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Exact Solution of the Ising Model on the 15×15 Square Lattice with Free Boundary Conditions

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Abstract—The square-lattice Ising model is the simplest system showing phase transitions (the transition between the paramagnetic phase and the ferromagnetic phase and the transition between the paramagnetic phase and the antiferromagnetic phase) and critical phenomena at finite temperatures. The exact solution of the square-lattice Ising model with free boundary conditions is not known for systems of arbitrary size. For the first time, the exact solution of the Ising model on the 15×15 square lattice with free boundary conditions is obtained after classifying all $2^{15\times15}(\approx 5.39 \times 10^{67})$ spin configurations with the microcanonical transfer matrix. Also, the phase transitions and critical phenomena of the square-lattice Ising model are discussed using the exact solution on the 15×15 square lattice with free boundary conditions.

Keywords—Phase transition, Ising magnet, Square lattice, Free boundary conditions, Exact solution.

I. Introduction

PHASE transitions and critical phenomena are the most universal phenomena in nature. The square-lattice Ising model is the simplest system showing phase transitions (the transition between the paramagnetic phase and the ferromagnetic phase and the transition between the paramagnetic phase and the antiferromagnetic phase) and critical phenomena at finite temperatures. The square-lattice 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.

The exact solution of the square-lattice Ising model with periodic boundary conditions is well known both in the thermodynamic limit (that is, the infinite-size system) [2] and in finite-size systems [3]. However, the exact solution of the square-lattice Ising model with free boundary conditions is not known for systems of arbitrary size. To overcome this, Ferdinand and Fisher [4] constructed the exact partition functions (that is, the exact solutions) of the Ising model on $L \times L$ square lattices with free boundary conditions up to $L = 4$. But their lattice sizes were too small and their results were not useful.

Bhanot [5] computed the exact partition functions of the Ising model on $L \times L$ square lattices with free boundary conditions up to $L = 10$ using Cray XMP. Bhanot counted all $2^{L\times L} = 2^{100}(\approx 1.27 \times 10^{30})$ states for $L = 10$, and began obtaining some useful results. Stosic *et al.* [6] calculated the exact partition functions up to $L = 12$ (corresponding to $2^{144} \approx 2.23 \times 10^{43}$ states) using IBM 3090, and tested finite-size scaling theory. Stodolsky and Wosiek [7] obtained the exact partition function for $L = 13$ (corresponding to $2^{169} \approx 7.48 \times 10^{50}$ states) using IBM RISC 6000, and studied phase transitions based on the entropy as a function of the energy. Recently, Kim [8]−[10] obtained the exact partition function of the Ising model on $L \times L$ square lattice with free boundary conditions for $L = 14$ (corresponding to $2^{196} \approx 1.00 \times 10^{59}$ states), and investigated the unknown properties of the antiferromagnetic phase transition.

In this work, for the first time, we evaluate the exact partition function of the Ising model on $L \times L$ square lattice with free boundary conditions for $L = 15$ (corresponding to $2^{225} \approx 5.39 \times 10^{67}$ states) using the microcanonical transfer matrix [5]−[29], and discuss its phase transition and critical behavior.

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II. Density of States

The Ising model on a lattice with N_s sites and N_b bonds is defined by the Hamiltonian

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

where J is the coupling constant ($J > 0$ for the ferromagnet and $J < 0$ for the antiferromagnet), $\langle i, j\rangle$ indicates a sum over all nearest-neighbor pairs of lattice sites, and $\sigma_i = \pm 1$. We define the density of states, $\Omega(E)$, with a given energy

$$E = -\sum_{\langle i,j\rangle} \sigma_i \sigma_j, \tag{2}$$

where E is integers $-N_b \le E \le N_b$. Then the partition function of the Ising model (a sum over 2^{N_s} possible spin configurations)

$$Z = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}}, \tag{3}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant, and T is temperature, can be written as

$$Z(T) = \sum_{E=-N_b}^{N_b} \Omega(E) e^{-\beta J E}. \tag{4}$$

Given the density of states $\Omega(E)$, the partition function is a polynomial in $e^{-\beta J}$. And the free energy per volume is given by

$$f = -\frac{k_B T}{N_s} \ln Z. \tag{5}$$

The microcanonical transfer matrix [5]−[29] is used to evaluate the *exact* integer values for the density of states $\Omega(E)$ of the Ising model on $L \times L$ (up to $L = 15$) square lattices with free boundary conditions ($N_s = L^2$ and $N_b = 2L^2 - 2L$).

