Time-Varying Energy Landscapes and Temperature Paths: Dynamic Transition Rates in Locally Ultrametric Complex Systems

Ángel Morán Ledezma

angel.ledezma@kit.edu

Institute of Photogrammetry and Remote Sensing
Karlsruhe Institute of Technology

NONLINEARITY, NONLOCALITY AND ULTRAMETRICITY

International Conference on the Occasion of Branko Dragovich 80th Birthday

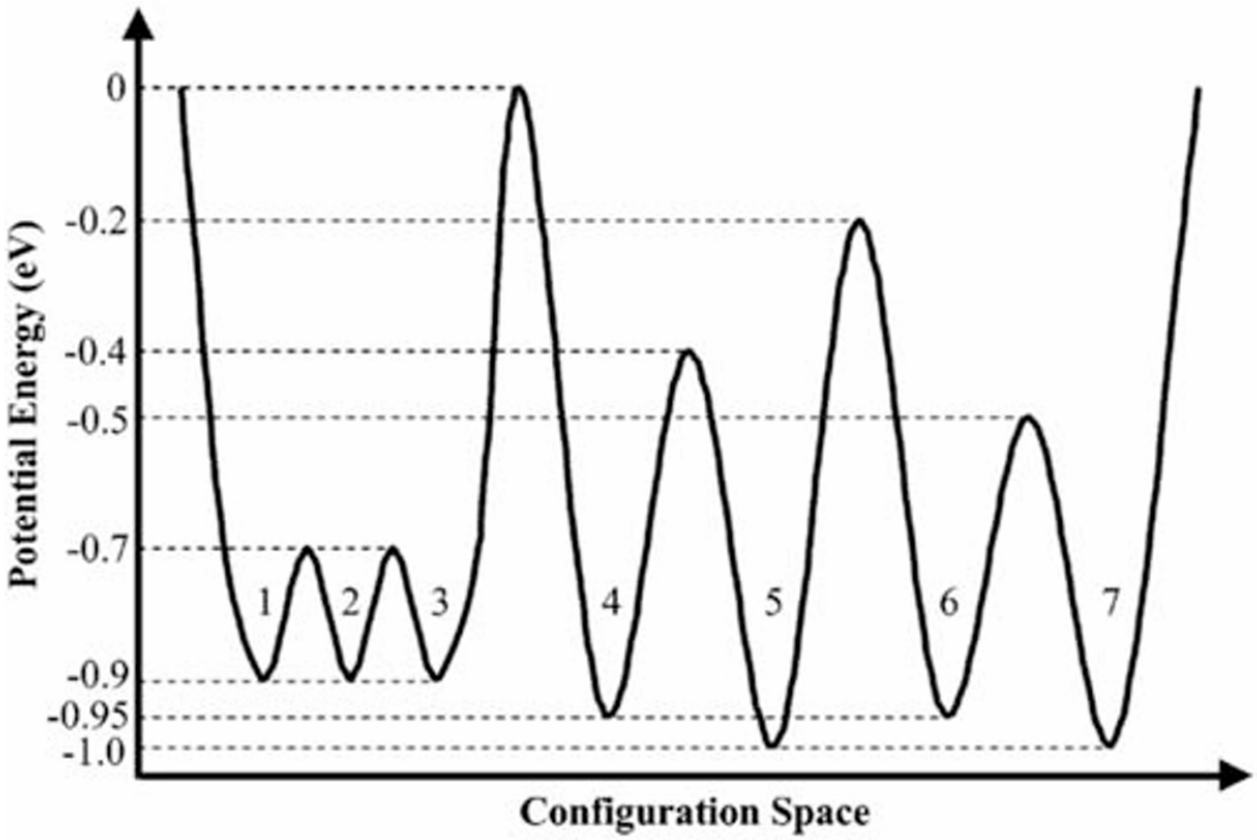
26 – 30.05.2025, Belgrade, Serbia

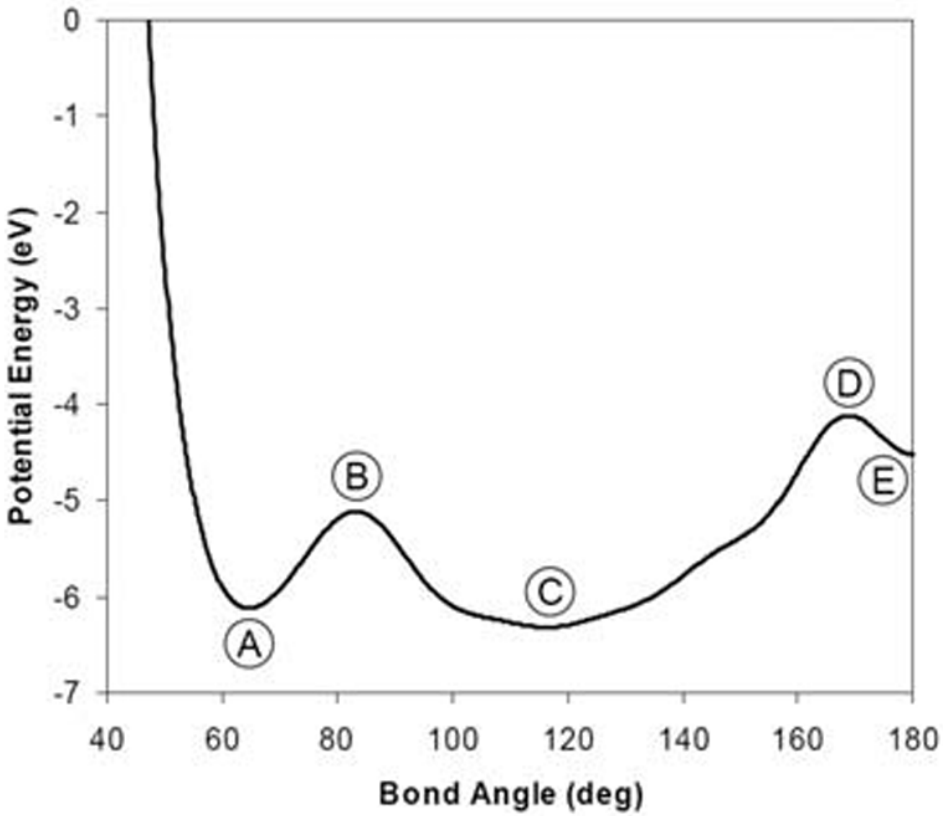
A central idea in physics of complex systems is that, non-equilibrium (relaxation) phenomena can be modeled by a CTMC where the states are local minima of a multidimensional surface called energy landscape.

The Energy Landscape Approach

- The energy landscape models all possible configurations as points on a multidimensional surface with many local minima (stable/metastable states) and barriers (transition states).
- This framework naturally separates:
  - **Fast** vibrational relaxations within basins.
  - **Slow** transitions between basins (configurational changes).
- It provides physical insight into how materials relax and evolve over time.

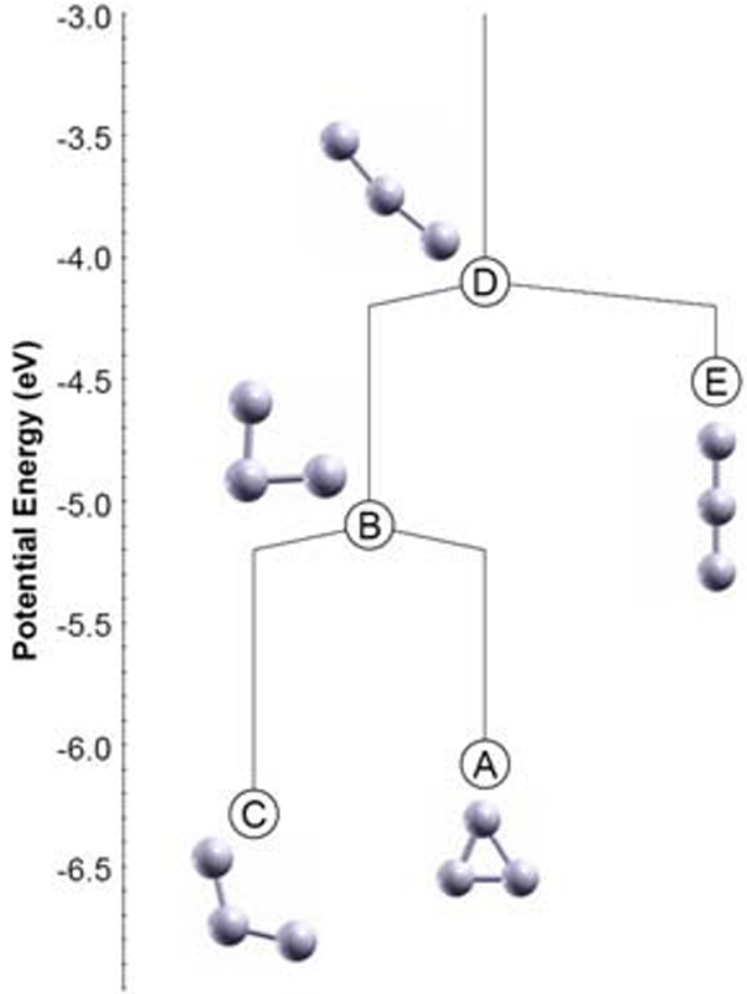
References: Stillinger & Weber, Science, 1984; Mauro et al., J. Chem. Phys., 2012.


0
-0.2
-0.4
-0.5
-0.7
-0.9
-0.95
-1.0
Potential Energy (eV)
1
2
3
4
5
6
7
Configuration Space



