

Stratified Sampling for the Ising Model: A Graph-Theoretic Approach*

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We present a new approach to a classical problem in statistical physics: estimating the partition function and other thermodynamic quantities of the ferromagnetic Ising model. Markov chain Monte Carlo methods for this problem have been well-studied, although an algorithm that is truly practical remains elusive. Our approach takes advantage of the fact that, for a fixed bond strength, studying the ferromagnetic Ising model is a question of counting particular subgraphs of a given graph. We combine graph theory and heuristic sampling to determine coefficients that are independent of temperature and that, once obtained, can be used to determine the partition function and to compute physical quantities such as mean energy, mean magnetic moment, specific heat, and magnetic susceptibility.

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I. INTRODUCTION

Computing thermodynamic quantities of the ferromagnetic Ising model has been a fundamental problem in statistical physics since the early 20th century [1], where the demonstration of the model's phase transition served as the first rigorous proof that small changes at an atomic scale can lead to large, observable changes [2]. Singularities in the thermodynamic quantities indicate the critical temperature at which the phase transition occurs. The partition function Z of the Ising model and its partial derivatives determine these quantities. While Z has been found exactly in special cases [3, 4], there is unlikely to exist an efficient method of finding Z in general [5]. Therefore, the task of estimating Z has drawn significant effort from the physics and computer science communities [6]. However, an algorithm that is truly practical has yet to be found. In this paper, we present a new heuristic sampling approach with the goal of solving real-world instances quickly.

The classical approach to this problem is to sample from the Gibbs distribution using a Markov chain [5, 7, 8]. Ideally, the algorithm will require only a polynomial number of samples to estimate Z at a particular temperature, but even then this process must be repeated

for each temperature of interest. In contrast, each run of our heuristic sampling algorithm, $\mathcal{A}_{\text{CYCLE}}$, estimates certain coefficients that are independent of temperature. Once obtained, these coefficients can be used to compute Z , mean energy, mean magnetization, specific heat, and magnetic susceptibility at all temperatures by simply evaluating polynomials with these coefficients.

For a fixed bond strength, computing Z is equivalent to counting subgraphs of a graph G . Let $x_{k,e}$ denote the number of subgraphs of G with $2k$ odd vertices and e edges. Using the high-temperature expansion, we can write Z and its derivatives as polynomials whose coefficients come from the set of $x_{k,e}$. For each k , $\mathcal{A}_{\text{CYCLE}}$ generates a search tree whose leaves are the set of subgraphs with $2k$ odd vertices, and then implements the stratified sampling method of Chen [9] to estimate the $x_{k,e}$. In the absence of an applied field, the problem of estimating Z reduces to estimating $x_{0,e}$ for all e . As will become clear, it is simple to restrict $\mathcal{A}_{\text{CYCLE}}$ to subgraphs with no odd-degree vertices, which significantly reduces the complexity of the algorithm in this special case.

II. DEFINITIONS AND TERMINOLOGY

In this section, we introduce important notions from statistical physics and graph theory.

A. Ising Model

Given a graph $G = (V, E)$ with $|V| = n$ and $|E| = m$, a *spin configuration* $\sigma = \sigma(G)$ is an assignment of spins in $\{+1, -1\}$ to the elements of V . The energy of σ is given by the Hamiltonian

$$H(\sigma) = -J \sum_{(x,y) \in E} \sigma_x \sigma_y - B \sum_{x \in V} \sigma_x,$$

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where J is the interaction energy (bond strength) and B is the external magnetic field. In this paper we restrict the ferromagnetic case, fixing $J = 1$. To model the physical reality of a ferromagnet, the probability assigned to state σ is given by the Gibbs distribution, defined as $e^{-\beta H(\sigma)} / Z$, where $\beta = (k_B T)^{-1}$ is proportional to inverse temperature and k_B is Boltzmann's constant. The normalizing constant $Z = \sum_{\sigma} \exp(-\beta H(\sigma))$ is also called the partition function.

