The Ehrenfest Diffusion Model in a 1-dimensional lattice

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Synopsis

In this work, I study the Ehrenfest diffusion model [7] and in the webEJS platform, I create a simulation of the diffusion of *N* particles along a 1-dimensional finite lattice, towards the state of equilibrium. The particles are distributed in a sequence of cells arranged along the lattice. In a time-interval of length *Dt*, each particle can perform just one jump between neighboring cells with a certain transition probability determined in the frame of the Ehrenfest model [1,2,7], which is described in paragraph 1. The initial state of the system and the number of the cells along the lattice, are selected by the user.
In a sequence of time-moments, the program of the simulation calculates the number of particles in every cell. The number of the particles in a cell is depicted by a certain cell-color. The intermediate states of the system between the initial state and the final state of equilibrium are depicted by a varying histogram and a sequence of changing cell-colors. On the other hand, the distribution of the particles at the equilibrium state has been determined according to the theoretical model and it is depicted in the same system of axes. The first objective of the applet is to compare the data obtained in real-time from the virtual environment, with the theoretical predictions of the model.
Furthermore, as a second objective, the user is getting able to confirm the theoretical proposition that "irrespectively of the form of the initial distribution, the system converges to a certain equilibrium state which is determined by the transition probabilities". In a separate window, the graph of a Lyapunov functional *H* corresponding to the system, is created in real time. Each time-moment, the value of *H* is uniquely determined by the corresponding distribution of the particles in the cells of the lattice. In addition, by using the graph of *H* over time, the user can estimate the relaxation time of the process towards the equilibrium-state.

Key concepts and their relationships

Probability - Conditional probability - Stochastic variable - Probability density - Distribution of a stochastic variable - Stochastic process - Chapman-Kolmogorov equation - Markov processes - The master equation - Equilibrium distribution - Lyapunov functional - The Ehrenfest model

The objectives of the simulation

The user is getting able to:
a) Describe the Ehrenfest model for a system of particles distributed in a 1d lattice of cells
b) Define the concept of the system's equilibrium state and derive its analytic form for the case of the Ehrenfest model
c) Compare the results achieved in real time in the virtual environment of the simulation, with the theoretical predictions of the model
d) Confirm the predicted by the model variation of the Lyapunov functional over time, from an initial state to the equilibrium state of the system, and estimate the relaxation time of the process.

Contents

1. Description of the model

1a. The Markov process

An aggregate of N discrete, but identical particles are confined in a region consisted of a sequence $0,1,\ldots j_{\max} < +\infty$ of similar, orthogonal cells placed next to each other along the x-axis of a Cartesian system of reference Oxy (figure 1). The number of particles that can be placed in each cell is unrestricted.

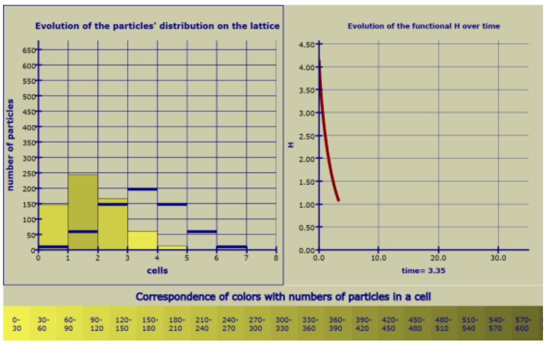

Figure 1: The cells are arranged along the x-axis. At time t_k the j-cell (j=0,1,…$j_{\max}$) contains $n_j(t_k)$ particles. In the time interval $[t_k, t_k+Dt)$, a particle is possible to jump from the j-cell into one of the two neighboring cells, or stay in the j-cell.

Consider a sequence of time-intervals, with equal lengths Dt:

$I_k = [t_k, t_{k+1}) = [kDt, (k+1)Dt)$, $k = 0,1,\ldots$

For each t_k , the position X of a particle is determined by the index j corresponding to the cell where the particle is in. Hence, the sample space of the stochastic process $X(t_k)$ is defined by the set Ω_X :

$X(t_k) = j \in \Omega_X = \{0,1,\ldots j_{max}\}$

The particles are characterized by an index s=1,2…N. It is assumed that at any time t_k the particles have the same probability distribution, which is determined by the same probability density [1,2,7] (I follow the symbolism of N.G. Van Kampen - see reference 1):

$p(j,t_k) \equiv P_1(j,t_k) = \Pr\{X(t_k) = j\}$ for any s=1, 2…N

The probability density in the initial state of the system is a given function of the position:

$p_{in.}(j) \equiv p(j,0) = P_1(j,0) = \Pr\{X(0) = j\}$

The joint probability density of the composite event:

"The location of the s-particle at time t_k is in the j_k-cell AND at time t_{k-1} it was in the j_{k-1}-cell AND… at time $t_0 = 0$ it was in the j_0-cell".

