Thermal statistics of small magnets

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While the canonical ensemble has been tremendously successful in capturing thermal statistics of macroscopic systems, deviations from canonical behavior exhibited by small systems are not well understood. Here, using a small two dimensional Ising magnet embedded inside a larger Ising magnet heat bath, we characterize the failures of the canonical ensemble when describing small systems. We find significant deviations from the canonical behavior for small systems near and below the critical point of the two dimensional Ising model. Notably, the agreement with the canonical ensemble is driven not by the system size but by the statistical decoupling between the system and its surrounding. A superstatistical framework wherein we allow the temperature of the small magnet to vary is able to capture its thermal statistics with significantly higher accuracy than the Gibbs-Boltzmann distribution. We discuss future directions.
I. INTRODUCTION

Recent advancements in magnetic resonance imaging have enabled individual spins in magnetic structures and atomic sized magnets to be observed\([1]\). Given their significant importance in miniaturization of electronic devices\([2]\), there is great theoretical interest in controlling the spin configurations of these small magnets using external control variables such as temperature and magnetic fields\([3]\).

In general, in order to manipulate the properties of a thermally fluctuating system, we first need to understand its statistics; the equilibrium probability distribution of its states as the system traverses through the phase space.

A natural choice to model the thermal statistics of small magnets (the ‘system’) embedded in and exchanging energy with a larger magnet (the ‘surroundings’) is the Gibbs-Boltzmann distribution. Here, the probability of observing any particular configuration of the system is given by

\[
p(x) = \frac{1}{Z(\beta)} \exp \left( -\beta \varepsilon(x) \right).
\]

In Eq. 1, \(x\) is the configuration of the system (for example, the collective state of all spins of a magnet), \(\varepsilon(x)\) is the Hamiltonian, and \(\beta\) is the inverse temperature. The Gibbs-Boltzmann distribution posits that the complex interactions between the system and its surroundings can be captured effectively by a single parameter; the inverse temperature \(\beta\). Remarkably, this simple description accurately predicts the thermal properties of a wide range of systems.

The Gibbs-Boltzmann distribution is derived with the help of two assumptions\([4]\). We imagine that the system and its surroundings whose configurations we denote by \(y\) are held at a constant energy \(\varepsilon_{\text{tot}}(x, y)\). First, we assume that the system under consideration is macroscopic. This assumption allows us to neglect the ‘boundary’ interactions between the system and the surroundings. That is, we can write:

\[
\varepsilon_{\text{tot}}(x, y) = \varepsilon(x) + \varepsilon_{\text{bath}}(y) + \varepsilon_{\text{int}}(x, y)
\]

\[
\approx \varepsilon(x) + \varepsilon_{\text{bath}}(y).
\]

The second assumption states that the system is much smaller compared to its surroundings, that is, \(\varepsilon_{\text{tot}}(x, y) \gg \varepsilon(x)\). With these two key assumptions, we can conclude that in the case when (1) the total energy \(\varepsilon_{\text{tot}}\) is kept constant and (2) all configurations of the universe
 SYSTEM + BATH) WITH ENERGY $\varepsilon_{\text{tot}}$ HAVE AN EQUAL PROBABILITY, THE NUMBER OF WAYS IN WHICH THE SYSTEM CAN BE IN CONFIGURATION $x$ IS EXACTLY EQUAL TO THE NUMBER OF WAYS IN WHICH THE BATH WILL HAVE ENERGY $\varepsilon_{\text{tot}} - \varepsilon(x)$. THIS NUMBER IS DIRECTLY PROPORTIONAL TO THE PROBABILITY OF OBSERVING THE SYSTEM IN CONFIGURATION $x$ AND IS GIVEN BY

$$p(x) \propto \Omega \left( \varepsilon_{\text{tot}} - \varepsilon(x) \right) = \exp \left( S_{\text{bath}} \left( \varepsilon_{\text{tot}} - \varepsilon(x) \right) \right)$$

$$\approx \exp \left( S_{\text{bath}} \varepsilon_{\text{tot}} - \beta \varepsilon(x) \right) \propto \exp \left( -\beta \varepsilon(x) \right).$$

(3)

Here, $S_{\text{bath}}$ is the microcanonical entropy of the bath and a Taylor series approximation is invoked to approximate $S_{\text{bath}}(\varepsilon_{\text{tot}} - \varepsilon(x))$. We note that for small systems, the second assumption is valid, but the first one breaks down because the strength of the system-surrounding interactions is of comparable magnitude to the interactions within the system. In fact, recent work using harmonic oscillators and hard sphere gasses has shown that the statistics of small systems differ considerably from the Gibbs-Boltzmann distribution; the fluctuations around the mean are much greater than the corresponding predictions. However, the potential failures of the Gibbs-Boltzmann distribution in describing small systems with realistic Hamiltonians, atomic sized magnets for example, are not well understood.

