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A single saddle model for the β-relaxation in supercooled liquids

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Abstract

We analyse the relaxational dynamics of a system close to a saddle of the potential energy function, within an harmonic approximation. Our main aim is to relate the topological properties of the saddle, as encoded in its spectrum, to the dynamical behaviour of the system. In the context of the potential energy landscape approach, this represents a first formal step to investigate the belief that the dynamical slowing down at T_c is related to the vanishing of the number of negative modes found at the typical saddle point. In our analysis we keep the description as general as possible, using the spectrum of the saddle as an input. We prove the existence of a timescale t_ϵ, which is uniquely determined by the spectrum, but is not simply related to the fraction of negative eigenvalues. The mean square displacement develops a plateau of length t_ϵ, such that a two-step relaxation is obtained if t_ϵ diverges at T_c. We analyse different spectral shapes and outline the conditions under which the mean square displacement exhibits a dynamical scaling identical to the β-relaxation regime of mode coupling theory, with a power-law approach to the plateau and power-law divergence of t_ϵ at T_c.

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1. Introduction

In recent years much attention has been devoted in the field of glass-forming liquids to the so-called 'energy landscape' paradigm. The main background of this approach is the existence of a strong relation between the topological properties of the potential energy landscape (i.e. the potential energy as a function of the system's coordinates) and the dynamical behaviour of the system.

Historically this idea goes back to Goldstein [1], who, in 1969, argued how at low enough temperatures supercooled liquids spend a long time in local minima of the potential energy, with rare activated jumps among minima [2–4]. According to Goldstein this low-T description breaks down at a temperature T_c above which activation is no longer the main mechanism of diffusion. This temperature T_c has been subsequently identified with the critical temperature where idealized mode coupling theory (MCT) locates a divergence of the relaxation time [5–7], supporting the view that T_c marks a crossover from a low-T activated hopping dynamics, to a continuous flow dynamics at higher T, which is well described by MCT [8–12].

According to this interpretation, from a topological point of view, it is clear that at low temperature the crucial role is played by the minima of the potential energy function, since the system spends most of the time close to them. This observation can be translated in quantitative terms and various approaches have been elaborated to use information available on the minima and their structure, to compute (thermo)dynamical quantities [2, 13, 14, 17].

On the other hand, above T_c the system is no longer confined around a minimum, but rather 'flows' in configuration space. From a topological point of view one may imagine that the system explores regions of the configuration space which are rich in negative modes. A confirmation of this perspective comes from the instantaneous normal modes (INM) approach [13, 14]: the INM spectrum, i.e. the average density of states of the Hessian matrix of the potential energy, displays above T_c a finite fraction of imaginary modes, indicating that the system at equilibrium explores regions of the landscape which have negative curvature [15–17]. There have been various attempts to use the INM analysis to identify diffusive modes [18–22], but it still remains unclear under what conditions this can be done, and how far the procedure can be pushed.

From a theoretical point of view, a crucial question is whether also above T_c the behaviour of the system can be characterized by well-defined topological entities, as happens at low temperature with minima. This point has been addressed in detail in mean-field disordered systems in the context of spin glasses [24–29], as well as in finite-dimensional ordered models [30]. Given the numerous analogies between the phenomenology of certain spin-glass models and that of structural glasses [31], and exploiting the results achieved in that field, a new topological interpretation of the dynamics above T_c has been developed by various authors. Within this scenario, above T_c it is still possible to describe the behaviour of the system in terms of well-defined topological entities. These are not minima, but rather *saddle points* of the potential energy function, that is stationary points with a non-zero fraction of unstable directions. More precisely, we can summarize this 'saddles interpretation' in a few main points:

- For $T > T_c$ at equilibrium the system is 'close' to a saddle point. The typical topological properties of this saddle point, for example its energy E and the number of unstable directions K, depend on the temperature T.
- Since $K \neq 0$ the system explores a region where negative (non-confining) modes are available. Diffusion can then in principle occur in two different ways: either via barrier hopping along the positive eigenvalues, or exploiting the presence of these free directions (see [34] for a discussion of this point). When $K(T)$ is large this second mechanism will be faster than the first one, and will reasonably prevail. However, upon lowering the temperature $K(T)$ decreases and it will become less and less efficient.
- As the temperature approaches T_c the typical saddles become less unstable, and at T_c they finally cease to have negative modes and turn into minima. Thus, as $T \to T_c$ the system finds fewer and fewer free directions in which to diffuse and the second mechanism of diffusion previously described will freeze. If barriers at T_c are relevant, as numerical simulations indicate for fragile systems [33], this implies a dramatic increase of the relaxation time and a slowing down of the dynamics as T_c is approached. Around T_c a crossover occurs to a different regime where, negative modes being extremely rare, the

main mechanism of diffusion becomes barrier crossing and the Goldstein scenario is thus recovered [34].

This scenario has been tested in different ways and up to now various indications in its favour have been gathered. Numerical experiments on glass forming fragile models [32, 33, 35–40] have shown that it is possible to identify relevant saddles at a given temperature T and classify them through their index $K(T)$. Also, and more importantly, $K(T) \to 0$ as $T \to T_c$, T_c being the mode coupling temperature. Besides, analytical computations in simple models [45] show that the system at equilibrium is truly close to a saddle according to a rigorous well-defined notion of distance in the configuration space. As in numerical experiments, the index of the closest saddle goes to zero as the critical temperature is approached.

Despite these encouraging results the saddle scenario is not immune to some criticisms. The results of numerical simulations [32, 33, 35] highly rely on numerical algorithms to locate the saddles, and the sampling procedure has been deeply questioned (see for example [39]). Also the whole energy landscape approach, even if supported by a great part of the community, has recently received many objections (see for example [41] where a description of the supercooled behaviour in terms of heterogeneities is preferred). Besides, the saddle scenario still remains from a theoretical point of view rather vague and incomplete. In particular, there are several questions which should be addressed, in our opinion, in a more formal and quantitative way:

(i) From an intuitive point of view and in the light of the numerical results, it is reasonable that saddles do play a crucial role in the dynamical behaviour of the system above T_c. However, is this just a useful qualitative interpretation, or can we push this approach further? In other words, is it possible to cast the ‘saddle dynamics’ into a formal description?
(ii) What is the precise relation between the vanishing of negative modes and the increase of the relaxation time as $T \to T_c$? In particular, what is the link between $K(T)$ and the relaxation time τ?
(iii) Is $K(T)$ really the topological quantity most relevant to the dynamics?
(iv) Is a saddle description compatible with mode coupling theory?