Minima: A C E

Transition States: B D



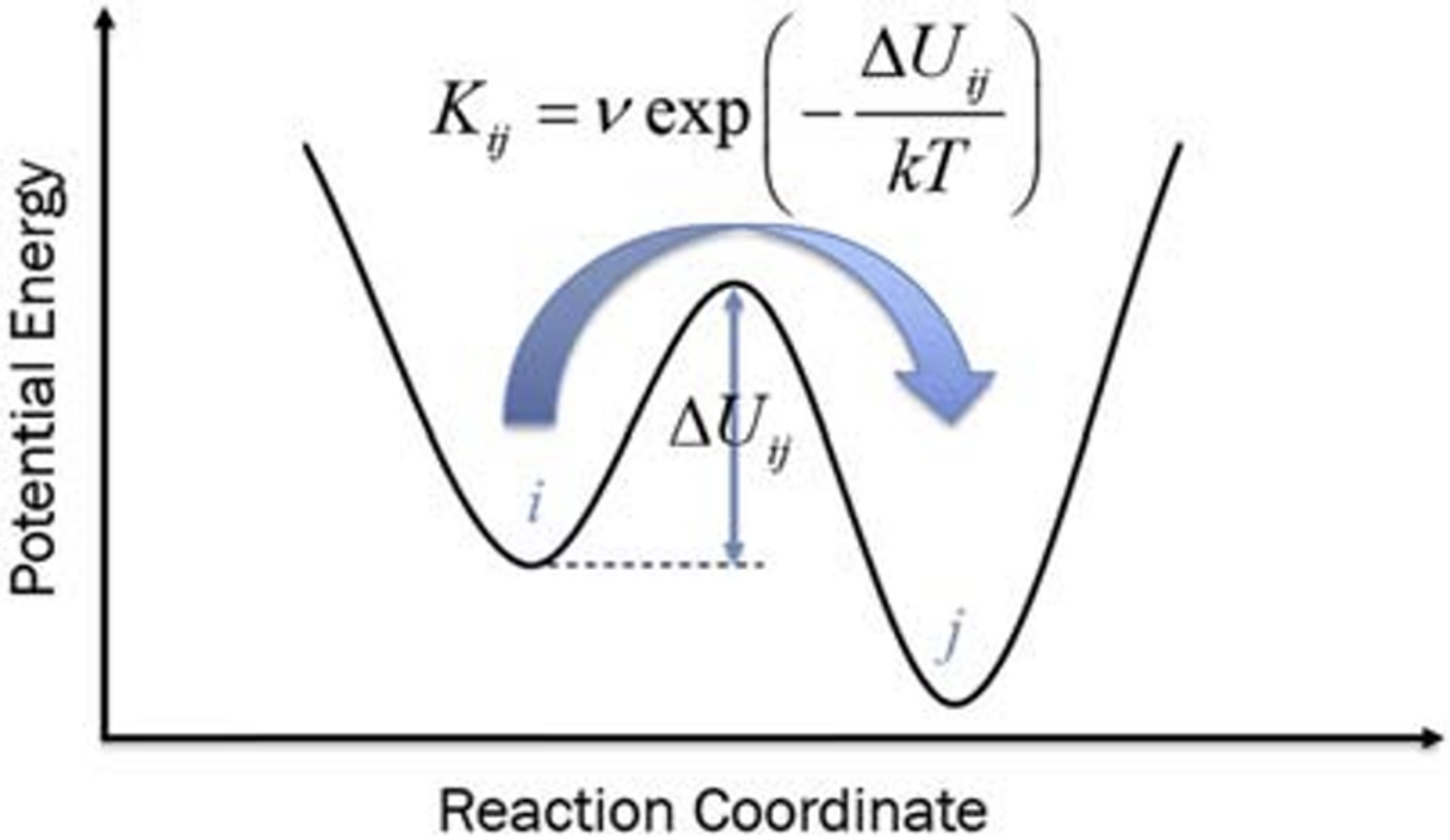
Master Equation

The evolution of the basin occupation probabilities over time, t, is governed by a set of coupled differential equations known as **master equations**:

$$\frac{d}{dt}p_i(t) = \sum_{j\neq i}^{\Omega} K_{ji}[T(t)]\, p_j(t) - \sum_{j\neq i}^{\Omega} K_{ij}[T(t)]\, p_i(t)$$

Using transition state theory, each element of the transition rate matrix can be calculated as:

$$K_{ij}[T(t)] = \nu_{ij} \exp\left[-\frac{U_{ij} - U_i}{kT(t)}\right]$$


$K_{ij} = \nu \exp\left(-\frac{\Delta U_{ij}}{kT}\right)$
Potential Energy
ΔU_{ij}
i
j
Reaction Coordinate

Q-Matrix Formulation

The master equation can be written in matrix form as a Q-matrix equation:

$$\frac{d}{dt}\mathbf{p}(t) = Q[T(t)]\,\mathbf{p}(t)$$

where $\mathbf{p}(t)$ is the vector of occupation probabilities and $Q[T(t)]$ is the transition rate matrix (Q-matrix).
The elements of the Q-matrix are given by:

$$Q_{ij}[T(t)] = \begin{cases} K_{ji}[T(t)] & \text{for } i \neq j, \\ -\sum_{k \neq i} K_{ik}[T(t)] & \text{for } i = j, \end{cases}$$

with $K_{ij}[T(t)]$ defined as before.

Solution via Matrix Exponential

For constant temperature T, the formal solution to the master equation is:

$$\mathbf{p}(t) = \exp(-Q[T]\,t)\,\mathbf{p}(0)$$

where $\exp(-Q[T]\,t)$ denotes the matrix exponential of $-Q[T]\,t$.

Why Solvable Mathematical Models for Glass Relaxation

- Glass relaxation is a key scientific and technological challenge—crucial for predicting stability and long-term behavior of materials.
- Direct simulations on experimental timescales are unfeasible for complex glasses.
- The system's enthalpy (energy) landscape is extremely complex, involving a huge number of possible configurations and transitions.

Reference: Mauro et al., *Minimalist Model of Relaxation in Glass*, J. Chem. Phys., 2012.

The Case for Minimalist (Solvable) Models

- **Too many states:** The number of energy minima and barriers is astronomically large—far too big to enumerate or analyze directly.
- **Simulations are limited:** Molecular Dynamics (MD) can only reach nanosecond timescales, but glass relaxation occurs over much longer periods (seconds to years).
- **Statistical models help... but:** They avoid the timescale problem, but are often very difficult to solve or generalize to real materials.

Solution:

Develop simple, analytically solvable models that:

- Capture the essential features of glass relaxation.
- Can be solved exactly (not only simulated).
- Allow us to study the influence of barriers, entropy, and temperature.

Reference: Mauro et al., J. Chem. Phys., 2012.

Contents lists available at SciVerse ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Minimalist landscape model of glass relaxation

John C. Mauro *, Morten M. Smedskjaer

Science and Technology Division, Corning Incorporated, Corning, NY 14831, USA

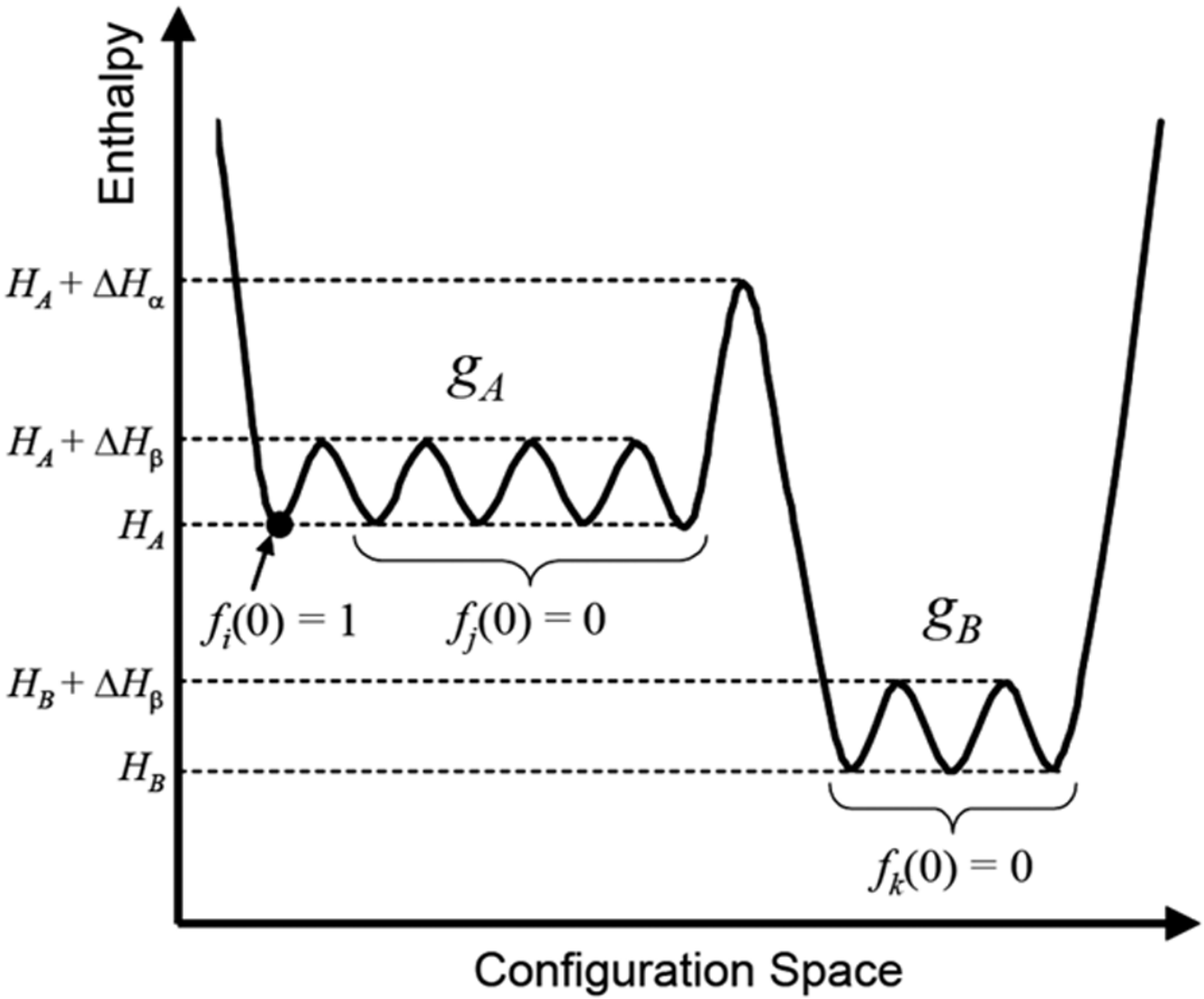
ARTICLE INFO

Article history:
Received 23 November 2011
Received in revised form 9 January 2012
Available online 3 February 2012

Keywords:
Enthalpy landscape
Glass relaxation
Modeling

ABSTRACT

The relaxation behavior of glass is of great scientific and technological importance. However, prediction of glass relaxation behavior using direct first principles techniques is currently infeasible for realistic laboratory time scales. The enthalpy landscape approach has proven to be successful in overcoming this time scale constraint and providing insights into the fundamental physics governing glass transition and relaxation behavior. However, it is still too computationally intensive to calculate representative enthalpy landscapes for multicomponent glasses of industrial interest. It is thus interesting to consider a simplified enthalpy landscape that captures the essential features of glass relaxation and can be solved analytically. Here, we present the analytical solution for such a "minimalist landscape" model that is complicated enough to capture both primary (α) and secondary (β) relaxation processes, yet simple enough to offer a closed-form solution. Using this minimalist landscape, we perform model calculations to illustrate the relative impact of activation barriers and entropy on glass relaxation behavior. The results of our model show that α and β relaxation processes are largely decoupled, in agreement with recently published experimental results.


Enthalpy
$H_A + \Delta H_\alpha$
$H_A + \Delta H_\beta$
H_A
$H_B + \Delta H_\beta$
H_B
g_A
g_B
$f_i(0) = 1$
$f_j(0) = 0$
$f_k(0) = 0$
Configuration Space

nature COMMUNICATIONS

ARTICLE

Received 31 Dec 2013 | Accepted 26 Mar 2014 | Published 24 Apr 2014

DOI: 10.1038/ncomms4725

Fractal free energy landscapes in structural glasses

Patrick Charbonneau[1,2,3], Jorge Kurchan[4], Giorgio Parisi[5,6], Pierfrancesco Urbani[7] & Francesco Zamponi[3]

Glasses are amorphous solids whose constituent particles are caged by their neighbours and thus cannot flow. This sluggishness is often ascribed to the free energy landscape containing multiple minima (basins) separated by high barriers. Here we show, using theory and numerical simulation, that the landscape is much rougher than is classically assumed. Deep in the glass, it undergoes a 'roughness transition' to fractal basins, which brings about isostaticity and marginal stability on approaching jamming. Critical exponents for the basin width, the weak force distribution and the spatial spread of quasi-contacts near jamming can be analytically determined. Their value is found to be compatible with numerical observations. This advance incorporates the jamming transition of granular materials into the framework of glass theory. Because temperature and pressure control what features of the landscape are experienced, glass mechanics and transport are expected to reflect the features of the topology we discuss here.

