The critical temperature of two-dimensional and three-dimensional Ising models

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(Received 20 June 2002; accepted 9 April 2003)

The critical temperatures of the Ising model can be obtained by considering the elementary cells of the corresponding lattice, namely the square lattice in two dimensions and the cube in three dimensions. The configurations in the statistical sum of a cell are divided into nondegenerate and degenerate cases. At the critical temperature of the infinite lattice the contributions of these two groups of configurations are assumed to be equal. This conjecture reproduces the exact Onsager result for two dimensions and the numerical result for the three-dimensional Ising lattices. Although this conjecture is not exact, it gives insight into the nature of the transitions. © *2003 American Association of Physics Teachers.*

[DOI: 10.1119/1.1579495]

The Ising model is one of the simplest models describing interacting particles. It is based on the assumptions that the particles (spins) are located on the sites of a lattice, each spin may be in one of two possible states characterized by the values $S_i=\pm 1$, and account is taken only of interactions between nearest neighbors. A given pair (i,j) contributes $-JS_iS_j$ to the energy, so that the Hamiltonian has the form

$$H=-J\sum_{(i,j)} S_iS_j. \tag{1}$$

The thermodynamic functions of the states described by the Hamiltonian in Eq. (1) can be easily found in one dimension. The two-dimensional Ising model was solved exactly by Onsager in 1944.[1] He found that for $T<T_c$, the system is ordered, in the sense that $\langle S\rangle\neq 0$ so that more spins are in one state than in the other, while for $T>T_c$ the ordering is absent. However, this exact solution has been found only for two dimensions, while we are interested mainly in three-dimensional systems. In the latter case only approximate results are available. Moreover, the Onsager solution is so complicated that even after some simplifications, the solution requires eight pages of the very concisely written Landau–Lifshitz textbook.[2] Other attempts to simplify the exposition[3,4] are still quite complicated. Due to this mathematical complexity, it is difficult to follow the underlying physical ideas.

Preparatory to our analysis, let us mention two simple physical arguments suggested for an estimate of the critical temperature, one proposed by Peierls[5] and cited in Ziman's book,[3] and the other formulated in the less widely known article of Svrakic.[6] The equilibrium state of a system is defined by the minimum of the free energy $F=E-TS$, which is, roughly speaking, a compromise between the ordered tendency of the energy E and the tendency toward disorder of the entropy S. Clearly, the former dominates at low temperatures, $T\to 0$, while the latter for $T\to\infty$. As a compromise, the phase transition from the disordered state to the ordered one occurs at some temperature T_c, where the changes of energy and entropy due, for example, to a single spin flip compensate each other, yielding

$$k_BT_c=\frac{\Delta E}{\Delta S}, \tag{2}$$

where k_B is the Boltzmann constant.

A square lattice is shown in Fig. 1 where the spins are shown by dots and circles. Let us compare the two states, one of which is fully ordered (all spins are parallel); the second one (shown in Fig. 1) is similar to the first, but contains an island of spins in the opposite direction. The question is whether the second state might appear spontaneously from the first one, thereby destroying the order. To provide the answer, we have to calculate the appropriate changes in the energy and the entropy. Then, the change of the free energy will show whether the transition between these two states is favorable, and Eq. (2) will give the temperature of the transition. The change of the energy E is equal to $2JL$, because each of the L changes from the parallel to the antiparallel orientation of spins costs energy $2J$. To calculate the change in the entropy, we can use the relation $S=\ln W$, where W is the number of ways required to build an island of perimeter L. S can be calculated approximately using the idea of random walks. If we come to a lattice site on the perimeter, we can continue outward along three other ways, then again along three ways, and so on. In order to build the closed island after L steps, we have to return to the initial lattice site. However, for large L, the neglect of the latter requirement will bring only a small error. Thus, we obtain $W=3^L$, so that $\Delta S=L\ln 3$. Then Eq. (2) gives

$$k_BT_c=\frac{2J}{\ln 3}. \tag{3}$$

This result is not too different from the exact Onsager's result,[1]

$$k_BT_c=\frac{2J}{\ln(1+\sqrt{2})},$$

when the crudeness of the approximations is considered. However, by similar hand-waving arguments we can obtain the exact result as well[6] (see also Refs. 7–9). The statistical sum that corresponds to the energy in Eq. (1) is given by