Following the notation of [5], let $\lambda = \tanh(\beta J)$ and $\mu = \tanh(\beta B)$. The high-temperature expansion is defined by $Z = AZ'$, where $A = (2 \cosh(\beta B))^n \cosh(\beta J)^m$ is an easily computed constant, and

$$Z' = \sum_{X \subseteq E} \lambda^{|E(X)|} \mu^{|\circ(X)|},$$

where the sum is taken over all subsets X of the edges of G . In a slight abuse of notation, we let X also refer to the graph with vertex-set V and edge-set X . In this manner, $E(X)$ is the edge-set of X , $\circ(X)$ is the set of odd-degree vertices in X , and all subgraphs in this paper are spanning and labeled.

Since all graphs have an even number of vertices of odd degree, Jerrum and Sinclair [5] write Z' as a polynomial in μ^2 : $Z' = \sum_{k=0}^{\lfloor n/2 \rfloor} c_k \mu^{2k}$, where $c_k = \sum_{X : |\circ(X)|=2k} \lambda^{|E(X)|}$. Notice that we can compute Z' for any choice of μ given the values of the c_k , making the c_k independent of the magnetic field. However, we wish to have full temperature-independence, so we write

$$c_k = \sum_{e=0}^m x_{k,e} \lambda^e \quad \text{and} \quad Z' = \sum_{k=0}^{\lfloor n/2 \rfloor} \sum_{e=0}^m x_{k,e} \lambda^e \mu^{2k}, \quad (1)$$

where $x_{k,e}$ is as defined in the introduction. As we shall see, $\mathcal{A}_{\text{CYCLE}}$ is designed to estimate the $x_{k,e}$. Thus, $\mathcal{A}_{\text{CYCLE}}$ yields an estimate of Z' , and hence Z as well, at all temperatures simultaneously.

While $\mathcal{A}_{\text{CYCLE}}$ is defined for all graphs G , the graphs with the most physical significance are the square lattices (grids) with periodic boundary conditions in two and three dimensions. Therefore, all of the computations provided in this paper utilize such graphs, and we shall refer to the $s \times s$ square lattice with periodic boundary conditions simply as the $s \times s$ grid.

B. Cycle Bases

We now introduce some elementary algebraic graph theory which $\mathcal{A}_{\text{CYCLE}}$ uses (for more on this topic, see [10]). The *symmetric difference* of two subgraphs X_1 and X_2 of G , written $X_1 \oplus X_2$, is the subgraph of G that contains precisely those edges in exactly one of X_1 and X_2 . One may consider this operation as addition of subgraphs over the field $\mathbb{F}_2 = \{0, 1\}$. Notice that an edge e is in $\bigoplus_{i=1}^t X_i$ if and only if e appears in an odd number of these subgraphs.

Let \mathcal{E}_0 be the set of *even subgraphs*, those subgraphs with no vertices of odd degree. Since the symmetric difference of two even subgraphs is again an even subgraph, we may view \mathcal{E}_0 as a vector space over \mathbb{F}_2 , called the *cycle space* of G . The dimension of the cycle space is $m - n + 1$. Hence, every set of $m - n + 1$ linearly independent even subgraphs forms a *cycle basis* \mathcal{C} of G . Further, every even subgraph has a *unique* representation using the elements of \mathcal{C} , and $|\mathcal{E}_0| = 2^{m-n+1}$.

When $X \in \mathcal{E}_0$, the parity of each vertex in $X \oplus Y$ is the same in Y . Now consider a subgraph P of G with $\circ(P) = \{v_1, v_2, \dots, v_{2k}\}$. The set

$$\mathcal{E}_0 \oplus P := \{X \oplus P : X \in \mathcal{E}_0\}$$

is exactly the 2^{m-n+1} subgraphs whose odd vertices are $\circ(P)$. Therefore, the set of subgraphs with $2k$ odd vertices, \mathcal{E}_k , is $\bigcup_S \mathcal{E}_0 \oplus P_S$, where the union is over all $S \subseteq V$ of size $2k$ and P_S is *any* subgraph with $\circ(P) = S$.