Degeneracy in Native and Unfolded Basins

- **Native basin:** The native state is not a single structure, but an ensemble of rapidly interconverting, nearly isoenergetic conformations.[1]
- **Unfolded basin:** The unfolded state also consists of a heterogeneous ensemble of conformations, separated by barriers of various heights, with rapid transitions between them.[2]
- **Modeling perspective:** Both basins can be described as clusters of (quasi-)degenerate states, justifying hierarchical models with multiple barrier scales.[3]

This supports the use of models with two metabasins, each containing many (nearly) degenerate substates separated by multi-scale energy barriers.

[1] A.N. Yakubovich et al., *Biochim. Biophys. Acta*, 2004; see also Onuchic & Wolynes, *Curr. Opin. Struct. Biol.*, 2004.
[2] L. S. Itzhaki et al., *Protein Science*, 2006; F. Ding et al., *PNAS*, 2005.
[3] J. E. Shea et al., *Annu. Rev. Phys. Chem.*, 1999; F. Ding et al., *PNAS*, 2005.

Why Study Time-Dependent Energy Landscapes?

- **Real materials and biomolecules experience changing environments.**
- In *glasses*, relaxation dynamics depend on the "temperature path"—the history of how temperature changes with time.[4]
- In *proteins*, both the energy landscape and transition rates can vary over time due to:
  - Artificial modulation (e.g., controlled temperature ramps)
  - Intracellular interactions and physiological processes
  - Environmental fluctuations
- Time-dependent rates are key to understanding non-equilibrium dynamics and memory effects.

[4] Mauro et al., J. Chem. Phys., 2012

The p-adic Numbers and the p-adic Norm

- Let $\mathbb{Q}$ be the set of rational numbers.
- For a prime p, the p-adic norm of $x = \frac{a}{b} \neq 0$ is defined as $|x|_p = p^{-\nu(x)}$, where $\frac{a}{b} = p^{\nu} \frac{a'}{b'}$ for some integer ν and coprime a', b'.
- The norm extends by setting $|0|_p := 0$.
- The completion of $\mathbb{Q}$ with respect to $|\cdot|_p$ gives the field $\mathbb{Q}_p$ of p-adic numbers.

Properties of $\mathbb{Q}_p$

- $(\mathbb{Q}_p, |\cdot|_p)$ is an ultrametric space:

$$|x+y|_p \leq \max\{|x|_p, |y|_p\}$$

- There is a Haar measure dx on $\mathbb{Q}_p$.
- Every $x \in \mathbb{Q}_p$ can be written as a convergent Laurent series:

$$x = \sum_{k=\nu}^{\infty} x_k p^k, \quad x_k \in \{0, \ldots, p-1\}$$

- The unit ball is $\mathbb{Z}_p := \{x \in \mathbb{Q}_p : |x|_p \leq 1\}$.
- A function $w : \mathbb{Q}_p \to \mathbb{R}$ is called **radial** if $w(x) = w(|x|_p)$.

Finite p-adic Groups and Ball Decomposition

- The finite group $G_n := \mathbb{Z}_p/p^n\mathbb{Z}_p$ consists of elements

$$G_n \ni x = a_0 + a_1 p + \cdots + a_{n-1}p^{n-1}, \quad a_i \in \{0, \ldots, p-1\}$$

- $\mathbb{Z}_p$ decomposes as a disjoint union:

$$\mathbb{Z}_p = \bigsqcup_{a \in G_n} a + p^n\mathbb{Z}_p$$

Tree Representation of G_n for $p = 2$

Level 0: radius $2^0 = 1$

Level 1: radius $2^{-1} = \frac{1}{2}$

Level 2: radius $2^{-2} = \frac{1}{4}$

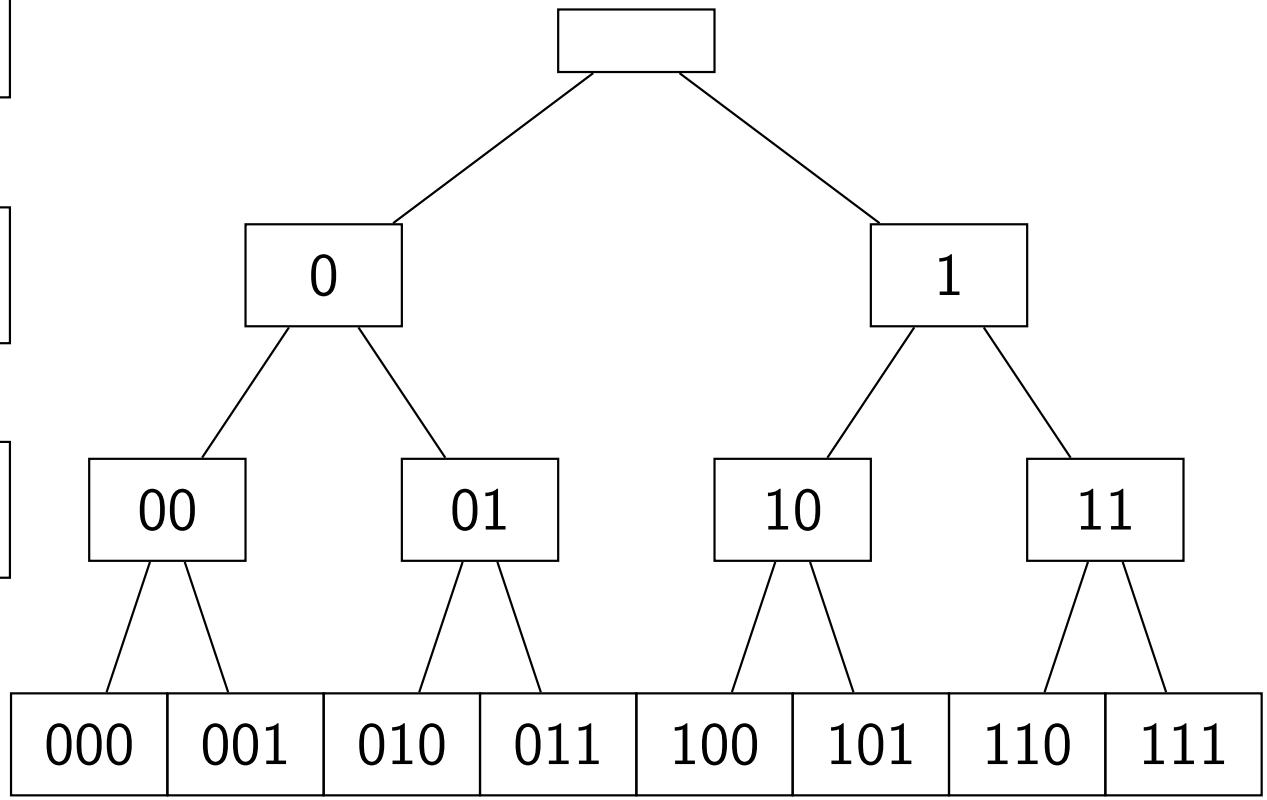


Figure: Tree representation of G_3 for $p = 2$

The p-adic Ball Operator

Let

$$W_{\mathbb{Z}_p} f(x,t) = \int_{\mathbb{Z}_p} w(|x-y|)\,[f(y,t) - f(x,t)]\; dy.$$

As $n \to \infty$, we obtain the evolution equation:

$$\frac{d}{dt} f(x,t) = \int_{\mathbb{Z}_p} w(|x-y|)\,[f(y,t) - f(x,t)]\; dy.$$

Finite Dimensional Approximation

- Let $V_n = \mathrm{Span}_{\mathbb{C}}\{\varphi_a(x) := p^n 1_{a+p^n\mathbb{Z}_p}(x)\}$, where $1_{a+p^n\mathbb{Z}_p}(x)$ is the indicator function of the ball $a + p^n\mathbb{Z}_p$.
- Then $V_n \cong \mathbb{C}^{p^n}$.

Matrix Representation

- With respect to the basis $\{\varphi_a\}_{a\in G_n}$, the matrix representation is

$$\langle \varphi_b, W_{\mathbb{Z}_p}\varphi_a\rangle_{L^2(\mathbb{Z}_p)} = w(|a-b|_p), \quad \text{for } a \neq b,$$

$$\langle \varphi_a, W_{\mathbb{Z}_p}\varphi_a\rangle_{L^2(\mathbb{Z}_p)} = -\gamma_a,$$

where $\gamma_a = \sum_{b\in G_n, b\neq a} w(|a-b|_p)$.

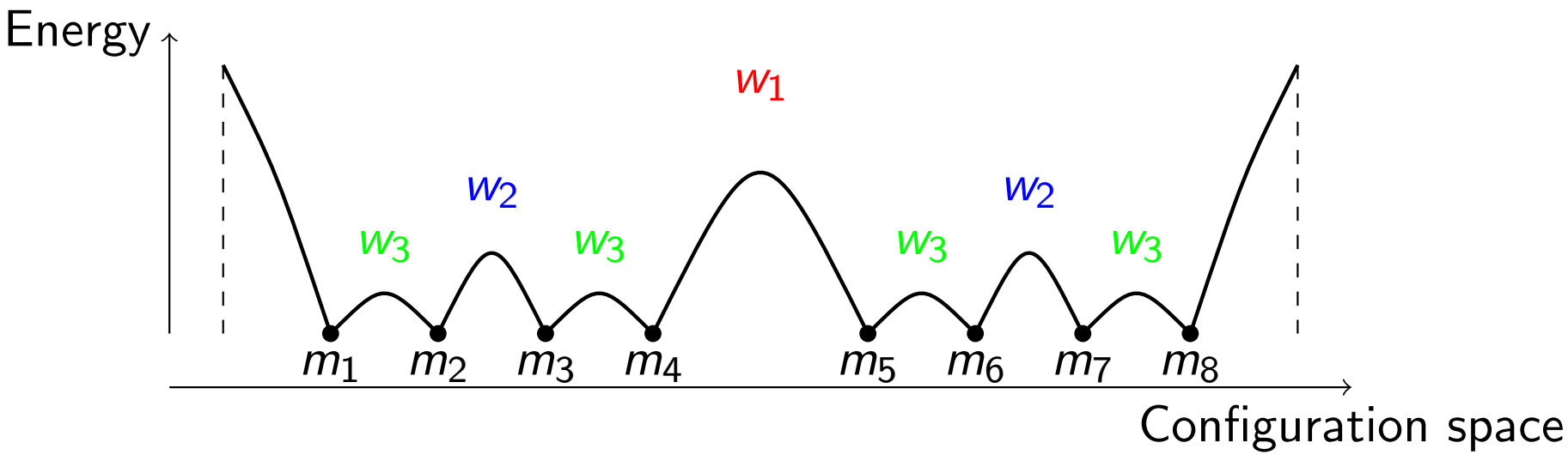
Master Equation for the Finite System

The system restricted to V_n yields a master equation for a continuous time Markov chain:

