# Machine learning topological phases in real space

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**[AU: Please check change to M. A. R. Griffith]** We develop a supervised machine learning algorithm that is able to learn topological phases of finite condensed-matter systems from bulk data in real lattice space. The algorithm employs diagonalization in real space together with any supervised learning algorithm to learn topological phases through an eigenvector ensembling procedure. We combine our algorithm with decision trees and random forests to successfully recover topological phase diagrams of Su-Schrieffer-Heeger (SSH) models from bulk lattice data in real space and show how the Shannon information entropy of ensembles of lattice eigenvectors can be used to retrieve a signal detailing how topological information is distributed in the bulk. We further use insights obtained from these information entropy signatures to engineer global topological features from real-space lattice data that still carry most of the topological information in the lattice, while greatly diminishing the size of feature space, thus effectively amounting to a topological lattice compression. Finally, we explore the theoretical possibility of interpreting the information entropy topological signatures in terms of emergent information entropy wave functions, which lead us to Heisenberg and Hirschman uncertainty relations for topological phase transitions. The discovery of Shannon information entropy signals associated with topological phase transitions from the analysis of data from several thousand SSH systems illustrates how model explainability in machine learning can advance the research of exotic quantum materials with properties that may power future technological applications such as qubit engineering for quantum computing.

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## I. INTRODUCTION

The quest for innovative materials that harness exotic quantum properties has lured physicists into the realm of topological insulators and topological states of matter [1]. These materials feature previously unthought-of traits like bulk insulation coupled with metallic conductance at the surface and the splitting of currents according to spin orientation. Adding to that, these properties are protected by nontrivial topology that renders them robust to many sources of perturbation like thermal noise. Such characteristics make them promising candidates to being the cornerstone of 21st century technologies like spintronics and quantum computing.

These new topological states of matter have been studied in several contexts in condensed-matter physics including superconductors [2–5], ultracold atoms [6–10], photonic crystals [11–13], photonic quantum walks [14–16], and Weyl semimetals [17, 18]. Among these, the Su-Schrieffer-Heeger (SSH) model [19] has attracted particular theoretical interest due to its simplicity and generality.

The SSH model is the simplest tight-binding model that exhibits a topological phase transition. As such, it can be viewed as the *Drosophila* of the field, providing a simple framework for testing new techniques. The model can be expressed in terms of creation and annihilation operators by the Hamiltonian

$$\mathbf{H}(\mathbf{t}) = \mathbf{c}^{\dagger} H(\mathbf{t})\mathbf{c} \tag{1}$$

and describes, e.g., the hopping of electrons along a one-dimensional chain comprising two atoms per unit cell (a brief discussion of the SSH model and its topological properties can be found in the ~~section **The SSH model**~~ in the Supplemental Material [20]). The SSH model has found several interesting applications in the ~~modelling~~modeling of diverse systems with nontrivial topology like optical lattices [21], polymeric materials [22], and topological mechanisms [23, 24].

Many recent papers have explored the possibility of treating the general problem of determining phase transition boundaries of physical systems as machine learning tasks [25]–[41].**[COMP: Please note that the reference ranges are not tagged properly]**In the particular case of topological phase transitions, the usual approach for supervised learning is to generate a data set $(H_1(k), W_1)$, ..., $(H_n(k), W_n)$ whose inputs are representations of Hamiltonians in wave-vector space $H_i(k)$ and targets are their corresponding topological invariants $W_i$ (for the SSH model the topological invariant is the winding number). Our paper extends this task to the case of learning topological phase diagrams from input data in real space. Strikingly, we find that information localized on a few lattice sites in the bulk is sufficient to predict with high accuracy which topological phase a particular Hamiltonian belongs to.

The main motivation for developing a data-driven approach based on real space is that the canonical method of choice for the analysis of topological systems, i.e., wave-vector space computations of topological invariants, is often only feasible for systems with translational symmetry, which many physical systems of current interest (e.g., disordered systems in condensed matter) do not have. Furthermore, it is not always granted that the topological invariants of a physical system being investigated are known in advance, as is presently the case for many gapless insulators. In such cases, being able to engineer topological features that encode the topological states of a system while at the same time reducing the system's complexity may provide an alternative strategy. Moreover, since real-space and wave-vector space eigenvectors are related by Fourier transforms, the latter are essentially delocalized and therefore so is any information recovered from them. Constructing theoretical methods to trace the distribution of information in topological systems may be an essential prerequisite to discovering new topological invariants and features. The data-driven approach designed in this ~~ar~~paper~~ticle~~ addresses these issues.

To investigate topological phases of matter in real space, we have designed a ~~novel~~ **[AU: Please note that the use of "novel" in this context is discouraged as it could lead to priority claims]**supervised learning algorithm (here called eigenvector ensembling algorithm) tailored for the task of learning phase transition boundaries from local features. The algorithm is based on eigenvector decomposition and eigenvector ensembling and therefore will require minimal changes to be applicable to a broader class of data-driven physics problems. We describe the algorithm in detail in ~~se~~Sec.~~ction~~ II and demonstrate its effectiveness by combining it with decision trees and random forests to recover the topological phase diagrams of SSH systems from local coordinates of eigenstates in real space. This is performed in ~~se~~Sec.~~ction~~ III.

The advantage of using decision-tree-based algorithms to learn topological phases from local eigenvector data is that their use of entropy-based cost functions (such as Shannon information entropy or Gini impurity) furnishes them with an intrinsic model explainability tool that summarizes how important each feature was to learning the desired patterns in the data. This makes it much easier to trace the localization of relevant information along the features of a data set. Here, we use the Shannon information entropy of ensembles of real-space eigenvectors to recover a signal quantifying the amount of topological information available from each lattice site. This is a highly nontrivial proposition since the topological phase of a system is a global property of the system as a whole emerging from complex interactions between its components, and therefore even defining a local topological signal is a daunting theoretical task. ~~To our knowledge this is the first time that~~We present **[AU: Please check changes. Use of the "first time" in**

FIG. 1. Phase diagrams in parameter space. (a) SSH model with first-neighbor hoppings $t_1$ and $t_2$. The (red) regions with winding number $W = 0$ are trivial, while the (blue) regions with winding number $W = 1$ are topologically nontrivial. (b) SSH model with first ($t_1$ and $t_2$) and second ($T_1$ and $T_2$) nearest-neighbor hoppings. In this ~~arti~~paper~~cle~~ we set $t_1 = t_2 = 1$ and renamed the variables $T_1 \rightarrow t_1$, $T_2 \rightarrow t_2$ for convenience. The (orange) region with winding number $W = 0$ is trivial while the others with winding numbers $W = -1$, $W = 1$, and $W = 2$ (red, green, and blue respectively) are topologically nontrivial.

**this context also could result in a claim of priority]**a signal describing the localization of topological information in the bulk of topological condensed matter systems~~ is presented in the literature~~. These topological signals, here called information entropy signatures, are the subject of ~~se~~Sec.~~ction~~ IV.