Cycle bases have a long history in combinatorics [11], and are used both in theory and applications [12]. A *fundamental cycle basis* is defined as the cycles in $T + e$ for each $e \in E(G) - E(T)$, for a spanning tree T of G . Since spanning trees can be found quickly (see e.g. [13]), so can fundamental bases. *Minimum cycle bases*, which are bases with the fewest total edges, have proven helpful in practice and can also be found in polynomial time [14].

III. ALGORITHMS

Our main data structure is a search-tree; a rooted tree in which each node represents a subgraph of G . For each k , we shall define a search-tree τ_k whose leaves are precisely \mathcal{E}_k . Our goal is to estimate $x_{k,e}$, the number of leaves of τ_k that have e edges.

Tree search algorithms have a lengthy history in computer science [15]. A classical example of such is an algorithm of Knuth [16] for estimating properties of a backtrack tree. To estimate the number of leaves, for example, Knuth's algorithm explores a random path down the tree from the root, choosing a child uniformly at random at each step. It then returns the product of the number of children of each node seen along the path. It is easy to see that this estimator is unbiased; i.e. the expected value is the number of leaves.

For our application, we want the number of leaves of τ_k of a certain type (with e edges). We achieve this via Chen's generalization of Knuth's algorithm, which was originally introduced to reduce the variance of the estimator. Since Chen's work lies at the heart of our approach, we take the next section to explain it in further detail. In Section III B, we describe $\mathcal{A}_{\text{CYCLE}}$. In [17], we present an alternative to $\mathcal{A}_{\text{CYCLE}}$, which is related to [5]. This approach, which we call $\mathcal{A}_{\text{EDGE}}$, may be more appropriate in the presence of an external field, but is outperformed by $\mathcal{A}_{\text{CYCLE}}$ when $B = 0$.

A. Stratified Sampling

We describe in Algorithm 1 a simplified version of the stratified sampling algorithm introduced by Chen [9]. Let τ be a search tree and choose a *stratifier* for τ — a way of partitioning the nodes into sets called *strata*.¹ For each stratum α , Algorithm 1 produces a representative $s_\alpha \in \alpha$ and a weight w_α , which is an unbiased estimate of the number of nodes in α .

For Algorithm 1, let Q_1 and Q_2 be queues. Each node s of τ has a weight w , and we write (s, w) to represent this pair. The input is the root r of τ , a method for determining the children of a node in τ , and the stratifier. The output is the set of (s_α, w_α) . If the algorithm never encounters an element of α , it returns $(\emptyset, 0)$ for α .

ALGORITHM 1: Chen's Algorithm

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initialize:  $Q_1 = \{(r, 1)\}$ ,  $Q_2 = \{\}$ ,  $i = 0$ .
while  $i < \text{number of levels in } \tau$  do
  while  $Q_1 \neq \emptyset$  do
    output the first element  $(s, w)$  of  $Q_1$ 
    for each child  $t$  of  $s$  in  $\tau$  do
      if  $Q_2$  contains an element  $(u, w_u)$  in the same stratum as  $t$  then
        update  $w_u = w + w_u$ 
        w. prob.  $w/w_u$  replace  $(u, w_u)$  with  $(t, w_u)$  in  $Q_2$ 
      else
        add  $(t, w)$  to  $Q_2$ 
    pop  $(s, w)$  off of  $Q_1$ 
  set  $Q_1 = Q_2$  and reset  $Q_2 = \emptyset$ 
   $i++$ 

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B. Cycle-Addition Algorithm

Let $S \subseteq V$ of size $2k$ and recall that P_S is any subgraph of G with $o(P) = S$. Let $\mathcal{C} = \{C_1, C_2, \dots, C_{m-n+1}\}$ be a cycle basis of G . Define $\tau(\mathcal{C}, P_S)$ as the search-tree determined by the following rules:

1. P_S is the root of $\tau(\mathcal{C}, P_S)$, and
2. each node X at level $0 \leq i < m - n + 1$ has two children: $X \oplus C_{i-1}$ and X .

