

Exact Computation of the Triangular-Lattice Ising Model with Eighteen Spins on a Side

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Abstract—The Ising model, consisting of magnetic spins, is the most important system in understanding phase transitions and critical phenomena. For the first time, the exact integer values for the density of states of the triangular-lattice Ising model with eighteen spins on a side and free boundary conditions are evaluated. Also, the exact specific heats are obtained for the triangular-lattice Ising ferromagnet and antiferromagnet at the same time.

Index Terms—Exact computation, triangular-lattice Ising model, density of states.

I. INTRODUCTION

Phase transitions and critical phenomena are the most universal phenomena in nature. The Ising model, consisting of magnetic spins, is the simplest system showing phase transitions and critical phenomena at finite temperatures. The Ising model has played a central role in our understanding of phase transitions and critical phenomena [1]. Also, the Ising model explains the gas-liquid phase transitions accurately. Based on the Ising model, various theoretical methods such as mean-field theory, power-series expansion and analysis, renormalization group, and canonical transfer matrix have been developed to understand phase transitions and critical phenomena.

In particular, computer simulations have been the most popular method in studying phase transitions and critical phenomena due to the recent fast growth of computer hardware and software technologies. To investigate the phase transition and critical behavior of a given system as a continuous function of temperature, to obtain the partition function zeros showing most effectively phase transitions and critical phenomena, and to perform microcanonical analysis for phase transitions and critical phenomena, we need to calculate the density of states as a function of energy. The most computational methods to calculate the density of states yield the approximate density of state [2]-[13].

On the other hand, the microcanonical transfer matrix [14]-[39] is an exact computation method to calculate the exact integer values for the density of states. Until now, the exact integer values for the density of states of the Ising model on equilateral triangular lattice with free boundary conditions have been obtained up to fifteen spins on a side

(corresponding to $2^{120} \approx 1.3 \times 10^{36}$ states) [15]. In this work, for the first time, we evaluate the exact integer values for the density of states of the triangular-lattice Ising model with eighteen spins on a side (corresponding to $2^{171} \approx 3.0 \times 10^{51}$ states). It is very difficult task to classify all 2^{171} spin configurations according to their energy values.

Using the exact density of states of the triangular-lattice Ising model with eighteen spins on a side, we obtain much more accurately the specific heats of two different systems (the triangular-lattice Ising ferromagnet and antiferromagnet) at the same time. Based on the specific heats of the triangular-lattice Ising ferromagnet and antiferromagnet, we discuss the phase transitions and critical phenomena of these systems.

II. ISING MODEL

The Ising model on the equilateral triangular lattice [15] with eighteen spins on a side and free boundary conditions is defined by the Hamiltonian

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

where J is the coupling constant, $\langle i, j \rangle$ indicates a sum over all bonds between any nearest-neighbor spin pairs σ_i and σ_j , and $\sigma_i = \pm 1$ (1 for upward magnetic spin and -1 for downward magnetic spin). On triangular lattice, each spin has the six nearest neighbor spins except for the spins on the boundary edges. The triangular-lattice Ising model with L spins on a side has $N=L(L+1)/2$ spins and $B=3(N-L)$ bonds. Therefore, there are $N=171$ spins and $B=459$ bonds for the equilateral triangular lattice with eighteen spins on a side ($L=18$) and free boundary conditions.

Next, we define the density of states, $\Omega(E)$, with a given energy

$$E = \sum_{\langle i, j \rangle} (1 - \sigma_i \sigma_j),$$

where E is integers between 0 and $4B/3=612$ for $L=18$. Then, the partition function of the triangular-lattice Ising model (a sum over all possible spin configurations)

$$Z = \sum_{\{\sigma\}} \exp(-\beta H),$$

where $\beta=1/kT$ (k is the Boltzmann constant and T is temperature), can be written as

$$Z(T) = \sum_{E=0}^{612} \Omega(E) \exp(-\beta E).$$

The partition function is the most important function in

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thermodynamics, statistical mechanics, and physical chemistry.