…is symbolized (see ref. 1):

$P_1(j_k,t_k; j_{k-1},t_{k-1};\ldots j_0,0)$ where: $t_{k'} = k'Dt$ and $j_{k'} \in \Omega_X$, $k' = 0,1\ldots k$

The probability density $p(j_k,t_k) \equiv P_1(j_k,t_k) = \Pr(X(t_k) = j_k \in \Omega_X)$ can be expressed by means of the joint probabilities of the system's evolution [1,2,3,7]. It always holds true that:

$$P_1(j_k,t_k) = \sum_{j_0,\ldots j_{k-1}} P_1(j_k,t_k; j_{k-1},t_{k-1};\ldots; j_0,0) =$$

$$= \sum_{j_0,\ldots j_{k-1}} P_{1|k}(j_k,t_k \mid j_{k-1},t_{k-1};\ldots; j_0,0)\, P_1(j_{k-1},t_{k-1}; j_{k-2},t_{k-2};\ldots; j_0,0) =$$

$$= \sum_{j_0,\ldots j_{k-1}} P_{1|k}(j_k,t_k \mid j_{k-1},t_{k-1};\ldots; j_0,0)\, P_{1|k-1}(j_{k-1},t_{k-1} \mid j_{k-2},t_{k-2};\ldots; j_0,0)\ldots P_{1|1}(j_1,t_1 \mid j_0,0)\, P_1(j_0,0)$$

…where, $P_{1|k}(j_k,t_k \mid j_{k-1},t_{k-1};\ldots j_0,t_0)$ is the conditional probability that the random variable X at time t_k has the value j_k given that at the previous times $t_{k-1} > t_{k-2} > \ldots > t_0$ has obtained the corresponding values $j_{k-1}, j_{k-2},\ldots j_0$ [1].

In the present model, I assume that the evolution of the system is a Markov process [1,2,3,7]: the conditional probability $P_{1|k}(j_k,t_k \mid j_{k-1},t_{k-1};\ldots j_0,t_0)$ depends only on what happened just in the previous time:

$$P_{1|k}(j_k,t_k \mid j_{k-1},t_{k-1}; j_{k-2},t_{k-2};\ldots; j_0,t_0) = P_{1|1}(j_k,t_k \mid j_{k-1},t_{k-1}) \qquad (1)$$

Under this assumption, the probability $p(j_k,t_k) = P_1(j_k,t_k)$ satisfies the equation:

$$p\left(j_{k+1},t_{k+1}\right)=\sum_{j_k\in\Omega_X}P_{1|1}\left(j_{k+1},t_{k+1}\mid j_k,t_k\right)p\left(j_k,t_k\right) \tag{2}$$

The evolution of the probability density $p\left(j_k,t_k\right)$ is a solution of equation 2, with initial condition:

$p(j,0)=p_{in.}(j)$

The conditional probability $P_{1|1}\left(j,t_{k+1}\mid l,t_k\right)$ is interpreted as the probability of a particle to jump from the l-cell where it was located at time t_k, to the j-cell, at time t_{k+1}. It is called "**transition-probability**" [1,2,7]. Equation 2 is an expression of the **Chapman-Kolmogorov equation** [1,2,7] which describes the evolution of any **Markov process**. In our model, it is also assumed that the transition probabilities are independent of the time t_k. They depend only on the length Dt of the time-intervals $I_k=\left[kDt,(k+1)Dt\right)$. Under this assumption, the stochastic process is called **static** and the transition probabilities can take the form [1]:

$$P_{1|1}\left(j,t_{k+1}\mid l,t_k\right)=Dt\,w_{lj}\ \text{for } j\neq l \tag{2a}$$

...where $w_{lj},\ j\neq l$ are positive or zero quantities, independent of time, named "transition probabilities per unit time".

Let $p_{ll}\equiv P_{1|1}\left(l,t_{k+1}\mid l,t_k\right)$ be the conditional probability "Given that at time t_k, the s-particle is in the l-cell, it is not being moved off the l-cell in the time interval $\left[t_k,t_k+Dt\right)$". From the identity:

$$\sum_{j\in\Omega_X}P_{1|1}\left(j,t_{k+1}\mid l,t_k\right)=1$$

...I infer that:

$$p_{ll}\equiv P_{1|1}\left(l,t_{k+1}\mid l,t_k\right)=1-Dt\sum_{j\in\Omega_X-\{l\}}w_{lj} \tag{2b}$$

Hence, from 2 it is implied that:

$$p\left(j_{k+1},t_{k+1}\right)=\sum_{j_k\in\Omega_X}P_{1|1}\left(j_{k+1},t_{k+1}\mid j_k,t_k\right)p\left(j_k,t_k\right)=$$

$$=Dt\sum_{j_k\in\Omega_X-\{j_{k+1}\}}p\left(j_k,t_k\right)w_{j_kj_{k+1}}+\left(1-Dt\sum_{j_k\in\Omega_X-\{j_{k+1}\}}w_{j_{k+1}j_k}\right)p\left(j_{k+1},t_k\right)\Rightarrow$$

$$p\left(j_{k+1},t_{k+1}\right)=p\left(j_{k+1},t_k\right)+Dt\sum_{j_k\in\Omega_X-\{j_{k+1}\}}\left(p\left(j_k,t_k\right)w_{j_kj_{k+1}}-p\left(j_{k+1},t_k\right)w_{j_{k+1}j_k}\right)\Rightarrow$$

$$p\left(j,t_{k+1}\right)-p\left(j,t_k\right)=Dt\sum_{l\in\Omega_X-\{j\}}\left(p\left(l,t_k\right)w_{lj}-p\left(j,t_k\right)w_{jl}\right) \tag{2c}$$

...or, equivalently:

$$p\left(j,t_{k+1}\right)-p\left(j,t_k\right)=\sum_{l\in\Omega_X}\left(p\left(l,t_k\right)p_{lj}-p\left(j,t_k\right)p_{jl}\right) \tag{2d}$$

Equation 2c (or 2d) is known as the "master" equation which describes the evolution of any static Markov process [1,2,3,7].

