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Search for stable skyrmion lattices at the ground state in a multiferroic nanofilm using artificial neural networks

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Magnetoelectric nanofilms are of great interest as functional elements of ultra-dense memory cells. In the ground state they may contain various topological magnetic vortex structures of several nanometers in size. The qualitative and quantitative properties of such structures strongly depend on a set of physical parameters. To calculate the ground state configuration with given parameters, we use the steepest descent method. However, to study a large parametric space significant computational resources are required. To solve this problem, we propose the use artificial neural networks (ANN), which can help us uncover the relationship between combinations of parameters and the corresponding ground state configurations using a relatively small number of pre-computed configurations as the training data. The application of the ANN allows one to avoid excessive computational costs in the study of the parametric space and narrow down the parametric area in which the existence of stable non-trivial ground state configurations in the form of a stable skyrmion crystal is possible.

Keywords: artificial neural networks, skyrmions, ground state, frustrated models, magnetoelectric interaction.

1. Introduction

A significant progress in the development of mathematical modeling methods using neural networks in the theory of condensed matter makes it possible to improve and achieve serious acceleration in methods for studying physical properties of materials. The wide interest in neural networks has led to the emergence of a large number of methods and approaches to their study (software, biological, chemical, physical, etc.). A striking example of this is the construction of a neural network to represent the quantum wave function, proposed by Carleo and Troyer [1], which has become a significant event in the field of modeling complex systems of many interacting bodies [2 – 5]. In Ref. [6], the authors discuss a new method of deep machine learning for the tasks of selecting the parameters of a multilayer photonic structure according to a given optical spectrum of the reflection coefficient, which makes it possible to apply the developed high-precision method for designing the structure using the characteristics of the optical signal, thereby solving the inverse problem.

The use of neural networks allows us to hope for success in modeling frustrated systems and nanofilms, the alternative being statistical methods, which requires sufficiently large computational resources. It is worth noting, though, that serious efforts are currently made to search for alternative models of information processing with high energy efficiency by analogy with the activity of the human brain [5,7]. One of the possible implementations of this type of cognitive computing is "accumulative" computing networks built from non-linear recursively connected resistive magnetic elements. It was proposed in [7] that a network of skyrmions formed in a frustrated magnetic film is capable of providing a suitable physical implementation for applications of a cumulative computing network.

It should be noted that numerous experimental studies have revealed the skyrmion state in metallic ferromagnets that allow the Dzyaloshinskii-Moriya interspin interaction, such as FeGe [8,9], Fe monolayer on various compounds [10 –13] in a narrow range of external parameters, magnetic fields and temperature. Reducing the size of skyrmions, increasing their stability to room temperatures, as well as reducing energy consumption for controlling skyrmions are topical problems in spintronics. To overcome these difficulties, it is proposed to use artificial antiferromagnets (SAF) [14], in which two ferromagnetic layers are coupled antiferromagnetically through a nonmagnetic layer; calculations show that skyrmions in such systems will be smaller, more stable, and require less energy for manipulation [15,16]. Experimental phase diagrams of a number of materials indicate significant transition regions between different phases (including skyrmion and paramagnetic), which poses the problem of accurately determining the phase boundaries of skyrmions and, say, a spin helix. Artificial neural networks are successfully used in the identification of the magnetic phases of spin Hamiltonians, which are widely used to describe strongly correlated materials [5,17– 22]. In [5], machine learning approach was applied to recognize and classify complex noncollinear magnetic structures in two-dimensional materials. It is shown that a standard feed-forward network can be effectively used for supervised learning on topologically protected states of a magnetic skyrmion and a spin helix. Having trained such a network on a limited set of configurations belonging to pure ferromagnetic, skyrmion and spiral states on a square lattice, the authors managed to recognize states from completely different parts of the phase diagram, including transition zones between different phases. The proposed work demonstrates a method for training an artificial neural network for solving the inverse problem of designing a multilayer multiferroic in the form of a composite film with alternating magnetic and ferroelectric layers (see Fig. 1a) according to a given distribution of the skyrmion structure.

