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# *p*-adic models of ultrametric diffusion constrained by hierarchical energy landscapes

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## Abstract

We demonstrate that the *p*-adic analysis is a natural basis for the construction of a wide variety of models of ultrametric diffusion constrained by hierarchical energy landscapes. A general analytical description in terms of the *p*-adic analysis is given for a class of models. Two exactly solvable examples, i.e. the ultrametric diffusion constrained by the linear energy landscape and the ultrametric diffusion with a reaction sink, are considered. We show that such models can be applied to both the relaxation in complex systems and the rate processes coupled to rearrangement of the complex surrounding.

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## 1. Introduction

The concept of a hierarchical energy landscape attracts a lot of interest in connection with relaxation phenomena in complex systems, in particular, glasses, clusters and proteins [1–12]. This concept can be outlined as follows. A complex system is assumed to have a large number of metastable configurations which realize local minima on the potential energy surface. The local minima are clustered in hierarchically nested basins of minima, namely, each large basin consists of smaller basins, each of these consisting of even smaller ones, and so on. To be more definite, the hierarchy of basins possesses ultrametric geometry. Finally, the basins of minima are separated from one another by a hierarchically arranged set of barriers, i.e. high barriers separate large basins and smaller basins within each larger one are separated by lower barriers. Transitions between the basins determine the rearrangements of the system configuration for different time scales.

Thus, two key points of the concept of a hierarchical energy landscape should be marked. First, the configuration space of the system is approximated by an ultrametric space; second, the configuration rearrangements of the system are described by stochastic motion in the ultrametric configuration space.

This concept has been implemented in a number of toy models referred to as random walks in ultrametric space, diffusion in ultrametric space and ultra-diffusion [13–17]. A recent term

for such processes is ‘basin-to-basin kinetics’ [9]. In fact, all these models deal with a certain type of stochastic motion, which in this paper we call diffusion in ultrametric space, or for short, ultrametric diffusion.

The toy models have definitely demonstrated that ultrametricity actually reflects the characteristic features of relaxation in complex systems. It is commonly recognized that relevant analytical tools should be developed for applying the concept of a hierarchical energy landscape to the description of relaxation phenomena in complex systems [7–9, 12].

In this paper, we show that  $p$ -adic analysis is an adequate analytical tool for studying these problems. The field of  $p$ -adic numbers is the most important example of ultrametric spaces (see, for instance, [18]). An introduction to  $p$ -adic analysis can be found in [19]. The  $p$ -adic mathematical physics attracts a great deal of interest in quantum mechanics, string theory, quantum gravity [19–22], spin-glass theory [23, 24] and theoretical biology [25]. We demonstrate here that the  $p$ -adic analysis can be efficiently applied to both the relaxation in complex systems and the rate processes coupled to the relaxation of complex environment.

This paper has the following structure. In section 2, a general analytical description in terms of  $p$ -adic analysis is given for a class of ultrametric diffusion models, the so-called pure models [18]. Since  $p$ -adic analysis seems to be a fairly new analytical tool, we thought it appropriate to describe the technique of solving the corresponding  $p$ -adic master equation. Specific examples are considered in the next two sections. In section 3, we give a complete description of the ultrametric diffusion constrained by the linear energy landscape. In section 4, we consider a special case where the rate process coupled to the configuration rearrangements can be described; we also introduce and study a model of ultrametric diffusion with a reaction sink. We show that such models can be applied, in particular, to the ligand rebinding kinetics in heme proteins.

## 2. Ultrametric diffusion

In this section, we describe a class of pure ultrametric diffusion models corresponding to regular hierarchical landscapes with degeneracy. First, we review a model of diffusion on an ultrametric lattice [13] (this model was considered in [23] with the help of  $p$ -adic analysis). Then, passing to a continuous description, we obtain the  $p$ -adic master equation. The last part of this section contains a brief description of the standard analytical technique for the investigation of such  $p$ -adic equations.

### 2.1. Ultrametric lattice and the master equation

Consider a system with the state space  $B_N$  consisting of the points  $i = 1, \dots, p^N$ , where  $p$  is a prime number. These points can be regarded as lattice sites. On this lattice, a regular hierarchical energy landscape can be constructed as follows (see figure 1). Let us divide the space  $B_N$  into  $p$  mutually disjoint subsets (basins)  $B_{N-1}(a_1)$ ,  $a_1 = 1, \dots, p$ , where each  $B_{N-1}(a_1)$  consists of  $p^{N-1}$  points

$$\bigcup_{a_1} B_{N-1}(a_1) = B_N.$$

Let us introduce activation barriers. The activation barrier for the transitions between the basins  $B_{N-1}(a_1)$  with different values of  $a_1$  is taken equal to  $H_N$ . Thus, the probability of transition between any two sites  $i \in B_{N-1}(a_1)$  and  $j \in B_{N-1}(a'_1)$  of different basins  $B_{N-1}$  is equal to  $\rho_N$ . In the Arrhenius case, we have  $\rho_N = \exp(-H_N/kT)$ . Further, let us divide each basin  $B_{N-1}(a_1)$  into  $p$  smaller basins  $B_{N-2}(a_1 a_2)$ ,  $a_2 = 1, \dots, p$ , each having  $p^{N-2}$  sites