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1b. The actual and the mean number of particles in each cell

In the virtual environment of the simulation, the particles jump from one cell to another, according to a random process running in the body of the program of the simulation. Hence, at every time-moment t_k, in every j-cell there exist some particles which are being counted by the program. This is the actual number of particles in each cell at time t_k. Let us symbolize it:

$n_{real}\left(j,t_k\right),\ j\in\Omega_X$

On the other hand, one can define the mean number of particles in each cell over time which is denoted by $n\left(j,t_k\right)$ The theoretical variation of $n\left(j,t_k\right)$ can be predicted in the context of our model. Hence, the user is able to compare the data issued by the virtual environment, with the theoretical predictions. In the following I show how to calculate the actual and the theoretical number of particles in the j-cell as functions of time.

Define the index-function:

$$\mathrm{Ind}_j(s,t_k) = \begin{cases} = 1 \text{ if at time } t_k\text{, the s-particle is in the j-cell} \\ = 0 \text{ if at time } t_k\text{, the s-particle is not in the j-cell} \end{cases} \qquad (3a)$$

At any time-moment t_k , the actual number $n_{real}(j;t_k)$ of particles in every cell is to be counted by applying the relation:

$$n_{real}(j,t_k) = \sum_{s=1}^{N} \mathrm{Ind}_j(s,t_k) \qquad (3b)$$

In the context of our model, $\mathrm{Ind}_j(s,t_k)$ can be considered as a random variable which takes the value 1 with probability $p(j,t_k)$ and the value 0 with probability $1-p(j,t_k)$, for any s-particle s=1,2…N.

The mean value of $\mathrm{Ind}_j(p,t_k)$ is:

$\langle \mathrm{Ind}_j(s,t_k) \rangle = p(j,t_k)$

Hence, the mean number $n(j,t_k)$ of particles in the j-cell, at time t_k , is given by the relation:

$$n(j,t_k) = \left\langle \sum_{s=1}^{N} \mathrm{Ind}_j(s,t_k) \right\rangle = Np(j,t_k) \qquad (3c)$$

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2. The 'master' equation for the Ehrenfest model

In this paragraph, by using the analytic expression of the transition probabilities for the Ehrenfest model [7], I obtain the specific form of equation 2c that describes the evolution of our system:

$$p(j,t_{k+1}) - p(j,t_k) = Dt \sum_{l \in \Omega_X - \{j\}} \left(p(l,t_k) w_{lj} - p(j,t_k) w_{jl} \right) \qquad (4)$$

…or, according to 3c:

$$n(j,t_{k+1}) = n(j,t_k) + Dt \sum_{i \in \Omega_X - \{j\}} \left(n(i,t_k) w_{ij} - n(j,t_k) w_{ji} \right) \qquad (4a)$$

…where $n(j,t_k)$ is the number of particles in the j-cell at time t_k.

I postulate that in the present model, the transition probabilities per unit time are given by the expressions [7]:

$$p_{jm} = \begin{cases} aDt \dfrac{2z-j}{2z} & \text{for } m = j+1 \text{ and any } j = 0,1,\dots 2z-1 \\ aDt \dfrac{j}{2z} & \text{for } m = j-1 \text{ and any } j = 1,3,\dots 2z \\ 1 - aDt & \text{for } m = j \text{ and any } j = 0,1,\dots 2z \\ 0 & \text{for any other case} \end{cases} \qquad (5)$$

or:

$$w_{jm} = \begin{cases} a \dfrac{2z-j}{2z} & \text{for } m = j+1 \text{ and any } j = 0,1,\dots 2z-1 \\ a \dfrac{j}{2z} & \text{for } m = j-1 \text{ and any } j = 1,2,\dots 2z \\ 0 & \text{for any other case} \end{cases} \qquad (5a)$$

…where a is a positive parameter, which satisfies the condition $aDt < 1$ The number of the cells in the lattice has been considered to be $j_{\max} = 2z$ where $z \in \mathbb{N}$ (see paragraph 1a). The sample space of the stochastic variable X is the set of integers:

$\Omega_X = \{0,1,\dots 2z\} \subset \mathbb{N}$

If a particle arrives at time t_k in one of the end-cells of the lattice; i.e. to the cell with index j=0 or j=2z, at the next time-moment t_{k+1} it will return with probability aDt to the cell with index j=1 or j=2z-1 respectively, or it will stay in the cell it was at t_k, with probability 1-aDt:

$$p_{01} = aDt,\ p_{00} = 1 - aDt,\ p_{2z\,2z-1} = aDt,\ p_{2z\,2z} = 1 - aDt \qquad (5b)$$

That means that the end-points of the lattice work like "reflecting barriers" [7].
It has to be noticed that in our model, it has been assumed that in any interval I_k, a particle can get a jump only between neighboring cells. The probability of a jump between non-neighboring cells, as well as the probability of a double or multiple jumps between cells, is negligible and it is not taken into account.

According to these remarks, equations 4 and 4a are taking the subsequent forms:

$$p(j,t_{k+1}) - p(j,t_k) = aDt\left(p(j-1,t_k)\frac{2z-j+1}{2z} - p(j,t_k) + p(j+1,t_k)\frac{j+1}{2z}\right) \qquad (6)$$

$$n(j,t_{k+1}) - n(j,t_k) = aDt\left(n(j-1,t_k)\frac{2z-j+1}{2z} - n(j,t_k) + n(j+1,t_k)\frac{j+1}{2z}\right) \qquad (6a)$$

...with initial conditions: $n(j,0) = n_{in}(j) : j \in \Omega_X,\ \sum_{j\in\Omega_X} n_{in}(j) = N = const$

...where $n_{in}(j)$ is a given function defined on Ω_X, and N is the initial number of particles moving in the lattice, which is a constant of the dynamical system 4a.