$$\frac{d}{dt}\varphi(t) = \mathbf{W}_{\mathbb{Z}_p}^{(n)}\varphi(t),$$

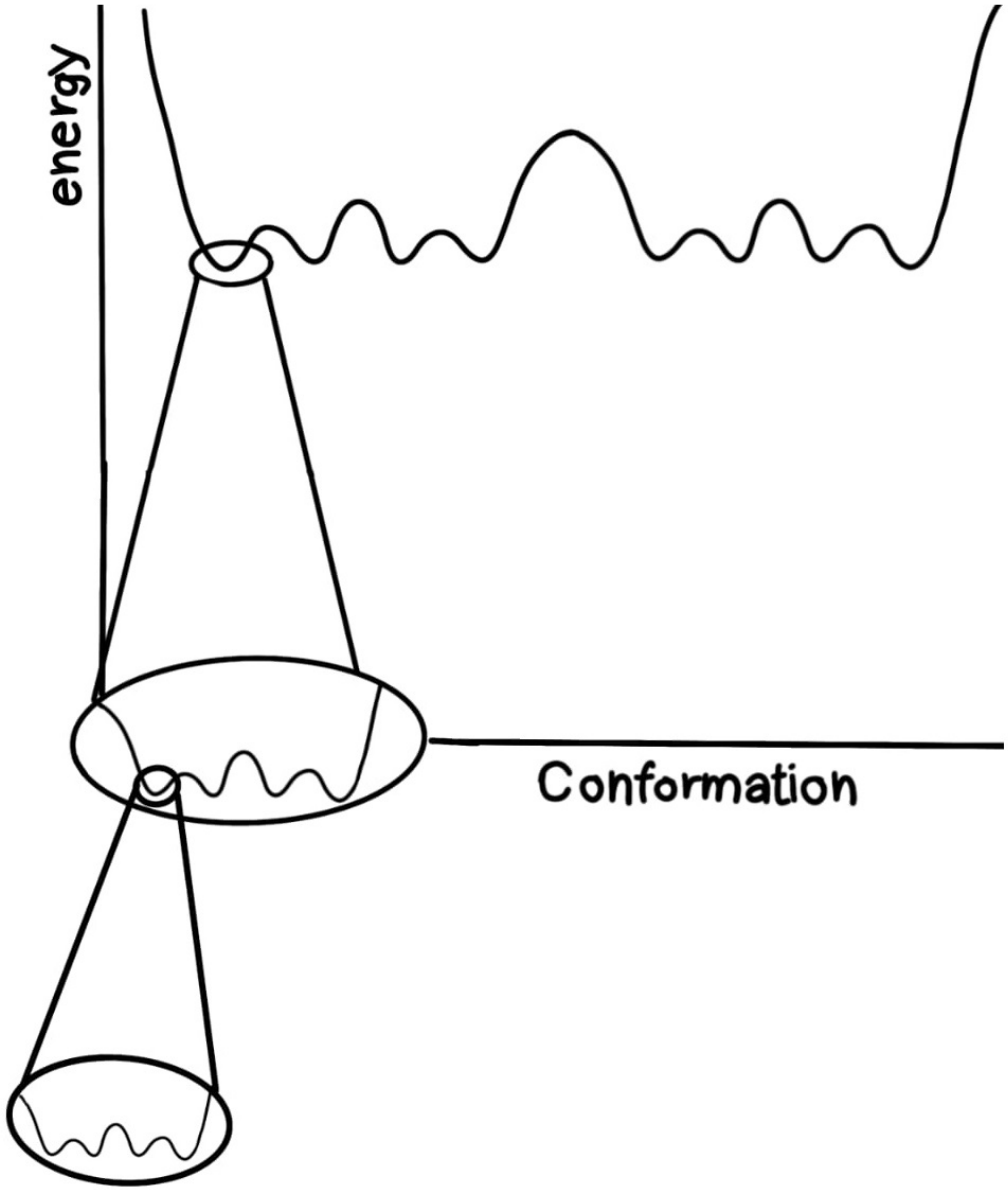
where $\varphi(t) \in \mathbb{C}^{p^n}$ and the matrix entries are

$$(\mathbf{W}_{\mathbb{Z}_p}^{(n)})_{a,b} = \begin{cases} w(|a-b|_p), & \text{if } a \neq b \\ -\gamma_a, & \text{if } a = b \end{cases}$$


Energy
w_1
w_2
w_2
w_3
w_3
w_3
w_3
m_1
m_2
m_3
m_4
m_5
m_6
m_7
m_8
Configuration space

$$\begin{bmatrix} w_0 & w_3 & w_2 & w_2 & w_1 & w_1 & w_1 & w_1 \\ w_3 & w_0 & w_2 & w_2 & w_1 & w_1 & w_1 & w_1 \\ w_2 & w_2 & w_0 & w_3 & w_1 & w_1 & w_1 & w_1 \\ w_2 & w_2 & w_3 & w_0 & w_1 & w_1 & w_1 & w_1 \\ w_1 & w_1 & w_1 & w_1 & w_0 & w_3 & w_2 & w_2 \\ w_1 & w_1 & w_1 & w_1 & w_3 & w_0 & w_2 & w_2 \\ w_1 & w_1 & w_1 & w_1 & w_2 & w_2 & w_0 & w_3 \\ w_1 & w_1 & w_1 & w_1 & w_2 & w_2 & w_3 & w_0 \end{bmatrix}$$

When n increase, the number number of barriers and the depth increase.



Master Equation with Time-Dependent Transition Function

We propose to study the dynamics generated by a master equation of the form:

$$\frac{d}{dt}f(x,t) = \int_{K_N} [w(x,y,t)f(y,t) - w(y,x,t)f(x,t)]\, dy,$$

where

$$K_N = \bigsqcup_{I \in V} I + \mathbb{Z}_p.$$

and $w : K_N \times K_N \times (0,\infty) \to (0,\infty)$ is a not necessarily symmetric function .

Ultrametric diffusion, rugged energy landscapes and transition networks☆

W.A. Zúñiga-Galindo

University of Texas Rio Grande Valley, School of Mathematical & Statistical Sciences, One West University Blvd, Brownsville, TX 78520, United States

ARTICLE INFO

Article history:
Received 17 January 2022
Received in revised form 7 March 2022
Available online 14 March 2022

MSC:
35S05
60J76
82C44

Keywords:
Ultrametricity
p-adic diffusion
Markov processes
Energy landscapes
Protein folding
p-adic mathematical physics

ABSTRACT

In this article we introduce the ultrametric networks which are *p*-adic continuous analogs of the standard Markov state models constructed using master equations. A *p*-adic transition network (or an ultrametric network) is a model of a complex system consisting of a hierarchical energy landscape, a Markov process on the energy landscape, and a master equation. The energy landscape consists of a finite number of basins. Each basin is formed by infinitely many network configurations organized hierarchically in an infinite regular tree. The transitions between the basins are determined by a transition density matrix, whose entries are functions defined on the energy landscape. The Markov process in the energy landscape encodes the temporal evolution of the network as random transitions between configurations from the energy landscape. The master equation describes the time evolution of the density of the configurations. We focus on networks where the transition rates between two different basins are constant functions, and the jumping process inside of each basin is controlled by a *p*-adic radial function. We solve explicitly the Cauchy problem for the master equation attached to this type of networks. The solution of this problem is the network response to a given initial concentration. If the Markov process attached to the network is conservative, the long term response of the network is controlled by a Markov chain. If the process is not conservative the network has absorbing states. We define an absorbing time, which depends on the initial concentration, if this time is finite the network reaches an absorbing state in a finite time. We identify in the response of the network the terms responsible for bringing the network to an absorbing state, we call them the fast transition modes. The existence of the fast transition modes is a consequence of the assumption that the energy landscape is ultrametric (hierarchical), and to the best of our understanding this result cannot be obtained by using standard methods of Markov state models. Nowadays, it is widely accepted that protein native states are kinetic hubs that can be reached quickly from any other state. The existence of fast transition modes implies that certain states on an ultrametric network work as kinetic hubs.

In this work, W.A. Zuñiga-Galinda use two functions $w(x|y), w(y,x) \in C(K_N \times K_N)$ satisfying $w(x|y) \leq w(y|x)$. Here $w(x,y) \geq 0$ is one function not necessarily symmetric.

