Problem 2: the free-energy & the freezing transition

1 THE CRITICAL TEMPERATURE & FREEZING TRANSITION

We have $Z_N = \sum_{\alpha=1}^{2^N} e^{-\beta E_\alpha} = \int dE\, \mathcal{N}_N(E)\, e^{-\beta E}$

↑ random variable

The free-energy:

$$f(\beta) = \lim_{N\to\infty} \left(-\frac{1}{\beta N}\right) \log Z_N^{typ} \quad \text{and using } \varepsilon = E/N:$$

$$Z_N^{typ} = \int dE\, \mathcal{N}_N^{typ}(E)\, e^{-\beta E} = N \int_{-\sqrt{2\log 2}}^{\sqrt{2\log 2}} d\varepsilon\, e^{N(\log 2 - \varepsilon^2/2) + o(N)}\, e^{-\beta N \varepsilon}$$

Saddle-point calculation:

$$Z_N^{typ} = e^{N \sup_{\varepsilon \in [-\sqrt{2\log 2}, \sqrt{2\log 2}]} \left(\log 2 - \frac{\varepsilon^2}{2} - \beta\varepsilon\right)}$$

Call ε_β^* the point where the maximum is attained.
The stationary point satisfies $\frac{\partial S(\varepsilon)}{\partial \varepsilon} - \beta = 0 = -\varepsilon - \beta$, meaning $\varepsilon = -\beta = -1/T$. This is acceptable if it belongs to the domain, i.e. $|\varepsilon| < \sqrt{2\log 2}$, which is true provided that

$$T \geq 1/\sqrt{2\log 2} = T_f.$$

For $T < T_g$, the maximum is attained at the boundary of the interval, $\varepsilon^*_\beta = -\sqrt{2\log 2}$.

Therefore:

$$\varepsilon^*_\beta = \begin{cases} -1/T & \text{for } T \geq T_g = 1/\sqrt{2\log 2} \\ -\sqrt{2\log 2} & \text{for } T < T_g = 2/\sqrt{2\log 2} \end{cases}$$

which gives:

$$f(\beta) = -\frac{1}{\beta}\left(S(\varepsilon^*_\beta) - \beta\varepsilon^*_\beta\right) = \begin{cases} -\frac{1}{\beta}\left(\log 2 - \beta^2/2 + \beta^2\right) & T \geq T_g \\ -\frac{1}{\beta}\left(\beta\sqrt{2\log 2}\right) & T < T_g \end{cases}$$

$$= \begin{cases} -T\log 2 - 1/2T & T \geq T_g \\ -\sqrt{2\log 2} & T < T_g \end{cases}$$

FREEZING! For all $T \leq T_g$, system behaves as if it was frozen at T_g

This transition is of 2nd order thermodynamically, in the sense that the derivative of the free-energy is continuous at $T = T_g$.