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3. The equilibrium state of the system

The equilibrium state of the system, if it exists, is defined by the requirement that the probability density $p^e(j,t_k)$ of the equilibrium distribution of the particles on the lattice is not changing with time:

$$p^e(j,t_{k+1}) = p^e(j,t_k) \equiv p^e(j) \text{ for any } j \in \Omega_X \text{ and } k = 0,1,..., \qquad (7)$$

Hence, according to 4, $p^e(j)$ is a solution of the subsequent equations:

$$\sum_{i\in\Omega_X-\{j\}}\left(n^e(i)w_{ij} - n^e(j)w_{ji}\right) = 0 \Leftrightarrow Dt\sum_{i\in\Omega_X-\{j\}} n^e(i)w_{ij} = n^e(j)Dt\sum_{i\in\Omega_X-\{j\}} w_{ji} \Leftrightarrow$$
$$Dt\sum_{i\in\Omega_X-\{j\}} n^e(i)w_{ij} = n^e(j)\left(1-p_{jj}\right) \Leftrightarrow n^e(j) = \sum_{i\in\Omega_X} n^e(i)p_{ij} \qquad (7a)$$

...and by using 5 or 6, I deduce that $p^e(j)$ should be a solution of the equation:

$$p^e(j) = p^e(j-1)\frac{2z-j+1}{2z} + p^e(j+1)\frac{j+1}{2z} \qquad (8)$$

To solve equation 8, I define the characteristic function of the distribution determined by $p^e(j)$, from the expression:

$$G(s) = \left\langle s^X\right\rangle = \sum_{j=0}^{2z} s^j p^e(j) \qquad (9)$$

In Appendix A, I formulate a differential equation which is to be satisfied by $G(s)$ and I proceed to the derivation of the analytic form of $G(s)$ and of the probability density $p^e(j)$, as well. I find out that:

$$G(s) = 2^{-2z}(s+1)^{2z} \qquad (10)$$

$$p^e(j) = \binom{2z}{j}2^{-2z},\ j = 0,1,...2z \qquad (11)$$

In Appendix B, it is being proved that the system of the particles on the cells-lattice, which is described by the present model, converges to the equilibrium state $p^e(j)$ irrespectively of its initial state:

$$\lim_{t_k \to +\infty} p\left(j,t_k\right) = p^e(j) \qquad (12)$$

That is, any solution $p(j,t_k)$ of equation 6, for $t_k \to +\infty$ converges to the $p^e(j)$, which is uniquely determined, irrespectively of the form of the system's initial state $p(j,0) = p_{in}(j)$

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4. Definition of a Lyapunov functional for the dynamical system

For a dynamical system which converges to its equilibrium state can be defined a certain functional, called "Lyapunov functional". The Lyapunov functional converges to a constant limit value if and only if the sequence of the system's probability densities converges to the equilibrium density function. In the present paragraph, I define a Lyapunov functional *H* for the Ehrenfest dynamical system, according the analysis developed in Appendix B and in ref.1: van Kampen chapter V, paragraph 5.

The analytic expression of *H* is determined by relation B8, in Appendix B, by choosing the function *f* as follows (figure 2):

$$f(x) = \begin{cases} x\ln x & \text{for } x \in (0,+\infty) \\ 0 & \text{for } x = 0 \end{cases} \qquad (13)$$

The real function *f* is strictly convex:

$$f''(x) = \frac{1}{x} > 0 \text{ for any } x \in (0,+\infty)$$

Hence the functional:

$$H\left[p^{(k)}\right] = \sum_{j\in\Omega_X} p_j^e x_j^{(k)} \ln\left(x_j^k\right) = \sum_{j\in\Omega_X} p_j^{(k)} \ln\left(\frac{p_j^{(k)}}{p_j^e}\right) \qquad (14)$$

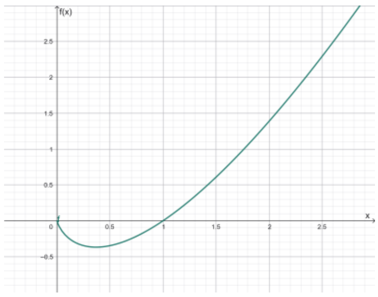

Figure 2.

…satisfies the conditions referred in Appendix B implying that it is an appropriate Lyapunov functional for the dynamical system of the Ehrenfest model (see equation 6, par.2).
The analytic expression of the equilibrium density function is given by the analytic expression 11, par.3.

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5. Activities implemented in the virtual environment of the simulation

Run the simulation for every combination of the available values of *z* and the initial states ('a', 'b', 'c', 'd'). For each case, carry out the following activities and answer to the questions.
a) Watch the evolution of the probability densities over time and the variation of the Lyapunov functional *H*.
b) Does the sequence of the probability densities converge to the theoretically predicted state of equilibrium?
c) By using the graph of *H* over time, calculate the required time for the system to attain the equilibrium state. Try to explain the differences and the similarities of the achieved values.
d) Did you confirm that the equilibrium state of the system is not dependent of the initial state? Explain your conclusion.

