Entropy of Ising model on Bethe lattice: how to define entropy on infinite system?

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We study the entropy of spins in Ising model defined on an infinite Bethe lattice. Thanks to the iterative branching structure of Bethe lattice, there is an exact solution of spin distribution for a cluster of spins. Based on that, Shannon entropy measurement of the spin cluster is obtained. It turns out that Shannon information diagram of spins have the same geometric structure as Bethe lattice. Two features are observed. Firstly, every spin has the same local environment in information diagram. Secondly, a pair of spins that are not nearest neighbors are shielded by any spin in the path linking them. In another word, there is no mutual information between non-nearest spins conditional on the spin in between. By that, the area corresponding to the additive information for each spin is regarded as entropy per spin. So we get one definition of density of entropy. Then a method only employing thermodynamic relationships is given also to get the density of entropy. Comparison indicates they are close. but numerically different. We think both of them are reasonable interpretations for entropy density. They both focus on central spins (those far away from boundaries at infinity), but at different levels. This is the reason of two distinct entropy density.

Entropy is an insightful indicator for disorder in a system. But the same entropy can be interpreted in two different ways. Microscopically, in the phase space for a canonical ensemble, entropy is the Shannon entropy for all accessible microscopic states. Macroscopically, as a thermodynamic quantity, entropy is regulated by thermodynamic relationships involving free energy, temperature and expectation of internal energy. For finite system, these two ways meet with the same value. For an infinite system , the definition of entropy is challenging. Since entropy is an extensive quantity, we have to define the density of entropy instead of total entropy. This method works well with bulky system where the bulk density is well-defined. However, things are different in the system in which surface sites are dominating, i.e., the ratio of surface area to the bulk volume does not vanish as size $\to \infty$. We need to be careful of the definition of entropy density: is that the entropy for bulk part or the whole system? Bethe lattice is a good example for this kind of infinite surface system. And Ising model is a well studied statistical model. So in this project we are going to discuss the entropy of Ising model on a Bethe lattice.

I. BACKGROUND

A. Ising model

Ising model and the generalized is statistical physics model of interacting spins on lattice. Some collective phenomena occur in these models including phase transition, universality in order parameter and frustration on specific lattice and. More importantly, it is a good scenario to understand how entropy regulate order and disorder in thermodynamic system.

In Ising model of N spins on lattice, each spin s_i can have 2 quantized values. The space of states is a discrete N dimensional one containing all possible spin configuration. With a configuration of spins S = $s_0, s_1, ...$, the Hamiltonian is:

$$H = -J \sum_{(i,j)} \delta(s_i, s_j) + h \sum_i s_i \qquad (1)$$

The interaction is only between nearest neighbor pairs (i,j). $\delta(s_i, s_j)$ is the Kronecker notation. With positive J (ferromagnetism), neighbors tend to have the same spin, hence less energy and more stable. With negative J (antiferromagnetism), the more stable configuration is associated with neighbors in different spins.Here we only consider the ferromagnetism scenario.

The second term is the coupling between each spin and external field h. With large h, spins will be forced into the same direction with h. Under critical temperature, a non-zero spontaneous magnetism exists while external field is gradually tuned to zero. Tuning from positive / negative external field leads to positive / negative spontaneous magnetism. So, $M|_{h\to h_+} \neq M|_{h\to h_-}$. This abrupt critical phenomena is a consequence from a bifurcation in partition function, which we will discuss later.

In fig. 1 and fig. 2, critical phenomenon of Ising model is shown. To be noticed, the phase transition does not emerge on every lattices in all dimensions. On Bethe lattice, there is a phase transition. But no phase transition shows up on the Cayley tree. So the infinite boundary distance is a key point here.

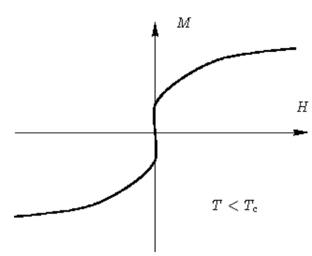

FIG. 1. Hysteresis phenomena at temperature below T_c. Even though the external field is tuned to zero, there is non-zero spontaneous magnetism.

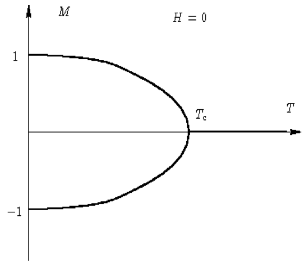

FIG. 2. Spontaneous magnetism versus temperature when external field is zero. Above T_c, it is zero. Below T_c, two non-zero values of spontaneous magnetism show up associated with hysteresis from positive or negative external field.