In possession of the information entropy signatures, we demonstrate how the symmetries in real and wave-vector space eigenvectors can be manipulated with signal processing tools commonly employed in audio and image processing to execute two standard unsupervised learning tasks, namely, dimensionality reduction and feature engineering. The topological features resulting from this analysis, here denominated discrete cosine transform and discrete sine transform topological features, are discussed in ~~section~~Sec. V.

The information entropy signatures are finally explored as theoretical constructs in terms of information entropy mass functions along the lattices. By taking their continuum limit and admitting that they are quantum in nature, we show how the information entropy signatures can be naturally understood in terms of emergent information entropy wave functions along the lattices. The theoretical formulation of the results obtained with machine learning in terms of emergent quantum mechanical wave functions allows us to establish Heisenberg and Hirschman uncertainty principles for the localizability of information entropy in topological phase transitions. The emergent information entropy wave functions are the theme of ~~sec~~Sec.~~tion~~ VI.

The discovery of information entropy signatures of topological phase transitions and their description as a measurable emergent phenomenon originating from the information entropy of ensembles of topological systems proximal to phase transition boundaries provide clear illustrations of how model explainability in machine learning can guide new discoveries in condensed matter and quantum materials physics since the existence of these signals was established by analyzing data from several thousand SSH systems which, taken individually, could not have provided any concrete hint of their existence.

As of yet, model explainability [42–44] is one of the topics at the edge of machine learning research that has been little explored by the physics community working at the interface between the two disciplines. This raises important questions as to whether machine learning can in fact help to advance theoretical investigation in physics since the majority of physics papers published on the subject are proofs of concept aimed at showing that modern machine learning techniques are capable of recognizing the relevant patterns in data from physical systems whose properties were known in advance. By proposing ~~new~~ concepts from the data analysis of physical systems of contemporary interest and knitting together ideas from topological phase transitions and information theory by dint of model explainability, we expect to draw the physics community's attention to this essential machine learning tool.

## II. EIGENVECTOR ENSEMBLING ALGORITHM

The eigenvector ensembling algorithm consists of five steps: (1) generating Hamiltonians in real space and their corresponding winding numbers; (2) creating training, validation, and test sets; (3) training on real-space eigenvectors of Hamiltonians in the training set; (4) eigenvector ensembling, and (5) bootstrapping. We describe here in detail each of these steps as they were implemented in this work. For a comprehensive introduction to the concepts referenced in the steps below, we recommend Ref. [45].

(1) *Generating Hamiltonians and winding numbers.* We start generating a number of ~~paremeterized~~parametrized Hamiltonians $H(\mathbf{t})$ in real space and their corresponding winding numbers $W(\mathbf{t})$, where ~~$\mathbf{t} = (t_1, t_2, , t_h)$~~$\mathbf{t} = (t_1, t_2, \ldots, t_h)$ is a vector of $h$ hopping parameters (in the simplest case of the SSH model ~~$h$~~$h = 2$). These Hamiltonians are $N \times N$ matrices, where $N$ is twice the number of unit cells in the chain.

(2) *Creating training, validation, and test sets.* We split our set of paramet~~e~~rized Hamiltonians and winding numbers into training, validation, and test sets, as is ~~usualy~~usually done in machine learning. More explicitly, assume our hopping parameter vector $\mathbf{t}$ takes on the values ~~$\mathbf{t}_1, \mathbf{t}_2, , \mathbf{t}_n$~~$\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_n$ corresponding to the Hamiltonian-winding number pairs $(H_1, W_1), \ldots, (H_n, W_n)$. We partition the set $\{(H_i, W_i)$~~$\mid i = 1, , n$~~$\mid i = 1, \ldots, n\}$ in three disjoint subsets: the training set, the validation set, and the test set.

(3) *Training on eigenvectors in real space.* Since each Hamiltonian $H_i$ is represented by an $N \times N$ matrix, each

one will provide $N$ eigenvectors $\cancel{\mathbf{v}_i^{(1)}, \mathbf{v}_i^{(2)}, , \mathbf{v}_i^{(N)}}\mathbf{v}_i^{(1)}, \mathbf{v}_i^{(2)}, \ldots, \mathbf{v}_i^{(N)}$ to our data set. Our supervised learning algorithm of choice will take as inputs the real-space eigenvectors $\mathbf{v}_i^{(j)}$ of each Hamiltonian $H_i$ in the training set and be trained to learn the winding number $W_i$ of their parent Hamiltonian $H_i$. Therefore, our ~~dataset~~data set will consist of eigenvector-winding number pairs $(\mathbf{v}_i^{(j)}, W_i)$.

(4) *Eigenvector ensembling.* In order to predict the phase of a system described by a particular Hamiltonian, we need to take into account how each of its eigenvectors were classified. This amounts to performing ensemble learning on the eigenvectors of each Hamiltonian. In this work we estimate the phase probabilities for each Hamiltonian as the fraction of its eigenvectors that were classified in each phase.

(5) *Bootstrapping.* We refine the phase probabilities for each Hamiltonian using a bootstrapping procedure, i.e., we repeat steps (1)–(4) $\cancel{n_{\text{exp}}}n_{\text{expt}}$ times, at each round sampling randomly a new training set from our grid in $\mathbf{t}$ space. The final estimated probabilities are then arrived at by averaging the probabilities obtained in each experiment.

Before continuing to the analyses of the SSH systems with the eigenvector ensembling algorithm, it will be timely to digress a moment and peek into the algorithm itself. The focus on eigenvectors (and hence the algorithm's name) as the input data to a machine learning algorithm of choice is a hallmark of the procedure as it differentiates it from related applications of machine learning to the study of phase transitions. The intuition that eigenvectors can be used in replacement of raw Hamiltonians can be grasped when we consider the spectral decomposition of a Hamiltonian $H$:

$$H = \sum_{i=1}^{N} \lambda^{(i)} \left|\mathbf{v}^{(i)}\right\rangle \left\langle \mathbf{v}^{(i)}\right| , \tag{2}$$

where $\lambda^{(i)}$ is the eigenenergy corresponding to the eigenstate $|\mathbf{v}^{(i)}\rangle$. It is therefore clear that all information available from a Hamiltonian can be recovered from its spectral decomposition. By expressing the eigenvectors in a basis suitable to a particular problem (e.g., the real-space basis chosen in this ~~article~~paper), it becomes possible to investigate the properties of a set of Hamiltonians using the coordinates of eigenvectors in the chosen basis as features. Thus, the eigenvector ensembling procedure described above provides a broad framework for the implementation of model explainability in applications to data-driven physics.