In this work, we use the two dimensional Ising model to study the thermal statistics of a small magnet embedded inside a larger magnet. The larger magnet (the ‘universe’) is kept at a constant energy, and the small magnet exchanges energy with its surroundings (the ‘bath’). In this setting, we systematically examine the ability of the Gibbs-Boltzmann distribution in capturing the thermal statistics of the small magnet. We find that there are large differences between the predictions from the Gibbs-Boltzmann distribution and the observed statistics of the magnet that depend on both magnet size and the temperature of the surroundings. Specifically, the high energy tails of the energy distribution are not well captured by the Gibbs-Boltzmann model. Our analysis suggests that the statistical coupling between the system Hamiltonian and the system-bath interaction Hamiltonian predicts whether Gibbs-Boltzmann distribution accurately describes the statistics of the small system. We also find that a superstatistical generalization of the Gibbs-Boltzmann distribution wherein the temperature of the system is allowed to fluctuate fits the statistics better. Future directions are discussed as well.
II. RESULTS

The Hamiltonian of a $N \times N$ two dimensional ferromagnetic Ising model is given by

$$\varepsilon(\bar{\sigma}) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

where $\bar{\sigma}$ is the configurational state of the magnet and $\langle i,j \rangle$ denotes that the summation is restricted over spin pairs $\sigma_i$ and $\sigma_j$ that are nearest neighbors. Individual spins can take on values $\sigma_i = \pm 1$, and the interaction between the spins is mediated by the coupling constant $J > 0$. Without loss of generality, in our calculations we choose $J = 1$. The schematic of our simulation system is shown in Fig. 1 and the simulation procedure is as follows. We construct a large $(100 \times 100)$ periodic two dimensional Ising lattice which represents the ‘universe’. The universe is held at a fixed energy $\varepsilon_{\text{tot}}$ and evolved using the Demon algorithm to sample configurations according to the microcanonical ensemble. Within this universe, we focus on small $n \times n$ sites, with $n \in [3, 10]$, that represent the ‘system’. The system exchanges energy with its surroundings as the universe samples equal-energy configurations. The energy is exchanged between the system and the bath through the spins at the boundary (see Fig. 1). This is exactly the setup of the canonical ensemble. Therefore, the statistics of the system should ideally be represented by the Gibbs-Boltzmann distribution.

We wanted to test the validity of the Gibbs-Boltzmann distribution for different system sizes and different average energies. To achieve this, we initialized the microcanonical universe at different constant energies by first running a small canonical simulation for the universe at a fixed temperature $T_{\text{universe}}$ and then switching over to the microcanonical simulation. Below, we use this temperature $T_{\text{universe}}$ to characterize the microcanonical universe. Alternatively, we can also characterize the universe by its average energy. The system exchanges energy with its surroundings as the universe samples equal-energy configurations. Relevant quantities are recorded: the system configuration, the system energy, and the interaction energy between the system and the surroundings. The details of the simulation procedure and location of scripts are provided in Appendix A.

Using these sampled spin configurations, we fit a Gibbs-Boltzmann model to the distribution of energies by tuning the inverse temperature $\beta$. The distribution is fit by matching the average energy of the system to the one predicted by the Gibbs-Boltzmann distribution. The exact procedure is outlined in more detail in Appendix B. The distribution of energies
FIG. 1. The schematic of our simulation. A large square microcanonical lattice is simulated. From the interior of that lattice small square spin sites are sampled (shaded in green). It is important to note that while spins that contribute to the boundary energy interact with spins outside of the system, the only interactions that contribute to the boundary energy are those that are across the boundary (shaded in red).

predicted by the Gibbs-Boltzmann model are of the form

\[ p(\varepsilon) \propto \Omega(\varepsilon) \exp (-\beta \varepsilon), \]  

where \( \Omega(\varepsilon) \) is the microcanonical partition function of the small system when held at a constant energy \( \varepsilon \).

