8 Complexity

We have seen that in the spherical spin glasses we have a kind of paradox: the statics predicts a thermodynamic transition from a paramagnetic state to a 1RSB spin glass state for temperatures lower than

$$\frac{f(q)}{f'(q)} = -(q + \log(1-q))\frac{1-q}{q} \qquad\qquad T_K = \sqrt{\frac{1-q}{q}f'(q)} \tag{1}$$

but that the dynamics predicts the loss of ergodicity and entry into a aging asymptotic dynamics for temperatures lower than

$$\frac{f'(q)}{f''(q)} = q(1-q) \qquad\qquad T_d = \sqrt{\frac{1-q}{q}f'(q)} \tag{2}$$

The aging dynamics is characterized by ever longer lingering at a marginal q and a long-time effective temperature $T_{\text{eff}} = T/x$ for

$$\beta^2 f''(q) = \frac{1}{(1-q)^2} \qquad\qquad \beta^2 f'(q) = \frac{q}{(1-q)(1-q(1-x))} \tag{3}$$

For pure p-spin models we combined these to find x as a function of q and show that the asymptotic energy reached was

$$x = \frac{(p-2)(1-q)}{q} \qquad\qquad E_\infty = -\frac{1}{2}\beta(1-q^p(1-x)) \tag{4}$$

Today we will see how this behavior can be explained by the structure of metastable states in the free energy.

First, let us be clear about what we mean by a state. A pure state is defined by a subregion of configuration space ω such that connected correlation functions vanish over that region:

$$\langle s_i s_j\rangle_\omega = \langle s_i\rangle_\omega \langle s_j\rangle_\omega \tag{5}$$

where

$$\langle f(\mathbf{s})\rangle_\omega = \int_\omega d\mathbf{s}\, e^{-\beta H(\mathbf{s})} f(\mathbf{s}) \tag{6}$$

In the standard ferromagnet, for instance, you have one or two pure states depending on the temperature: the paramagnetic Gibbs state is a pure state, and there is one pure state corresponding to each of positive and negative magnetization.

Our goal is to count the number of pure states in the spherical models. We start by decomposing the Gibbs measure into pure states:

$$Z(\beta) = \int_\Omega d\mathbf{s}\, e^{-\beta H(\mathbf{s})} = \sum_{\omega\subseteq\Omega}\int_\omega d\mathbf{s}\, e^{-\beta H(\mathbf{s})} = \sum_{\omega\subseteq\Omega} Z_\omega(\beta) \tag{7}$$

We can define the free energy density of a pure state by $F_\omega(\beta) = -\frac{1}{N}\frac{1}{\beta}\log Z_\omega(\beta)$, which gives

$$Z(\beta) = \sum_{\omega \subseteq \Omega} e^{-\beta N F_\omega(\beta)} \tag{8}$$

Suppose that there are many pure states, and we define their density $\rho(F)$. Then we have

$$Z(\beta) = \int dF\, \rho(F,\beta) e^{-\beta N F} = \int dF\, e^{-\beta N (F - T\Sigma(F,\beta))} \tag{9}$$

where we have defined $\Sigma(F,\beta) = \frac{1}{N}\log\rho(F,\beta)$ as the entropy of pure states with free energy F. We call this the *complexity*. In a mean-field approach, we would evaluate this integral by taking a saddle-point with respect to F, yielding

$$\beta = \frac{\partial \Sigma}{\partial F} \tag{10}$$

and

$$\Phi = F - T\Sigma \tag{11}$$

a generalization of the standard relationship between temperature, entropy, and energy density. However, we don't know Σ – this is what we want to find! We can extract it by the following trick. We compute the sum

$$Z(\beta, x) = \sum_{\omega \subseteq \Omega} Z_\omega(\beta)^x \tag{12}$$

in which every pure state partition function is raised to the power x. Then, following the same logic, we have

$$Z(\beta, x) = \int dF\, e^{-\beta N (xF - T\Sigma(F,\beta))} \tag{13}$$

In this form, we can extract $\Sigma(F,\beta)$ by Legendre transform: if $\Phi(\beta, x) = -\frac{1}{N}\beta^{-1}\log Z(\beta, x)$, then