Time-Dependent p-adic Transition Function

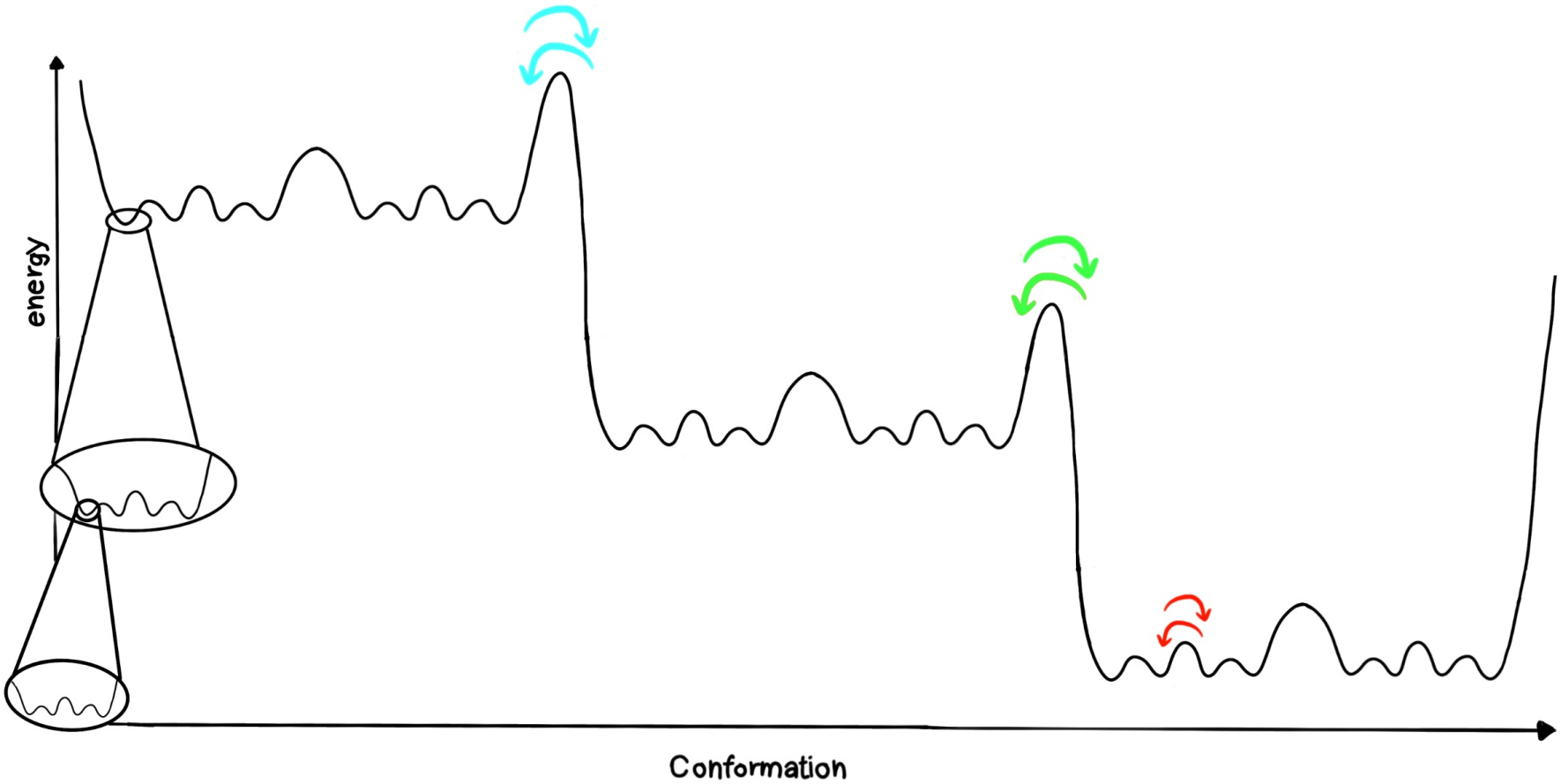
Definition

A time-dependent p-adic transition function
$w : K_N \times K_N \times (0, \infty) \to (0, \infty)$ is a function of the form:

$$w(x, y, t) = \sum_{I,J \in V} w_{I,J}(x, y, t)\, \Omega(p^N |x - I|_p)\, \Omega(p^N |y - J|_p)$$

where:

- $w_{I,I}(x, y, t) = w(|x - y|_p, t)$ are bounded radial functions,
- $w_{I,J}(x, y, t) = w_{I,J}(t)$ for $I \neq J$.


energy
Conformation

Block Structure of the Transition Rate Matrix

The transition rate matrix is given by

$$\mathbf{W}(t) = \left(P_{I,J}(t)\right),$$

where each diagonal block $P_{II}(t)$ has the Parisi matrix form:

$$\begin{bmatrix}
w_0(t) & w_3(t) & w_2(t) & w_2(t) & w_1(t) & w_1(t) & w_1(t) & w_1(t) \\
w_3(t) & w_0(t) & w_2(t) & w_2(t) & w_1(t) & w_1(t) & w_1(t) & w_1(t) \\
w_2(t) & w_2(t) & w_0(t) & w_3(t) & w_1(t) & w_1(t) & w_1(t) & w_1(t) \\
w_2(t) & w_2(t) & w_3(t) & w_0(t) & w_1(t) & w_1(t) & w_1(t) & w_1(t) \\
w_1(t) & w_1(t) & w_1(t) & w_1(t) & w_0(t) & w_3(t) & w_2(t) & w_2(t) \\
w_1(t) & w_1(t) & w_1(t) & w_1(t) & w_3(t) & w_0(t) & w_2(t) & w_2(t) \\
w_1(t) & w_1(t) & w_1(t) & w_1(t) & w_2(t) & w_2(t) & w_0(t) & w_3(t) \\
w_1(t) & w_1(t) & w_1(t) & w_1(t) & w_2(t) & w_2(t) & w_3(t) & w_0(t)
\end{bmatrix}$$

Off-Diagonal Blocks

The off-diagonal blocks are given by

$$P_{IJ}(t) = \begin{bmatrix} w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \\ w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) & w_{IJ}(t) \end{bmatrix}$$

for $I \neq J$.

Theorem

Let $w(x,y,t)$ be a time-dependent p-adic transition function such that the functions $w(x,y,t)$ is uniformly continuous. Then there exists a probability transition function $P(t,x;s,\cdot)$, where $(t,x,s) \in [0,T] \times K \times [0,T]$, and $s \leq t$, on the Borel σ-algebra of K, such that the Cauchy problem

$$\begin{cases} \frac{\partial u}{\partial t}(x,t) = \int_{K_N} [w(x,y,t)u(y,t) - w(y,x,t)u(x,t)]\, dy \\ u(x,s) = u(x) \in C(K_N), \end{cases}$$

has a unique solution satisfying:

$$\mathbb{E}[\varphi(X_t) \mid X_s \sim u(x)\, dx] = \int_{K_N \times K_N} \varphi(y) P(t,x;s,dy) u(x) dx = \int_{K_N} \varphi(x) u(x,t) dx$$

In addition, $P(t,x;s,\cdot)$ is the transition function of a strong Markov process.

Summary of the Proof

- Fix $t_0 > 0$ and define $w_0(x, y) = w(x, y, t_0)$.
- The operator $\mathbf{W}^* u(x) = \int_{K_N} w_0(x, y)[u(y) - u(x)]dy$ generates a Feller semigroup (Hille-Yosida theorem):
  - (a) The range of $\lambda_0 - \mathbf{W}^*$ is dense in $C(K_N)$.
  - (b) Maximum principle: if f attains its maximum at x_0, then $\mathbf{W}^* f(x_0) < 0$.
- The time-dependent operator $\mathbf{W}^*(t)$ generates a Feller evolution, yielding a strong Markov process with transition probabilities $P(t, x; s, dy)$.
- The evolution families of $\mathbf{W}(t)$ and its adjoint $\mathbf{W}^*(t)$ are dual in $L^2(K_N)$:

$$\int_{K_N} (P_{\mathbf{W}^*}(t, s)f)(x)g(x)dx = \int_{K_N} f(x)(P_{\mathbf{W}}(t, s)g)(x)dx$$

- Consequently, for a solution $u(x, t)$ of the Cauchy problem,

$$\mathbb{E}[\varphi(X_t)|X_s \sim u(x)dx] = \int_{K_N} \varphi(x)u(x, t)dx$$

Theorem

Let $w(x,y,t)$ be a time-time dependent p-adic transition function satisfying the hypothesis of Theorem 2. Then the solution of the Cauchy problem (with initial condition at s) is given by

$$u(x,t+s)u_0(x) = \hat{u}(x,t+s) + \sum_{supp(\Psi_{j,I,r})\subset K_N} C_{r,I,j}(s)e^{-\int_s^t \gamma_{I,r}(\tau)d\tau}\psi_{j,I,r}(x),$$

where $t \geq s$, and the coefficients $C_{r,I,j}(s)$ are uniquely determined by the initial condition.

Here:

$$\gamma_{I,r}(t) = \int_{\mathbb{Z}_p \setminus p^{r-1}\mathbb{Z}_p} w_{II}(|x|_p,t)dx + p^{r-1}w(p^r,t) + \sum_{J\in V} w_{IJ}(t)$$

Frame Title

Where

$$\hat{u}(x,t)$$

is the solution of the CTMC attached to the matrix $w_{I,J}(t)$ (the transitions between metabasins only.

We have the decomposition

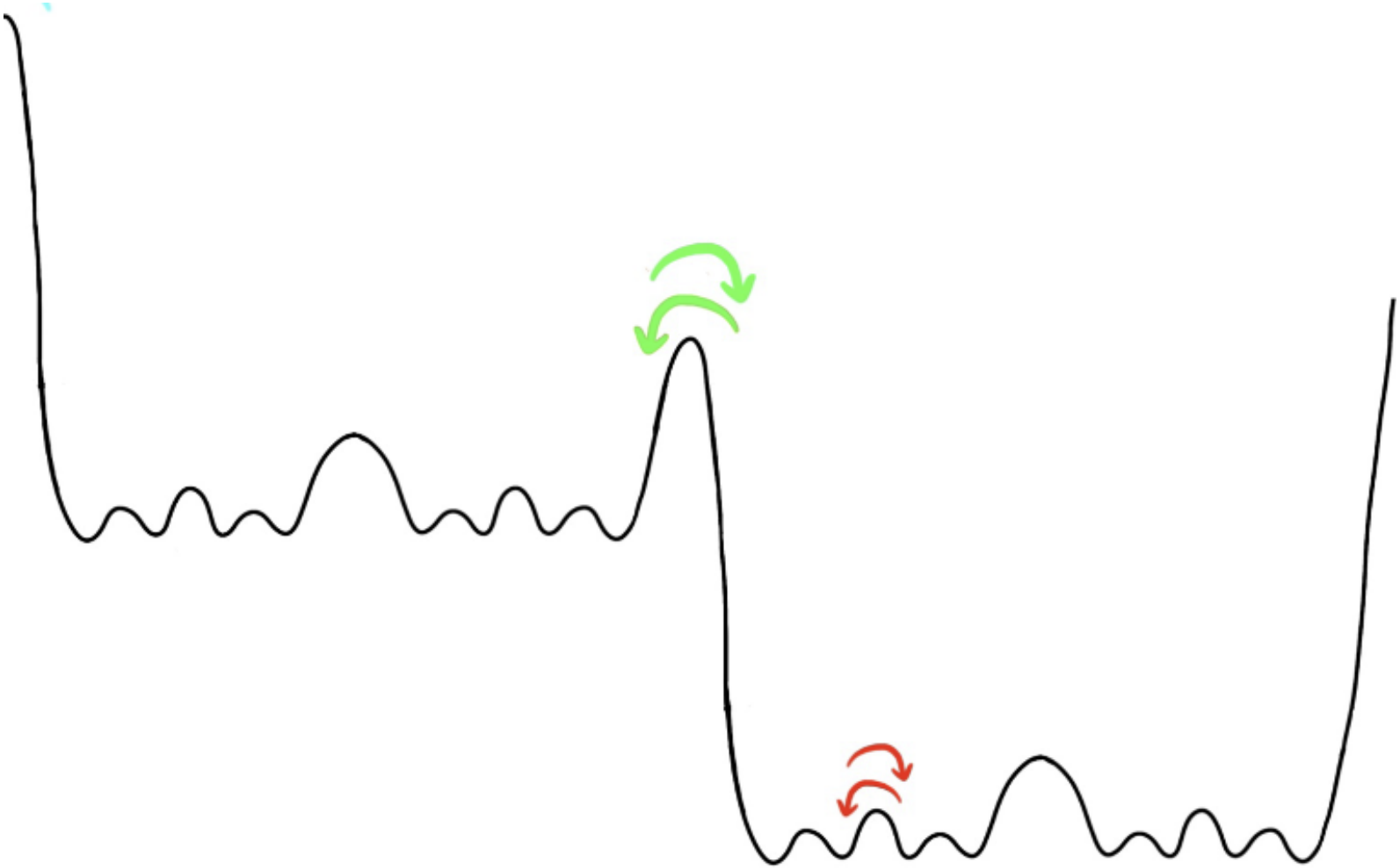
$$L^2(K_N) = \mathbb{C}^{|V|} \oplus \mathcal{L}_0(K_N).$$

