Locating analytically critical temperature in some statistical systems

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Abstract

We have found a simple criterion which allows for the straightforward determination of the order-disorder critical temperatures. The method reproduces exactly results known for the two dimensional Ising, Potts and $Z(N < 5)$ models. It also works for the Ising model on the triangular lattice. For systems which are not selfdual our proposition remains an unproven conjecture. It predicts $\beta_c = 0.2656...$ for the two coupled layers of Ising spins. Critical temperature of the three dimensional Ising model is related to the free energy of the two layer Ising system.

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Classical method of determining critical temperature in statistical physics consists of locating singularities of the largest eigenvalue of the corresponding transfer matrix $T$. To this end one has to study the high power of $T$, e.g. $T^L$ with $L$ being the linear size of the system. This amounts to investigate the $d$ dimensional euclidean system in its full complexity. On the other hand it is conceivable that the information about the phase transition is also encoded in all other eigenvalues, i.e. that the whole spectrum of the transfer matrix is sensitive to its location. This observation is confirmed by the famous example of the two dimensional Ising model where all eigenvalues show the extremal behaviour at $\beta = \beta_c \ [1]$. Therefore we propose to search for the extremum of some simpler function which characterizes the system, which however is not dominated solely by the largest eigenvalue. The advantage of such an approach is that one may infer a nontrivial information from ”characteristic” functions which are much easier to calculate. To be specific we propose to study the following characteristic function of a $d$ dimensional system

$$\rho(\beta) = \lim_{L \to \infty} \left( \frac{\text{Tr}T^2}{\text{Tr}T^2} \right)^{\frac{1}{L^{d-1}}} ,$$

and analogous higher, moments of the transfer matrix. Following simple properties of $\rho$ can be easily proven.

a) $\rho(0) = 1,$  
b) $\rho(\infty) = 1,$  
c) $\rho(\beta) \geq 1.$

(2)

To see a) consider the normalized second moment at finite $L$

$$r_L(\beta) = \frac{(\text{Tr}T)^2}{\text{Tr}T^2} = \frac{(Z_1)^2}{Z_2},$$

(3)

where $Z_1$ and $Z_2$ are the partition functions of the $d - 1$ dimensional system and of the two coupled $d - 1$ dimensional systems respectively. For simplicity we shall use the terminology of the $d=2$ spin system. Hence $Z_1$ and $Z_2$ describe one dimensional spin chain and two coupled chains of spins. Periodic boundary conditions are implied in both directions, even for the single chain. With these definitions a) follows immediately from the observation that $Z_2(\beta = 0) = N_2 = (N_1)^2,$ where $N_1, N_2$ denote the total number of
microscopic states of single and double chain. At low temperatures \((\beta \to \infty)\) fully ordered states dominate, hence
\[
\rho(\beta = \infty) = \lim_{L \to \infty} g^{L^{d-1}} L^{d-1} = 1. \tag{4}
\]
Where \(g\) denotes degeneracy factor of the ordered states. The last equality requires finite \(g\) (and \(d > 1\)), therefore \(b\) holds only for systems with the discrete internal symmetry. Finally the property \(c\) follows directly from the positivity of the eigenvalues of the transfer matrix since
\[
\rho_L(\beta) = \frac{\sum_{\alpha,\beta} \lambda_\alpha \lambda_\beta}{\sum_\alpha \lambda_\alpha^2} > 1. \tag{5}
\]
Characteristic function, Eq.(1), is sensitive to the whole spectrum of the transfer matrix. However in view of our earlier discussion supplemented with the properties \(a)\) – \(c)\) it is natural to expect that the maximum of \(\rho\) occurs at the phase transition point,
\[
\beta_{\text{max}} = \beta_c. \tag{6}
\]
Surprisingly this simple proposition is true in many, sometimes nontrivial, cases. We shall discuss them in the order of increasing complexity.

Two dimensional Ising model. For \(d = 2\), calculation of \(\rho(\beta)\) is easily reduced to solving a straightforward two spin problem. Indeed the partition functions \(Z_i(i = 1, 2)\) are readily written as
\[
Z_i = Tr(T_i)^L, \tag{7}
\]
where \(T_i\) are the transfer matrices propagating one/two spins horizontally, c.f. Fig.1.