In Fig. 2 we present the distribution of energies \( p(\varepsilon) \) as obtained from the simulations and the corresponding Gibbs-Boltzmann fits for a 4 × 4 and a 8 × 8 site at temperatures \( T = 1.9 \) and \( T = 2.7 \). We see clearly that for temperatures well above the critical point of the infinite two dimensional Ising model (\( T \approx 2.27 \)), the Gibbs-Boltzmann distribution accurately describes the distribution of energies, even for very small systems. At the same time, there are systematic deviations for temperatures below the critical point. First, there is a significant deviation at low energies. This arises because of the idiosyncrasies of the definition of the boundary in the Ising model (see Appendix C). Second, and most importantly, the Gibbs-Boltzmann distribution is unable to capture the high energy tail of the
FIG. 2. Distribution of energies in the small system and comparison with the predictions from the Gibbs-Boltzmann distribution. The energy distributions $p(\varepsilon)$ for $4 \times 4$ Ising sites at temperatures (a) $T = 1.9$ and (b) $T = 2.7$, and for $8 \times 8$ Ising sites at temperatures (c) $T = 1.9$ and (d) $T = 2.7$. The Gibbs-Boltzmann distributions were fitted by tuning $\beta$ to match the average energy.

distribution.

For a more insightful analysis, we fit the Gibbs-Boltzmann distribution to simulated energy distributions for a range of temperatures and systems sizes. In Fig. 3, we plot the absolute difference in standard deviation of the energy distribution, normalized by $n$, as estimated from the simulation and the Gibbs-Boltzmann fit. As above, the Gibbs-Boltzmann fit was obtained by tuning the system temperature to match the average energy estimated from the simulation. We note that the best fit temperatures were consistently lower than the temperature of the universe. This discrepancy of differences in temperatures of a small system embedded inside a larger system have been previously described as well.

The standard deviation of the energy distribution for canonical system grows as the square root of the system size $\sigma \propto \sqrt{n \times n} \propto n$. Therefore, this normalization ensures that there are no system-size based artifacts. We observe two trends. First, the degree of convergence of the Gibbs-Boltzmann fit depends on both the system size and the temperature of the bath. Notably, as the size of the system increases the deviations between the Gibbs-Boltzmann and simulated distribution occurs at successively lower temperatures, until for an $10 \times 10$
FIG. 3. **Accuracy of the Gibbs-Boltzmann distribution in fitting the energy distribution.** The absolute difference in the standard deviation of the simulated energy distribution and the corresponding Gibbs-Boltzmann fit.

sample we observe the deviations become negligible across all temperatures tested. This size potentially marks the convergence of the system to the canonical ensemble.

Additionally, we see the Gibbs-Boltzmann distribution fits the simulated energy distribution for sufficiently high temperatures, even for the smallest system sizes. The high temperature convergence for all system sizes tested indicates that the assumption of a macroscopic systems may not be necessary in order to apply the Gibbs-Boltzmann model. We hypothesize that the accuracy of the Gibbs-Boltzmann distribution is driven also by the decoupling between the system and the bath. We quantify this decoupling using the mutual information between the internal energy distribution for the system $\varepsilon$, and the system-bath interaction energy distribution $\varepsilon_{\text{int}}$. For the joint distribution $p(\varepsilon, \varepsilon_{\text{int}})$ of system size $n \times n$ and temperature $T$, the mutual information is defined as

$$I(n, T) = \sum_{\varepsilon, \varepsilon_{\text{int}}} p(\varepsilon, \varepsilon_{\text{int}}) \log \left( \frac{p(\varepsilon, \varepsilon_{\text{int}})}{p(\varepsilon)p(\varepsilon_{\text{int}})} \right).$$  

(6)

The mutual information quantifies the covariance between the two variables $\varepsilon$ and $\varepsilon_{\text{int}}$, and is zero iff the two variables are statistically independent of each other. Fig. 4 displays the mutual information between the boundary and internal energy of the system for the range of system sizes and temperatures tested. To avoid system size effects, the mutual information is normalized by the logarithm of the total number of different energy states for the system. The region in which there is a high degree of mutual information between the two distri-
FIG. 4. Mutual information between system energy and the strength of the system-
bath boundary interactions. We have normalized the mutual information by $\log(n_E)$, the
number of discrete energies for a $n \times n$ Ising model.

butions coincides with the region where deviations from the Gibbs-Boltzmann distribution
are high (see Fig. 3 and Fig. 4). Indeed, the Spearman correlation between the mutual
information and divergence from the Gibbs-Boltzmann distribution across all temperatures
and system sizes is 0.8 ($p < 10^{-20}$). This observation suggests that the decoupling be-
tween the system and the bath could be a predictor of convergence to the Gibbs-Boltzmann
distribution.