2 FLUCTUATIONS, & BACK TO AVERAGE vs TYPICAL

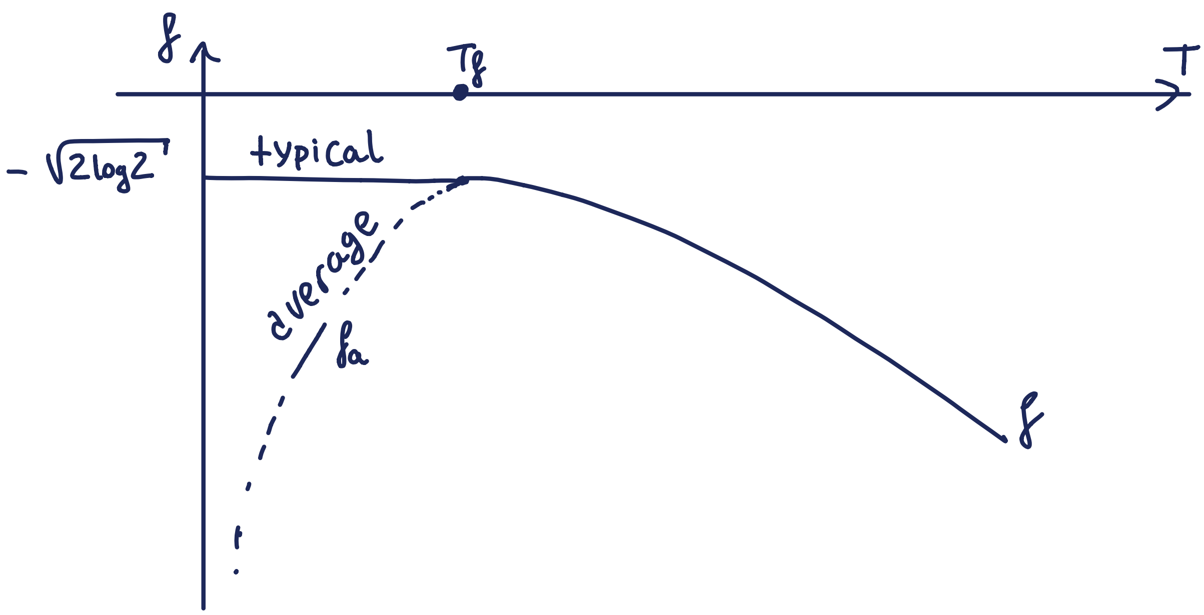
Let us compute the average of the partition function:

$$\overline{Z_N} = \int dE\, \overline{\mathcal{N}_N(E)}\, e^{-\beta E} = \int d\varepsilon\, e^{N\left[\log 2 - \frac{\varepsilon^2}{2} - \beta\varepsilon\right] + o(N)}$$

In this case, there is no restriction to the domain, and the saddle point value is always $\varepsilon^*_\beta = -\beta$

Then $$f_a = -\left(\frac{\log 2}{\beta} + \frac{\beta}{2}\right)$$

which coincides with the quenched free-energy of the model only when $T \geq T_g$. In the low-T phase, this is smaller than the quenched free-energy:



The average $\overline{Z_N}$ is much larger than its typical value, because is dominated by rare events: realizations of the randomness for which there are energies $E_\alpha < -N\sqrt{2\log 2}$, which occur with exponentially small probability.

However, this exponential smallness is compensated by the largeness of the Boltzmann weight when computing the average:

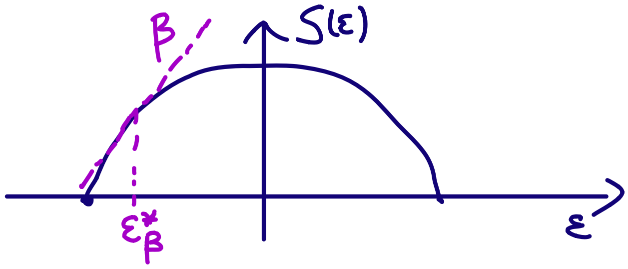
$$\overline{Z} = N \int d\varepsilon \; \underbrace{\overline{\mathcal{N}_N(\epsilon)}}_{\substack{\text{exponentially small} \\ \text{when } T<T_g:\ \text{RARE}}} \; \underbrace{e^{-\beta N \varepsilon}}_{\text{exponentially large}}$$

The typical value Z_N^{typ} accounts only for instances occurring with probability of $O(1)$ when $N \to \infty$.

3 ENTROPY CRISIS

Let us look at the entropy in the two phases.

The equation for ε^*_β graphically corresponds to choosing ε^*_β such that the tangent of $S(\varepsilon)$ at ε^*_β has slope β:



As β increases, ε^*_β decreases until one reaches a maximal value: $\beta_g = 1/T_g$

The maximal slope corresponds to $\varepsilon^* = -\sqrt{2\log 2}$, where $S(\varepsilon)$ vanishes: for $\beta > \beta_g$, the saddle point is stuck there an $S(\varepsilon)=0$. At T_g one also has a transition from positive to zero entropy:

FREEZING TRANSITION :

- $T > T_g$: $S(\varepsilon^*_\beta) > 0$: exponentially-many configurations contribute to Z_N
- $T \leq T_g$: $S(\varepsilon^*_\beta) = 0$: sub-exponential number of configurations contribute to Z_N: Condensation! Extreme values dominate.