$$\bigcup_{a_2} B_{N-2}(a_1 a_2) = B_{N-1}(a_1).$$

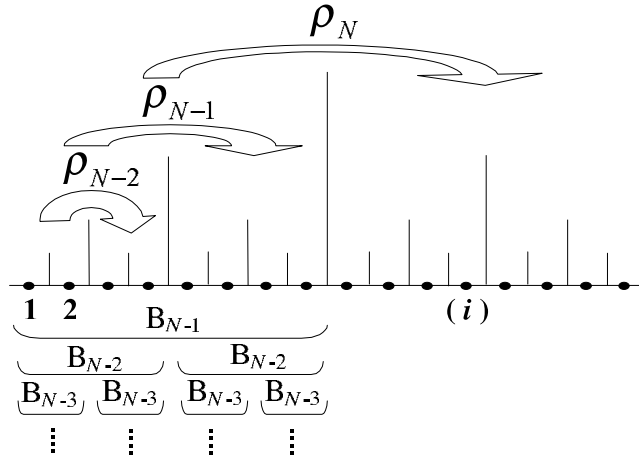


Figure 1. Basin-to-basin transitions on an ultrametric lattice ( $p = 2$ ).

Assume that the activation barriers within each larger basin  $B_{N-1}(a_1)$  are equal to  $H_{N-1}$ . Moreover, assume that the probability of transition between any two sites  $i \in B_{N-2}(a_1 a_2)$  and  $j \in B_{N-2}(a'_1 a'_2)$  of different basins  $B_{N-2}$  is equal to  $\rho_{N-1}$  for  $a_1 = a'_1$ , and is equal to  $\rho_N$  for  $a_1 \neq a'_1$ . In other words, the probability of transition between sites of different basins  $B_{N-2}$  depends on the hierarchical level,  $N - 1$  or  $N$ , at which these basins merge into a single super basin. We proceed like this until we reach the first level with each basin  $B_1(a_1 a_2 \dots a_N)$  having only one site. As a result, the probability of transition between any two sites is specified by a single value  $\rho_\gamma$  among  $\rho_1 > \dots > \rho_\gamma > \dots > \rho_N$ , according to the level  $\gamma = 1, 2, \dots, N$  on which these two sites happen to be in a single basin  $B_\gamma$ .

Denote by  $f_i(t)$  the probability of finding the system in the site  $i$  at time  $t$ . Using the equivalence between the transition probability matrix and the Parisi matrix, we can write the master equation for the evolution of probabilities in the form

$$\frac{d}{dt} \mathbf{f}(t) = (\mathbf{Q} - \lambda_0 \mathbf{I}) \mathbf{f}(t) \tag{1}$$

where  $\mathbf{f}(t) = \{f_1(t), \dots, f_{p^N}(t)\}$  is the state vector,  $\mathbf{Q}$  is the transition  $p^N \times p^N$  matrix of the Parisi type [26],  $\mathbf{I}$  is the unity matrix and  $\lambda_0 = \sum_{\gamma=1}^N p^{\gamma-1} \rho_\gamma$  is the eigenvalue of the matrix  $\mathbf{Q}$  corresponding to the eigenvector with equal components. For instance, the transition matrix  $\mathbf{Q}$  for  $p = 2$  has the form

$$\mathbf{Q} = \begin{pmatrix} 0 & \rho_1 & \rho_2 & \rho_2 & \rho_3 & \rho_3 & \rho_3 & \rho_3 & \dots \\ \rho_1 & 0 & \rho_2 & \rho_2 & \rho_3 & \rho_3 & \rho_3 & \rho_3 & \dots \\ \rho_2 & \rho_2 & 0 & \rho_1 & \rho_3 & \rho_3 & \rho_3 & \rho_3 & \dots \\ \rho_2 & \rho_2 & \rho_1 & 0 & \rho_3 & \rho_3 & \rho_3 & \rho_3 & \dots \\ \rho_3 & \rho_3 & \rho_3 & \rho_3 & 0 & \rho_1 & \rho_2 & \rho_2 & \dots \\ \rho_3 & \rho_3 & \rho_3 & \rho_3 & \rho_1 & 0 & \rho_2 & \rho_2 & \dots \\ \rho_3 & \rho_3 & \rho_3 & \rho_3 & \rho_2 & \rho_2 & 0 & \rho_1 & \dots \\ \rho_3 & \rho_3 & \rho_3 & \rho_3 & \rho_2 & \rho_2 & \rho_1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{2}$$

This form of the transition probability matrix  $\mathbf{Q}$  is a direct consequence of the hierarchical picture of basin-to-basin transitions.

The master equation (1) coincides with the equation of ultrametric diffusion considered in [13].

## 2.2. Continuum limit

The continuum limit for the above hierarchical lattice model is realized by  $p$ -adic parameterization of the Parisi matrix discussed in [23, 24]. The results obtained in [23] can be summarized as follows. We introduce the following one-to-one mapping of integers  $i$  enumerating the lattice sites onto a set of rational numbers:

$$i = 1 + p^{-1} \sum_{j=1}^n x_j^{(i)} p^j \rightarrow \sum_{j=1}^N x_j^{(i)} p^{-j} = x^{(i)} \quad 0 \leq x_j^{(i)} \leq p - 1.$$

The value  $x^{(i)}$  is regarded as a coordinate of the site  $i$ . Then, in the continuum limit, the set of coordinates  $x$  is extended to the field of  $p$ -adic numbers  $\mathcal{Q}_p$ , the matrix  $(\mathbf{Q} - \lambda_0 \mathbf{I})$  turns into an integral operator and the master equation (1) transforms into the following equation:

$$\frac{d}{dt} f(x, t) = \int_{\mathcal{Q}_p} (f(y, t) - f(x, t)) \rho(|x - y|_p) d\mu(y). \quad (3)$$

Here, the operator on the right-hand side is called the ultrametric diffusion operator, the function  $\rho(|x - y|_p): \mathcal{Q}_p \times \mathcal{Q}_p \mapsto \mathbf{R}$  ( $\mathbf{R}$  is the field of real numbers) is the kernel of the ultrametric diffusion operator, the function  $f(x): \mathcal{Q}_p \mapsto \mathbf{R}$  is the probability density distribution and  $d\mu(y)$  is the Haar measure on the field of  $p$ -adic numbers  $\mathcal{Q}_p$ .