## III. NUMERICAL EXPERIMENTS

We performed two numerical experiments with the eigenvector ensembling algorithm. The first experiment deals with the simplest case, the SSH model with nearest-neighbor hopping [here called SSH 1, Fig. 1(a)], while the second Fig. 1
experiment uses the SSH model with first- and second-nearest-neighbor hoppings [here called SSH 2, ~~figure~~Fig. 1(b)].

In each experiment our grid consisted of 6561 Hamiltonians uniformly distributed in the closed square $[-2, 2] \times [-2, 2]$ in the $t_1$-$t_2$ plane in parameter space. The goal in each experiment is to recover the corresponding phase diagram in 2D (two-dimensional) parameter space ~~figures~~[Figs. 1(a) and 1(b)] from local lattice data in the much higher-dimensional real space (100 D, in both experiments lattices have 50 unit cells, yielding $\cancel{\times 100}100 \times 100$ Hamiltonian matrices).

This task is particularly hard near phase transition boundaries, where numerical computation of winding numbers becomes less stable. For this reason, when sampling the training set we only consider those Hamiltonians in the grid whose numerically computed winding numbers lie in a minimum range of $\epsilon = 0.01$ from the correct winding-number values. Therefore, a good performance metric is the accuracy measured at those Hamiltonians near phase transitions that are never used for training, and thus we assign them to the test set. The remaining Hamiltonians in the grid are split into training and validation sets as detailed in the sections below.

As performance metrics, we report here both accuracy of predicted classes for eigenvectors as well as accuracy of predicted classes for Hamiltonians obtained from eigenvector ensembling. These accuracy scores are to be gauged against the baseline of a system that simply guesses the most frequent class for all Hamiltonians. Checking against this baseline is important because it indicates whether the decision trees are in fact learning the underlying patterns that relate real-space coordinates to winding numbers, and therefore whether the associated information entropy signature is meaningful or not.

When generating the Hamiltonians we applied periodic boundary conditions to eliminate border effects. This should make recovering a topological signal from local eigenvector coordinates even harder since, in this case, the translational symmetry of the systems should allow for no obvious way to distinguish between unit cells. The choice of periodic

FIG. 2. Visualization of a single iteration of experiment 1 (~~section~~Sec. III A) as seen from 2D parameter space. (a) Train/validation/test split. (b) Distribution of winding numbers in the training set. (c) Phase diagram learned from real-space lattice data by combining a decision tree with eigenvector ensembling.

boundary conditions also implies that the information recovered from real-space data comes from the bulk of the topological systems considered and therefore provides strong evidence for the existence of topological signatures in the bulk of such systems.

Figures 2 and 3, respectively, illustrate single iterations of experiment 1 (Sec. III A) and experiment 2 (Sec. III B) Figs.
as seen from parameter space. The accuracy statistics presented in the following subsections, as well as the probability 2,3
~~heatmaps~~heat maps and recovered phase diagrams shown in ~~f~~Figs.~~igures~~ 4 and 5 were obtained after bootstrapping Figs.
each experiment $\cancel{n_{exp}} n_{\mathrm{expt}} = 100$ times. Thus, each probability ~~heatmap~~heat map shown in ~~figures~~Figs. 4(a), 4(b) 4,5
and 5(a)–5(d) represents the averaged fraction of eigenvectors of each Hamiltonian in the grid that were classified with a given winding number across 100 experiments. The recovered phase diagrams 4(c) and 5(d) are constructed by superposing the corresponding probability ~~heatmaps~~heat maps. As these figures make clear, the recovered phase diagrams faithfully portray the true phase diagrams in ~~f~~Fig.~~igure~~ 1, with clear phase transition lines appearing in the regions of highest uncertainty.

The numerical experiments with the eigenvector ensembling algorithm described in the next subsections were implemented in Python using the SCIKIT-learn module [46, 47].

### A. Experiment 1: Learning a first-neighbor hopping SSH model with decision trees

Our test set in this experiment contained 1005 Hamiltonians (approximately 15.32% of all data). Of the remaining 5556 Hamiltonians, 556 were randomly assigned to the training set (approximately 8.47%) and 5000 (approximately 76.21%) were used to compute validation scores at each iteration. These proportions between training and validation sets are such that approximately 10% of Hamiltonians from outside of the test set were used for training at each iteration. The composition of the train + validation set for this experiment was 50.79% of Hamiltonians with winding number $\cancel{W} W = 0$ and 49.21% with winding number $\cancel{W} W = 1$. The composition of the test set was 44.79% of Hamiltonians with winding number $\cancel{W} W = 0$ and 55.21% with winding number $W = 1$. Our learning algorithm of choice for this experiment was a simple decision-tree model [48].

The bootstrap allows us to collect several statistics to evaluate performance. In particular, we report mean accuracies on training eigenvectors (0.9814), validation eigenvectors (0.9639), and test eigenvectors (0.7897). Eigenvector ensembling substantially improved mean accuracies for Hamiltonians. These were 1.000 for training Hamiltonians, 1.000 for validation Hamiltonians, and 0.9919 for test Hamiltonians. When compared with the baseline test accuracy of 0.5521 of a system that predicts the whole test set as having winding number $W = 1$, the accuracy achieved on test Hamiltonians indicates that the decision trees indeed learned the patterns that relate real-space coordinates to winding numbers.

The probability ~~heatmaps~~heat maps and phase diagram learned by the combination of decision trees with eigenvector ensembling used in experiment 1 are shown in ~~fi~~Fig.~~gure~~ 4.

### B. Experiment 2: Learning a first- and second-neighbor hopping SSH model with random forests

This task is considerably more difficult than the previous one due to the higher number of classes and the fact that some of the labels encompass disconnected regions. For this reason, instead of using a single decision tree, we upgraded our model to a random forest [49] with 25 decision trees. Our data set consisted of 1040 (15.85%) test Hamiltonians. The remaining 5521 Hamiltonians are randomly split in half between training and validation sets at each iteration, giving 2761 (42.08%) training Hamiltonians and 2760 (42.07%) validation Hamiltonians. The distribution of winding numbers for the Hamiltonians in the train + validation set for this experiment was $W = -1$ (17.90%), $W = 0$ (32.51%), $W = 1$ (32.26%), and $W = 2$ (17.33%). The distribution of winding numbers for the Hamiltonians in the test set was $W = -1$ (36.32%), $W = 0$ (11.06%), $W = 1$ (12.69%), and $W = 2$ (39.93%).

Mean accuracies across 100 repetitions of experiment 2 were 0.9997 for training eigenvectors, 0.9709 for validation eigenvectors, and 0.6634 for test eigenvectors. Mean accuracies resulting from eigenvector ensembling were 1.000 for training Hamiltonians, 0.9972 for validation Hamiltonians, and 0.8797 for test Hamiltonians. The large accuracy gain achieved by eigenvector ensembling in the test set (going from 0.6634 eigenvector accuracy to 0.8797 Hamiltonian accuracy) attests to its power. The effectiveness of eigenvector ensembling is also evident from the much worse

FIG. 3. Visualization of a single iteration of experiment 2 (~~section~~Sec. III B) as seen from 2D parameter space. (a) Train/validation/test split. (b) Distribution of winding numbers in the training set. (c) Phase diagram learned from real-space lattice data by combining a random forest with eigenvector ensembling.

performance (0.3993) achieved by a baseline system that simply guesses $W = 2$ for all test Hamiltonians in this experiment.

