ICFP M1 - Phase Transitions – TD n$^{\text{o}}$ 1 – Solution
The Curie-Weiss Model

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1. The scaling with N of the coupling constant ensures that the Hamiltonian is an extensive quantity, i.e. proportional to the system size N. As an example, imagine all spins are aligned and there is no magnetic field. Then the Hamiltonian of the Curie-Weiss model takes its minimal value $H_{\min} = -\frac{J}{2N}N^2$, which is indeed proportional to N.

2. We can rewrite the Hamiltonian as a function of the average magnetization $m(\underline{\sigma}) = \frac{1}{N}\sum_{i=1}^{N}\sigma_i$, with $H(\underline{\sigma}) = N\left(-\frac{J}{2}m(\underline{\sigma})^2 - hm(\underline{\sigma})\right)$. Decomposing the sum over the configurations according to their average magnetization the partition function then becomes

$$Z = \sum_{\underline{\sigma}} e^{-\beta H(\underline{\sigma})} = \sum_{m\in\mathcal{M}_N} e^{-\beta N[-\frac{J}{2}m^2-hm]} \sum_{\underline{\sigma}} \delta_{m,m(\underline{\sigma})} = \sum_{m\in\mathcal{M}_N} \mathcal{N}_m^N\, e^{-\beta N[-\frac{J}{2}m^2-hm]} \ ,$$

where $\mathcal{M}_N = \{-1, \frac{-N+2}{N}, ..., \frac{N-2}{N}, 1\}$ contains the $(N+1)$ possible values of the average magnetization, and $\mathcal{N}_m^N$ denotes the number of spin configurations that have the average magnetization m. Such a configuration is produced when there are $\frac{N}{2} + \frac{mN}{2}$ spins up and $\frac{N}{2} - \frac{mN}{2}$ spins down. The degeneracy $\mathcal{N}_m^N$ of these configurations is thus the number of ways that $\frac{N}{2} + \frac{mN}{2}$ spins can be selected from a total of N spins, i.e. the binomial factor $\mathcal{N}_m^N = \binom{N}{\frac{1+m}{2}N}$.

3. According to Stirling's formula, for $N \to \infty$ we have the approximation $N! \sim \sqrt{2\pi N}N^N e^{-N}$ which can be rewritten as

$$\ln(N!) = N\ln(N) - N + \mathcal{O}(\ln(N)).$$

Then it follows that

$$\begin{aligned}\ln\binom{N}{\alpha N} &= \ln\left(\frac{N!}{(\alpha N)!(N(1-\alpha))!}\right)\\ &= -\alpha N\ln\alpha - (1-\alpha)N\ln(1-\alpha) + \mathcal{O}(\ln N)\,,\end{aligned}$$

from which we get the result.

Now we compute the free energy per spin in the thermodynamic limit. By definition we have

$$\begin{aligned}f_{\text{CW}}(\beta,h) &= \lim_{N\to\infty} -\frac{1}{\beta N}\ln Z\\ &= \lim_{N\to\infty} -\frac{1}{\beta N}\ln\left(\sum_{m\in\mathcal{M}_N} e^{-N\left[\beta(-\frac{J}{2}m^2-hm)-\ln(\mathcal{N}_m^N)/N\right]}\right)\,. \end{aligned} \tag{1}$$

Note that the term $\ln(\mathcal{N}_m^N)/N = -\frac{1+m}{2}\ln(\frac{1+m}{2}) - \frac{1-m}{2}\ln(\frac{1-m}{2}) + \mathcal{O}(\ln N/N)$ (where we inserted $\alpha = \frac{1+m}{2}$) is independent of N for large N. Therefore, once we take the large N limit, only the term with the largest exponential will contribute to the sum. Such an asymptotic expansion of the sum goes under the name "Laplace's method". Thus we find

$$f_{\text{CW}}(\beta,h) = \inf_{m\in[-1,1]} \underbrace{\left(-\frac{J}{2}m^2 - hm + \frac{1+m}{2\beta}\ln(\frac{1+m}{2}) + \frac{1-m}{2\beta}\ln(\frac{1-m}{2})\right)}_{\equiv \widehat{f}_{\text{CW}}(m;\beta,h)}$$