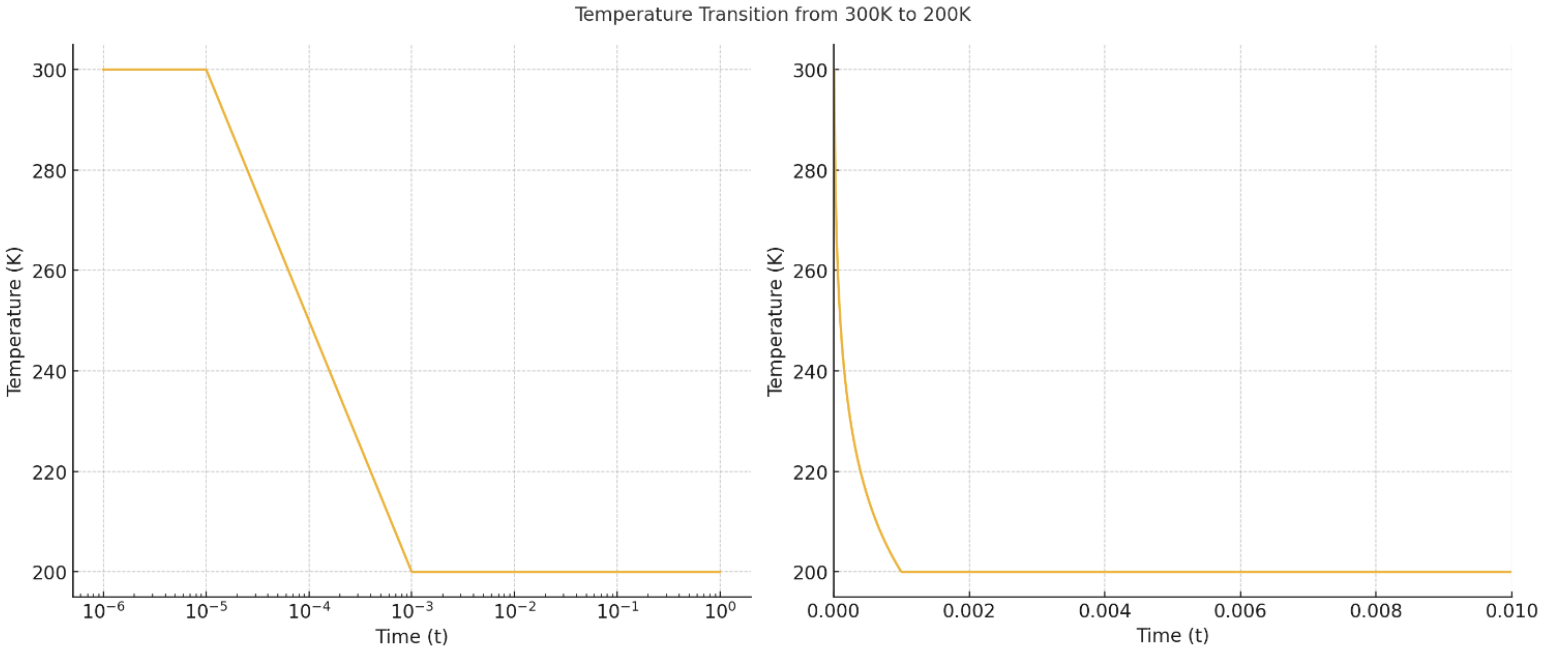
For any $f \in L^2(K_N)$ denote by $\hat{f}$ the projection of f in the space $\mathbb{C}^{|V|} \cong span\{1_{a+\mathbb{Z}_p}\}_{a \in V}$. Then, we have

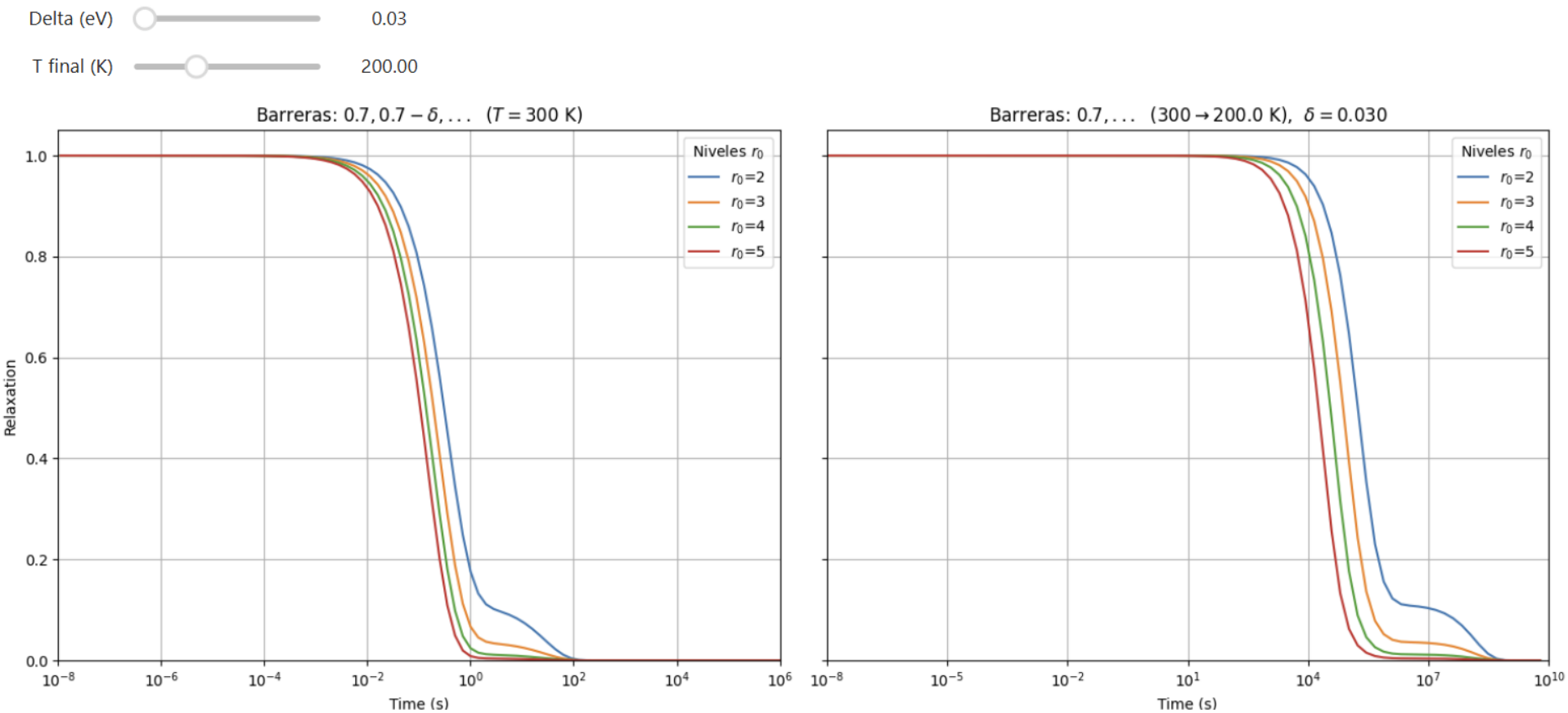
$$f(x) = \hat{f} + \sum_{supp(\Psi_{j,I,r}) \subset K_N} C_{j,I,r}\psi_{j,I,r}.$$

In a two metabasin model: $\mathbb{Z}_p$ and $a + \mathbb{Z}_p$, with initial condition $u(x) = 1_{p^{-r_0}\mathbb{Z}_p}(x)$ the characteristic relaxation is given by

$$S(t) = p^{-r_0} p_1(t) + p^{-r_0} \sum_{Supp\ \psi_{r,j,n} \not\subset B_U} |C_{r,j,n}|^2 e^{-\int_0^t \gamma_{r,U}(\tau) d\tau}$$

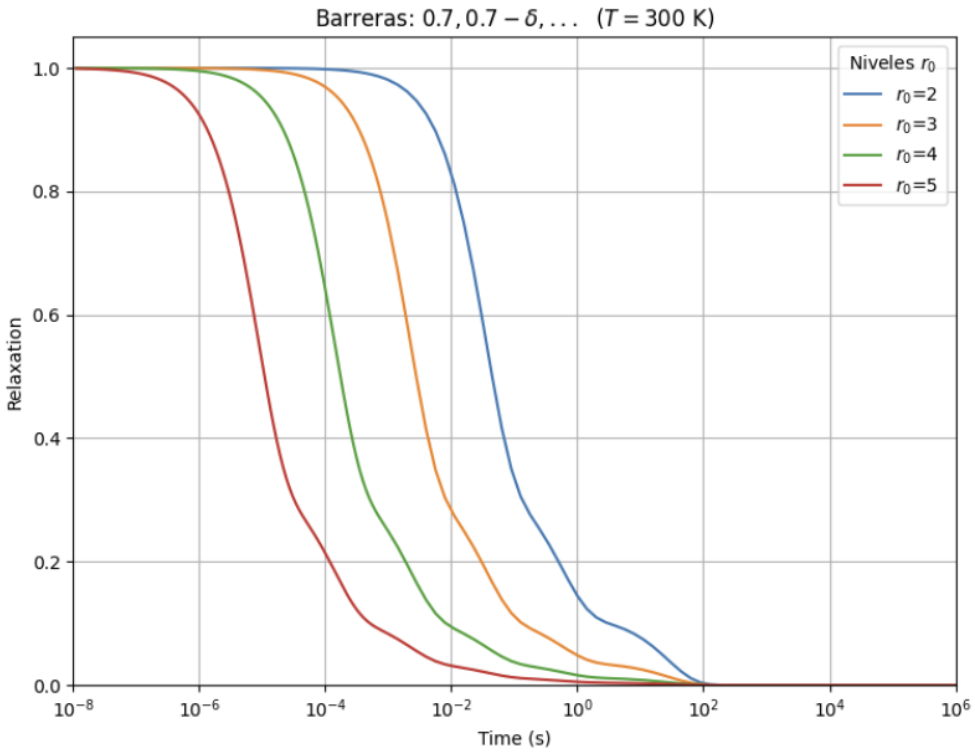


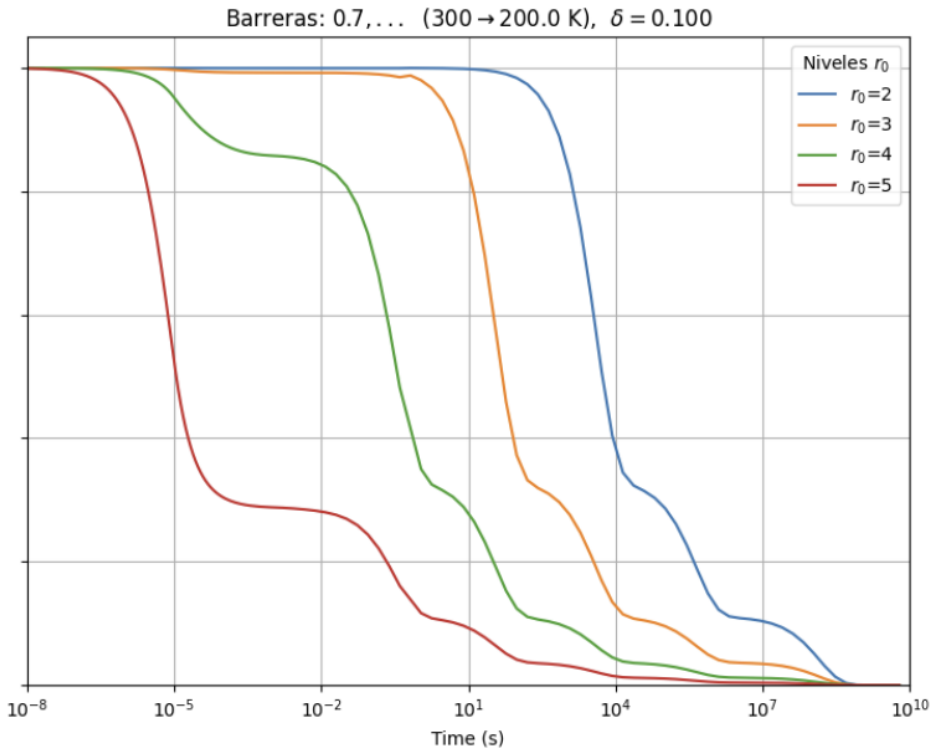

Temperature Transition from 300K to 200K
Temperature (K)
Time (t)
300
280
260
240
220
200
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
0.000
0.002
0.004
0.006
0.008
0.010