Expression (3) specifies the general form of ultrametric diffusion operators. A special case of the operator on the right-hand side of (3) should be mentioned, namely, the Vladimirov operator

$$D_x^\alpha f(x, t) = \frac{1}{\Gamma_p(-\alpha)} \int_{\mathcal{Q}_p} \frac{f(y) - f(x)}{|x - y|_p^{1+\alpha}} d\mu(y) \quad (4)$$

where  $\alpha > 0$  and  $\Gamma_p(\alpha) = \frac{1-p^{\alpha-1}}{1-p^{-\alpha}}$  is the  $p$ -adic gamma function. This operator is an analogue of the differentiation operator in  $p$ -adic analysis. For this reason, the equation

$$\frac{d}{dt} f(x, t) = -D_x^\alpha f(x, t) \quad (5)$$

is interpreted in  $p$ -adic mathematical physics as the equation of Brownian motion on a  $p$ -adic line. More details concerning pseudo-differential operators and equation (5) can be found in the monograph [19]. It is interesting to note that an equation of type (5) is the master equation for the model in which the height of the barriers separating the basins of states has linear growth with respect to the hierarchy level number [23].

## 2.3. Solution technique

Next, we give a brief review of the standard technique for solving equations of type (3). We investigate the Cauchy problem for equation (3) with the initial condition  $f(x, 0) = \delta(x)$ , where  $\delta(x)$  is the  $p$ -adic delta function [19]. Let us find a fundamental solution of equation (3). Applying the  $p$ -adic Fourier transformation to (3), we obtain the following equation:

$$\frac{\partial \tilde{f}(\xi, t)}{\partial t} = -\tilde{\rho}(|\xi|_p) \tilde{f}(\xi, t) \quad (6)$$

where

$$\tilde{\rho}(|\xi|_p) = \int_{\mathcal{Q}_p} \rho(|x|_p) (1 - \chi(\xi x)) d\mu(x) \quad (7)$$

and  $\tilde{f}(\xi, t)$  is the Fourier transform of the distribution  $f(x, t)$ . Hence, it is easy to find the Fourier transform

$$\tilde{f}(\xi, t) = \exp(-\tilde{\rho}(|\xi|_p)t). \tag{8}$$

Applying the inverse Fourier transformation to (8), we obtain the fundamental solution

$$f(x, t) = \int_{Q_p} \exp(-\tilde{\rho}(|\xi|_p)t)\chi(-\xi x) d\mu(\xi) \tag{9}$$

where  $\chi(\xi x)$  is the additive character of the field of *p*-adic numbers.

Equation (3) is defined on the whole field of *p*-adic numbers  $Q_p$ . Therefore, the solution (9) describes the diffusion process in an unbounded ultrametric space. However, for some applications, it is important to study the ultrametric diffusion in a bounded region. In this case, the following procedure can be used.

Consider diffusion in the *p*-adic disc  $B_r = \{x : |x|_p \leq p^r\}$  of radius  $p^r$  with centre at zero. In this case, the master equation reads

$$\frac{\partial f(x, t)}{\partial t} = \int_{B_r} (f(y, t) - f(x, t))\rho(|x - y|_p) d\mu(y). \tag{10}$$

Changing the variables,  $x = p^{-r}z$ , we transform this equation to

$$\frac{\partial f(z, t)}{\partial t} = \int_{Z_p} (f(z', t) - f(z, t))\rho(|z - z'|_p) d\mu(z').$$

This equation can be investigated by means of *p*-adic Fourier series

$$\phi(z, t) = \sum_{k \in I} \tilde{\phi}_k(t)\chi(-kz)$$

where the characters  $\{\chi(kz)\}$  form an orthonormal basis in  $L^2(Z_p)$  labelled by

$$\begin{aligned} k = 0 & \quad k = p^{-\gamma}(k_0 + k_1p + \dots + k_{\gamma-1}p^{\gamma-1}) \\ \gamma = 1, 2, \dots & \quad k_0 = 1, 2, \dots, p - 1 \quad k_j = 0, 1, \dots, p - 1 \quad j = 1, 2, \dots, \gamma - 1. \end{aligned}$$