The probability ~~heatmaps~~heat maps and phase diagram learned by the combination of random forests with eigenvector ensembling used in experiment 2 are shown in ~~fi~~Fig.~~gure~~ 5.

## IV. INFORMATION ENTROPY SIGNATURES

We now analyze how the algorithm was able to recover a global property of the Hamiltonians (their topological phase) from bulk local features (real-space eigenvector coordinates on each lattice site). Alongside the fact that decision trees and random forests are very easy to train and visualize, the other reason that led us to test the eigenvector ensembling algorithm with them was that they allow us to check which features (and thus which lattice sites) were most informative in training.

The (normalized) relevance of a feature is given by how much it reduces a loss function (in this paper, the Shannon information entropy of ensembles of eigenvectors). By averaging normalized relevances as measured by reduction in the information entropy of ensembles of real-space eigenvectors across ~~$n_{exp}$~~$n_{\mathrm{expt}} = 100$ iterations of both experiment 1 (~~section~~Sec. III A) and experiment 2 (~~section~~Sec. III B) we recovered Shannon entropy signals that reveal which lattice sites were consistently more relevant in learning topological phases from data in real space for each experiment. These signals are the information entropy signatures of each topological phase transition.

We should briefly comment on the possibility of using the Gini impurity of ensembles of eigenvectors [45] instead of their Shannon entropy as cost function. This would similarly lead us to Gini impurity signatures of topological phase transitions. Given that in the examples analyzed in this paper the Gini impurity signatures and the Shannon entropy signatures were very similar, the larger familiarity of a general physics audience with the latter influenced us to choose it over the former. Nevertheless, the question of which split criterion should be used when training decision trees is as of yet largely undecided [50] and may be of relevance in the analysis of other physical systems than the ones studied here.

The bar plots in ~~fig~~Fig.~~ure~~ 6 show how informative each lattice site was in learning topological phases for each Fig. 6
experiment. They represent the information entropy signatures along the lattices in each SSH system. For experiment 1 (~~sec~~Sec.~~tion~~ III A), only six lattice sites (0, 1, 3, 50, 51, 53) corresponding to the two sharp peaks seen in ~~figur~~Fig.~~e~~ 6(a) contributed approximately 70% of total reduction in Shannon entropy. Similarly, approximately 30% of total reduction in the Shannon information entropy of eigenvector data from experiment 2 (~~sec~~Sec.~~tion~~ III B) was achieved by ~~eighteen~~18 lattice sites (0, 1, 2, 3, 4, 5, 46, 48, 49, 50, 51, 53, 94, 95, 96, 97, 98, 99) distributed along the three peaks in ~~figu~~Fig.~~re~~ 6(b). As we shall see in ~~s~~Sec.~~ection~~ V, the information entropy signatures can be used to compress the topological information in SSH lattices.

The information entropy signatures presented here have some interesting subtleties. Although they give us a visualization of how important each lattice site was in determining the topological phases of Hamiltonians, they actually express a global property of the whole lattice. In ~~se~~Sec.~~ction~~ VI, where we develop a quantum formalism for the information entropy signatures obtained in this section, these seemingly antagonistic conceptions shall be harmonized. What is important to emphasize at this point is that an information entropy signature should not be naively taken at face value: a lattice site that appears unimportant in an information entropy signature plot may not be unimportant or void of topological information by itself.

To give a concrete example, reduction in Shannon entropy tends to be distributed among highly correlated variables. This implies that if only a single lattice site in a highly correlated subset is used by a learning algorithm, it will likely inherit most of the reduction in Shannon entropy from the other correlated lattice sites that were not taken into account by the algorithm. The corollary of this fact is that lattice sites that carry redundant information that is also available from other lattice sites tend to have decreased importance in the information entropy signature. In this regard, the information entropy signatures presented here express a summary of relations between lattice sites and are therefore intrinsically global.

Each of the information entropy signatures shown in ~~fig~~Fig.~~ure~~ 6 captures a general pattern that persists regardless of the length of the lattice (i.e., the number of unit cells) used to compute them. In fact, by rerunning each experiment with longer lattices we have verified that the signals in ~~f~~Figs.~~igures~~ 6(a) and 6(b) appear to converge to well-defined continuous density functions in the macroscopic limit. They are not, therefore, artifacts of particular choices of hyperparameters used to run the eigenvector ensembling algorithm. The information entropy signatures for longer

FIG. 4. Probability ~~heatmaps~~heat maps learned by a combination of decision trees with eigenvector ensembling from bulk real-space eigenvector data in experiment 1 (~~sec~~Sec.~~tion~~ III A). ~~Heatmaps~~Heat maps were averaged across all 100 iterations of the experiment. (a) Probability ~~heatmap~~heat map showing the probability that a Hamiltonian in the grid has winding number equal to 0. (b) Probability ~~heatmap~~heat map showing the probability that a Hamiltonian in the grid has winding number equal to 1. (c) The phase diagram resulting from ~~heatmaps~~heat maps (a) and (b).

FIG. 5. Probability ~~heatmaps~~heat maps learned by a combination of random forests with eigenvector ensembling from bulk real-space eigenvector data in experiment 2 (~~sec~~Sec.~~tion~~ III B). ~~Heatmaps~~Heat maps were averaged across all 100 iterations of the experiment. (a) Probability ~~heatmap~~heat map showing the probability that a Hamiltonian in the grid has winding number equal to ~~-1~~$-1$. (b) Probability ~~heatmap~~heat map showing the probability that a Hamiltonian in the grid has winding number equal to 0. (c) Probability ~~heatmap~~heat map showing the probability that a Hamiltonian in the grid has winding number equal to 1. (d) Probability ~~heatmap~~heat map showing the probability that a Hamiltonian in the grid has winding number equal to 2. (e) The phase diagram resulting from ~~heatmaps~~heat maps (a)–(d).

lattices are presented in the ~~section **Numerical explorations on longer lattices** in the~~ Supplemental Material [20].

## V. TOPOLOGICAL FEATURE ENGINEERING AND LATTICE COMPRESSION

In this section, we explore the information entropy signatures obtained in ~~se~~Sec.~~ction~~ IV from a signal processing perspective. As we shall see, this will enable us to perform two important unsupervised learning tasks on topological systems: dimensionality reduction and data compression.

