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# Anatomy of a Spin: The Information-Theoretic Structure of Classical Spin Systems

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Collective organization in matter plays a significant role in its expressed physical properties. Typically, it is detected via an order parameter, appropriately defined for a given system’s observed emergent patterns. Recent developments in information theory suggest how to quantify collective organization in a system- and phenomenon-agnostic way: decompose the system’s thermodynamic entropy density into a *localized entropy*, that solely contained in the dynamics at a single location, and a *bound entropy*, that stored in space as domains, clusters, excitations, or other emergent structures. We compute this decomposition and related quantities explicitly for the nearest-neighbor Ising model on the 1D chain, the Bethe lattice with coordination number  $k = 3$ , and the 2D square lattice, illustrating its generality and the functional insights it gives near and away from phase transitions. In particular, we consider the roles that different spin motifs play (cluster bulk, cluster edges, and the like) and how these affect the dependencies between spins.

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## I. INTRODUCTION

Collective behavior underlies a vast array of fascinating phenomena, many of critical importance to contemporary science and technology. Unusual material properties—such as superconductivity, metal-insulator transitions, and heavy fermions—have been attributed to collective behavior arising from the compounded interaction of system components [1]. Collective behavior is by no means limited to complex materials, however: the behavior of financial markets [2], epileptic seizures [3] and consciousness [4], and animal flocking behavior [5] are all now also seen as examples. And, we now appreciate that it appears most prominently via phase transitions [6, and references therein]. Operationally, collective behavior is detected and quantified using correlations or, more recently, by mutual information [7], estimated either locally via pairwise component interactions or globally. Exploring spin systems familiar from statistical mechanics, here we argue that these diagnostics can be substantially refined to become more incisive tools for quantifying collective behavior. This is part of the larger endeavor of discovering ways to automatically detect collective behavior and the emergence of organization [8].

Along these lines, much effort has been invested to study information-theoretic properties of the Ising model of statistical mechanics. Both Shaw [9] and Arnold [10]

studied information in 1D spin-strips within the 2D Ising model. Feldman and Crutchfield [11–13] explored several generalizations of the excess entropy, a well known mutual information measure for time series, in 1D and 2D Ising models as a function of coupling strength, showing that they were sensitive to spin patterns and can be used as a generalized order parameter. In one of the more thorough-going studies to date, Lau and Grassberger [14] computed the excess entropy using adjacent rings of spins to probe criticality in the 2D cylindrical Ising model. Barnett *et al.* [6] tracked information flows in a kinetic Ising system using both the pairwise and global mutual informations (generalized as the total correlation [15], it appears below) and the transfer entropy [16]. Abdallah and Plumbley [17] employed an extensive version of the bound information [15] on small, random spin glasses. Despite their successful application, the measures used to monitor collective phenomena in these studies were motivated information theoretically rather than physically, and so their thermodynamic relevance and structural interpretation have remained unclear.

To address this we decompose the thermodynamic entropy density for spin systems into a set of information measures, some already familiar in information theory [18], complex systems [19], and elsewhere [17]. For example, one measure that falls out naturally—the bound entropy—is that part of the thermodynamic entropy accounting for entropy shared *between* spins. This is in contrast to monitoring collective behavior as the difference between the thermodynamic entropy and the entropy of a hypothetical distribution over uncorrelated spins—the total correlation mentioned above. In this way, the decomposition

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provides a physical basis for informational measures of collective behavior, in particular showing how the measures lead to interpretations of emergent structure in system configurations.

To make this argument and illustrate its consequences, Section II first defines notation and lays the groundwork for our decomposition. Section III then derives the decomposition. Section IV outlines the computational methods for estimating the resulting quantities, using them to interpret emergent organization in the nearest-neighbor ferromagnetic Ising model in one dimension (Section IV A), in the Bethe lattice with coordination number  $k = 3$  (Section IV B), and in the two-dimensional square Ising lattice (Section IV C). Having established the different types of entropy in spin systems and connections to their underlying physical structures, we conclude by suggesting applications and future directions.

## II. SPIN ENTROPIES

We write  $\sigma$  to denote a configuration of spins on a lattice  $\mathcal{L}$ ,  $\sigma_i$  for the particular spin state at lattice site  $i \in \mathcal{L}$ , and  $\sigma_{\setminus i}$  the collection of all spin states in a configuration excluding  $\sigma_i$  at site  $i$ . The random variable over all possible spin configurations is denoted  $\sigma$ , for a particular spin variable  $\sigma_i$ , and for all spin variables but the one at site  $i$ ,  $\sigma_{\setminus i}$ . As a shorthand, we write  $\sigma \in \sigma$  and similar to mean indexing into the event space of the random variable  $\sigma$ .

