ICFP M2 - Statistical physics 2 – TD n° 6
The trap model – Solution

Grégory Schehr, Francesco Zamponi

1. The trap model is a Markov dynamics on the wells $E_\alpha \geq 0$, specified by the following transition probabilities $W(\alpha \to \gamma)$, from the well of depth E_α to the one of depth E_γ, within the time interval t and $t + \mathrm{d}t$

$$W(\alpha \to \alpha) = 1 - r(E_\alpha)\mathrm{d}t + \frac{1}{N} r(E_\alpha)\mathrm{d}t \tag{1}$$
$$W(\alpha \to \gamma) = \frac{1}{N} r(E_\alpha)\mathrm{d}t \;, \; \gamma \neq \alpha \;,$$

with $r(E_\alpha) = e^{-\beta E_\alpha}$. The corresponding master equation satisfied by $\widehat{P}(\alpha, t)$, the probability to find the particle in the α-th well at time t reads

$$\widehat{P}(\alpha, t + \mathrm{d}t) = \widehat{P}(\alpha, t) W(\alpha \to \alpha) + \sum_{\gamma \neq \alpha} \widehat{P}(\gamma, t) W(\gamma \to \alpha) \;. \tag{2}$$

Using the expressions of the transition probabilities (1), one finds

$$\widehat{P}(\alpha, t + \mathrm{d}t) = \widehat{P}(\alpha, t)(1 - r(E_\alpha)\mathrm{d}t) + \frac{1}{N} \sum_{\gamma=1}^{N} \widehat{P}(\gamma, t) r(E_\gamma)\mathrm{d}t \;. \tag{3}$$

Taking the limit $\mathrm{d}t \to 0$, one obtains the master equation

$$\frac{\partial \widehat{P}(\alpha, t)}{\partial t} = -r(E_\alpha)\widehat{P}(\alpha, t) + \frac{1}{N} \sum_{\gamma=1}^{N} r(E_\gamma) \widehat{P}(\gamma, t) \;. \tag{4}$$

Note that by summing the above equation over $\alpha = 1, \cdots, N$ one easily checks that $\sum_{\alpha=1}^{N} \widehat{P}(\alpha, t)$ is conserved, as it should, since $\sum_{\alpha=1}^{N} \widehat{P}(\alpha, t) = 1$ for all time $t \geq 0$.

2. Denoting the Gibbs-Boltzmann distribution $\widehat{P}_{\rm eq}(\alpha) = e^{\beta E_\alpha}/Z$ with $Z = \sum_{\alpha=1}^{N} e^{\beta E_\alpha}$, it is easy to check that

$$-r(E_\alpha)\widehat{P}_{\rm eq}(\alpha) + \frac{1}{N} \sum_{\gamma=1}^{N} r(E_\gamma)\widehat{P}_{\rm eq}(\gamma) = -\frac{1}{Z} + \frac{1}{Z} = 0 \;. \tag{5}$$

Note that from Eq. (1) one can check that the dynamics actually satisfies detailed balance, i.e., $W(\alpha \to \gamma)\widehat{P}_{\rm eq}(\alpha) = W(\gamma \to \alpha)\widehat{P}_{\rm eq}(\gamma) = 1/(N\,Z)$, for all α, γ.

3. The probability density $P(E, t)$ to find the particle in a well of depth E at time t is given, in terms of the $\widehat{P}(\alpha, t)$, by

$$P(E, t) = \sum_{\alpha=1}^{N} \widehat{P}(\alpha, t)\, \delta(E - E_\alpha) \;. \tag{6}$$

Therefore, taking a time derivative of Eq. (6) and using the master equation (4), one gets

$$\begin{aligned} \frac{\partial P(E,t)}{\partial t} &= \sum_{\alpha=1}^{N} \delta(E-E_\alpha)\left[-r(E_\alpha)\widehat{P}(\alpha,t) + \frac{1}{N}\sum_{\gamma=1}^{N} r(E_\gamma)\widehat{P}(\gamma,t)\right] && (7) \\ &= \underbrace{-r(E)P(E,t)}_{\text{rate of exit from depth } E} + \underbrace{\left(\frac{1}{N}\sum_{\alpha=1}^{N}\delta(E-E_\alpha)\right)}_{\text{uniform choice of a well after an escape}} \underbrace{\left(\int_0^\infty r(E')P(E',t)\,\mathrm{d}E'\right)}_{\text{total rate of escape}} , && (8) \end{aligned}$$

where in the last line we have used Eq. (6), together with the fact that, by convention, $E_\alpha \geq 0$ for all $\alpha = 1, \cdots, N$.

