STATISTICAL MECHANICS - EXERCISE 4

1. Consider the space $\Omega = \{-1,1\}^{\mathbb{Z}^d}$ as a topological space where the topology is given by the product topology and the topology of $\{-1,1\}$ is the discrete topology. Show that this topology is metrizable and a compatible metric is

$$d(\sigma, \sigma') = \sum_{x \in \mathbb{Z}^d} 2^{-|x|} |\sigma_x - \sigma'_x|. \tag{1}$$

Moreover, show that Ω is compact in this topology.

Solution: By the definition of the product topology, a set $U \subset \Omega$ is open if it is a union of sets of the form

$$\prod_{x \in \mathbb{Z}^d} U_x, \tag{2}$$

where U_x are open sets and $U_x = \{-1,1\}$ for all but finitely many x. To show that the topology given by the metric is equivalent to the product topology, we have to show that each open set in the product topology is open in the metric topology and vice versa.

Fix $\sigma \in \{-1,1\}^{\mathbb{Z}^d}$ and let $U = B(\sigma, \epsilon)$, i.e. a ball of radius ϵ around the point σ and let $V = \{\sigma' : \sigma_x = \sigma'_x \text{ for } |x| < M\}$. Clearly V is an open set in the product topology and we can of course choose M so large that $V \subset U$. So we see that for any set U' which is open in the metric topology, for each point $\sigma \in U'$ we can find a set V which is open in the product topology and $\sigma \in V \subset U'$. Thus U' is open in the product topology (each point has a neighborhood contained in the set).

For the other direction, let V be in the standard basis of the product topology, i.e. it is of the form $V = \prod_{x \in \mathbb{Z}^d} V_x$, where $V_x \neq \{-1,1\}$ for only finitely many $x \in \mathbb{Z}^d$. Let $I \subset \mathbb{Z}^d$ be a finite set of points so that $V_x = \{-1,1\}$ for $x \neq I$ and

$$M = \sup_{x \in I} |x|. \tag{3}$$

Then pick some $\sigma \in V$ and let $\epsilon = 2^{-M-1}$. Then for any $\sigma' \in B(\sigma, \epsilon)$, $\sigma'_x = \sigma_x$ if $|x| \leq M$. So in particular, $\sigma_x = \sigma'_x$ for $x \in I$ and we see that $\sigma' \in V$. Thus for each $\sigma \in V$, there exists a positive ϵ so that $B(\sigma, \epsilon) \subset V$ and V is open in the metric topology. Thus any set open in the product topology is also open in the metric topology.

Compactness follows of course from Tychonoff's theorem, though in the case of a countable product of compact metric spaces, one does not have to rely on the axiom of choice. The proof is still standard and can be found in most books on topology of metric spaces.

2. Let Ω be as in the previous problem and define

$$C_0(\Omega) = \{f : \Omega \to \mathbb{R} |\ f \text{ depends on only finitely many } \sigma_x\}. \tag{4}$$

Show that $C_0(\Omega)$ is dense in $C(\Omega)$ (the space of real valued continuous functions defined on Ω) if we equip $C(\Omega)$ with the topology given by the sup-norm.

Solution: What we wish to show is that for any $f \in C(\Omega)$ and any $\epsilon \in (0, \infty)$, there exists a $g \in C_0(\Omega)$ such that $||f - g|| \leq \epsilon$. So fix any such f and ϵ. Since Ω is compact, f is uniformly continuous. Thus we can find a positive δ so that $|f(\sigma) - f(\sigma')| \leq \epsilon$ when $d(\sigma, \sigma') \leq \delta$.

Fix some finite M so that $\sum_{|x|\geq M} 2^{-|x|+1} \leq \delta$ and define $\sigma'_x = \sigma_x$ for $x \leq M$ and $\sigma'_x = 1$ for other x. Now define $g(\sigma) = f(\sigma')$. Clearly g satisfies the desired properties.

3. Consider a system of Ising spins with a translation invariant finite range potential on $\Lambda \subset \mathbb{Z}$. Show that $\langle \sigma_x \rangle_\Lambda^{\bar{\sigma}}$ converges as $\Lambda \to \mathbb{Z}$ and the limit is independent of the boundary conditions. Show also that the two point function $\langle \sigma_x \sigma_y \rangle_\Lambda^{\bar{\sigma}} - \langle \sigma_x \rangle_\Lambda^{\bar{\sigma}} \langle \sigma_y \rangle_\Lambda^{\bar{\sigma}}$ converges, is independent of boundary conditions and decays exponentially.

Hint: The approach is basically the same as in the case of the 1-d Ising model. The generalization to a finite range potential makes the transfer matrix larger, but it is still a useful quantity. You will also need some version of Perron-Frobenius.