We study the ferromagnetic spin-1/2 Ising model with nearest-neighbor interactions in the thermodynamic limit whose Hamiltonian is given by:

$$\mathcal{H}(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad (1)$$

where  $\langle i, j \rangle$  denotes all pairs  $(i, j)$  such that the sites  $i$  and  $j$  are directly connected in  $\mathcal{L}$  and the interaction strength  $J$  is positive. We assume the system is in equilibrium and isolated. And so, the probability of configuration  $\sigma$  occurring is given by the Boltzmann distribution:

$$p(\sigma) = \frac{1}{Z} e^{-\mathcal{H}(\sigma)/k_B T}, \quad (2)$$

where  $Z$  is the partition function.

The *Boltzmann entropy* of a statistical mechanical system assumes the constituent degrees of freedom (here spins) are uncorrelated. To determine it, we use the *isolated spin entropy*:

$$H[\sigma_0] = -p(\uparrow) \log_2 p(\uparrow) - p(\downarrow) \log_2 p(\downarrow),$$

where  $p(\uparrow) = (1 + m)/2$  is the probability of a spin being up,  $p(\downarrow) = (1 - m)/2$  is the probability of a spin being down, and  $m = (\#\uparrow - \#\downarrow)/|\mathcal{L}|$  is average magnetization in a configuration. The site index 0 was chosen arbitrarily and represents any single spin in the lattice. The system's Boltzmann entropy is then the extensive quantity  $H_B = |\mathcal{L}| \cdot H[\sigma_0]$ .

As Jaynes [20] emphasizes, though correct for an ideal gas,  $H_B$  is not the empirically correct system entropy if a system develops internal correlations. In our case, if spins are correlated across the lattice, one must consider entire configurations, leading to the *Gibbs entropy*:

$$H[\sigma] = - \sum_{\sigma \in \sigma} p(\sigma) \log_2 p(\sigma) \quad (3)$$

and the *thermodynamic entropy density*  $h$ , the entropy per spin when the entire lattice is considered:

$$h = \frac{H[\sigma]}{|\mathcal{L}|}.$$

Note that we dropped the factor  $k_B$  and used the base-2 logarithm. Our use of the letter  $h$  as opposed to  $s$  is meant to reflect this multiplicative constant difference. It is easy to see that  $H[\sigma] \leq H_B$ . Thus, the Boltzmann entropy is typically an overestimate of the true thermodynamic entropy.

More to the point, in the thermodynamic limit the Boltzmann entropy  $H_B$  and Gibbs entropy  $H[\sigma]$  differ substantially. As Jaynes shows [20], the difference directly measures the effect of internal correlations on total energy and other thermodynamic state variables. Moreover, the difference does not vanish, rather it increases proportionally to system size  $|\mathcal{L}|$ .

Before leaving the differences between entropy definitions, it is important to note that Boltzmann's more familiar definition— $S = k_B \ln W$ —via the number of microstates ( $W$ ) associated with a given thermodynamic macrostate is consistent with Gibbs' definition [20]. This follows from Shannon's deep insight on the *asymptotic equipartition property* that  $2^{h|\mathcal{L}|}$  measures the volume of *typical* microstates: the set of equiprobable configurations that are simultaneously most numerous *and* capture the bulk of the probability—those that are typically realized. (See Refs. [21, Sec. 21], [7, Ch. 3] and [22, 23].) Thus, Boltzmann's  $W$  should be interpreted as the size (phase space volume) of the typical set associated with a particular thermodynamic macrostate. Given this agreement, we focus Gibbs' approach. Though, as we now note, the contrast between Gibbs' entropy  $H[\sigma]$  and Boltzmann's  $H_B$  leads directly to our larger goals.

### III. DECOMPOSING A SPIN'S THERMODYNAMIC ENTROPY

Since we are particularly interested here in monitoring the appearance of internal correlations, the difference between the Boltzmann and Gibbs entropies suggests itself as our first measure of a system's internal organization. If each spin were independent,  $H[\sigma_0] = h$ . For example, this is true at  $T = \infty$  for the Ising model and for site percolation models. If there are correlations between spins, however, then  $h < H[\sigma_0]$ , as just noted for the extensive quantities. Their difference is the *total correlation density* [15]:

$$\begin{aligned} \rho &= H[\sigma_0] - h \\ &= \frac{T[\sigma]}{|\mathcal{L}|} , \end{aligned}$$

$T[\sigma]$  here is the Kullback-Leibler divergence [7] between the distribution over entire configurations and the product of isolated-spin marginal distributions. Now called the *total correlation* [15], this measure of internal correlation was wholly anticipated by Gibbs, as Jaynes notes [20, Eq. (4)]. Since  $\rho$  vanishes only when each spin is independent, one might consider it a measure of pattern or structure in a spin system. While this is certainly reasonable as an operational definition, our next step decomposes both  $h$  and  $\rho$  into more nuanced quantities.

