



**Università degli Studi di Trento**

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DIPARTIMENTO DI FISICA  
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**Ehrenfest Chains and  
Poincaré's Recurrence Theorem**

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# 1 Introduction

The relation between mathematics and physics is way younger than both of the subjects: they have existed separately for millennia before bonding together in the XVII century, and together they have been from that time on; the advantages of the union became evident as years passed by, the former developing new ideas for theories and structures and the latter having at his disposal powerful tools to express the surrounding world.

It is no coincidence that physics was previously called “natural philosophy”: most of its principles arises with a philosophical flavour rather than a mathematical one, and these philosophical observation are later made into mathematical statements, getting modified and somehow sharpened.

In this guise, a principle becomes part of a mathematical structure, and as such one can try to understand whether it's coherent or not with the axioms of the structure itself: Poincaré's Recurrence Theorem, for instance, was firstly proved in the framework of classical mechanics. In the same paper in which the theorem is proven, the mathematician remarks that

The world [...] tends at first towards a state where it remains for a long time without apparent change; and this is consistent with experience; but it does not remain that way forever, if the theorem cited above is not violated; it merely stays there for an enormously long time, a time which is longer the more numerous are the molecules. This state will not be the final death of the universe, but a sort of slumber, from which it will awake after millions of millions of centuries. According to this theory, to see heat pass from a cold body to a warm one, it will not be necessary to have the acute vision, the intelligence and dexterity of Maxwell's demon: it will suffice to have a little patience.<sup>1</sup>

Thus the theorem shows there exists a contradiction between the Second Law of Thermodynamics and Classical Mechanics: anyway, one may hope this is due to flaws in the theory of Classical Mechanics, and try to show that taking other points of view the contradiction disappears.

This is the aim of the paper, which consists of two independent sections, the first one approaching the problem by means of probability theory following a model proposed by Ehrenfest, the second one employing quantum mechanics: as the purpose is to prove the existence - or the lack - of a contradiction in these structures with respect to the Second Law, a special emphasis is given to the mathematical aspects of the theories involved, clarifying the physical correspondences whenever needed.

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<sup>1</sup>H. Poincaré. Le mécanisme et l'expérience. *Revue de Métaphysique et de Morale*, **4**, 534.



## 2 Stochastic approach

Consider the typical thermodynamic example of a box divided in half by an internal septum, and let an ideal gas be put in one of the two halves: we want to study the temporal evolution of the system when the septum is taken away, exploiting a stochastic approach. We will be using a modeling due to Ehrenfest: imagine the two halves of the box to be two urns  $A$  and  $B$ , and put in each urn as many balls as many are the gas particles in the respective half of the box; for instance, at time  $t = 0$ , when the septum has just been removed, all the balls are in  $A$ . Say that the total number of balls is  $2N$ , and label each ball by a different number.

Now, after a fixed time  $n$  randomly choose a number between 1 and  $2N$ , pick the ball with that number on from the corresponding urn and move it to the other urn. Repeat the process at times  $2n, 3n, \dots$

We want to study the evolution of this system, called an *Ehrenfest chain*, in its most natural environment, that of the Markov chains.

The chapter is structured as follows:

1. The first paragraph contains some recalls of probability theory;
2. The second introduces Markov chains and some of their features;
3. The third formalizes the concepts of *recurrence* and *transience* in this context;
4. The fourth defines an equivalence class and analyzes some of its properties;
5. The fifth takes advantages of the results of the previous one to develop some fundamental identities;
6. The last paragraph is dedicated to the analysis of the Ehrenfest chain.

### 2.1 Recalls of probability theory

We summarize hereby some basic definitions of probability theory.

**Definitions.** (i) Let  $\Omega$  be a set and  $\mathcal{P}$  a  $\sigma$ -algebra of subsets of  $\Omega$ : the couple  $(\Omega, \mathcal{P})$  is called a *probabilizable space*.

(ii.1) Let  $P$  a probability measure on  $\mathcal{P}$ , namely  $P : \mathcal{P} \rightarrow [0,1]$  with the requirements

$$P(\Omega) = 1, \quad P(A) \geq 0 \quad \forall A \in \mathcal{P} \tag{1}$$

and  $\forall \{A_n\}_n$  sequence of mutually disjoint subsets of  $\mathcal{P}$

$$P(\cup_{n \geq 1} A_n) = \sum_{n \geq 1} P(A_n) \tag{2}$$

Then the triple  $(\Omega, \mathcal{P}, P)$  is called a *probability space*.

(ii.2) A probability space is said to be complete if every subset of a negligible set for  $P$  (i.e.  $A \in \mathcal{P}$  s.t.  $P(A) = 0$ ) is contained in  $\mathcal{P}$  himself.

We won't address this requirement more specifically, as it's rather technical and it will not be needed explicitly in the following sections; completion of the probability space is nonetheless a compulsory request in order to avoid undesirable situation, and in the following the probability spaces are always assumed to be complete.

(iii.1) Let  $(\Omega, \mathcal{P}, P)$  be a probability space and  $(S, \mathcal{S})$  a probabilizable space.

By a random element  $X$  we understand a function  $X : \Omega \rightarrow S$  such that

$$\{\omega \in \Omega : X(\omega) \in B\} \in \mathcal{P} \quad \forall B \in \mathcal{S} \quad (3)$$

$\Omega$  and  $S$  are respectively called sample space and state space of  $X$ , while their element are respectively called sample events and states.

(iii.2) Set  $S$  discrete, and  $\mathcal{S}$  its power set. Then a function  $X : \Omega \rightarrow S$  is said to be a (discrete) random variable if

$$\{\omega \in \Omega : X(\omega) = s\} \in \mathcal{P} \quad \forall s \in \mathcal{S} \quad (4)$$

Henceforth we will only be dealing with discrete random variable, abbreviating the term by RV.

**[Notation]** From now on  $X$  denotes an RV,  $(\Omega, \mathcal{P}, P)$  a probability space and  $(S, \mathcal{S})$  a probabilizable space with discrete state space.

Furthermore, we shorten statements as  $\{\omega \in \Omega : X(\omega) = s\}$  by  $\{X = s\}$ , and write  $P\{X = s\}$  rather than  $P(\{X = s\})$ .

(iv) The expectation  $E(X)$  of an RV taking the values  $\{s_k\}$  is defined by

$$E[X] \doteq \sum_k s_k P\{X = s_k\} \quad (5)$$

(v) Let  $B \in \mathcal{P}$  such that  $P(B) > 0$ . Then the mapping  $P_B(\cdot) : \mathcal{P} \rightarrow [0, 1]$  defined by

$$P_B(A) = P(A \cap B) / P(B) \quad (6)$$

is a measure on  $\mathcal{P}$ . The value  $P_B(A)$  is called conditional probability of  $A$  given  $B$  and is written as  $P(A|B)$ .

(vi) Let  $\{B_n\}_n$  be a partition of  $\Omega$  such that  $P(B_n) > 0 \forall n$ .

If  $A \in \mathcal{P}$ , then

$$P(A) = \sum_n P(B_n)P(A|B_n) \quad (7)$$

We will refer to the above identity as Formula of total probability.

(vii) By a discrete stochastic process we understand a sequence of random variables sharing the same probability and probabilizable space, indexed by a discrete parameter set.

We are now ready to introduce Markov chains.



## 2.2 Markov chains: definitions and first properties

In order to get a grasp of the idea behind Markov chains one may make an analogy with the evolution of a classical physical system: if at time  $n$  all the physical coordinates - the initial values - of the system are known, one doesn't need any further information to predict the evolution of the system at time  $n + 1$ ; stochastically the system is described at each  $n, n + 1, \dots$  by some  $X_n, X_{n+1}, \dots$ , and the corresponding assumption is that to predict the probability of  $X_{n+1}$  taking any fixed value one just needs knowing the probability of  $X_n$  taking the initial value.

Namely, one doesn't need to investigate the probability distributions of  $X_{n-1}$  and such, just as physically one doesn't need to know the past of the system to predict its future evolution: the present suffices.

On with the definition:

**Definition** (Markov chain). *A discrete stochastic process  $X = \{X_n, n \geq 0\}$  on the state space  $S$  is said to be a Markov chain, or MC, if for any sequence  $\{x_i\}_i \subset S$*

$$P\{X_{n+1} = x_{n+1} \mid X_k = x_k, 0 \leq k \leq n\} = P\{X_{n+1} = x_{n+1} \mid X_n = x_n\} \doteq p(n, x_n, x_{n+1}) \quad (8)$$

We call the indexes of the sequence  $\{X_n\}_n$  *time points*, and  $\forall x, y \in S$  we call  $p(n, x, y)$  the *one step transition probability from  $x$  to  $y$  at time  $n$* . When this probability is independent of  $n$  we say that the Markov chain is *homogeneous*.

For homogeneous Markov Chain a notion of  *$n$ -step transition probability from  $x$  to  $y$*  is given:

$$p^n(x, y) = P\{X_n = y \mid X_0 = x\} \quad \forall x, y \in S, n \in \mathbb{N} \quad (9)$$

The initial distribution of an MC is defined as  $p_0(x) \doteq P\{X_0 = x\} \quad \forall x \in S$ .

Please note that from now on we will only be dealing with homogenous MC, which will be referred at just by MC.

We are ready to prove a preliminary result.

**Proposition 2.2.1.** *Let  $\{X_n, n \geq 0\}$  be an homogeneous MC with an initial distribution  $\{p_0(x)\}$  and  $n$ -step transition probabilities  $p^n(x, y) \quad \forall x, y \in S$ . Then the following holds:*

$$(i) \quad P\{X_n = y\} = \sum_{x \in S} p_0(x) p^n(x, y)$$

$$(ii) \quad p^{n+m}(x, y) = \sum_{z \in S} p^m(x, z) p^n(z, y) \quad (\text{Chapman-Kolmogorov relation})$$

*Proof.* Ad (i). Fix  $m \in \mathbb{N}$  and let  $\{Q_x^m\}_{x \in S}$  be the countable family of pairwise, disjoint measurable sets with generic element  $Q_x^m \doteq \{X_m = x\}$ , observe  $\cup_{x \in S} Q_x^m = \Omega$  and  $P(Q_x^m) > 0 \quad \forall x \in S$ .