Now τ_k is the tree with artificial root node R whose $\binom{n}{2k}$ children correspond to the roots of $\tau(\mathcal{C}, P_S)$, one for each distinct subset of size $2k$.

In order to implement Algorithm 1, we define the stratifier for each $\tau(\mathcal{C}, P_S)$ by: the nodes X and Y in $\tau(\mathcal{C}, P_S)$ belong to the same stratum if and only if X and Y are in the same level of $\tau(\mathcal{C}, P_S)$, and $|E(X)| = |E(Y)|$.

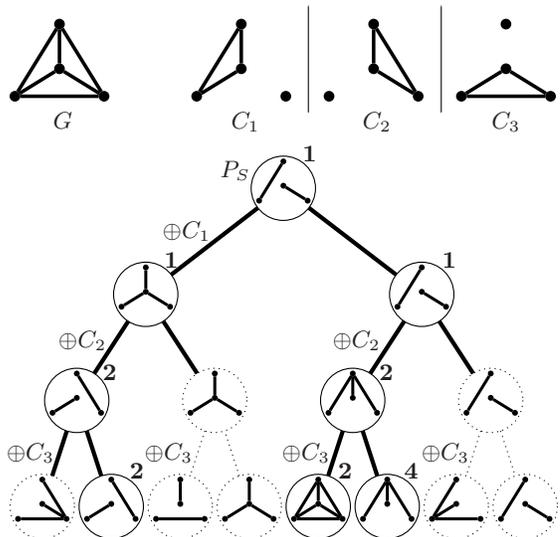


FIG. 1

The inputs to $\mathcal{A}_{\text{CYCLE}}$ are a graph G , an integer k in $[0, n/2]$, and an integer N . The output of each of the N runs of Algorithm 1, as a subroutine of $\mathcal{A}_{\text{CYCLE}}$, is a set of (s_α, w_α) pairs. Consider a representative s_α that is a leaf node in the tree $\tau(\mathcal{C}, P_S)$, and suppose s_α has e edges. Then $\binom{n}{2k} w_\alpha$ is our estimate of $x_{k,e}$, since each sample represents all $\binom{n}{2k}$ choices of S .

ALGORITHM 2: $\mathcal{A}_{\text{CYCLE}}$

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Choose a cycle basis  $\mathcal{C}$  of  $G$ 
for  $j \in [1, N]$  do
  Choose  $S \subseteq V$  with  $|S| = 2k$ 
  Find  $P_S$ 
  Run Algorithm 1 on  $\tau(\mathcal{C}, P_S)$ 
for  $e \in [0, m]$  do
  Let  $\alpha$  be the stratum corresponding to the bottom level
  of  $\tau(\mathcal{C}, P_S)$  and  $e$  edges, and output  $\binom{n}{2k}$  times the average
  of the  $N$  estimates of  $w_\alpha$  as  $x_{k,e}$ 

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Figure 1 shows an example of $\mathcal{A}_{\text{CYCLE}}$ with $k = 2$, $S = V(G)$, $N = 1$, and $G, P_S, \mathcal{C} = \{C_1, C_2, C_3\}$, and $\tau(\mathcal{C}, P_S)$ as depicted. The graphs bounded by solid circles are the strata representatives, and their weights are in bold just above. The solid edges of $\tau(\mathcal{C}, P_S)$ connect the nodes seen by $\mathcal{A}_{\text{CYCLE}}$. The output is $x_{2,2} = 2$, $x_{2,3} = 4$, $x_{2,6} = 2$, and $x_{2,e} = 0$ for $e \in \{0, 1, 4, 5\}$.