Continuing, we recast the Gibbs thermodynamic entropy  $H[\sigma]$  as the sum of two nonnegative terms; starting from the configuration entropy in its standard statistical form Eq. (3) and manipulating it into two terms:

$$\begin{aligned} H[\sigma] &= - \sum_{\sigma \in \sigma} p(\sigma) \log_2 \left[ p(\sigma) \frac{\prod_{i=1}^{|\mathcal{L}|} p(\sigma_i | \sigma_{\setminus i})}{\prod_{i=1}^{|\mathcal{L}|} p(\sigma_i | \sigma_{\setminus i})} \right] \\ &= R[\sigma] + B[\sigma] , \end{aligned} \quad (4)$$

where  $R[\sigma]$  and  $B[\sigma]$ , known as the *residual entropy* and *bound information* [15, 17, 18], are the following measures:

$$\begin{aligned} R[\sigma] &= \sum_{i=1}^{|\mathcal{L}|} \left[ - \sum_{\sigma \in \sigma} p(\sigma) \log_2 p(\sigma_i | \sigma_{\setminus i}) \right] \\ &= \sum_{i=1}^{|\mathcal{L}|} H[\sigma_i | \sigma_{\setminus i}] , \end{aligned} \quad (5)$$

and

$$\begin{aligned} B[\sigma] &= - \sum_{\sigma \in \sigma} p(\sigma) \log_2 \frac{p(\sigma)}{\prod_{i=0}^{|\mathcal{L}|} p(\sigma_i | \sigma_{\setminus i})} \\ &= H[\sigma] - \sum_{i=0}^{|\mathcal{L}|} H[\sigma_i | \sigma_{\setminus i}] . \end{aligned} \quad (6)$$

Note that both  $R[\sigma]$  and  $B[\sigma]$  are nonnegative and bound from above by  $H[\sigma]$ . Spatial densities are denoted in lower case:  $h = H[\sigma]/|\mathcal{L}|$ ,  $r = R[\sigma]/|\mathcal{L}|$ , and  $b = B[\sigma]/|\mathcal{L}|$ . We consider their thermodynamic limit, where  $|\mathcal{L}| \rightarrow \infty$ .

Similarly, we can begin with the total correlation of spins  $T[\sigma]$  and break it in to two terms:

$$\begin{aligned} T[\sigma] &= \sum_{\sigma \in \sigma} p(\sigma) \log_2 \frac{p(\sigma)}{\prod_{i=1}^{|\mathcal{L}|} p(\sigma_i)} \\ &= B[\sigma] + Q[\sigma] , \end{aligned} \quad (7)$$

where  $B[\sigma]$  is as above. Though perhaps not clear here,  $B[\sigma]$  is naturally a component of  $T[\sigma]$ ; see Ref. [15, Figs. 7c and 7d].  $Q[\sigma]$  is the *enigmatic information* [15]:

$$\begin{aligned} Q[\sigma] &= \sum_{\sigma \in \sigma} p(\sigma) \log_2 \frac{p(\sigma)^2}{\prod_{i=1}^{|\mathcal{L}|} p(\sigma_i) \prod_{j=1}^{|\mathcal{L}|} p(\sigma_j | \sigma_{\setminus j})} \\ &= T[\sigma] - B[\sigma] , \end{aligned} \quad (9)$$

and again, we consider the spatial density  $q = Q[\sigma]/|\mathcal{L}|$  in the thermodynamic limit.

Let us now interpret the physics captured by these entropy components. First,  $H[\sigma_0]$  quantifies the entropy per spin ignoring any dependencies (*e.g.*, correlations) between spins. The thermodynamic entropy density  $h$ , however, is the entropy per spin including dependencies. Continuing in this way, from Eq. (5)  $r$  is the entropy per spin remaining after these dependencies have been factored out, meaning it is the average amount of *independent* entropy, entropy per spin when we know the state of the other spins in the lattice. With this logic,  $b$  is the portion of the thermodynamic entropy density that comes from dependencies and is, therefore, the average amount of *dependent* entropy per spin. As we shall see, compared to  $\rho$  this provides a complementary, quantitatively different, and more physically grounded approach to quantifying dependencies among spins.