Then the Formula of Total Probability holds, and we may safely write

$$P(Q_y^n) = \sum_{x \in S} P(Q_x^m) P(Q_y^n \mid Q_x^m) \quad (10)$$

by choosing  $m = 0$  we get

$$P\{X_n = y\} = P(Q_y^n) = \sum_{x \in S} P(Q_x^0)P(Q_y^n | Q_x^0) = \sum_{x \in S} p_0(x)p^n(x, y) \quad (11)$$

Ad (ii). Observe that by the formula of total probability and by definition of conditioned probability the following holds  $\forall A, B \in \mathcal{S}$ :

$$\begin{aligned} P(A|B) &= \frac{P(A \cap B)}{P(B)} = \sum_{x \in S} \frac{P(Q_x^m)}{P(B)} P(A \cap B | Q_x^m) = \sum_{x \in S} \frac{P((A \cap B) \cap Q_x^m)}{P(B)} \\ &= \sum_{x \in S} \frac{P(A \cap (B \cap Q_x^m))}{P(B \cap Q_x^m)} \frac{P(B \cap Q_x^m)}{P(B)} = \sum_{x \in S} P(A | B \cap Q_x^m) P(Q_x^m | B) \end{aligned} \quad (12)$$

This can be used to our advantage. In fact by the previous identity

$$P(Q_y^{n+m} | Q_x^0) = \sum_{z \in S} P(Q_y^{n+m} | Q_z^m \cap Q_x^0) P(Q_z^m | Q_x^0) \quad (13)$$

But now

1. by the Markov property  $P(Q_y^{n+m} | Q_z^m \cap Q_x^0) = P(Q_y^{n+m} | Q_z^m)$
2. by homogeneity  $P(Q_y^{n+m} | Q_z^m) = P(Q_y^n | Q_z^0)$

Hence

$$\begin{aligned} p^{n+m}(x, y) &= P(Q_y^{n+m} | Q_x^0) = \\ &= \sum_{z \in S} P(Q_z^m | Q_x^0) P(Q_y^n | Q_z^0) = \sum_{z \in S} p^m(x, z) p^n(z, y) \end{aligned} \quad (14)$$

■

In order to investigate the phenomenon of recurrence, we need to formalize the idea of probability for an event to happen at time  $n$ : time must then be thought as a random variable, and it's called *Markov time*.

**Definition** (Markov time). *Let  $\mathcal{P}_n$  be the  $\sigma$ -algebra generated by the events  $\{X_k \in B\}_{k=0, \dots, n} \forall B \in \mathcal{S}$ . A random variable  $t : \Omega \rightarrow \mathbb{N} \cup \{+\infty\}$  is called a Markov time relative to  $\{X_n\}_n$  if*

$$\{t = n\} \in \mathcal{P}_n \quad \forall n \in \mathbb{N} \quad (15)$$

An useful notion is that of *hitting time* of a set  $A \in \mathcal{S}$ , defined as

$$t_A \doteq \min\{n > 0 : X_n \in A\} \quad (16)$$

The hitting time of a set is indeed a Markov time, as

$$\begin{aligned} \{t_A = n\} &= \{\omega \in \Omega : t_A(\omega) = n\} = \\ &= \{\omega \in \Omega : X_n(\omega) \in A, X_k(\omega) \notin A, 0 \leq k \leq n-1\} \in \mathcal{P}_n \end{aligned} \quad (17)$$

We get to see how important the notion of hitting time in the next paragraph.

## 2.3 Recurrence and transience

Denote by  $P_x(A)$  the probability of some event  $A$  with respect to the MC  $\{X_n\}_n$  taking the initial value  $x \in S$ , namely

$$P_x(A) \doteq P(A \mid X_0 = x) \quad (18)$$

Then we define the following probabilities  $\forall x, y \in S$ :

- (i)  $f^n(x, y) \doteq P_x\{t_y = n\}$   
That is, the probability that the first passage from  $x$  to  $y$  occurs at time  $n$ ;
- (ii)  $f^*(x, y) \doteq P_x\{t_y < +\infty\}$   
That is, the probability that a passage from  $x$  to  $y$  eventually occurs.

Now let  $\nu(x) : S \rightarrow \mathbb{N} \cup \{+\infty\}$  such that

$$\nu(x) \doteq \sum_{n \geq 1} I_x(X_n(\Omega)) \quad \forall x \in S \quad (19)$$

where  $I_x : \mathcal{S} \rightarrow \{0, 1\}$  denotes the *indicator function of  $x$* , namely

$$I_x(S) \doteq \begin{cases} 1 & \text{if } x \in S \\ 0 & \text{if } x \notin S \end{cases} \quad (20)$$

As time passes,  $\nu(x)$  increases its value by 1 if  $X_n$  may take the value  $x$ , thus making for a (stochastic) visit counter to  $x$ . It doesn't take in account the initial value of the MC, though, so that the following definition is far more useful in applications:

- $g(x, y) \doteq P_x\{\nu(y) = +\infty\}$   
That is, the probability of infinitely many visits to the state  $y$  for an MC starting from  $x$ .

The following proposition collects some useful identities related to the definitions we have just given:

**Proposition 2.3.1.** *Let  $x, y \in S$ . Then*

- (i)  $f^*(x, y) = \sum_{n \geq 1} f^n(x, y)$
- (ii)  $P_x\{\nu(y) = n\} = f^*(x, y)[f^*(y, y)]^{n-1}[1 - f^*(y, y)]$ , provided  $n \geq 1$
- (iii)  $g(x, y) = f^*(x, y)g(y, y)$
- (iv)  $g(x, x) = \lim_{n \rightarrow +\infty} [f^*(x, x)]^n$

*Proof.* Ad (i). Observe that the sets  $\{t_y = n\}_{n \geq 1}$  form a countable family of pairwise disjoint sets, as  $t$  is an RV. Then

$$f^*(x, y) = P_x\{t_y < +\infty\} = P_x\{\cup_{n \geq 1} \{t_y = n\}\} = \sum_{n \geq 1} P_x\{t_y = n\} = \sum_{n \geq 1} f^n(x, y) \quad (21)$$

Ad (ii). First let us prove that

$$P_x\{\nu(y) \geq n\} = f^*(x, y)[f^*(y, y)]^{n-1}, \quad n \geq 1 \quad (22)$$

For  $n = 1$ ,  $P_x\{\nu(y) \geq 1\} = P_x\{t_y < +\infty\} = f^*(x, y)$ , namely the probability of having at least one visit to  $y$  is equal the probability of transition from  $x$  to  $y$  in a finite time. For greater  $n$  we have to take into consideration the probability of  $y$  returning on itself in a finite time: as an example for  $n = 2$  we have

$$P_x\{\nu(y) \geq 2\} = P_x\{t_y < +\infty\}P_y\{t_y < +\infty\} = f^*(x, y)f^*(y, y) \quad (23)$$

and thus we have by induction equation (22). Now observe

$$\begin{aligned} P_x\{\nu(y) = n\} &= \sum_{k \geq n} P_x\{\nu(y) = k\} - \sum_{k \geq n+1} P_x\{\nu(y) = k\} = \\ &= P_x\{\nu(y) \geq n\} - P_x\{\nu(y) \geq n+1\} = f^*(x, y)[f^*(y, y)]^{n-1}[1 - f^*(y, y)] \end{aligned} \quad (24)$$

Ad (iii). Let us denote by  $\nu(y, n)$  the number of visits to the state  $y$  up to the time  $n$ . Then we may calculate  $g(x, y)$  as the probability of a transition from  $x$  to  $y$  at time  $n$  times the probability that infinitely many visits are paid to  $y$  from that time on. Namely

$$g(x, y) = \sum_{n \geq 1} P_x\{t_y = n\}P_y\{\nu(y) - \nu(y, n) = +\infty\} \quad (25)$$

But we're considering an homogenous MC, thus

$$\begin{aligned} \sum_{n \geq 1} P_x\{t_y = n\}P_y\{\nu(y) - \nu(y, n) = +\infty\} &= \\ &= \sum_{n \geq 1} P_x\{t_y = n\}P_y\{\nu(y) = +\infty\} = f^*(x, y)g(y, y) \end{aligned} \quad (26)$$

Ad (iv). Take  $x = y$  in (22). Then

$$g(x, x) = P(\nu(x) = +\infty) = \lim_{n \rightarrow +\infty} P_x\{\nu(x) \geq n\} = \lim_{n \rightarrow +\infty} [f^*(x, x)]^n \quad (27)$$

■

Now we are all set to state the definition of recurrent state and prove an important recurrence criterion.

**Definition.** A state  $x \in S$  is called recurrent if  $f^*(x, x) = 1$ , and transient otherwise.

**Theorem 1** (Recurrence criterion). A state  $x$  is recurrent if and only if

$$\sum_{n \geq 0} p^n(x, x) = +\infty \quad (28)$$

*Proof.* First we claim that  $\forall x, y \in S$  we have

$$f^*(x, y) = \lim_{N \rightarrow +\infty} \frac{\sum_{n=1}^N p^n(x, y)}{\sum_{n=0}^N p^n(y, y)} \quad (29)$$

indeed observe that any  $n$ -step transition from  $x$  to  $y$  may be thought as a composition of a transition from  $x$  to  $y$  in  $n - m$  steps ( $n > m$ ) and a permanence of  $y$  in the same state for the remaining  $m$  steps; in order to range over all the possible transitions  $m$  should be allowed to vary from 0 to  $n - 1$ , namely

$$p^n(x, y) = \sum_{m=0}^{n-1} P_x\{t_y = n - m\} p^m(y, y) = \sum_{m=0}^{n-1} f^{n-m}(x, y) p^m(y, y) \quad (30)$$

then

$$\begin{aligned} \sum_{n=1}^N p^n(x, y) &= \sum_{n=1}^N \sum_{m=0}^{n-1} f^{n-m}(x, y) p^m(y, y) = \\ &= \sum_{m=0}^{N-1} p^m(y, y) \sum_{n=m+1}^N f^{n-m}(x, y) = \sum_{m=0}^{N-1} p^m(y, y) \sum_{n=1}^{N-m} f^n(x, y) \end{aligned} \quad (31)$$

Now define

1.  $\{b_n\}_n \doteq \{\sum_{k=0}^n f^k(x, y)\}_n$ ,  $b_0 \doteq 0$ , and observe  $b_n \rightarrow f^*(x, y) \doteq b$  as  $n \rightarrow +\infty$  by (i) of the previous proposition;
2.  $\{a_n\}_n \doteq \{p^n(y, y)\}_n < 1$ , and observe  $a_n \leq 1 \forall n \in \mathbb{N}$

Our claim can be now written as

$$b = \lim_{N \rightarrow +\infty} \frac{\sum_{m=0}^N a_m b_{N-m}}{\sum_{m=0}^N a_m} \quad (32)$$

In order to show that it is indeed true we examine the two cases

- (i)  $\sum_{m \geq 0} a_m = +\infty$
- (ii)  $\sum_{m \geq 0} a_m < +\infty$

Suppose (i). Then

$$\left| b - \frac{\sum_{m=0}^N a_m b_{N-m}}{\sum_{m=0}^N a_m} \right| = \frac{|\sum_{m=0}^N a_m (b - b_{N-m})|}{\sum_{m=0}^N a_m} \quad (33)$$

but now, for  $N$  sufficiently large,  $\forall \epsilon > 0 \exists \bar{n} = \bar{n}(\epsilon) > 0$  s.t.  $|b - b_{N-m}| < \epsilon$ ,  $0 \leq m < N - \bar{n}$ ; since  $\epsilon$  is arbitrary we may safely choose  $\epsilon = \hat{\epsilon} \cdot 2^{-N} < \hat{\epsilon} \cdot 2^{-m}$ ,  $0 \leq m < N - \bar{n}$ , for some  $\hat{\epsilon} > 0$ . Then

$$\begin{aligned} \frac{|\sum_{m=0}^N a_m (b - b_{N-m})|}{\sum_{m=0}^N a_m} &< \hat{\epsilon} \frac{|\sum_{m=0}^{N-\bar{n}-1} a_m 2^{-m}|}{\sum_{m=0}^N a_m} + \frac{|\sum_{m=N-\bar{n}}^N a_m (b - b_{N-m})|}{\sum_{m=0}^N a_m} < \\ &< \frac{\hat{\epsilon}}{\sum_{m=0}^N a_m} + \max_{0 \leq n \leq \bar{n}} |b - b_n| \frac{\bar{n}}{\sum_{m=0}^N a_m} \xrightarrow{N \rightarrow +\infty} 0 \end{aligned} \quad (34)$$