4 THE OVERLAP DISTRIBUTION (ORDER PARAMETER)

Recall: in a spin-glass, because of the disorder, the magnetization is NOT a good order parameter.

We introduce instead the overlaps:

$$q_N(\vec{\sigma}^\alpha, \vec{\sigma}^\beta) = \frac{1}{N} \sum_i \sigma_i^\alpha \sigma_i^\beta = q_N^{\alpha\beta}$$

The overlap distibution is:

$$P_{N,\beta}(q) = \sum_{\alpha,\beta=1}^{2^N} \frac{z_\alpha z_\beta}{\underbrace{Z_N^2}_{\text{partition function}}} \delta(q - q_N^{\alpha\beta}) \qquad z_\alpha = e^{-\beta E(\vec{\sigma}^\alpha)}$$

It is convenient to split the cases $\alpha \neq \beta$ and $\alpha = \beta$:

$$P_{N,\beta}(q) = \underbrace{\sum_\alpha \sum_{\beta:\, \beta\neq\alpha} \frac{z_\alpha z_\beta}{Z_N^2}}_{\substack{\text{probability to extract two}\\ \neq \text{ configurations when}\\ \text{sample twice with}\\ \text{Boltzmann weight}}} \delta(q - q_N^{\alpha\beta}) + \underbrace{\sum_\alpha \frac{z_\alpha^2}{Z_N^2}}_{\substack{\text{probability to extract}\\ \text{the same configuration.}}} \delta(q - \underbrace{1}_{\substack{\text{overlap}\\ \text{of a configuration}\\ \text{with itself}}})$$

For large N:

- When extract two configurations with Boltzmann measure, when $N \gg 1$ they will have similar energy density, close to equilibrium one: $\frac{E_\alpha}{N} \simeq \frac{E_\beta}{N}$ $\left(= \epsilon^*_\beta \text{ in REM}\right)$

- In REM, energies E_α independent of configurations $\vec{\sigma}^\alpha$: Two configurations $\vec{\sigma}^\alpha$ and $\vec{\sigma}^\beta$ such that $E_\alpha \simeq E_\beta$ are like two random vectors of ± 1, statistically

- When $N \to \infty$, two random vectors are orthogonal:

$$q_N^{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} \underbrace{\sigma_i^\alpha \sigma_i^\beta}_{\pm 1} \underset{\substack{\uparrow \\ \text{central limit} \\ \text{theorem}}}{\sim} \frac{1}{\sqrt{N}} \xrightarrow{N \to \infty} 0.$$

Therefore in the REM

$$P_{N,\beta}(q) \overset{N \gg 1}{\approx} \sum_\alpha \sum_{\beta (\neq \alpha)} \frac{Z_\alpha Z_\beta}{\mathcal{Z}_N^2} \delta(q) + \sum_{\alpha=1}^{2^N} \frac{Z_\alpha^2}{\mathcal{Z}_N^2} \delta(q-1)$$

Call $\boxed{I_2^{(N)}(\beta) := \sum_{\alpha=1}^{2^N} \frac{Z_\alpha^2}{\mathcal{Z}_N^2} \quad \text{inverse participation ratio} \quad \text{Herfindhal index}}$

Here: probability to extract same config twice with Boltzmann.

How $I_2^{(N)}(\beta)$ scales with N?

- When $N\to\infty$, Boltzmann weight selects configs with $\frac{E_\alpha}{N} \simeq \frac{E_\beta}{N} = \mathcal{E}^*_\beta$.

Given $\vec{\sigma}^\alpha$, the probability to extract $\vec{\sigma}^\beta = \vec{\sigma}^\alpha$ is:

$$I_2^{(N)}(\beta) \sim \frac{1}{\mathcal{N}_N^{typ}(\mathcal{E}^*_\beta)} = e^{-N\, S(\mathcal{E}^*_\beta)}$$

When $|\mathcal{E}^*_\beta| < \sqrt{2\log 2}$, $S(\mathcal{E}^*_\beta) > 0$ and thus

$$I_2^{(N)}(\beta) \xrightarrow{N\to\infty} 0.$$

This happens when $\beta \leq \beta_c = \sqrt{2\log 2}$.