This completes, in effect, our decomposition of the isolated-spin entropy  $H[\sigma_0]$ , shown schematically in Fig. 1. To take stock, let's back up a bit. Recall that  $\rho$  is the

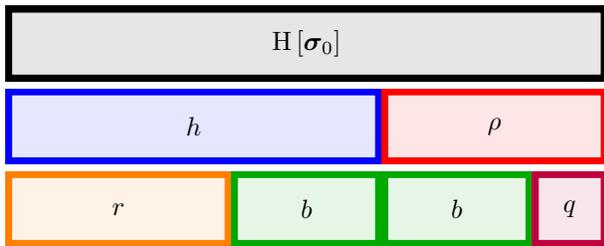


FIG. 1. Decomposition of the isolated-spin entropy  $H[\sigma_0]$ . First, into the Gibbs thermodynamic entropy density  $h$  and the total correlation  $\rho$ . Second, the thermodynamic entropy into the localized density  $r$  and the bound information density  $b$ , and the total correlation density  $\rho$  into  $b$  and the enigmatic information density  $q$ .

difference between  $H[\sigma_0]$ , which ignores the dependencies between the spins, and the thermodynamic entropy density  $h$ . That is,  $\rho$  is the difference between the isolated-spin entropy and how much entropy ( $h$ ) there actually is. Whereas,  $b$  is the difference between the thermodynamic entropy  $h$  and the amount of independent entropy  $r$  there is. In addition,  $b$  is also part of  $\rho$  [15], leaving  $q$  which therefore quantifies potential dependencies not present in the thermodynamic entropy.

Let’s explore the consequences of this decomposition. Although  $r$  and  $b$  are components of the thermodynamic entropy density  $h$ —itself a measure of the irreducible per-spin randomness—individually they have very different meanings that give insight into the interplay of randomness and ordering. The first,  $r$ , is the average amount of unshared entropy, quantifying randomness remaining in a single spin given the exact configuration of the rest of the lattice. For this reason we refer to it as the *localized entropy*. In the limit of high and low temperature,  $r$ ’s behavior is intuitive. At low temperature the lattice is entirely aligned, and so there is no randomness in individual sites given the global alignment. At high temperatures, each spin is independent, and so there is full randomness in a site, even knowing its surroundings.

The other quantity  $b$  is the entropy remaining in a spin when the localized entropy is removed, and so it captures the thermodynamic entropy shared between a spin and the rest of the lattice. We refer to it as the *bound entropy*. Its limits are similarly intuitive. At low temperatures there is no randomness to share, and so  $b = 0$ . Similarly, at high temperatures all randomness is localized, and so no entropy can be shared and bound entropy also vanishes. At intermediate temperatures, though spins are in flux, a spin’s context does at least in part influence its alignment and so  $b > 0$ . We refer to the temperature at which  $b$  is maximized by  $T_b$ .

Finally, we consider the enigmatic information density  $q$ . As a component of  $\rho$  it also reflects dependencies, but

in a way different from  $b$ . The bound entropy captures dependencies that are also part of the thermodynamic entropy, but  $q$  captures those that are not. As we shall see in Section V, this means it is sensitive to the interior of clusters. At low temperatures, we expect  $q$  to be small, since  $H[\sigma_0]$  is small. At high temperatures, there are no dependencies between spins, and so we also expect  $q$  to be small. At intermediate temperatures, just like  $b$ , we expect  $q$  to take larger values. This suggests that  $q$  effectively captures the effect of clusters beyond what is expected if the spins were independent; *e.g.*, as in a site percolation model. In short, this says that  $q$  behaves as a sort of generalized order parameter, peaking at  $T_c$ .

## IV. RESULTS

To explore what the entropy components reveal, we simulated the ferromagnetic spin-1/2 Ising model on one-(1D) and two-dimensional (2D) square lattices and on the Bethe lattice. As part of this, we provide analytical results for the 1D chain and the Bethe lattice and show that they match results from simulation.

And, we use analytic results whenever possible for the 2D lattice. For example, only  $r$  needs to be estimated from simulation and that result is then combined with analytic values (for  $h$ ,  $H[\sigma_0]$ , and  $\rho$ ) to compute  $b$  and  $q$ . All simulation results were obtained using the Wolff algorithm [24]. Estimating  $b$  requires estimating both  $h$  and  $r$  accurately. To do so, we make use of the global Markovian property of spin lattices [25]. In the case of  $r$  we merely condition a spin on all its nearest neighbors—spins directly coupled via the Hamiltonian Eq. (1). For  $h$  we use the method of Ref. [26]. In both cases, Ref. [27]’s entropy estimator  $\hat{H}_2$  was used to decrease the number of configuration samples needed to converge to known analytic results. In cases where analytic results are available, simulation results match to within standard error bars smaller than plot line widths.

