

LETTER TO THE EDITOR

Entropy barriers and slow relaxation in some random walk models

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Abstract. We study the zero temperature limit of a simple model of slow relaxation without energy barriers, recently proposed by Ritort, as well as two other closely related models with a much faster relaxation. These models can be mapped onto random walk problems, which allows for their analytic study. We analyse, in particular, a specific aspect of the former model, namely the existence of a bias leading to 'entropy barriers' and to a very slow relaxation.

The study of off-equilibrium dynamics, characteristic of the glassy state, has recently seen an upsurge of interest [1–6]. A very widespread phenomenon in this context is the existence of a slow relaxation together with an aging effect, where the correlation function of the system at two times t, t' becomes approximately a function of t'/t , instead of the usual equilibrium, time-translation invariant, behaviour in $t - t'$. Recent works have made it clear that this phenomenon may be present in a variety of physical situations, for example, domain growth or spin-glass dynamics.

One simple mechanism for slow relaxation and aging, recently put forward (among several others [5–8]), is the existence of entropy barriers [9, 10]. This term characterizes a situation where the system becomes trapped in some regions of phase space without energy barriers: some paths out of these regions without any energy cost exist, but they are rare and difficult to find. It has been shown in [10] that the low-temperature evolution of such systems can become very slow and show an aging effect, because the number of accessible escape paths decreases with energy, and therefore it decreases when time increases. In general, one may expect that both entropy and energy barriers to be present. It is, however, interesting to consider a model where only entropy barriers are present.

The first explicit example of such a model was recently proposed by Ritort [9]. One considers N distinguishable particles distributed among M boxes. The energy is defined as minus the number of empty boxes (the dynamics of this model at zero temperature will be defined in more detail below, where it is called model A). While the ground state can always be found without encountering any energy barrier (i.e. without having to put a particle into an empty box), the simulations in [9] clearly show a slowing down of the dynamics together with hysteresis and aging effects.

In this note we study model A, together with two closely related models (called B and C). We show that these models may be mapped onto random walk problems. We concentrate on the relaxation of the energy and point out the mechanism leading to the slow

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relaxation in model A. We identify the bias in the random walk describing model A as being responsible for the existence of entropy barriers. In a continuum version of this model the entropy barriers are due to an effective potential in the associated Fokker–Planck equation. We also discuss the origin of the quantitative discrepancy between this continuum model and the original discrete model A. In a very recent paper, Franz and Ritort [11] give an adiabatic approximate solution of model A, using different methods (see below).

The three models we shall study are:

Model A. Consider N distinguishable particles. At zero time these particles are distributed amongst M boxes. At each time step a particle is chosen at random and put in one of the non-empty boxes chosen at random. This is the zero-temperature version of the model introduced in [9]†.

Model B. The particles are now considered to be indistinguishable. At each time step a box is chosen at random among the non-empty boxes. A particle is withdrawn from this box and put into one of the other non-empty boxes chosen at random.

Model C. The particles are again distinguishable. At each time step two particles are chosen at random. One of the particles is put in the box to which the second one belongs.

At a qualitative level, it is clear why the relaxation should be much slower in model A than in models B and C. In model A, the box from which a particle is withdrawn is selected with a probability proportional to the number of particles it contains (hereafter called the ‘size’ of the box), therefore the largest boxes are emptied preferentially. In contrast, in model B this probability is uniform, since a particle is withdrawn from a box independently of its size. For these two models the particle which is withdrawn is then put in any of the other non-empty boxes with equal probability. Hence the lifetime of small boxes will be much larger for model A. In model C, the largest boxes are emptied *and* filled preferentially. We will see that in this case small boxes disappear almost as rapidly as for model B.

Models B and C may be mapped onto classical random walk problems (known in the mathematical literature as birth–death processes), which are solvable. Model A, though it may also be mapped onto a random walk problem, is much more difficult. We found it instructive to put model A in perspective with the other two simpler ones, in order to characterize the nature of its difficulty.