III. DENSITY OF STATES

The microcanonical transfer matrix [14]-[39], an exact computation method, is applied to calculate the exact integer values for the density of states of the Ising model on the equilateral triangular lattice with eighteen spins on a side ($L=18, N=171, B=459$). First, an array $\omega^{(1)}$, which is indexed by energy E and the eighteen spin variables $\sigma_i^{(1)} (1 \leq i \leq 18)$ for the first row, is initialized with the seventeen horizontal bonds as

$$\omega^{(1)}(E; \sigma^{(1)}) = \delta(E + \sum_{n=1}^{17} \sigma_n^{(1)} \sigma_{n+1}^{(1)} - 17),$$

where δ is the Kronecker delta. Second, by introducing the seventeen spin variables $\sigma_i^{(2)} (1 \leq i \leq 17)$ for the second row and considering the thirty-four vertical bonds between the first and second rows, the array $\omega^{(1)}$ is modified into

$$\varpi^{(2)}(E; \sigma^{(2)}) = \omega^{(1)}(E + \sum_{n=1}^{17} \sigma_n^{(2)} (\sigma_n^{(1)} + \sigma_{n+1}^{(1)}) - 34; \sigma^{(1)}).$$

After taking the sixteen horizontal bonds of the second-row spins, we obtain

$$\varpi^{(2)}(E; \sigma^{(2)}) = \varpi^{(2)}(E + \sum_{n=1}^{16} \sigma_n^{(2)} \sigma_{n+1}^{(2)} - 16; \sigma^{(2)}).$$

Next, for the third row, if we introduce the sixteen spin variables $\sigma_i^{(3)} (1 \leq i \leq 16)$ and consider the thirty-two vertical bonds, we have

$$\varpi^{(3)}(E; \sigma^{(3)}) = \varpi^{(2)}(E + \sum_{n=1}^{16} \sigma_n^{(3)} (\sigma_n^{(2)} + \sigma_{n+1}^{(2)}) - 32; \sigma^{(2)}).$$

Now, the fifteen horizontal bonds connecting the spins in the third row are taken into account by shifting the energy:

$$\omega^{(3)}(E; \sigma^{(3)}) = \varpi^{(3)}(E + \sum_{n=1}^{15} \sigma_n^{(3)} \sigma_{n+1}^{(3)} - 15; \sigma^{(3)}).$$

After repeating these steps, the final spin $\sigma_1^{(18)}$ in the eighteenth row is introduced with the two vertical bonds such as

$$\varpi^{(18)}(E; \sigma^{(18)}) = \omega^{(17)}(E + \sigma_1^{(18)} (\sigma_1^{(17)} + \sigma_2^{(17)}) - 2; \sigma^{(17)}).$$

Finally, the exact integer values for the density of states of the triangular-lattice Ising model with eighteen spins on a side is given by

$$\Omega(E) = \sum_{\sigma} \varpi^{(18)}(E; \sigma_1^{(18)}),$$

as shown in Table I, II, and III. The sum over all densities of states is exactly equal to the number of all possible spin configurations:

$$\sum_E \Omega(E) = 2^{171} \approx 3.0 \times 10^{51}.$$

TABLE I: EXACT INTEGER VALUES FOR THE DENSITY OF STATES $\Omega(E)$ OF THE ISING MODEL ON THE EQUILATERAL TRIANGULAR LATTICE WITH EIGHTEEN SPINS ON A SIDE AND FREE BOUNDARY CONDITIONS, AS A FUNCTION OF ENERGY E ($=0\sim 248$)