In this paper we will address these questions in a formal way by considering a very simple model of harmonic relaxation in a saddle. In our analysis we only assume as starting hypotheses two facts which have been numerically or analytically tested up to now: (1) the system above T_c is close to a saddle point with non-zero index $K(T)$, and (2) the number of negative modes of this saddle goes to zero as $T \to T_c$. The first assumption will enable us to perform an harmonic expansion of the potential energy around a saddle point, while the second will be used as a constraint on the behaviour of the saddle spectrum close to T_c.

Our aim is to find an explicit and quantitative link between the topological properties of the energy landscape and the dynamical behaviour of the system. The input of our model is then the spectrum of the saddle, while our results concern the relation between this spectrum and the relaxation time of the system. We will leave the shape of this spectrum unspecified as long as we can (apart from the above-mentioned constraints) in order to make our statements as general as possible. Only after will we discuss specific cases and their physical relevance. We will then show how even a simple relaxational dynamics is able to provide precise answers to the previous questions, and in certain cases, even approximately reproduce the results of more complicated dynamical theories such as mode coupling.

The paper is organized in the following way. In section 2 we introduce our model and the main quantity to be considered, namely the mean square distance (MSD) (in configuration space) of the system from the typical reference saddle point at temperature $T = (1 + \epsilon)T_c$.

The MSD will be expressed in terms of the topological properties of the saddle, more precisely its spectrum. In section 3 we use the Laplace method to find a relation between the asymptotic dynamical behaviour of the MSD and the spectrum of the saddle point. In section 4 we analyse the consequences of our result, and discuss how the shape of the spectrum may determine qualitatively and quantitatively the long-time dynamics. We look at different classes of spectra and focus on the conditions under which a two-step relaxation with a diverging timescale is obtained. In section 5 we compare our results with the prediction of mode coupling theory. Section 6 is devoted to our conclusions.

2. The harmonic saddle model

Let us consider a glass forming system with N particles and potential energy $V(\mathbf{r})$, where $\mathbf{r} = \{r_i\}$ is the (mass-weighted) vector of the particle positions and $i = 1, \ldots, N$ is a particle index[4]. As explained in the introduction, the stationary points of V are, from a topological point of view, the quantities of interest to describe the behaviour of the system.

At equilibrium in the low-temperature phase $T < T_c$, the system (i.e. its representative point $\underline{r}$) explores for most of the time a region close to a minimum of V, only occasionally jumping via barrier crossing into the basin of another minimum. This separation of timescales between intra and inter basin motion has been exploited by both the INM and the inherent structure [2] approaches to compute dynamic (velocity autocorrelation) and thermodynamic quantities (equilibrium energy, entropy, etc) via a harmonic expansion of the potential energy around a reference configuration. On the other hand, above T_c the system is typically close to a stationary point which is not a minimum, but a saddle with a certain number of negative modes. One can wonder whether also in this case it is possible to use this information to simplify the computations with a reasonable approximation, such as the harmonic one adopted in the low-temperature phase. If the relevant saddles have a large instability index $K(T)$, the system very easily finds escape directions to flow from one region of the phase to another one: even if the closest stationary point will typically be a saddle with the same statistical properties (index, energy, etc), it will not be the *same* saddle even for relatively short times. However, we know from the numerical and analytical works quoted in the introduction that when $T \to T_c$, $K(T) \to 0$, thus close enough to T_c the relevant saddles have a very small instability index. Then, if at some time the system is close to a given saddle it will take a long time before finding one of the few available escape directions and flowing away. In this case the system remains close to the *same* saddle (we could say in its 'basin') for some time, and a harmonic expansion seems justified, at least on timescales shorter than the time when the saddle is definitely left.

Given that, we shall now consider our system at a temperature $T = (1+\epsilon)T_c$ where ϵ is a small parameter, and assume that at time $t = 0$ it is close to a saddle point whose coordinates are r_0 in configuration space. We wish to examine the dynamical behaviour of the system and to do that we resort to a simplified treatment where we use a harmonic expansion of the potential V around r_0. Our starting point is then the following Langevin equation:

$$\dot{x}_i = -\sum_{k=1}^{N} M_{ik} x_k + \xi_i(t) \qquad (1)$$

[4] The particle position r_i is still a vector in three dimensions, i.e. $x_i = \{x_i^a\}$ with $a = 1, \ldots, 3$; however we will indicate it with a roman variable in order to keep the notation simple.

where $x_i(t) = r_i(t) - r_i^0$ are the displacements from the saddle, the matrix M_{ik} is the second derivative of the potential V at the saddle point and ξ is a δ-correlated noise, $\langle \xi_i(t)\xi_k(t')\rangle = 2T\delta_{ik}\delta(t-t')$.[5]

This equation has formally a very simple form of the Ornstein–Ulhenbeck type in $3N$ dimensions. Of course, it is not as trivial as it may seem at first sight in that the matrix M_{ik} is not known. This is not only a consequence of having left the potential V unspecified, since even when an explicit energy function is assumed, still the exact position $\mathbf{r}_0$ of a typical saddle at temperature T is not determinable. This is the glassy nature of the system we are considering: even if the Hamiltonian is deterministic, as the temperature is lowered particles tend to arrange in disordered configurations. Thus M_{ik} has rather to be considered a disordered matrix whose distribution is determined in a complicated way by the equilibrium Boltzmann measure (see e.g. [44, 45]). Thus in the following the Hessian matrix $\mathbf{M}$ will be treated as a random variable whose statistical properties are in principle accessible. In particular, we will express the dynamics in terms of the density of eigenvalues (spectrum) of $\mathbf{M}$:

$$\rho(\lambda; r_0) = \frac{1}{3}N \sum_\alpha \delta(\lambda - \lambda_\alpha) \tag{2}$$

where λ_α are the eigenvalues of M_{ik}. Of course, $\rho(\lambda; r_0)$ also depends on the precise saddle where it is evaluated, and it is thus a stochastic quantity, as is the Hessian. However, its statistical properties are in general more easily computed via numerical simulations [32, 35] or analytical procedures [46, 47, 50] and we have more information on its typical behaviour. For example, we know from previous works that the instability degree of a typical saddle decreases as the critical temperature is approached, which means that the spectrum evaluated in a typical saddle has fewer and fewer negative modes. Consequently, we will assume that the *average* spectrum $\rho(\lambda)$ depends parametrically on $\epsilon \equiv (T - T_c)/T_c$, and that its negative support vanishes for $T \to T_c$, i.e.

