# ICFP M1 - Phase Transitions – TD n° 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

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

from which we get the result.

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

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

Note that the term $\ln(\mathcal{N}_m^N)/N = -\frac{1+m}{2}\ln(\frac{1+m}{2}) - \frac{1-m}{2}\ln(\frac{1-m}{2}) + \mathcal{O}\left(\ln N/N\right)$ (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

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

*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

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

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 $\widehat{f}_{\mathrm{CW}}(m;\beta,h=0) = e(m) - Ts(m)$, 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 $m=\pm 1$, where it vanishes with infinite derivatives (vertical slopes). The shape of $\widehat{f}_{\mathrm{CW}}(m;\beta,h=0)$ 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 $\widehat{f}_{\mathrm{CW}}$ has two global minima in $m = \pm m_{\mathrm{sp}}(\beta)$, as can be seen on the following curves :

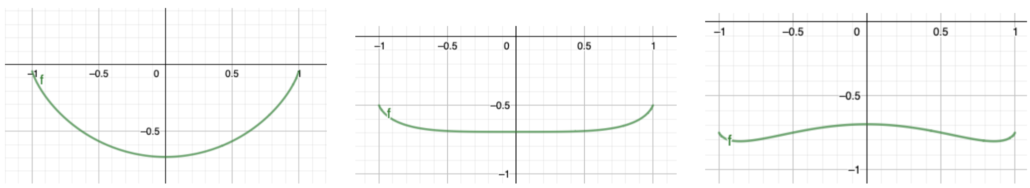


Figure 1: The free energy per spin $\widehat{f}_{\mathrm{CW}}(m;\beta,h=0)$ as a function of the magnetization $m$ for $T > T_c$, $T = T_c$, $T < T_c$ (from left to right)

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

According to the previous question the partition function is dominated by configurations with average magnetization $m$ that minimize $\widehat{f}_{\mathrm{CW}}(m)$. The physical interpretation of the transition is thus that above $T_{\mathrm{c}}$ 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 $|m| \approx m_{\mathrm{sp}}(\beta) > 0$, 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 $T < T_{\mathrm{c}}$ and $h = 0$ is now lifted, for $h \neq 0$ the global minimum of $\widehat{f}_{\mathrm{CW}}(m)$ is always unique and depends smoothly on the temperature.

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

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

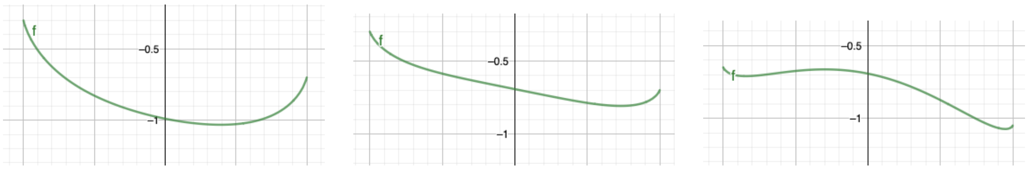


Figure 2: The free energy per spin $\widehat{f}_{\text{CW}}(m;\beta,h)$ as a function of the magnetization $m$ for $T > T_c$, $T = T_c$, $T < T_c$ (from left to right)

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 $T > T_{\text{c}}$ 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 $\widehat{f}_{\text{CW}}(m)$, $m_*(\beta,h)$ is the one corresponding to the global minimum).

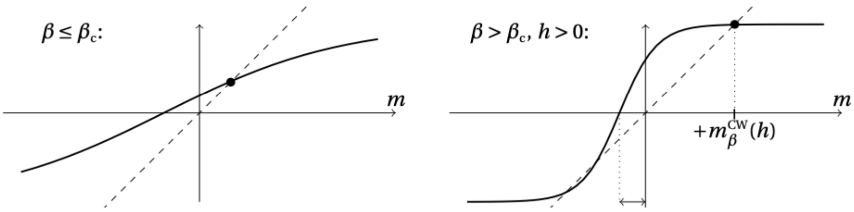


Figure 3: Graphical solution of $\tanh(\beta(Jm+h)) = m$.

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

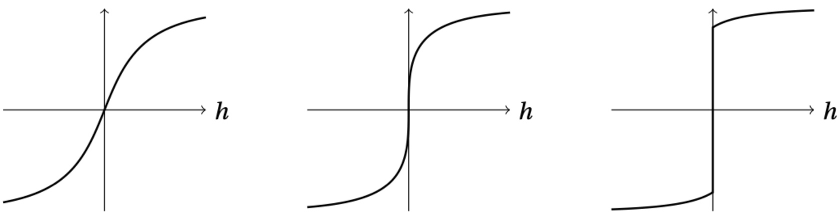


Figure 4: The magnetization $m_*(\beta,h)$ as a function of the applied magnetic field $h$ for $T > T_{\text{c}}$, $T = T_{\text{c}}$ and $T < T_{\text{c}}$ (from left to right).

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

   To find the exponent $\beta_{\text{mf}}$ that controls the behaviour of the magnetization close to the critical temperature, $m_{\text{sp}}(T) \propto (T_{\text{c}} - T)^{\beta_{\text{mf}}}$ for $T \to T_{\text{c}}^-$, 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 $T_{\text{c}} = J$, we have

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

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

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

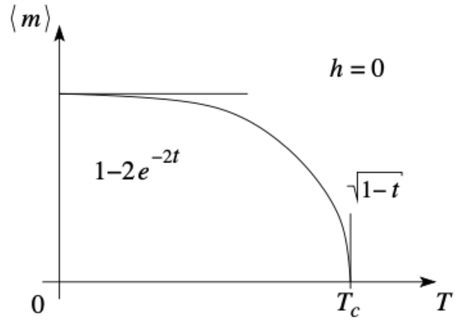


Figure 5: The spontaneous magnetization $m_{\rm sp}$ as a function of the temperature.

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 $\beta J = 1$:

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

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

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

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 $\chi$ 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 $C \propto |T - T_{\rm c}|^{-\alpha}$.