B. Bethe Lattice

Bethe lattice is a generalization from Cayley tree. It is a tree-like structure in which each node is equivalent to each other. All nodes have the same degree of q, which is called degree coordination. Starting from one node as a root, q nearest neighbors consist of the first shell. Every nearest neighbors have $q-1$ neighbors except the root one, then we have the second shell. We can pick any node as the root and will get the same Bethe lattice. To show the equivalence between node, Bethe lattice can be drawn on the hyperbolic plane. It is an infinite non-Euclidean plane with curvature in which every point is equivalent, like the feature of Bethe lattice. In fig. 3, fig. 4, a Bethe lattice with coordination 3 is shown on normal 2D plane and hyperbolic plane.

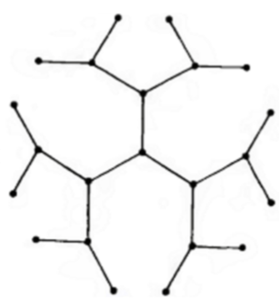

FIG. 3. Bethe lattice with coordination $q = 3$. Only the first 3 shells are shown. The whole lattice expands to infinity

C. Entropy density versus entropy rate

Shannon entropy measures the disorder of a system. If the probability distribution $Pr(S_i)$ of all state S_i is known, Shannon entropy is defined as:

$$H = -\sum_i Pr(S_i) log(Pr(S_i)) \tag{2}$$

In Ising model, those states S_i are every configurations of all spins in the phase space. So H grows with the size

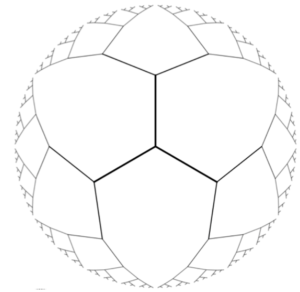

FIG. 4. Bethe lattice with $q = 3$ on a hyperbolic plane. If we zoom into every node, they have the same local structure with a 3 fold rotational symmetry and the same edge length.

of lattice. The density of entropy can be defined as a straightforward way:

$$h = \frac{H}{N} \tag{3}$$

Where N is the number of site in lattice. h is the effective entropy for each site. This definition assumes that each site has the same entropy. Actually, there is no physics meaning of entropy on one site. The motivation for entropy density is that we can show the whole entropy scales as N.

As a consequence, entropy density should be equivalent to the concept that how much entropy is gained when one more site is added in. Instead of investigating all spins, now we regard spins as a sequence of process site by site. In a 1D lattice, the process is scanning all spins from left to right. The entropy $H(N)$ in the state space corresponds to block entropy of length N. When $N \to \infty$, we know that these two definitions are really equivalent:

$$h = h_\mu = H(s_i|s_{i-1}s_{i-2}...) = H(s_i|s_{i-1}) \tag{4}$$

where h_μ is the entropy rate. Markov order equals 1 because only nearest neighbor interaction exists. For all square lattices in any dimensions, the equation above is valid. So entropy density is just entropy rate for those systems. In a Bethe lattice, a natural way to scan all sites is exploration of the whole lattice shell by shell from a root. Since it is not a stochastic process with a forward time direction, how should we define the rate? The Shannon information diagram unveils the fact that entropy grows in a branching way just like the Bethe lattice grows.

II. EXACT SOLUTION OF ISING MODEL ON BETHE LATTICE

Owing to the simple and iterative structure of Bethe lattice, there is a analytic exact solution of Ising model on it [1]. For a statistical model, knowing the partition function is the key to all thermodynamic quantities including entropy and free energy. Here, instead of solving the partition function of the whole system, we focus on it of subsystems. Define $g_n(s_i)$ as the partition function of a branch rooted at site i with spin s_i. To be noticed, the root i itself is not include into the subsystem. site i has one nearest neighbor $s_j$in that branch. Then partition function for this branch can be rewritten as product of partition functions for its own $q-1$ branches. In fig. 5, the g_n corresponding to different branches are shown.

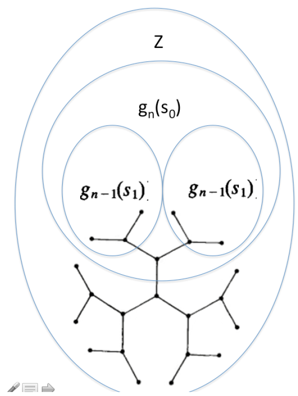

FIG. 5. g_n as partition function for branches and sub-branches. Here we choose root site $i = 0$. The first branch is the upward one with site $j = 1$ in it. Then this branch is decomposed into two sub-branches rooted at site $j = 1$. The partition function for the whole system is Z including all sites.