Due to the presence of several competing interactions, the coexistence of two or more types of ordering is possible in multiferroics in certain ranges of external fields and temperatures, including the appearance of topologically protected vortex nanoobjects [21–22].

This work is devoted to the search for such values of the interaction parameters and the intensity of external fields in a three-layer multiferroic film (Fig. 1a), at which nontrivial topological magnetic structures are stable in the ground state. To reduce the computational complexity of searching in the parametric space, we use the apparatus of artificial neural networks.

2. Model and ground state of a skyrmion crystal

We define the Hamiltonian of the simulated multiferroic as follows:

$$\mathcal{H} = -\sum_{i=1,9}\left[\vec{S}_i \cdot \left(J_m^1 \sum_{j1=1,6} \vec{S}_{j1} + J_m^2 \sum_{j2=1,6} \vec{S}_{j2} + J_m^3 \sum_{j3=1,6} \vec{S}_{j3} + \vec{H}\right) + \right. \\ \left. + \sum_{k=1,2} P_i^k \cdot \sum_{j1=1,6}\left(J_f P_{j1}^k + J_{mf} \vec{S}_i \cdot \vec{S}_{j1}\right)\right], \quad (1)$$

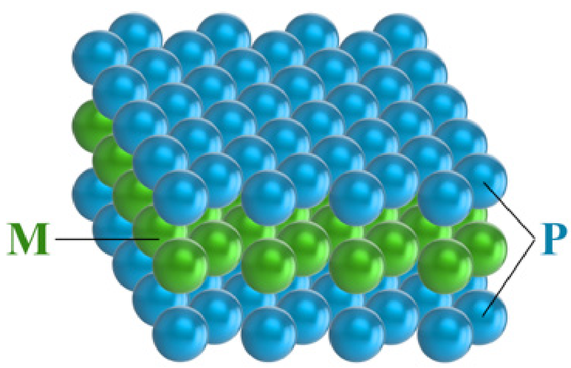
where J_m, J_f, J_{mf} are parameters of antiferromagnetic exchange, ferroelectric exchange and Dzyaloshinskii-Moriya magnetoelectric interactions, $\vec{S}_i$ — magnetic spin, P_t^k — electric dipole on layer k, $\vec{H}$ — external magnetic field. We will assume that both systems have hexagonal crystal symmetry and consider three exchange interactions in the magnetic subsystem: J_m^1, J_m^2, J_m^3 (Fig. 1b).

The ground state of magnetic subsystem is determined by the energy minimum described in Hamiltonian (1). Our task is to find such combinations of parameters for which nontrivial stable skyrmion-like topological structures arise in the ground state (an example of such a structure is shown in Fig. 2a).

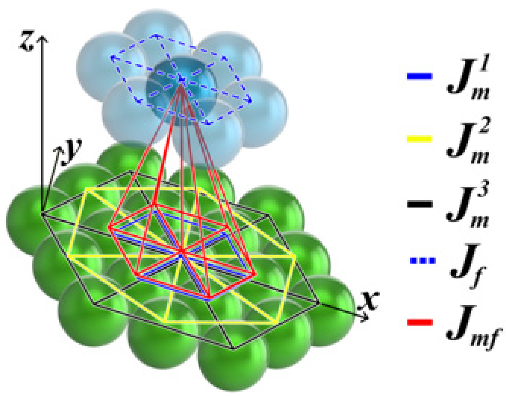
Search for the global minimum of the energy function with a large number of variables ($4N^2$ components of unit magnetic spins in the central magnetic layer and $4N^2$ one-dimensional electric polarization vectors in two outer ferroelectric films, where N is the linear size of a square nanofilm) is extremely resource-intensive task. For this research of a multiferroic nanofilm with hexagonal symmetry and three exchange interaction parameters we will consider the system of 400 cells, each cell contains only 9 spins and two layers of 9 local electric polarization vectors, applying periodic in-plane boundary conditions (Fig. 2b). This number of variables of the cell is quite small but it allows all nodes to interact with each other through different ranges while providing relevant information about ground states and quick search through parametric space (see Conclusions). In this study we consider a three-layer multiferroic film, each magnetic layer is coupled antiferromagnetically in-plane, and antiferromagnetically to both the one above and below with nonmagnetic layer. The three layer multiferroic film is a 180×180 nm square composed of 400 cells. These sizes were chosen to represent the typical lattice sizes of multilayer systems, which, as shown in the literature, contain skyrmions [15,16,7]. This number of variables is quite small but it allows all nodes to interact with each other through different ranges while providing relevant information about ground states and quick search through parametric space (see Conclusions).