### A. 1D Ising Model

Simple Ising models have been broadly adapted to understand simple collective phenomena in fields ranging from surface physics [28, 29] and biophysics [30, 31] to economics [32]. The Ising model on a one-dimensional lattice ( $\mathcal{L} = \mathbb{Z}$ ) can be fully analyzed in closed form. Unfortunately, its emergent patterns are rather limited; for example, it does not exhibit a phase transition [33]. However, the exact solutions provide an important benchmark and so it is an excellent candidate with which to

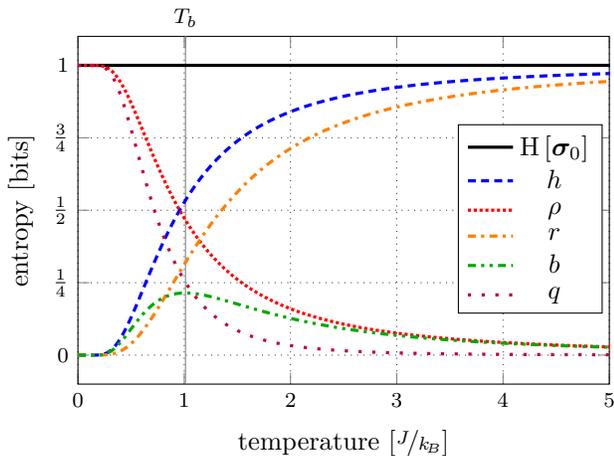


FIG. 2. Thermodynamic entropy decomposition for the 1D, nearest neighbor, ferromagnetic spin-1/2 Ising model: Entropy density  $h$  and the localized entropy density  $r$  both monotonically increase with temperature, but the bound entropy density  $b$  is maximal near  $T_b \approx 1.0117 J/k_B$ , indicating that thermodynamic entropy is mostly shared across nearby spins at that temperature.

start and provides a base from which to generalize [34–37]. Simulations were performed on a lattice of size  $N = 1024$  and the analytic results computed using a transfer matrix approach combined with the aforementioned Markovian property.

Independent of sporting a phase transition or not, the argument that  $b$  maximizes between temperature extremes still holds and Fig. 2 verifies this. The bound entropy  $b$  reaches a maximal value at  $T_b \approx 1.0117 J/k_B$  and this is not (cannot be) associated with a phase transition. At lower temperatures,  $b$  is the dominant contributor to the thermodynamic entropy density  $h = r + b$ . Whereas at higher temperatures,  $r$  is the dominant contributor. Similarly, at lower temperatures  $q$  is the dominant contributor to  $\rho$ , and  $b$  is the dominant contributor at higher temperatures. Section V below demonstrates why  $b$  peaks where it does and to which spin-configuration features each measure is sensitive. For now, let’s continue with system phenomenology.

### B. Bethe Lattice Ising Model

What role does the underlying lattice topology play in determining the balance between local randomness and spatially shared information that configurations achieve? Spins on the Bethe lattice, in which  $\mathcal{L}$  is an infinite Cayley tree with coordination number  $k$ , is an ideal candidate since the absence of loops makes it possible to compute quantities analytically. Moreover, spin configurations

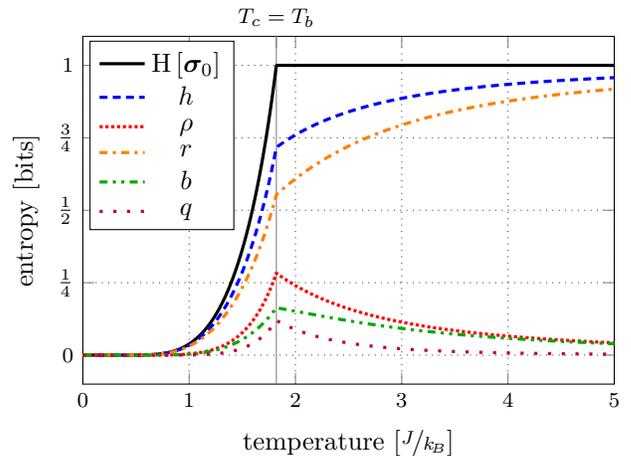


FIG. 3. Thermodynamic entropy decomposition for the Ising model on a Bethe lattice. By far and away, and unlike the 1D spin lattice, the individual spin disorder  $r$  is the dominant contributor to entropy density  $h$  over the entire temperature range. Of the information generated, relatively little ( $b$ ) is stored in patterns.

exhibit a phase transition at critical temperature [34]:

$$T_c = 2J \left[ k_B \ln \left( \frac{k}{k-2} \right) \right]^{-1}. \quad (10)$$

We analytically computed the entropy decomposition for a Bethe lattice with coordination number  $k$ , the details of which appear in Appendix A. The simulation results, matching the analytic to high precision, were performed on a 1,000 node 3-regular random graph, which has no boundary and is locally Bethe lattice-like.