In Figure 2a, we show the output of many runs of $\mathcal{A}_{\text{CYCLE}}$ on a 4×4 grid for $k \in [0, 4]$, and use this output (and that for $k \in [5, 8]$) with Equation 1 to get Figure 2a, using four values of λ . While the c_k are log-concave [5], the $x_{k,e}$ may not be.

¹In general, the stratifier must satisfy a few technical conditions. However, as long as we require each strata to contain nodes from a single level of τ , we are guaranteed that these conditions are met.

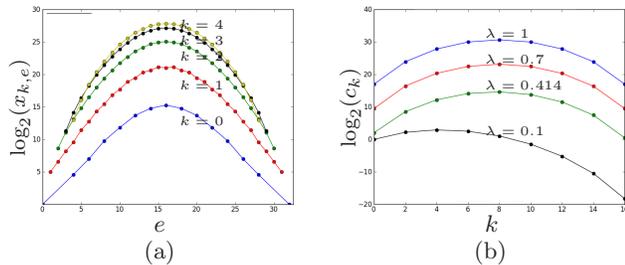


FIG. 2: (Color online)

C. No external field

In the absence of an external field, we only need to run $\mathcal{A}_{\text{CYCLE}}$ for $k=0$. This represents a huge time savings in comparison to the case $B \neq 0$, as then we need to run $\mathcal{A}_{\text{CYCLE}}$ for all $k \in [0, n/2]$. Furthermore, we must choose $S = \emptyset$, which eliminates this step from the algorithm.

D. Details

The algorithm $\mathcal{A}_{\text{CYCLE}}$ is really a class of algorithms, each corresponding to the choice of cycle basis, the order of the subgraphs in the basis, the subsets S , and the roots P_S . We briefly discuss these choices here and elaborate further in [17].

The choice of cycle basis is central to the performance of $\mathcal{A}_{\text{CYCLE}}$. Experimentally, minimum cycle bases have outperformed fundamental and random cycle bases in terms of overall speed and variance. However, it remains an interesting open problem to determine the optimal basis for $\mathcal{A}_{\text{CYCLE}}$.

As for the choice of S , we know that $k=0$ implies $S = \emptyset$. But for $k > 0$, we must choose S .² We would like every subset of $V(G)$ of size $2k$ to appear as S at least once. However, when k is near $n/4$, $\binom{n}{2k}$ is exponentially large in n .³ So instead we are forced to select a reasonable number of such subsets that work well in $\mathcal{A}_{\text{CYCLE}}$.

Once $S = \{v_1, v_2, \dots, v_{2k}\}$ is chosen, we must find P_S . One such method is to use a spanning tree T of G to create $P_S = \bigoplus_{i=1}^k \mathcal{P}_{2i-1, 2i}$, where $\mathcal{P}_{2i-1, 2i}$ is the path from v_{2i-1} to v_{2i} in T .

IV. PERFORMANCE

A. Convergence

In Section V, we show how to get unbiased estimates of Z' from our unbiased estimates of the $x_{k,e}$. To evaluate the efficiency of the algorithm, we need to know how many samples (N) we need to be reasonably confident about our estimate of Z' . The answer depends on the relative variance of our estimate of Z' .⁴ As heuristic sampling methods are relatively new, there are not many tools for computing the variance of these algorithms. Experimentally, such methods have been shown to work well in practice, but a robust theoretical foundation is lacking [15, 18]. Therefore, analyzing the variance for this problem remains an important open question which deserves further study.