Now suppose (ii). Then  $\forall \eta > 0 \exists \bar{N} = \bar{N}(\eta) > 0$  s.t.  $\sum_{n=\bar{N}}^q a_n < \eta \forall q \geq \bar{N}$ . Choose an  $\eta$  and pick  $N > \bar{N}$ , then

$$\left| b - \frac{\sum_{m=0}^N a_m b_{N-m}}{\sum_{m=0}^N a_m} \right| < \left| \frac{\sum_{m=0}^{\bar{N}} a_m (b - b_{N-m})}{\sum_{m=0}^N a_m} + \frac{\eta}{\sum_{m=0}^N a_m} \right| \quad (35)$$

Now recall that for  $N$  sufficiently large,  $\forall \epsilon > 0 \exists \bar{n} = \bar{n}(\epsilon) > 0$  s.t.  $|b - b_{N-m}| < \epsilon$ ,  $0 \leq m < N - \bar{n}$ ; pick an  $\epsilon$ , by choosing  $N$  sufficiently large we may satisfy  $\bar{N} < N - \bar{n}$ . Then we may proceed as previously and prove

$$\sum_{m=0}^{\bar{N}} a_m (b - b_{N-m}) < \sum_{m=0}^{N-\bar{n}} a_m (b - b_{N-m}) < \epsilon \quad (36)$$

If  $\bar{\epsilon} \doteq \epsilon + \eta$  we have

$$\left| b - \frac{\sum_{m=0}^N a_m b_{N-m}}{\sum_{m=0}^N a_m} \right| < \frac{\bar{\epsilon}}{a_0} \quad (37)$$

The thesis follows taking the infimum on  $\bar{\epsilon}$  on both sides of the equality.

Now that our first claim is proven, we can choose  $x = y$  and observe that (i)  $\Rightarrow x$  recurrent, while (ii)  $\Rightarrow x$  transient, hence the thesis.  $\blacksquare$

This criterion enables us to prove that the visits paid to a transient state are always finite, and to give an explicit expression for its expected value. The first result is quite intuitive, and important nonetheless, whereas the second will be particularly useful in the next paragraph.

**Proposition 2.3.2.** *Let  $u, x$  be states, denote by  $\mu(u, x) \doteq E_u(\nu(x))$ , the expected number of visits to  $x$  for an MC starting from  $u$ . Let  $x$  be transient, then the following holds:*

$$(i) \quad g(u, x) = 0$$

$$(ii) \quad \mu(u, x) = \frac{f^*(u, x)}{1 - f^*(x, x)} < +\infty$$

*Proof.* Ad (i). By Proposition 5.2.2 (iii)-(iv) and the transience of  $x$  we have

$$g(u, x) = f^*(u, x)g(x, x) = f^*(u, x) \lim_{n \rightarrow +\infty} [f^*(x, x)]^n = 0 \quad (38)$$

Ad (ii). By Proposition 5.2.2 (ii) we have

$$\begin{aligned} \mu(u, x) &= \sum_{n \geq 1} n P_u(\nu(x) = n) = f^*(u, x) [1 - f^*(x, x)] \sum_{n \geq 1} n f^*(x, x)^{n-1} \\ &= f^*(u, x) \frac{1 - f^*(x, x)}{(1 - f^*(x, x))^2} = \frac{f^*(u, x)}{1 - f^*(x, x)} < +\infty \end{aligned} \quad (39)$$

$\blacksquare$

## 2.4 Communication between states

We want to study the structure of the state space of an MC. It turns out that there is an equivalence relation linking communicating states, and more precisely:

**Definition.** We say that a state  $x$  leads to state  $y$  and write  $x \longrightarrow y$  if  $\exists n \geq 0 : p^n(x, y) > 0$ . If both  $x \longrightarrow y$  and  $x \longleftarrow y$  hold, we say that  $x$  and  $y$  communicate, and write  $x \longleftrightarrow y$ .

The relation ‘communication’ is indeed an equivalence relation in the state space of an homogeneous MC, as it is

1. Reflexive:  $p^0(x, x) = 1 > 0 \forall x \in S$ ;
2. Symmetric: by definition;
3. Transitive: if  $x \longleftrightarrow y$  and  $y \longleftrightarrow z$  for some  $x, y, z \in S$ , then  $\exists m, n \in \mathbb{N}$  such that  $p^m(x, y)p^n(y, z) > 0$ . Then by the Chapman-Kolmogorov relation we have

$$p^{n+m}(x, z) = \sum_{u \in S} p^n(x, u)p^m(u, z) \geq p^m(x, y)p^n(y, z) > 0 \quad (40)$$

that is,  $x \longrightarrow z$ . Similarly  $z \longrightarrow x$ .

When the state space of an MC is an equivalence class with respect to  $\longleftrightarrow$ , we say that the corresponding MC is *irreducible*. It is natural to expect that an irreducible MC over a finite state space contains just recurrent states: we state the result as a theorem for its future importance.

**Theorem 2.** Let  $\{X_n\}_n$  be an irreducible MC with finite space  $S$ : then all the states of  $\{X_n\}_n$  are recurrent, and the MC is said to be recurrent.

*Proof.* We divide the proof in two steps:

- (i)  $S$  contains at least one recurrent state;
- (ii) For any  $x, y \in S$  if  $x$  is recurrent and  $x \longrightarrow y$  then  $y$  is recurrent.

Ad (i). Ad absurdum: suppose that all the states in  $S$  are transient, then  $\forall x, y \in S$  we have from Proposition 5.2.3 (ii) that

$$+\infty > \mu(x, y) = E_x\left[\sum_{n=1}^{+\infty} I_y(X_n)\right] = \sum_{n=1}^{+\infty} P_x\{X_n = y\} = \sum_{n=1}^{+\infty} p^n(x, y) \quad (41)$$

Hence  $\lim_{n \rightarrow +\infty} p^n(x, y) = 0$ . As this limit exists and the state space is finite we may write

$$0 = \sum_{x \in S} \lim_{n \rightarrow +\infty} p^n(x, y) = \lim_{n \rightarrow +\infty} P_x\{X_n \in S\} = \lim_{n \rightarrow +\infty} 1 = 1. \quad (42)$$

Hence (i).

Ad (ii). As  $x \longrightarrow y$ , there exists  $m \in \mathbb{N}$  such that  $p^m(x, y) > 0$ . Let us define

$$M \doteq \min\{m : p^m(x, y) > 0\} \quad (43)$$

We proceed claiming  $f^*(y, x) = 1$ .

Indeed, assume the contrary: then  $1 - f^*(y, x) > 0$ , namely there is a positive probability for a particle starting in  $y$  of never visiting  $x$ . Then  $p^M(x, y)(1 - f^*(y, x)) > 0$ , that is, there is a positive probability for a particle starting from  $x$  to get to  $y$  in  $M$  steps and then never coming back to  $x$ .

But we know from Proposition 5.2.2 (iv) that  $P\{\nu(x) = +\infty\} = 1$ , hence a contradiction and  $f^*(y, x) = 1$ .

Observe that  $f^*(y, x) = 1 \Rightarrow \exists N \in \mathbb{N} : p^N(y, x) > 0$ . By an obvious extension of the Chapman-Kolmogorov relation we have

$$\begin{aligned} p^{N+n+M}(x, y) &= \sum_{u, v \in S} p^N(y, u)p^n(u, v)p^M(v, y) \geq \\ &\geq p^N(y, x)p^n(x, x)p^M(x, y) \quad \forall n \in \mathbb{N} \end{aligned} \quad (44)$$

Hence

$$\begin{aligned} \sum_{n=0}^{+\infty} p^n(y, y) &= \sum_{n=0}^{N+M} p^n(y, y) + \sum_{n=0}^{+\infty} p^{N+n+M}(y, y) \\ &\geq \sum_{n=0}^{+\infty} p^{N+n+M}(y, y) \geq p^N(y, x)p^M(x, y) \sum_{n=0}^{+\infty} p^n(x, x) = +\infty \end{aligned} \quad (45)$$

where we have used

- (a)  $p^N(y, x) > 0, p^M(x, y) > 0$  by construction;
- (b)  $\sum_{n=0}^{+\infty} p^n(x, x) = +\infty$  by the recurrence criterion.

We can use the recurrence criterion again to conclude that  $y$  is recurrent as well, and thus complete the proof. ■

In the next paragraph we work with irreducible MCs over finite state spaces, giving the last definitions and proving one important identity.

## 2.5 Stationary distributions

Consider an MC  $\{X_n\}_n$  over a finite state space. By Proposition 2.2.1(i)

$$P\{X_n = y\} = \sum_{x \in S} p_0(x)p^n(x, y) \quad (46)$$

Now suppose that the system evolves so that  $P\{X_n = y\} = p_0(y) \quad \forall y \in S$ . If this is the case we denote  $\pi(x) \doteq p_0(x)$ , and (46) becomes

$$\pi(x) = \sum_{u \in S} \pi(u)p^n(u, x) \quad (47)$$

Let us show that if the above equality is valid for  $n = 1$ , then it is  $\forall n \in \mathbb{N}$ , provided we're working in a finite state space. Indeed, if (46) holds for  $n = 1$ , let us prove our



claim by induction: that is, we suppose it holds for  $n$  and show that then it does hold for  $n + 1$  too. The proof is straightforward:

$$\sum_{u \in S} \pi(u) p^{n+1}(u, x) = \sum_{u \in S} \sum_{v \in S} \pi(u) p^n(u, v) p(v, x) = \sum_{v \in S} \pi(v) p(v, x) = \pi(x) \quad (48)$$

We're ready to give the definition of *stationary distribution*.

**Definition** (Stationary distribution). *Let  $S$  be a finite state space, let  $\pi : S \rightarrow [0, 1]$  such that*

$$(i) \sum_{x \in S} \pi(x) = 1$$

$$(ii) \pi(x) = \sum_{u \in S} \pi(u) p(u, x) \quad \forall x \in S$$

*then  $\{\pi(x)\}_{x \in S}$  is called a stationary distribution.*

The definition has an immediate physical meaning, but before proceeding we'd rather clarify some language issues.

**Definitions.** (i) *We say that a physical quantity related to a particle obey to some distribution  $\{p^*(x)\}_{x \in S}$  if when a measurement of the said quantity is made it yields the result  $x$  with a probability  $p^*(x)$ . We call  $x$  a state of the particle. When there is no need to refer to a particular physical quantity, we will simply say that the particle obeys to the distribution  $\{p^*(x)\}_{x \in S}$ .*

(ii) *Many particles make up a system; if all of them obey the same distribution  $\{p^*(x)\}_{x \in S}$ , we say that the system obeys to the distribution  $\{p^*(x)\}_{x \in S}$ .*

Now observe that no matter the value of  $n$  in (47),  $\pi(x)$  stays constant, that is, if a particle obeys  $\{\pi(x)\}_{x \in S}$  the probability of finding it in some state  $x$  is time independent; a direct consequence of this fact is that if a system obeys to  $\{\pi(x)\}_{x \in S}$ , the fraction of particles in each of the possible states of the system is “more or less” constant - namely, we are assuming that if the number of particles  $N$  is large enough  $N\pi(x) \in \mathbb{N} \quad \forall x \in S$ . Thus the notion of stationary distribution is closely related to that of macroscopic equilibrium: even if there may be transitions of the single particles from one state to another, the number of particles in the state is overall the same.