A. Superstatistics confers a better fit to the statistics of small systems

How do we fix the discrepancy between the Gibbs-Boltzmann distribution and the ob-
served statistics? One way forward is as follows: from Eq. 3, we write the probability of
observing the system configuration

$$p(\mathbf{x}) \propto \Omega (\varepsilon_{\text{tot}} - \varepsilon(\mathbf{x}) - \varepsilon_{\text{int}}(\mathbf{x}, y))$$
$$= \exp (S_{\text{bath}} (\varepsilon' - \varepsilon(\mathbf{x})))$$
$$\approx \exp (S_{\text{bath}} (\varepsilon') - \beta' \varepsilon(\mathbf{x})) \propto \exp (-\beta' \varepsilon(\mathbf{x})).$$

(7)

Here, we denote by $\varepsilon'$ sum total of the energy of the bath $\varepsilon_{\text{bath}}(y)$ and the interaction energy
$\varepsilon_{\text{int}}(\mathbf{x}, y)$. For small systems, this term is not negligible. Therefore, the specific value of
the Taylor series coefficient $\beta'$ will depend on the specific realization of the system-bath
FIG. 5. **Superstatistical fits to energy distributions.** Panels (a) and (b), superstatistical fits to the energy distribution $p(\varepsilon)$ for two system sizes shown in Fig. 2. Panel (c), the heatmap of the absolute difference of normalized standard deviation of the energy distributions from the simulation and the superstatistical fit.

interaction energy. Moreover, for a given system energy, multiple different values of the system-bath interaction may be permitted. Therefore, the variability in system-bath interactions may be captured by allowing the temperature of the system to vary. This approach is called superstatistics\textsuperscript{10} and has been previously used to model the thermodynamics of small systems\textsuperscript{5–7}. Specifically, we have for any configuration of the system $x$,

$$p(x) = \int p(x|\beta)p(\beta)d\beta$$

(8)

where $p(x|\beta)$ is the Gibbs-Boltzmann distribution. The distribution over temperatures is usually taken to be the gamma or the inverse gamma distribution. This choice is often justified using the maximum entropy principle\textsuperscript{5} but can also be derived from first principles\textsuperscript{10}. Here, we choose $p(\beta)$ to be the inverse gamma distribution:

$$p(\beta; \alpha, \lambda) = \frac{\lambda^\alpha}{\Gamma(\alpha)} \beta^{-\alpha-1} e^{-\lambda/\beta}.$$  

(9)

We fit the parameters $\alpha$ and $\lambda$ of the superstatistical distribution by minimizing the Kullback-Leibler divergence between the energy distributions (see Appendix B). In Fig. 5, we show the energy distributions observed in the simulation and the corresponding fit from the superstatistical model for the same system sizes in panels (a) and (b) of Fig. 2. Unlike the canonical Gibbs-Boltzmann distribution, the superstatistical distribution tends better predict the high energy tail of the distribution. Moreover, the absolute difference in the
variance in energy between the simulated data and the superstatistical model is smaller for all system sizes, as shown in panel (c) of Fig. 5. The heatmap shows that the superstatistical fit is uniformly better than the Gibbs-Boltzmann distribution. Is this surprising? After all, we are introducing additional complexity to the model. We note that because the Dirac Delta function $\delta(\beta)$ is a special case of the inverse gamma distribution, the Gibbs-Boltzmann distribution is a sub-family of the superstatistical distribution. Therefore, the superstatistical approach is guaranteed to be at least as accurate as the canonical ensemble. Yet, given that these two are nested models, we can statistically evaluate whether it is justifiable to include additional complexity to the model. We use the likelihood ratio test to test whether the fit given by the superstatistical approach is statistically significant. Indeed, we find that for all tested distributions, the chi-squared test derived from the likelihood ratio indicates that the superstatistical model fits the data better in a statistically significant manner ($\chi^2 > 6000, p < 10^{-20}$).