In a tree, branches are independent to each other. So sub-branches are independent sub-systems. The whole partition function is the product of sub-partition functions. So $g_n(s_0)$ can be rewritten as:

$$g_n(s_0) = \sum_{s_1} exp(Js_0s_1 - hs_1)g_{n-1}(s_1)^{q-1} \quad (5)$$

This iterative relationship is valid from any node in shell n to its neighbor in shell n+1. By that, we can get the joint distribution for any local connected cluster of spins. Typically, we investigate the root spin s_0 and all spins in the first shell $s_1, s_2, ..., s_q$. The joint distribution is[2]:

$$p(s_0, s_1, s_2, ..., s_q) = exp(\beta J \sum_{i\in[1,q]} s_0s_i) \prod_{i\in[1,q]} [g_{n-1}(s_i)]^{q-1}/Z \quad (6)$$

Where Z is the total partition function as:

$$\begin{aligned} Z &= \sum_{s_0} exp(-hs_0)g_n(s_0)^q \\ &= \sum_{s_0}\{\sum_{s_1} exp(Js_0s_1 - hs_1 - hs_0)g_{n-1}(s_1)^{q-1}\}^q \end{aligned} \quad (7)$$

Notice that $n \to \infty$, so g_n is also approaching to infinity. However, the ratio $x_n = \frac{g_n(s_i=+1)}{g_n(s_i=-1)}$ can be obtained by eq. (5). It is reasonable to assume $x_n \sim x_{n+1} \sim x$ when $n \to \infty$. From that, x is obtained by the relationship:

$$x = \frac{e^{-J} + e^J x^{q-1}}{e^J + e^{-J} x^{q-1}} \quad (8)$$

Solving this equation, we can get x numerically. There is only one solution when temperature is above T_c. There is a bifurcation at T_c, so two more solutions x_+ and x_- show up below T_c. These two non-zero solutions correspond to spontaneous magnetism. Substitute x back into eq. (6), the joint distribution is known.

III. SHANNON INFORMATION DIAGRAM

With the joint distribution of a cluster of spins. We can do Shannon entropy partition for them to get a information diagram. Let us focus on Bethe lattice with coordination 3. For a root spin 0 and its nearest neighbors $1, 2, 3$, Shannon partition of these four variables is shown in fig. 6. By the chain rule of conditional entropy, we can get:

$$I[1:2|0] = I[1:2|3,0] + I[1:2:3|0] = 0 \quad (9)$$

So there is no mutual information between two spins in first shell conditional on the root spin. Though the mutual information between them are not zero. Spins in the first shell are correlated, but the correlation is shielded by the spin in between them. In fig. 6, information diagram is shown. Be aware, there is a non-zero overlap between 1 and 2 inside 0. The graph is incorrect for the part inside 0. However, if we only care about how much entropy is gained from spin 1,2,3. The conclusion is each of them contribute $I[1|0,2,3] = I[1|0]$ as an entropy rate.

Also, entropy for each spin itself is the same. We can regard any of spins 0,1,2,3 as the root and get the same information diagram.

$$\begin{aligned} &I[0] = I[1] = I[2] = I[3] \\ &I[1|0] = I[0|1] \end{aligned} \quad (10)$$

Till now, we can use the expansion process to explore all spins on Bethe lattice. The entropy gain every time a new spin is added is the entropy of the new spin conditional on the spin from which it grows. The direct father spin is the casual state for the new spin. However, it is not a standard Markov order 1 process. New spins only depend on one past spin, but not the most recent past one.

$$I[s_{new}|S_{past}] = I[s_{new}|s_{directfather}] \quad (11)$$

To prove it, we also show the Shannon partition and information diagram of the second shell. fig. 8,fig. 9. Now we choose one root, all of the first shell and two spins in the second shell. Still, the previous conclusion is true. Information diagram has the same geometrical structure as Bethe lattice. fig. 10

measure	bits
H[0|1,2,3]	0.233
H[1|0,2,3]	0.313
H[2|0,1,3]	0.313
H[3|0,1,2]	0.313
I[0:1|2,3]	0.037
I[0:2|1,3]	0.037
I[0:3|1,2]	0.037
I[1:2|0,3]	0.000
I[1:3|0,2]	0.000
I[2:3|0,1]	0.000
I[0:1:2|3]	0.006
I[0:1:3|2]	0.006
I[0:2:3|1]	0.006
I[1:2:3|0]	0.000
I[0:1:2:3]	0.002

FIG. 6. Shannon partition of root spin and the first shell. Several zero mutual information are marked.