Figure 3 presents the results for a Bethe lattice with coordination number  $k = 3$ , though other  $k$ s behave similarly. Interestingly, the information measures have a discontinuity in their first derivatives, and this happens at the phase transition  $T_c$ . Furthermore, the bound entropy is maximized there:  $T_b = T_c \approx 1.8205 J/k_B$ . Opposite the 1D lattice, at small  $T$  the dominant contributor to  $h$  is the local randomness  $r$ . Thus, not only does this change in lattice topology induce a phase transition, but it also inverts the components’ contributions to thermodynamic entropy density. This, in turn, indicates a rather different underlying mechanism that supports entropy production. Also, unlike 1D,  $b$  is the dominant contributor to  $\rho$  at both low and high temperatures.

### C. 2D Ising Model

Unlike its 1D sibling, the nearest-neighbor ferromagnetic Ising model in two dimensions ( $\mathcal{L} = \mathbb{Z}^2$ ) has a phase transition at a finite critical temperature  $T_c = 2/\ln(1+\sqrt{2}) \approx$

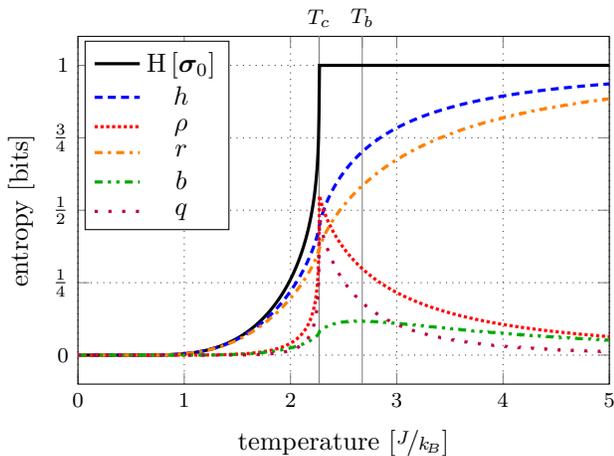


FIG. 4. Thermodynamic entropy decomposition for the 2D, nearest neighbor, ferromagnetic Ising model. Curves are from numerical simulation with sufficient size that standard errors are much smaller than the line widths. As in 1D, the entropy density  $h$  and the localized entropy density  $r$  monotonically increase with temperature. Here, also, the bound entropy density  $b$  reaches a maximal value at a nonextremal temperature: near  $T_b \approx 2.675 J/k_B$ , but this peak value is not at the critical temperature  $T_c \approx 2.2692 J/k_B$ , where domain sizes become scale-free.

$2.2692 J/k_B$ . In the 2D case, although Onsager's solution lets us calculate  $H[\sigma_0]$ ,  $h$ , and  $\rho$  [34], we do not have an analytic form for  $r$  and so the curves for  $r$ ,  $b$ , and  $q$  in Fig. 4 partly rely on estimates from a simulation on a  $128 \times 128$  lattice that averaged over 200,000 configuration updates. The resulting standard error bars were smaller than the line width.

Phase transition aside, the behaviors of  $h$ ,  $r$ , and  $b$ , seen in Fig. 4, are qualitatively similar to those in the 1D lattice. However, unlike 1D, at low temperatures  $r$  is the dominant contributor to  $h$ , similar to the Bethe lattice below its transition. Also, paralleling the Bethe lattice,  $b$  is the dominant contributor to  $\rho$  at both low and high temperatures. Like the 1D system, bound entropy is maximized in the disordered phase at  $T_b \approx 2.675 J/k_B$ , above  $T_c$ . Let us now turn to what configurational structures lead to the overall behaviors of these measures.

## V. DISCUSSION

At first, it may seem odd that  $T_b$  is not generically identical to  $T_c$ . To understand why, we need to investigate to which local spin-motifs the various measures are sensitive. To accomplish this, we take a pointwise approach. Each of the measures examined above is an average density, which is important when discussing the lattice as a whole and bulk thermodynamic properties. However, each local spin

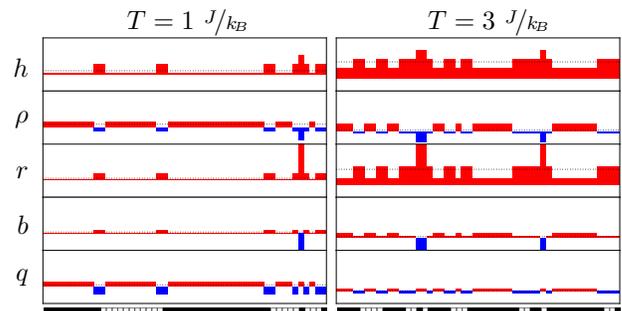


FIG. 5. Pointwise entropy-component analysis of the 1D Ising model at two temperatures. A segment of a spin configuration showing up spins (white cells) and down spins (black cells) is shown at the bottom.