Here, the microcanonical transfer matrix is briefly described for the Ising model on the 3×3 square lattice. First, an array $\omega^{(1)}$, which is indexed by energy E and spin variables $\sigma_i^{(1)}$ $(1 \leq i \leq 3)$ for the first row, is initialized as

$$\omega^{(1)}(E; \sigma_1^{(1)}, \sigma_2^{(1)}, \sigma_3^{(1)}) = \delta\big(E + \sigma_1^{(1)}\sigma_2^{(1)} + \sigma_2^{(1)}\sigma_3^{(1)}\big), \quad (6)$$

where δ is the Kronecker delta. Next, by introducing a new spin variable ($\sigma_1^{(2)}$) from the second row, each spin in the first row is traced over in turn

$$\tilde{\omega}^{(2)}(E; \sigma_1^{(2)}, \sigma_2^{(1)}, \sigma_3^{(1)}) = \sum_{\sigma_1^{(1)}} \omega^{(1)}\big(E + \sigma_1^{(1)}\sigma_1^{(2)}\big). \quad (7)$$

This procedure is repeated until all the spins in the first row have been traced over, leaving a new function of the three spins $(\sigma_1^{(2)}, \sigma_2^{(2)}, \sigma_3^{(2)})$ in the second row. Now, the horizontal bonds connecting the spins in the second row are then taken into account by shifting the energy,

$$\omega^{(2)}(E; \sigma_1^{(2)}, \sigma_2^{(2)}, \sigma_3^{(2)}) = \tilde{\omega}^{(2)}\big(E + \sigma_1^{(2)}\sigma_2^{(2)} + \sigma_2^{(2)}\sigma_3^{(2)}\big). \quad (8)$$

These two procedures, Eqs. (7) and (8), are then applied to each row in turn until the final (3rd) row is reached. Finally, the density of states is given by

$$\Omega(E) = \sum_{\sigma_1^{(3)}} \sum_{\sigma_2^{(3)}} \sum_{\sigma_3^{(3)}} \omega^{(3)}(E; \sigma_1^{(3)}, \sigma_2^{(3)}, \sigma_3^{(3)}). \quad (9)$$

The sum over all densities of states is equal to 2^{N_s} (all possible spin configurations).

For the Ising model on the 3×3 square lattice with free boundary conditions, we obtain $\Omega(-12) = 2$ (corresponding to the ferromagnetic ground states), $\Omega(-8) = 8$, $\Omega(-6) = 32$, $\Omega(-4) = 46$, $\Omega(-2) = 96$, $\Omega(0) = 144$, $\Omega(2) = 96$, $\Omega(4) = 46$, $\Omega(6) = 32$, $\Omega(8) = 8$, and $\Omega(-12) = 2$ (corresponding to the antiferromagnetic ground states). In general, $\Omega(E) = 0$ for $E =$ odd numbers, and $\Omega(E) = \Omega(-E)$. And we have

$$\sum_E \Omega(E) = 2^{N_s} = 512 \quad (10)$$

for $L = 3$. Then the exact partition function is given by

$$\begin{aligned} Z &= 2e^{12\beta J} + 8e^{8\beta J} + 32e^{6\beta J} + 46e^{4\beta J} + 96e^{2\beta J} \\ &+ 144 + 96e^{-2\beta J} + 46e^{-4\beta J} + 32e^{-6\beta J} \\ &+ 8e^{-8\beta J} + 2e^{-12\beta J} \end{aligned} \quad (11)$$

for $L = 3$.

III. 15 × 15 SQUARE LATTICE

We have classified all $2^{225} (\approx 5.39 \times 10^{67})$ spin configurations according to their E values using the microcanonical transfer matrix, and obtained the exact integer values for the density of states $\Omega(E)$ of the Ising model on 15×15 square lattice with free boundary conditions for the first time. The largest density of states is

$$\begin{aligned} \Omega(E = 0) &= 2105045165715689383461560790938809759 \\ &\quad 321645387068435547845740402832, \end{aligned} \quad (12)$$

which is approximately 2.105×10^{66}.