In view of the discussion on the Ehrenfest chain, we would like to give a definition of *mean recurrence time* of a state  $x$ , that is, we would like to know on average how long does it take to a particle in state  $x$  to get back to  $x$  during its temporal evolution. The rough idea is to consider the ratio of the time elapsed in the complete evolution of the system to the number of visits paid to  $x$  during that time: for our purposes the evolution process is infinitely long, and the definition needs some mathematical refinements, but essentially it still works.

We give the definition and then show it is indeed well-posed.

**Definition.** Let  $x, y$  states,  $\{X_n\}$  an irreducible, recurrent MC. Recall that  $\nu(y) \doteq \sum_{n \geq 1} I_y(X_n)$  denotes the number of visits paid to  $y$  after  $n$  steps, whereas  $E_x[\nu(y, n)]$  denotes the expected number of visits paid to  $y$  after  $n$  steps for a particle starting with state  $x$ . It is easy to see, by definition of  $\nu(y, n)$

$$E_x(\nu(y, n)) = \sum_{m=1}^n p^m(x, y) \quad (49)$$

Define then

$$\bar{\nu}(x, y) \doteq \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{m=1}^n p^m(x, y) \quad (50)$$

Then the mean recurrence time  $\tau(y)$  of the state  $y$  is, by definition,

$$\tau(y) \doteq \begin{cases} [\bar{\nu}(x, y)]^{-1} & \text{if } \bar{\nu}(x, y) \neq 0 \\ +\infty & \text{otherwise} \end{cases} \quad (51)$$

Now for some comments.

- (i) First of all, note that  $\tau(y)$  is by definition independent of the choice of  $x$ . That's actually the case: to prove it, let  $x, u, v$  states and observe

$$\begin{aligned} \frac{1}{n} \sum_{m=1}^n (p^m(x, y) - p^m(u, y)) &= \underbrace{\frac{p(x, y) + p(u, y)}{n}}_{=a(n)} + \frac{1}{n} \sum_{m=1}^n (p^{m+1}(x, y) - p^{m+1}(u, y)) \\ &= a(n) + \frac{1}{n} \sum_{m=1}^n \sum_{v \in S} (p(x, v) - p(u, v)) p^m(v, y) \\ &= a(n) + \sum_{v \in S} (p(x, v) - p(u, v)) \frac{1}{n} \sum_{m=1}^n p^m(v, y) \end{aligned} \quad (52)$$

The exchange of sums is justified as they're both finite. Now take the limit for  $n \rightarrow +\infty$ , and for the moment assume that  $\bar{\nu}(\cdot, y)$  exists no greater than 1 on both sides of the equation - we will show it does in (ii). Then

$$\begin{aligned} |\bar{\nu}(x, y) - \bar{\nu}(u, y)| &= \left| 0 + \sum_{v \in S} (p(x, v) - p(u, v)) \bar{\nu}(v, y) \right| \leq \left| \sum_{v \in S} (p(x, v) - p(u, v)) \right| = \\ &= \left| \sum_{v \in S} p(x, v) - \sum_{v \in S} p(u, v) \right| = 0 \end{aligned} \quad (53)$$

- (ii) For the definition to make sense, the limit denoted by  $\bar{\nu}(x, y)$  has to exist for any two states  $x, y$ . We claim it does, and that furthermore  $\bar{\nu}(x, y) \in [0, 1]$ . Indeed

$$0 \leq \frac{1}{n} \sum_{m=1}^n p^m(x, y) \leq \frac{1}{n} \sum_{m=1}^n 1 = 1 \quad \forall n \in \mathbb{N} \quad (54)$$

moreover, it is easily seen that the sequence is non-decreasing, and made up of positive terms. Then it converges.

(iii) There is a simple identity linking the stationary distribution of an *MC* to its mean recurrence times, namely

$$\tau(x) = \frac{1}{\pi(x)} \quad (55)$$

indeed, recall that for a stationary distribution

$$\pi(x) = \sum_{u \in S} \pi(u) p^m(u, x) \quad \forall m \in \mathbb{N} \quad (56)$$

then

$$\pi(x) = \frac{1}{n} \sum_{m=1}^n \sum_{u \in S} \pi(u) p^m(u, x) = \sum_{u \in S} \pi(u) \frac{1}{n} \sum_{m=1}^n p^m(u, x) \quad (57)$$

and by letting  $n \rightarrow +\infty$  we get our identity.

Now we have all the results we need to examine the Ehrenfest chain in detail.

## 2.6 Ehrenfest chain

First of all, let's make sure we are working with an *MC*.

Recall that the total number of balls is  $2N$  and focus on urn *A*: the possible states of the urn - that is, the number of balls contained in it - ranges from 0 to  $2N$ , extremes included, spanning all the integers.

Let  $\{X_n\}_n$  be the RVs related to the state of the urn at any time  $n \in \mathbb{N}$ : by construction

$$P\{X_{n+1} = x_{n+1} \mid X_k = x_k, 0 \leq k \leq n\} = P\{X_{n+1} = x_{n+1} \mid X_n = x_n\} \quad (58)$$

in fact at time  $n + 1$  the number of balls in urn *A* either increase by 1 or decrease by 1, unless we're in the extremes, with a probability that varies according to the same number before the extraction. The probability of the number of balls increasing equals the probability of extracting a number corresponding to a ball not contained in the urn; vice versa, the probability of losing a ball equals the probability of the extraction of a number whose ball is contained in the urn: there aren't any other possibilities. Note that the process is time homogeneous.

The transition probabilities look like

$$\begin{aligned} p(m, m-1) &= \frac{m}{2N} \\ p(m, m+1) &= \frac{2N-m}{2N} \\ p(m, k) &= 0, \quad k \neq m \pm 1 \end{aligned} \quad (59)$$

To sum it up, we have a time homogeneous *MC* over a finite state space. Is it irreducible? It is: as we have just seen each state communicates with the previous and following one, namely

$$p(m, m-1) = \frac{m}{2N} > 0; \quad p(m-1, m) = \frac{2N+1-m}{2N} > 0 \quad (60)$$

unless  $m = 0$ . But  $p(0, 1) = 1 > 0$ , and for  $m = 1$  the inequalities above are verified: by transitivity all the states are communicating, and the Ehrenfest chain is irreducible.

By Theorem 2 an irreducible MC over a finite state space is a recurrent MC. Indeed observe that to have a nonzero probability of a state recurring we need just two steps:

$$\begin{aligned} p^2(m, m) &= \sum_{l \in S} p(m, l)p(l, m) = p(m, m+1)p(m+1, m) + p(m, m-1)p(m-1, m) \\ &= \frac{2Nm - m^2 + N}{2N^2} = \frac{2N - m}{2N^2}m + \frac{1}{2N} > 0 \quad \forall m = 0, 1, \dots, 2N \end{aligned} \quad (61)$$

Now we want to estimate the mean recurrence times of the states of the Ehrenfest chain: it is most convenient to do so by computing the stationary distribution  $\pi(x)$  of the chain, in order to exploit the relation

$$\tau(x) = \frac{1}{\pi(x)} \quad (62)$$

Observe that  $\tau(x)$  is well defined since we proved the chain to be irreducible and recurrent; as for  $\pi(x)$ , we know that by definition two conditions must hold:

- (i)  $\sum_{x \in S} \pi(x) = 1$
- (ii)  $\pi(x) = \sum_{u \in S} \pi(u)p(u, x) \quad \forall x \in S$

Let's focus on (ii). We have recursively

$$\begin{aligned} \pi(0) &= \frac{1}{2N}\pi(1) \Rightarrow \pi(1) = 2N\pi(0) \\ \pi(1) &= \pi(0) + \frac{2}{2N}\pi(2) \Rightarrow \pi(2) = \frac{2N(2N-1)}{2}\pi(0) \\ \pi(2) &= \frac{2N-1}{2N}\pi(1) + \frac{3}{2N}\pi(3) \Rightarrow \frac{2N(2N-1)(2N-2)}{6}\pi(0) \end{aligned} \quad (63)$$

We see that generally

$$\pi(x) = \binom{2N}{x} \pi(0), \quad x = 0, 1, \dots, 2N \quad (64)$$

Now observe

$$\sum_{i=0}^K \binom{K}{i} = 2^K \quad (65)$$

Indeed, by the binomial theorem  $(x+y)^k = \sum_{i=0}^k \binom{k}{i} x^i y^{k-i}$ , and by choosing  $x = y = 1$  (65) follows.

Then (i) yields  $\pi(0)2^{2N} = 1$ . In conclusion

$$\pi(x) = \binom{2N}{x} 2^{-2N} \quad (66)$$

Thus the mean recurrence time of the generic state  $x$  is

$$\tau(x) = 2^{2N} \frac{x!(2N-x)!}{2N!} \quad (67)$$

Observe that for  $x = 0$  and  $x = 2N$  the mean recurrence is time is enormous:

$$\bar{\tau} \doteq \tau(0) = \tau(2N) = 2^{2N} \quad (68)$$

In order to give a rough estimate, take for instance  $N \simeq 10^{23}$  and let  $2^{10} = 1024 \simeq 10^3$ : then  $\bar{\tau} \simeq 10^{(10^{22})}$ .

Now this is just the number of “extractions” it takes to have a recursion: by multiplying it for a typical time of the system one can try to convert the result in seconds; we may choose as a typical time the inverse of the collision frequency. Suppose to work with Helium at STP, what we get is  $\Delta t_{typ,He} \simeq 10^{-13} s$ <sup>2</sup>.

Then the mean recurrence time is  $T_{He} = \Delta t_{typ,He} \cdot \bar{\tau} \simeq 10^{(10^{22}-13)} s \simeq 10^{(10^{22})} s$ . Observe that for  $x = N$  the same computation yields, by making use of the Stirling approximation,  $t_{He} \simeq \sqrt{\frac{\pi 10^{23}}{2}} 10^{-13} s \simeq 10^{-2} s!$

Asking for the mean recurrence time of the state 0 or  $2N$  is equivalent to ask the frequency at which the gas is found all contained in one half of the box: the time we obtain is so large that we may safely consider the process of a gas previously enclosed in an half of the box spreading all over the box to be irreversible.

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<sup>2</sup>see HyperPhysics, <http://hyperphysics.phy-astr.gsu.edu>



### 3 Quantum approach

While the Ehrenfest chain has the advantages of giving a simple model, it lacks both accuracy and depth: the dynamics of the system is totally neglected in favour of a stochastic viewpoint, and the very ideas of "extractions" and discrete time are quite far from the actual behavior of the system.

On the other hand, the quantum theory is less simple both in terms of understanding of the model and mathematics implied, but it lets us push our analysis further by elaborating more information about the system and giving a fuller response.