### 3. Diffusion on linear hierarchical landscape

In this section, we examine ultrametric diffusion in the case of a linear landscape with the height of activation barriers  $H_\gamma$  having a linear growth with respect to the number  $\gamma$  of the hierarchical level. Since  $|x - y|_p = p^\gamma$ , for the linear landscape we have

$$H_\gamma = H_0 \ln(|x - y|_p) \tag{11}$$

where  $H_0$  is a scale parameter. Suppose that the probability of transition between the states separated by the activation barrier  $H_\gamma$  is defined by

$$\rho_\gamma = w_0 p^{-\gamma} \exp\left(-\frac{H_\gamma}{kT}\right) \tag{12}$$

where  $w_0$  is a pre-exponential factor,  $T$  is temperature and  $k$  is the Boltzmann constant. As noted in section 2, under these assumptions, the kernel of the ultrametric diffusion operator coincides with the kernel of the Vladimirov operator (see also [23])

$$\rho(|x - y|_p) = \frac{w_0}{|x - y|_p^{\alpha+1}}$$

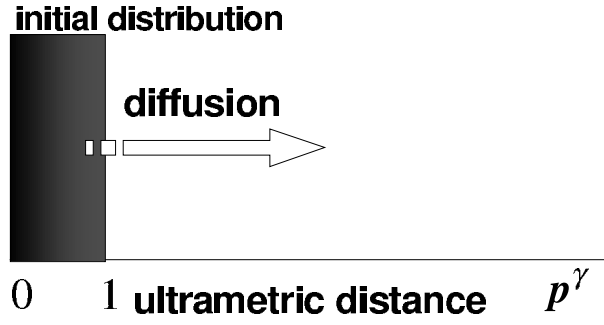


Figure 2. Diagram of the ultrametric diffusion model with initial distribution on  $Z_p$ .

where  $\alpha = H_0/kT$ . The Fourier transform of this kernel is

$$\tilde{\rho}(\xi) = -w_0 \Gamma_p(-\alpha) |\xi|_p^\alpha. \quad (13)$$

Thus, in the case of a linear hierarchical landscape (11) (under the assumption (12)), the master equation of ultrametric diffusion coincides with the equation of Brownian motion on the  $p$ -adic line (see relations (4) and (5) in section 2)

$$\frac{\partial f(x, t)}{\partial t} - w_0 \Gamma_p(-\alpha) D_x^\alpha f(x, t) = 0. \quad (14)$$

Let us examine the solutions of this equation. As the initial value we take  $f(x, 0)$  which is constant inside a bounded set in  $Q_p$  and vanishes outside. For instance, we can take as the initial function the indicator of  $Z_p$

$$f(x, 0) = \Omega(|x|_p) = \begin{cases} 1 & |x|_p \leq 1 \\ 0 & |x|_p > 1. \end{cases} \quad (15)$$

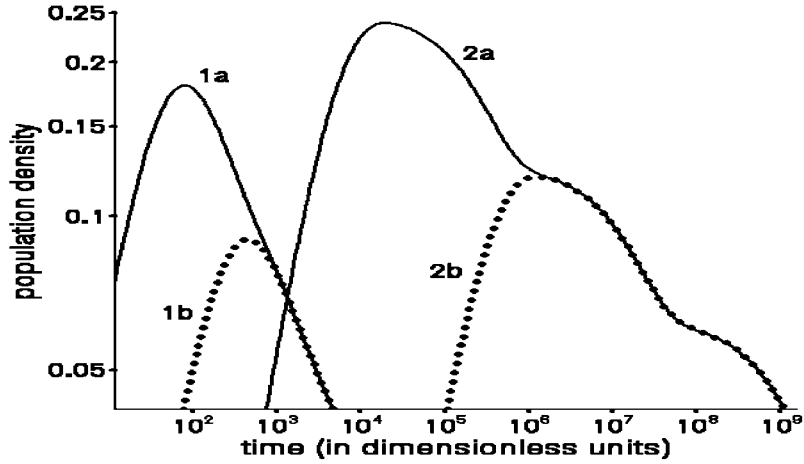
Note that the  $p$ -adic Fourier transform of this indicator function is the same function. The diagram of the model with this initial condition is given in figure 2. Using the fundamental solution (9), one can construct the solution of equation (14) with the initial condition (15)

$$f(x, t) = \int_{Q_p} \chi(-\xi x) \Omega(|\xi|_p) \exp\{\Gamma_p(-\alpha) |\xi|_p^\alpha w_0 t\} d\mu(\xi). \quad (16)$$

Calculating the integral, we obtain

$$f(x, t) = (1 - p^{-1}) |x|_p^{-1} \sum_{\gamma=0}^{+\infty} p^{-\gamma} \Omega\left(\frac{p^{-\gamma}}{|x|_p}\right) \exp\left\{\frac{p^{-\alpha\gamma}}{|x|_p^\alpha} \Gamma_p(-\alpha) w_0 t\right\} - |x|_p^{-1} \Omega\left(\frac{p}{|x|_p}\right) \exp\left\{\frac{p^\alpha}{|x|_p^\alpha} \Gamma_p(-\alpha) w_0 t\right\}. \quad (17)$$

The solution (17) describes the diffusion process in the unbounded ultrametric space. As an illustration, the time-dependence of population densities for different states is shown in figure 3. It is easy to see that at fairly low temperatures (with  $\alpha$  much larger than unity) the decay of the population density of the states has a discrete character due to the hierarchy of the characteristic times of transition through the respective activation barriers. As the temperature increases, the discrete nature of decay becomes less and less noticeable and at sufficiently high temperatures (with  $\alpha$  of the order of or less than unity) the population density of the states is governed by the power law.



**Figure 3.** Evolution of the population density at two points: (a) solid curves,  $\gamma_a = 2$ ; (b) dotted curves,  $\gamma_b = 3$ . The curves 1a and 1b ( $\alpha = 2.5$ ) are transformed into the curves 2a and 2b ( $\alpha = 6.0$ ) when the temperature decreases.

