Machine-learning Skyrmions

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Introduction: The basic idea behind teaching machine learning (ML) algorithm to recognize various phases of many-body systems, whether classical or quantum, is to input the many-body configuration together with an "answer" to the phase to which it belongs. After such supervised learning is implemented successfully, the ML algorithm can recognize a new input configuration, not drawn from the previous training set, as belonging to a certain phase, say A or B. If the input is drawn from states close to some phase transition, the prediction will be either A or B phase with certain probability distribution. The continuous change in the probability with temperature or tuning parameter for different system sizes can be used to correctly identify the critical temperature (classical phase transition) or the interaction strength (quantum phase transition). Most studies in the recent years along this line of thinking have focused on the transition between ordered and disordered phase, with a second-order critical point separating them. For first-order phase transition, the prediction changes abruptly from 100% A to 100% B across the critical point. Following a natural progression, models that were studied with the ML method have evolved from Ising[1–6] to XY[4,7,8] spins, and most recently to Heisenberg[9] spins.

Here we address various aspects of the Heisenberg-Dzyaloshinskii-Moriya-Zeeman (HDMZ) spin Hamiltonian by the ML method:

$$H_{\rm HDMZ} = -J\sum_{i\in L^2}\mathbf{n}_i\cdot(\mathbf{n}_{i+\hat{x}}+\mathbf{n}_{i+\hat{y}}) + D\sum_i(\hat{y}\cdot\mathbf{n}_i\times\mathbf{n}_{i+\hat{x}} - \hat{x}\cdot\mathbf{n}_i\times\mathbf{n}_{i+\hat{y}}) - \mathbf{B}\cdot\sum_i\mathbf{n}_i. \quad (1)$$

This lattice model, usually solved in two-dimensional $L\times L$ square lattice, is known to describe the magnetic interaction at the interface of a magnetic layer with a non-magnetic layer, or a magnetic layer exposed to vacuum. Its phase diagram, by now well-known, includes the skyrmion crystal over some intermediate field range, flanked by spiral phase at low field and ferromagnetic phase at high field[10–14].

Classifying intermediate phases: As an initial application of the ML ideas to the study of the HDMZ model and its phases, we created a training set of configurations drawn from deep inside the spiral, skyrmionic, and ferromagnetic phases of the model (1) by the Monte Carlo (MC) method. The training data was initially prepared in terms of spin angles (θ_i,ϕ_i), which gave far poorer results than if the data was prepared in terms of the magnetization $\mathbf{n}_i = (\sin\theta_i\cos\phi_i, \sin\theta_i, \sin\phi_i, \cos\theta_i)$. All the ML analysis presented in this paper is thus based on the magnetization inputs. Only its z-component was used for training in earlier work[9].

After training, the validation procedure gave nearly 100% correct values for the phase labels. This is not surprising given the fact that validation sets also came from deep inside one of the three phases. The next logical step is to generate configurations that have mixed characters and ask the ML program to predict the phases to which they belong. It is well-known both experimentally and from simulations that a substantial mixed phase or intermediate phase region exists in two dimensional skyrmion matter[15]. They are mixed spiral and skyrmion (SpSk) regions at low fields, and mixed skyrmion and ferromagnetic (SkFm) regions at higher fields. Because of their presence, a sharp phase boundary separating one phase from another is difficult to define. The ML prediction is expected to reflect this degree of uncertainty.

Our training set was generated on 24×24 lattice with $D/J=\sqrt{6}$, corresponding to the spiral period $\lambda=6$. The inter-skyrmion distance in the skyrmion phase is also of the same order, giving rise to the nucleation of about $(L/\lambda)^2$ number of skyrmions. The average spin chirality distribution [see (??) for definition] over the (T,B) plane is presented in Fig. ??. The region $T\in[0,0.5]$ with $B=$?? can be said to clearly belong to the spiral phase, as the $T\in[0,0.5]$ region with $B=$? belongs clearly to the ferromagnetic phase. The robust skyrmion phase can be assigned to $T\in[0,0.5]$ at $B=$??. After using a total of ?? configurations from various parts of this phase diagram to train labelling, we generate a new batch of MC configurations at $T=$?? and $B\in[xx,xx]$ which belongs to the SpSk mixed phase, and another batch of configurations at $T=$?? and $B\in[y,yy]$ belonging to the SkFm mixed phase. The machine prediction for the phase labels, averaged over all the input test configurations at the same (T,B) values, is shown as a function of the magnetic field in

Fig. ?? for several temperatures. (**test for higher temperature required**)

Feature predictions: The main characteristics of the ferromagnetic and the skyrmion phases are the average magnetization and the chirality, respectively, defined as (N=number of lattice sites)

$$m = (1/N)\sum_i n_i^z,$$
$$\chi = (1/N)\sum_i (\mathbf{n}_i \cdot \mathbf{n}_{i+\hat{x}} \times \mathbf{n}_{i+\hat{y}}). \quad (2)$$

The spiral phase is the one where none of these features takes on significant values. Instead of training the algorithm on the "labels" of the phases as spiral, skyrmion, or ferromagnet, we might train it on their features such as m and χ. Once the ML algorithm could be trained to correctly predict such values for input configurations, the problem of labeling them is as good as solved, since an input whose m (χ) is predicted to be close to the maximum allowed value can have no other label than ferromagnet (skyrmion). Intermediate values of m and χ signify the SkFm mixed phase. Finally, a configuration with small but non-negligible χ and m are likely associated with the SpSk mixed phase. In addition to m and χ, the temperature (T) and the magnetic field (B) from which the configuration originated can be trained as well. In total we carry out supervised learning of the four features (m, χ, T, B) on the configurations from a wide temperature range $0 < T \leq 2.0$ and magnetic field $0 \leq B \leq 3.5$. For each (T, B) we collect 100 MC-annealed configurations for training purpose. After training, those configurations not included in the training set are used to compare the machine-predicted (m, χ, T, B) against the actual values. As shown in Fig. ?? the agreement between predicted and actual values are very good across the whole phase diagram.

Prediction for adiabatically connected phases: The HDMZ Hamiltonian (1) represents the simplest case of spin interaction that supports the skyrmion phase. Various modifications can be added to it, and one that reflects the disorder in the actual material is given by

$$H_K = -K \sum_{i\in\text{random}} (S_i^z)^2. \quad (3)$$

The magnetic anisotropy term of strength K is added at the random sites occupying a fraction p of the whole lattice. The model $H(K, p) = H_{\text{HDMZ}} + H_K$ represents an adiabatically connected family of Hamiltonians as long as K is sufficiently small compared to other energy scales. It is interesting to ask whether the ML algorithm, trained solely on the configurations drawn from $H(0, 0) = H_{\text{HDMZ}}$, can have predictive power over those generated from arbitrary $H(K, p)$. It is also a pragmatic question, when it comes to addressing the machine's predictive power over the experimental data. The real materials are never as simple as the HDMZ Hamiltonian, and there is always some degree of disorder one does not know a priori. If the model Hamiltonian used for training is somehow adiabatically connected to the real Hamiltonian governing physical systems, one expects the predictive power of the ML to hold sway over the real-life data as well.

A large number of configurations at $K = 0.5$ and $p = 0.5$ were generated by MC and tested by the ML algorithm, which was trained solely on the pristine Hamiltonian H_{HDMZ}. As shown in Fig. ??, very good fits of all features (m, χ, T, B) were obtained, in a nice demonstration of the adiabatic continuity of the ML's predictive power. Another test was conducted on configurations generated by $H(0.5, 1)$, which is the anisotropic version of the HDMZ Hamiltonian without disorder. The results are ....

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