Optional Comment: The statement above that only the term with the largest exponent contributes to the sum in (1) (Laplace's method) can be explained more rigorously. For simplicity consider a sum of the form

$$S_N = \sum_{m \in \mathcal{M}_N} e^{-Nf(m)} \tag{2}$$

for some arbitrary, but continuous function $f\colon [-1,1] \to \mathbb{R}$, where for each N we define its infimum as

$$f_N^\star = \inf_{m \in \mathcal{M}_N} f(m)$$

Since f is continuous, $f_N^* \to f^* := \inf_{m\in[-1,1]} f(m)$ for $N \to \infty$. The idea is now to find two sequences a_N and b_N that sandwich S_N between them for all N such that $(-\frac{1}{N}\ln a_N)$ and $(-\frac{1}{N}\ln b_N)$ converge for large N to the same desired value, namely $f^\star$. Concretely, we choose

$$a_N := e^{-Nf_N^\star} \leq S_N \leq (N+1)e^{-Nf_N^\star} =: b_N \ .$$

Then we find $-\frac{1}{N}\ln a_N = f_N^\star \to f^\star$ and $-\frac{1}{N}\ln b_N = f_N^\star + \frac{\ln(N+1)}{N} \to f^\star$ (for $N \to \infty$). This shows that $\lim_{N\to\infty} -\frac{1}{N}\ln S_N = f^\star$.

4. One can decompose the free-energy as $\widehat{f}_{\rm CW}(m;\beta,h=0) = e(m) - Ts(m)$, with the energy $e(m) = -\frac{J}{2}m^2$ and the entropy $s(m) = -\frac{1+m}{2}\ln(\frac{1+m}{2}) - \frac{1-m}{2}\ln(\frac{1-m}{2})$; we set the Boltzmann constant to 1 for simplicity. The energy is maximal in $m=0$ and minimal in $m=\pm 1$; the entropy is maximal in $m=0$ and minimal in $m=\pm1$, where it vanishes with infinite derivatives (vertical slopes). The shape of $\widehat{f}_{\rm CW}(m;\beta,h=0)$ thus arises from the competition between the entropy and the energy; at high temperature the entropy wins and the free-energy has a unique global minimum in $m=0$, whereas at low temperatures $m=0$ becomes a local maximum and $\widehat{f}_{\rm CW}$ has two global minima in $m = \pm m_{\rm sp}(\beta)$, as can be seen on the following curves :

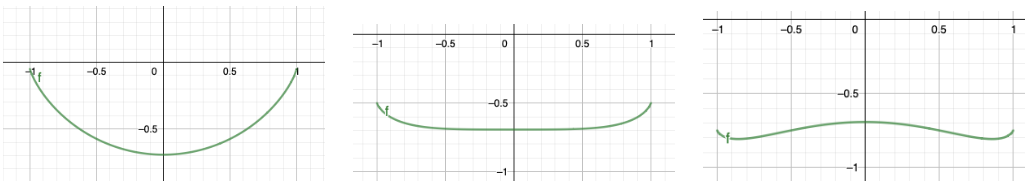

Figure 1: The free energy per spin $\widehat{f}_{\rm CW}(m;\beta,h=0)$ as a function of the magnetization m for $T > T_c$, $T = T_c$, $T < T_c$ (from left to right)

The critical temperature $T_{\rm c}$ at which there is a qualitative change in the behavior of $\widehat{f}_{\rm CW}$ marks the birth of the minima in $m \neq 0$, it can thus be defined as the temperature at which the second derivative of $\widehat{f}_{\rm CW}$ goes from positive (for $T > T_{\rm c}$) to negative (for $T < T_{\rm c}$). Computing the second derivative of $\widehat{f}_{\rm CW}(m;\beta,h=0)$ with respect to m in $m=0$ one finds $T - J$, hence $T_{\rm c} = J$.

According to the previous question the partition function is dominated by configurations with average magnetization m that minimize $\widehat{f}_{\rm CW}(m)$. The physical interpretation of the transition is thus that above $T_{\rm c}$ the system is in a paramagnetic phase, with only configurations with $m \approx 0$ populated. On the contrary below the critical temperature the system will be found in configurations with $|m| \approx m_{\rm sp}(\beta) > 0$, i.e. in a ferromagnetic phase.

5. The magnetic field adds a linear term $-hm$ in the expression of the free-energy, the previous curves are thus tilted, as plotted in Figure 2.

For $h > 0$ the configurations with larger magnetizations have their free-energies lowered more strongly, and hence are more probable. The degeneracy between minima seen previously for $T < T_{\rm c}$ and $h = 0$ is now lifted, for $h \neq 0$ the global minimum of $\widehat{f}_{\rm CW}(m)$ is always unique and depends smoothly on the temperature.