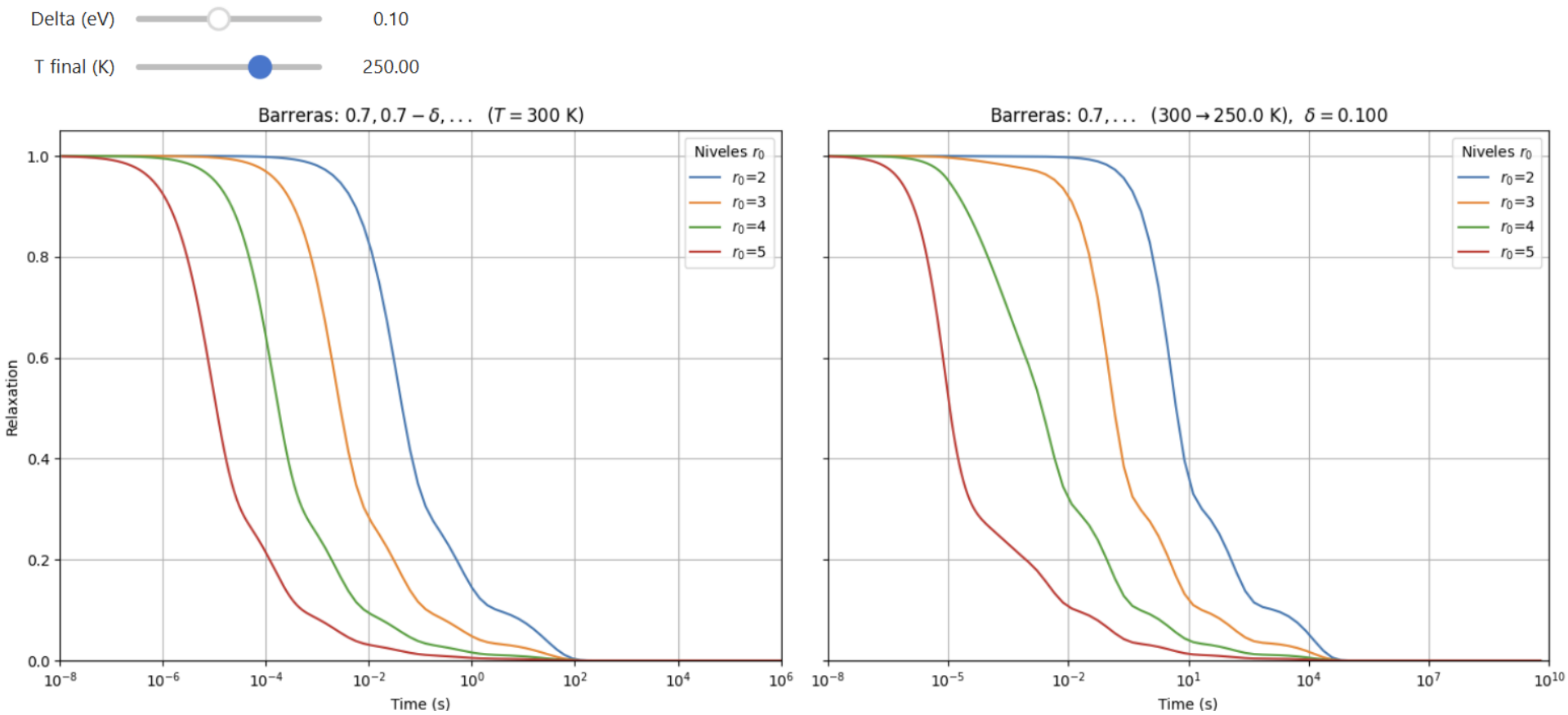

Delta (eV)
0.03
T final (K)
200.00
Barreras: 0.7, 0.7 − δ, . . . (T = 300 K)
Barreras: 0.7, . . . (300 → 200.0 K), δ = 0.030
Niveles r0
r0=2
r0=3
r0=4
r0=5
Relaxation
Time (s)