This conclusion can also be obtained by analytical means. Now, let us estimate the solution (17) for  $|x|_p > 1$ . Using the Abel transformations

$$\begin{aligned}
 f(x, t) &= |x|_p^{-1} \sum_{\gamma=0}^{+\infty} p^{-\gamma} \left[ \exp \left\{ \frac{p^{-\alpha\gamma}}{|x|_p^\alpha} \Gamma_p(-\alpha) w_0 t \right\} - \exp \left\{ \frac{p^{-\alpha(\gamma-1)}}{|x|_p^\alpha} \Gamma_p(-\alpha) w_0 t \right\} \right] \\
 &= |x|_p^{-1} \sum_{\gamma=0}^{+\infty} p^{-\gamma} \int_{\gamma-1}^{\gamma} \frac{d}{dz} \left[ \exp \{ p^{-\alpha z} |x|_p^{-\alpha} \Gamma_p(-\alpha) w_0 t \} \right] dz
 \end{aligned}$$

and the estimate

$$p^{-m} \int_{m-1}^m g(z) dz \leq \int_{m-1}^m p^{-z} g(z) dz \leq p^{-m+1} \int_{m-1}^m g(z) dz$$

we get

$$\begin{aligned}
 &\frac{(w_0 t)^{-1/\alpha}}{p(-\Gamma_p(-\alpha))^{1/\alpha}} \gamma \left( 1 + \frac{1}{\alpha}, -\Gamma_p(-\alpha) w_0 t \left( \frac{p}{|x|_p} \right)^\alpha \right) \\
 &\leq f(x, t) \leq \frac{(w_0 t)^{-1/\alpha}}{(-\Gamma_p(-\alpha))^{1/\alpha}} \gamma \left( 1 + \frac{1}{\alpha}, -\Gamma_p(-\alpha) w_0 t \left( \frac{p}{|x|_p} \right)^\alpha \right)
 \end{aligned}$$

where  $\gamma(a, b)$  is the incomplete gamma function. If

$$w_0 t \gg \left( \frac{|x|_p}{p} \right)^\alpha \frac{1}{-\Gamma_p(-\alpha)}$$

then

$$\gamma \left( 1 + \frac{1}{\alpha}, -\Gamma_p(-\alpha) w_0 t \left( \frac{p}{|x|_p} \right)^\alpha \right) \approx \Gamma \left( 1 + \frac{1}{\alpha} \right)$$

where  $\Gamma(a)$  is the gamma function. Thus, for any state  $x$ , there is a characteristic time

$$\tau(x, \alpha) = \left( \frac{|x|_p}{p} \right)^\alpha \frac{w_0^{-1}}{-\Gamma_p(-\alpha)}$$



such that the population density  $f(x, t)$ , for  $t \gg \tau(x, \alpha)$ , can be estimated by power functions

$$\frac{\Gamma\left(1 + \frac{1}{\alpha}\right)}{p(-\Gamma_p(-\alpha))^{1/\alpha}}(w_0 t)^{-1/\alpha} \leq f(x, t) \leq \frac{\Gamma\left(1 + \frac{1}{\alpha}\right)}{(-\Gamma_p(-\alpha))^{1/\alpha}}(w_0 t)^{-1/\alpha}. \quad (18)$$

Let us calculate the average of the distribution (17). Note that the moment integrals

$$\langle |x|_p^\beta \rangle = \int_{Q_p} |x|_p^\beta f(x, t) d\mu(x)$$

are divergent for all  $\beta \geq \alpha$ , and therefore, neither the mean  $p$ -adic distance nor the mean square of the  $p$ -adic distance contain any information on the distribution  $f(x, t)$  if, for instance,  $\alpha \leq 1$ . To describe the ultrametric diffusion process in terms of mean values, some meaningful characteristics should be introduced. The mean value of the activation barrier to be overcome by the system by the instant  $t$  can be taken as one such characteristic. In the case of a linear hierarchical landscape (see (11)), the mean value of the activation barrier is

$$\langle H(t) \rangle = H_0 \int_{Q_p} \ln|x|_p f(x, t) d\mu(x). \quad (19)$$

Note that the integral on the right-hand side of (19) should be understood as the limit

$$\int_{Q_p} \ln|x|_p f(x, t) d\mu(x) = \lim_{n \rightarrow +\infty} \int_{|x|_p \leq p^n} \ln|x|_p f(x, t) d\mu(x).$$

Let

$$L^{(n)}(t) = \int_{|x|_p \leq p^n} \ln|x|_p f(x, t) d\mu(x). \quad (20)$$

From (16) we get

$$L^{(n)}(t) = p^n(n(1 - p^{-1}) - p^{-1}) \ln p \sum_{\gamma=-\infty}^{-n} p^\gamma \exp\{\Gamma_p(-\alpha)p^{\alpha\gamma} w_0 t\} \\ - \ln p \sum_{\gamma=-n+1}^{+\infty} \exp\{\Gamma_p(-\alpha)p^{\alpha\gamma} w_0 t\}.$$

Therefore, the quantities  $L^{(n)}(t)$  satisfy the recurrent relations

$$L^{(n)}(p^\alpha t) = L^{(n-1)}(t) + p^{n-1}(1 - p^{-1}) \ln p \sum_{\gamma=-\infty}^{-n+1} p^\gamma \exp\{\Gamma_p(-\alpha)p^{\alpha\gamma} w_0 t\}.$$

Passing to the limit as  $n \rightarrow +\infty$ , we obtain the following functional equation:

$$L(p^\alpha t) = L(t) + \ln p$$

with the solution

$$L(t) = \alpha^{-1} \ln t.$$

Therefore,

$$\langle H(t) \rangle = kT \ln t. \quad (21)$$

Thus, the linear hierarchical landscape has a remarkable feature, namely, the mean value of the activation barrier to be overcome by the instant  $t$  has logarithmic growth with respect to time.