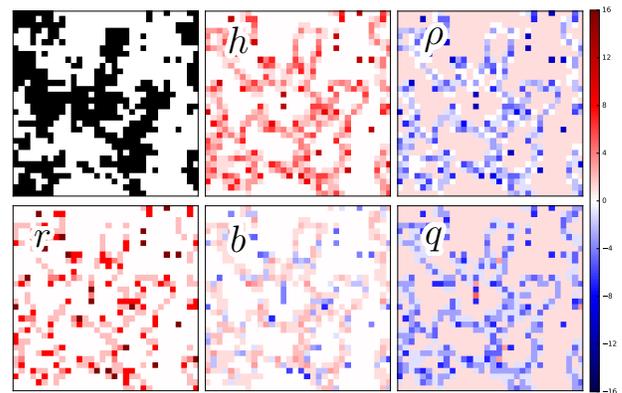


FIG. 6. Pointwise entropy-component analysis of the 2D Ising model at  $T_b$ .

configuration contributes differently to this average. For example, an up spin surrounded by down spins contributes to the measures differently than an up spin surrounded by other up spins.

To quantify this, we appeal to local forms of the densities we are considering. This is possible on square lattices  $\mathcal{L} = \mathbb{Z}^d$ , due to the existence of conditional forms of the entropy density; see Ref. [38, Thm. 2.9]. The conditional forms for each of the component quantities are weighted averages over quantities of the form  $\log_2(\bullet)$  [15]. The latter quantities are known as *pointwise measures*. We can more directly understand how local motifs contribute entropy and what kind of entropy by plotting the pointwise measures over a given lattice configuration.

Figures 5 and 6 show the results of the pointwise analysis in 1D and 2D lattices. In all cases, the spatial average of the displayed quantities corresponds (in the thermodynamic limit) with the values reported in Figs. 2 and 4.

There are several immediate similarities that allow for structural interpretation. For example, pointwise  $q$  is positive within the bulk of a cluster and negative on

its edges. Highlighting opposite features, pointwise  $r$  is negligible within the bulk, but positive along edges, particularly corners and isolated spins. The pointwise bound entropy  $b$ , however, is more nuanced in its behavior. Considering Figure 5, at lower temperatures it is sensitive to cluster edges more so than cluster bulk. At higher temperatures, however, this relationship flips and it is more sensitive to the bulk. For all temperatures, it is negative for isolated spins (clusters of size 1).

In contrast, we see that at not-too-high temperatures pointwise  $b$  is largely sensitive to cluster boundaries. We speculate that, as in Ref. [6], the maximization of  $b$  in the disordered phase is due to complex interactions between cluster sizes and their surface area. This may also shed light on why  $b$  does in fact peak at  $T_c$  on the Bethe lattice. On the square lattice, cluster boundaries have a tendency to smooth due to the presence of correlations flowing along short loops in the lattice topology. The Bethe lattice has no such loops, and so there is no pressure to reduce surface area. This suggests that  $b$  will generically peak at  $T_c$  for systems where boundaries are not constrained by system energetics and that the energetic smoothing of cluster boundaries drives  $b$  to peak in the more “textured” disordered phase.

Interestingly, local (conditional) forms of the thermodynamic entropy density and other measures are unknown, and may not exist, for general lattices such as the Bethe lattice, let alone random graphs. While techniques such as that in Ref. [39] exist that can estimate the thermodynamic entropy density for a ferromagnetic Ising model on an arbitrary graph, the interpretation of an entropy density in such systems is problematic as each node may have differing connectivity. Therefore, while global averages may exist for arbitrary topologies and may even be tractably estimated, their structural meaning is vastly more challenging. If local estimates, such as those used for the pointwise analyses above, existed then studies such as which nodes in a graph contribute most to collective behavior could be undertaken. These concerns are touched on by the informational analyses of frustration in spin glasses by Robinson *et al.* [40]. More study is required, however.