E	$\Omega(E)$
0	2
4	6
8	120
12	698
16	4926
20	32898
24	183598
28	1077360
32	5732928
36	29742908
40	149995056
44	725682150
48	3441025398
52	15850948398
56	71378421714
60	314842377450
64	1360270736442
68	5773198112370
72	24079429379534
76	98835422837142
80	399631763275344
84	1593020943584184
88	6266017974032538
92	24336615611053698
96	93394373030137502
100	354349069960204254
104	1329908486113610586
108	4939747629298345624
112	18166324908534247938
116	66172517125822650006
120	238828273199602595280
124	854324137189574254854
128	3029724735335329863798
132	10654321072330846416222
136	37159871767171454952942
140	128563609273897927138074
144	441279588731867009146194
148	1502816275339314440210718
152	5078404212126656898914814
156	17029451373598977602838314
160	56668176518722621470880116
164	187131754821406286835976524
168	613227992362498144545682982
172	1994123411279023994947380294
176	6434584028140782226639532112
180	20601752121939915250005359616
184	65444705313464469115525800978
188	206251950660318896085506890758
192	644817488924589508544194155446
196	1999625296622038907636275808550
200	6150176507800464864457145926374
204	18758764707707840199874164120552
208	56734322502598178279959938358008
212	170120524893135900490975462542828
216	505682708225017649369928170719504
220	1489870977644177452447531651457436
224	4350151776353064838774025656713900
228	12585743860761393660220709604901732
232	36074742254773441282921967499712296
236	102425068949841268490650936689064146
240	288014606367086068382310243413145754
244	801959230924593393823151339228959818
248	2210760545258121573655221760353521826

The ferromagnetic ($J > 0$) ground states correspond to

$$\Omega(E = 0) = 2,$$

and the antiferromagnetic ($J < 0$) ground states are quite degenerate such as

$$\Omega(E = 612) = 23665003296449525435806996826,$$

corresponding approximately to 2.4×10^{28} .

The largest density of states is

$$\Omega(E = 460) = 223344742615528798625291061965 \\ 299440306354840893412,$$

corresponding approximately to 2.2×10^{50} . This kind of a large integer number is stored in a computer by using a positional numeral system with a radix (or base) of 2^{31} such as

$$\Omega(E = 460) = \sum_j P_j (2^{31})^{j-1}.$$

Here, we need the six P_j 's as follows:

$$P_1 = 143620068,$$

$$P_2 = 1321816796,$$

$$P_3 = 1227133195,$$

$$P_4 = 1023651300,$$

$$P_5 = 424290496,$$

and

$$P_6 = 4890.$$

It should be noted that the exact integer values for the density of states of the Ising model on the equilateral triangular lattice with eighteen spins on a side and free boundary conditions are obtained for the first time. Even the approximate values for the density of states of the triangular-lattice Ising model with eighteen spins on a side and free boundary conditions have never been calculated by using other non-exact methods.

IV. EXACT SPECIFIC HEATS

Given the exact integer values for the density of states $\Omega(E)$, the free energy F is exactly given by

$$F = -kT \ln Z(T).$$

From the exact free energy, the exact thermodynamic functions can be obtained. For example, the exact specific heat can be expressed as [32], [37]

$$C(T) = (NkT^2)^{-1} \frac{\partial^2}{\partial \beta^2} \ln Z(T).$$

It should be noted that the exact specific heats of two different systems (the ferromagnet and the antiferromagnet) can be obtained at the same time in this work.

Fig. 1 shows the exact specific heat of the Ising ferromagnet ($J > 0$) on the equilateral triangular lattice with eighteen spins on a side and free boundary conditions. The specific heat shows the sharp peak at $T = 3.232J/k$, signaling the phase transition between the low-temperature ferromagnetic phase and the high-temperature paramagnetic

phase.