Summing up the results of this section, we emphasize three important features of ultrametric diffusion. The first and foremost is that the evolution of the population density

in any state has a discrete nature and is determined by the hierarchy of the relaxation time scales. This feature stems from the concept of the hierarchical energy landscape and is typical for ultrametric diffusion. The discrete pattern of ultrametric diffusion can be observed at sufficiently low temperatures (with the dependence of  $\alpha$  on  $T$  considered above). Next, in the case of a linear hierarchical landscape, the long-time behaviour of the population density of states is described by the power law. Finally, the mean value of activation barriers overcome by the time  $t$  is logarithmically increasing with the time.

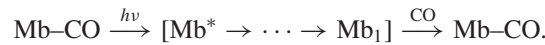
For glasses and proteins, relaxation processes with similar properties are discussed in [2, 4, 6–9, 27–29].

#### 4. Rate processes coupled to configuration rearrangements

In this section, we apply the *p*-adic analysis to describe the kinetics of transformations coupled to configuration rearrangements of the surrounding. We consider a well-known example of such processes, namely, the ligand rebinding kinetics of myoglobin (Mb) [4, 6, 7, 27, 30]. In this case, the object of investigation is the rebinding process governed by conformational rearrangements of the protein itself. These investigations were the origin of the concept of a hierarchical energy landscape in the conformational dynamics of proteins.

The experiment is as follows. The myoglobin is transformed by a laser pulse from the ground state [Mb–CO] into the excited unbound state [Mb\*–]. Then the protein macromolecule relaxes into the functionally active state [Mb<sub>1</sub>–]. From this state, the myoglobin can go back to the ground state [Mb–CO] owing to the binding of the CO.

This process can be represented as the following sequence



The rebinding kinetics is described by the survival probability function  $S(t)$ , i.e. the probability of the fact that myoglobin is still unbound by time  $t$  after being exposed to the laser pulse. Thus, the quantity observed in these experiments is the total population of the conformational states [Mb\*– → … → Mb<sub>1</sub>–] through which the protein macromolecule relaxes from the excited state [Mb\*–] to the functionally active state [Mb<sub>1</sub>–].

Similar types of processes correlate with the models of ultrametric diffusion described by the master equation in the following form:

$$\frac{\partial f(x, t)}{\partial t} = \int_{Q_p} (f(y, t) - f(x, t)) \rho(|x - y|_p) d\mu(y) + \int_{Q_p} K(x, y) f(y, t) d\mu(y). \quad (22)$$

The last integral in the right-hand side of (22) can be thought of as a reaction sink distributed over a bounded region in the conformational space. In this case, the survival probability function is

$$S(t) = \int_{Q_p} f(x, t) d\mu(x). \quad (23)$$

The procedure for solving equations of type (22) is as follows. Let us take  $f(x, 0) = f_0(x)$  in the initial condition. Consecutively applying the *p*-adic Fourier transformation to  $x$  and the Laplace transformation to the real variable  $t$ , we obtain from (23)

$$\hat{f}(\xi, s) = \frac{\tilde{f}_0(\xi)}{s + \tilde{\rho}(|\xi|_p)} + \frac{1}{s + \tilde{\rho}(|\xi|_p)} \tilde{K}(\xi, \zeta) \hat{f}(\zeta, s) d\mu(\zeta). \quad (24)$$

where the symbol  $\hat{\phantom{x}}$  marks the Laplace transform with respect to the variable  $s$ , and  $\tilde{\rho}(|\xi|_p)$  is given by (7). Next, we note that equation (24) is a heterogeneous Fredholm equation of the second kind.

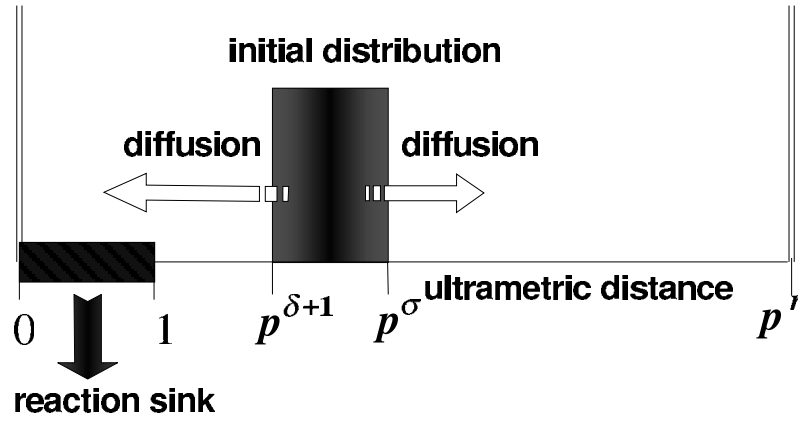


Figure 4. Diagram of ultrametric diffusion model with a reaction sink.

Consecutively, applying the inverse Laplace transformation and the inverse  $p$ -adic Fourier transformation to  $\hat{f}(\xi, s)$ , we obtain the solution  $f(x, t)$  and the function  $S(t)$ .