TABLE I
EXACT INTEGER VALUES FOR THE DENSITY OF STATES $\Omega(E)$ OF THE ISING MODEL ON THE 15×15 SQUARE LATTICE WITH FREE BOUNDARY CONDITIONS, AS A FUNCTION OF ENERGY $E(= -420 \sim -282)$.

E	$\Omega(E)$
−420	2
−416	8
−414	120
−412	478
−410	720
−408	6404
−406	30240
−404	91762
−402	301840
−400	1424652
−398	4991560
−396	16140716
−394	57144080
−392	209081096
−390	682422320
−388	2239506328
−386	7486962928
−384	24651289964
−382	78192052120
−380	249194057452
−378	789333745232
−376	2467673528752
−374	7606128234760
−372	23380750236690
−370	71216175150152
−368	215056197414004
−366	644040639564872
−364	1918339626058576
−362	5670286716774976
−360	16651964841981840
−358	48585295056689136
−356	140969121525380038
−354	406500613098304192
−352	1165816394094955208
−350	3325182520753643800
−348	9436374842660011746
−346	26641427103949458704
−344	74858227117775444096
−342	209344574298194390872
−340	582820167551704738498
−338	1615377498547676050464
−336	4458347645197136668492
−334	12253466031085041469016
−332	33542747485545525915386
−330	91457551129666383965304
−328	248415283260870627084624
−326	672203007725851484253304
−324	1812299156194400877647788
−322	4868442304330442051558568
−320	13032131980866730237247448
−318	34763712358867916609368728
−316	92416304486415786528175540
−314	244849423415614604938108288
−312	646543091517232270918450764
−310	1701594866301099819604828016
−308	4463641665390829763325869638
−306	11670934766287055922638006656
−304	30416863362698135594355703868
−302	79017064768726909997235465976
−300	204611570353466548157242747176
−298	528134279938407828078376549992
−296	1358829590494664612282872229764
−294	3484907896246088552695756532840
−292	8908854118143532068299562539974
−290	22701435175128566494202570456760
−288	57660935095798202254435232213924
−286	145982715804623832111134863295336
−284	368388750009407563591786675051084
−282	926593006924278224186073977697240

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TABLE II
DENSITY OF STATES $\Omega(E)$ FOR $E = -280 \sim -142$.

E	$\Omega(E)$
−280	2322957728266961481107171696851188
−278	5804357346624774911884514207499624
−276	14454990352505300976332450217441476
−274	35877467434475718891205721469071312
−272	88747262050921383477263205753793804
−270	218778979883379279381079164155148576
−268	537478853907536762469454738065292012
−266	1315859379774808487532230971273083328
−264	3210233134388163599014094353210292932
−262	7804208451711297526470688395188242648
−260	18904801956995833315014615054142823468
−258	45630135148423868799938771007592884272
−256	109736910357317496141919904371596730616
−254	262941831721522480601894974930598571600
−252	627706927266480788376249376554068950798
−250	1492892085537193063547980393432692410456
−248	3537185547666884907353555981672976479340
−246	8348887030886627238185919867864455688720
−244	19630156248022841131904697866573692755786
−242	45975473075498814081249465789710915532720
−240	107255244263446995420242866337119053031372
−238	249220122759516035036327543223402371116928
−236	576769180600012902783375316897541043410870
−234	1329404875477179075473311744071484857223128
−232	3051620094658243699008603729105777074856348
−230	6975946371308371427712542697538750126151736
−228	15880221666611494410635027384550907618220186
−226	35997458959983408941237557652894604720236840
−224	81251221414116542876019463915270048181655748
−222	182604487666256260401325145397906727701567800
−220	408598754763429651437632056374065038198938120
−218	910263334060798303231047269418231399045344648
−216	2018838984171896278174169466935064080050888012
−214	4457393489932959107345324585254611310243655960
−212	9796812540383324471133391500499019381205817078
−210	21433488609238599719953695382325939068084901288
−208	46675042975023246361558767007230566154992096332
−206	101167211666162588005606563845016160974608874256
−204	218241464819124671778442095856916865444052582168
−202	468550363548423247530625474294231097516438505504
−200	1001096062743760248272974887595477446623307891012
−198	2128504049620757536875448601755902435997221800800
−196	4503302333373191635993383251784391393173642544466
−194	9480344567792052001442563072871018865441969770424
−192	19857834464797005863574229312692352473895101617912
−190	41384013338884544141027809658699275854281070797192
−188	85803370336455849282102373628642576252396045783230
−186	176980345004088581867855911600699731817315518054840
−184	363138639295384297132810870209181506198255854721768
−182	741180982863074592060242668398046798815692015990696
−180	1504727866168962944368192646121867201295840781184408
−178	3038441801163536239432432699841057341997904527990632
−176	6102114876136836615025707600552987144589522343457628
−174	12187747168693423228203083969604934677378813043898768
−172	24207896907986367233657995437524431947432540480212252
−170	47814331587687653134824153962884430993775846968232232
−168	93908136723642769027334752278138015493951213570396264
−166	183387208014625010209971844235921075480008178924951056
−164	356067207903025591289040842589020355824040347837929220
−162	687334846728750977998322663524619879413862362535094488
−160	1319029111310672890909098233280605742387818552730272264
−158	2516321342645253858999502476577774805843809639361541136
−156	4771769635222409604561627635268174995218346384973439884
−154	8994360896498331181802951488073739401535204408794836368
−152	16850559602566924720311864256151565483951645871285702848
−150	31375244243415568638750246408084854684371716429502592112
−148	58058277487452104960179721525995601099323094939642052626
−146	106763004535908831128833775952491439561657257806255428184
−144	195088780039500495802658884112753258678200983479885203564
−142	354220599946934867213918973725479721245175911312632793064