$$\Sigma(F,\beta) = \sup_x [x\beta F - \beta\Phi(\beta, x)] \tag{14}$$

and therefore be evaluated at x such that

$$F = \frac{\partial \Phi(\beta, x)}{\partial x} \tag{15}$$

To compute this, we note that the power x looks an awful lot like a replication. Consider replicating $Z(\beta, x)$ in order to calculate the quenched average:

$$\overline{\Phi(\beta, x)} = -\frac{T}{N}\lim_{n\to 0}\frac{\partial}{\partial n}\overline{Z(\beta, x)^n} = -\frac{T}{N}\lim_{n\to 0}\frac{\partial}{\partial n}\overline{\left(\sum_{\omega \subseteq \Omega} Z_\omega(\beta)^x\right)^n} \tag{16}$$

In this light, we have nx total replicas, where groups of x of them are restricted to lie in the same pure state. But, we know what it looks like when replicas lie in the same pure state: they belong to the same block of the replica matrix! We are therefore facing a replica calculation where the size m of the blocks is fixed from the outset to be equal to x.

From previous work, we already know what the 1RSB effective action looks like in general. Writing it for nx total replicas and with $m = x$ gives

$$\overline{\Phi(\beta, x)} = -\frac{T}{N} \lim_{n\to 0} \frac{\partial}{\partial n} \int dq\, e^{Nn\mathcal{S}_x(q)} \tag{17}$$

where

$$\mathcal{S}_x(q) = \frac{1}{2}\left[\beta^2 x[f(1) - (1-x)f(q)] + x\log(1-q) + \log\frac{1-(1-x)q}{1-q}\right] \tag{18}$$

Minimizing this over q gives

$$0 = -\beta^2 x(1-x)f'(q) + \frac{qx(1-x)}{(1-q)(1-q(1-x))} \tag{19}$$

which simplifies to

$$\beta^2 f'(q) = \frac{q}{(1-q)(1-q(1-x))} \tag{20}$$

exactly the same condition between q and x we found in the aging solution. Then if $q^*(x)$ solves this, we are basically done:

$$\overline{\Phi(\beta, x)} = -\beta^{-1}\mathcal{S}_x(q^*(x)) \tag{21}$$

Finally we have to find x such that

$$F = \frac{\partial\overline{\Phi}}{\partial x} = -\beta^{-1}\left(\frac{\partial\mathcal{S}_x(q^*)}{\partial x} + \frac{\partial\mathcal{S}_x(q)}{\partial q}\frac{\partial q^*}{\partial x}\right) = -\beta^{-1}\frac{\partial\mathcal{S}_x(q^*)}{\partial x} \tag{22}$$

where we have used the fact that $\mathcal{S}_x(q)$ is stationary with respect to q at q^*. We then have

$$\begin{aligned}\beta F &= -\frac{\partial\mathcal{S}_x(q)}{\partial x} \\ &= -\frac{1}{2}\left(\beta^2[f(1) - (1-x)f(q)] + \beta^2 x f(q) + \log(1-q) + \frac{q}{1-q(1-x)}\right) \\ &= -\frac{1}{2}\left[\beta^2[f(1) - (1-x)f(q)] + \beta^2 x f(q) + \log(1-q) + \beta^2 f'(q)(1-q)\right]\end{aligned} \tag{23}$$

where in the second line we used the equation for q. Now this is linear in x and can be solved to give

$$x = \frac{1}{f(q)}\left[-TF - \frac{1}{2}\left(f(1) - f(q) + (1-q)f'(q) + T^2\log(1-q)\right)\right] \tag{24}$$