TABLE II: EXACT INTEGER VALUES FOR THE DENSITY OF STATES $\Omega(E)$ OF THE ISING MODEL ON THE EQUILATERAL TRIANGULAR LATTICE WITH EIGHTEEN SPINS ON A SIDE AND FREE BOUNDARY CONDITIONS, AS A FUNCTION OF ENERGY E ($=252 \sim 500$)

E	$\Omega(E)$
252	6032574296702207567992159617631054388
256	16291195531867254409681753011959573286
260	43531947414286528716741831764080745418
264	115075126573566581358408907157488958812
268	300873678653252315209962248506197217320
272	777902547118917508886357885597026371366
276	1988433439781483966312131893603101542126
280	5023958673368655601048981585747322922204
284	12543885244867446025652519130032502285132
288	30943435281169248372287421652274949167448
292	75396697989825485392612164879262241525340
296	181416915513496537802958960691994207820984
300	430959549961245438057562394617210011264808
304	1010455910177551377990340814506184069953140
308	2337794510734717746244322204432816224734456
312	5335638573482537573490477967589333546397300
316	12009846987882627333999323765431938145155756
320	26652393902684429250696803548595613647326734
324	58298310736110255123305274354978237303067770
328	125651170264436331856921237358213453896069668
332	266768220748538447476589754247011255114467706
336	557726120368120620395722344793580882465983536
340	1147851147704756884493869558888840041533574048
344	232478092992574532523529638049595520750686530
348	4631910578468230284770764119614881772222106046
352	907538736279688330336224354705276013549719348
356	17479838923327154950510934380492643075364900888
360	33083560464058716419199680375817998937570681962
364	61506299526417504864955335620459187482958031548
368	112275207284978890115800573591860818881023776790
372	201151604933687224887819792212492026300496077482
376	353549914805816553550110672952201751485673345844
380	609356184799887613362709199930535233554098666606
384	102939883000162555975376200800372922640666522202
388	1703646342247042457834241306547706659577566228218
392	2760845787272406555573996114171202185297260231814
396	4378719827587143093460219433647641846027105118498
400	6792992427163107607330591388598583409311604038806
404	10302472823119506572551114792442523831590149014978
408	15266370194980358625705190888815790266438642426302
412	22089262612143002704248051819439686486356276466066
416	31189169632766629985795474696554089831603362694564
420	42945512870251241349677149761961196285738164376340
424	57626836356124675863137961179245217030105494120710
428	75303113020939996316545143187513130695899814814958
432	95753806349040845154443893768987044017052089168192
436	118389329416043473011419930462233300764094757778936
440	142208141171905046740916723511813585532991827339074
444	165812058367006765384057007646193071136749750987574
448	187496418825096013726516930528609480748581983635754
452	205418817021640234882736178728743807730007752178450
456	217831755706261800880699734153843652400701430461078
460	223344742615528798625291061965299440306354840893412
464	221166015404198799821872320331558576084831981659624
468	211269309152492812119488374854525701462767985296124
472	194440864822807089868319235365666649412871411180940
476	172185929905909902442436348164816469818599994947408
480	146506912841695542187622155503529962943797769036172
484	119597709009310355684848476855733332051653835280332
488	93520159958647237984995369509626383559951598328372
492	69931766814162508421556977727470656380144332831802
496	49917393007869262174557191391305210208311870740686
500	33947391382667604774400754087373481647747354286902

TABLE III: EXACT INTEGER VALUES FOR THE DENSITY OF STATES $\Omega(E)$ OF THE ISING MODEL ON THE EQUILATERAL TRIANGULAR LATTICE WITH EIGHTEEN SPINS ON A SIDE AND FREE BOUNDARY CONDITIONS, AS A FUNCTION OF ENERGY E (=504~612)