3. Training and application of artificial neural network (ANN)

Calculating ground states for a large number of combinations of exchange parameters and the magnetic field requires significant computational resources, so we propose the ANN-based approach. ANN is a universal approximating blackbox function emulating biological neural structures which allows us to predict the ground state for specific parameters without directly calculating the minimum energy of the system. Before using it, we need to prepare a training sample of data by calculating ground states for randomly generated parameters (withing a region of [−1, 1] for each parameter). Each element of the training data consists of a pair of vectors: input (physical parameters) and output (ground state in the form of projections of magnetic spins

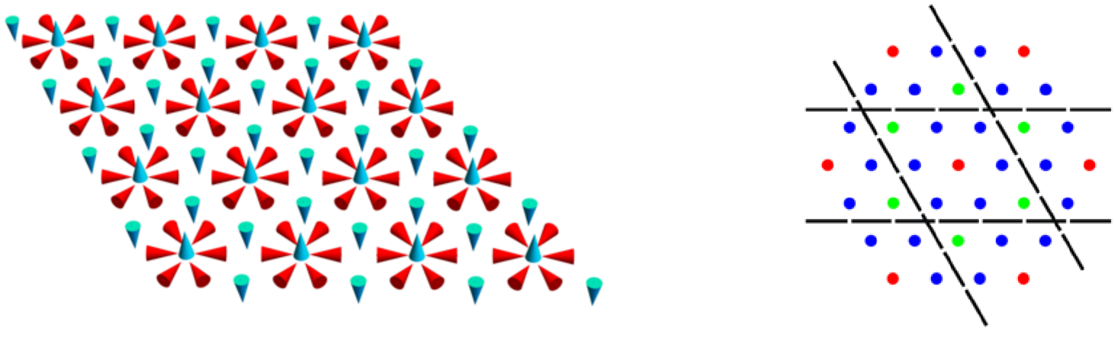


a



b

Fig. 1. (Color online) Composite multiferroic film consists of one magnetic (M) and two ferroelectric layers (P) (a), interaction scheme at the boundary of nanofilm layers (interface) (b).



a b

Fig. 2. (Color online) Skyrmion lattice of magnetic layer with hexagonal symmetry in the ground state (a) and the scheme of a cell (Red dotes indicate the central site, blue dotes — nearest neighbors, green dotes — next nearest neighbors) with 9 independent nodes and periodic boundary conditions (b).

and one-dimensional polarization vectors). We "train" the ANN with this data, training being a process of algorithmic search for internal parameters of ANN such that the error between the result of applying ANN to the input and the output is minimized. The huge advantage of using ANN for a search in high-dimensional parametric space (8 in our case) is that is evaluates output much faster than any optimization method, giving correct predictions for known inputs and approximating for unknown, thus offering an effective solution of the inverse problem of searching parameters corresponding to certain non-trivial ground state configurations that were not present in training data.

ANN takes an array as input (also called "input signal") and processes it in a certain way to yield an output array (or "output signal"). ANN is trained using training data, a combination of "input signal"+"output signal" of arbitrary dimensions. In our case input signal is a vector of $L_{in}=8$ parameter values, output signal contains 9 spin unit vectors (expressed as spherical angles θ, φ) and 2 layers of 9 ferroelectric scalars with a total of $L_{out}=36$ components. ANN consists of 3 or more "layers": input, output and one or more "hidden" layers which are sequentially organized (Fig. 3). Each layer receives a signal from the previous layer, processes it and passes to the next layer. Processing usually consists of applying a linear transformation $\widehat{W}$, adding a "bias" vector $\vec{B}$ and applying a nonlinear "activation" function σ to the result [23].

