SOLUTIONS TD2

Problem 2: the free-energy & the freezing transition

1 THE CRITICAL TEMPERATURE & FREEZING

We have $\mathcal{Z} = \sum_{\alpha=1}^{2^N} e^{-\beta E_\alpha} = \int dE\, \mathcal{N}(E)\, e^{-\beta E} = \int_{-N\sqrt{2\log 2}}^{N\sqrt{2\log 2}} dE\; e^{N S(E/N) - \beta E + o(N)}$

Change variables to $\varepsilon = E/N$:

$$\mathcal{Z} = \int d\varepsilon\; e^{N[S(\varepsilon) - \beta\varepsilon] + o(N)} \overset{\text{saddle-point calculation}}{=} e^{N \max\limits_{|\varepsilon| < \sqrt{\log 2}} (S(\varepsilon) - \beta\varepsilon) + o(N)}$$

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

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

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:

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

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

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

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

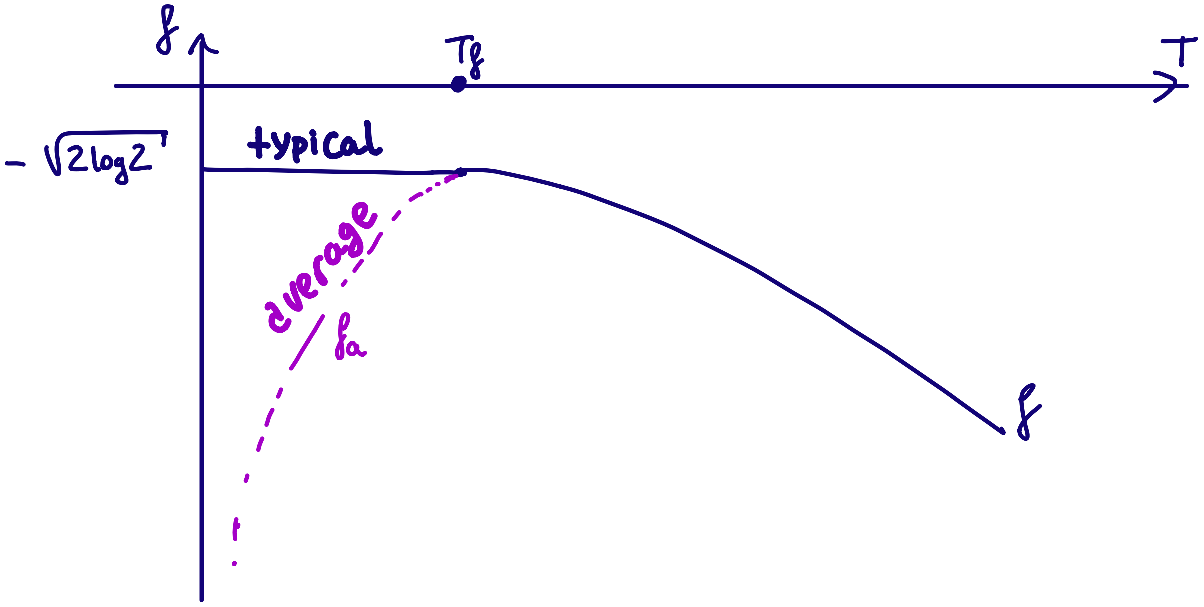
Let us compute the average of the partition function:

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

In this case, there is no restriction to the domain, and the saddle point value is always $\varepsilon^* = -1/T$

Then $$f_a = -\left(T\log 2 + \frac{1}{2T}\right)$$

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



The average $\overline{Z}$ 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.

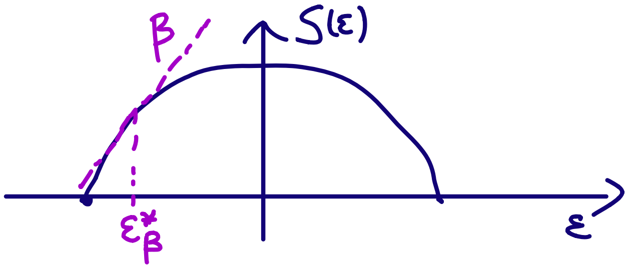
However, this exponential smallness is compensated by the largeness of the Boltzmann weight when computing the average.