## VI. CONCLUSIONS

As noted in the beginning, even the earliest debates over entropy’s statistical foundation turned on contrasting its thermodynamic components—Boltzmann’s isolated-spin entropy versus the Gibbs global entropy. From a modern perspective their difference, well known to Gibbs, is a generalized mutual information that measures the degree

of individual-component independence, now called the total correlation. Keying off this, we showed that the thermodynamic entropy density naturally decomposes further into two functionally distinct informational components: one quantifying independence among constituent spins and the other, dependence. The one quantifying dependence, the bound entropy  $b$ , quantifies collective behavior by expressing how much of the thermodynamic entropy density is locally shared. We then demonstrated the behavior of the bound entropy and related quantities for the nearest-neighbor ferromagnetic Ising model on a variety of lattices. We found that it does tend to a maximum at intermediate temperatures, though not always at the magnetic phase transition. We also found that the enigmatic information  $q$  generically is maximized at critical points, consistent with its interpretation in Ref. [41] as the component of the persistent mutual information [42] which identifies a certain kind of emergent noisy-periodic structure.

This brief phenomenological study of thermodynamic entropy components served to give a physical grounding for information measures and what they can reveal in spin systems on various lattice topologies. The results suggest many avenues of potential research. One topic to explore is the behavior of  $b$  in the Potts model, which switches from having a second-order phase transition in the magnetization to a first-order transition when the number of spin states exceeds four. Another setting of particular interest is to study the behavior of  $b$  in a frustrated system, such as the antiferromagnetic Ising model on a triangular lattice, paralleling Ref. [40]. Finally, as alluded to above, although beyond the present scope of this work, a next step is to consider informational measures for spins on arbitrary graphs, with the goal of providing insight into the roles that different nodes play in information processing and storage in complex dynamical networks.

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## Appendix A: Bethe Lattice Spin-Neighborhood Probabilities

Consider a Cayley tree with coordination number  $k$  and  $n$  shells. The total number of spins in such a tree is  $N = k[(k-1)^n - 1]/(k-2)$ . We denote the spins in the lattice using  $\sigma_i$ ,  $i \in [0, N-1]$ . Let us use the index 0 for the central spin and indices  $[1, k]$  for its neighbors. We use  $\sigma$  to denote a configuration—the state of all spins present in the Cayley tree. Following Ref. [34], we write the partition function for the Ising model on the Bethe lattice as:

$$Z = \sum_{\sigma \in \mathcal{C}} p(\sigma),$$

where  $p(\sigma) = \exp(\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j)$  is the unnormalized probability of the system being in a state  $\sigma$  and  $\mathcal{C}$  denotes the set of all possible configurations. As shown in Ref. [34], due to the Bethe lattice topology, the above expression

can be written as:

$$Z = \sum_{\sigma_0 \in \mathcal{C}_0} g_n(\sigma_0)^k,$$

where  $g_n(\sigma_0)$  is the partition function of the branch of the Cayley tree with its root at  $\sigma_0$ . Let  $g_n(\sigma_0) \rightarrow g(\sigma_0)$  in the limit of  $n \rightarrow \infty$  shells. Then, the spins not *close* to the Cayley tree leaves behave like those on the Bethe lattice with the same coordination number. In this limit, by explicitly accounting for the bonds between the central spin and its neighbors, we can write the partition function as:

$$Z = \sum_{\sigma_i \in \mathcal{L}} \exp\left(\beta J \sum_{i \in [1,k]} \sigma_0 \sigma_i\right) \prod_{i \in [1,k]} [g(\sigma_i)]^{k-1}.$$

From this, we obtain the joint probability of the central spin  $\sigma_0$  and its  $k$  neighbors as:

$$\begin{aligned} p(\sigma_0, \sigma_1, \dots, \sigma_k) &= \exp\left(\beta J \sum_{i \in [1,k]} \sigma_0 \sigma_i\right) \prod_{i \in [1,k]} [g(\sigma_i)]^{k-1} / Z. \end{aligned}$$

Dividing both numerator and denominator by  $[g(1)]^{k-1}$  we obtain:

$$p(\sigma_0, \sigma_1, \dots, \sigma_k) = \frac{\exp\left(\beta J \sum_{i \in [1,k]} \sigma_0 \sigma_i\right) \prod_{i \in [1,k]} \left[\frac{g(\sigma_i)}{g(1)}\right]^{k-1}}{\left[e^{\beta J} + e^{-\beta J} \left[\frac{g(-1)}{g(+1)}\right]^{k-1}\right]^k + \left[e^{-\beta J} + e^{\beta J} \left[\frac{g(\sigma_i)}{g(-1)}\right]^{k-1}\right]^k}. \quad (\text{A1})$$

This is the joint probability distribution of the central spin and its neighbors. We evaluate the above expression numerically by defining  $g(-1)/g(+1) = x$ . From Ref. [34, Eq. (4.3.14)], we know that  $x$  is the “stable” root of the

equation:

$$x = \frac{e^{-\beta J} + e^{\beta J} x^{k-1}}{e^{\beta J} + e^{-\beta J} x^{k-1}}. \quad (\text{A2})$$

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