Problem 2: the free-energy & the freezing transition

1 THE CRITICAL TEMPERATURE & FREEZING TRANSITION

We have $\mathcal{Z}_N = \sum_{\alpha=1}^{2^N} e^{-\beta E_\alpha} = \int dE \, \underbrace{\mathcal{N}_N(E)}_{\text{random variable}} \, e^{-\beta E}$

The free-energy:

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

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

Saddle-point calculation:

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

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:

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

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

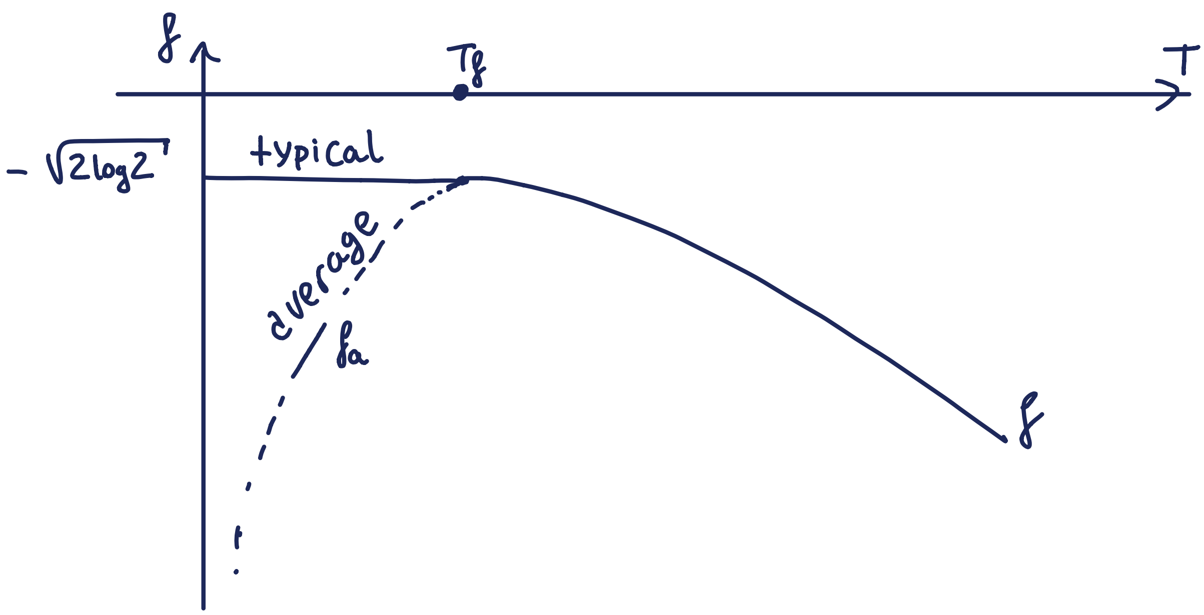
Let us compute the average of the partition function:

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

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 $T \geq T_f$. In the low-T phase, this is smaller than the quenched free-energy (Jensen's inequality!)



The annealed and quenched free-energies differ when $T<T_g$ because of RARE EVENTS: they imply that $\overline{Z_N}$ is (exponentially) larger then Z_N^{typ}.

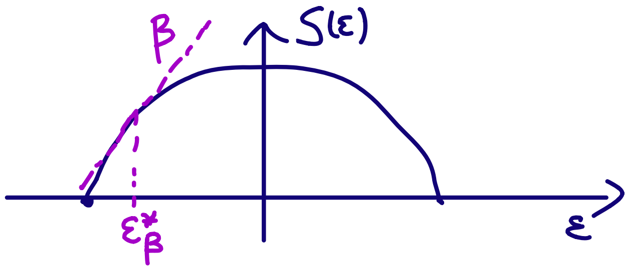
The average $\overline{Z_N}$ is "dominated by rare events": realizations of the randomness for which there are energies $E_\alpha < -N\sqrt{2\log 2}$, which occur with exponentially small probability.
However, this exponential smallness is compensated by the largeness of the Boltzmann weight when computing the average:

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

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:



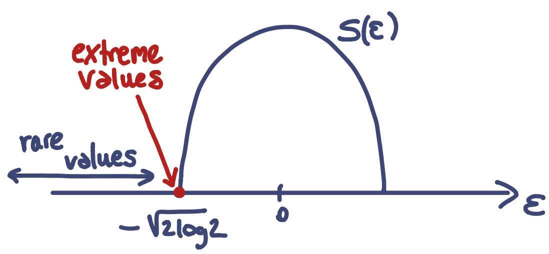
As β increases, ε^*_β decreases until one reaches a maximal value: $\beta_g = 1/T_g$

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.

Recall Alberto's lecture: extreme values are the energy levels close to E_{min}: $E_\alpha = E_{min} + X$, with $X \sim O(N^0)$. Their energy density is $\varepsilon = E/N = \varepsilon_{GS} = -\sqrt{2\log 2}$



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:

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

The overlap thermal distribution is

$$P_{N,\beta}(q) = \sum_{\alpha,\gamma=1}^{2^N} \frac{e^{-\beta E[\vec{\sigma}^\alpha]}\, e^{-\beta E[\vec{\sigma}^\gamma]}}{\underbrace{Z_N^2(\beta)}_{\text{partition function}}} \delta\left(q - q(\vec{\sigma}^\alpha, \vec{\sigma}^\gamma)\right)$$

Set $z_\alpha = e^{-\beta E(\vec{\sigma}^\alpha)}$ and split the cases $\alpha \neq \gamma$ and $\alpha = \gamma$:

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

For large N, in the REM

- 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:

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

Therefore in the REM

$$P_{N,\beta}(q) \overset{N \gg 1}{\approx} \sum_{\alpha} \sum_{\gamma (\neq \alpha)} \frac{z_\alpha z_\gamma}{Z_N^2(\beta)} \delta(q) + \sum_{\alpha=1}^{2^N} \frac{z_\alpha^2}{Z_N^2(\beta)} \delta(q-1)$$

Call $\boxed{I_2^{(N)}(\beta) := \sum_{\alpha=1}^{2^N} \frac{z_\alpha^2}{Z_N^2} \quad \text{inverse participation ratio, Herfindhal index}}$

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 $\vec{\sigma}^\gamma = \vec{\sigma}^\alpha$ is:

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

number of equilibrium configurations

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

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

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

- High-T phase: $P_\beta(q) = \delta(q)$ 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.

- Low-T phase: The value $\overline{I_2(\beta)}$ (averaged over the disorder) can be computed for the REM, using tools of probability. One finds:

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

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 measure is dominated by sub-exponentially many configurations: the probability to pick up twice the same is large, $\mathcal{O}(1)$. 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 $E_\alpha = E(\vec{\sigma}^\alpha)$ and $E_\beta = E(\vec{\sigma}^\beta)$ are 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 lectures gives an alternative way to do so!