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TABLE III
DENSITY OF STATES $\Omega(E)$ FOR $E = -140 \sim -2$.

E	$\Omega(E)$
−140	639028752623901398334284829032383819605895145331133059044
−138	1145373147552635550852176439649702485082613739053209728184
−136	2039522315125452473431404851344886670715906829615947801480
−134	3607775910960077406229583674789641331903455575465030704656
−132	6339499199513246044456843529359549164412713477835291841002
−130	11064944616977836166877038962659524288041055145021073924152
−128	19182135238789456449783645907264499410335582583318261983572
−126	33027256956677531702022866375740903485392602690799834017792
−124	56474226260814566169184896625448055917245433224254634924106
−122	95896910155057255512557660780338501202818272667264177055408
−120	161699894887512737959161427856377794969035604179773330347968
−118	270732172965460392237814230508559490234719465546449694252848
−116	450058715519058385258678864561680024997237617253610336477782
−114	742799825719252287278989327375216376429982402410770060539848
−112	1217087569095059520265220303061276229361523173564623214809780
−110	1979672572472963652818101135739484236005681023144589933642320
−108	3196395358337446864538433360275360808036931249553446228021684
−106	5122680642372803848736922109197772018508798704581512929680944
−104	8148502956521498824814147859339071934931068286903126168521804
−102	12864006089458016038947338081726200542968953755731877211040112
−100	20154250417142515309368935808612522123268048203644567063716248
−98	31334534648120243522078324367671428511622128666234530852629432
−96	48341516381351646518754428980575918854722726592119545164025480
−94	74000049749318383352566284018075126756587855074591606630098576
−92	112391342068552472151469412911807975292269900796511168655667968
−90	169354709726532401649433597190236038963686838828327158452338848
−88	253162780211609731414084278378963698094589373164786049857291224
−86	375418172412818518237910761626115931743932052723380996689558720
−84	552227997051466469821994736010365902946061976083582383543038234
−82	805720170420098592904429449468770432379875356506159520357370064
−80	1165971394254308607922230352723267518804240796774478889425035864
−78	1673419191955075235208469378144486071441502037869632110510547008
−76	2381827660771162730195130397050368153142791269878320860820181542
−74	3361866269816113206628962554844710407309846464953004270632990688
−72	4705340486172910863760460979267380047642653487207219733465666440
−70	6530079525301012364797760562634959702977825359577005677503917712
−68	8985437565381677636604458089522899285802727126061914629995733086
−66	12258298396417552882808796266317237952612197088683738009217805136
−64	16579388849702276511695817589265379770552949270956478050572631344
−62	22229604310783364118529173865862866544645777124129545032591626288
−60	29545933294590012893479184242399525722612474394660077919404032946
−58	38926443448826825031880019987149909386688575867536523197834932832
−56	50833667711332990922553488468283329543398399731733830942809278128
−54	65795619336977193817646056842784992469019362055477705552620601456
−52	84403583912570824868113761611924118683307655538945896205340374378
−50	107305803409733626788408032869588138240006773899327604356837567856
−48	135196200847067341090223710178612939660506507613804952997630848120
−46	168797412259291366608161992835128802086159225368441968772614156512
−44	208837609852224591754560918721645319423891555328765954112318564970
−42	256020924488187448717943945149931188262258035843083094122022687552
−40	310991705714745477366536144740796218986302159963480862401134421616
−38	374293380303907717680329328495398089739093447461996449290089882192
−36	446323259067084762568118286660594203189736378781836998373527022282
−34	527285256002833404027839011419832374017636834420173250660681248656
−32	617143070486334736638055514682864760950083169227484094822934814776
−30	715576879788576857801499276933979908578588063276799574462741301360
−28	821946929239404248184447109972491802709856143459675410102013651154
−26	935267527234926611640899288994488416181225385379912091635387474480
−24	1054194799367354843104368259917356969035758379492797819085637588944
−22	1177031096691327172547215993245413047887494035761722861183088379840
−20	1301748180448220942178216987048076918454667295322988092300720857214
−18	1426030244036262884999800467736880887890210748657760009359329917104
−16	1547336540978084923059143165304840143547461365323493409517483714696
−14	1662981955333378788503074379098573990791559983249639455770999986416
−12	1770232394456850845025067960164694117715372818181404263097605852242
−10	1866410534927532989386347955954703847353464999231055246229071968304
−8	1949006345072735666356463791969066698711952112953732463849573001936
−6	2015786063566382859083764584943047754072252817562284490136618574736
−4	2064893027730983732423216013975507220497395242943584361779035913358
−2	2094933972277576103737861740869564503926883254008137691828506024128

