Journal of Theoretical Physics

Founded and Edited by M. Apostol

ISSN 1453-4428

On the critical temperature of the Ising ferromagnets M. Apostol Department of Theoretical Physics, Institute of Atomic Physics, Magurele-Bucharest Mg-6, POBox Mg-35, Romania email: apoma@theory.nipne.ro

Abstract

The critical temperature of the two-dimensional Ising ferromagnet is computed by a simple method, which can be extended to various others lattice models, including the Ising ferromagnet in three dimensions.

The well-known Ising ferromagnet in two dimensions consists of a regular square lattice of twovalued spin variables $\mu_i = \pm 1$, i = 1, ...N, whose energy is given by

$$E = -\frac{1}{2}J\sum_{\langle ik\rangle}\mu_i\mu_k - mH\sum_i\mu_i \quad ; \tag{1}$$

in eq.(1) J is a coupling constant, $\langle ik \rangle$ are the nearest-neighbours, m is the magnetic moment of each spin and H is the applied magnetic field. The problem is to compute the partition function

$$Z = \sum_{\{\mu_i = \pm 1\}} \exp\left(\frac{1}{2} K \sum_{\langle ik \rangle} \mu_i \mu_k + C \sum_i \mu_i\right) \quad , \tag{2}$$

where the summation extends over all spin configurations, K = J/T, C = mH/T, T being the temperature.

Kramers and Wannier[1] succeeded to exactly locate the critical temperature at $K_c = 0.44$, and to show that the specific heat is singular at the critical point, by using a particular matricial method which may be termed the V-matrix technique. The location of the critical temperature is attained by using a so-called duality argument, which is neither transparent, nor practical. Subsequently, Onsager[2] gave the exact solution for the partition function in vanishing magnetic field, by a quaternion algebra, rotation matrices have successfully been used to the same effect,[3] and, finally, the magnetization (announced by Onsager) has been reported by Yang.[4] All these techniques are exceedingly laborious, and, worth-remarking, they all contain, more or less implicitly, the duality argument. Various simplifications have been attempted during the time[5], of not much avail, so that it might be preferrable sometime to resort to approximate methods.[6] Such a method is presented here, which gives the critical temperature of the two-dimensional Ising ferromagnet surprisingly accurate ($K_c = 0.44$), and which can be extended to other lattice models; for instance, the method predicts a critical point $K_c = 0.26$ for the (simple cubic) Ising ferromagnet in three dimensions.

26 (1997)

The method is based on the transfer matrix introduced by Kramers and Wannier[1], following, it seems, a suggestion of Montroll.[7] We consider a strip of N_2 chains, each with N_1 spins, such as $N = N_1 N_2$. Suppose that at one end the strip has a row of spins $\mu' = (\mu'_1, \mu'_2, ..., \mu'_{N_1})$, and we connect at this end another raw of spins $\mu = (\mu_1, \mu_2, ..., \mu_{N_1})$. For large N_2 and with cyclic boundary conditions along each chain $(\mu_{N_1+1} = \mu_1)$ we get from eq.(2)

$$Z(\mu) = \exp\left[K\left(\mu_{1}\mu_{2} + ...\mu_{N_{1}}\mu_{1}\right) + C\left(\mu_{1} + ...\mu_{N_{1}}\right)\right] \cdot \sum_{\mu'} \exp\left[K\left(\mu_{1}\mu'_{1} + ...\mu_{N_{1}}\mu'_{N_{1}}\right)\right] \cdot Z(\mu') \quad ,$$
(3)

which, introducing the scalar product, can be written symbolically as

$$Z(\mu) = e^{K(\mu, D\mu) + C(1,\mu)} \cdot \sum_{\mu'} e^{K(\mu, \mu')} \cdot Z(\mu') \quad , \tag{4}$$

or

$$Z(\mu) = e^{\varepsilon(\mu)} \cdot \sum_{\mu'} e^{K(\mu,\mu')} \cdot Z(\mu') \quad , \tag{5}$$

where

$$\varepsilon(\mu) = K(\mu, D\mu) + C(1, \mu) \tag{6}$$

is the one-chain energy divided by temperature, D is a shift operator, $D\mu = (\mu_2, \mu_3, ..., \mu_{N_1}, \mu_1)$, and 1 = (1, 1, ...1). Introducing $Z^*(\mu) = \exp[-\varepsilon(\mu)/2] Z(\mu)$ eq.(5) becomes

$$Z^{*}(\mu) = \sum_{\mu'} T(\mu, \mu') Z(\mu') \quad ,$$
(7)

where the transfer matrix

$$T(\mu, \mu') = (\mu, T\mu') = e^{K(\mu, \mu') + \frac{1}{2}\varepsilon(\mu) + \frac{1}{2}\varepsilon(\mu')}$$
(8)

has been introduced. With cyclic boundary conditions across the strip we get from eq.(7) the partition function

$$Z = \sum_{\mu\mu_1...\mu_{N_2-1}} T(\mu, \mu_1) T(\mu_1, \mu_2) \dots T(\mu_{N_2-1}, \mu) =$$

= $tr(T^{N_2}) = \lambda_1^{N_2} + \lambda_2^{N_2} + \dots,$ (9)

where λ 's are the eigenvalues of the transfer matrix T. We note that T is a $2^{N_1} \times 2^{N_1}$ matrix.

