Tutorial 6, Statistical Mechanics: Concepts and applications
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Tutorial exercises

I. ISING MODEL IN $D \geq 2$ – THE PEIERLS ARGUMENT

1. **Peierls argument for the Ising model in $D > 2$** *C. Bonati, Eur. J. Phys.* **35***, 035002 (2014)*

The model: Consider a classical Ising ferromagnet, defined for spins $\sigma \in \{+1, -1\}$:

$$E = -J \sum_{(i,j)} \sigma_i \sigma_j - h \sum_i \sigma_i \ , \tag{1}$$

where J is assumed to be positive and we set the applied magnetic field h to zero. We define the average magnetization per lattice site as

$$m = \frac{1}{N} \sum_i \sigma_i = \frac{N_+ - N_-}{N} = 1 - 2\frac{N_-}{N} \tag{2}$$

where N is the total number of spins and $N_\pm$ is the number of ± 1 spins. In $D \geq 2$, this system undergoes a phase transition at the critical temperature T_c. In the paramagnetic phase ($T > T_c$), the average magnetization in thermodynamic limit $\langle m \rangle$ vanishes, whereas in the ferromagnetic phase ($T < T_c$) it does not. The Peierls argument allows one to show that $\langle N_- \rangle / N < 1/2 - \epsilon$ (for every N) in ferromagnetic phase, from which it follows that $\langle m \rangle > 0$. The argument in $D = 2$ has been presented in the lecture: in this exercise we generalize it to the case $D > 2$.

Peierls argument for the Ising model in $D \geq 3$: Consider a three dimensional cubic lattice of dimensions $N^{1/3} \times N^{1/3} \times N^{1/3}$. The Peierls contours are in this case surfaces, but their construction proceeds along the same lines as in the two dimensional case.

(a) Label an arbitrary Peierls surface by γ_S^i , where S is the surface area measured in units of elementary squares. Show that for a fixed spin configuration, the following bound holds:

$$N_- \leq \sum_{S \geq 6, \text{even}} \sum_{i=1}^{N(S)} V(\gamma_S^i) X(\gamma_S^i) \tag{3}$$

where $X(\gamma_S^i)$ is non-zero iff γ_S^i belongs to the configuration, $V(\gamma_S^i)$ is the volume enclosed by the Peierls surface and $N(S)$ the total number of surfaces or area S.

: *In a fixed configuration, each negative spin is enclosed within at least one Peierls surface, but the latter can include also positive spins (see Fig. 1 of Bonatti's paper for a $D = 2$ example). Thus the sum of the volumes enclosed in all Peierls surfaces gives an upper bound to N_-.*

(b) Give an upper bound on the volume inside a surface $V(\gamma_S^i)$ as a function $V(S)$ depending only the surface area S.

: *Let $\mathcal{R}$ be the smallest parallelogram containing the surface γ_S^i. Its edges x_1, x_2, x_3 must satisfy $x_i \leq S/4$, and each x_i can be at most $(S-2)/4$. This gives:*

$$V(\gamma_S^i) \leq \max_{x_i \leq (S-2)/4} x_1 x_2 x_3 \leq \max_{x_1 \leq S/4} x_1 \max_{x_2 \leq S/4} x_2 \max_{x_3 \leq S/4} x_3 = \left(\frac{S}{4}\right)^3 . \tag{4}$$

(c) Find an upper bound $X(S)$ on the thermal average $\langle X(\gamma_S^i)\rangle$.

: *With exactly the same argument as for $D = 2$ we get:*

$$\langle X(\gamma_S^i)\rangle \leq \frac{\sum_{c\in\mathscr{C}} e^{-\beta E(c)}}{\sum_{\bar{c}\in\bar{\mathscr{C}}} e^{-\beta E(\bar{c})}} \tag{5}$$

and

$$E(c) = E(\bar{c}) + 2JS . \tag{6}$$

Substituting this into the above inequality we get

$$\langle X(\gamma_L^i)\rangle \leq \frac{e^{-2J\beta L} \sum_{c\in\mathscr{C}} e^{-\beta E(\bar{c})}}{\sum_{\bar{c}\in\bar{\mathscr{C}}} e^{-\beta E(\bar{c})}}$$

where the two sums are equal to each other because for a given surface, for every configuration c, there is exactly one configuration $\bar{c}$. This results in the following upper bound on $\langle X(\gamma_S^i)\rangle$:

$$\langle X(\gamma_S^i)\rangle \leq X(S) \equiv e^{-2J\beta S} . \tag{7}$$

(d) Derive an upper bound on the number $N(S)$ of closed surfaces of area S.

: *This is obtained bounding the number of ways in which a closed surface of size S can be built by combining S faces of unit area. At the first step, the first face can be placed around any of the N lattice sites, in 3 possible orientations. At any subsequent step n, one additional face is attached to each of the s_n links left open at the previous step: for each added face there are at most 3 possible orientations. This is iterated until the step $\overline{n}$ such that $1 + \sum_{n=2}^{\overline{n}} s_n = S$. Therefore we get:*

$$N(S) \leq N\frac{3^S}{S}, \tag{8}$$

where the additional factor of S in the denominator accounts for the different possible choices of which is the first one out of the S faces.

(e) Use the quantities you calculated to write down an expression for $\langle N_-\rangle$, which will be proportional to a sum over surface areas S. The final result should be of the form $\langle N_-\rangle \leq N f_3(x)$ where $x = 9e^{-4J\beta}$ and $f_3(x)$ is a continuous function of x.

: *Combining all estimates one gets*

$$\langle N_-\rangle \leq \sum_{S\geq 6,\text{even}} V(S)N(S)X(S) = \frac{N}{4^3} \sum_{S\geq 6,\text{even}} S^2 (3\, e^{-2\beta J})^S \tag{9}$$

Writing $S = 2k$ we get

$$\langle N_- \rangle \le \frac{N}{16} \sum_{k \ge 3} k^2 (9\, e^{-4\beta J})^S = \frac{N}{16} \left[\sum_{k \ge 1} k^2 x^k - x - 4x^2 \right]. \tag{10}$$

Using that

$$\sum_{k \ge 1} k^2 x^k = \frac{x(1+x)}{(1-x)^3} \tag{11}$$

one gets $\langle N_- \rangle \le N f_3(x)$ with

$$f_3(x) = \frac{x^3}{16(1-x)^3}(9 - 11x + 4x^2). \tag{12}$$

(f) Use the same reasoning to arrive at a similar result for the general $D > 3$ case.

: *In D dimensions, let γ_H^i denote a Peierls hypersurface of area H. The bounds generalize to:*

$$V(\gamma_H^i) \le V(H) = \left(\frac{H}{2(D-1)} \right)^D, \qquad N(H) \le DN \frac{3^H}{3H} \tag{13}$$

and $\langle X(\gamma_H^i) \rangle \le X(H) = e^{-2J\beta H}$, so that

$$\langle N_- \rangle \le \frac{ND}{6(D-1)^D} \sum_{k \ge D} k^{D-1} x^k, \tag{14}$$

and the sum is convergent.

(g) Why cannot the Peierls argument be applied to the one dimensional Ising model?

: *In $D = 1$ the domains are segments of length H: while $V(H)$ and $N(H)$ grow with H, $X(H) = e^{-4\beta J}$ does not: the upper-bound is thus a diverging series.*