The aim of the chapter is to build a wave function for a quantum gas of non-interacting particles and show that a recurrence theorem holds, giving an estimate of the recurrence time for a sample system.

The chapter is structured as follows:

1. The first paragraph introduces the problem from a physical point of view, emphasizing the concepts we need to formalize;
2. The second paragraph collects some results on tensors;
3. The third paragraph collects some results on groups;
4. The fourth paragraph proves and comments the recurrence theorem;

#### 3.1 Quantum gases and exchange degeneracy

Consider a system of  $N$  non-interacting particles with the same mass, and label their positions by  $\mathbf{r}_1, \dots, \mathbf{r}_n$ , setting  $t$  as the time coordinate for the system. Spin is not relevant by now, and we ignore it; we suppose the particles to be confined in a finite volume  $\mathcal{V}$ . The state function of the system may be written in the spatial coordinates framework as some  $\psi = \psi(\mathbf{r}_1, \dots, \mathbf{r}_n, t)$  satisfying the Schrödinger equation

$$i\hbar\partial_t\psi = H\psi \tag{69}$$

where  $H$  is the Hamiltonian operator for the system. As the particles do not mutually interact we may write it down as

$$H = \sum_{i=1}^N H_i \tag{70}$$

with the  $H_i$ s being the Hamiltonians for the single particles. The normalization request for the spatial parts reads out

$$\int_{\mathcal{V}_x \dots \mathcal{V}_x} |\psi(\mathbf{r}_1, \dots, \mathbf{r}_n, t)|^2 d^{3N}\mu = 1 \quad \forall t \in \mathbb{R} \tag{71}$$

with  $d^{3N}\mu$  denoting the  $3N$ -dimensional Lebesgue measure. We conclude  $\psi(\cdot, t) \in L^2(\mathcal{V}^N, d^{3N}\mu) \forall t \in [0, +\infty)$ .

For our purposes it is not restrictive to assume the Hamiltonian to be time independent; furthermore, we consider only systems with a *discrete* energy eigenvalues set  $\mathcal{E}$ . When these hypotheses are made we know that the the general solution of the Schrödinger equation may be written as

$$\sum_{E \in \mathcal{E}} a_E \phi_E(\mathbf{r}) \exp(-iEt) \quad (72)$$

Where  $\mathbf{r}$  collects all the  $N$ -tuple of coordinates,  $\hbar = 1$ , and

$$H\phi_E(\mathbf{r}) = E\phi_E(\mathbf{r}) \forall E \in \mathcal{E} \quad (73)$$

Now we would like to use at our advantage equation (70). In order to do so, consider the  $i$ th particle's stationary Schrödinger equation

$$H_i \varphi_i(\mathbf{r}_i) = E_i \varphi_i(\mathbf{r}_i) \quad (74)$$

and observe that the  $i$ th Hamiltonian will regard the  $j$ th particle's stationary wave function as a constant whenever  $i \neq j$ . Now observe that  $\forall E \in \mathcal{E}$  we can find an eigenvalue  $N$ -tuple  $(E_1, \dots, E_n)$  such that  $\sum_{i=1}^N E_i = E$ , then it is easily seen that

$$\phi_E(\mathbf{r}) \doteq \prod_{i=1}^N \varphi_i(\mathbf{r}_i) \quad (75)$$

satisfies equation (73).

Mathematically this solution makes sense - indeed, it solves the equation of motion. But what about the physical meaning? Our simple model of a quantum gas is that of a system made up of  $N$  "equivalent" particles, that is, particles with the same physical properties (e.g. mass, charge...): therefore the single particle Hamiltonians  $H_i$  have all the same form, and the domain is the same as well, namely  $L^2(\mathcal{V}^N)$ . They are, indeed, all the same operator, and it is just *us* making a distinction by assigning each of them to a different particle: but this is just a virtual difference, a problem of bookkeeping without any correspondence in the physical reality.

Now we may expect this misunderstanding to have consequences on the mathematical form of the solution too. That's the direction we'll be investigating on.

Before addressing the quandary, let's clarify the meaning of  $\phi_i(\mathbf{r}_j)$  for  $i \neq j$ : it is the wave function with energy  $E_i$  assigned to the framework of the  $j$ th particle, namely it satisfies

$$H_j \phi_i(\mathbf{r}_j) = E_i \phi_i(\mathbf{r}_j) \quad (76)$$

as all the Hamiltonians have the same form and therefore the same eigenvalues.

A direct consequence of this fact is that any permutation of particle, any reordering of the function's indexes, yields another possible solution of the equation of motion. If a permutation is defined, naturally, as a bijection of the form

$$\sigma : \{1, \dots, N\} \rightarrow \{1, \dots, N\} \quad (77)$$



we may conclude that if  $\prod_{i=1}^N \varphi_i(\mathbf{r}_i)$  solves the stationary equation of motion then

$$\prod_{i=1}^N \varphi_{\sigma(i)}(\mathbf{r}_i) \quad (78)$$

does too, yielding the same eigenvalue.

We have found a degeneracy, but this is not a problem: the problem is that it cannot be solved, for it doesn't exist an operator who can distinguish any two of those degenerate solutions, for *we made up the degeneracy in first place*: the particles are not distinguishable.

A good way to get out of this is to select from the set of all possible solutions a smaller class of solutions who have the physical meaning we ask for. When making measurement what we determine is not the wave function, but rather its absolute value: therefore we would like wave functions whose absolute value does not to change under swaps, namely

$$\left\| \prod_{i=1}^N \varphi_i(\mathbf{r}_i) \right\|^2 = \left\| \prod_{i=1}^N \varphi_{\sigma(i)}(\mathbf{r}_i) \right\|^2 \quad (79)$$

for any possible permutations.

Now the question is: is there a way to obtain solutions of this form from the solution we got before? And how do we transfer the idea of swapping indexes to the idea of swapping single particle wave functions? Is there a way to do so?

What we had was a good mathematical solution with physical problems. Now we have the physical solution, but we lack the proper mathematical tools for an in-depth analysis. The next paragraph is devoted to the construction of these tools.

### 3.2 Some recalls about tensors on Hilbert spaces

Firstly some basic definitions (and a fact) about tensors:

**Definitions.** Let  $V_1, \dots, V_n$  ( $n \geq 1$ ) vector spaces on  $\mathbb{K} = \mathbb{R}$  or  $\mathbb{C}$ ,  $\mathcal{L}(V_1^*, \dots, V_n^*)$  the linear space of multilinear maps from  $V_1^* \times \dots \times V_n^*$  to  $\mathbb{K}$ ,  $V^*$  denoting the dual space of  $V$ . Then

(i) if  $(u_1, \dots, u_n) \in V_1 \times \dots \times V_n$ ,  $\mathcal{L}(V_1^*, \dots, V_n^*) \ni u_1 \otimes \dots \otimes u_n$  is defined as

$$u_1 \otimes \dots \otimes u_n(v_1, \dots, v_n) \doteq \langle u_1, v_1 \rangle \dots \langle u_n, v_n \rangle \quad \forall (v_1, \dots, v_n) \in V_1^* \times \dots \times V_n^* \quad (80)$$

where  $\langle, \rangle$  is the pairing between elements of  $V$  and  $V^*$  respectively.

We call  $u_1 \otimes \dots \otimes u_n$  tensor product of  $(u_1, \dots, u_n)$ .

(ii) The map  $\otimes : V_1 \times \dots \times V_n \rightarrow \mathcal{L}(V_1^*, \dots, V_n^*)$  such that  $\otimes((u_1, \dots, u_n)) = u_1 \otimes \dots \otimes u_n$  is called tensor product map.

(iii) The vector subspace  $Im(\otimes)$  of  $\mathcal{L}(V_1^*, \dots, V_n^*)$  is denoted by  $V_1 \otimes \dots \otimes V_n$  and is called tensor product of the spaces  $V_1, \dots, V_n$ .

(Universality) Let  $W$  a vector space,  $f : V_1 \times \dots \times V_n \rightarrow W$  a multilinear mapping.

Then there exists an unique linear mapping  $f^\otimes \doteq f \circ \otimes : V_1 \otimes \dots \otimes V_n \rightarrow W$ .

From now on we will be working on  $N$  copies of the Hilbert space  $(\mathcal{H}, (\cdot|\cdot))$  on  $\mathbb{C}$ , denoting  $\underbrace{\mathcal{H} \otimes \dots \otimes \mathcal{H}}_{N \text{ times}} \doteq \mathcal{H}^N$ .

The next proposition collects some useful properties of  $\mathcal{H}^N$ .

**Proposition 3.2.1.** Let  $(\mathcal{H}, (\cdot|\cdot))$  an Hilbert space on  $\mathbb{C}$ , consider its tensor product  $\mathcal{H}^N$ . Then

- $\mathcal{H}^N$  can be enriched with an Hermitean scalar product  $(\cdot|\cdot)_\otimes$  defined as

$$(u_1 \otimes \dots \otimes u_N | v_1 \otimes \dots \otimes v_N)_\otimes \doteq (u_1 | v_1) \dots (u_N | v_N) \quad \forall u_i, v_i \in \mathcal{H}, \quad i = 1, \dots, N \quad (81)$$

- The completion of  $\mathcal{H}^N$  with respect to  $(\cdot|\cdot)_\otimes$  is an Hilbert space, which we will denote by  $\mathcal{H}_\otimes^N$  and call Hilbertian tensor product;
- If  $\{e_i\}_{i \in I}$  is an Hilbert basis for  $\mathcal{H}$ , then  $\{e_{i_1} \otimes \dots \otimes e_{i_N}\}_{i_1, \dots, i_N \in I}$  is an Hilbert basis for  $\mathcal{H}_\otimes^N$ .

The reason for which we want to work with spaces of this sort is that permutations may be conveniently represented - in a sense that we'll see more precisely in a while - on the tensor product of vectorial spaces.

We have already observed that our wave function's spatial part belongs to the space  $L^2(\mathcal{V}, d^{3N}\mu)$ : we would like to prove that  $L^2(\mathcal{V}, d^{3N}\mu)$  can be seen - i.e.: is isomorphic to - some Hilbertian tensor product. That's the content of the following theorem.

**Theorem 3.** Let  $\mathcal{V}$  a bounded subset of  $\mathcal{V}$ ,  $\mathcal{H} \doteq L^2(\mathcal{V}, d^3\mu)$ . Then  $\mathcal{H}_\otimes^N$  is naturally isomorphic to  $L^2(\mathcal{V}^N, d^{3N}\mu)$ .

*Proof.* We know that  $\mathcal{H}$  admits an Hilbert basis  $\{e_i\}_{i \in I}$ , then by proposition (3.2.1)  $\mathcal{H}_\otimes^N$  admits a basis  $\{e_{i_1} \otimes \dots \otimes e_{i_N}\}_{i_1, \dots, i_N \in I}$ .

As  $\{e_{i_1} \cdot \dots \cdot e_{i_N}\}_{i_1, \dots, i_N \in I}$  is a basis for  $L^2(\mathcal{V}^N, d^{3N}\mu)$ , it sounds quite natural to propose an association of the form

$$\mathcal{H}_\otimes^N \ni e_{i_1} \otimes \dots \otimes e_{i_N} \xrightarrow[A]{} e_{i_1} \cdot \dots \cdot e_{i_N} \in L^2(\mathcal{V}^N, d^{3N}\mu) \quad (82)$$

and try to extend it on the whole space.