4. We denote by $\tau(E)$ the time of first escape from a well of depth E. Let us compute first the cumulative probability $\mathbb{P}(\tau(E) \geq t)$. We divide the time interval $[0,t]$ in $n = t/\mathrm{d}t$ infinitesimal intervals, each of size $\mathrm{d}t$. During each of these intervals, the probability to escape is thus $r(E)\mathrm{d}t$ (independently of what happens before). Therefore, the probability not to escape in any of these intervals is

$$\mathbb{P}\left[\tau(E) \geq t\right] = \left[1 - r(E)\mathrm{d}t\right]^n = \left[1 - r(E)\mathrm{d}t\right]^{\frac{t}{\mathrm{d}t}} \underset{\mathrm{d}t\to 0}{=} e^{-r(E)t} \ . \tag{9}$$

Hence the probability law of $\tau(E)$, which is minus the derivative of $\mathbb{P}\left[\tau(E) \geq t\right]$ with respect to t, is an exponential distribution with parameter $r(E)$. Its expectation value $\overline{\tau}(E)$ is thus given by

$$\overline{\tau}(E) = \int_0^\infty e^{-r(E)t}\, r(E)\, t\, \mathrm{d}t = \frac{1}{r(E)} = e^{\beta E} \ , \tag{10}$$

which has an Arrhenius form: the deeper the well, the longer the time spent (on average) in it.

5. We now consider that the depths E_α are i.i.d. random variables, which amounts to assume that at each escape a new well with depth E_γ is found, neglecting the possibility to visit twice, or more, the same well, which is justified in the limit $N \to \infty$. Moreover, in the limit $N \to \infty$, one has

$$\lim_{N\to\infty} \frac{1}{N}\sum_{\alpha=1}^{N} \delta(E - E_\alpha) = \rho(E) \ , \tag{11}$$

from which it follows that Eq. (8) becomes, in the limit $N \to \infty$

$$\frac{\partial P(E,t)}{\partial t} = -r(E)P(E,t) + \rho(E)\left(\int_0^\infty r(E')P(E',t)\,\mathrm{d}E'\right) . \tag{12}$$

6. If we set $P_{\mathrm{st}}(E) = \frac{\rho(E)}{r(E)}$ it is easy to check that

$$-r(E)P_{\mathrm{st}}(E) + \rho(E)\left(\int_0^\infty r(E')P_{\mathrm{st}}(E')\mathrm{d}E'\right) = -\rho(E) + \rho(E)\int_0^\infty \rho(E')\mathrm{d}E' = 0 \ , \tag{13}$$

where we have used that $\int_0^\infty \rho(E')\mathrm{d}E' = 1$, which follows straightforwardly from Eq. (11).

7. The correlation function $C(t_{\mathrm{w}}+t, t_{\mathrm{w}})$ is defined by the following probability

$$C(t_{\mathrm{w}}+t, t_{\mathrm{w}}) = \mathbb{P}[\text{particle stays in the same trap in the time interval } [t_{\mathrm{w}}, t_{\mathrm{w}}+t]] \tag{14}$$

which can be computed by integrating over energy depths E as

$$\begin{aligned} C(t_{\mathrm{w}}+t, t_{\mathrm{w}}) &= \int_0^\infty \mathbb{P}[\text{part. stays in the same trap of depth in } [E, E+\mathrm{d}E] \text{ within } [t_{\mathrm{w}}, t_{\mathrm{w}}+t]]\mathrm{d}E \\ &= \int_0^\infty P(E,t_{\mathrm{w}})\mathbb{P}\left[\tau(E) \geq t\right]\mathrm{d}E = \int_0^\infty P(E,t_{\mathrm{w}})\, e^{-t\, e^{-\beta E}}\mathrm{d}E \ , && (15) \end{aligned}$$

where we have used Eq. (9).

8. If one assumes that $\rho(E) = e^{-E}$ for $E \geq 0$ — and of course $\rho(E) = 0$ if $E < 0$ — the stationary distribution $P_{\rm st}(E)$ defined above in question 6 is given by

$$P_{\rm st}(E) = \frac{\rho(E)}{r(E)} = e^{-(1-\beta)E} \; , \; E \geq 0 \; . \tag{16}$$

Hence, if $\beta < 1$ (i.e. at high temperature), $P_{\rm st}(E)$ can be normalized and $\widehat{P}_{\rm st}(E) = (1-\beta)e^{-(1-\beta)E}$ is a well normalized stationary distribution. However, for $\beta \geq 1$ the integral $\int_0^\infty P_{\rm st}(E){\rm d}E$ diverges, which means that there is no stationary state in the low temperature phase $\beta \geq 1$, i.e. $T \leq T_c = 1$.