Remark: The original formulation of the problem was for a general bounded spin model. Of course the two point function defined the way it is as a product makes no sense in a general metric space. One could consider some other forms of correlation functions or perhaps a metric space with a structure of an algebra and try to prove similar results. Also, note that translation invariance is important for transfer matrix methods to work the way we use them.

Solution: Let R be the range of the potential and for simplicity consider $\Lambda = \{-NR, ..., NR-1\}$. Recall that our Hamiltonian is

$$\mathcal{H}_\Lambda^{\bar{\sigma}}(\sigma) = \sum_{X: X \cap \Lambda \neq \emptyset} \Phi_X(\sigma \vee \bar{\sigma}), \tag{5}$$

where $\Phi_X = 0$ is $\mathrm{diam}(X) > R$. As usual, we begin by calculating the partition function

$$Z_{\beta,\Lambda}^{\bar{\sigma}} = \sum_\sigma e^{-\beta \mathcal{H}_\Lambda^{\bar{\sigma}}(\sigma)}. \tag{6}$$

Let us split the Hamiltonian into a sum over clusters containing interactions. Define $\mathcal{H}_{k,k+1}$ to be the part of $\mathcal{H}_\Lambda^{\bar{\sigma}}$ containing the interactions between spins in $\{kR, ..., (k+1)R-1\}$ and $\{(k+1)R, ..., (k+2)R-1\}$. Note that this representation is not unique: interactions within a block $\{kR, ..., (k+1)R-1\}$ can be put into different parts, but we shall pick one where $\mathcal{H}_{k,k+1}$ is independent of k - by translation invariance this is possible. We shall still carry the index k with us even though it is redundant. We also interpret $\mathcal{H}_{-N-1,-N}$ and $\mathcal{H}_{N-1,N}$ to contain the boundary conditions. Let us also write σ_k for $\{\sigma_x : x \in \{kR, ..., (k+1)R-1\}\}$. So we have

$$Z_{\beta,\Lambda}^{\bar{\sigma}} = \sum_{\sigma_{-N}} \sum_{\sigma_{-N+1}} \cdots \sum_{\sigma_{N-1}} e^{-\beta \mathcal{H}_{-N-1,-N}(\bar{\sigma}_{-N-1},\sigma_{-N})} e^{-\beta \mathcal{H}_{-N,-N+1}(\sigma_{-N},\sigma_{-N+1})} \cdots e^{-\beta \mathcal{H}_{N-1,N}(\sigma_{N-1},\bar{\sigma}_N)}. \tag{7}$$

Due to this form of the partition function, it is natural to define the transfer matrix $T(\sigma, \sigma') = e^{-\beta \mathcal{H}_{k,k+1}(\sigma,\sigma')}$ and we see that $Z_{\beta,\Lambda}^{\bar{\sigma}} = (f^-, T^{2N} f^+)$, where $f^-(\sigma) = e^{-\beta \mathcal{H}_{-N-1,-N}(\bar{\sigma}_{-N-1},\sigma)}$ and $f^+(\sigma) = e^{-\beta \mathcal{H}_{N-1,N}(\sigma,\bar{\sigma}_N)}$.

Now that we have the transfer matrix representation, the rest of the problem is very similar to problem 1.3. Perron-Frobenius implies that T has a largest positive eigenvalue λ and $\lambda^{-2N} Z_{\beta,\Lambda}^{\bar{\sigma}} \to (f^-, v)(w, f^+)$ for some right and left eigenvectors v, w with positive entries. Also if $x = kR + l$ with $l \in \{1, ..., R-1\}$ we have

$$\langle \sigma_x \rangle_{\lambda,\beta}^{\bar{\sigma}} = \frac{1}{Z_{\beta,\Lambda}^{\bar{\sigma}}} \sum_{\sigma_{-N}} \sum_{\sigma_k} \sum_{\sigma_{N-1}} f^-(\sigma_{-N}) T^{N+k}(\sigma_{-N}, \sigma_k)(\sigma_k)_l T^{N-k}(\sigma_k, \sigma_{N-1}) f^+(\sigma_{N-1}) \tag{8}$$

and Perron-Frobenius gives us

(9) $$\lim_{N\to\infty}\langle\sigma_x\rangle^{\bar\sigma}_{\beta,\Lambda}=\sum_{\sigma_k} w_{\sigma_k}(\sigma_k)_l v_{\sigma_k},$$

which is independent of the boundary conditions. Note that we do not assume that the Hamiltonian is invariant under spin flips so we can not argue that this limit is zero.

The treatment of the two-point function is similar to problem 1.3 and we shall not repeat the argument here. Note that the result on the exponential decay of the correlation function will be something like if $x=kR+l$ and $y=k'R+l'$, we'll find that the correlation function can be bounded by $\lambda^{|k-k'|}$ for some $\lambda\in(0,1)$, but this of course implies a similar result where k and k' are replaced by x and y.