TABLE I. Accuracy scores of numerical experiments. The features used to train the decision trees (SSH 1) or random forests (SSH 2) in the numerical experiments with SSH systems were as follows. Real-space features: all real-space lattice sites ($X_\alpha$) (~~sections~~Secs. III A and III B); real-space lattice sites from subset $\mathcal{S}_\alpha$ ($X_{\mathcal{S}_\alpha}$) [Eq. (7)]. DCT topological features: all DCT topological features ($\hat{X}^c_\alpha$) [Eq. (5)]; DCT topological features from subset $\mathcal{E}_\alpha$ ($\hat{X}^c_{\mathcal{E}_\alpha}$) [Eq. (8)]; DCT topological features from subset $\mathcal{E}_\alpha$ computed using only real-space lattice sites $\mathcal{S}_\alpha$ ($\hat{X}^c_{\mathcal{S}_\alpha,\mathcal{E}_\alpha}$) [Eq. (10)]. DST topological features: all DST topological features ($\hat{X}^s_\alpha$) [Eq. (6)]; DST topological features from subset $\mathcal{O}_\alpha$ ($\hat{X}^s_{\mathcal{O}_\alpha}$) [Eq. (9)]; DST topological features from subset $\mathcal{O}_\alpha$ computed using only real-space lattice sites $\mathcal{S}_\alpha$ ($\hat{X}^s_{\mathcal{S}_\alpha,\mathcal{O}_\alpha}$) [Eq. (11)].

| SSH system | Features | Val. eigenvectors | Test eigenvectors | Val. Hamiltonians | Test Hamiltonians |
|---|---|---|---|---|---|
| 1 | $X_1$ | 0.9639 | 0.7897 | 1.000 | 0.9919 |
| 1 | $X_{\mathcal{S}_1}$ | 0.9444 | 0.7763 | 0.9853 | 0.9853 |
| 1 | $\hat{X}^c_1$ | 0.9521 | 0.7374 | 0.9976 | 0.9916 |
| 1 | $\hat{X}^c_{\mathcal{E}_1}$ | 0.8280 | 0.6067 | 0.9979 | 0.9191 |
| 1 | $\hat{X}^c_{\mathcal{S}_1,\mathcal{E}_1}$ | 0.9444 | 0.8176 | 0.9853 | 0.9934 |
| 1 | $\hat{X}^s_1$ | 0.9533 | 0.7314 | 0.9906 | 0.9856 |
| 1 | $\hat{X}^s_{\mathcal{O}_1}$ | 0.6942 | 0.5420 | 0.7088 | 0.4798 |
| 1 | $\hat{X}^s_{\mathcal{S}_1,\mathcal{O}_1}$ | 0.9456 | 0.7818 | 0.9854 | 0.9399 |
| 2 | $X_2$ | 0.9709 | 0.6634 | 0.9972 | 0.8797 |
| 2 | $X_{\mathcal{S}_2}$ | 0.9590 | 0.6168 | 0.9961 | 0.9961 |
| 2 | $\hat{X}^c_2$ | 0.9740 | 0.6895 | 0.9976 | 0.8862 |
| 2 | $\hat{X}^c_{\mathcal{E}_2}$ | 0.8990 | 0.5357 | 0.9955 | 0.7897 |
| 2 | $\hat{X}^c_{\mathcal{S}_2,\mathcal{E}_2}$ | 0.8999 | 0.5030 | 0.9956 | 0.7671 |
| 2 | $\hat{X}^s_2$ | 0.9735 | 0.6878 | 0.9971 | 0.8899 |
| 2 | $\hat{X}^s_{\mathcal{O}_2}$ | 0.9042 | 0.5527 | 0.9918 | 0.7427 |
| 2 | $\hat{X}^s_{\mathcal{S}_2,\mathcal{O}_2}$ | 0.8204 | 0.4127 | 0.9942 | 0.5903 |

As a cursory glance at ~~fig~~Figs.~~ures~~ 6(a) and 6(b) seems to suggest, the existence of peaks and symmetries in information entropy signatures can be exploited as a powerful dimensionality reduction tool: by keeping only the most relevant lattice sites in an information entropy signature, the amount of data needed to characterize the topological phase of a SSH system can be largely decreased with little loss of information. Nevertheless, given that the topological phase of a SSH system is a global property of the whole lattice, it is natural to expect that it should be possible to engineer global features from real-space coordinates. Here, we show how the symmetries in real-space eigenvectors and information entropy signatures can be exploited to engineer new global topological features, leading to an effective compression of topological information.

Given a real-space eigenvector $x[m]$, we can compute its coordinates in ~~wavevector~~wave vector space using the discrete Fourier transform (DFT)

$$\hat{x}[n] = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} x[m] e^{-i\frac{2\pi}{N}nm}, \quad n = 0, \dots, N-1. \tag{3}$$

Since the choice of phase of the real-space eigenvectors was such that they were all in $\mathbb{R}^N$, the eigenvectors in wave-vector space computed from ~~equa~~Eq.~~tion~~ (3) will be Hermitian vectors in $\mathbb{C}^N$. The Hermitian symmetry of the wave-vector space eigenvectors manifests itself mathematically in closed lattices with periodic boundary conditions as

$$\hat{x}[\overline{k}] = \hat{x}^*[\overline{N-k}], \quad k = 0, \dots, N-1 \tag{4}$$

where we have used the notation $\overline{k} = k \mod N$.

Equation (4) forks into two natural paths to topological feature engineering. In the first path, we exploit the fact that the real part of $\hat{x}[m]$ is even symmetric around the reciprocal lattice sites 0 and $\frac{N}{2}$. This leads us to the discrete cosine transform (DCT) topological features

$$\hat{x}^c[n] = x[0] + (-1)^n x[M-1] + \sum_{m=1}^{M-2} 2x[m] \cos\left(\frac{\pi}{M-1} nm\right), \quad n = 0, \dots, M-1 \tag{5}$$

where $M = \frac{N}{2} + 1$. The second path capitalizes on the fact that the imaginary part of $\hat{x}[m]$ is odd ~~symetric~~symmetric around the reciprocal lattice sites 0 and $\frac{N}{2}$, thus yielding the discrete sine transform (DST) topological features

$$\hat{x}^s[n] = \sum_{m=0}^{M-1} 2x[m+1] \sin\left(\frac{\pi}{M+1}(n+1)(m+1)\right), \quad n = 0, \dots, M-1 \tag{6}$$

where $M = \frac{N}{2} - 1$.

The topological features in both ~~equa~~Eqs.~~tions~~ (5) and (6) are generated from only half of the real-space lattice, i.e., the sites $0 \leq l \leq \frac{N}{2}$. This is due to the fact that each equation assumes that the eigenvectors are even symmetric (DCT topological features) or odd symmetric (DST topological features) around the lattice sites 0 and $\frac{N}{2}$ in real space as well. While these assumptions are strictly true for the eigenvector representations in wave-vector space, they are not generally true for the real-space representations. Therefore, ~~eq~~Eqs.~~uations~~ (5) and (6) achieve lattice compression by keeping only half of the real-space eigenvector coordinates and imposing the corresponding boundary conditions (even symmetry or odd symmetry) on the lattice sites 0 and $\frac{N}{2}$ to extrapolate the information from one half of the lattice to the other.