In order to do so, observe that  $\forall v \in \mathcal{H}_\otimes^N$  there exists a sequence of scalars such that  $v = \sum_{i_1, \dots, i_N \in I} c_v^{i_1, \dots, i_N} e_{i_1} \otimes \dots \otimes e_{i_N}$ ; then we define  $\tilde{A} : \mathcal{H}_\otimes^N \rightarrow L^2(\mathcal{V}^N, d^{3N}\mu)$  as

$$\tilde{A}(v) \doteq \sum_{i_1, \dots, i_N \in I} c_v^{i_1, \dots, i_N} A(e_{i_1} \otimes \dots \otimes e_{i_N}) = \sum_{i_1, \dots, i_N \in I} c_v^{i_1, \dots, i_N} e_{i_1} \cdot \dots \cdot e_{i_N} \quad (83)$$

observe that  $\tilde{A}(v) < +\infty \quad \forall v \in \mathcal{H}_\otimes^N$ , as the series on the right side must converge by definition of  $A$  and by the fact that  $\{e_{i_1} \cdot \dots \cdot e_{i_N}\}_{i_1, \dots, i_N \in I}$  is a basis for  $L^2(\mathcal{V}^N, d^{3N}\mu)$ ; moreover  $\tilde{A}$  is linear by construction, then we may conclude it is continuous.

Such an extension is unique. Indeed, let  $B$  be another linear, continuous extension of  $A$ , then:

$$\begin{aligned} B(v) &= \sum_{i_1, \dots, i_N \in I} c_v^{i_1, \dots, i_N} B(e_{i_1} \otimes \dots \otimes e_{i_N}) = \sum_{i_1, \dots, i_N \in I} c_v^{i_1, \dots, i_N} B(e_{i_1} \otimes \dots \otimes e_{i_N}) \\ &= \sum_{i_1, \dots, i_N \in I} c_v^{i_1, \dots, i_N} A(e_{i_1} \otimes \dots \otimes e_{i_N}) = \tilde{A}(v) \end{aligned} \quad (84)$$

Now let's show that  $\tilde{A}$  is an isomorphism.

- Injectivity: suppose  $\tilde{A}(v) = y = \tilde{A}(w)$  for some  $v, w \in \mathcal{H}_\otimes^N$ ,  $y \in L^2(\mathcal{V}^N, d^{3N}\mu)$ , then

$$0 = \tilde{A}(v) - \tilde{A}(w) = \tilde{A}(v - w) = \sum_{i_1, \dots, i_N \in I} (c_v^{i_1, \dots, i_N} - c_w^{i_1, \dots, i_N}) e_{i_1} \dots e_{i_N} \quad (85)$$

but  $\{e_{i_1} \cdot \dots \cdot e_{i_N}\}_{i_1, \dots, i_N \in I}$  is a basis for  $L^2(\mathcal{V}^N, d^{3N}\mu)$ , so that

$$c_v^{i_1, \dots, i_N} - c_w^{i_1, \dots, i_N} = 0 \quad \forall i_1, \dots, i_N \in I \quad (86)$$

therefore  $v = w$ .

- Surjectivity: pick  $y \in L^2(\mathcal{V}^N, d^{3N}\mu)$ . We may write it in terms of the basis, therefore

$$\begin{aligned} y &= \sum_{i_1, \dots, i_N \in I} c_y^{i_1, \dots, i_N} e_{i_1} \dots e_{i_N} = \sum_{i_1, \dots, i_N \in I} c_y^{i_1, \dots, i_N} A(e_{i_1} \otimes \dots \otimes e_{i_N}) = \\ &= \tilde{A} \left( \sum_{i_1, \dots, i_N \in I} c_y^{i_1, \dots, i_N} e_{i_1} \otimes \dots \otimes e_{i_N} \right) = \tilde{A}(v) \end{aligned} \quad (87)$$

for some  $v \in \mathcal{H}_\otimes^N$ , by its completeness.

- Scalar product preservation: let  $(\cdot|\cdot)_\otimes$  the scalar product of  $\mathcal{H}_\otimes^N$ ,  $(\cdot|\cdot)$  the one of  $L^2(\mathcal{V}^N, d^{3N}\mu)$ . Then

$$(A(v)|A(w)) = \sum_{i_1, \dots, i_N \in I} \sum_{j_1, \dots, j_N \in I} c_v^{i_1, \dots, i_N} c_w^{j_1, \dots, j_N} \delta_{i_1 j_1} \dots \delta_{i_N j_N} = (v|w)_\otimes \quad (88)$$

■

This theorem lets us choose a more convenient domain for our wave function, that is - we write it explicitly once and for all -  $\underbrace{L^2(\mathcal{V}, d^3\mu) \otimes \dots \otimes L^2(\mathcal{V}, d^3\mu)}_{N \text{ times}} \doteq \mathcal{L}^N(\mathcal{V})$ .

Furthermore, we denote  $\underbrace{L^2(\mathcal{V}, d^3\mu) \times \dots \times L^2(\mathcal{V}, d^3\mu)}_{N \text{ times}} \doteq \mathcal{L}_\times^N(\mathcal{V})$

### 3.3 The group of permutations

We defined a permutation as a bijection of a set of indexes  $\{1, \dots, N\} \subset \mathbb{N}$  into itself: with this definition we can permute indexes, but what we would like to have is an object that swaps the wave functions generating in turn other wave functions, just as the original permutation generates sets of indexes from sets of indexes.

First of all, let  $I_N \doteq \{1, \dots, N\}$  and observe that the set of all permutations  $\sigma : I_n \rightarrow I_n$  makes up a group when endowed with the usual composition rule for maps  $\circ$ .

The group structure is self-evident, indeed

- (i)  $\circ$  is associative by definition;
- (ii) the group unit is  $I_\sigma$ , the identity on  $I_N$ ;
- (iii) each  $\sigma$  is invertible, as it is bijective.

We denote the group of permutations on  $I_N$  by  $\mathcal{P}_N$ .

The group structure allows us to explore representations of the group in other spaces. More precisely,

**Definitions.** 1. Let  $(G_1, \circ_1), (G_2, \circ_2)$  groups.

A group homomorphism from  $(G_1, \circ_1)$  to  $(G_2, \circ_2)$  is a mapping  $h$  which preserves the group structure, that is

$$h(g_a \circ_1 g_b) = h(g_a) \circ_2 h(g_b) \quad (89)$$

2. Let  $(G, \circ_G)$  a group,  $V$  a vector space and  $(GL(V), \circ)$  the group made up by the set of automorphisms of  $V$  with the usual composition rule for maps.

A representation of  $(G, \circ_G)$  on  $V$  is a group homomorphism from  $(G, \circ_G)$  to  $(GL(V), \circ)$ .

Now for the main goal, namely a representation of  $\mathcal{P}_N$  on  $\mathcal{L}^N(\mathcal{V})$ : we want to associate to each  $\sigma \in \mathcal{P}_N$  some  $\sigma^\otimes \in GL(\mathcal{L}^N(\mathcal{V}))$ . That's not hard when observing that we can easily build a  $\sigma^\times : \mathcal{L}_\times^N(\mathcal{V}) \rightarrow \mathcal{L}^N(\mathcal{V}) : (v_1, \dots, v_N) \mapsto v_{\sigma^{-1}(1)} \otimes \dots \otimes v_{\sigma^{-1}(N)}$ , and then determine uniquely the linear map we looked for by universality:

$$\sigma^\otimes : \mathcal{L}^N(\mathcal{V}) \rightarrow \mathcal{L}^N(\mathcal{V}) : v_1 \otimes \dots \otimes v_N \mapsto v_{\sigma^{-1}(1)} \otimes \dots \otimes v_{\sigma^{-1}(N)} \quad (90)$$

And here's the crucial result:

**Theorem 4.** *The mapping*

$$\mathcal{P}_N \ni \sigma \xrightarrow{A} \sigma^\otimes \in GL(\mathcal{L}^N(\mathcal{V})) \quad (91)$$

is a representation of  $\mathcal{P}_N$  on  $\mathcal{L}^N(\mathcal{V})$ .

*Proof.* Two steps:

- Let us show the group structure is preserved, that is

$$A(\sigma_1 \circ \sigma_2) = A(\sigma_1) \circ A(\sigma_2) \quad (92)$$

to have it proven, we should show it holds for any  $v_1 \otimes \dots \otimes v_N \in \mathcal{L}^N(\mathcal{V})$  applied on the left and right side of the equation. Indeed

$$\begin{aligned} (A(\sigma_1) \circ A(\sigma_2))(v_1 \otimes \dots \otimes v_N) &= \sigma_1^\otimes(\sigma_2^\otimes(v_1 \otimes \dots \otimes v_N)) = \sigma_1^\otimes(v_{\sigma_2^{-1}(1)} \otimes \dots \otimes v_{\sigma_2^{-1}(N)}) \\ &= v_{\sigma_2^{-1}(\sigma_1^{-1}(1))} \otimes \dots \otimes v_{\sigma_2^{-1}(\sigma_1^{-1}(N))} = v_{(\sigma_1 \circ \sigma_2)^{-1}(1)} \otimes \dots \otimes v_{(\sigma_1 \circ \sigma_2)^{-1}(N)} \\ &= A(\sigma_1 \circ \sigma_2)(v_1 \otimes \dots \otimes v_N) \end{aligned} \quad (93)$$

by choosing as  $v_1 \otimes \dots \otimes v_N$  the Hilbert basis elements of  $\mathcal{L}^N(\mathcal{V})$  and observing that  $\sigma^\otimes$  is bounded - an isometry, actually -, hence continuous, the thesis follows.

- Let us show  $\sigma^\otimes \in GL(\mathcal{L}^N(\mathcal{V}))$ . Linearity is given by construction, as for bijectivity observe that by the first step

$$\sigma^\otimes \circ (\sigma^\otimes)^{-1} = (\sigma \circ \sigma^{-1})^\otimes = (I_\sigma)^\otimes = I_{\sigma^\otimes} \quad (94)$$

The last equality is easily proven to be true when noticing  $(I_\sigma)^\otimes : v_1 \otimes \dots \otimes v_N \mapsto v_1 \otimes \dots \otimes v_N$ , and the existence of left inverse is analogously verified.

■

Now that we have learned to swap functions, it's time to find out what kind of permutations generates the wave functions we look for.