$$Z=\sum \exp\left(J\sum_{(i,j)}\frac{S_iS_j}{k_BT}\right), \tag{4}$$

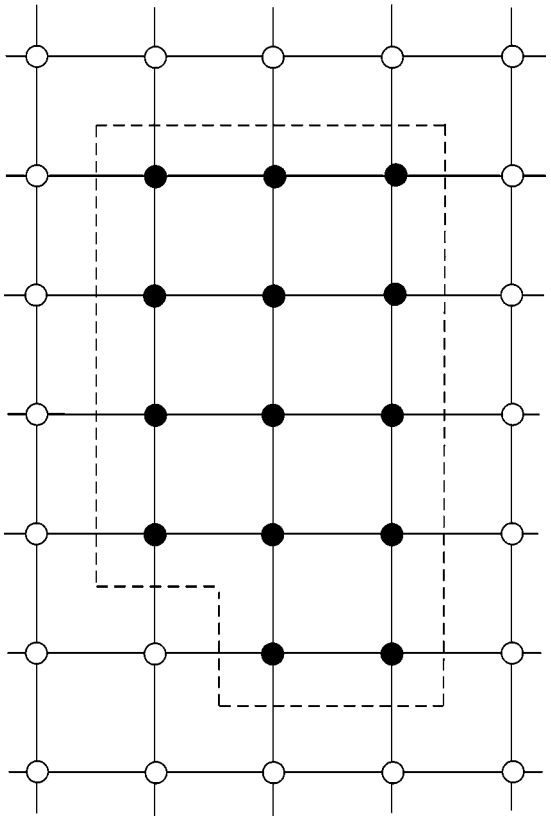

Fig. 1. Two-dimensional Ising square lattice with an island of opposite spins (indicated by black solid dots) of perimeter L.

where the outer sum has to be performed over all 2^N configurations of N spins.

Let us consider the elementary cell of the square lattice containing only four spins. Then, the sum in Eq. (4) will contain only the configurations

$$Z=\sum_{S_1,S_2,S_3,s_4=\pm 1}\exp\left[\frac{J}{k_BT}\sum_{(i,j)}(S_1S_2+S_2S_3+S_3S_4+S_4S_1)\right] \tag{5}$$

shown in four different groups in Fig. 2 with n the number of the equivalent configurations. For instance, $n=2$ for group a means that the configuration is equivalent to one obtained by replacing all circles by dots. Following Ref. 6 we call the first two configurations ''ordered,'' and the remaining two ''disordered.'' The reasoning behind this division is based on

configuration	a	b	c	d
E	-4 J	4 J	0	0
n	2	2	4	8

Fig. 2. Different configurations of an elementary cell of a two-dimensional Ising square lattice divided in four groups, when the energy E and number of configurations n are shown for each group. Groups a and b contain nondegenerate configurations while degeneracies are inherent in groups c and d.

	configuration	n	E	W_G	W_N		configuration	n	E	W_G	W_N
a		2	-12 J	0	1	b		2	12 J	0	1
c		6	-4 J	0	1	d		6	4 J	0	1
e		8	0	0	1	f		8	0	0	1
g		24	0	1	0	h		24	0	1	0
i		16	-6 J	$\frac{2}{8}$	$\frac{6}{8}$	j		16	6 J	$\frac{2}{8}$	$\frac{6}{8}$
k		24	-4 J	$\frac{4}{8}$	$\frac{4}{8}$	l		24	4 J	$\frac{4}{8}$	$\frac{4}{8}$
m		48	-2 J	$\frac{6}{8}$	$\frac{2}{8}$	n		48	2 J	$\frac{6}{8}$	$\frac{2}{8}$

Fig. 3. Different configurations of the elementary cell of a three-dimensional Ising cube lattice with n being the number of equivalent configurations in each group, and E is their energy. Groups $a-f$ contain nondegenerate (stable) configurations, while configurations composing groups g and h are degenerate (unstable). Groups $i-n$ make a contribution to statistical sum of both degenerate and nondegenerate states which are characterized by the statistical weight W_G and W_N, respectively.

the fact that by filling the entire plane by such squares, we obtain the fully ordered state for the first two configurations, and a disordered state for the last two configurations. However, as noted above, the phase transition is defined as a compromise between order and disorder. Let us assume, therefore, that the temperature of the phase transition can be obtained from the equality of the statistical sum of the ordered configurations (a and b) and the disordered configurations (c and d),

$$Z_{\text{order}}=Z_{\text{disorder}}. \tag{6}$$

If we substitute the appropriate number of configurations from Fig. 2, we obtain $Z_{\text{order}}=2e^{4\beta J}+2e^{-4\beta J}$, and $Z_{\text{disorder}}=12$, where $\beta=1/k_BT$. The equality $Z_{\text{order}}=Z_{\text{disorder}}$ gives the exact Onsager result $k_BT_c=2J/\ln(1+\sqrt{2})$. Exact results have been also obtained for the triangle lattice,[6,7] but the application of this method to *the* q-state Potts model gives only approximate although quite reasonable results.[7–9]

It is intriguing to extend this approach to three-dimensional lattices and to find the critical temperature of these lattices by considering just one elementary cell. All possible $2^8=256$ configurations of such a cell for a simple cubic lattice are shown in Fig. 3, where, as in Fig. 2, n stands for the number of equivalent configurations associated with the appropriate group. By following the reasoning of Ref. 6, we see that the fully ordered states in three dimensions can be obtained from the configurations associated with groups a and b, that is, the statistical sum of the ordered configura-

tions Z_{order} is equal to $Z_{\text{order}}=2e^{12\beta J}+2e^{-12\beta J}$. All other configurations are related to disordered configurations, and Z_{order} is equal to

$$Z_{\text{disorder}}=16e^{6\beta J}+16e^{-6\beta J}+30e^{4\beta J}+30e^{-4\beta J}+48e^{2\beta J}+48e^{-2\beta J}+64. \tag{7}$$

The critical temperature is given by the condition (6), which gives $k_BT_c/J=2.030$. This result is significantly different from the approximate result $k_BT_c/J=4.511$ (see Ref. 10 for a recent review of results obtained by the high-temperature series and different forms of Monte Carlo calculations).