$$\rho_\epsilon(0) \to 0 \qquad \text{for} \quad \epsilon \to 0. \tag{3}$$

From equation (1) we can easily compute the mean square displacement (MSD),

$$d_2(t) \equiv \frac{1}{3N}\sum_{i=1}^{N}\sum_{a=1}^{3}\left\langle x_i^a(t)^2\right\rangle = \frac{T}{3N}\sum_{\alpha=1}^{3N}\frac{1-\mathrm{e}^{-2\lambda_\alpha t}}{\lambda_\alpha} = T\int_{-\infty}^{+\infty}\mathrm{d}\lambda\,\rho_\epsilon(\lambda)\frac{1-\mathrm{e}^{-2\lambda t}}{\lambda} \tag{4}$$

where we have only assumed that in the thermodynamic limit fluctuations of the spectrum around its average value are negligible (as indicated by numerical simulations), and we have therefore substituted $\rho(\lambda; r_0)$ with $\rho_\epsilon(\lambda)$. Also, we have considered as initial conditions $x_i(0) = 0$, that is we have assumed the system to start exactly on the top of the saddle. As we shall see, the initial condition is not important as long as the system does not start too far from the saddle (in section 3 we will say exactly how far). Indeed, the additional term arising in equation (4) when $x_i(0) \neq 0$ can be shown in this case to be exponentially small at large times.

This equation is the starting point of our analysis. All the physics is clearly encoded in the behaviour of the spectrum, both in its shape as a function of λ and in its dependence on the temperature. We immediately see that if $\rho_\epsilon(\lambda)$ has some negative support the integral will diverge for $t \to \infty$, meaning that the system asymptotically leaves the saddle if there are some negative eigenvalues, as expected. As already said, since we want our harmonic approximation to be reasonable, we are working in the regime $\epsilon \ll 1$, when the support of $\rho_\epsilon(\lambda)$ is almost entirely positive. In this case the systems remain a long time close to

[5] We assume that the system is at the top of the saddle at $t = 0$, i.e. $x_i(0) = 0\,\forall i$. This will be justified later.

the saddle and we can study what happens in the large time limit, but *before* the saddle is left.

3. The asymptotic dynamics

For mathematical convenience it is better to look at the time derivative of $d_2(t,\epsilon)$,

$$\dot{d}_2(t,\epsilon) = 2T \int_{-\infty}^{+\infty} \mathrm{d}\lambda\, \rho_\epsilon(\lambda)\, \mathrm{e}^{-2\lambda t}. \tag{5}$$

Since the MSD is a well-defined physical quantity at any given time t, this integral should converge for any value of t. Convergence for $\lambda \to -\infty$ requires that

$$\log \rho_\epsilon(\lambda) < 2\lambda t \qquad \text{for} \quad \lambda \to -\infty. \tag{6}$$

If we exclude oscillating functions this implies a concavity condition on $\rho(\lambda)$ (this is obvious graphically): a $\lambda_0(\epsilon)$ must exist such that

$$\frac{\mathrm{d}^2}{\mathrm{d}\lambda^2} \log \rho_\epsilon(\lambda) < 0 \qquad \text{for} \quad \lambda < \lambda_0(\epsilon). \tag{7}$$

The support of the spectrum must be entirely positive for $\epsilon = 0$, and this implies that $\lambda_0(\epsilon) > 0$ for ϵ small enough. We can split the integral in (5) separating the domains $\lambda < \lambda_0$ and $\lambda > \lambda_0$. We have

$$\mathcal{R} \equiv 2T \int_{\lambda_0}^{+\infty} \mathrm{d}\lambda\, \rho_\epsilon(\lambda)\, \mathrm{e}^{-2\lambda t} \leqslant \rho_{\max} \frac{\mathrm{e}^{-2\lambda_0 t}}{t} \tag{8}$$

where $\rho_{\max}$ is the maximum of $\rho_\epsilon(\lambda)$. As we shall see, the remaining part of the integral in $\dot{d}_2(t,\epsilon)$ is much larger than $\mathcal{R}$ for $t \gg 1$. We can thus disregard $\mathcal{R}$ and write

$$\dot{d}_2(t,\epsilon) = 2T \int_{-\infty}^{\lambda_0} \mathrm{d}\lambda\, \rho_\epsilon(\lambda) \exp(-2\lambda t) = 2T \int_{-\infty}^{\lambda_0} \mathrm{d}\lambda \exp(-t S_\epsilon(\lambda, t))$$

with $S_\epsilon(\lambda,t) = 2\lambda - \log \rho_\epsilon(\lambda)/t$. Thus, only the left tail of the spectrum contributes to the behaviour of $\dot{d}_2(t,\epsilon)$.

To evaluate this integral in the regime $t \gg 1$ we can use the Laplace (saddle-point) method [48] to find

$$\dot{d}_2(t,\epsilon) = d_0 T \frac{\exp(-t S_\epsilon(\hat{\lambda}_\epsilon(t), t))}{\sqrt{t S''_\epsilon(\hat{\lambda}_\epsilon(t), t)}} \tag{9}$$

where d_0 is a constant independent of t and ϵ, the prime indicates the derivative with respect to λ and $\hat{\lambda}_\epsilon(t)$ is the solution of the saddle-point equation $S'_\epsilon(\hat{\lambda}_\epsilon, t) = 0$, namely

$$\frac{\rho'_\epsilon(\hat{\lambda}_\epsilon)}{\rho_\epsilon(\hat{\lambda}_\epsilon)} = 2t. \tag{10}$$

From the convergence condition (7) we see that $\rho'_\epsilon(\lambda)/\rho_\epsilon(\lambda)$ is a monotonically decreasing function of λ, and therefore equation (10) has a unique solution $\hat{\lambda}_\epsilon(t)$. Besides, we see that $\hat{\lambda}_\epsilon(t)$ changes sign at a well-defined time: if we define

$$t_\epsilon = \frac{1}{2} \frac{\rho'_\epsilon(0)}{\rho_\epsilon(0)} \tag{11}$$

we have that

$$\hat{\lambda}_\epsilon(t) > 0 \qquad \text{for} \quad t < t_\epsilon \tag{12}$$

$$\hat{\lambda}_\epsilon(t) < 0 \qquad \text{for} \quad t > t_\epsilon. \tag{13}$$

If we interpret the saddle value $\hat{\lambda}(t)$ as the relevant mode at time t, this result translates the intuitive fact that while at short times the system does not realize the presence of escape directions and 'relaxes' in the pseudo-basin around the saddle given by the positive modes, as time increases it finally finds the unstable modes and exploits them to flow away. This argument already tells us that t_ϵ represents a crucial dynamical timescale in our problem. This can be appreciated in a more explicit and quantitative way if we analyse in detail the behaviour of $\dot{d}_2(t, \epsilon)$.