**Definitions.** 1. We call *transposition* a permutation that swaps just two elements. Furthermore, it holds true that any permutation may be expressed as composition of a finite number  $\eta$  of transpositions, whose parity is independent from the chosen composition; the parity  $\epsilon_\sigma$  of a permutation is defined as

$$\epsilon_\sigma = \begin{cases} 1 & \text{if } \eta \text{ is even} \\ -1 & \text{if } \eta \text{ is odd} \end{cases} \quad (95)$$

2.  $\phi \in \mathcal{L}^N(\mathcal{V})$  is said to be *symmetric* if  $\sigma^\otimes \phi = \phi \quad \forall \sigma \in \mathcal{P}_N$ ;
3.  $\phi \in \mathcal{L}^N(\mathcal{V})$  is said to be *anti symmetric* if  $\sigma^\otimes \phi = \epsilon_\sigma \phi \quad \forall \sigma \in \mathcal{P}_N$ ;

The good news is that whenever  $\phi$  is either symmetric or antisymmetric

$$\|\sigma^\otimes \phi(\mathbf{r})\|^2 = \|\phi(\mathbf{r})\|^2 \quad (96)$$

and now we can state more precisely what kind of wave function we want: a symmetric or anti symmetric wave function. The bad news is that we don't know how to get one. Luckily, the following proposition holds:

**Proposition 3.3.1.** *Define the linear operators*

$$\mathcal{A} : \mathcal{L}^N(\mathcal{V}) \rightarrow \mathcal{L}^N(\mathcal{V}) : \phi \mapsto \frac{1}{N!} \sum_{\sigma \in \mathcal{P}_N} \epsilon_\sigma \sigma^\otimes \phi \quad (97)$$

and

$$\mathcal{S} : \mathcal{L}^N(\mathcal{V}) \rightarrow \mathcal{L}^N(\mathcal{V}) : \phi \mapsto \frac{1}{N!} \sum_{\sigma \in \mathcal{P}_N} \sigma^\otimes \phi \quad (98)$$

then  $\forall \phi \in \mathcal{L}^N(\mathcal{V})$

- (i)  $\mathcal{A}\phi$  is anti symmetric;
- (ii)  $\mathcal{S}\phi$  is symmetric.

*Proof.* Ad (i). We have to show that

$$\tau^\otimes(\mathcal{A}\phi) = \epsilon_\tau \mathcal{A}\phi \quad \forall \tau \in \mathcal{P}_N \quad (99)$$

Indeed observe that  $\mathcal{P}_N$  has a finite number of elements, and therefore we can compute the summation after the action of  $\tau^\otimes$ :

$$\tau^\otimes(\mathcal{A}\phi) = \frac{1}{N!} \sum_{\sigma \in \mathcal{P}_N} \epsilon_\sigma \tau^\otimes \sigma^\otimes \phi = \frac{1}{N!} \sum_{\sigma \in \mathcal{P}_N} \epsilon_\sigma (\tau \circ \sigma)^\otimes \phi \quad (100)$$

Now observe that

- $\epsilon_{\tau \circ \sigma} \epsilon_\sigma = \epsilon_{\tau \circ \sigma \circ \sigma} = (\epsilon_\tau)^2 \epsilon_\sigma = \epsilon_\sigma$ ;
- if  $\sigma$  spans over all  $\mathcal{P}_N$ , so does  $\tau \circ \sigma \doteq \sigma'$ .

Therefore

$$\tau^\otimes(\mathcal{A}\phi) = \frac{\epsilon_\tau}{N!} \sum_{\sigma' \in \mathcal{P}_N} \epsilon_{\sigma'} \sigma'^\otimes \phi = \epsilon_\tau \mathcal{A}\phi \quad (101)$$

Ad (ii). The proof is essentially the same: we have to show that

$$\tau^\otimes(\mathcal{S}\phi) = \mathcal{S}\phi \quad \forall \tau \in \mathcal{P}_N \quad (102)$$

Indeed, as before:

$$\tau^\otimes(\mathcal{S}\phi) = \frac{1}{N!} \sum_{\sigma \in \mathcal{P}_N} \tau^\otimes \sigma^\otimes \phi = \frac{1}{N!} \sum_{\sigma \in \mathcal{P}_N} (\tau \circ \sigma)^\otimes \phi = \frac{1}{N!} \sum_{\sigma' \in \mathcal{P}_N} \sigma'^\otimes \phi = \mathcal{S}\phi \quad (103)$$

■

Furthermore, it can be shown that if  $\mathcal{A}\phi = 0 = \mathcal{S}\phi$  then necessarily  $\phi = 0$ .

To sum things up: we had a mathematical solution for the equation of motion of our gas, but it lead to an unpleasant exchange degeneracy; we moved the wave functions on another environment, and managed to describe on that environment the exchange of particle, that is, the permutation of wave functions.

At the end of the day what we have is that there exists a standard procedure by means of the operator  $\mathcal{A}$  or  $\mathcal{S}$  which transforms the unpleasant wave function into another wave function which still solves the equation of motion, being a linear combination of permutations of a solution, and hasn't got any exchange degeneracy. Moreover, if the wave function has a trivial symmetrization - namely,  $\mathcal{S}\phi = 0$  -, the anti symmetrization is not trivial, and vice versa: one way or the other we can obtain a "good" solution.

Now that we are all set with the state function of the gas, let's have a look at the recurrence problems.

### 3.4 The recurrence theorem

Before stating and proving the theorem, it is convenient to do a quick résumé of the physical conclusions - and notations - of the first paragraph: we had an Hamiltonian of the form  $H = \sum_{i=1}^N H_i$  with a discrete set of eigenvalues  $\mathcal{E}$  and eigenvectors  $\phi_E$ ,  $E \in \mathcal{E}$ . Then we expressed the eigenvectors as  $\phi_E \doteq \prod_{i=1}^N \varphi_i$ , with the requests

$$\begin{aligned} (1) \quad & H_i \varphi_i = E_i \varphi_i \quad i = 1, \dots, N \\ (2) \quad & \sum_{i=1}^N E_i = E \end{aligned} \tag{104}$$

Now we know we can express  $\phi_E$  as  $\varphi_{i_1(E)} \otimes \dots \otimes \varphi_{i_N(E)}$ .

Furthermore, we observed that solutions of this kind had an exchange degeneracy. With the formalism we have developed in the previous paragraphs we can write equivalently

$$H[\sigma^\otimes \phi_E] = E \sigma^\otimes \phi_E \quad \forall \sigma \in \mathcal{P}_N, \forall E \in \mathcal{E} \tag{105}$$

This is the starting point of the recurrence theorem.

**Theorem 5.** Fix  $\Pi = \mathcal{A}$  or  $\mathcal{S}$ ,  $\mathcal{V}$  a bounded subset of  $\mathbb{R}^3$ ,  $\{\varphi_i\}_{i \in I}$ ,  $H$ ,  $\{\phi_E\}_{E \in \mathcal{E}}$  as in the comments above. Let  $\ell^2 \ni \{a_E\}_{E \in \mathcal{E}} \subset \mathbb{C}$  and define  $\psi \in L^N(\mathcal{V}) \cap C^{1,t}([0, +\infty))$  as

$$\psi(\mathbf{r}, t) \doteq \sum_{E \in \mathcal{E}} a_E \Pi[\phi_E(\mathbf{r})] \exp(-iEt) : \mathcal{V}^N \times [0, +\infty) \rightarrow \mathbb{C} \tag{106}$$

that is, the general solution of the Schrödinger equation related to  $H$ .

Then  $\forall \varepsilon > 0, \forall t_0 \geq 0 \exists T = T(\varepsilon, t_0) \in (t_0, +\infty)$  such that

$$\|\psi(\cdot, t_0) - \psi(\cdot, T)\|_{\mathcal{L}^N(\mathcal{V})} < \varepsilon \tag{107}$$

Before proceeding with the proof we state and prove a lemma.

**Lemma.**—Let  $b \in \mathbb{R} \setminus \{0\}$  a fixed constant,  $(a_1, \dots, a_m) \in \mathbb{R}^m \setminus \{0\}$  such that

$$q_j \doteq \frac{a_1}{a_j} \in \mathbb{Q}, \quad j = 2, \dots, m \tag{108}$$

then  $\exists t \in \mathbb{R} \setminus \{0\}$ ,  $(k_1, \dots, k_m) \in \mathbb{N}^m \setminus \{0\}$  such that

$$ta_i = bk_i, \quad i = 1, \dots, m \tag{109}$$

*Proof.* Equation (109) is equivalent to the following requests:

$$(i) \quad ta_1 = bk_1$$

$$(ii) \quad q_j = \frac{k_1}{k_j} \quad \forall j = 2, \dots, m$$

Indeed

$$\frac{a_1}{a_j} = \frac{k_1}{k_j} \iff \frac{ta_1}{ta_j} = \frac{bk_1}{bk_j} \quad (110)$$

Now define

$$\begin{aligned} r_i &\doteq \min\{n \in \mathbb{N} \setminus \{0\} : n/q_i \in \mathbb{N}\} \\ r &\doteq \text{LCM}\{r_i : i = 2, \dots, m\} \end{aligned} \quad (111)$$

and let  $k_1 = r$ ,  $k_j = r/q_j$  for  $j = 2, \dots, m$ : then  $(k_1, \dots, k_m) \in \mathbb{N}^m \setminus \{0\}$  and it satisfies (ii). Finally, set  $t = br/a_1$ .  $\blacksquare$

Now for the proof of the theorem.

*Proof.* We divide the proof in steps.

*Step 1.* The vectors in  $\{\Pi(\phi_E)\}_{E \in \mathcal{E}} \subset L^N(\mathcal{V})$  are pairwise normal. In order to prove it, choose  $E_1, E_2 \in \mathcal{E}$ ,  $E_1 \neq E_2$ . Then

$$(\Pi[\phi_{E_1}] | \Pi[\phi_{E_2}])_{\mathcal{L}^N(\mathcal{V})} = \frac{1}{(N!)^2} \sum_{\sigma_a, \sigma_b \in \mathcal{P}_N} \pi_{\sigma_a} \pi_{\sigma_b} (\sigma_a^\otimes \phi_{E_1} | \sigma_b^\otimes \phi_{E_2})_{\mathcal{L}^N(\mathcal{V})} \quad (112)$$

where  $\pi_\sigma = \epsilon_\sigma$  if  $\Pi = \mathcal{A}$ , and 1 if  $\Pi = \mathcal{S}$ . But now

$$\begin{aligned} (\sigma_a^\otimes \phi_{E_1} | \sigma_b^\otimes \phi_{E_2})_{\mathcal{L}^N(\mathcal{V})} &= (\varphi_{\sigma_a^{-1}(i_1(E_1))} \otimes \dots \otimes \varphi_{\sigma_a^{-1}(i_N(E_1))} | \varphi_{\sigma_b^{-1}(i_1(E_2))} \otimes \dots \otimes \varphi_{\sigma_b^{-1}(i_N(E_2))})_{\mathcal{L}^N(\mathcal{V})} \\ &= \prod_{k=1}^N (\varphi_{\sigma_a^{-1}(i_k(E_1))} | \varphi_{\sigma_b^{-1}(i_k(E_2))})_{L^2(\mathcal{V})} = \prod_{k=1}^N \delta_{\sigma_a^{-1}(i_k(E_1)), \sigma_b^{-1}(i_k(E_2))} \end{aligned} \quad (113)$$

We proceed ad absurdum: suppose  $\exists \sigma_a, \sigma_b$  such that  $(\sigma_a^\otimes \phi_{E_1} | \sigma_b^\otimes \phi_{E_2}) \neq 0$ , then we must have  $\sigma_a^{-1}(i_k(E_1)) = \sigma_b^{-1}(i_k(E_2)) \quad \forall k = 1, \dots, N$ , hence by definition

$$\sigma_a^\otimes \phi_{E_1} = \sigma_b^\otimes \phi_{E_2} \quad (114)$$

Now it descends from  $H[\sigma^\otimes \phi_E] = E\sigma^\otimes \phi_E$  that

$$E_1 \sigma_b^\otimes \phi_{E_2} = E_1 \sigma_a^\otimes \phi_{E_1} = H \sigma_a^\otimes \phi_{E_1} = H \sigma_b^\otimes \phi_{E_2} = E_2 \sigma_b^\otimes \phi_{E_2} \quad (115)$$

But  $\sigma_b^\otimes \phi_{E_2} \neq 0$ , as a tensorial product of non-zero terms, then our identity is contradictory and we conclude that if  $E_1 \neq E_2$  then  $(\sigma_1^\otimes \phi_{E_1} | \sigma_2^\otimes \phi_{E_2}) = 0 \quad \forall \sigma \in \mathcal{P}_N$ , whence  $(\Pi[\phi_{E_1}] | \Pi[\phi_{E_2}])_{\mathcal{L}^N(\mathcal{V})} = 0$ .