We therefore have

$$\begin{aligned}\Sigma &= x\beta F - \beta\overline{\Phi} = x\beta F + \mathcal{S}_x \\ &= x\beta F + \frac{1}{2}\left[\beta^2 x[f(1) - (1-x)f(q)] + x\log(1-q) + \log\frac{1-(1-x)q}{1-q}\right] \\ &= x\beta F + \frac{1}{2}\left[\beta^2 x[f(1) - (1-x)f(q)] + x\log(1-q) - \log\frac{\beta^2 f'(q)(1-q)^2}{q}\right] \\ &= \frac{1}{8\beta^2 f(q)}\left[(1-q)^2\beta^4 f'(q)^2 - \left[2\beta F + \beta^2[f(1)-f(q)] + \log(1-q)\right]^2\right] - \log(1-q) - \frac{1}{2}\log\frac{\beta^2 f'(q)}{q}\end{aligned} \tag{25}$$

where in the last step we inserted the solution for x and made some simplification. The complexity of metastable states at a given free energy F can be numerically studied at a given temperature by solving the equation for q with our formula for x inserted, then plugging this into the expression above.

When this is evaluated as a function of F, there are two possibilities: either Σ has no solution or is negative everywhere, which indicates that it is vanishingly unlikely to find pure states at any free energy at that temperature, or it is positive for some interval of F, which indicates that there is a range of pure states with an entropy. When there is such an interval, it terminates suddenly at its maximum, due to the solution to the equation for q vanishing. We want to ask the question: what is the value of q, x, and F where solutions first appear for a given β?

We can first answer this at zero temperature. In that limit, recall that q asymptotically approaches 1, which we write as $q = 1 - yT$. Inserting this into the equation for x and expanding in small T, we find

$$x = -\frac{T}{f(1)}(F + yf'(1)) + O(T^2) \tag{26}$$

Inserting this into the equation for q and expanding gives

$$\begin{aligned}0 &= \beta^2 f'(q)(1 - q(1-x)) - \frac{q}{1-q} \\ &= \beta\left(\frac{f'(1)}{f(1)}[-F - y(f'(1) - f(1))] - \frac{1}{y}\right) + O(T^0)\end{aligned} \tag{27}$$

This gives a quadratic equation for y that can be solved to give

$$y = \frac{1}{2}\frac{F + \sqrt{F^2 - 4\frac{f(1)}{f'(1)}[f'(1) - f(1)]}}{f'(1) - f(1)} \tag{28}$$

Finally, the same expansion applied to the complexity Σ gives

$$\Sigma = \frac{1}{2}\left[-\frac{1}{f(1)}F(F + yf'(1)) - \log(y^2 f'(1))\right] \tag{29}$$

This gives in closed form the complexity of zero-temperature states, or the complexity of *minima of the energy*, where the energy density of a minimum is given by F. The ground state of the model can be worked out simply, since it is the place where the entropy of minima vanishes, or $\Sigma = 0$, which for $p = 3$ is around $E = -1.17167$. Plotting the complexity curve as a function of energy density, it abruptly ends at

$$E_{sh}(T = 0) = -2\sqrt{\frac{f(1)}{f'(1)}[f'(1) - f(1)]} = -\sqrt{\frac{2(p-1)}{p}} \tag{30}$$

This is the energy density where in pure models the minima become unstable. In mixed models this isn't quite right: we need to look explicitly at the stability condition

$$0 \geqslant \beta^2 f''(q) - \frac{1}{(1-q)^2} = \beta^2 \left(f''(1) - \frac{1}{y^2}\right) + O(T^{-1}) \tag{31}$$

which instead is saturated for

$$E_{th}(T = 0) = -\frac{1}{\sqrt{f''(1)}}\left(f'(1) + \frac{f(1)}{f'(1)}(f''(1) - f'(1))\right) = -\sqrt{\frac{2(p-1)}{p}} \tag{32}$$

which is the same as the expression above for pure models. Recall that in the aging solution, we found the asymptotic energy density is

$$E_\infty = -\frac{1}{2}\beta\left[1 - q^p\left(1 - \frac{(p-2)(1-q)}{q}\right)\right] \tag{33}$$

for q satisfying the stability condition

$$\beta^2 f''(q) = \frac{1}{(1-q)^2} \tag{34}$$

Making the same limit of $q \to 1$ as $T \to 0$ using $q = 1 - yT$, this condition gives

$$y^2 = \frac{1}{f''(1)} = \frac{2}{p(p-1)} \tag{35}$$

and

$$E_\infty(T = 0) = -(p-1)y = -\sqrt{\frac{2(p-1)}{p}} \tag{36}$$

exactly the same is the maximum energy at which minima are found!