Importantly, the superstatistical approach allows us to not only fit the simulated distributions better, but also provides a quantitative characterization of the departure from Gibbs-Boltzmann distribution. As mentioned above, the Gibbs-Boltzmann distribution with a unique temperature is a subset of the superstatistical distribution with the temperatures distributed according to a Dirac Delta function. Therefore, we can use the width (coefficient of variation) of the $p(\beta)$ distribution to measure the departure from canonical behavior. Indeed, we find that the coefficient of variation, defined as $\sigma/\mu$ of $p(\beta)$, is significantly correlated with the error in the Gibbs-Boltzmann fit (the absolute difference of normalized standard deviations, see Fig. 3) with a Spearman correlation of 0.75 ($p \sim 10^{-17}$).

III. DISCUSSION

We studied the performance of the Gibbs-Boltzmann distribution in modeling thermal statistics of small Ising models. We showed that systematic deviations exist that depend on both the size and temperature of the system. We also showed that a superstatistical approach that allows the temperature of the system to fluctuate was a superior descriptor of its statistics. Notably, the superstatistical approach has the Gibbs-Boltzmann statistics as a special case and can thus be viewed as a generalization of the canonical ensemble that is useful to model systems that exchange energy with their surroundings, regardless of their
size. However, this is not to say that the superstatistical model is perfectly able to model the data. In the cases where the canonical distribution fails to model the simulated data, the superstatistical model also fails to model the simulated data, but to a far lesser extent.

Regardless, generalizing the Gibbs-Boltzmann distribution by superstatistics has been shown to result in a increase in our ability to model the energy distribution of a small Ising model, beyond the mere addition of degrees of freedom. Taking the superstatistical approach to modeling small systems requires further consideration. In particular, investigating the ability of the superstatistical distribution to model other types of small systems, both strongly and weakly interacting, would provide a clearer picture of the limitations of the superstatistical approach. Additionally, investigating the precise ways in which the canonical model fails may lead to a more concrete way of determining when the Gibbs-Boltzmann distribution may be applied. We have shown that for the Ising model the degree of deviation is dependent of both the temperature and size of the system. Furthermore, we have proposed examining the mutual information between the boundary and internal energy of the system to gauge the degree of decoupling between the system and its environment, and consequently the degree of deviation from the canonical distribution.

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Appendix A: Simulation Procedure

The procedure used for simulating a microcanonical universe is as follows. We initialize a $100 \times 100$ lattice with spins randomly initialized with values $+1$ or $-1$, corresponding to spin up and spin down respectively. This lattice will have a high temperature since the spins are randomly initialized. We then anneal the lattice to a desired temperature using the Metropolis-Hastings algorithm\(^\text{5}\) for $10^5$ steps. At the end of this simulation, we use a snapshot of the $100 \times 100$ lattice, with energy $E_0$ as the starting point of the microcanonical simulation.

The lattice is evolved microcanonically according to the Demon algorithm\(^\text{5}\), which allows for efficient simulation at an approximately constant energy. This is achieved by the introduction of an energy “bank” that acts as a bookkeeping device. We denote the energy contained in the bank as $E_B \in [0, E_M]$. A brief outline of the algorithm is as follows. A spin is randomly selected from the lattice, and a spin flip is proposed. If the spin flip requires energy $E'$, the flip is only accepted if $E_B \geq E'$, and in accepting the spin flip we deduct $E'$ from the bank. If the proposed spin flip decreases the energy of the lattice, we accept the spin flip only if $E_B + E' \leq E_M$. When the spin flip is accepted, $E'$ is added to the bank. Using this algorithm the energy of the microcanonical lattice $E$ is restricted to $E \in [E_0, E_0 + E_M]$. Importantly, the results of the sampling procedure are robust with respect to choice of $E_M$ so long as $E_M \ll E_0$.

We evolved the microcanonical universe for $10^9$ steps. We randomly sampled small $n \times n$ sites every 100 steps from the interior of the lattice. The sampling frequency was determined by the decorrelation time of the energy of successive samples. For each sample we recorded the internal energy of the $n \times n$ site, and the interaction energy across the system-bath boundary.