As it is well-known, if the matrix T is non-singular and has a maximum eigenvalue $\lambda_{\max} \equiv \lambda$ then the partition function is given by

$$Z \simeq \lambda^{N_2} \quad . \tag{10}$$

The maximum eigenvalue of a large matrix like the matrix T is given by

$$\lambda = (\mu_0, T\mu_0) \quad , \tag{11}$$

where μ_0 is the positive-valued vector of highest symmetry.[8] In our case $\mu_0 = (1, 1, ...1)$, such that

$$\lambda = (1, T1) = e^{(2K+C)N_1} \tag{12}$$

and

$$Z = e^{(2K+C)N} {.} {(13)}$$

From eq.(13) we get the magnetization

$$M = m \frac{\partial \ln Z}{\partial C} = mN \tag{14}$$

and the energy

$$E = -MH - J\frac{\partial \ln Z}{\partial K} = -mNH - 2JN \quad , \tag{15}$$

which show that $Z = \exp\left[(2K + C)N\right] = Z_{ord}$ is the partition function of the ordered, ferromagnetic state.

Slightly above the critical temperature the spins are all disordered, such as the energies of all configurations in eq.(2) may be replaced by zero (as if the temperature goes to infinite). The transfer matrix T has then all the elements equal to unity, it is a singular matrix, and all its eigenvalue vanish except one which is $\lambda = 2^{N_1}$. We have therefore

$$Z_{dis} = 2^N \quad . \tag{16}$$

In order to get the critical temperature we may equate (in vanishing magnetic field C = 0) $Z_{ord} = Z_{dis}$ obtained above, leading to $K_c = \ln 2/2 = 0.35$. However, we can improve upon the partition function of the disordered state by expanding the expnentials in eq.(2) for small energies:

$$Z_{dis} = \sum_{\{\mu_i = \pm 1\}} \left[1 + \frac{1}{2} K \sum_{\langle ik \rangle} \mu_i \mu_k + \frac{1}{8} K^2 \left(\sum_{\langle ik \rangle} \mu_i \mu_k \right)^2 + \dots \right] = 2^N \left[1 + \frac{1}{8} K^2 \left\langle \left(\sum_{\langle ik \rangle} \mu_i \mu_k \right)^2 \right\rangle + \dots \right] = 2^N \left(1 + N K^2 \dots \right) \quad ,$$
(17)

which is nothing else but the high-temperature expansion.[9] The critical temperature is now given by

$$e^{2K} = 2\left(1+K^2\right) \quad ,$$
 (18)

which yields a surprisingly accurate result $K_c = 0.43.[10]$

Replacing the chains by planes the transfer matrix method can obviously be extended to the three-dimensional Ising ferromagnet. We obtain in this case (for a simple cubic lattice) $Z_{ord} = \exp\left[(3K+C)N\right]$, whence the critical temperature would be given in the first approximation by $K_c = \ln 2/3 = 0.23$. However, the low=energy series expansion gives $Z_{dis} = 2^N \left(1 + \frac{3}{2}NK^2 + ...\right)$, so that the critical temperature is given by

$$e^{3K} = 2\left(1 + \frac{3}{2}K^2\right) \quad , \tag{19}$$

i.e. $K_c = 0.26$.

It is a straightforward matter to see that the method can also be applied to various other versions of the Ising ferromagnet, as well as to some others lattice models for computing their critical temperature.

References

- [1] H. A. Kramers and G. H. Wannier, Phys. Rev. 60 252, 263 (1941).
- [2] L. Onsager, Phys. Rev. 65 117 (1944).
- [3] B. Kaufman, Phys. Rev. 76 1232 (1949); B. Kaufman and L. Onsager, Phys. Rev. 76 1244 (1949).
- [4] C. N. Yang, Phys. Rev. 85 808 (1952); the magnetization has previously been announced by L. Onsager, Nuovo Cim. (Suppl.) 6 261 (1949).
- [5] See, for example, N. Vdovitchenko's method of graph summation quoted in L. Landau and E. Lifshitz, *Statistical Physics*, Mir (1967), p. 538.
- [6] Various approximate treatments are quoted in Ref. 1; see, also, C. Domb's review article in *Phase Transitions and Critical Phenomena*, ed. by C. Domb and M. S. Green, Academic (1974), p. 357.
- [7] E. Montroll, J. Chem. Phys. 9 706 (1941); 10 61 (1942).
- [8] This assertion seems to be traced back to S. B. Frobenius, Preuss. Akad. Wiss. 514 (1909).
- [9] W. Opechowski, Physica 4 181 (1937).
- [10] Higher-order terms in the high-temperature expansion, as well as Bloch's low-temperature expansion (F. Bloch, Z. Physik 61 206 (1930)), would bring only minor corrections, for obvious reasons.

[©] J. Theor. Phys. 1997, apoma@theor1.theory.nipne.ro