Let us give an example of a model of this type (see figure 4) by making the following assumptions:

- (i) Conformational rearrangements are restricted to a bounded region of the conformational space of the system and this region is the  $p$ -adic disc  $B_r = \{x : |x|_p \leq p^r, r > 1\}$ .
- (ii) The hierarchical landscape is linear, i.e. conformational rearrangements are described by the ultrametric diffusion operator of type (4) defined on the disc  $B_r$ .
- (iii) In the region  $B_r$ , there is a certain set of conformational states in which the system can undergo irreversible transformations. This set of states is described by the unit disc  $Z_p$ . In other words, there is a reaction-type sink at each point of the disc  $Z_p$ .
- (iv) The rate of the reaction sink at each point of the disc  $Z_p$  is proportional to the mean value of the population density on that disc.
- (v) The initial distribution  $f(x, 0)$  is constant on the  $p$ -adic layer

$$R_{\sigma\delta} = \{x : p^{\delta+1} \leq |x|_p \leq p^{\sigma}, 0 \leq \delta < \sigma < r\}$$

and vanishes outside the layer.

The master equation for the model with the above assumptions is

$$\frac{\partial f(x, t)}{\partial t} = \int_{B_r} \frac{f(y, t) - f(x, t)}{|x - y|_p^{\alpha+1}} d\mu(y) - \lambda \Omega(|x|_p) \int_{B_r} \Omega(|y|_p) f(y, t) d\mu(y) \quad (25)$$

and the initial conditions have the form

$$f(x, 0) = AG_{\delta}^{\sigma}(x) \equiv A [\Omega(|x|_p p^{-\sigma}) - \Omega(|x|_p p^{-\delta})] \quad A^{-1} = p^{\sigma} - p^{\delta} \quad 0 \leq \delta < \sigma$$

where  $\lambda$  is the rate parameter of the reaction sink. Let us use the technique of section 2 to solve equation (25). First, we pass from the disc  $B_r$  to the disc  $Z_p$  by letting  $x = p^{-r}z$ . Then the Cauchy problem takes the form

$$\begin{aligned} \frac{\partial \phi(z, t)}{\partial t} &= p^{-r\alpha} \int_{Z_p} \frac{\phi(z', t) - \phi(z, t)}{|z - z'|_p^{\alpha+1}} d\mu(z') \\ &\quad - \lambda p^r \Omega(|z|_p p^r) \int_{Z_p} \Omega(|z'|_p p^r) \phi(z', t) d\mu(z') \end{aligned}$$

$$\phi(z, 0) = AG_{\delta-r}^{\sigma-r}(z).$$

Using the  $p$ -adic Fourier series for  $Z_p$  (see section 2) and reasoning as above, we obtain a system of equations for the Laplace transforms  $\hat{\phi}_k(s)$  of the coefficients of the  $p$ -adic Fourier series

$$\begin{aligned}
 k = 0: \quad s\hat{\phi}_0(s) &= p^{-r} - \lambda p^{-r} \left[ \hat{\phi}_0(s) + \sum_{q \in I \setminus \{0\}} \Omega(|q|_p p^{-r}) \hat{\phi}_q(s) \right] \\
 k \neq 0: \quad s\hat{\phi}_k(s) &= A\tilde{G}_{\delta-r}^{\sigma-r}(k) + p^{-\alpha r} \Gamma_p(-\alpha) (g_\alpha - |k|_p^\alpha) \hat{\phi}_k(s) \\
 &\quad - \Omega(|k|_p p^{-r}) \lambda p^{-r} \left[ \hat{\phi}_0(s) + \sum_{q \in I \setminus \{0\}} \Omega(|q|_p p^{-r}) \hat{\phi}_q(s) \right]
 \end{aligned}$$

where

$$g_\alpha = \frac{1 - p^{-1}}{1 - p^{-(1+\alpha)}} \quad \tilde{G}_{\delta-r}^{\sigma-r}(k) = p^{\sigma-r} \Omega(|k|_p p^{\sigma-r}) - p^{\delta-r} \Omega(|k|_p p^{\delta-r}).$$

It is easy to find the solution to this system and write the equations for  $\hat{\phi}_0(s)$  and  $\hat{\phi}_k(s)$ . If we note that in this case the following equations hold:

$$S(t) = p^r \int_{Z_p} \phi(z, t) d\mu(z) = p^r \tilde{\phi}_0(t) \quad S(s) = p^r \hat{\phi}_0(s)$$

we can find the Laplace transform of the survival probability function

$$\hat{S}(s) = \frac{1}{s + \lambda p^{-r}} \left[ 1 + \lambda^2 p^{-2r} \frac{J_r(s)}{s + \lambda p^{-r} (1 + s J_r(s))} \right] - \frac{\lambda A [p^{\sigma-r} J_{r-\sigma}(s) - p^{\delta-r} J_{r-\delta}(s)]}{s + \lambda p^{-r} (1 + s J_r(s))} \tag{26}$$

where

$$J_l(s) = \sum_{k \in I \setminus \{0\}} \frac{\Omega(|k|_p p^{-l})}{s + p^{-\alpha r} \Gamma_p(-\alpha) (|k|_p^\alpha - g_\alpha)}.$$

Applying the inverse Laplace transformation to (26), we find  $S(t)$ .