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Appendix A: Derivation of the probability density in the equilibrium state

The probability density in the equilibrium state for the Ehrenfest model, if it exists, should be a solution of equation 8, par. 3:

$$p^e(j) = p^e(j-1)\frac{2z-j+1}{2z} + p^e(j+1)\frac{j+1}{2z} \qquad (8)$$

To solve this equation, I first derive the analytic expression of the characteristic function $G(s)$ corresponding to the probability density $P_X^e(j) \equiv p^e(j)$ The characteristic function $G(s)$ is defined by the expression:

$$G(s) = \langle s^X \rangle = \sum_{j=0}^{2z} s^j p^e(j) \qquad (A1)$$

The functions $G(s)$ and $p^e(j)$ satisfy the conditions:

$$p^e(j) = 0 \text{ for } j < 0 \text{ or } j > 2z,\ \sum_{j=0}^{2z} p^e(j) = 1 \Rightarrow G(1) = 1 \qquad (A2)$$

From 11, A1 and A2, I deduce the truth of the subsequent relations:

$$\sum_{j=0}^{2z} s^j p^e(j) = \sum_{j=0}^{2z} s^j p^e(j-1)\frac{2z-j+1}{2z} + \sum_{j=0}^{2z} s^j p^e(j+1)\frac{j+1}{2z} \qquad (A3)$$

$$G'(s) = \sum_{j=0}^{2z} j s^{j-1} p^e(j) \qquad (A3a)$$

$$\begin{aligned}\sum_{j=0}^{2z} s^j p^e(j-1) &= \sum_{j=1}^{2z} s^j p^e(j-1) = \sum_{m=0}^{2z-1} s^{m+1} p^e(m) = s\left(\sum_{m=0}^{2z} s^m p^e(m) - s^{2z} p^e(2z)\right) = \\ &= s\sum_{m=0}^{2z} s^m p^e(m) - s^{2z+1} p^e(2z) = sG(s) - s^{2z+1} p^e(2z)\end{aligned} \qquad (A3b)$$

$$\begin{aligned}\frac{1}{2z}\sum_{j=0}^{2z} s^j (j-1) p^e(j-1) &= \frac{1}{2z}\sum_{j=1}^{2z} s^j (j-1) p^e(j-1) = \frac{1}{2z}\sum_{m=0}^{2z-1} s^{m+1} m p^e(m) = \\ &= \frac{s^2}{2z}\left(\sum_{m=0}^{2z} s^{m-1} m p^e(m) - s^{2z-1} 2z p^e(2z)\right) = \frac{s^2}{2z}\left(G'(s) - s^{2z-1} 2z p^e(2z)\right)\end{aligned} \qquad (A3c)$$

$$\frac{1}{2z}\sum_{j=0}^{2z} s^j p^e(j+1)(j+1) = \frac{1}{2z}\sum_{m=1}^{2z+1} s^{m-1} p^e(m) m = \frac{1}{2z}\sum_{m=0}^{2z} s^{m-1} p^e(m) m = \frac{1}{2z} G'(s) \qquad (A3d)$$

According to the identities A3a, A3b, A3c, A3d, equation A3 is transformed to a differential equation with unknown the characteristic function $G(s)$, as follows:

$$2zG(s) = 2zsG(s) - 2zs^{2z+1} p^e(2z) - s^2\left(G'(s) - s^{2z-1} 2z p^e(2z)\right) + G'(s)$$

…which is simplified to the equation:

$$G'(s)\left(1+s\right) - 2zG(s) = 0 \qquad (A4)$$

I solve A4 by using condition A2. I deduce that:

$\frac{dG}{G} = \frac{2z}{s+1} \Rightarrow \ln\left(\frac{G(s)}{C}\right) = \ln(s+1)^{2z} \Rightarrow G(s) = C(s+1)^{2z}$, where: C=constant

$$G(1) = 1 \Rightarrow C\left(1+1\right)^{2z} = 1 \Rightarrow C = 2^{-2z}$$

Hence:

$$G(s) = 2^{-2z}\left(s+1\right)^{2z} \qquad (A5)$$

From A5 and A1, I infer that:

$$2^{-2z}\left(s+1\right)^{2z} = \sum_{m=0}^{2z} s^m p^e(m) \Rightarrow \sum_{m=0}^{2z} 2^{-2z}\binom{2z}{m} s^m = \sum_{m=0}^{2z} s^m p^e(m) \Rightarrow$$

$$p^e(j) = \binom{2z}{j} 2^{-2z} \qquad (A6)$$

It is concluded that in our model there exists an equilibrium state, which is determined by the probability density given by analytic expression A6.

Verification:
I verify that the probability density A6 is indeed a solution of equation A1:

$$p^e(j) = \frac{(2z)!}{j!(2z-j)!}2^{-2z} \stackrel{?}{=}$$

$$\stackrel{?}{=} \frac{(2z)!}{(j-1)!(2z-j+1)!}2^{-2z} - \frac{(2z)!}{(j-1)!(2z-j+1)!}2^{-2z}\frac{j-1}{2z} + \frac{(2z)!}{(j+1)!(2z-j-1)!}2^{-2z}\frac{j+1}{2z} =$$

$$= 2^{-2z}\frac{(2z)!}{j!(2z-j)!}\left(\frac{j}{2z-j+1} - \frac{j}{2z-j+1}\frac{j-1}{2z} + \frac{2z-j}{j+1}\frac{j+1}{2z}\right) =$$

$$= 2^{-2z}\frac{(2z)!}{j!(2z-j)!}\left(\frac{j+2z-j}{2z}\right) = 2^{-2z}\frac{(2z)!}{j!(2z-j)!} = p^e(j) \quad \text{QED}$$