If layer i receives signal $\vec{a}_{i-1}$ it will pass signal $\vec{a}_i$ to layer $(i+1)$ given by:

$$\vec{a}_i = \sigma\left(\widehat{W}_i \vec{a}_{i-1} + \vec{B}_i\right). \quad (2)$$

Dimensions of weight and bias massives correspond to the number of components ("nodes") or the "width" of each layer. The set of elements $\left\{\widehat{W}_i, \vec{B}_i\right\}$ are internal parameters of ANN to be trained, i. e. changed in that way which minimizes the error of ANN predictions for given training data.

ANN training is based on the gradient descent method, in which ANN is viewed as a nested function with input signal X and internal parameters subject to training $\widehat{\Theta}=\left\{\widehat{W}_i, \vec{B}_i\right\}$ as arguments and output signal F as its value $F=F(\Theta, X)$. The "error function" C of ANN is usually calculated as standard deviation of predicted signal F from expected output Y: $C=\|F-Y\|_2$. Dependence of F on internal parameters $\widehat{\Theta}$ is known (2), so we can calculate the gradient of error function:

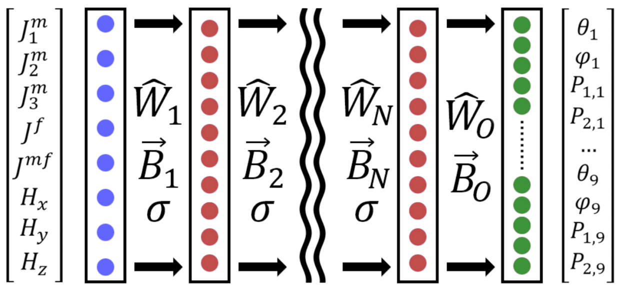


Fig. 3. (Color online) Structure of the ANN. The input layer is marked blue, the hidden layers are red, and the output layer is green.

$\vec{\nabla}C = \partial C/\partial\widehat{\Theta}_k$, thus we changing $\widehat{\Theta}$ in the opposite to gradient direction will lower error function:

$$\widehat{\Theta}^{t+1} = \widehat{\Theta}^t - \eta\vec{\nabla}C. \quad (3)$$

Formula (3) reflects one step of ANN training, where parameter $\eta>0$ is "learning rate". With large value of η error function oscillates around the minimum, while the very small learning rate guarantees slow and smooth approach to the local minimum, which may not coincide with the global one, so finding the optimal value for a particular training data requires some fine tuning.

4. Results of ANN application and discussion

We set initial magnetic configuration in the form shown in Fig. 2, initial values for ferroelectric layers to vacuum: P_{11}, P_{12}, …, P_{19}, $P_{29}=0$, and denote these initial states as SP_0. The search for stable solutions we start by generating random sets of parameters A_i in the range $[-1, 1]$ and minimizing the total energy $\mathcal{H}(A_i, SP_0)$ (1) by Newton method with as SP_0 first approximation. Obtained solutions SP_i are stable, but are not necessarily the ground states of the multiferroic for the parameters A_i. We have generated a total of 2^8 different solutions $\{A_i, SP_i\}$ as training data for the ANN. Then we choose such SP_i which has minimal Euclidean norm with initial state SP_0: $M_0=\|SP_i-SP_0\|_2$ and call corresponding parameters A_0. This allows us to stochastically search for stable states close to SP_0 in the parametric space while simultaneously retraining ANN according to following steps:

1. Generate sets of parameters $\{A_i\}$ as small random modifications to A_0, apply ANN to $\{A_i\}$ and calculate

the Euclidean norm between outputs and target state $\{M_i\} = ||F(\{A_i\}) - SP_0||_2$;

2. Find minimal M'_i, directly calculate stable state SP'_i for corresponding A'_i, add $\{A'_i, SP'_i\}$ to training data and retrain ANN;

3. Calculate norm $M'_0 = ||SP'_i - SP_0||_2$ and compare it to M_0: if $M'_0 < M_0$ then new state is closer to target state and we reassign, $M_0 \to M'_0$, $A_0 \to A'_0$.