E	$\Omega(E)$
504	21950781726445057354293572646890974133910427062586
508	13465804322590765693109900843417171490205709454840
512	7818704538801627208348282883093631189281721542472
516	4286118920863464319012351239079820313385928372184
520	2212305652992360430441136002143791362484968188504
524	1072041653307650893550563631998246073083876491714
528	486181006450383850841607109660327484773133664052
532	205649417094675483217121122612034006852750305776
536	80835122735378429057361360565289896153212053658
540	29408820840369626431217743962720078903176877928
544	9859751964338024711704821054735749328800880912
548	3031755345218311633082572397197569224058917256
552	850526355685300635904139272904828377861799116
556	21643949177571394524726780347735395063388510
560	49642320030960240892240905384932124041386758
564	10188582054939574080136950772359492660736290
568	1856076608608365806023004991979821849783174
572	297351124582870094358418260738393802564494
576	41444399841439401286605731668575495441304
580	4962271488410140540704733439860177529052
584	502673946829119573918563783000154607602
588	42275793284432184726316549690456143940
592	2881565478570894451055004821430792480
596	154143255292560847456301000415328128
600	6182853767838614190348673645213992
604	173315951796170858726377113576180
608	2994826377002713783475651283510
612	23665003296449525435806996826

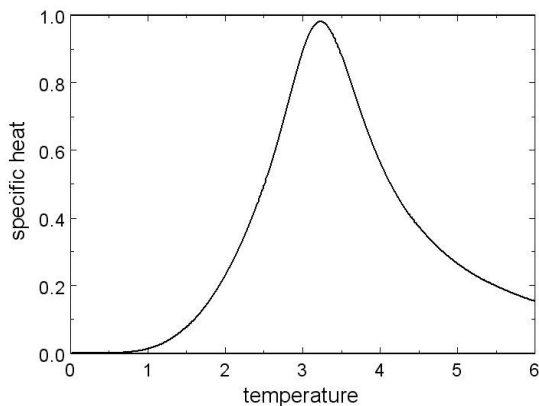


Fig. 1. Exact specific heat (in units of the Boltzmann constant k) per volume as a function of temperature (in units of J/k) for the triangular-lattice Ising ferromagnet ($J > 0$) with eighteen spins on a side.

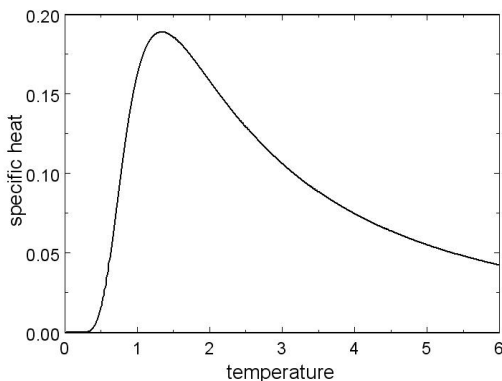


Fig. 2. Exact specific heat (in units of k) per volume as a function of temperature (in units of $|J/k|$) for the triangular-lattice Ising antiferromagnet ($J < 0$) with eighteen spins on a side.

Fig. 2 shows the exact specific heat of the Ising antiferromagnet ($J < 0$) on the equilateral triangular lattice with eighteen spins on a side and free boundary conditions. The specific heat shows a peak at $T=1.340|J/k$. But the peak of the triangular-lattice Ising antiferromagnet is not sharp, compared to the peak of the triangular-lattice Ising ferromagnet. Rather, the peak for the specific heat of the triangular-lattice Ising antiferromagnet resembles the Schottky-anomaly peak for the specific heat of the one-dimensional Ising model [40].

V. CONCLUSION

For the first time, we have evaluated the exact integer values for the density of states of the Ising model on the equilateral triangular lattice with eighteen spins on a side and free boundary conditions, by classifying all $2^{171} \approx 3.0 \times 10^{51}$ spin configurations according to their energy values. Using the exact density of states of the triangular-lattice Ising model with eighteen spins on a side, we have obtained much more accurately the specific heats of two different systems (the triangular-lattice Ising ferromagnet and antiferromagnet) at the same time. Based on the specific heats of the triangular-lattice Ising ferromagnet and antiferromagnet, we have investigated the phase transitions and critical phenomena of these systems. The specific heat of the triangular-lattice Ising ferromagnet has shown a sharp peak, signaling the phase transition between the low-temperature ferromagnetic phase and the high-temperature paramagnetic phase. On the other hand, the specific heat of the triangular-lattice Ising antiferromagnet has shown the Schottky-anomaly peak.

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