Some properties of the equilibrium distribution

$$\left.\begin{array}{l} G'(s) = 2^{-2z}2z(s+1)^{2z-1} \\ \langle X \rangle = G'(1) \end{array}\right\} \Rightarrow \langle X \rangle = 2^{-2z}2z2^{2z-1} = 2z/2 = z \qquad \text{(A7)}$$

$$G''(1) = \frac{z}{2}(2z-1)$$

$$G''(s) = \sum_{m=0}^{2z} m(m-1)s^{m-2}p^e(m) = \sum_{m=0}^{2z} m^2 s^{m-2}p^e(m) - \sum_{m=0}^{2z} m s^{m-2}p^e(m)$$

$$G''(1) = \langle X^2 \rangle - \langle X \rangle \Rightarrow \langle X^2 \rangle = G''(1) + \langle X \rangle = \frac{z}{2}(2z-1) + z = z^2 + \frac{z}{2}$$

$$\sigma_X^2 = \langle X^2 \rangle - \langle X \rangle^2 = z^2 + \frac{z}{2} - z^2 = \frac{z}{2} \Rightarrow \sigma_X = \sqrt{\frac{z}{2}} \qquad \text{(A8)}$$

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Appendix B: Convergence of the stochastic process to the equilibrium distribution

In Appendix A, it has been proved that for the stochastic process described by the Ehrenfest model, there exists an equilibrium distribution which is a solution of equation 8, par.3.
In the present Appendix B, I am proving that in general, if the Markov chain described by the Chapman-Kolmogorov equation:

$$p(m,t_k) = \sum_{j\in\Omega_X} p(j,t_{k-1})\,p_{jm} \qquad \text{(B1)}$$

…has an equilibrium distribution specified by the probability density $p^e(j),\, j \in \Omega_X$ which is a solution of the equation:

$$p^e(m) = \sum_{j\in\Omega_X} p^e(j)\,p_{jm} \qquad \text{(B2)}$$

…then, the sequence of the probability densities $p(m,t_k),\ t_k = kDt,\ k = 0,1,...$ converges to the equilibrium probability density $p^e(m)$ [1]:

$$\lim_{k\to+\infty} p(m,t_k) = p^e(m) \text{ for any } m \in \Omega_X \qquad \text{(B3)}$$

Proof:
I show that there exists a Lyapunov functional H corresponding to the dynamical system defined by equation B1, with the following properties [1,4]:

a) The domain of H is the compact set [5,6] $[0,1]^{2z+1}$ and its codomain a subset of the real numbers:

$$[0,1]^{2z+1} \ni p \to H[p] \in \mathbb{R}$$

where: $p = (p_0, p_1, ...p_{2z}),\ p_j \in [0,1],\ j \in \Omega_X$

b) H is a continuous function for any $p \in [0,1]^{2z+1}$ Hence, it is bounded [5,6], i.e. there are real numbers $h_1 < h_2$ such that:

$H[p] \in [h_1, h_2]$ for every $p = (p_0, p_1, ...p_{2z}) \in [0,1]^{2z+1}$

c) For every sequence $p^{(k)} = \left(p_0^{(k)}, p_1^{(k)}, ...p_{2z}^{(k)}\right) \in \left[0,1\right]^{2z+1}$, where: k=0,1,... and $p_j^{(k)} \equiv p^{(k)}(j)$, which is a solution of the Chapman-Kolmogorov equation B1, the sequence $H[p^{(k)}]$ is strictly monotone; for example, strictly decreasing: $H[p^{(k)}] > H[p^{(k+1)}]$ If this is true, then the sequence $H[p^{(k)}]$ converges to a certain point h of the compact set $\left[h_1, h_2\right]$ (5,6):

$$\lim_{k \to +\infty} H[p^{(k)}] = h \in \left[h_1, h_2\right]$$

d) Given that H is strictly decreasing, it is implied that $p^{(k)}$ is a sequence with infinite number of terms, different of each other (6):

$$k' > k \Rightarrow H\left[p^{(k)}\right] > H\left[p^{(k')}\right] \Rightarrow p^{(k)} \neq p^{(k')}$$

The set $\left\{p^{(k)} : k = 1,2,...\right\}$ is infinite and bounded. Hence, according to the Bolzano-Weierstrass theorem, it has a limiting point (6) $p^{\infty} \in \left[0,1\right]^{2z+1}$. There exists a subsequence $p^{(k_s)}$, $s = 1,2,...$ of $p^{(k)}$ which converges to p^{∞}:

$$\lim_{s \to \infty} p^{(k_s)} = p^{\infty} \qquad \text{(B4)}$$

...and consequently, given that H is continuous, it holds:

$$\lim_{s \to +\infty} H\left[p^{(k_s)}\right] = H[p^{\infty}]$$

But the sequence $H\left[p^{(k)}\right]$ is convergent and has a unique limit. Hence:

$$\lim_{k \to +\infty} H\left[p^{(k)}\right] = H[p^{\infty}] \qquad \text{(B5)}$$

From B4 and B1 it is implied that:

$$p^{k_s}(m) = \sum_{j \in \Omega_X} p^{k_{s-1}}(j)\, p_{jm} \Rightarrow \lim_{s \to \infty} p^{k_s}(m) = \sum_{j \in \Omega_X} \left(\lim_{s \to \infty} p^{k_{s-1}}(j)\right) p_{jm} \Rightarrow$$

$$\Rightarrow p^{\infty}(m) = \sum_{j \in \Omega_X} p^{\infty}(j)\, p_{jm} \qquad \text{(B6)}$$