The dynamics of the three models can be written in a unified way as follows. The number of active (i.e. non-empty) boxes at time τ is denoted by $M(\tau)$, the number of active boxes at time τ with k particles by $n_k(\tau)$. The latter are normalized as follows

$$\begin{aligned} \sum_{k \geq 1} n_k(\tau) &= M(\tau) \\ \sum_{k \geq 1} k n_k(\tau) &= N. \end{aligned} \tag{1}$$

One may also denote by $n_0^*(\tau)$ the number of inactive (empty) boxes, such that $M(\tau) + n_0^*(\tau) = M$ (whereas the number of *active* empty boxes $n_0(\tau) = 0$). We take as initial condition $n_k(0) = \delta_{k,1}M$, i.e. each box initially contains one particle and $M = N$. The fraction $\lambda(\tau) = N/M(\tau)$ represents the mean number of particles in the active boxes. Next, one defines $f_k(\tau)$, the density of active boxes with k particles, at time τ , by

† We thus disregard moves from boxes containing one particle to empty boxes, which are allowed by the definition given in [9] since they do not increase the energy. The two definitions are nevertheless equivalent for one-time quantities, up to a rescaling of time.

$f_k(\tau) = n_k(\tau)/N$. It is normalized such that

$$\sum_{k \geq 1} f_k(\tau) = \frac{M(\tau)}{N} = \frac{1}{\lambda(\tau)} = 1 - f_0^*(\tau) \quad (2)$$

$$\sum_{k \geq 1} k f_k(\tau) = 1.$$

We also define the energy density of the system as $E(\tau) = -f_0^*(\tau)$.

As will be shown below, these models may be described in terms of random walks on the half line, with an absorbing site at the origin, the size k of boxes playing the role of the position of the random walker. Indeed the density $f_k(\tau)$ obeys the equation

$$\frac{d}{d\tau} f_k(\tau) = \mu_{k+1} f_{k+1}(\tau) + \lambda_{k-1} f_{k-1}(\tau) - (\mu_k + \lambda_k) f_k(\tau) \quad (3)$$

where μ_k and λ_k are the hopping rates at site k , to the left and to the right, respectively, given by

$$\begin{array}{lll} \mu_k = k & \lambda_k = \lambda(\tau) & (\text{model A}) \\ \mu_k = \lambda(\tau) & \lambda_k = \lambda(\tau) & (\text{model B}) \\ \mu_k = k & \lambda_k = k & (\text{model C}). \end{array} \quad (4)$$

Hence the walk is symmetric for models B and C, while it is biased for model A. In addition, the boundary condition $f_0(\tau) = 0$ is imposed by the fact that empty boxes become inactive. The unit of time chosen in (3) closely follows the definition of the models. It corresponds to N successful moves of a particle to one of the $M(\tau)$ active boxes. The time variable t defined below corresponds to another possible choice for model A (or B) where one makes N attempts to move a particle to one of the M boxes [9, 11].

We first study model B. The evolution in time of $f_k(\tau)$ is given by the equation

$$\frac{d}{d\tau} f_k(\tau) = \lambda(\tau) [f_{k+1}(\tau) + f_{k-1}(\tau) - 2f_k(\tau)]. \quad (5)$$

This last equation is found by an analysis of the balance between the gains and losses to the density $f_k(\tau)$. Indeed, $n_k(\tau)$ increases by one unit, either if one selects a box of size $k+1$ to which a particle is withdrawn and put in a box of size $l \neq k-1, k$, corresponding to a probability

$$\frac{n_{k+1}(\tau)}{M(\tau)} \left(1 - \frac{n_{k-1}(\tau)}{M(\tau)} - \frac{n_k(\tau)}{M(\tau)} \right) \quad (6)$$

or if one selects a box of size $l \neq k, k+1$ to which a particle is withdrawn and put in a box of size $k-1$, corresponding to a probability with a similar form. All the probabilities of the events such that n_k increases or decreases by one or two units can be computed similarly and add up to give equation (5). The balance equations for models A and C are found in a similar way. Summing both sides of this equation on k gives the evolution in time of $1/\lambda(\tau)$

$$-\frac{d}{d\tau} (1/\lambda(\tau)) = \frac{d}{d\tau} f_0^*(\tau) = \lambda(\tau) f_1(\tau). \quad (7)$$