The main aim of this note is to suggest a new method of calculating the critical temperature of the two- and three-dimensional Ising models from the analysis of elementary cells. This method differs from that proposed in Ref. 6, although it is also nonrigorous and is based on physical arguments. Consider first the different configurations of the two-dimensional Ising lattice shown in Fig. 2. We call the configurations of groups *a* and *b* ''nondegenerate'' in the sense that all neighboring states that can be obtained from a given one by the flipping of a single spin are distinguished from the original one by their energy. By contrast, all the configurations in group *c* do not change their energy if one of the spins is flipped. Hence, these configurations have adjacent states of the same energy, and we call these configurations ''degenerate.'' The situation is slightly more complicated for the configurations belonging to group *d*. Indeed, flipping spin 1 will change the energy to $-4J$, while flipping spin 4 will result in the energy change $4J$. Due to the symmetry of these two states with respect to the original one with $E=0$, we place the original ''quasi-degenerate'' configuration in the degenerate group. Note, that flipping spins 2 or 3 will not change the energy, and hence, all configurations of group *d* are related, along with those of group *c* to degenerate configurations. Our conjecture is that the phase transition occurs when the statistical sum of nondegenerate states is equal to that of degenerate states,

$$Z_{\text{degenerate}}=Z_{\text{nondegenerate}}. \tag{8}$$

Because our criterion (8) coincides with that of Eq. (6) for the two-dimensional Ising lattice, it yields the exact Onsager solution for the critical temperature. However, in contrast to Eqs. (3)–(6), the criterion (8) can be applied to three-dimensional lattices as well.

All possible configurations of a three-dimensional Ising cubic lattice are shown in Fig. 3. Groups $a-f$ of Fig. 3 are nondegenerate, because a flip of the spin of each site will change the energy of the cell, and no quasi-degenerate states are observed in these configurations. Groups *g* and *h* are degenerate according to our criterion. Indeed, a flip of each spin of group *g* results in the change of energy $\Delta E=2J$, $-2J$, $2J$, $-2J$, $2J$, $-2J$, $2J$, $-2J$, while a flip of each spin of group *h* change the energy by $6J$, $-6J$, $6J$, $-6J$, $2J$, $-2J$, $2J$, $-2J$. Hence, these two groups are quasi-degenerate. However, groups $i-n$ contribute to both degenerate and nondegenerate states. Let us consider, as an example, group *i*. The flip of each of the eight spins changes the energy by $-6J$, $6J$, $6J$, $6J$, $6J$, $2J$, $2J$, $2J$, respectively. The first two excited states are symmetric, and, according to our classification, they are quasi-degenerate, while the remaining six states are nondegenerate. The numbers $W_G=\frac{2}{8}$ and $W_N=\frac{6}{8}$ shown in Fig. 3 for group *i* show the statistical weight of degenerate and nondegenerate states. Analogous analysis could be easily performed for each of the groups $j-n$. The result of this analysis is the following form of Eq. (8) for the cubic Ising lattice:

$$2e^{12\beta J}+2e^{-12\beta J}+12e^{6\beta J}+12e^{-6\beta J}+18e^{4\beta J}+18e^{-4\beta J}+12e^{2\beta J}+12e^{-2\beta J}+16=4e^{6\beta J}+4e^{-6\beta J}+12e^{4\beta J}+12e^{-4\beta J}+36e^{2\beta J}+36e^{-2\beta J}+48. \tag{9}$$

The solution of Eq. (9), $k_BT_c/J=4.277$, is much closer to the numerical result[10] $k_BT_c/J=4.511$ than that obtained by the method of Ref. 6.

In conclusion, we have shown that the critical temperature of two- and three-dimensional Ising models can be obtained by simple physical arguments based on the compromise between configurations that are degenerate or nondegenerate with respect to a single spin-flip excitation. As a graduate student homework problem, we suggest expanding our analysis to other elementary cells of the two-dimensional lattice (say, 3×3, 3×2) and to other types of three-dimensional lattices (bcc, fcc, etc). Results for the latter should be compared with the precise numerical results $k_BT_c/J=6.235$ and 9.792 for the bcc and fcc lattices, respectively.[11] Results of such a comparison are not known *a priori* because it is not clear how well this method will work in general. For example, the method does not give the exact result for the honeycomb lattice.

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