From B6 it is resulted that p^{∞} is a solution of equation 7a which has the unique solution $p^e(m)$, the probability density in the equilibrium state. I infer that every subsequence of the sequence $p^{(k)}(m)$ converges to $p^e(m)$. Hence, $p^{(k)}(m)$ is convergent and its limit is the equilibrium probability density:

$$\lim_{k \to \infty} p^{(k)}(m) = p^e(m), \text{ for every } m \in \Omega_X \qquad \text{(B7)}$$

Construction of the functional H

I construct the analytic expression of H by following a procedure similar to the one sited in ref.1: N.G. Van Kampen, Stochastic Processes in Physics and Chemistry, North-Holland Personal Library 2007 third edition, page 111. H define the functional H by the expression:

$$H\left[p^{(k)}\right] = \sum_j p^e(j) f\left(x_j^{(k)}\right) \qquad \text{(B8)}$$

...where: $x_j^{(k)} = p_j^{(k)} / p^e{}_j$, $p^{(k)} = \left(p_0^{(k)}, p_1^{(k)}, ...p_{2z}^{(k)}\right)$

The real function f is defined in the interval $\left[0, +\infty\right)$ and it is strictly convex:

$$\left[0, +\infty\right) \ni x \to f(x) \in \mathbb{R},\ f''(x) > 0$$

Lemma B1

The function f satisfies the inequalities (Figures B1, B2, B3):

$f(y) - f(x) > (y - x)f'(x)$ or: $f(x) - xf'(x) < f(y) - yf'(x)$

...for every $x, y \in \left[0, +\infty\right)$

<u>Proof</u>:

Figures B1, B2 and B3 depict a strictly convex real function. In any case, one can confirm the truth of the subsequent relations:

$$f''(x) > 0 \Rightarrow \{x < y \Rightarrow f'(x) < f'(y)\}$$

$$\{x, y \in [0, +\infty), \, x < y\} \Rightarrow f(y) - f(x) > (y - x) f'(x)$$

$$x > y \Rightarrow f(x) - f(y) < (x - y) f'(x) \Rightarrow$$

$$f(y) - f(x) > (y - x) f'(x)$$

Finally, it holds true that for any $x, y \in [0, +\infty)$:

$$f(y) - f(x) - (y - x) f'(x) > 0 \qquad \text{(B9)}$$

QED

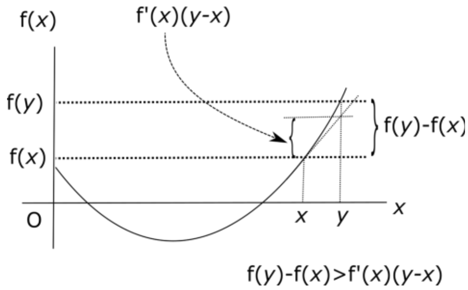

Figure B1: *f* is convex, *y*>*x*

Lemma B2

In the equilibrium state, the probability density is not being changed with time:

$$p^e(j, t_{k+1}) = p^e(j, t_k) = p^e_j$$
$$\text{for every } j \in \Omega_X = \{0, 1, \ldots 2z\} \qquad \text{(B10)}$$

Hence, from equation 2d, par.1a and condition B10, the truth of the subsequent relations is implied:

$$p(j, t_{k+1}) = p(j, t_k) + \sum_{l \in \Omega_X} \left(p(l, t_k) p_{lj} - p(j, t_k) p_{jl} \right) \Rightarrow$$

$$p^{(k+1)}_m = p^{(k)}_m + \sum_{j \in \Omega_X} \left(p^{(k)}_j p_{jm} - p^{(k)}_m p_{mj} \right) \Rightarrow$$

$$\sum_{j \in \Omega_X} p^e_j p_{jm} = \sum_{j \in \Omega_X} p^e_m p_{m\,j} \qquad \text{(B11)}$$

Let $\psi : \Omega_X \ni m \to \psi_m \in \mathbb{R}$ be a real function defined on Ω_X

I multiply both members of B11 with ψ_m and add over m:

$$\sum_{m, j \in \Omega_X} p^e_j p_{jm} \psi_m = \sum_{m, j \in \Omega_X} p^e_m p_{m\,j} \psi_m \Rightarrow$$

$$\Rightarrow \sum_{m, j \in \Omega_X} p^e_m p_{mj} \psi_j = \sum_{m, j \in \Omega_X} p^e_m p_{m\,j} \psi_m \Rightarrow$$

$$\sum_{m, j \in \Omega_X} p^e_m p_{mj} \left(\psi_j - \psi_m \right) = 0 \qquad \text{(B12)}$$