The topological feature engineering techniques described above are commonly employed in several applications of digital signal processing like audio and image processing and, most importantly here, data compression. As ~~equations~~Eqs. (4)–(6) show, signal transforms such as the DCT and DST profit from the redundance of information arising from the existence of certain symmetries in signals, allowing us to write a signal of length $N$ in terms of at most $M = \frac{N}{2} + 1$ features.

We ran several numerical experiments to evaluate if the DCT and DST topological features defined in ~~equations~~Eqs. (5) and (6) are able to efficiently encode the topological information existing in SSH lattices. The accuracy scores obtained in each experiment are listed in Table I, where we also report the accuracy scores of the numerical experiments Table I of ~~sect~~Sec.~~ion~~ III.

The lattice compression strategies tested in this work were as follows: (i) learning topological phases from only a subset of real-space lattice sites; (ii) learning topological phases from the DCT or DST engineered features of ~~equ~~Eqs.~~ations~~ (5) and (6); (iii) learning topological phases from a fraction of the DCT or DST topological features; and (iv) learning topological phases from a fraction of the DCT or DST features, computed from only a fraction of real-space lattice sites.

In strategy (i) the lattice sites used in the SSH 1 and SSH 2 systems were

$$\mathcal{S}_1 = (0, 1, 3, 50) \quad \text{and} \quad \mathcal{S}_2 = (0, 1, 2, 3, 4, 5, 6, 7, 46, 48, 49, 50). \tag{7}$$

Note that for the nearest-neighbor SSH systems $\mathcal{S}_1$ corresponds to the four most informative sites such that $0 \leq l \leq 50$ as indicated by the information entropy signature in ~~figu~~Fig.~~re~~ 6(a). Similarly, for the first- and second-nearest-neighbor SSH systems $\mathcal{S}_2$ corresponds to the 12~~twelve~~ most informative sites such that $0 \leq l \leq 50$ in the corresponding information entropy signature in ~~f~~Fig.~~igure~~ 6(b). In Table I, the features used in strategy (i) are referred to as $X_{\mathcal{S}_1}$ and $X_{\mathcal{S}_2}$, according to the SSH systems they relate to. In strategy (ii), the full set of DCT or DST topological features written in ~~equa~~Eqs.~~tions~~ (5) and (6) were used. These features are denoted in Table I by $\hat{X}^c_1$, $\hat{X}^s_1$, $\hat{X}^c_2$, $\hat{X}^s_2$, according to which set of topological features and SSH systems they refer to.

Similarly to strategy (i), in strategy (iii) we selected the most informative DCT topological features of both SSH 1 and SSH 2 systems that were obtained from strategy (ii),

$$\mathcal{E}_1 = (1, 2, 36, 49) \quad \text{and} \quad \mathcal{E}_2 = (0, 1, 2, 3, 4, 5, 6, 7, 47, 48, 49, 50) \qquad \text{(DCT)} \tag{8}$$

and the most informative DST topological features of both systems that were obtained from strategy (ii) as well,

$$\mathcal{O}_1 = (0, 18, 28, 30) \quad \text{and} \quad \mathcal{O}_2 = (0, 1, 2, 3, 4, 5, 43, 44, 45, 46, 47, 48) \qquad \text{(DST).} \tag{9}$$

The features in strategy (iii) are denoted in Table I by $\hat{X}^c_{\mathcal{E}_1}$, $\hat{X}^s_{\mathcal{O}_1}$, $\hat{X}^c_{\mathcal{E}_2}$, $\hat{X}^s_{\mathcal{O}_2}$, according to the topological features and wave-vector space subset used with each SSH system.

The most aggressive lattice compression strategy tested in this work was strategy (iv). It consists of using the DCT (DST) topological features of ~~equa~~Eq.~~tion~~ (8) [Eq. (9)], but having computed these topological features using only the real-space lattice sites given in ~~equ~~Eq.~~ation~~ (7). Thus, in strategy (iv) a lossy compression is performed both on real-space features and the engineered DCT (DST) topological features. Mathematically, we can express the topological features used in strategy (iv) as follows:

$$\hat{x}^c_{\mathcal{S},\mathcal{E}}[n] = \mathbb{1}_{\mathcal{S}}[0]x[0] + (-1)^n \mathbb{1}_{\mathcal{S}}[M-1]x[M-1] + \sum_{m \in \mathcal{S}^*} 2x[m] \cos\left(\frac{\pi}{M-1} nm\right), \quad n \in \mathcal{E} \qquad \text{(DCT)} \tag{10}$$

$$\hat{x}^s_{\mathcal{S},\mathcal{O}}[n] = \sum_{m \in \mathcal{S}} 2x[m+1] \sin\left(\frac{\pi}{M+1}(n+1)(m+1)\right), \quad n \in \mathcal{O} \qquad \text{(DST)} \tag{11}$$

where in ~~equ~~Eq.~~ation~~ (10) the notation $\mathbb{1}_{\mathcal{S}}[l]$ stands for the indicator function of the lattice subset $\mathcal{S}$ and $\mathcal{S}^*$ is the complement of $\{0, M-1\}$ with respect to $\mathcal{S}$:

$$\mathbb{1}_{\mathcal{S}}[l] = \begin{cases} 1 & \text{if } l \in \mathcal{S}, \\ 0 & \text{otherwise,} \end{cases} \qquad \mathcal{S}^* = \mathcal{S} \backslash \{0, M-1\}. \tag{12}$$

The features engineered in strategy (iv) are denoted in Table I by $\hat{X}^c_{\mathcal{S}_1,\mathcal{E}_1}$, $\hat{X}^s_{\mathcal{S}_1,\mathcal{O}_1}$, $\hat{X}^c_{\mathcal{S}_2,\mathcal{E}_2}$, $\hat{X}^s_{\mathcal{S}_2,\mathcal{O}_2}$, again referencing the type of topological features used, which components in real and wave-vector space engineered them and the appropriate SSH systems.

The results shown in Table I bring some startling surprises. For example, the topological phase transition boundaries of SSH 1 systems can be learned using only the four real-space lattice sites $\mathcal{S}_1$ with virtually no loss in accuracy, as seen from eigenvector and Hamiltonian accuracy scores for the features $X_{\mathcal{S}_1}$. The same appears to be true to SSH 2 systems, where the ~~tw~~12~~elve~~ real-space lattice sites $\mathcal{S}_2$ corresponding to the features $X_{\mathcal{S}_2}$ in the table produce accuracy scores at near the same level as using the whole lattice.