As we show in appendix A, it is possible to rewrite (9) as

$$\dot{d}_2(t, \epsilon) = D_0 T \sqrt{-\dot{\hat{\lambda}}_\epsilon(t)} \exp\left(-2 \int_1^t \mathrm{d}t'\, \hat{\lambda}_\epsilon(t')\right) \tag{14}$$

where D_0 is a constant. This equation shows that the sign of $\hat{\lambda}_\epsilon(t)$ is the key factor determining the asymptotic behaviour of $\dot{d}_2(t, \epsilon)$ and thus, depending on the value of t compared to t_ϵ, we find two time regimes:

- *Early time region* ($1 \ll t < t_\epsilon$). In this regime $\hat{\lambda}_\epsilon(t) > 0$ and thus $\dot{d}_2(t, \epsilon)$ is a decreasing function of t, reaching its minimum at $t = t_\epsilon$. From (14) we see that $\dot{d}_2(t_\epsilon, \epsilon) \to 0$ for $t_\epsilon \to \infty$. This means that if the timescale t_ϵ diverges at T_c, then $d_2(t, \epsilon)$ develops a plateau, whose length is of order t_ϵ.[6] The value of d_2 at the plateau is given by

$$d_p(\epsilon) = T \int_{1/t_\epsilon}^{\infty} \frac{\mathrm{d}\lambda}{\lambda} \rho_\epsilon(\lambda). \tag{15}$$

  The demonstration of this expression is sketched in appendix B. Physically, it is rather intuitive from equation (4) if one remembers that at $t = t_\epsilon$ only positive modes contribute, and makes the additional approximation that those with $\lambda > 1/t_\epsilon$ have reached their asymptotic value, while the rest do not contribute at all. Since the length of the plateau is proportional to t_ϵ, it is clear that the plateau itself is better defined the closer we are to T_c. Note also that for large t_ϵ, the expression for the plateau is just the value of $d_2(t, \epsilon)$ which would be obtained for a strictly positive spectrum by taking the limit $t \to \infty$ in (4). This means that for $1 \ll t < t_\epsilon$ the system 'thermalizes' in the saddle using only the positive eigenvalues, and d_2 reaches the value it would have reached in a purely harmonic well. This justifies our initial condition $x_i(0) = 0$: any other choice with $d_2(t, \epsilon) \leqslant d_p$ would have been the same. The average energy density is given by $E(t) = E_0 + \frac{1}{2} T[1 - \dot{d}_2(t, \epsilon)]$, where E_0 is the bare energy of the saddle. Therefore, at the plateau, that is for $t \sim t_\epsilon$, the corrections to the harmonic thermal energy $T/2$ are small if $t_\epsilon \gg 1$.
- *Late time region* ($t \gg t_\epsilon$). In this regime we have that $\hat{\lambda}_\epsilon(t) < 0$. Now the system has finally found the unstable directions and its dynamics is ruled by the escape from the saddle basin. The integral in the exponential of (14) changes sign at a time τ defined by $\int_1^\tau \mathrm{d}t'\, \hat{\lambda}_\epsilon(t') = 0$. Besides, in appendix C we show that the prefactor in the square root does not go to zero exponentially for $t \to \infty$. Thus, $\dot{d}_2(t, \epsilon) \to \infty$ for $t \gg \tau$, corresponding to $d_2(t, \epsilon)$ leaving the plateau, i.e. to the system leaving the saddle. We could in principle identify τ as an 'escape' time and consider it as a second relevant dynamical timescale. However, as we have stressed in the introduction, our harmonic expansion is meaningful as long as the system remains close to the saddle, therefore it is not clear whether τ has a genuine physical meaning or whether other terms in the potential expansion should already be considered on these timescales.

We stress that these results are valid for a general $\rho_\epsilon(\lambda)$, with minimal requirements on its behaviour dictated by physical consistency. To summarize, the most important result is

[6] For a numerical study of the plateau developed by the MSD in LJ systems close to T_c, see [43].

the existence of a relevant timescale t_ϵ, directly expressed in terms of topological properties of the landscape (the spectrum at the saddle point). This result answers one of the questions discussed in the introduction, namely the relation between a topology and a relaxation time. Contrary to the naive expectation, the relaxation time t_ϵ is *not* naturally related to the fraction of negative eigenvalues $k_\epsilon = \int_{-\infty}^{0} \rho_\epsilon(\lambda)\,\mathrm{d}\lambda$. Rather, if there is a degree of universality in saddle dynamics, the correct scaling variable seems to be $\rho'_\epsilon(0)/\rho_\epsilon(0)$ (see equation (11)). A second general result is that the MSD exhibits a two-step relaxation close to the critical temperature, provided the relevant timescale t_ϵ diverges at T_c. Given the expression for t_ϵ and given that $\rho_\epsilon(0) \to 0$ for $\epsilon \to 0$, it is likely that this is actually the most general scenario for most reasonable spectra shapes (even if there are simple counter-examples, such as the case $\rho_\epsilon(\lambda) = \epsilon f(\lambda)$).

On the other hand, the way the system approaches and leaves the plateau, which is encoded in expression (14), depends on the specific form of $\rho_\epsilon(\lambda)$. Therefore, to extend our analysis further we need at this point to specify the spectrum in some detail. Thus in the next section we shall consider different spectral shapes.

4. Specific spectra

Let us now consider some specific forms for the spectrum $\rho(\lambda)$ and compute explicitly the behaviour of $d_2(t)$. Since we are interested in the asymptotic behaviour we shall specify the spectrum only in the left tail, that is for $\lambda < \lambda_0$.

4.1. Exponential case

Let us consider

$$\rho_\epsilon(\lambda) \sim \rho_\epsilon(0)\exp(a\lambda) \tag{16}$$

where $\lim_{\epsilon\to 0}\rho_\epsilon(0) = 0$ in order to ensure a positive definite spectrum at T_c. This spectrum is of the form $\rho_\epsilon(\lambda) = \epsilon f(\lambda)$ and, as noted in the previous section, it has a non-diverging timescale $t_\epsilon = a/2$. Besides, from expression (4) we see that $d_2(t)$ diverges at a finite time $t = t_\epsilon$. Equation (5) can be easily integrated and we get

$$\dot{d}_2(t,\epsilon) \sim 2T\rho_\epsilon(0)\,\mathrm{erfc}(\lambda_0(a-2t)) + \mathcal{R}. \tag{17}$$

Therefore in this case we do not get any diverging timescale as a function of ϵ nor a two-step dynamics. Rather what happens is that $d_2(t,\epsilon)$ diverges at the same time for any temperature above T_c, but in a steeper and steeper way as T_c is approached.