In order to solve (5) it is convenient to define a new time variable t by $dt = \lambda(\tau) d\tau$. We denote by $g_k(t) = f_k(\tau)$ the density in this new variable. Equation (5) becomes

$$\frac{d}{dt} g_k(t) = g_{k+1}(t) + g_{k-1}(t) - 2g_k(t). \quad (8)$$

This equation, together with the boundary condition $g_0(t) = 0$, describes a one-dimensional symmetric random walk with an absorbing site at the origin. This problem may be solved in this discrete formulation. However, its solution is simpler in its continuum version:

$$\frac{\partial g(h, t)}{\partial t} = \frac{\partial^2 g(h, t)}{\partial h^2} \quad (9)$$

where h is now a continuum variable. The solution of (9) is given by

$$g(h, t) = \int_0^\infty dh' p(h, t|h', 0)g(h', 0) \quad (10)$$

where

$$p(h, t|h', 0) = \frac{1}{\sqrt{4\pi t}} \{ \exp[-(h-h')^2/4t] - \exp[-(h+h')^2/4t] \} \quad (11)$$

is the probability of finding the random walker at a distance h of the origin at time t if it started at a distance h' at time 0, without ever passing through the origin. This result may be easily found by the method of images. With the initial condition $g(h', 0) = \delta(h' - 1)$ and using (2), one gets

$$\frac{1}{\lambda(t)} = \int_0^\infty g(h, t) dh = \frac{2}{\sqrt{\pi}} \int_0^{1/\sqrt{4t}} \exp(-x^2) dx = \operatorname{erf}\left(\frac{1}{2\sqrt{t}}\right). \quad (12)$$

For t large this implies that $\lambda(t) \approx \sqrt{\pi t}$. The original time variable τ is given by the integral

$$\tau = \int_0^t \operatorname{erf}\left(\frac{1}{2\sqrt{u}}\right) du = \left(\frac{1}{2} + t\right) \operatorname{erf}\left(\frac{1}{2\sqrt{t}}\right) + \sqrt{\frac{t}{\pi}} \exp\left(-\frac{1}{4t}\right) - \frac{1}{2}. \quad (13)$$

Equation (12) together with (13) provide a parametric representation of $1/\lambda$. When t is large (13) gives $\tau \approx 2\sqrt{t/\pi}$ hence

$$\lambda(\tau) \approx \frac{\pi}{2} \tau \quad (14)$$

so that the energy density decreases asymptotically as $E(\tau) \simeq -1 + 2/(\pi\tau)$. This behaviour is confirmed numerically with high accuracy. Finally we note that the density of active boxes has a scaling form at large times: $f(h, \tau) = F(x)/\lambda^2(\tau)$ where $x = h/\lambda$ and where

$$F(x) = \frac{\pi}{2} x \exp(-\pi x^2/4) \quad (15)$$

normalized to 1, is obtained from (10), (11), (13).

Let us point out that there is a simple connection between this process and the zero temperature coarsening dynamics of a one-dimensional Potts model with an infinite number of states [12]. The domain walls perform random walks. When two domain walls meet, they coalesce into one. Their number therefore decreases in time. In the mean field case the density of domains of length h obeys equation (8). The mean field theory gives the exact scale invariant distribution of domains (15) [12]. Therefore the model described here, which does not possess any spatial structure, should have the same behaviour as its one-dimensional version, at least for the dependence of $\lambda(\tau)$ with time. We checked the validity of this point numerically.

Let us now turn to model C. The equation for $f_k(\tau)$ is

$$\frac{d}{d\tau} f_k(\tau) = (k+1)f_{k+1}(\tau) + (k-1)f_{k-1}(\tau) - 2kf_k(\tau) \quad (16)$$

with $f_0(\tau) = 0$. Summing both sides of (16) on k yields

$$-\frac{d}{d\tau}(1/\lambda(\tau)) = \frac{d}{d\tau}f_0^*(\tau) = f_1(\tau). \quad (17)$$

One deduces from (16) that the generating function $G(y, \tau) = f_0^*(\tau) + \sum_{k \geq 1} f_k(\tau)y^k$ satisfies the equation

$$\frac{\partial}{\partial t}G(y, \tau) = (y - 1)^2 \frac{\partial}{\partial y}G(y, \tau) \quad (18)$$

which is solved using the method of characteristics with the boundary condition $G(y, 0) = y$. One finds

$$G(y, \tau) = \frac{\tau(1-y) + y}{\tau(1-y) + 1} = \frac{\tau}{1+\tau} + \sum_{k \geq 1} \frac{1}{(1+\tau)^2} \left(\frac{\tau}{1+\tau} \right)^{k-1} y^k. \quad (19)$$

The first term of the expansion is $f_0^*(\tau)$. Hence $\lambda(\tau) = 1 + \tau$. Note that, at large times, the behaviour of $\lambda(\tau)$ is linear in time as for model B. The energy converges to -1 as $1/\tau$. Again $f(h, \tau)$ has a scaling form at large times with $F(x) = \exp(-x)$, obtained from (19).