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

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

$\boxed{3}$ ENTROPY CATASTROPHE

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
- $T \leq T_g$: $S(\varepsilon^*_\beta) = 0$: sub-exponential number of configurations contribute to Z : **Condensation**

$\boxed{4}$ THE OVERLAP DISTRIBUTION

The overlap distibution is:

$$P(q) = \sum_{\alpha,\beta} \frac{Z_\alpha Z_\beta}{Z^2}\,\delta\left(q - q(\vec\sigma^\alpha, \vec\sigma^\beta)\right) \qquad Z_\alpha = e^{-\beta E(\vec\sigma^\alpha)}$$

Partition function

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

$$P(q) = \underbrace{\sum_{\alpha}\sum_{\beta:\,\beta\neq\alpha} \frac{Z_\alpha Z_\beta}{Z^2}}_{\text{probability to extract two } \neq \text{ configurations when sample twice with Boltzmann weight}} \delta(q - q_{\alpha\beta}) + \underbrace{\sum_{\alpha} \frac{Z_\alpha^2}{Z^2}}_{\text{probability to extract the same configuration.}} \delta(q - 1)$$

overlap of a configuration with itself

- Now, if one extracts two different configurations $\vec{\sigma}^\alpha$ and $\vec{\sigma}^\beta$ with a Boltzmann measure, in the REM the overlap between them is independent of their energies, because the energies E_α are assigned randomly to the configurations. The two configurations $\vec{\sigma}^\alpha$ and $\vec{\sigma}^\beta$ are uncorrelated random vectors of ±1; their overlap is a sum of uncorrelated ±1 variables: its typical value is zero. Therefore:

$$P(q) = \sum_\alpha \sum_{\beta:\, \beta\neq\alpha} \frac{Z_\alpha Z_\beta}{Z^2} \delta(q) + \sum_\alpha \frac{Z_\alpha^2}{Z^2} \delta(q-1)$$

- Call $I_2 = \sum_\alpha \frac{Z_\alpha^2}{Z^2}$.

Then, averaging over all possible realizations of the model:

$$\overline{P(q)} = \overline{I_2}\, \delta(q-1) + (1-\overline{I_2})\, \delta(q)$$

- Let us compute the probability to extract the same configuration from a Boltzmann measure at temperature T.

When $N \to \infty$, the Boltzmann weight Z_α / Z selects configurations with the equilibrium energy density ε_β^*. With prob $\simeq 1$, $\vec{\sigma}^\alpha$ and $\vec{\sigma}^\beta$ will have this energy. Given $\vec{\sigma}^\alpha$, the probability to re-extract $\vec{\sigma}^\alpha$ from the family of $N(\varepsilon_\beta^*)$ configurations with the correct energy density is:

$$\overline{I_2} = \frac{1}{N(\varepsilon_\beta^*)} = e^{-N S(\varepsilon_\beta^*) + o(N)}$$

Therefore, when $|\varepsilon_\beta^*| < \sqrt{2 \log 2}$, since $S(\varepsilon_\beta^*) > 0$ this probability decays to zero exponentially fast when $N \to \infty$. This is what happens for $T > T_c$. Thus

$$\boxed{\overline{P(q)} = \delta(q) \qquad \text{for } T > T_f}$$

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.

When $T<T_c$, $S(\varepsilon^*_\beta)=0$ and $I_2 \sim O(1)$: our large-N expansion is not enough to compute the average.

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

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

One has:

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

Using that $\boxed{\Gamma(z) = \int_0^\infty dt\, t^{z-2}\, e^{-t}}$ 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 $\frac{\Gamma(2-z)}{-\Gamma(-z)} = z(1-z)$ we find:

$$\overline{I}_2 = \frac{T_f}{T}\frac{T}{T_f}\left(1-\frac{T}{T_f}\right) = 1-T/T_f$$

$$\Rightarrow \boxed{\overline{P}(q) = \left(1-\frac{T}{T_f}\right)\delta(q-1) + T/T_f\,\delta(q) \qquad T<T_f}$$

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 catastrophe! 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!