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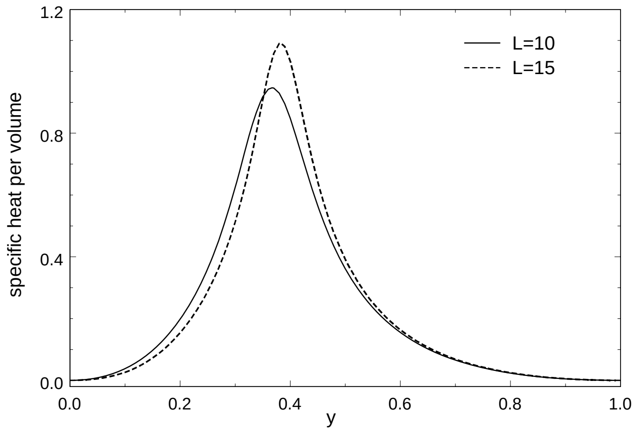

Fig. 1. Exact specific heat (in unit of k_B) per volume of the Ising model, as a function of $y = e^{-2\beta J}$, on the $L \times L$ square lattice with free boundary conditions for $L = 10$ and 15.

Tables I, II, and III show the exact integer values for the density of states $\Omega(E)$ of the Ising model on the 15×15 square lattice with free boundary conditions, as a function of energy $E(= -420 \sim -2)$. The values for $E = 2 \sim 420$ are easily obtained using $\Omega(E) = \Omega(-E)$.

IV. Specific heat

The square-lattice Ising model has the paramagnetic-ferromagnetic phase transition at the critical temperature (the so-called Curie temperature)

$$T_C = 2J/k_B \ln(\sqrt{2}+1) = 2.26919(J/k_B) \qquad (13)$$

for the ferromagnetic interaction ($J > 0$) and the paramagnetic-antiferromagnetic transition at T_N (Néel temperature)

$$T_N = 2J/k_B \ln(\sqrt{2}-1) = 2.26919(-J/k_B) \qquad (14)$$

for the antiferromagnetic interaction ($J < 0$). Because of the symmetry of the density of states, $\Omega(E) = \Omega(-E)$, for the Ising model, the critical phenomena at Néel temperature is the same as the critical behaviors at Curie temperature.