Even more striking is the performance achieved by the compressed DCT topological features $\hat{X}^c_{\mathcal{S}_\alpha,\mathcal{E}_\alpha}$ defined in ~~equa~~Eq.~~tion~~ (10). For SSH 1 systems, they perform on par with using the full set of real-space features $X_1$, while for SSH 2 systems a small loss in accuracy is incurred relative to the full set of real-space features $X_2$.

Another interesting insight comes from comparing the accuracy scores obtained with the DCT topological features versus the DST topological features. The latter have poorer performance than the former, as is indicated by the sharp drops in accuracy scores obtained with the DST topological features in both SSH 1 and SSH 2 systems. This may be related to the fact that the odd-symmetric boundary conditions imposed on DST topological features imply discarding the lattice sites 0 and 50, which correspond to sharp peaks in the information entropy signatures of ~~figures~~Figs. 6(a) and 6(b).

The accuracy scores obtained with the real-space features $X_{\mathcal{S}_\alpha}$ and the DCT topological features $\hat{X}^c_{\mathcal{S}_\alpha,\mathcal{E}_\alpha}$, both of which use information from a small fraction of real-space lattice sites, demonstrate that learning topological phases from local real-space data in the bulk is still possible even for small subsets of lattice sites. In this sense, key topological information can be said to be localized on few sites in the lattice. We refer the reader to ~~the section Learning topological phases from real space data in~~ the Supplemental Material [20] for a discussion of how this is possible.

## VI. EMERGENT INFORMATION ENTROPY WAVE FUNCTIONS

The information entropy signatures that we have been investigating pose an immediate theoretical question: How can a signal that is locally defined arise from a global property of the whole SSH lattice? In this section we venture into a theoretical exploration of the information entropy signatures in the hope of elucidating this issue. Our goal is to arrive at a theoretical framework that will allow us to interpret the information entropy signatures in terms of quantum mechanics.

We can think of the Shannon information entropy signatures in ~~fig~~Figs.~~ures~~ 6(a) and 6(b) as discrete information entropy mass functions that, in the continuum (i.e., macroscopic) limit of an infinite chain, lead to local entropy density functions along the lattices, which themselves become 1D manifolds. By mapping the lattice to a partition of the 1D manifold, the cumulative distribution of topological information in the continuum limit will be given by

$$F_S(x) = \int_\ell^{(x)} \rho_S(x')dx', \tag{13}$$

where $\rho_S(x)$ is the local information entropy density function in the continuum limit and $x$ is defined by the coordinate system specified on the 1D manifold $\ell$. The index $S$ is meant to emphasize that in this paper we have used Shannon's definition of entropy to arrive at the information entropy signatures as opposed to, e.g., Gini impurity.

Our use of periodic boundary conditions implies that the coordinate $x$ should be defined on the circle $S^1 = [0,1]/R$, where $R$ is the equivalence relation in $[0,1]$ defining the circle $S^1$,

$$x \; R \; y \iff x = y \text{ or } (x,y) \in \{(0,1),(1,0)\}. \tag{14}$$

For open boundary conditions, the spatial coordinate $x$ is defined on the closed interval $[0,1]$ or, in the case of infinite systems, $\mathbb{R}$. However, for the sake of generality, we shall continue to use the ~~caligraphic~~calligraphic $\ell$ to denote an arbitrary 1D manifold in this section.

Given the quantum nature of the phase transitions being discussed, the information entropy density function $\rho_S(x)$ can be naturally interpreted as the squared magnitude of a spatial information entropy wave function,

$$\rho_S(x) = |\psi_S(x)|^2, \tag{15}$$

the local density of topological information available from a single point in the 1D manifold then being expressed in bra-ket notation by Born's rule

$$\rho_S(x) = |\langle x|\psi_S\rangle|^2. \tag{16}$$

The counterpart of the spatial information entropy wave function $\psi_S(x)$ in wave-vector space is its Fourier transform

$$\hat{\psi}_S(k) = \int_\ell \psi_S(x) e^{-2\pi i k x} dx \tag{17}$$

from which the information entropy density function in wave-vector space can be computed:

$$\hat{\rho}_S(k) = |\hat{\psi}_S(k)|^2. \tag{18}$$

The interpretation of information entropy signatures in terms of information entropy wave functions opens several avenues of investigation of possible connections between exotic states of matter and quantum information theory. Here, we explore its most forthright corollary, which is the establishment of uncertainty relations for topological phase transitions.

Let us denote the mean, the variance, and the entropy associated with the probability distribution $\rho_S$ by $\mu_{\rho_S}$, $\sigma^2_{\rho_S}$, and $H_{\rho_S}$, respectively. Explicitly, we have

$$\mu_{\rho_S} = \int_\ell x\rho_S(x)dx, \tag{19a}$$

$$\sigma^2_{\rho_S} = \int_\ell (x-\mu_{\rho_S})^2\rho_S(x)dx, \tag{19b}$$

$$H_{\rho_S} = \int_\ell \rho_S(x)\ln\big(\rho_S(x)\big)dx, \tag{19c}$$

with analogous equations for the wave-vector space counterparts $\mu_{\hat{\rho}_S}$, $\sigma^2_{\hat{\rho}_S}$, and $H_{\hat{\rho}_S}$ in terms of $\hat{\rho}(k)$.

In possession of this quantum formalism, we may write topological versions of two canonical uncertainty relations that bind together the real space and wave-vector space information entropy density functions (15) and (18):

(i) *The Heisenberg uncertainty principle:*

$$\sigma_{\rho_S}\sigma_{\hat{\rho}_S} \geq \frac{1}{4\pi}. \tag{20}$$

(ii) *The Hirschman entropic uncertainty:*

$$H_{\rho_S} + H_{\hat{\rho}_S} \geq \ln\left(\frac{e}{2}\right). \tag{21}$$

The information entropy density function $\rho_S$ devised in this section furnishes a physics-grounded interpretation of the information entropy signatures obtained in ~~secti~~Sec.~~on~~ IV from sheer data analysis of finite SSH systems in real space. In particular, the uncertainty relations (20) and (21) express concisely the tradeoff between the localizability of information in topological phase transitions in real space and wave-vector space.

Perhaps the fundamental consequence of interpreting the information entropy density function $\rho_S(x)$ as the probability distribution resulting from an information entropy wave function $\psi_S(x)$ defined on a 1D manifold is that it reconciles the apparently conflicting notions of a local topological signal arising from a global property of the SSH systems. Indeed, while $\psi_S(x)$ is defined locally at every point of the 1D manifold, it is a single, global wave function encoding the spatial distribution of topological information of an ensemble of SSH Hamiltonians close to phase transition boundaries in parameter space. Therefore, the information entropy wave function $\psi_S(x)$ and its corresponding information entropy density function $\rho_S(x)$ can be pictured as emergent properties of an ensemble of quantum many-body systems near phase transitions.