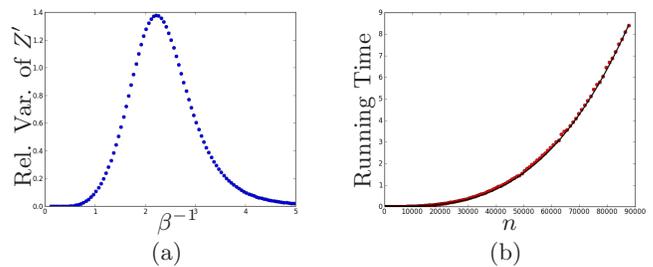


FIG. 3: (Color online)

In our simulations, we find that although $\mathcal{A}_{\text{CYCLE}}$ is temperature independent, the variance is not. Figure 3a shows the relative sample variance of our estimate of Z' as a function of temperature, for a 4×4 grid with no external field. The highest sample variance occurs at the critical temperature, $\beta^{-1} \approx 2.269$. However, even at the critical temperature, our estimate of Z' converges quickly. Figure 4 presents six separate runs of $\mathcal{A}_{\text{CYCLE}}$ with $B = 0$, and shows the convergence to Z' for each run as a function of the number of samples. The exact value of Z' is displayed as the straight black line.

²Except if G itself is even, in which case there is no choice for $k = n/2$ either.

³Ideally, we would partition the subsets of $V(G)$ into isomorphism classes $\{V_i\}_{i=1}^t$ and choose a representative for class V_i to act as S in $|V_i|N/\binom{n}{2k}$ instances. However, the number of such classes can also be exponentially large.

⁴By the Central Limit Theorem, we need $N = \frac{z_{\delta/2}^2}{\epsilon^2} \left(\frac{E[(Z')^2]}{E^2[Z']} - 1 \right)$ to be within ϵ with probability $1 - \delta$, where $z_{\delta/2}$ comes from the normal distribution, and $\frac{E[(Z')^2]}{E^2[Z']} - 1$ is precisely relative variance.

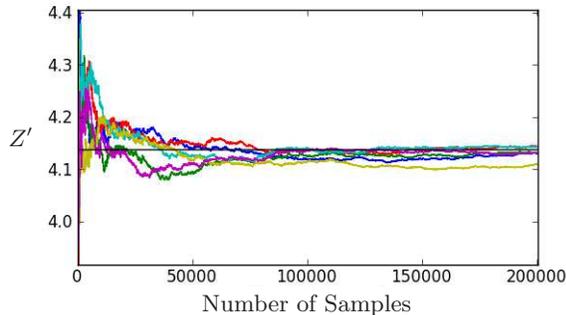


FIG. 4: (Color online)

B. Running time

The number of operations of a single run of Algorithm 1 as a subroutine of $\mathcal{A}_{\text{CYCLE}}$ is a function of the number of strata used in $\tau(\mathcal{C}, P_S)$ and the number of operations performed to process each node in Q_1 . Recall that our stratifier partitions nodes according to their level in $\tau(\mathcal{C}, P_S)$ and number of edges. Clearly, each level has at most $m+1$ strata. Further, there are $m-n+2$ levels. Hence, the number of strata used is at most $(m-n+2)(m+1)$. For each node in Q_1 , $\mathcal{A}_{\text{CYCLE}}$ examines its two children, so the total number of nodes of $\tau(\mathcal{C}, P_S)$ used by the subroutine is at most $2(m-n+2)m = O(m^2)$. For each of these nodes, we take the symmetric difference of two subgraphs and count the number of edges remaining, each of which is an $O(m)$ operation. Thus, each run of Algorithm 1 as a subroutine of $\mathcal{A}_{\text{CYCLE}}$ terminates after $O(m^3)$ operations. For square lattices in dimension d , the number of operations is $O(d^3 n^3)$, as $m = dn$.

C. Implementation

We implemented $\mathcal{A}_{\text{CYCLE}}$ in C, using GMP to deal with the large weights generated by the algorithm. In Figure 3b, we plot our experimental running times for $\sqrt{n} \times \sqrt{n}$ grids against the curve $f(n) = 1.25 \cdot 10^{-14} n^3$, which matches up well with our bound of $O(n^3)$.

Typically, one stores graphs as matrices or lists. However, we greatly improve the running time of $\mathcal{A}_{\text{CYCLE}}$ by storing each subgraph X as an integer whose bitstring b_X has length m ; $b_X(e) = 1$ if and only if $e \in E(X)$. Here, $b_{X \oplus Y} = b_X \text{ XOR } b_Y$, so taking symmetric differences is quite fast. Further, $|E(X)|$ is simply the number of ones in the bitstring, which can also be computed quickly.