In the thermodynamic limit, the specific heat per volume of the square-lattice Ising ferromagnet (or antiferromagnet) becomes infinite at the critical point (Curie or Néel temperature) where the transition between the paramagnetic phase and the ferromagnetic (or antiferromagnetic) phase emerges. In finite systems, the specific heat per volume shows a sharp peak but is not infinite. At the same time, the location (the so-called effective critical point) of the sharp peak of the specific heat in a finite system is different from the critical point at the inifinite system. As the system size increases, the effective critical point approaches the critical point. The characteristic of the approach to the critical point is determined by the shift exponent whose value is not known and depends on the types of boundary conditions.

TABLE IV
The values of the effective critical point $y_p(L)$ and the effective shift exponent $\lambda(L)$ of the Ising model on $L \times L$ square lattices with free boundary conditions for $L = 3 \sim 15$.

L	$y_p(L)$	$\lambda(L)$
3	0.264609	0.915894
4	0.299262	0.944940
5	0.321115	0.961422
6	0.336084	0.972301
7	0.346959	0.980061
8	0.355209	0.985847
9	0.361677	0.990290
10	0.366883	0.993773
11	0.371160	0.996547
12	0.374736	0.998785
13	0.377769	1.000609
14	0.380374	1.002108
15	0.382634	

Given the density of states, we obtain the specific heat per volume

$$\begin{aligned} C(y) &= (N_s k_B T^2)^{-1} \frac{\partial^2}{\partial \beta^2} \ln Z \\ &= \frac{k_B}{N_s} (\ln y)^2 (\langle E^2 \rangle - \langle E \rangle^2), \end{aligned} \qquad (15)$$

where $y = e^{-2\beta J}$. For a ferromagnetic interaction ($J > 0$), the physical interval is $0 \le y \le 1$ ($0 \le T \le \infty$). That is, y is a convenient temperature variable, confined to a short interval $[0, 1]$. Figure 1 shows the exact specific heat of the Ising ferromagnet on the $L \times L$ square lattice (for $L = 10$ and 15), as a function of y. As the system size L increases, the specific-heat peak positions (that is, the effective critical points) $y_p(L)$ approach the critical point $y_c = \sqrt{2} - 1 = 0.41421$, and the specific-heat heights $C_p(L)$ increase. The effective critical point $y_p(L)$ of the specific heat scales as

$$y_c - y_p(L) = \Delta y_p(L) \sim L^{-\lambda}, \qquad (16)$$

where λ is the shift exponent [4] whose exact value is not known for the square-lattice Ising model with free boundary conditions. And we can define the effective shift exponent

$$\lambda(L) = -\frac{\ln[\Delta y_p(L+1)/\Delta y_p(L)]}{\ln[(L+1)/L]} \qquad (17)$$

for finite lattices. Table IV shows the values of $y_p(L)$ and $\lambda(L)$ for $L = 3 \sim 15$.

By using the Bulirsch-Stoer (BST) method [30], we have extrapolated the values for finite lattices to infinite size ($L \to \infty$), and the extrapolated value of the shift exponent is $\lambda = 1.00(2)$, implying the possibility of $\lambda = 1$ for the square-lattice Ising ferromagnet with free boundary conditions. The error estimates are twice the difference between the ($n-1$,1) and ($n-1$,2) approximants. From the specific-heat peak positions, the BST estimate of the critical point is precisely obtained to be $y_c = 0.41424(4)$, in excellent agreement with the exact value $y_c = \sqrt{2} - 1 = 0.41421$.

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V. Conclusion

Phase transitions and critical phenomena are the most universal phenomena in nature. The square-lattice Ising model is the simplest system showing phase transitions and critical phenomena at finite temperatures. The square-lattice Ising model has played a central role in our understanding of phase transitions and critical phenomena. The exact solution of the square-lattice Ising model with free boundary conditions is not known for systems of arbitrary size. For the first time, we have obtained the exact solution of the Ising model on the 15×15 square lattice with free boundary conditions after classifying all $2^{225}(\approx 5.39 \times 10^{67})$ spin configurations with the microcanonical transfer matrix. We have also discussed the phase transitions and critical phenomena of the square-lattice Ising model using the exact solution on the 15×15 square lattice with free boundary conditions.

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