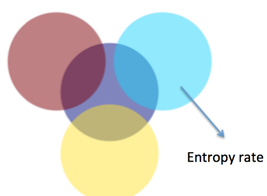

FIG. 7. Information diagram of root spin and the first shell. The half-moon area is the entropy rate.

IV. ENTROPY FROM THERMODYNAMIC VIEW

Entropy, as a thermodynamic quantity, is regulated by thermodynamic relationship:

$$F =< E > -TS - \frac{\partial F}{\partial H} = M \tag{12}$$

Where F is the free energy. Since every spin is equivalence, a concept of density of free energy can also be applied here. So the equation above is converted into:

$$f =< e > -Ts - \frac{\partial f}{\partial H} = m =< s_i > \tag{13}$$

f, e, s, m are all corresponding quantity for a single spin. Based on that, another entropy density s can be obtained. If we compare it with our previous entropy rate, they look similar in the trend from low temperature to high temperature. They even have the same critical temperature $T_c$and phenomenon. However, numerically they are distinct, especially for temperature around T_c. In fig. 11, both of them are shown. Entropy rate from information

measure	bits
H[0|1,2,3,4,5]	0.233
H[1|0,2,3,4,5]	0.233
H[2|0,1,3,4,5]	0.313
H[3|0,1,2,4,5]	0.313
H[4|0,1,2,3,5]	0.313
H[5|0,1,2,3,4]	0.313
I[0:1|2,3,4,5]	0.026
I[0:2|1,3,4,5]	0.037
I[0:3|1,2,4,5]	0.037
I[0:4|1,2,3,5]	0.000
I[0:5|1,2,3,4]	0.000
I[1:2|0,3,4,5]	0.000
I[1:3|0,2,4,5]	0.000
I[1:4|0,2,3,5]	0.037
I[1:5|0,2,3,4]	0.037
I[2:3|0,1,4,5]	0.000
I[2:4|0,1,3,5]	0.000
I[2:5|0,1,3,4]	0.000
I[3:4|0,1,2,5]	0.000
I[3:5|0,1,2,4]	0.000
I[4:5|0,1,2,3]	0.000

FIG. 8. Shannon partition of root spin and the first and second shells.

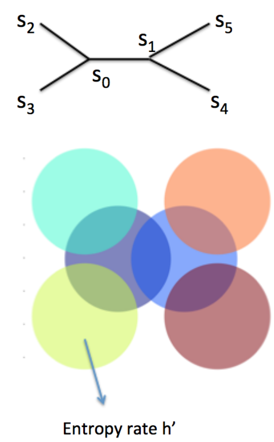

FIG. 9. Information diagram of root spin and the first and second shells. The half-moon area is the entropy rate.

measurement is slightly larger than the entropy density from thermodynamic relationship.

In both methods, we only concern about spins far away from boundary. In information measurement, the joint distribution is obtained from partition function rooted at spin s_i. And the assumption $x_n = x_{n+1}$ infers that only central spins are considered in entropy rate. The range on which information method is valid is smaller than the range on which thermodynamic method is valid. Though the latter one also calculates the density for central spins, they have different standards of "central".

In the future, I would like to explore the entropy of

FIG. 10. Information diagram has the same structure as Bethe lattice

Ising model on a very large Cayley tree. On such a finite system, $g_0(s) = 1$ is a seed for the iterative map from g_{n-1} to g_n. All the g_n can be obtained in a numerical way. Then we can see how the difference between entropy for boundary spins and central spins scale as size of lattice grows. It can help us to understand more about entropy distribution in infinite system.

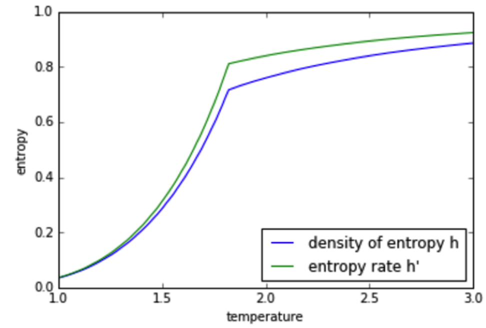

FIG. 11. Comparison between entropy density from thermodynamic view and entropy rate from information view

[1] R. Baxter, *Exactly Solved Models in Statistical Mechanics*, Dover books on physics (Dover Publications, 2007).

[2] V. S. Vijayaraghavan, R. G. James, and J. P. Crutchfield, ArXiv e-prints (2015), arXiv:1510.08954 [cond-mat.stat-mech].