This algorithm provides a quick search for certain stable states in parametric space, since each new element of the training data increases the accuracy of ANN prediction, which in turn increases the accuracy of searching, narrowing down the areas of desired parameters' values. A typical example of the obtained states is shown in Fig. 4.

This ANN-enhanced search allowed us to determine the ranges of parameter values (Table 1) which correspond to stable magnetic states with skyrmion lattice.

With increasing the magnitude of interface coupling J_{mf}, the spins form a magnetic vortex in the plane of the magnetic layer — a Neel-type skyrmion. A typical example (zoom of two skyrmions) of the obtained states is shown in Fig. 5. The results for radius of skyrmions are shown in Fig. 6 as a function of interface coupling J_{mf}. One can see that the radius of skyrmions increases when we increase the values of J_{mf}. In the region of the magnetoelectric interaction $J_{mf} \in (-0.7; 0)$ the radius of the skyrmions increases to 3 sites at $J_{mf} = -0.45$, and for $J_{mf} \in (0; 1.9)$ the radius of skyrmions the radius of skyrmions tends towards 5.8 atomic sites atomic units, and then the size of the skyrmions is reduced to zero.

Note that the nearest and second nearest neighbors' exchange parameters J_m^1 and J_m^2 are negative, which leads to frustration in magnetic layer, while negative values of J_f force the antiferroelectric ordering. It is also worth noting that the range of stable values of J_m^2 is much wider than that of other parameters, which hints at the weak dependence of stability on it. Third nearest neighbors' interaction J_m^3 doesn't significantly affect results, so it and farther exchange parameters can be ignored.

5. Conclusions

With the help of ANN we have built a relationship between combinations of multiferroic parameters and the corresponding ground state configurations using a relatively small number of pre-computed configurations as training data. The application of ANN allowed us to avoid excessive computational costs in the study of the parametric space and to find such parameters for which the existence of stable non-trivial ground state configurations in the form of a stable skyrmion crystal is possible. We show in this article that a lattice of skyrmions can be generated by the magnetic field applied perpendicularly to a multiferroic nanofilm with a hexagonal lattice. The skyrmion cristall stabilized by frustrated exchange interaction in a magnetic layer with perpendicular magnetoelectric interaction, which are important for practical applications based on the manipulation of skyrmions by the electric field.

The obtained results allow us to make certain observations about the studied model.

Table 1. Values of parameters corresponding to stable skyrmion lattices.

Parameter	Min. value	Max. value
J_m^1	−1.01	−0.903
J_m^2	−9.975	−0.954
J_m^3	−1.055	1.005
J_f	−1.007	−0.802
J_{mf}	−0.725	1.887
H_x	−0.5	0.5
H_y	−0.5	0.5
H_z	−1.0	1.0

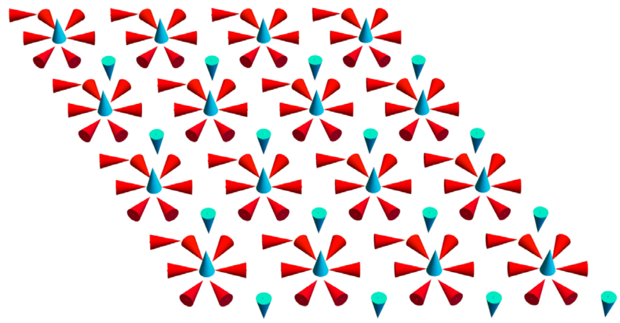


Fig. 4. (Color online) Stable state of the magnetic layer of a multiferroic with parameters $J_m^1 = -0.93$, $J_m^2 = -1.0$, $J_m^3 = -0.59$, $J_f = -0.97$, $J_{mf} = 0.14$, $H^z = 0.3$.