4.2. The Gaussian case

The Gaussian tail is less trivial. In this case we consider

$$\rho_\epsilon(\lambda) \sim \exp\left(-\frac{b}{2}(\lambda - \bar{\lambda}_\epsilon)^2\right) \tag{18}$$

with $\lim_{\epsilon\to 0}\bar{\lambda}_\epsilon^{-1} = 0$. By applying the Laplace method we find $\hat{\lambda}_\epsilon(t) = \bar{\lambda}_\epsilon - 2t/b$ and $t_\epsilon = b\bar{\lambda}_\epsilon/2$. Then $\dot{d}_2$ is given by

$$\dot{d}_2(t,\epsilon) \sim D_0 T \exp\left[\frac{2t^2}{b} - 2\bar{\lambda}_\epsilon t\right] \tag{19}$$

and

$$d_2(t,\epsilon) \sim d_p(\epsilon) + D_0 T \exp(\bar{\lambda}_\epsilon t_\epsilon)\int_0^{t-t_\epsilon} \exp\left(\frac{2\tau^2}{b}\right)\mathrm{d}\tau. \tag{20}$$

(The same expressions can of course be obtained by exactly solving the Gaussian integral equation (5).) Therefore for a Gaussian tail we get a two-step dynamics with a plateau and a diverging timescale. The plateau is approached exponentially, as we see from equation (20).

4.3. The power-law case

This is actually the most interesting case, since it gives predictions compatible with MCT. Besides, the *p*-spin spherical model which has been widely used as a mean-field description of glassy physics and exactly obeys MCT equations, has a spectrum belonging to this class (see section 5.3).

Let us consider

$$\rho_\epsilon(\lambda) = (\epsilon^\mu + \lambda)^\eta \tag{21}$$

with $\mu\eta > 0$, such that $\rho_\epsilon(0) = \epsilon^{\mu\eta} \to 0$, for $\epsilon \to 0$. From equation (10) we have $\hat{\lambda}_\epsilon(t) = -\epsilon^\mu + \eta/2t$, while equation (14) gives

$$\dot{d}_2(t, \epsilon) = D_0 T \frac{\exp(2\epsilon^\mu t)}{t^{\eta+1}}. \tag{22}$$

By integrating from t_ϵ (given by (11)) up to t, we find

$$d_2(t, \epsilon) = d_p(\epsilon) + \epsilon^{\mu\eta} h(t/t_\epsilon) \qquad t_\epsilon = \frac{\eta}{2}\epsilon^{-\mu} \tag{23}$$

where $h(x)$ is a scaling function obtained by the expansion of the exponential in (22). The approach to the plateau can be found by noting that for $x \ll 1$ we have $h(x) \sim -1/x^\eta$, and thus

$$d_2(t, \epsilon) - d_p(\epsilon) \sim -t^{-\eta}. \tag{24}$$

These three general shapes of the spectrum give rise to different dynamical behaviour. In particular, only a power spectrum gives rise to a diverging timescale *and* a power-law approach to the plateau. This fact is particularly important when comparing the predictions of this simple model with those of the MCT, as we shall do in the next section.

To conclude, we note that a useful quantity to characterize the approach to the plateau is the time-dependent effective exponent [49],

$$\nu_{\mathrm{eff}}(t, \epsilon) = 1 + \frac{\mathrm{d}\log \dot{d}_2(t, \epsilon)}{\mathrm{d}\log t} = 1 + \frac{t}{2}\frac{\ddot{\hat{\lambda}}_\epsilon(t)}{\dot{\hat{\lambda}}_\epsilon(t)} - 2t\hat{\lambda}_\epsilon(t).$$

If in some time regime the MSD has a power-law dependence on time, $d_2(t, \epsilon) = d_p \pm t^\nu$, this must show up as a constant contribution to the effective exponent in some extended region of time, that is $\nu_{\mathrm{eff}}(t) = \nu$. If we apply this definition to the previous cases, we see easily that the only one exhibiting a constant region for $\nu_{\mathrm{eff}}(t)$ is the third one (see figure 1), for which we find $\nu_{\mathrm{eff}}(t) = -\eta(1 - t/t_\epsilon)$.

5. Comparison with MCT

Mode coupling theory (MCT) [5–7] is a dynamical approach which has been widely tested on a wide range of glass forming systems. It is not an exact theory, in that it makes some assumptions on the memory functions entering the exact dynamical equations, but it deals with the complete dynamics of the system and takes into account in detail its structural properties. For structural fragile glasses it is now commonly accepted that MCT represents an excellent description of the supercooled liquid system for $T \geqslant T_c$ (see e.g. [43]).

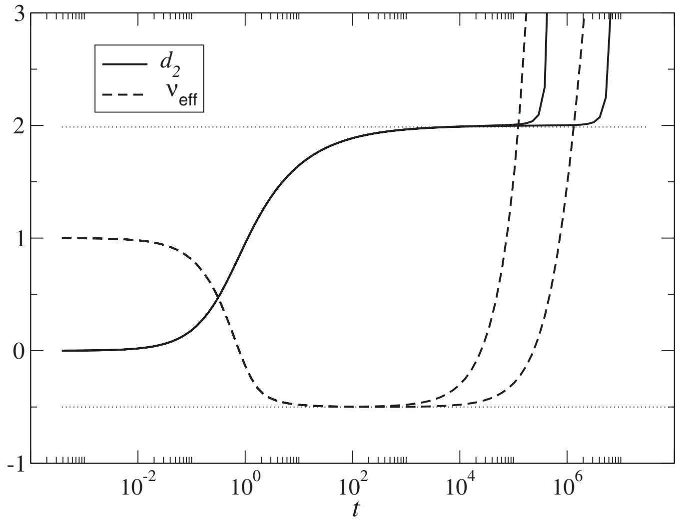

Figure 1. The MSD (continuous line) and effective exponent (dashed line) for a power-law spectrum with $\eta = 1/2$ and $\mu = 1$, for $\epsilon = 10^{-5}$ and $\epsilon = 10^{-6}$. Dotted lines indicate the plateau of d_2 from equation (15), and the plateau of ν_{eff}.

Our single saddle model is, on the other hand, a much more simplified approach and we cannot expect it to reproduce the whole set of MCT results. However, if we believe that close to T_c the main mechanism driving the dynamical slowing down is the vanishing of the negative modes available to the system, our model should describe reasonably the behaviour of the system in this temperature range and should therefore reproduce at least the main MCT predictions.

5.1. MCT predictions

The MCT predicts the existence of a critical temperature T_c where the relaxation time of the system diverges. In real systems a real dynamical transition is not observed, however T_c still represents a well-defined relevant temperature where a slowing down of the dynamics takes place and a clear crossover to a different dynamical regime arrives.