Appendix B: Data Analysis Procedure

To mitigate the effect of undersampling, we restricted the simulated distributions to energies $\varepsilon$ such that $p(\varepsilon) > 10^{-7}$. Then, to fit the Gibbs-Boltzmann distribution to the simulated energy distribution, we tune the inverse temperature $\beta$ so that the average energies of the two distributions are the same.
The exact procedure is different for sites smaller and larger than $4 \times 4$. For sites of size $4 \times 4$ and below, we are able to enumerate each microstate, and are thus able to directly compute the prediction from the Gibbs-Boltzmann distribution. For sites larger than $4 \times 4$, it is not computationally feasible to enumerate all microstates. Here, we fit the simulated site energy distribution by simulating an aperiodic canonical system of equal size as the system over a range of inverse temperatures from $\beta = 0.01$ to $\beta = 5$. We find the temperature of the canonical simulation that best matches the average energy of the distribution generated during our main simulation procedure. The parallel simulations used for fitting the Gibbs-Boltzmann distribution are also used in fitting the superstatistical model (see below), and are run over $5 \times 10^8$ time steps.

To fit the superstatistical distribution, we fit the free parameters $\lambda$ and $\alpha$ of the inverse gamma distribution $p(\beta; \alpha, \lambda)$. Given that there are only two parameters, we fit them using exhaustive search on a two dimensional grid, equally spaced in the log space. We then minimize the Kullback-Leibler divergence to fit the superstatistical model. The KL divergence is defined as

$$D(P_{\text{sim}}(\varepsilon)||P_{\text{model}}(\varepsilon)) = \sum_{\varepsilon} P_{\text{sim}}(\varepsilon) \log \left( \frac{P_{\text{sim}}(\varepsilon)}{P_{\text{model}}(\varepsilon)} \right),$$

where $P_{\text{sim}}(\varepsilon)$ and $P_{\text{model}}(\varepsilon)$ are the probabilities of observing energy $\varepsilon$ in the simulated distribution and superstatistical model respectively. The KL divergence was specifically chosen because minimizing $D(P_{\text{sim}}(\varepsilon)||P_{\text{model}}(\varepsilon))$ is equivalent to maximizing the data likelihood of $P_{\text{sim}}(\varepsilon)$ given $P_{\text{model}}(\varepsilon)$. This ensures that when we are using the likelihood ratio test to see if our results are significant we are using the maximum likelihood superstatistical model.

**Appendix C: Low Energy Deviations**

The low energy deviations that are present for all site size and temperatures tested. These arise due to the way in which the boundary is defined for an embedded two dimensional Ising models. Consider two identical Ising models $A$ and $B$, except system $A$ is not embedded in bath, and system $B$ is embedded in a bath. The evolution of both systems may be described by the Metropolis-Hastings algorithm. Note that the lowest energies occur when site is magnetized - most of the spins face the same direction. In particular, the lowest energy
state occurs when the site is completely magnetized. The next few lowest energy states occur when spins along the boundary are flipped. To illustrate why the probabilities of the lowest energy states differ between the simulated and Gibbs-Boltzmann distribution, consider the probability that a corner spin is flipped in systems $A$ and $B$. More specifically, consider the situation where $A$ and $B$ are at the same temperature and completely magnetized, and the corner spin is flipped so that the energy of the system increases.

According to the Metropolis-Hastings algorithm, when a proposed spin flip increases the energy of the system by $\Delta E$, the spin flip is accepted only if a uniformly distributed random variable $x \in [0,1]$ satisfies $x < \exp(-\beta \Delta E)$. Let us examine the average positive $\Delta E$, denoted as $\langle \Delta E^+ \rangle$, for a corner spin in systems $A$ and $B$. For system $A$, which is not embedded in a bath, the corner spin has two nearest neighbors so that $\langle \Delta E^+ \rangle = 4J$. And for embedded system $B$, the corner spin has four nearest neighbors so that $\langle \Delta E^+ \rangle = 4.8J$. Thus, we can expect that a corner spin in an embedded canonical system will be flipped more often than a corner spin in an isolated canonical system, which the Gibbs-Boltzmann distribution describes. This is the only way that the second lowest energy state in a square Ising model can occur, and is exactly what we observe in our analysis (see Fig. 2).

Appendix D: Scripts

All scripts can be found at https://github.com/lukasherron/ising-model.