One may achieve another increase in speed if machine-level instructions for the operation XOR are used for large integers. Most modern micro-processors have such capabilities, as they are used in scientific computing [19].

V. PHYSICAL QUANTITIES

In this section, we show how to use the estimates of the $x_{k,e}$ to calculate physical quantities. Let $f(X) = f(|o(X)|, |E(X)|)$ be any function on subgraphs X which depends only on the number of odd vertices and the number of edges of X . We can calculate the expected value of f with respect to the distribution $\pi'(X) = \lambda^{|E(X)|} \mu^{|o(X)|} / Z'$ from our estimates of the $x_{k,e}$ by

$$\mathbb{E}[f] = \frac{1}{Z'} \sum_{k=0}^{\lfloor n/2 \rfloor} \sum_{e=0}^m f(k, e) x_{k,e} \lambda^e \mu^{2k}. \quad (2)$$

Notice if f is identically 1, $Z' \mathbb{E}[f] = Z'$, and so we can approximate Z' , and hence Z , by simply looking at the double sum. In Theorem 1, we show that important physical quantities can also be expressed as $\mathbb{E}[f]$ for suitable choices of f . The proof of Theorem 1 involves taking partial derivatives of $\ln Z$ with respect to β and B following the method of [5]. As these calculations are tedious but easy, we leave the details to [17].

Theorem 1. *The mean magnetic moment, mean energy, magnetic susceptibility, and specific heat can each be written as sums of expectations of random variables over the distribution π' .*

In Figure 5, we show estimates of mean energy and specific heat from $\mathcal{A}_{\text{CYCLE}}$ with $N = 50,000,000$ on a 16×16 grid as a function of β^{-1} . These figures match those of [20, p. 252] nicely.

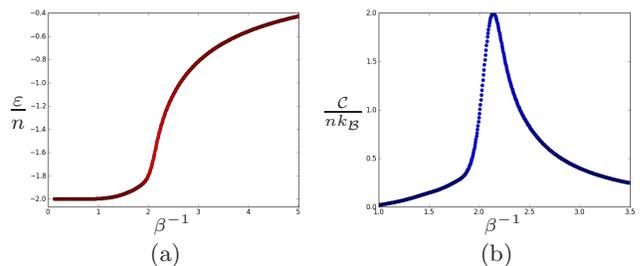


FIG. 5: (Color online)

VI. CONCLUSIONS

The algorithm $\mathcal{A}_{\text{CYCLE}}$ is a completely new approach to the problem of estimating Z . To our knowledge it is the first heuristic sampling method for this problem. For this reason, it is difficult to compare the running time of $\mathcal{A}_{\text{CYCLE}}$ with the current best-known algorithms, which are all Markov chain Monte Carlo methods. What is clear is that $\mathcal{A}_{\text{CYCLE}}$ gives us an estimate of Z at *all temperatures simultaneously* in only $O(m^3)$ operations, where the constant hidden by the big-O notation is small. Bounding the variance of $\mathcal{A}_{\text{CYCLE}}$ is an important open problem

which is necessary to give a real understanding of its efficiency. However, if the goal is to get *some* estimate as fast as possible, $\mathcal{A}_{\text{CYCLE}}$ is an excellent choice.

Besides analyzing the variance of $\mathcal{A}_{\text{CYCLE}}$, there are several other directions for future work. For example, there are many choices made in $\mathcal{A}_{\text{CYCLE}}$ which could be optimized, such as the choice of cycle basis. These choices could affect the variance significantly. One might consider other tree-search algorithms and compare their performance with that of $\mathcal{A}_{\text{CYCLE}}$ and $\mathcal{A}_{\text{EDGE}}$. We also plan

to investigate more extensively the connections between our heuristic method and MCMC methods.

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