Explicitly for Ising spins
\[
T_1 = \begin{pmatrix} x^2 & x \\ x & x^2 \end{pmatrix}, T_2 = \begin{pmatrix} x^4 & x^2 & x^2 & x^2 \\ x^2 & x^2 & 1 & x^2 \\ x^2 & 1 & x^2 & x^2 \\ x^2 & x^2 & x^2 & x^4 \end{pmatrix}, x = e^{\beta}. \tag{8}
\]
We have chosen the interaction energy
\[
E(s) = -\sum_{<nm>} \delta_{s_n,s_m}, \tag{9}
\]
and \( s_n = \pm 1 \). In the thermodynamical limit the largest eigenvalues of \( T_i \) dominate and we get

\[
\rho_{\text{Ising}2}(\beta) = \frac{t_{1\text{max}}^2}{t_{2\text{max}}} = \frac{x^2(x+1)^2}{\frac{1}{2}(x^2+1)^2 + \sqrt{\frac{1}{4}(x^2-1)^4 + x^2(x^2+1)^2}}. \tag{10}
\]

Since the \( L \to \infty \) limit was already performed, \( \rho(\beta) \), as given by Eq.(10), is the nontrivial characteristic of the infinite system. As conjectured \( \rho(\beta) \) has a single maximum at \( x_c = 1 + \sqrt{2} \) which corresponds to the famous Onsager value \([2,3]\).

**Potts and equivalent \( Z(N) \) models.** The energy of the \( q \) state Potts model is given by Eq.(9) with \( s_n \) assuming \( q \) different values. Transfer matrices for one and two spin system are again simple

\[
\begin{align*}
<s|T_1|s'> &= \exp \beta(\delta_{s,s'} + 1), \\
<s_1,s_2|T_2|s_1',s_2'> &= \exp \beta(\delta_{s_1,s_2} + \delta_{s_1,s_1'} + \delta_{s_2,s_2'} + \delta_{s_1',s_2'}). \tag{11}
\end{align*}
\]

For \( q = 3 \) the diagonalization is tractable \([4]\) and the final result for the characteristic function reads

\[
\rho_{\text{Potts}3}(\beta) = \frac{2x^2(x+2)^2}{x^4 + 3x^2 + 2x + 3 + \sqrt{x^8 + 2x^6 - 4x^5 + 27x^4 + 28x^3 + 6x^2 + 12x + 9}}.
\]

Again it has a single maximum at \( x_c = 1 + \sqrt{3} \) which agrees with the known location of the transition temperature \([4]\).

For \( q = 4,5 \) we have used standard numerical methods to diagonalize transfer matrices. In both cases \( \rho(x) \) has a single maximum located at \( x_c = 1 + \sqrt{q} \) in accord with known results. For \( q > 4 \) the transition is first order \([4]\) and consequently our method seems to apply to both kinds of transitions. We have not attempted algebraic diagonalization of \( T_i \) for arbitrary \( q \).

Low \( N \) (\( N < 5 \)) \( Z(N) \) (clock) models are equivalent to Potts3 (\( N=3 \)) and Ising (\( N=4 \)) systems. Not surprisingly the maximum of \( \rho(\beta) \) again agrees with known results. We obtain \( x_c^{Z(3)} = (1 + \sqrt{3})\frac{5}{11} \) and \( x_c^{Z(4)} = 1 + \sqrt{2} \) within the accuracy of our numerical procedures.

\[^1\text{Note the difference by a factor of 2 which is caused by our choice of the Potts-like interactions in Eq.(9).}\]

\[^2\text{All algebraic calculations were done with the aid of MATHEMATICA.}\]
All previously considered systems were selfdual. Therefore one may justifiably wonder if our principle is not yet another manifestation of the selfduality. Next example demonstrates that the “maximum rule”, Eq.(6), is at least more general than the simple duality.

**Ising model on a triangular lattice.** Transfer matrices $T_{1,2}$ (see Fig.2.)

$$< s_1 | T_1 | s'_1 > = \exp \beta (2s_1 s'_1 + 1),$$ (12)

$$< s_1, s_2 | T_2 | s'_1, s'_2 > = \exp \beta (s_1 s'_1 + s_2 s'_2 + s_1 s_2 + s'_1 s'_2 + s_1 s'_1 + s_2 s'_1),$$

can be simply diagonalized. We get

$$t_{1,2}^{max} = x^3 + x^{-1},$$ (13)

$$= \frac{1}{2x^2} (3 + x^8 + \sqrt{x^{16} - 2x^8 + 16x^4 + 1}).$$ (14)

The maximum of the characteristic function is located at $x_{max} = 3^{\frac{1}{4}}$. This agrees with the critical temperature first derived for this system by Onsager [2]. One should remember however that Ising models on triangular and hexagonal lattices are interrelated via the duality and star-triangle relations, hence effectively there exists a symmetry which determines transition points in both systems [3]. Our maximum rule could in principle be a consequence of such a symmetry in this case. Next application provides more stringent test of this possibility.