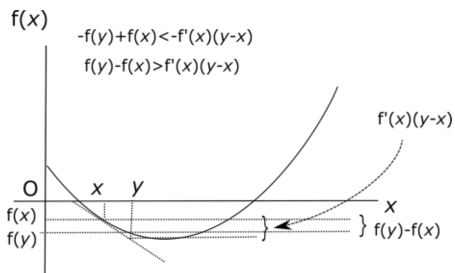

Figure B2: *f* is convex, *y*>*x*

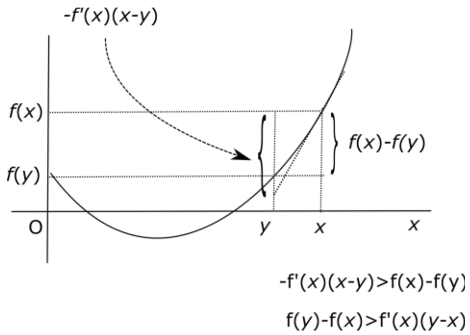

Figure B3: *f* is convex, *x*>*y*

The functional defined by B8 satisfies conditions (a) and (b), straight by its analytic form: its domain is the compact set $[0,1]^{2z+1}$; it is continuous and bounded [5,6], i.e. there are real numbers $h_1 < h_2$ such that: $H[p] \in [h_1, h_2]$ for every $p = (p_0, p_1, \ldots p_{2z}) \in [0,1]^{2z+1}$

I am proving the truth of condition (c). From B8, and Lemmas B1 and B2, the truth of the following relations is deduced:

$$H\left[p^{(k+1)}\right] - H\left[p^{(k)}\right] = \sum_j p^e_j f\left(x^{(k+1)}_j\right) - \sum_j p^e_j f\left(x^{(k)}_j\right) =$$

$$= \sum_j p^e_j \left(f\left(x^{(k+1)}_j\right) - f\left(x^{(k)}_j\right) \right) \approx$$

$$\approx \sum_j p^e_j f'\left(x^{(k)}_j\right) \left(x^{(k+1)}_j - x^{(k)}_j \right) = \sum_j \left(p^{(k+1)}_j - p^{(k)}_j \right) f'\left(x^{(k)}_j\right) \Rightarrow$$

$$H\left[p^{(k+1)}\right]-H\left[p^{(k)}\right]=\sum_j\left(p_j^{(k+1)}-p_j^{(k)}\right)f'\left(x_j^{(k)}\right) \quad \text{(B13)}$$

By using B1, B13 takes the form:

$$H\left[p^{(k+1)}\right]-H\left[p^{(k)}\right]=\sum_j\left(p_j^{(k+1)}-p_j^{(k)}\right)f'\left(x_j^{(k)}\right)=\sum_j\left(p_j^{(k+1)}-p_j^{(k)}\right)f'\left(x_j^{(k)}\right)=$$

$$=\sum_{j,m}p_j^{(k)}\,p_{jm}\left(f'\left(x_m^{(k)}\right)-f'\left(x_j^{(k)}\right)\right)=\sum_{j,m}\;p_j^e p_{jm}\left(x_j^{(k)}f'\left(x_m^{(k)}\right)-x_j^{(k)}f'\left(x_j^{(k)}\right)\right)\Rightarrow$$

$$=\sum_{j,m}\left(p_m^{(k)}\,p_{mj}-p_j^{(k)}\,p_{jm}\right)f'\left(x_j^{(k)}\right)=\sum_{j,m}p_j^{(k)}\,p_{jm}f'\left(x_m^{(k)}\right)-\sum_{j,m}p_j^{(k)}\,p_{jm}f'\left(x_j^{(k)}\right)=$$

$$H\left[p^{(k+1)}\right]-H\left[p^{(k)}\right]=\sum_{j,m}\;p_j^e p_{jm}\left(x_j^{(k)}f'\left(x_m^{(k)}\right)-x_j^{(k)}f'\left(x_j^{(k)}\right)\right) \qquad \text{(B13a)}$$

I check if the terms of the sums, in the second part of B13a have all the same sign. This is achieved by using the procedure sited in ref.1, N.G. Van Kampen, Stochastic Processes in Physics and Chemistry, page 111:

I apply Lemma 2, by setting: $\psi_j=f(x_j^{(k)})-x_j f'(x_j^{(k)})$ Then, from B12 I deduce the truth of the identity:

$$0=\sum_{j,m}p_m^e p_{mj}\left(f(x_j^{(k)})-x_j^{(k)}f'(x_j^{(k)})\right)-\sum_{j,m}p_j^e p_{jm}\left(f(x_j^{(k)})-x_j^{(k)}f'(x_j^{(k)})\right) \qquad \text{(B13b)}$$

I add B13a and B13b member by member:

$$H\left[p^{(k+1)}\right]-H\left[p^{(k)}\right]=-\sum_{j,m}\;p_j^e p_{jm}\left(f(x_j^{(k)})-f(x_m^{(k)})-\left(x_j^{(k)}-x_m^{(k)}\right)f'\left(x_m^{(k)}\right)\right) \qquad \text{(B13c)}$$

From relation B9, in Lemma B1, it is immediately implied that:

$$H\left[p^{(k+1)}\right]-H\left[p^{(k)}\right]<0 \qquad \text{(B14)}$$

Hence, for every sequence $p^{(k)}=\left(p_0^{(k)},p_1^{(k)},\ldots p_{2z}^{(k)}\right)\in\left[0,1\right]^{2z+1}$ which is a solution of equation B1, the sequence $H[p^{(k)}]$ is strictly decreasing, resulting that the sequence $H[p^{(k)}]$ converges to a certain point h of the compact set $\left[h_1,h_2\right]$ [5,6].

Given that conditions (a), (b) and (c) are fulfilled, condition (d) comes out as a result of these: The sequence $p_m^{(k)}\equiv p^{(k)}(m)$ is convergent and its limit is the equilibrium probability density:

$$\lim_{k\to\infty}p^{(k)}(m)=p^e(m),\ \text{for every } m\in\Omega_X \qquad \text{(B15)}$$

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