To make this connection at finite temperature, we need to make use of another way of studying metastable states. This is the Thouless–Anderson–Palmer

(TAP) free energy, which is defined using a standard mean-field approach. Suppose we are in a thermodynamic pure state, so that averages factorize, and define the magnetizations in that state as

$$\langle s_i \rangle = m_i \tag{37}$$

We want to make the standard field-theoretic transformation from the free energy as a function of external field

$$F(\mathbf{h}) = -T \log \int_{\circ} d\mathbf{s}\, e^{-\beta[H(\mathbf{s}) - \mathbf{h}\cdot\mathbf{s}]} \tag{38}$$

to the free energy as a function of $\mathbf{m}$

$$G(\mathbf{m}) = -T \log \int d\mathbf{h}\, e^{-\beta[F(\mathbf{h}) - \mathbf{h}\cdot\mathbf{m}]} = F(\mathbf{h}^*) - \mathbf{h}^* \cdot \mathbf{m} \tag{39}$$

where we have evaluated the integral by saddle point with

$$0 = \frac{\partial F}{\partial \mathbf{h}}(\mathbf{h}^*) - \mathbf{m} \tag{40}$$

which implies that $\langle \mathbf{s} \rangle = \mathbf{m}$, as desired. We do this by expanding G in a high-temperature series.

$$G(\mathbf{m}) = G(\mathbf{m})\Big|_{\beta=0} + \beta \frac{\partial}{\partial \beta} G(\mathbf{m})\Big|_{\beta=0} + \beta^2 \frac{1}{2} \frac{\partial^2}{\partial \beta^2} G(\mathbf{m})\Big|_{\beta=0} + O(\beta^3) \tag{41}$$

In general models, this would be an approximation. However, it can be shown that in fully-connected models, higher order in β implies higher order in N^{-1}, and therefore truncating the series at quadratic order is exact. Each order can be calculated explicitly, since it amounts to connected expectation values over the infinite-temperature ensemble in the presence of a field that keeps $\langle \mathbf{s} \rangle = \mathbf{m}$. This is called the Plefka expansion in this context.

Here we do not go into detail into the calculation. The result is

$$G(\mathbf{m}) = -NT \left[\frac{1}{2} \log \left(1 - \frac{\|\mathbf{m}\|^2}{N} \right) - \beta \frac{1}{N} H(\mathbf{m}) + \frac{1}{2} \beta^2 \left(f(1) - f\left(\frac{\|\mathbf{m}\|^2}{N} \right) - \left(1 - \frac{\|\mathbf{m}\|^2}{N} \right) f'\left(\frac{\|\mathbf{m}\|^2}{N} \right) \right) \right]$$

or writing $q = \frac{1}{N}\|\mathbf{m}\|^2$,

$$G(\mathbf{m}, q) = -NT \left[\frac{1}{2} \log (1 - q) - \beta \frac{1}{N} H(\mathbf{m}) + \frac{1}{2} \beta^2 \left(f(1) - f(q) - (1 - q) f'(q) \right) \right]$$

Given this, pure states are found as solutions to

$$0 = \frac{\partial G}{\partial \mathbf{m}} = \frac{\partial H}{\partial \mathbf{m}} \qquad 0 = \frac{\partial G}{\partial q} \qquad 0 = \frac{1}{N}\|\mathbf{m}^2\| - q \tag{42}$$