**Two layer Ising model.** This system consists of the two planes of Ising spins coupled by the nearest neighbour ferromagnetic interaction, also along the vertical (between the planes) direction. Periodic boundary conditions are assumed in all three directions, which amounts to doubling the strength of interaction between the planes. The system in not selfdual and to our knowledge no other more complicated symmetries are known. Consequently its critical temperature was never derived. On the contrary our method provides relatively simple analytic predictions for $\beta_{max}$. We proceed analogously to the previous cases. Transfer matrices $T_{1,2}$ propagate now states of two and four spins respectively (see Fig.3). $T_1$ reads

$$< s_1 s_2 | T_1 | s'_1 s'_2 >= \exp \beta (s_1 s_2 + s_1 s'_1 + s_2 s'_2 + s'_1 s'_2 + 2), \quad s_i = \pm 1,$$ (15)

\footnote{From now on we use the standard Ising energy $E(s) = -\sum_{<ij>} s_i s_j$.}
and its largest eigenvalue is
\[ t_{1}^{\text{max}} = \frac{x^2}{2}(x^4 + 2 + x^{-4} + \sqrt{x^8 + 14 + x^{-8}}). \] (16)

Matrix elements of \( T_2 \) are
\[ \langle s_1 s_2 s_3 s_4 | T_2 | s'_1 s'_2 s'_3 s'_4 \rangle = \exp(\beta(s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_1)) \exp(\beta(s'_1 s'_2 + s'_2 s'_3 + s'_3 s'_4 + s'_4 s'_1)). \]

Diagonalisation of this 16 \times 16 matrix is simplified noting that \( T_2 \) conserves the \( U \)-parity, \( [T_2, U] = 0, U = \prod_{i=1}^{4} \sigma_i^x \). The largest eigenvalue belongs to the \( U = +1 \) sector. Final expression is little more complicated
\[ t_{2}^{\text{max}} = \frac{(1 + x^4)^2}{4x^{12}} q_3 + \frac{1 + x^8}{4x^{12}} \sqrt{q_3} + \frac{1 + x^4 + \sqrt{q_2 + (1 + x^8)}q_3 \sqrt{q_1}}{2\sqrt{2}x^{12}} q_1. \] (17)
\[ q_1(x) = x^{32} - 4x^{24} + 70x^{16} - 4x^8 + 1, \] (18)
\[ q_2(x) = x^{40} - 2x^{36} + 5x^{32} + 26x^{24} + 4x^{20} + 26x^{16} + 5x^8 - 2x^4 + 1, \]
\[ q_3(x) = x^{16} - 2x^{12} + 6x^8 - 2x^4 + 1. \]

Resulting characteristic function \( \rho(\beta) \) is shown in Fig.4. It has the single maximum located at
\[ \beta_{\text{max}} = 0.2656 \ldots . \] (19)

According to our proposition, Eq. (16), this gives the transition temperature of the two layer Ising system. For comparison:
\[ \beta_{\text{Ising}^2} \simeq 0.4407 \ldots \] and
\[ \beta_{\text{Ising}^3} \simeq 0.221652(3) \] \cite{[6]}. Confronting this number with the results from MC simulations would provide the crucial test of our hypothesis. It would be also very interesting to search for the "generalized selfduality" - the invariance which would assure existence of a single maximum at the transition point. An attractive possibility is to use the characteristic function given by Eqs. (16,18) to define such a mapping. This assumption has many verifiable consequences. For example, all higher normalized moments of \( T \) should respect the same symmetry.

**Three dimensional Ising model.** According to our proposition the transition temperature of the \( d \) dimensional system is determined by the \( \beta \) dependence of the free energies \( \beta F_{1,2} = -\log Z_{1,2} \) of the corresponding \( d - 1 \) dimensional systems. In particular, the problem of finding \( \beta_c \) for the three
| $L$ | 3    | 4    | 5    | 6    | 7    |
|-----|------|------|------|------|------|
| $\beta_{\text{max}}(L)$ | 0.3317 | 0.3067 | 0.2938 | 0.2859 | 0.2698 |

Table 1: Volume dependence of the pseudocritical temperature for the three dimensional Ising model.

dimensional Ising model would be reduced to finding the free energy of the two coupled layers of the Ising spins. Indeed in this case the full transfer matrix $T$ propagates the whole plane of spins, say, vertically, while the reduced transfer matrices $T_{1,2}$ propagate one (two) rows horizontally. No analytic solution of this system exists up to date. However exact expressions for the complete partition functions $Z_{1,2}(\beta, L)$ in the finite volume are available for not so large $L$. We have therefore calculated the exact locations $\beta_{\text{max}}(L)$ of the ratio $r_L(\beta)$, c.f. Eq. (3), which define the pseudocritical temperature at finite volume, c.f. Table I.

