI) is similar to that in the triangular lattice. However, in the second case (with both planar and out-ofplane DMI) there is a clear region at low temperature and higher fields where the error raises, indicating the possibility of a different type of phase. In fact, previous studies in this model [35] show that there is a high field bimeron glass phase. Moreover, this model also has a variety of phases at higher temperature, which is reflected in both the RMSE and BCE. Our analysis also suggests that the spread of the RMSE, considering independent realizations for the MC data, may also be a tool to distinguish between different low temperature phases.

Finally, we apply the skyrmion-lattice trained CAE to snapshots from two models in the antiferromagnetic triangular lattice: one with in-plane DMI, where antiferromagnetic skyrmion lattices are stabilized, and the pure exchange model, which presents a well known *uud* plateau at M = 1/3. Given that the CAE is trained with ferromagnetic skyrmion lattices, a good decodification of the input data is not expected. Nonetheless, the low-temperature RMSE curves have features that suggest possible different phases. In particular, in the pure antiferromagnetic exchange model, the RMSE is maximum for values of the magnetic field where the pseudo-plateau emerges.

In conclusion, we have shown how the anomaly detection technique, which we have applied resorting to a very simple Convolutional Autoencoder trained with analytically generated skyrmion lattices and choosing the RMSE to measure the error between input and output data, may give relevant information on skyrmion systems. We have demonstrated that it was able to distinguish the three typical phases in a skyrmion phase diagram (helices, skyrmions and field-polarized spins), and to spot regions in parameter space where there may be exotic behavior. Additionally, we have seen how it may also hint the existence of different phases in other types of models. Thus, we expect our work to support and further promote the exploration and use of machine learning techniques in different magnetic models.

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