We finally study model A. The evolution in time of $f_k(\tau)$ is now given by the equation

$$\frac{d}{d\tau}f_k(\tau) = (k+1)f_{k+1}(\tau) + \lambda(\tau)f_{k-1}(\tau) - (k+\lambda(\tau))f_k(\tau) \quad (20)$$

with the boundary condition $f_0(\tau) = 0$. Summing both sides of (20) on k yields

$$-\frac{d}{d\tau}(1/\lambda(\tau)) = \frac{d}{d\tau}f_0^*(\tau) = f_1(\tau). \quad (21)$$

Equation (20) describes an asymmetric random walk with transition rates $\mu_k = k$, $\lambda_k = \lambda(\tau)$ and with an absorbing site at the origin. The k -dependent velocity and diffusion coefficient of this random walk read

$$V_k = \lambda_k - \mu_k = \lambda(\tau) - k \quad D_k = (\lambda_k + \mu_k)/2 = (\lambda(\tau) + k)/2. \quad (22)$$

Hence, according to whether k (the size of the box) is smaller or larger than $\lambda(\tau)$ (the mean size of the boxes), the bias $V_k/(2D_k) = (\lambda(\tau) - k)/(\lambda(\tau) + k)$ is positive or negative. The existence of such a bias, which is the main difference between model A and the two previous models, has far reaching consequences.

(i) The random walker is attracted towards $\lambda(\tau)$, by a restoring force corresponding to a confining potential (see equation (29)). This potential is responsible for the existence of 'entropy barriers': configurations for which one of the boxes is nearly empty (i.e. the random walker is located near the origin) are much less numerous than those where all boxes are roughly equally occupied (i.e. the random walker is located around $\lambda(\tau)$), and thus harder to reach by the dynamics.

(ii) As a consequence, the random walker is absorbed by the origin at an extremely slow rate, and therefore its mean position $\lambda(\tau)$, which evolves by (21), increases extremely slowly with time, i.e. the minimum of the potential is moving slowly to the right. In other words, the relaxation of $1/\lambda(\tau) = M(\tau)/N$, i.e. of the energy, is very slow.

(iii) In principle, in order to solve (20), one could integrate the equation obeyed by the generating function $G(y, \tau) = \sum_{k \geq 1} f_k(\tau)y^k$, as was done for model C. The solution thus obtained is not explicit. Instead, the former analysis suggests that an adiabatic approximation to this process should be very accurate, at least at large enough times. It consists in considering that the system is always in a quasi-stationary state obtained by solving (20)

with a vanishing left-hand side and with no absorption at the origin. On this scale of time $\lambda(\tau)$ is considered as constant. One finds

$$f_k(\tau) = \exp(-\lambda) \frac{\lambda^{k-1}}{k!} \quad (k \geq 1) \quad (23)$$

which, up to the normalizing factor λ coming from the definition (2) of f_k , is the discrete Poisson distribution. It is easy to show that the approach to this equilibrium distribution is exponential, with a relaxation time t_0 equal to 1. The only dependence in time of this distribution comes from λ , which evolves through (21). Therefore in this approximation, using (23),

$$\frac{d\tau}{d\lambda} \simeq \frac{\exp(\lambda)}{\lambda^2}. \quad (24)$$

As a consequence, the energy decreases asymptotically as $E(\tau) \sim -1 + 1/\ln(\tau)$. A similar result is given in [11].

An improved treatment of the adiabatic approximation is as follows. The average duration of time before absorption for a random walker initially at position k reads [13]

$$T_k = \frac{1}{\lambda} \sum_{j=0}^{k-1} \frac{j!}{\lambda^j} \sum_{i=j+1}^{\infty} \frac{\lambda^i}{i!}. \quad (25)$$

Averaging over the starting position k , using (23), yields

$$\bar{T} = \frac{\exp(-\lambda)}{\lambda} \left[(\exp(\lambda) - 1)^2 + \frac{1}{\lambda} (\exp(\lambda) - 1 - \lambda)^2 + \frac{2!}{\lambda^2} \left(\exp(\lambda) - 1 - \frac{\lambda}{2!} \right)^2 + \dots \right]. \quad (26)$$