In the thermodynamical limit $\beta_{\text{max}}(L)$ should converge to the true transition temperature. Even though the available range of $L$ values is rather limited one sees the proper trend in the $L$ dependence. Our values definitely move toward $\beta_c^{\text{Ising}^3}$ which was quoted above. One needs larger sizes to test quantitatively the $L$ dependence against the finite size scaling predictions.

Variety of approximate methods (Monte Carlo, high temperature expansion) can be also employed to test predictions of Eq.(6), in this case.

Limits of applicability. We have also investigated situations where the maximum rule does not work. The regularity emerging from this study indicates that the method does not apply to systems with more than two phases. We have calculated the characteristic function for the variety of models with the intermediate Kosterlitz-Thouless (KT) phase. The maximum always occurred inside the KT region. This phenomenon was found for $Z(N)$ models with $N=5-19$, and for the icosahedron and dodecahedron models in two dimensions. For the O(2) model $\beta_{\text{max}} = 1.35...$ well above the known MC estimate for the transition between the disordered and KT phases $\beta_c = 1.1197(5)$. Interpretation of $\beta_{\text{max}}$ located inside the KT phase remains an open and interesting problem. On the other hand in the two dimensional O(3) model $\rho(\beta)$ does not have any maximum in accord with the common wisdom.

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4In our previous application we have derived the transition temperature only.
about the lack of a phase transition in this model. Note that for $O(2)$ and $O(3)$ models the property c) is not satisfied and indeed calculated $\rho(\infty) > 1$. Nevertheless the characteristic function has a maximum for $O(2)$ while it is monotonic for $O(3)$. This parallels the difference of the phase structures of both models.

Summary. We have found a surprisingly simple criterion for locating order-disorder transition. It is exact for selfdual models. The method allows for the analytic calculation in variety of more complicated systems. In particular we give the analytic estimate of the critical temperature of the two layer Ising system. Monte Carlo check of this prediction should be the first step towards more advanced applications.

Our proposition reduces determination of the critical temperature of the three dimensional Ising model to finding the $\beta$ dependence of the free energy of the two coupled planes of Ising spins.

While we are lacking the complete proof of our hypothesis in general case, many approximated methods can be employed to test it in specific applications. High temperature expansion is one interesting possibility.

One can reformulate the maximum principle in other equivalent ways. Differentiating the logarithm of Eq.(3) gives as the condition for the maximum

$$u_2(\beta_c) = u_1(\beta_c),$$

(20)

where $u_{1,2}$ denotes the density of the internal energy for the one (two) layer system. Analogous relations follow from applying our proposition to higher moments of transfer matrix. They all say that at the bulk ($d = 3$ say) critical temperature internal energies of the interacting and noninteracting planes are equal. According to our earlier discussion this statement follows from duality for the two dimensional Ising and Potts models with planes replaced by the spin chains. Perhaps the most interesting formulation of Eq.(20) for higher moments of the transfer matrix results in the limit of infinite number of planes. Then we recover the original two dimensional system and our criterion reads

$$u_d(\beta_c^{(d)}) = u_{d-1}(\beta_c^{(d)}),$$

(21)

where $u_d$ denotes the internal energy density of the $d$ dimensional system, and $\beta_c^{(d)}$ corresponds to its critical temperature. As emphasized before, this statement follows from selfduality in the case of the two dimensional Ising
model. It can be also checked directly. Indeed

$$u_2(\beta_c) = u^{\text{Onsager}}_{2\beta = \log(1+\sqrt{2})} = -\sqrt{2} = u_1(\beta_c), \quad (22)$$

where $u^{\text{Onsager}}(\beta) = -\text{ctgh}(2\beta) \left[ 1 + \frac{2\kappa'}{\pi} K_1(\kappa) \right]$, $\kappa' = 2 \tanh(2\beta)^2 - 1$, $\kappa^2 + \kappa'^2 = 1$, $K_1$ is the elliptic function of the first kind [1], and $u_1(\beta) = -\tanh(\beta) - 1$. For $d > 2$ Eq.(21) remains unproven similarly to Eq.(8).

To conclude, there are many unanswered questions and much more work is to be done, but we feel that it is certainly worth to undertake this effort.

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**Figure Captions**

**Fig.1.** Construction of the transfer matrices $T$ and $T_2$ for the two dimensional Ising model. Periodic boundary conditions are understood.

**Fig.2.** Same as Fig.2 but for the triangular lattice. Bonds impiled by the periodic boundary conditions are shown explicitly.

**Fig.3.** Same as Fig.3 but for the two layer Ising model.

**Fig.4.** Characteristic function for the two layer Ising model.
Fig. 1
Fig. 2
Fig. 3
This figure "fig1-1.png" is available in "png" format from:

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