We can think of the first condition as saying that the energy H has a minimum, but at a radius $\sqrt{N}q$ potentially different from the radius $\sqrt{N}$ of the configuration space. However, since in *pure* p-spin models $H(\mathbf{m}) = q^{\frac{p}{2}} H(\mathbf{s})$, it follows that *all pure states correspond one-to-one with minima of the energy.* Note that this is a very special property of the pure models, which isn't even shared by mixed spherical models. However, it allows us to easily analyze the free energy landscape at nonzero temperature. Suppose that we have a minimum at position $\mathbf{s}^*$ on the sphere with energy density $E(T=0) = \frac{1}{N}H(\mathbf{s}^*)$. Then the free energy density of that pure state is

$$\begin{aligned}
F &= -\left[\frac{1}{2\beta}\log\left(1-q\right) - \frac{1}{N}H(\mathbf{m}^*) + \frac{1}{2}\beta\left(f(1) - f\left(q\right) - \left(1-q\right)f'\left(q\right)\right)\right] \\
&= -\left[\frac{1}{2\beta}\log\left(1-q\right) - q^{\frac{p}{2}}\frac{1}{N}H(\mathbf{s}^*) + \frac{1}{2}\beta\left(f(1) - f\left(q\right) - \left(1-q\right)f'\left(q\right)\right)\right] \\
&= -\left[\frac{1}{2\beta}\log\left(1-q\right) - q^{\frac{p}{2}}E(T=0) + \frac{1}{2}\beta\left(f(1) - f\left(q\right) - \left(1-q\right)f'\left(q\right)\right)\right]
\end{aligned}$$

which depends only on the q characterizing the state and the energy density E of the energy minimum it is connected to. The corresponding value of x is

$$\begin{aligned}
x &= \frac{1}{f(q)}\left[-TF - \frac{1}{2}\left(f(1) - f(q) + (1-q)f'(q) + T^2\log(1-q)\right)\right] \\
&= -2Tq^{-\frac{p}{2}}E(T=0) - (1-q)\frac{f'(q)}{f(q)} = -2Tq^{-\frac{p}{2}}E(T=0) - p\frac{1-q}{q}
\end{aligned}$$

The highest energy density of minima is $E_{th}(T=0)$, and therefore this will be the highest free energy density at which pure states can exist at a given temperature. The energy density associated with those finite-temperature pure states is

$$\begin{aligned}
E(T) = \frac{\partial(\beta F)}{\partial\beta} &= q^{\frac{p}{2}}E_{th}(T=0) - [f(1) - f(q) - (1-q)f'(q)] \\
&= -\frac{1}{2}\beta q^p\left(x + p\frac{1-q}{q}\right) - \frac{1}{2}\beta\left[1 - q^p\left(1 + \frac{p(1-q)}{q}\right)\right] \\
&= -\frac{1}{2}\beta q^p\left(\frac{(p-2)(1-q)}{q} + p\frac{1-q}{q}\right) - \frac{1}{2}\beta\left[1 - q^p\left(1 + \frac{p(1-q)}{q}\right)\right] \\
&= -\frac{1}{2}\beta q^p\frac{2(p-1)(1-q)}{q} - \frac{1}{2}\beta\left[1 - q^p\left(1 + \frac{p(1-q)}{q}\right)\right] \\
&= -\frac{1}{2}\beta\left[1 - q^p\left(1 - \frac{(p-2)(1-q)}{q}\right)\right] = E_\infty
\end{aligned}$$

Thus we see that at every temperature where $q < 1$ and therefore marginal pure states are defined and exist in exponential quantity, the asymptotic energy reached by aging dynamics is the same as their energy density.

What is the interpretation aging posed by this picture? The real equilibrium states of the system at low temperature are few in number ($\Sigma = 0$) and are separated by high $O(N)$ barriers from each other. However, at a higher free energy density there exist extremely many marginal pure states with small $o(N)$ barriers. The aging dynamics consists of ergodic exploration of a given pure state, then on a longer timescale hopping to a nearby pure state with slightly ($o(N)$) lower free energy. As this process goes on, one explores pure states with lower and lower free energy and takes a longer time to escape each successive one, but one doesn't actually move any lower in free energy *density*. The effective temperature on long timescales is set by the change in complexity of marginal pure states with energy density, since hopping between these pure states is the relevant dynamics on these long timescales.