Noting that $d\bar{T}/d\lambda = (\exp(\lambda) - 1)/\lambda \equiv T_1$, one gets

$$\bar{T} = \text{Ei}(\lambda) - \ln \lambda - \gamma = \sum_{n \geq 1} \frac{\lambda^n}{nn!} \quad (27)$$

(Ei(x) is the exponential integral, γ the Euler constant). This quantity represents the average length of time between two events where a box becomes empty. In the limit where these events are very rare, the distribution of these lengths of time is exponentially distributed, with a density $1/\bar{T}$, therefore

$$\frac{d(1/\lambda)}{d\tau} = -\frac{1/\lambda}{\bar{T}} \quad \text{i.e.} \quad \frac{d\tau}{d\lambda} = \frac{\bar{T}}{\lambda}. \quad (28)$$

This equation is far more accurate than the leading order estimate (24): the difference between the exact result and our improved adiabatic approximation is exponentially small in λ [14], while equation (28) shows that the leading correction to (24) is of order $1/\lambda$.

To summarize, the adiabatic approximation relies on the existence of two different time scales in this model: the average time \bar{T} for the walker to be absorbed at the origin, of the order $\exp(\lambda)/\lambda \sim \tau/\ln(\tau)$, much larger than the relaxation time $t_0 = 1$ needed to reach equilibrium, at a given value of λ .

(iv) Another consequence of the existence of a bias in model A is the fact that the dynamics is not governed by the scaling regime of the f_k 's. More precisely, for large times (large λ), the distribution f_k possesses a scaling form, which is a Gaussian of width $\sqrt{\lambda}$ centred around λ . However, the time evolution of λ , given by (21), is driven by $f_1(\tau)$ which is exponentially small in λ and lies in the non-universal tail of the distribution. Hence this time evolution is governed by rare events. By contrast, models B and C possess a scale

invariant density $F(x)$, thus $f_1(\tau)$ is inversely proportional to a power of λ . This ensures a fast relaxation, by (7) and (17).

The same features may be seen in a continuum version of model A. Taking the gradient expansion of equation (20) to second order yields the Fokker-Planck equation

$$\begin{aligned} \frac{\partial f(h, \tau)}{\partial \tau} &= \frac{1}{2} \frac{\partial^2}{\partial h^2} [(h + \lambda) f(h, \tau)] - \frac{\partial}{\partial h} [(\lambda - h) f(h, \tau)] \\ &= \frac{\partial^2}{\partial h^2} [D(h) f(h, \tau)] - \frac{\partial}{\partial h} [V(h) f(h, \tau)]. \end{aligned} \quad (29)$$

In the adiabatic approximation one may estimate the typical time needed to reach $h = 0$ by an Arrhenius barrier crossing argument. The equilibrium distribution for this process is

$$f_{\text{eq}}(h) = \frac{\mathcal{N}}{D(h)} \exp\left(\int_0^h \frac{V(h')}{D(h')} dh'\right) = \frac{\mathcal{N}}{D(h)} \exp\{-[U(h) - U(0)]\} \quad (30)$$

where \mathcal{N} is determined by the normalization condition: $\int_0^\infty dh f_{\text{eq}}(h) = 1/\lambda$, and $U(h) = 2h - 4\lambda \ln(\lambda + h)$ is the 'effective potential'—which gives an intuitive meaning to the idea of entropy barriers. Note that the potential is, up to a factor 2, the integral of the bias. The rate at which boxes become empty can be approximated by $f_{\text{eq}}(0)$, which leads to an estimate $\bar{T} \approx \exp(\alpha\lambda)$, where $\alpha = 2(2\ln 2 - 1) \simeq 0.77$. So this continuous version leads again to an exponential increase with λ of the time constant \bar{T} , but with a different coefficient, $\alpha = 2(2\ln 2 - 1)$ instead of $\alpha = 1$ in the discrete version.

This discrepancy between model A and its continuum version (although both lead to a very slow decay $E(\tau) \simeq -1 + \alpha/\ln(\tau)$) can be traced back to the dominance of rare events in this process, mentioned above. Indeed one cannot expect any universal property far away from the scaling region (i.e., for $k - \lambda \gg \sqrt{\lambda}$), where the occurrence of rare events takes place. Phrased differently, the continuum limit of model A cannot be valid outside of the scaling region, where the bias is not small.