6. We find the magnetization $m_*(\beta,h)$ which minimizes $\widehat{f}_{\rm CW}(m;\beta,h)$ by taking its derivative w.r.t m, which yields an implicit equation:

$$0 = \frac{\partial \widehat{f}_{\rm CW}(m;\beta,h)}{\partial m} = -Jm - h + \frac{1}{2\beta}\ln\left(\frac{1+m}{1-m}\right) \ \Leftrightarrow\ \tanh(\beta(Jm+h)) = m \ .$$

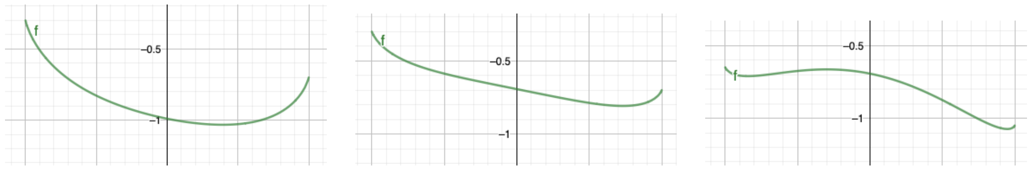

Figure 2: The free energy per spin $\widehat{f}_{\mathrm{CW}}(m;\beta,h)$ as a function of the magnetization m for $T > T_c$, $T = T_c$, $T < T_c$ (from left to right)

7. The implicit equation can be solved graphically studying the intersections between the graph of $\tanh(\beta(Jm+h))$ and m. Above the critical point $T > T_{\mathrm{c}}$ this equation admits only one solution for $m_*(\beta,h)$ that varies smoothly with h. Below the critical point there are up to three solutions and $m_*(\beta,h)$ will take the value of the intersection with positive magnetisation if $h > 0$, but if $h < 0$ it will take the value of the intersection with negative magnetisation (the solutions of the implicit equation corresponds to the critical points of $\widehat{f}_{\mathrm{CW}}(m)$, $m_*(\beta,h)$ is the one corresponding to the global minimum).

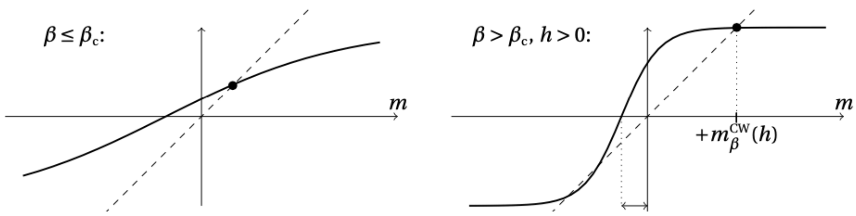

Figure 3: Graphical solution of $\tanh(\beta(Jm+h)) = m$.

This implies that $m_*(\beta,h)$ jumps discontinuously between $h = 0^-$ and $h = 0^+$ if $T < T_{\mathrm{c}}$.

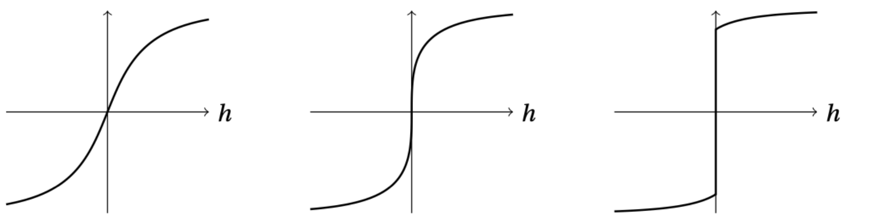

Figure 4: The magnetization $m_*(\beta,h)$ as a function of the applied magnetic field h for $T > T_{\mathrm{c}}$, $T = T_{\mathrm{c}}$ and $T < T_{\mathrm{c}}$ (from left to right).

8. From the previous discussion one can infer that the spontaneous magnetization $m_{\mathrm{sp}}(\beta) = \lim_{h\to 0^+} m_*(\beta,h)$ will vanish for $T > T_{\mathrm{c}}$ and grow continuously when T is reduced below T_{c}, towards its maximal value 1 at zero temperature. This behavior is shown below in Figure 5.