4. Consider the so called mean field Ising model:

(10) $$H=-\frac{J}{N}\sum_{(x,y)}\sigma_x\sigma_y,$$

where N is the number of spins we are considering (if you want take this to be in 1-d and consider an interval of length N) and J is a constant you can set to 1 if you don't want to carry it around and the σ_x are Ising spins and we consider free boundary conditions. Note that we are not summing over nearest neighbours but all possible pairs (x,y) where $x\neq y$.

Remark: In the original formulation of the problem, there was a slight error. The summation was not over all pairs, but over all x and y. This makes a slight difference to how the diagonal terms are weighted. Also in part e), the correct statement is that the free energy density can be approximated by considering only the maximal summand.

a) What do you think the term mean field refers to?

b) With a brief calculation, show that

(11) $$H=-\frac{J}{2N}\left(\left(\sum_x\sigma_x\right)^2-N\right).$$

c) Let $M=\frac{1}{N}\sum_x\sigma_x$ be the average magnetization (spatial average - not average with respect to the Gibbs measure). Show that the number of spin configurations with average magnetization M is given by

(12) $$W(M)=\frac{N!}{\left(\frac{N}{2}(1+M)\right)!\left(\frac{N}{2}(1-M)\right)!}.$$

d) Show that the partition function can be written as

(13) $$Z=\sum_M W(M)e^{-\beta H(M)}.$$

e) Estimate $W(M)e^{-\beta H(M)}$ in the limit of large N by using Stirling's approximation. Show that it is maximized by optimizing

(14) $$-F(M)=JM^2-\frac{1}{\beta}((1+M)\log(1+M)+(1-M)\log(1-M)).$$

Moreover, show that the free energy density can be approximated by considering only the maximal term in the sum for the partition funciton.

Do you know what the physical quantity F is?

f) By studying the maximum of $-F(M)$, prove that there is a phase transition in the model and try to find the critical temperature.

g) Expand $F(M)$ around $M = 0$ and try to evaluate few of the lowest order coefficients as functions of the temperature.

h) Think a bit about what changes and what doesn't change if we couple the spins to a uniform magnetic field (i.e. add a term $-h\sum_x \sigma_x$ to the Hamiltonian).

Solution: a) Compared to the normal Ising model, we have substituted an the interaction between nearest neighbors with an interaction with the average value of the spins. In more general models, one substitutes a local interaction between fields with an interaction with the average value of the field. This is where the name mean field comes from.

b)

(15)
$$H = -\frac{J}{2N}\left(\sum_{(x,y)}\sigma_x\sigma_y + \sum_{(y,x)}\sigma_x\sigma_y\right) = -\frac{J}{2N}\left(\sum_x\sum_y \sigma_x\sigma_y - \sum_x \sigma_x^2\right) = -\frac{J}{2N}\left(\left(\sum_x \sigma_x\right)^2 - N\right).$$

c) Let $S = NM$. Then the number positive spins is $\frac{1}{2}(N+S)$ and the number of negative spins is $\frac{1}{2}(N-S)$. The number of ways we can pick $\frac{1}{2}(N+S)$ positive spins and $\frac{1}{2}(N-S)$ negative spins is

(16)
$$\frac{N!}{(\frac{1}{2}(N+S))!(\frac{1}{2}(N-S))!} = \frac{N!}{(\frac{N}{2}(1+M))!(\frac{N}{2}(1-M))!}$$

d) Note that in b) we in fact proved that $H = -\frac{J}{2N}(N^2M^2 - N) = H(M)$ so the Hamiltonian is in fact only a function of M. Thus

(17)
$$Z = \sum_\sigma e^{-\beta H(\sigma)} = \sum_M |\{\sigma : \sum_x \sigma_x = MN\}| e^{-\beta H(M)} = \sum_M W(M) e^{-\beta H(M)}.$$

e) So far we have $e^{-\beta H(M)} = e^{-\frac{J}{2}(NM^2-1)}$ and by Stirling (valid when N is large and $M \neq \pm 1$):

$$\begin{aligned}
W(M) &= \frac{N!}{(\frac{N}{2}(1+M))!(\frac{N}{2}(1-M))!)} \\
&\approx \frac{\sqrt{2\pi N}\left(\frac{N}{e}\right)^N}{\sqrt{2\pi\frac{N}{2}(1+M)}\left(\frac{\frac{N}{2}(1+M)}{e}\right)^{\frac{N}{2}(1+M)}\sqrt{2\pi\frac{N}{2}(1-M)}\left(\frac{\frac{N}{2}(1-M)}{e}\right)^{\frac{N}{2}(1-M)}} \\
&= \sqrt{\frac{2}{\pi}}\frac{1}{\sqrt{(1-M^2)N}}\frac{1}{(\frac{1}{2}(1+M))^{\frac{N}{2}(1+M)}(\frac{1}{2}(1-M))^{\frac{N}{2}(1-M)}} \\
&= e^{\frac{1}{2}(\log 2 - \log\pi - \log(1-M^2) - \log N) - \frac{N}{2}(1+M)\log(\frac{1}{2}(1+M)) - \frac{N}{2}(1-M)\log(\frac{1}{2}(1-M))} \\
&= e^{\frac{1}{2}(\log 2 - \log\pi - \log(1-M^2) - \log N)} e^{N\log 2} e^{-\frac{N}{2}((1+M)\log(1+M) + (1-M)\log(1-M))}.
\end{aligned}$$