In the low-T phase, $S(\mathcal{E}^*_\beta) = 0$ and thus

$$I_2^{(N)}(\beta) \xrightarrow{N\to\infty} I_2(\beta) = \mathcal{O}(1)$$

$$\Rightarrow \boxed{\lim_{N\to\infty} P_{N,\beta}(q) = \begin{cases} \delta(q) & \beta \leq \beta_c \\ I_2(\beta)\,\delta(q-1) + (1 - I_2(\beta))\,\delta(q) & \beta > \beta_c \end{cases}}$$

$$P_\beta(q) = \delta(q) \qquad \text{for } T > T_f$$

The system is in a "paramagnetic" phase: equilibrium configurations (i.e., extracted from Boltzmann measure) are uncorrelated, $q=0$. Like in high-T phase of ferromagnet.

- The value $\overline{I_2(\beta)}$ (averaged) can be computed for the REM: one finds

$$\boxed{\overline{I_2(\beta)} = 1 - \beta_c/\beta = 1 - T/T_c \qquad T \leq T_c}$$

It can be shown that for $T<T_c$:

$$\overline{I_2} = \frac{T_f}{T} \frac{d}{d\mu} \log \int_0^\infty \left(1 - e^{-u-\mu u^2}\right) u^{-\frac{T}{T_f}-1} du \Bigg|_{\mu=0}$$

One has:

$$\frac{d}{d\mu} \log(\cdots)\Bigg|_{\mu=0} = \frac{\int_0^\infty e^{-u} u^{-T/T_f+1} du}{\int_0^\infty (1-e^{-u}) u^{-T/T_f-1} du} = \frac{\Gamma\left(2-\frac{T}{T_f}\right)}{-\Gamma(T/T_f)}$$

Using that $\Gamma(z) = \int_0^\infty dt\, t^{z-1} e^{-t}$ and that

$$\int_0^\infty (1-e^{-u}) u^{-z-1} du = \cancel{\frac{u^{-z}}{-z}(1-e^{-u})\Big|_0^\infty} - \int_0^\infty \frac{e^{-u} u^{-z}}{-z} = +\frac{e^{-u} u^{-z}}{-z}\Big|_0^\infty$$

$$- \int_0^\infty e^{-u} u^{-z-1} du = -\Gamma(-z)$$

Since $\dfrac{\Gamma(2-z)}{-\Gamma(-z)} = z(1-z)$ we find:

$$\overline{I_2} = \frac{T_f}{T}\frac{T}{T_f}\left(1-\frac{T}{T_f}\right) = 1 - T/T_f$$

Therefore:

$$\boxed{\overline{P_\beta(q)} = \left(1 - T/T_f\right)\delta(q-1) + T/T_f\, \delta(q) \qquad T \leq T_f}$$

Interpretation: glass phase!

In the low-T phase, the Boltzmann weight is dominated by sub-exponentially many configurations. The probability to pick up the same is $O(1)$. Consistent with entropy crisis! However, there are more than one configuration, and they are very different from each others: thus, there is also a finite probability to extract two of them at $q=0$. (this is not the case in a ferromagnet!). Only for $T \to 0$, the probability to pick up the same goes to one: this configuration is the ground state.

Comments:

(A) In this calculation we used the fact that $q_{\alpha\beta}$ and E_α, E_β are unrelated to each others: this is a peculiarity of the REM!
In other models, the larger is $q_{\alpha\beta}$ (the more $\vec{\sigma}^\alpha$ and $\vec{\sigma}^\beta$ are similar), the more the energies $E_\alpha = E(\vec{\sigma}^\alpha)$ and $E_\beta = E(\vec{\sigma}^\beta)$ will be correlated.

(B) Deriving the expression for $\overline{I_2}$ for $T<T_c$ is not trivial with a direct approach.
The replica method that we discuss in next TDs gives an alternative way to do so!