A general prediction of MCT is the presence, as T approaches T_c from above, of a two-step relaxation of the relevant dynamical quantities, such as correlation, response functions and the MSD. More than this, MCT provides detailed predictions about the approach and escape from the plateau and the final relaxation to the equilibrium asymptotic value. It distinguishes two dynamical regimes, both of which become critical at the transition: the so-called β-relaxation regime, which concerns the dynamics around the plateau, and the α-relaxation regime, which is related to structural relaxation to the ergodic values. Here, we will be concerned with the β-relaxation, since, as already underlined, our model is a reasonable approximation only until the plateau is left.

According to MCT, in the β-relaxation regime the correlation function $C(t)$ has the following scaling form (as usual $t \gg 1$),

$$C(t) = C_p + \epsilon^{1/2} g(t/t_\epsilon) \qquad t_\epsilon = \epsilon^{-1/2a}. \tag{25}$$

The correlation function has a plateau C_p of length t_ϵ, and t_ϵ diverges as a power law for $\epsilon \to 0$. Moreover, MCT predicts a power-law approach to the plateau (early β regime), that is,

$$C(t) - C_p \sim t^{-a} \qquad 1 \ll t \ll t_\epsilon \tag{26}$$

whereas for times larger than t_ϵ the correlation function leaves the plateau as (late β regime)

$$C(t) - C_p \sim -(t/t_0)^b \qquad t_\epsilon < t \ll \tau \tag{27}$$

where $t_0 = \epsilon^{-(a+b)/2ab}$, and τ is the α-relaxation time.

For the supercooled system studied in [43] the value of the exponent a is $a = 0.28$.

5.2. *Some general requirements*

Among the spectral shapes we have considered, only the power case gives a scaling compatible with MCT. Looking at equations (23) and (24), we conclude that the dynamical scaling of MCT is reproduced by spectra of the form

$$\rho_\epsilon(\lambda) = (\epsilon^\mu + \lambda)^\eta \qquad \mu\eta = \tfrac{1}{2} \tag{28}$$

the predicted dynamical exponent being $\alpha = \eta$.

Equation (28) also implies a simple condition on the behaviour of the spectrum in $\lambda = 0$: only spectra that behave as

$$\rho_\epsilon(0) \sim \epsilon^{1/2} \tag{29}$$

are compatible with MCT. This seems to be quite a strong topological requirement, very easy to check in specific cases.

Finally, we note that the important point is that the power-law behaviour is obeyed in the main range of the negative support as T_c is approached. The presence of small correcting tails around the lower band edge $\lambda = -\epsilon^\mu$ is not important if they arise in a vanishing (as $\epsilon \to 0$) region. Indeed, let us imagine that the power-law behaviour (28) holds down to a certain value $\bar{\lambda} > -\epsilon^\mu$. It is simple to show that the dynamical behaviour predicted by a power-law spectrum still holds up to timescales $t \sim \bar{t}$ with $\bar{t} = \rho'_\epsilon(\bar{\lambda})/2\rho_\epsilon(\bar{\lambda})$, while for greater times the tail effect starts dominating. Therefore if $t_\epsilon/\bar{t} = (\epsilon^\mu + \bar{\lambda})/\epsilon^\mu$ vanishes as $\epsilon \to 0$, the dynamical scaling still holds in a diverging time window. In finite-dimensional systems one usually gets small tails in the spectrum where localized modes are concentrated. The previous observation suggests that for a supercooled liquid, where we may expect small tails to smoothen the spectrum close to the lower band edge, only the extended modes representing the main negative support are truly relevant for diffusion.

5.3. *The p-spin spherical model*

To perform a real comparison between MCT and our simplified harmonic model we need to consider specific cases. In particular, an excellent test would be a system where both approaches can be fully applied. That is, we need a model where (i) the MCT dynamical phenomenology is reproduced and (ii) information on the local topology is analytically available.

The p-spin spherical model (PSM) [49] satisfies both these requirements. Indeed, it can be shown that the *exact* dynamical equations for this model have a MCT structure [51], that is for the PSM the MCT is *exact* (in contrast to structural glasses where it represents an approximation). Besides, for this model saddles have been shown analytically to play a relevant role [44] and the spectrum of a typical saddle at temperature $T = (1+\epsilon)T_c$ is exactly known [52, 53]. Its left tail is

$$\rho_\epsilon(\lambda) = (\epsilon + \lambda)^{1/2}. \tag{30}$$

Since in the PSM[7] $d_2(t) = 2[1 - C(t)]$, the MCT scaling forms of equations (25)–(27) directly apply also to the mean-square displacement. The exact resolution of the dynamical MCT equations for $C(t)$ can be found in [49] and gives $a_{\rm PSM} \sim 0.4$.

On the other hand the behaviour predicted by our harmonic model can be simply inferred by the results of the previous subsection with $\mu = 1$ and $\eta = 1/2$. We get

$$d_2(t,\epsilon) = d_p(\epsilon) \sim +\epsilon^{1/2} h(t/t_\epsilon) \qquad t_\epsilon = \frac{1}{4\epsilon} \tag{31}$$

and a power-law approach to the plateau:

$$d_2(t,\epsilon) - d_p(\epsilon) \sim -t^{-1/2}. \tag{32}$$

This behaviour is consistent with a MCT scaling form with an exponent $a = 1/2$, to be compared with the exact value $a_{\rm PSM} \sim 0.4$. Our conclusion is then that for the PSM the single saddle model correctly reproduces the general dynamical scaling of the complete MCT dynamics and the power-law approach to the plateau of the early β regime. The power-law approach to the plateau can also be seen by setting $t \ll t_\epsilon$ in the effective exponent. This gives $\nu_{\rm eff}(t,\epsilon) = -1/2(1 - t/t_\epsilon)$. From this expression we see that for $t > t_\epsilon$ the model gives no power-law departure from the plateau (see figure 1)[8]. This must not be regarded as significant since the model itself loses validity at large times (for this reason we have only focused on the early β regime).

Unfortunately, our model does not exactly reproduce the exponent a (or, in other terms, it does not give the correct form of the scaling function $g(x)$ (25), which is responsible for the value of the exponent a). Of course, this leaves us partly unsatisfied. However, it is known that anharmonicities are very strong in the PSM, and it is reasonable that they are already relevant close to the saddle. If this is the case one should be able to show that taking into account anharmonicities, for example via a perturbative approach, modifies the exponent in the correct direction. We are now working in this direction.