Thus

$$\begin{aligned}
W(M)e^{-\beta H(M)} &\approx e^{\frac{1}{2}(\log 2 - \log\pi - \log(1-M^2) - \log N) + N\log 2 + \frac{J}{2}} e^{-\frac{N}{2}((1+M)\log(1+M) + (1-M)\log(1-M) - J\beta M^2)} \\
&= e^{\frac{1}{2}(\log 2 - \log\pi - \log(1-M^2) - \log N) + N\log 2 + \frac{J}{2}} e^{-\beta\frac{N}{2}F(M)}.
\end{aligned}$$

Thus the maximum of $W(M)e^{-\beta H(M)}$ will be at the maximum of $-F(M)$.

To see that for the free energy density, only the extremum counts, let M_0 be the extremal point. We have

$$Z = W(M_0)e^{-\beta H(M_0)} \sum_M \frac{W(M)}{W(M_0)} e^{-\beta(H(M)-H(M_0))} \tag{18}$$

and

$$\mathcal{F} = -\frac{\log Z}{\beta N} = -\frac{\log(W(M_0)e^{-\beta H(M_0)})}{\beta N} - \frac{1}{\beta N} \log\left(\sum_M \frac{W(M)}{W(M_0)} e^{-\beta(H(M)-H(M_0))}\right). \tag{19}$$

By definition, the summand in the second term is at most one and the entire sum is at least one so we see that (since there are $2N+1$ terms in the sum) that

$$0 \leq \frac{1}{\beta N} \log\left(\sum_M \frac{W(M)}{W(M_0)} e^{-\beta(H(M)-H(M_0))}\right) \leq \frac{\log(2N+1)}{\beta N} \tag{20}$$

which implies that as $N \to \infty$

$$\mathcal{F} = -\frac{\log 2}{\beta} + \frac{1}{2}F(M_0) + o(1). \tag{21}$$

f)

$$-F'(M) = 2JM - \frac{2}{\beta}\text{artanh}M. \tag{22}$$

Thus at an extremum, we must have the equation $\beta JM = \text{artanh}M$. At a maximum, we have the condition

$$-F''(M) = 2J - \frac{2}{\beta}\frac{1}{1-M^2} \leq 0. \tag{23}$$

Thus we are concerned with the behavior of the solutions to the equation $\tanh(\beta JM) = M$ with the constraints $M^2 \geq 1 - \frac{1}{\beta J}$.

Using some elementary calculus, one can check that for $\beta J \leq 1$, the equation $\tanh(\beta JM) = M$ has only one solution: $M = 0$ and this indeed is a maximum of $-F$.

For $1 < \beta J$, one finds that there are three solutions: $M = 0$ and $M = \pm M_0$. We see from the form of $F''(M)$ that in this case $M = 0$ is a minimum for $-F$ and $\pm M_0$ are the maxima. Thus $F(M)$ is a constant in β for small β but then starts depending on β once we reach $\beta = \frac{1}{J}$. Thus $F(M)$ is non-analytic and we have a phase transition at $\beta = \frac{1}{J}$.

g) $-F(0) = 0$, $-F'(0) = 0$, $-F''(0) = 2J - \frac{2}{\beta}$, $-F'''(0) = 0$, $-F''''(0) = -\frac{4}{\beta}$. Thus

$$-F(M) = \left(J - \frac{1}{\beta}\right)M^2 - \frac{1}{6\beta}M^4 + \mathcal{O}(M^5). \tag{24}$$

Note that the M^2 term vanishes at the critical point. As a side remark: if the free energy is of this form, where there is no M or M^3 present, the free energy is said to be of Landau form and there is a 'Landau theory' for studying phase transitions in systems where the free energy has a certain symmetry. Note that this is similar also to the Ginzburg-Landau model.

h) Note that this amounts to the following change in the Hamiltonian: $H(M) = -\frac{J}{2}(NM^2 - 1 + \frac{2h}{J}NM)$ so we simply replace JM^2 with $JM^2 + 2hM$. One can again formulate a similar equation that the maximum must satisfy and one uses elementary calculus to analyze its solutions. With some tedious calculations, one finds that there is in fact a unique solution and the free energy is an analytic function of the temperature.