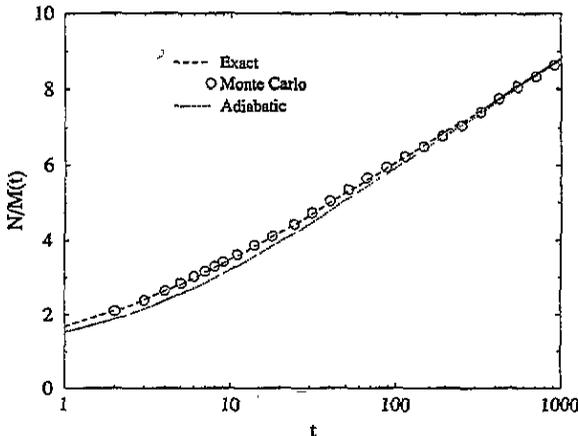


Figure 1. Exact result for $\lambda(t) = N/M(t)$ obtained by the integration of equation (20), compared to a Monte Carlo simulation, and to the adiabatic approximation equation (28). ($N = 10\,000$.)

Let us finally compare our predictions to numerical computations. The analytic predictions found for $f_k(\tau)$ or $\lambda(\tau)$ in models B and C are in total agreement with the Monte Carlo simulations of the models. We do not include these results here. Let us focus on model A. Figure 1 shows a comparison of the exact result for $\lambda(\tau) = N/M(\tau)$ obtained

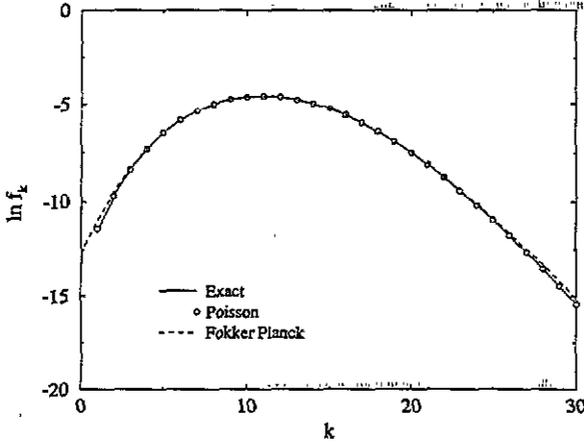


Figure 2. Exact density f_k obtained from equation (20) compared to the quasi-stationary Poisson distribution (23) and to the Fokker-Planck equilibrium distribution $f_{eq}(h)$ (30) ($\lambda = 11.44$).

by numerical integration of equation (20), with a Monte Carlo simulation, and with the adiabatic approximation equation (28). We chose to represent the data in the time scale t , where $dt = \lambda d\tau$, hence (28) yields $t(\lambda) = \sum_{n \geq 1} (\lambda^{n+1} - 1)/n(n+1)!$. Figure 2 depicts a comparison of the exact density f_k obtained from equation (20) with the quasi-stationary Poisson distribution (23) and with the Fokker Planck equilibrium distribution $f_{eq}(h)$ (30). (Here $\lambda = 11.44$ corresponding to $\tau = 1000$.) Even on a logarithmic scale, the discrepancy is hardly visible, except in the tails. This is due to the fact that the ratio $\ln(f_{eq}(1))/\ln(f_1)$ converges to α very slowly when λ increases. At this value of λ , this ratio is equal to 0.96. It is equal to 0.824 for $\lambda = 100$ and to 0.79 for $\lambda = 400$.

Let us conclude with some comments. An interesting point would be to better understand the nature of the corrections to the adiabatic approximation done above. Another point of interest is the t'/t aging behaviour reported in [9, 11]. These points will be the subject of further work [14].

The correspondence between model B and the infinite states Potts model has already been pointed out. More generally, the models studied here are reminiscent of coarsening models where the dynamics is driven by the coalescence of the smallest domains [12, 15–17]. For example, in [15], the average size of domains scales as $\ln t$, akin to the behaviour of λ in model A.

Another interesting situation is that of a polymer in a plane which would like to adsorb strongly on a line, but with the constraint that the total area between the line and the polymer is fixed (corresponding to, say, the incompressibility of the solvent). The size of a box corresponds in this case to the distance between the polymer and the wall. The polymer will then grow longer and longer localized ‘hairpins’. Our solution corresponds to an idealized, mean-field description of the resulting dynamics where the one dimensional structure of the problem has been lost. It would be interesting to pursue this particular model or higher dimensional versions further.

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