6. Conclusions

In this paper we have analysed a simple model of relaxational dynamics around an harmonic saddle. The physical problem we wanted to address was the description of supercooled liquids close to the crossover temperature T_c, and our main purpose was to model in a formal way the connection between topological properties of the potential energy and dynamical behaviour which is at the basis of the energy landscape approach.

Despite the extreme simplicity of our model and the generality of our assumptions our results are not trivial. We have obtained a general expression which relates the spectrum of the saddle and a relevant timescale, and we have outlined the conditions under which such a timescale diverges giving rise to a two-step dynamics with a well defined plateau at T_c. This timescale is related to unstable modes, however it is not proportional to the instability index, as naive expectation would have suggested. Rather, it is related to the behaviour of the spectrum close to zero: since negative modes tend to disappear as T_c is approached it is the way they turn into soft modes that determines the long time dynamics.

[7] In the PSM we have simply $d_2(t) = 2[1 - C(t)]$.

[8] In fact, the effective exponent in the PSM shows that even for $t_\epsilon \gg 1$ there is no extended time region where $\nu_{\rm eff} = b$ (figure 6 of [49]), and thus the departure from the plateau is not really power law in the PSM.

The precise way the system relaxes to the plateau depends on the shape of the saddle spectrum. We have analysed different spectral shapes and have shown that power-law spectra give rise to the same dynamical scaling as the one predicted by MCT in the β-regime. For this kind of spectra then our model seems to be consistent with MCT.

Beside these general qualitative predictions we have also looked at the specific case of the p-spherical model, where both the spectrum and the dynamics can be analytically computed. Here the saddle model reproduces the dynamical scaling predicted by the MCT, which is in this case exact. The p-spin spherical model is interesting because it represents a concrete model where the two approaches, MCT and single-saddle relaxation, can be independently performed and ultimately compared. Our analysis indicates that, despite its brutal disregard of anharmonic contributions, the single saddle model already reproduces the main features of the complete exact dynamics, namely the dynamical scaling and power-law approach to the plateau. Our interpretation of this result has been sketched in the introduction: the presence of the plateau and the slowing down of the dynamics described by the MCT equations are mainly due to the vanishing of the negative modes close to the transition temperature T_c, and these effects are already taken into account at the harmonic level in the single saddle model. In the PSM we have explicitly demonstrated this, however we expect the same to hold whenever MCT is a good description of the problem, as for structural fragile glasses. To support this conclusion we should in principle proceed as we did for the PSM: compute the dynamical quantities using the single saddle model and compare them with the MCT predictions. The problem is that, in contrast to the p-spin case, the spectrum of a typical saddle is not in general known for models of glass forming systems. We may expect that numerical simulations or analytic computations will provide this topological information and our analysis be completed in the future. On the other hand, there is something important we have already done at this stage: we have outlined under what general conditions for $\rho(\lambda)$ our single saddle model is compatible with the MCT predictions. If the spectra of real glass systems turn out to satisfy these conditions we will then have very strong support for our arguments.

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Appendix A. Computation of the MSD

Here we show how to derive expression (14) for the MSD. For convenience we omit in the following the sub-index ϵ. We recall that the dot indicates a derivative with respect to time, while the prime indicates a derivative with respect to λ. Let us call $N(t) = \exp(-tS(\hat{\lambda}))$. By deriving $N(t)$ with respect to time, the numerator of equation (9) and using the saddle-point equation (10) we obtain

$$\dot{N}(t) = -2\hat{\lambda}(t)N(t) \tag{A1}$$

and thus

$$N(t) = N(t_0)\exp\left(-2\int_{t_0}^{t} \mathrm{d}t'\,\hat{\lambda}(t')\right). \tag{A2}$$

Concerning the denominator of (9), we have to evaluate

$$tS''(\hat{\lambda}) = \left(\frac{\rho'^2}{\rho^2} - \frac{\rho''}{\rho}\right) = t^2 - \frac{\rho''(\hat{\lambda})}{\rho(\hat{\lambda})} \tag{A3}$$

where we have used again the saddle-point equation. We define $f(t) = \rho(\hat{\lambda}(t))$. Derivatives of $f(t)$ with respect to time give

$$\dot{f}(t) = t\dot{\hat{\lambda}} f(t) \tag{A4}$$

$$\frac{1}{f(t)}\ddot{f}(t) = \frac{\rho''(\hat{\lambda})}{\rho(\hat{\lambda})}\dot{\hat{\lambda}}^2 + t\ddot{\hat{\lambda}} \tag{A5}$$

$$\frac{1}{f(t)}\ddot{f}(t) = \dot{\hat{\lambda}} + t\ddot{\hat{\lambda}} + t^2\dot{\hat{\lambda}}^2. \tag{A6}$$

Putting together these relations we have

$$tS''(\hat{\lambda}) = -\frac{1}{\dot{\hat{\lambda}}}. \tag{A7}$$

So finally equation (9) becomes

$$\dot{d}_2(t,\epsilon) = d_0\sqrt{-\dot{\hat{\lambda}}(t)}\exp\left(-2\int_1^t \mathrm{d}t'\,\hat{\lambda}(t')\right) \qquad t \gg 1 \tag{A8}$$

where we have fixed $t_0 = 1$ for convenience, and $d_0 = N(1)$.

We recall that this formula is valid for $t \gg 1$, and on the assumption that the integral for $\lambda > \lambda_0$ is sub-dominant. We can see from (4) that this is actually true. Indeed, since the saddle-point solution $\hat{\lambda}$ is a decreasing function of time, it will surely become smaller than λ_0, for t large enough, therefore

$$\int_1^t \mathrm{d}t'\,\hat{\lambda}(t') \ll \lambda_0 t \tag{A9}$$

at large times and $\mathcal{R}(t)$ is exponentially sub-dominant with respect to (A8).