   To find the exponent β_{mf} that controls the behaviour of the magnetization close to the critical temperature, $m_{\mathrm{sp}}(T) \propto (T_{\mathrm{c}} - T)^{\beta_{\mathrm{mf}}}$ for $T \to T_{\mathrm{c}}^-$, we expand the implicit equation $\tanh(\beta J m) = m$ to third order in m, using $\tanh(x) = x - x^3/3 + \mathcal{O}(x^5)$ as $x \to 0$, which yields

$$\beta J m - (\beta J m)^3/3 + \mathcal{O}(m^5) = m \ .$$

   Then, recalling that $T_{\mathrm{c}} = J$, we have

$$\beta J = \frac{T_{\mathrm{c}}}{T} = 1 + \frac{T_{\mathrm{c}} - T}{T} = 1 + \frac{T_{\mathrm{c}} - T}{T_{\mathrm{c}}} + \mathcal{O}((T_{\mathrm{c}} - T)^2) \ ,$$

   hence equating the non-trivial terms of the implicit equation at the lowest order:

$$m \sim \sqrt{3}\left(\frac{T_{\mathrm{c}} - T}{T_{\mathrm{c}}}\right)^{1/2} \propto (T_{\mathrm{c}} - T)^{1/2} \ ,$$

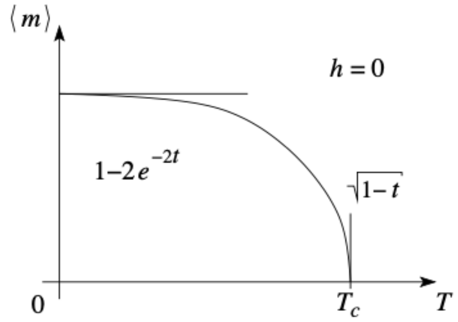

Figure 5: The spontaneous magnetization $m_{\rm sp}$ as a function of the temperature.

from which we find $\beta_{\rm mf} = 1/2$.

9. From Figure (4) we see that the isotherm $m(h)$ at the critical temperature T_c and $h \to 0^+$ can be modelled as $m(h) \propto h^{1/\delta}$. To derive the exponent we expand again $\tanh(\beta(Jm+h)) = m$ with $T = T_{\rm c}$, hence $\beta J = 1$:

$$
\begin{aligned}
m &= \tanh(m + h/T_{\rm c}) \sim m + h/T_{\rm c} - \frac{1}{3}(m + h/T_{\rm c})^3 \ , \\
m &\sim \left(\frac{3h}{T_{\rm c}}\right)^{1/3} - h/T_{\rm c} \ .
\end{aligned}
$$

For small h the contribution of the first term is much larger and therefore $\delta = 3$.

10. Taking the derivative with respect to h of the implicit equation satisfied by m_*, and using the fact that $\tanh(x)' = 1 - \tanh(x)^2$ one obtains

$$
\frac{\partial m_*}{\partial h} = (1 - m_*^2)\beta\left(J\frac{\partial m_*}{\partial h} + 1\right) \ , \qquad \text{hence} \qquad \chi = \frac{\beta(1-m_*^2)}{1-\beta J(1-m_*^2)} \ . \tag{3}
$$

For $h = 0^+$ the susceptibility diverges when $T \to T_{\rm c}$, as can be seen on Figure (4), this quantity corresponding to the slope of the curve in 0^+. In the expression (3) of χ one sees that the numerator is finite at $T_{\rm c}$, while the denominator vanishes linearly in $|T - T_{\rm c}|$ (both from the low and high temperature phases), which gives $\gamma = 1$.

11. As $\frac{1}{N}H(\underline{\sigma}) = -\frac{J}{2}m(\underline{\sigma})^2 - h\, m(\underline{\sigma})$ one has

$$
u = \lim_{N\to\infty} \frac{\sum\limits_{m\in\mathcal{M}_N} \left(-\frac{J}{2}m^2 - hm\right) \mathcal{N}_m^N e^{-\beta N[-\frac{J}{2}m^2 - hm]}}{\sum\limits_{m\in\mathcal{M}_N} \mathcal{N}_m^N e^{-\beta N[-\frac{J}{2}m^2 - hm]}} = -\frac{J}{2}m_*(\beta,h)^2 - h\, m_*(\beta,h) \ ,
$$

evaluating both sums with the Laplace method.

For $h = 0$, in the high-temperature phase u is constant and equal to 0. As the spontaneous magnetization vanishes with a square root $u = -\frac{J}{2}m_{\rm sp}(\beta)^2$ vanishes linearly in $T_{\rm c} - T$ when $T \to T_{\rm c}^-$. Differentiating u with respects to T one obtains that the specific heat is equal to 0 in the high-temperature phase, and goes to a strictly positive constant as $T \to T_{\rm c}^-$. This discontinuity of C at $T_{\rm c}$, without a divergence, corresponds to $\alpha = 0$ in $C \propto |T - T_{\rm c}|^{-\alpha}$.