The numerical results are as follows. The typical curves  $S(t)$  within a certain time window are shown in figures 5 and 6. It is clearly seen that there are three characteristic kinetic modes. At high temperatures (curve 1 in figure 5), the kinetics  $S(t)$  is governed by the exponential law. This mode is observed in the case of  $\tau_{\text{eq}} \ll \lambda^{-1}$ , where  $\tau_{\text{eq}}$  is the characteristic time during which the distribution  $f(x, t)$  reaches quasi-equilibrium and  $\lambda$  is the reaction sink parameter. In this case, during the observation periods  $t \gg \tau_{\text{eq}}$ , the function  $f(x, t)$  is close to a homogeneous distribution and the population of the reaction sink area (disc  $Z_p$ ) is equal to  $p^{-r} S(t)$ . Therefore,  $S(t)$  is determined by the kinetic equation

$$\frac{dS(t)}{dt} = -\lambda p^{-r} S(t)$$

which describes the exponential relaxation  $S(t) = \exp(-t/\tau)$  with the relaxation time  $\tau = p^r/\lambda$ . Since the limiting kinetic stage here is the reaction sink, this mode may be called the reaction control mode. As the temperature decreases (curves 2 and 3 in figure 5), a small section of power relaxation appears on the curve  $S(t)$  and then extends to the major part of the time window of observation. This change in the curve  $S(t)$  corresponds to the transition regime for which, with the decrease in temperature, the time of relaxation to equilibrium  $\tau_{\text{eq}}$  and the time parameter of the reaction sink  $\lambda^{-1}$  become commensurable. In this case, the kinetics of  $S(t)$  is limited first by the ultrametric diffusion (power section of the curve  $S(t)$ ), and

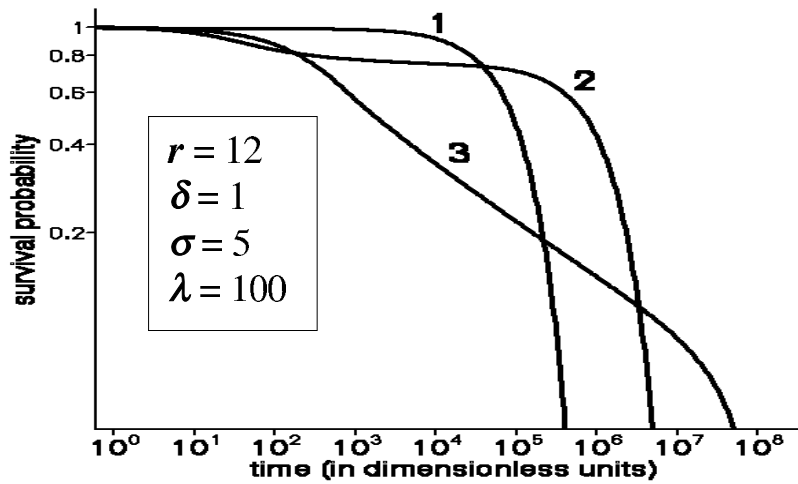


Figure 5. Typical curves  $S(t)$  for the model shown in figure 4 in the high temperature regime:  $\alpha = 0.1$  (1),  $\alpha = 0.7$  (2) and  $\alpha = 1.2$  (3). The values of other parameters are given in the inset.

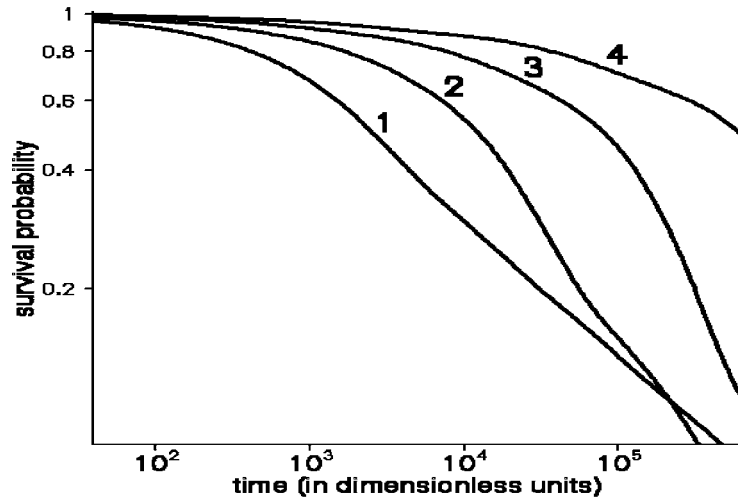


Figure 6. Typical curves  $S(t)$  for the model shown in figure 4 in the low temperature regime:  $\alpha = 1.5$  (1),  $\alpha = 2.0$  (2),  $\alpha = 2.5$  (3) and  $\alpha = 3.0$  (4). The values of other parameters are given in the inset to figure 5.

then by the reaction sink (the exponential decay). Note that if the time window of observation shows only the power section of the curve  $S(t)$ , it seems that the decay rate  $S(t)$  is growing with the decrease of temperature.

With further decrease of temperature (curves 1–3 in figure 6), a beak-shaped section appears on the curve  $S(t)$  which then extends to the entire time window under observation. This mode corresponds to situations with  $\tau_{\text{eq}} \gg \lambda^{-1}$ . In this case, the decay rate  $S(t)$  is limited by filling of the reaction sink area due to ultrametric diffusion. It is natural to call such a mode the diffusion control mode. Now, there are no ‘anomalous’ kinetic effects in the time window of observation, the rate of decay  $S(t)$  decreases as the temperature decreases.

It is interesting to note that the peculiarities of the kinetic curves for the model considered above are also typical for the ligand rebinding kinetics of myoglobin [4, 27]. Naturally, this gives grounds for some optimism. Nevertheless, we would like to stress that the main objective of this paper is to demonstrate a method for the construction of ultrametric diffusion models based on  $p$ -adic analysis. The examples given above should be considered as a mere illustration of the possibilities offered by this approach, rather than particular models giving a quantitative description of particular experiments. The development of such models seems to be a special task in each particular case.

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