## VII. DISCUSSION

Given the increasing complexity of systems studied in condensed-matter physics and the rising demand for materials with exotic and robust properties to power future technological progress, it is only expected that data-driven approaches to physics will grow in demand. Our work represents a step in this direction, as we have devised (~~section~~Sec. II) and implemented (~~section~~Sec. III) a data-driven approach to the discovery of previously unknown properties of topological materials from real-space data.

By starting from eigenvector data generated from the simulation of SSH systems in real space, proposing an approach based on eigenvector ensembling and decision trees and using model explainability to uncover the information entropy signatures presented in this ~~a~~paper~~rticle~~, and then exploring the numerical and theoretical possibilities offered by the information entropy signatures, our work exemplifies a full cycle of data-driven physics and illustrates how the interactions between machine learning and physics can be enriching to both disciplines.

The development of data-driven methods based on real-space lattice data will be particularly relevant to the study of disordered systems in condensed matter. Such systems usually break translational symmetry and therefore are not amenable to canonical wave-vector space methods. Thus, the discovery and engineering of topological features from real-space data as demonstrated in this work carries great promise to the theoretical investigation of these systems.

Furthermore, as is generally the case in engineering, the evolution of quantum technologies such as quantum computing and quantum communication will likely depend on a delicate balance between simplicity and robustness of components such as topological qubits. On the simplicity side, engineers try to build their systems with as little redundancy as possible to reduce design complexity, while for robustness redundancy is a necessary commodity to ensure error correction within the system. We expect that information-theoretic approaches to quantum materials such as the one advanced by this paper shall eventually become a staple of quantum engineering.

As we have seen, the use of real-space data enabled us to investigate how topological information is spatially distributed in SSH systems. This was demonstrated by the information entropy signatures of ~~se~~Sec.~~ction~~ IV, which were recovered from the Shannon entropy of ensembles of eigenvectors in each numerical experiment executed in ~~sec~~Sec.~~tion~~ III and led us to the ~~new~~ topological features of ~~sec~~Sec.~~tion~~ V and the emergent information entropy wave functions of ~~sec~~Sec.~~tion~~ VI. The existence of such signals that can be recovered from data from many distinct physical systems but are hard to conceptualize from sheer theoretical reasoning provides a clear example of how machine learning and model explainability can be important tools in the investigation of quantum materials.

The accuracy scores obtained in the numerical experiments performed in this paper were comparable to those reported in [30], where dense and convolutional neural networks were trained on wave-vector space data to predict the winding numbers of SSH Hamiltonians via supervised learning. This high accuracy level serves as a strong evidence that the entropy signatures presented here indeed express where topological information is most readily available in the SSH lattices investigated.

This paper should also be contrasted with [51], where the subject of investigation is the interpretability of neural network models trained to recognize topological phase transitions in some condensed-matter systems. In [51], interesting visualizations are shown demonstrating that the patterns captured by a single-layer feedforward neural network indeed map directly to known physical quantities that are relevant to the problems at hand. We agree that such tasks should be called *model interpretability*, as in that case the authors introspect into their models to make sure that they are learning patterns of physical pertinence to the systems being investigated. In our paper we preferred the term *model explainability*, as we used similar model introspection tools to propose previously unknown concepts and properties of the physical systems being investigated. While the nuances in the semantics of these two terms are the subject of often heated philosophical debates in the artificial intelligence community, this choice of nomenclature suits the practical application of these model introspection techniques to physics well.

Recent works have demonstrated the existence of local topological markers in real space that carry important information on the topological state of a system [52, 53]. Given the ~~new~~ DCT and DST topological features introduced in ~~sec~~Sec.~~tion~~ V which were shown to carry relevant topological information and the theoretical interpretation of the topological signals in terms of information entropy wave functions given in ~~s~~Sec.~~ection~~ VI, the results presented here suggest a ~~new~~different road for the theoretical exploration of local topological markers in terms of information theory as well. Whether there is any relationship between the local topological markers of [52, 53] and the information entropy wave functions discussed here is left for speculation.

The eigenvector ensembling algorithm employed in this work is likely to have further applications in data-driven physics. This is because most of physics is based on eigenvector decomposition, and statistical physics itself can be seen as an application of similar ensembling principles.

As a concrete example, the study of several many-body systems of current interest in condensed-matter physics is hindered by their large dimensionality. This problem, known as *the curse of dimensionality* in the scientific computing community, arises from the necessity of collecting or processing exponentially larger amounts of data as the feature space dimensionality of a problem grows. An approach based on eigenvector ensembling can be of use in such situations both as a dimensionality reduction tool and as a sampling strategy. The first case was illustrated in this work, where it was shown that relevant topological information of SSH systems can be retrieved from few sites in a lattice, which can be exploited as a dimensionality reduction strategy. The latter case, which was not explored here, also poses interesting possibilities, such as sampling eigenstates according to a desired distribution in Monte Carlo simulations of condensed-matter systems. Indeed, sampling eigenvectors from a carefully designed probability distribution can ultimately lead to a great reduction in dimensionality while still capturing all the relevant physics of a system. We therefore expect that a much broader class of data-driven physics problems could benefit from the techniques described in this paper.

Another interesting prospect is the combination of eigenvector ensembling with unsupervised learning algorithms. In the paper, our preference for decision trees and random forests was based on their powerful and accessible model explainability aptitudes. This choice was made in conformity with our main purpose, which was to exploit model explainability tools to investigate how topological information is distributed along a spatial lattice in SSH systems. Nevertheless, the eigenvector ensembling procedure we described here is flexible and can easily be repurposed for other supervised or unsupervised learning tasks.

One final comment should be made about the flourishing relationship between physics and machine learning. In this work we have demonstrated how a machine learning approach can provide ~~new~~ insights into complex physical phenomena of current interest. The other direction of this relationship (physics enhancing understanding in machine learning) is equally important. As the need for ever more powerful machine learning algorithms continues to grow,

FIG. 6. Information entropy signatures of the topological phase transitions from the numerical experiments of ~~sec~~Sec.~~tion~~ III. (a) In experiment 1 (~~section~~Sec. III A), the two sharp peaks in the Shannon entropy signal account for approximately 70% of reduction in information entropy. (b) In experiment 2 (~~section~~Sec. III B), the three visible peaks account for approximately 30% of reduction in information entropy.

the development of mathematical frameworks for understanding general data spaces (i.e., a physics of data) will be of crucial relevance. This pursuit is seen in many theoretical works investigating the intriguing connections between geometry, topology, and data [54–58].**[AU: Please note that Refs. 59–64 have not been cited. Please cite as appropriate, in consecutive order]**The detailed study of data generated by physical models with nontrivial geometrical and topological properties such as the SSH model may provide invaluable insights into the structure and shape of real-world high-dimensional data, since these models usually underscore well-known mathematical frameworks behind the data generating process, a feature that is often absent from machine learning applications. Thus, far from being restricted to applications in physics, the study of the topological and geometrical properties of data sets generated by physical models will also be of great value to the machine learning and artificial intelligence communities.

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