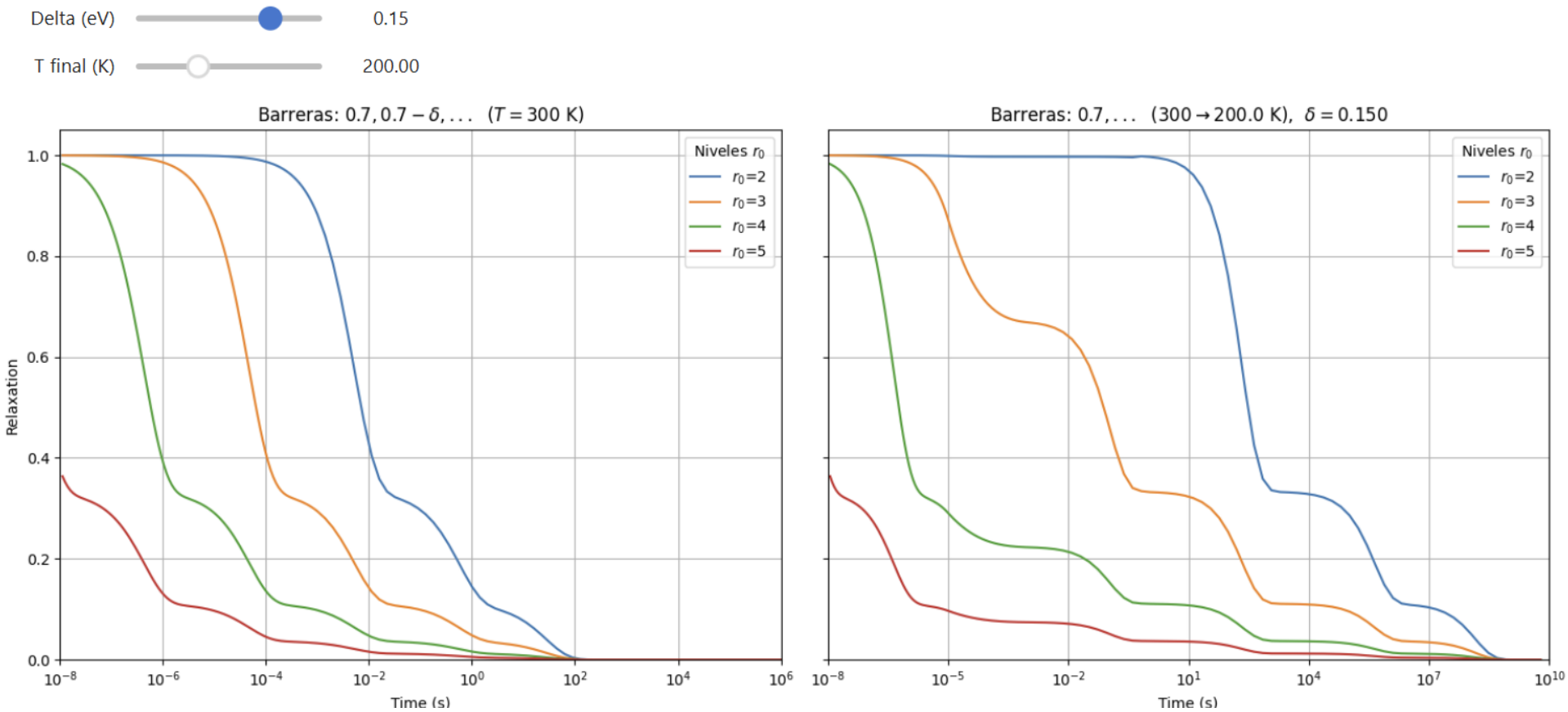
Delta (eV) 0.10

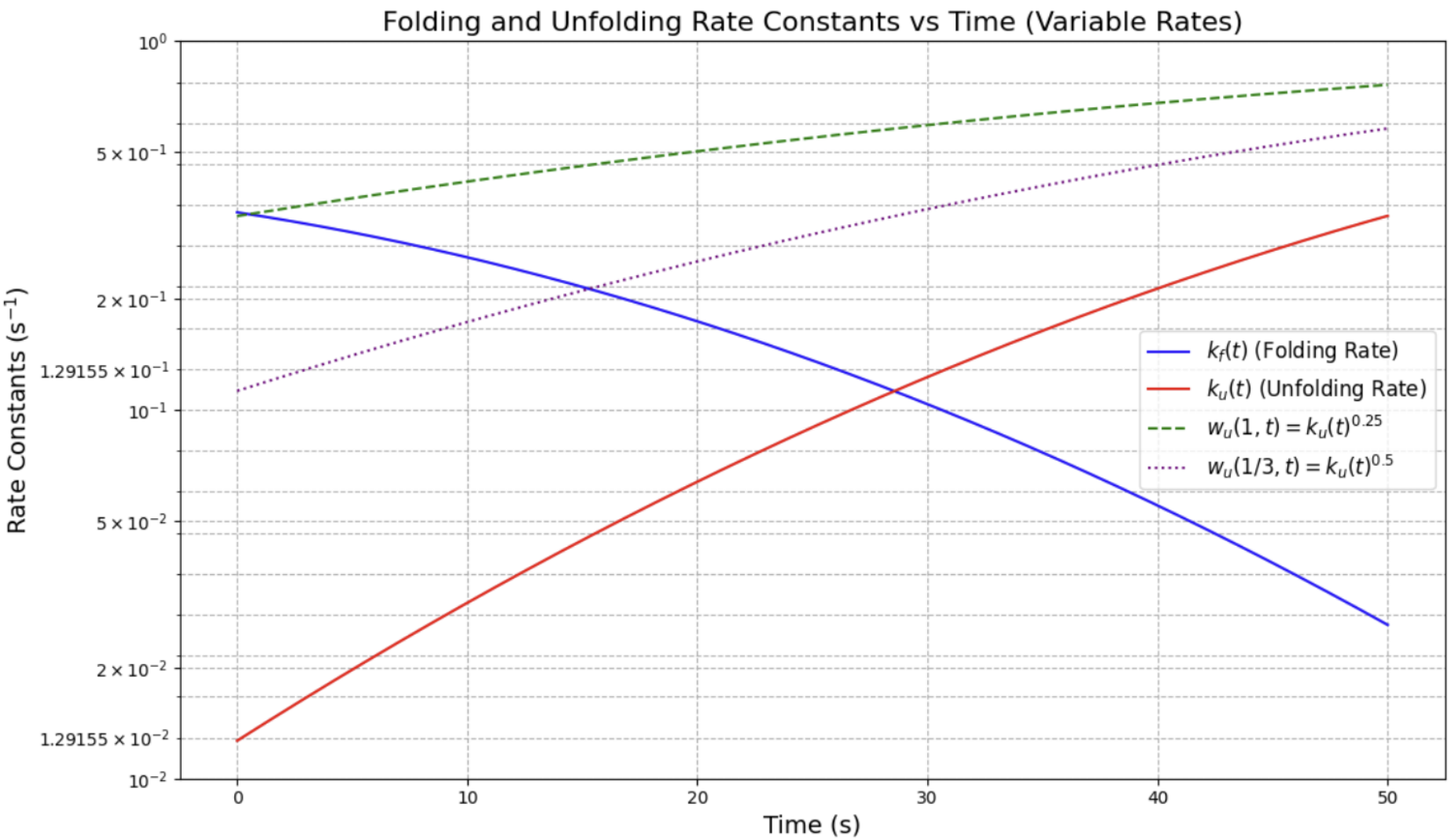
T final (K) 200.00

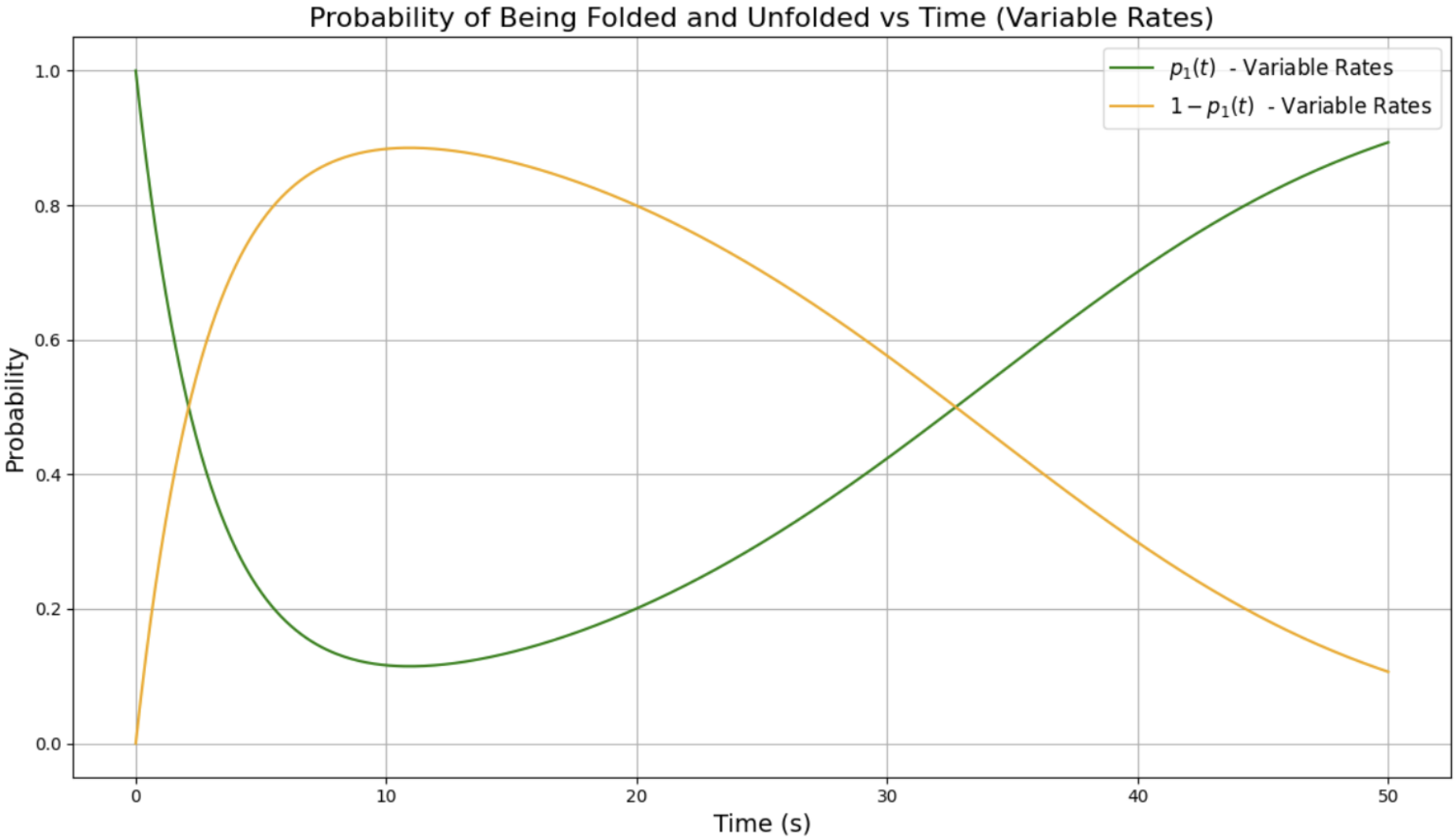


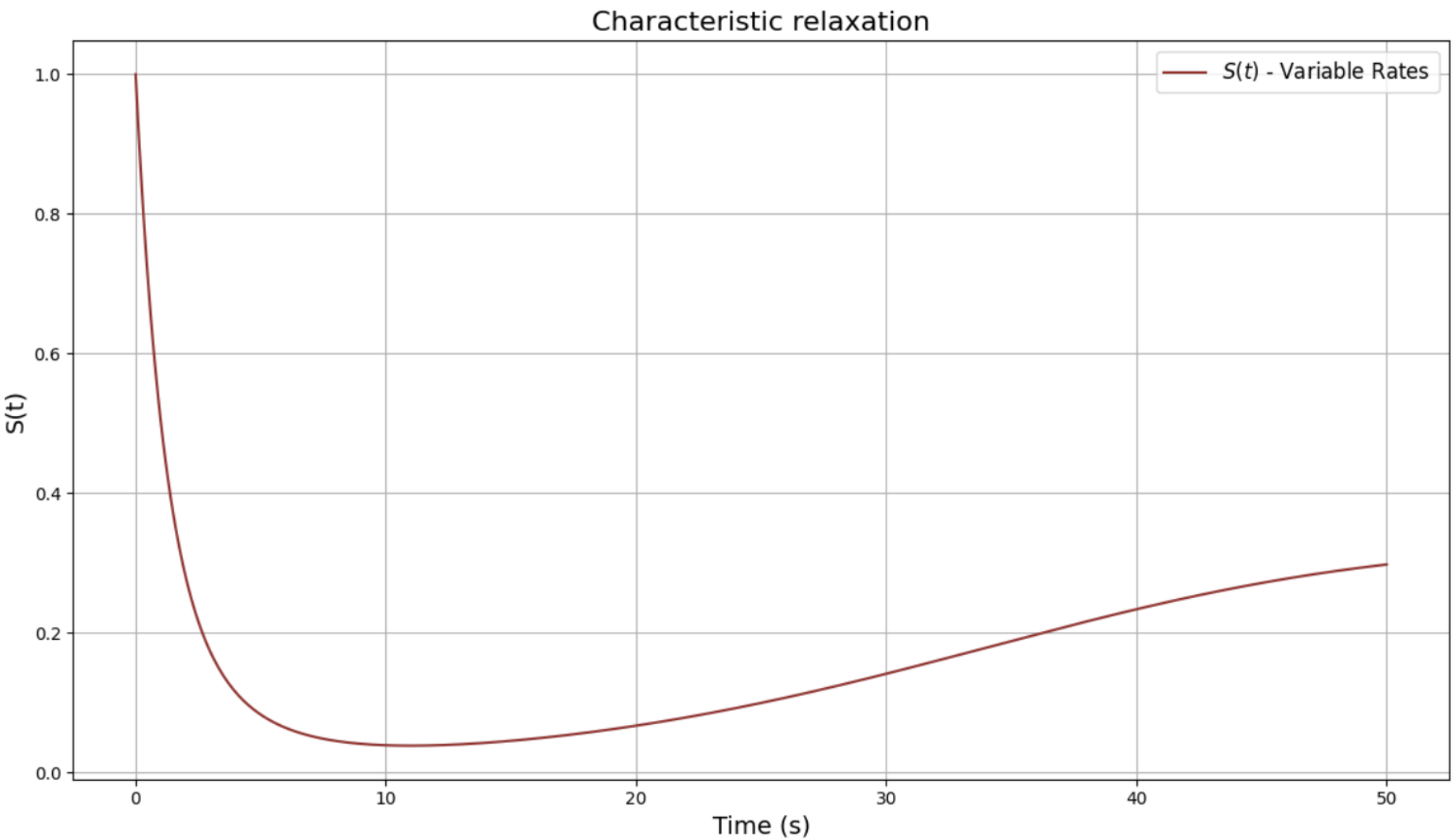



Delta (eV)
0.10
T final (K)
250.00
Barreras: 0.7, 0.7 − δ, . . . (T = 300 K)
Barreras: 0.7, . . . (300 → 250.0 K), δ = 0.100
Niveles r0
r0=2
r0=3
r0=4
r0=5
Relaxation
Time (s)


Delta (eV)
0.15
T final (K)
200.00
Barreras: 0.7, 0.7 − δ, . . . (T = 300 K)
Barreras: 0.7, . . . (300 → 200.0 K), δ = 0.150
Niveles r0
r0=2
r0=3
r0=4
r0=5
Relaxation
Time (s)


Folding and Unfolding Rate Constants vs Time (Variable Rates)
Rate Constants (s^{-1})
Time (s)
10^0
5×10^{-1}
2×10^{-1}
1.29155×10^{-1}
10^{-1}
5×10^{-2}
2×10^{-2}
1.29155×10^{-2}
10^{-2}
0
10
20
30
40
50
$k_f(t)$ (Folding Rate)
$k_u(t)$ (Unfolding Rate)
$w_u(1, t) = k_u(t)^{0.25}$
$w_u(1/3, t) = k_u(t)^{0.5}$


Probability of Being Folded and Unfolded vs Time (Variable Rates)
$p_1(t)$ - Variable Rates
$1 - p_1(t)$ - Variable Rates
Probability
Time (s)
0.0
0.2
0.4
0.6
0.8
1.0
0
10
20
30
40
50


Characteristic relaxation
S(t) - Variable Rates
S(t)
Time (s)
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50

Thank you!!