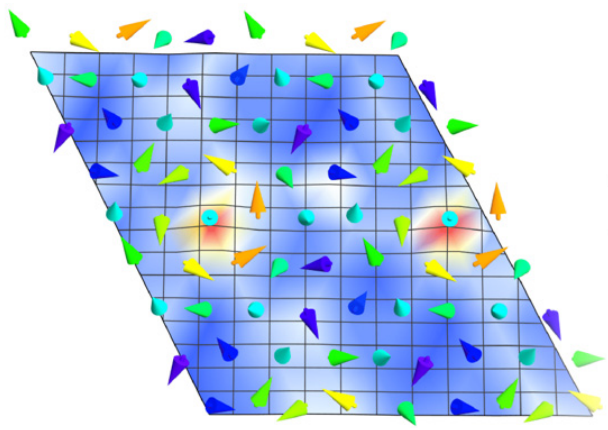


Fig. 5. (Color online) Stable state of the magnetic layer of a multiferroic with parameters $J_m^1 = -0.93$, $J_m^2 = -1.0$, $J_m^3 = -0.59$, $J_f = -0.97$, $J_{mf} = 1.14$, $H^z = 0.3$.

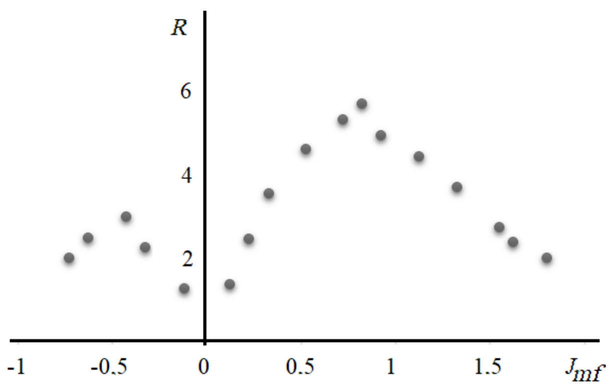


Fig. 6. Radius of skyrmions versus interface coupling J_{mf}. Here $J_m^1 = -0.93$, $J_m^2 = -1.0$, $J_m^3 = -0.59$, $J_f = -0.97$, $H_z = 0.3$.

1. The sign of magnetoelectric interaction J_{mf} does not affect skyrmion-like states due to its symmetry, which is broken only by external magnetic field $\vec{H}$. The considered model is interesting when the magneto-electric interaction is sufficiently large, in the order of the magnetic exchange interaction between nearest and next nearest neighbors. We note that this condition is realizable using the magneto-electric coupling in multilayer composed of magnetic layers separated by ferroelectric films. Let us mention a number of works showing strong and very strong magneto-electric coupling between the magnetic moments and the ferroelectric polarizations to justify the applicability of our model (see Ref. [19] and references cited in Ref. [12]). Very strong magneto-electric interactions at the interface leads to the disappearance of the phase transition in magnetic layers, unlike the case of simple cubic lattice where we observed at previous investigation very strong first-order phase transitions at large values of the interface coupling in form of Dzyaloshinskii-Moriya magnetoelectric interaction. The existence of skyrmions at the magneto-ferroelectric interface in the ground state in the absence external magnetic field is very interesting and may have practical applications in memory devices, data storage and spintronics.

2. The obtained values for external magnetic field $\vec{H}$ are very weak compared to other parameters and difficult to generate in real materials. Its stabilizing effect on vortical structures can be provided through magnetoelectric interaction with ferroelectric layers, which values linearly depend on easy to control external electric field. We note that ideal multiferroic memory cell could offer the possibility to electrically write the magnetic state. The realization of such devices requires an electrical control of magnetism.

3. Third nearest neighbors' J_m^3 interaction doesn't significantly affect results, so it and farther exchange parameters can be ignored. Note that the minimum required value of J_m^2 for stabilizing skyrmion lattice decreases with increasing the value of J_{mf} since J_m^2 and J_m^1 are antiferromagnetic exchange interactions that compete with magnetoelectric coupling.

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