9. We recall that the average trapping time $\overline{\tau}(E)$ within a well of depth E is given by $\overline{\tau}(E) = e^{\beta E}$ (here the average has to be understood as an average over different realizations of the Markov dynamics defined by Eq. (1) for a fixed realisation of the depths E_α). The probability distribution of $\overline{\tau}$ can be simply obtained by writing $p(\overline{\tau}){\rm d}\overline{\tau} = \rho(E){\rm d}E$ which leads to

$$p(\overline{\tau}) = \frac{1}{\beta}\frac{1}{\overline{\tau}^{1+\frac{1}{\beta}}} \; , \; \overline{\tau} \in [1, +\infty) \; . \tag{17}$$

This distribution in Eq. (17) shows that at high temperature $\beta < 1$, $p(\overline{\tau})$ decays sufficiently fast such that at least the first moment of $p(\overline{\tau})$ exists (and possibly higher moments if β is sufficiently small). On the other hand, at low temperature $\beta \geq 1$ the distribution $p(\tau)$ has a very heavy tail such that the average trapping time is infinite, which means physically that the particle stays trapped in the same (deep) well for very long times.

10. For $\beta < 1$, in the limit $t_{\rm w} \to \infty$, $P(E, t_{\rm w}) \to \widehat{P}_{\rm st}(E) = (1-\beta)e^{-(1-\beta)E}$. Hence, substituting $P(E, t_{\rm w})$ by its stationary value in Eq. (15) one obtains

$$\begin{aligned} \lim_{t_{\rm w}\to\infty} C(t_{\rm w}+t, t_{\rm w}) = C_{\rm st}(t) &= \int_0^\infty (1-\beta)e^{-(1-\beta)E}\, e^{-t\,e^{-\beta E}}{\rm d}E \\ &= \frac{1-\beta}{\beta}\frac{1}{t^{\frac{1}{\beta}-1}}\int_0^t v^{\frac{1}{\beta}-2}e^{-v}\,{\rm d}v \; , \end{aligned} \tag{18}$$

where, in the last line, we have performed the change of variable $v = t\,e^{-\beta E}$. Note that the integral over v in Eq. (18) is well defined for $\beta < 1$ since the integrand behaves as $v^{\frac{1}{\beta}-2}$ as $v \to 0$, which is integrable for $v \to 0$. On the other hand, this integral over v is well defined as $t \to \infty$ (due to the exponential factor), which implies that $C_{\rm st}(t)$ decays to zero, for large t, as

$$C_{\rm st}(t) \underset{t\to\infty}{\sim} \Gamma(\beta)\frac{1}{t^{\frac{1}{\beta}-1}} \; , \tag{19}$$

where we have used $\int_0^\infty v^{1/\beta-2}e^{-v}{\rm d}v = \Gamma(1/\beta-1)$ with $\Gamma(z)$ the gamma function, together with the functional identity $z\Gamma(z) = \Gamma(z+1)$.

11a. Let us denote by $\tau_1, \tau_2, \cdots, \tau_n$ the times spent in the n wells visited by the particle up to time t, such that $\tau_1 + \tau_2 + \cdots + \tau_n = t$. Since the τ_i's are i.i.d. random variables drawn from the heavy tailed distribution in Eq. (17), $p(\overline{\tau}) \propto \overline{\tau}^{-1-\alpha}$ for $\overline{\tau} \geq 1$ with $\alpha = 1/\beta < 1$, from the first lecture and TD, we have

$$S_n = \tau_1 + \tau_2 + \cdots \tau_n = \mathcal{O}(n^{1/\alpha}) \tag{20}$$

$$\tau_{\rm max} = \max\{\tau_1, \tau_2, \cdots, \tau_n\} = \mathcal{O}(n^{1/\alpha}) \; . \tag{21}$$

Hence, $\tau_{\rm max} \sim n^\beta \sim t$ and if we define $E_{\rm max}$ such that $e^{\beta E_{\rm max}} = \tau_{\rm max}$ this means that

$$E_{\rm max} \sim (\log t)/\beta \sim \log n \; , \tag{22}$$

which shows that, as time goes on, the particle finds deeper and deeper wells and that is why the dynamics never reaches a stationary state.

11b. Under the assumption that $P(E,t)$ reaches a stationary solution in terms of the variable $e^{\beta E}/t$, it is natural to perform the change of variable $E \to u = e^{\beta E}/t_{\mathrm{w}}$ in Eq. (15) such that $P(E,t_{\mathrm{w}})\mathrm{d}E = \phi(u)\mathrm{d}u$ – with $\phi(u)$ being independent of time. This yields, taking the limit $t, t_{\mathrm{w}} \to \infty$ but keeping the ratio $\theta = t/t_{\mathrm{w}}$ fixed

$$\lim_{t_{\mathrm{w}}\to\infty} C(t_{\mathrm{w}} + \theta t_{\mathrm{w}}, t_{\mathrm{w}}) = C_{\mathrm{ag}}(\theta) \; , \qquad C_{\mathrm{ag}}(\theta) = \int_0^\infty \phi(u) e^{-\frac{\theta}{u}} \mathrm{d}u \; . \tag{23}$$

This dependence of the correlation function on t/t_{w} is characteristic of the *aging* regime – in contrast to the *stationary* regime where it depends only on t, see Eq. (18).