Appendix B. The plateau of the MSD

We now want to determine the value of the plateau. First, we need to appropriately define what we mean by plateau. We have seen that $\dot{d}_2(t)$ has a minimum for $t \sim t_\epsilon$. This means that $d_2(t_\epsilon)$ is as close as possible to the limiting value where $d_2(t)$ would go if there were no negative eigenvalues. Thus, we may define an effective plateau for $\epsilon \neq 0$ (but very small) as

$$q_\epsilon = d_2(t_\epsilon). \tag{B1}$$

In this way, for $\epsilon \to 0$ q_ϵ approaches a well-defined value $q(T_c)$ related to relaxation in a harmonic well. We now show that

$$q_\epsilon = \int_{1/t_\epsilon}^{\infty} \frac{\rho(\lambda)}{\lambda} + O\left[\rho(1/t_\epsilon)\right] + O[\rho(-1/t_\epsilon)] \tag{B2}$$

and thus

$$q_\epsilon \to q(T_c) = \int_0^\infty \frac{\rho(\lambda)}{\lambda} \qquad \text{for} \quad \epsilon \to 0 \tag{B3}$$

as expected. To prove (B2) we proceed as follows. We split $d_2(t)$ into different parts

$$\begin{aligned} d_2(t) = \int_{-\infty}^{\infty}\mathrm{d}\lambda\,\rho(\lambda)\frac{1-\mathrm{e}^{-2\lambda t}}{\lambda} &\equiv A + B + C + D + E + F \\ = \int_{1/t_\epsilon}^{\infty}\frac{\rho(\lambda)}{\lambda}\,\mathrm{d}\lambda - \int_{1/t_\epsilon}^{\infty}\frac{\rho(\lambda)\,\mathrm{e}^{-2\lambda t}}{\lambda}\,\mathrm{d}\lambda &+ \int_0^{1/t_\epsilon}\rho(\lambda)\frac{1-\mathrm{e}^{-2\lambda t}}{\lambda}\,\mathrm{d}\lambda \\ + \int_{-\infty}^{-1/t_\epsilon}\frac{\rho(\lambda)}{\lambda}\,\mathrm{d}\lambda - \int_{-\infty}^{-1/t_\epsilon}\frac{\rho(\lambda)\,\mathrm{e}^{-\lambda t}}{\lambda}\,\mathrm{d}\lambda &+ \int_{-1/t_\epsilon}^{0}\rho(\lambda)\frac{1-\mathrm{e}^{-2\lambda t}}{\lambda}\,\mathrm{d}\lambda \end{aligned} \tag{B4}$$

and evaluate the different integrals. By using the saddle-point method for $t > t_\epsilon$ we find

$$B \sim -\frac{t}{t_\epsilon}\rho(1/t_\epsilon)\,\mathrm{e}^{-2t/t_\epsilon} \qquad \Longrightarrow \qquad B \sim \rho(1/t_\epsilon) \qquad \text{for} \quad t \sim t_\epsilon. \tag{B5}$$

C is easy:

$$C \leqslant \rho(1/t_\epsilon)\int_0^{t/t_\epsilon} \mathrm{d}x\,\frac{1-\mathrm{e}^{-2x}}{x} \qquad \Longrightarrow \qquad C \sim c\rho(1/t_\epsilon) \qquad \text{for} \quad t \sim t_\epsilon \tag{B6}$$

where c is a constant prefactor. To evaluate D we note that to ensure the convergence of $d_2(t)$ the function $f(\lambda) = \rho(\lambda)\,\mathrm{e}^{-2\lambda t}$ should go to zero for $\lambda \to -\infty$. We can thus estimate D with the saddle-point method:

$$D = \int_{-\infty}^{-1/t_\epsilon} f(\lambda)\frac{\mathrm{e}^{2\lambda t}}{\lambda}\,\mathrm{d}\lambda \sim \frac{t_\epsilon}{t} f(-1/t_\epsilon)\,\mathrm{e}^{-2t/t_\epsilon}$$
$$\Longrightarrow \qquad D \sim \rho(-1/t_\epsilon) \qquad \text{for} \quad t \sim t_\epsilon. \tag{B7}$$

The integral E is trickier. Once again we use the saddle-point method. The procedure is the same as the one used for $\dot{d}_2(t)$. Since the factor $1/\lambda$ is algebraic it can be discarded in the evaluation of the maximum so that the maximum of the integrand still occurs for a value $\hat{\lambda}(t)$ as given by equation (10). But, by definition, $\hat{\lambda}(t_\epsilon) = 0$. So for t close enough to t_ϵ the real maximum lies outside the integration range and the integral is dominated by the upper integration limit. Thus we have

$$E \sim \frac{-t_\epsilon}{-t + \rho'(-1/t_\epsilon)/\rho(-1/t_\epsilon)}\,\mathrm{e}^{2t/t_\epsilon}\rho(-1/t_\epsilon) \qquad \Longrightarrow \qquad E \sim \rho(-1/t_\epsilon) \qquad \text{for} \quad t \sim t_\epsilon. \tag{B8}$$

Finally, exactly as for C we have

$$F \leqslant \rho(-1/t_\epsilon)\int_{-t/t_\epsilon}^{0} \mathrm{d}x\,\frac{1-\mathrm{e}^{-x}}{x} \qquad \Longrightarrow \qquad F \sim \rho(-1/t_\epsilon) \qquad \text{for} \quad t \sim t_\epsilon. \tag{B9}$$

Appendix C. The prefactor of equation (14)

We now argue that the prefactor of the square root of equation (14) does not go to zero exponentially for $t \to \infty$, at least for physical spectra shapes. Let us suppose that for $t \to \infty$ we have

$$-\dot{\hat{\lambda}}(t) \leqslant A\,\mathrm{e}^{-at}. \tag{C1}$$

This implies that

$$\hat{\lambda}(t) \to \lambda_\infty \qquad t \to \infty \tag{C2}$$

that is, if we define $g(\lambda) = \rho'(\lambda)/2\rho(\lambda)$,

$$g(\lambda) \to \infty \qquad \lambda \to \lambda_\infty \tag{C3}$$

with $\lambda_\infty < 0$. This is what happens when ρ has a cut in the left tail (semicircle). Condition (C1) implies (we integrate between t and ∞)

$$\hat{\lambda}(t) \leqslant \lambda_\infty + A/a\,\mathrm{e}^{-at}. \tag{C4}$$

Given that $g(\lambda)$ is a decreasing function of λ, using the saddle-point equation we find

$$2t = g(\hat{\lambda}) \geqslant g\left(\lambda_\infty + A/a\,\mathrm{e}^{-at}\right). \tag{C5}$$

Calling $x \equiv \lambda_\infty + A/a\, e^{-at}$, and for $x \sim \lambda_\infty$, this relation gives

$$g(x) \leqslant -\frac{1}{a}\log(x-\lambda_\infty). \qquad \text{(C6)}$$

If we now recall that $g(x) = \rho'(x)/\rho(x)$, and integrate between λ and 0 and take the limit $\lambda \to \lambda_\infty$, we find

$$\rho(\lambda_\infty) > 0. \qquad \text{(C7)}$$

Thus, if equation (C1) holds, the spectrum must be nonzero at the left cut (the converse is not true). Therefore, if we discard this unphysical case, we are sure that for $t \to \infty$ the Gaussian fluctuations do not go to zero exponentially. It is possible that for spectra of the kind we exclude, the exponential factor increases faster than a simple exponential and therefore still kills the prefactor contribution, but we have not been able to prove under what conditions this happens.

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