Similarly it can be proven that  $\|\Pi[\phi_E]\|^2 \leq 1$ : essentially, the worst possible case in this sense is to have  $\phi_E = \underbrace{\varphi_k \otimes \dots \otimes \varphi_k}_{N \text{ times}}$ , which yields  $\|\Pi[\phi_E]\|^2 = 1$ . All the other possibilities



return smaller norms due to  $\{\phi_i\}_{i \in I}$  being an orthonormal basis.

*Step 2.* First part of the inequality. From step 1 we have

$$\|\psi(\cdot, t)\|_{\mathcal{L}^N(\mathcal{V})}^2 = \sum_{E \in \mathcal{E}} |a_E|^2 \|\Pi[\phi_E]\|_{\mathcal{L}^N(\mathcal{V})}^2 \quad (116)$$

then for some  $T > t_0$

$$\begin{aligned} \|\psi(\cdot, t_0) - \psi(\cdot, T)\|_{\mathcal{L}^N(\mathcal{V})}^2 &= 2 \sum_{E \in \mathcal{E}} |a_E|^2 \|\Pi[\phi_E]\|_{\mathcal{L}^N(\mathcal{V})}^2 (1 - \cos[E(T - t_0)]) \\ &\leq 4 \sum_{E \in \mathcal{E}} |a_E|^2 < +\infty \end{aligned} \quad (117)$$

As the set  $\mathcal{E}$  is discrete, we can label each of his components by an integer - in case  $\mathcal{E}$  is finite, add to the set a countable number of zeros from the last non-zero element on. Then the last inequality reads

$$\sum_{n=1}^{+\infty} |a_n|^2 \|\Pi[\phi_n]\|_{\mathcal{L}^N(\mathcal{V})}^2 (1 - \cos[E(T - t_0)]) < +\infty \quad (118)$$

Then  $\forall \varepsilon > 0 \exists M = M(\varepsilon) > 0$  such that

$$\sum_{n=M+1}^{+\infty} |a_n|^2 \|\Pi[\phi_n]\|_{\mathcal{L}^N(\mathcal{V})}^2 (1 - \cos[E(T - t_0)]) < \frac{\varepsilon}{2} \quad (119)$$

*Step 3.* Set  $\tau \doteq T - t_0$ , we want to prove the remaining side of the inequality, that is

$$\sum_{n=1}^M |a_n|^2 \|\Pi[\phi_n]\|_{\mathcal{L}^N(\mathcal{V})}^2 (1 - \cos[E_n \tau]) < \frac{\varepsilon}{2} \quad (120)$$

As a first estimate, set  $a \doteq \max_{1 \leq n \leq M} |a_n|$  and observe

$$\sum_{n=1}^M |a_n|^2 \|\Pi[\phi_n]\|_{\mathcal{L}^N(\mathcal{V})}^2 (1 - \cos[E_n \tau]) \leq a \sum_{n=1}^M (1 - \cos[E_n \tau]) \quad (121)$$

Whenever  $E_n = 0$  the corresponding term does not contribute to the sum, thus from now we restrict to the case  $E_n \neq 0$ ; furthermore, observe that by parity of the cosine we can take all the  $E_n$  to be positive.

By continuity of the cosine we have that  $\forall n \in \mathbb{N}, \forall \varepsilon > 0 \exists \delta_n = \delta_n(\varepsilon) > 0$  such that

$$1 - \cos[E_n \tau] < \varepsilon/M \quad \text{if} \quad \tau \in \cup_{k \in \mathbb{N}} (2k\pi/E_n - \delta_n, 2k\pi/E_n + \delta_n) \quad (122)$$

We would like the inequality to hold simultaneously for all the terms for some  $\tau$ , namely

$$\exists \tau > 0 : \forall n = 1, \dots, M \quad 1 - \cos[E_n \tau] < \varepsilon/M \quad (123)$$

this claim implies (120) and thus our final thesis.

Now we examine two different cases: the special case identified by the Lemma, which

turns out to be of great physical importance, and the general case.  
In order to prove the special case, observe that

$$\forall \bar{\varepsilon} > 0 \exists \bar{E}_n \in \mathbb{Q} : \left| \frac{1}{E_n} - \frac{1}{\bar{E}_n} \right| < \bar{\varepsilon} \quad \forall n = 1, \dots, M \quad (124)$$

thus  $\bar{E}_1/\bar{E}_n \in \mathbb{Q}$ : then apply the lemma with  $b = 2\pi$ . As a result there exist  $(k_1, \dots, k_M) \in \mathbb{N}^M \setminus \{0\}$ ,  $\tau \in \mathbb{R} \setminus \{0\}$  such that

$$\bar{E}_n \tau = 2k_n \pi \quad \forall n = 1, \dots, M \quad (125)$$

or equivalently

$$\forall n, m = 1, \dots, M \exists k_n, k_m \in \mathbb{N} : \frac{k_n}{\bar{E}_n} - \frac{k_m}{\bar{E}_m} = 0 \quad (126)$$

hence (123), hence the final thesis.

Notice that we obtained something way stronger than (123):

$$\exists \tau > 0 : \forall n = 1, \dots, M \quad 1 - \cos[E_n \tau] = 0 \quad (127)$$

We'll come back to this after the proof is finished.

*Step 4.* Now for the general case. We want to show

$$\forall m, n = 1, \dots, M \exists \eta_{m,n} > 0, k_m, k_n \in \mathbb{N} : \left| \frac{k_m}{E_m} - \frac{k_n}{E_n} \right| < \frac{\eta_{m,n}}{\pi \sqrt{2M}} \quad (128)$$

We'll prove this claim in a moment; for now observe that as a consequence we have that  $\exists \tau$  such that  $(1 - \cos[E_n \tau]) < \varepsilon/M \quad \forall n = 1, \dots, M$ . Indeed, choose  $(\bar{m}, \bar{n})$  such that  $\eta_{\bar{m}, \bar{n}} = \max!$  and set

$$\tau = 2\pi \left[ \frac{1}{2} \left( \frac{k_{\bar{m}}}{E_{\bar{m}}} + \frac{k_{\bar{n}}}{E_{\bar{n}}} \right) \right] \quad (129)$$

therefore we have the fundamental inequality

$$\left| \frac{\tau}{2\pi} - \frac{k_n}{E_n} \right| < \frac{\eta_{\bar{m}, \bar{n}}}{\pi M} \quad \forall n = 1, \dots, M \quad (130)$$

hence

$$|1 - \cos(E_n \tau)| = \left| 1 - \cos \left( 2\pi E_n \frac{\tau}{2\pi} \right) \right| \leq \frac{E_n^2 \eta^2}{M} \quad (131)$$

hence (123), by choosing  $\varepsilon = (\eta \cdot \max_{1 \leq n \leq M} E_n)^2$ .

Now we prove (128). Choose  $m, n = 1, \dots, M$  and observe that

$$\left| \frac{k_n}{E_n} - \frac{k_m}{E_m} \right| = \frac{1}{E_m} \left| k_n \frac{E_m}{E_n} - k_m \right| \quad (132)$$

and let

$$\begin{aligned} [E_{m,n}] &\doteq \max \left\{ n \in \mathbb{N} : \frac{E_m}{E_n} \geq 0 \right\} \\ \{E_{m,n}\} &\doteq \frac{E_m}{E_n} - [E_{m,n}] \end{aligned} \quad (133)$$

Observe  $\{E_{m,n}\} \in [0, 1)$  by construction and partition  $[0, 1)$  into  $Q$  subintervals of length  $1/Q$ :  $[1, 1/Q)$ ,  $[1/Q, 2/Q)$ , ...,  $[(Q-1)/Q, 1)$ . By the pigeonhole principle at least two of the numbers in the set

$$\{qE_{m,n}\}_{0 \leq q \leq Q} = \{0, \{E_{m,n}\}, \{2E_{m,n}\}, \dots, \{(Q-1)E_{m,n}\}, \{QE_{m,n}\}\} \quad (134)$$

belong to the same interval, that is

$$\exists p, q = 0, \dots, Q, p \neq q : |\{pE_{m,n}\} - \{qE_{m,n}\}| < 1/Q \quad (135)$$

then let  $k_n = |p-q|$ ,  $k_m = [E_{m,n}]k_n$  and observe that  $\left|k_n \frac{E_m}{E_n} - k_m\right| < \frac{1}{Q}$ ,  $Q$  being arbitrarily large. This result is known as *Dirichlet's approximation theorem*.

Observe then

$$\left|\frac{k_n}{E_n} - \frac{k_m}{E_m}\right| = \frac{1}{E_m} \left|k_n \frac{E_m}{E_n} - k_m\right| < \frac{1}{E_m Q} < \frac{\eta_{m,n}}{\pi \sqrt{2M}} \quad (136)$$

for some suitable  $\eta_{m,n}$ , hence (128), (123), and lastly the main thesis. ■

This result is impressive by itself, implying we may have recurrence phenomenons at any accuracy scale, but it's even more surprising when one takes a closer look at the hypothesis of step 3, that is, the allowed energies of the system are in rational proportion. Actually, this is the case for many simple physics models: as an example, for a system of  $N$  boson-like particles under the action of a 3D harmonic potential with frequency  $\omega$  we have

$$q_n = \frac{E_1}{E_n} = \frac{\frac{3N\hbar\omega}{2}}{\frac{\hbar\omega(2n+3N)}{2}} = \frac{3N}{2n+3N} \in \mathbb{Q} \quad (137)$$

applying the lemma with  $b = 2\pi$  we can get the exact recurrence time for the first  $M$  energy levels: we have  $\tau = \frac{4\pi}{3\hbar\omega} \hbar r = \frac{4\pi}{3\omega} r$ , where we have restored the  $\hbar$  previously set to 1 and  $r$  is uniquely determined by the requests

$$\begin{aligned} r_n &\doteq \min\{m \in \mathbb{N} \setminus \{0\} : m/q_n \in \mathbb{N}\} \\ r &\doteq \text{LCM}\{r_i : i = 2, \dots, M\} \end{aligned} \quad (138)$$

as it is easily seen,  $r = 3N$  for every value of  $M$ , that is, the harmonic oscillator has an exact recurrence time: any state of the harmonic oscillator returns exactly in his original configuration regardless of its composition in terms of stationary solutions.

We can have a look at the recurrence time, then. As a typical value, set  $\hbar\omega = K_b T \simeq 4 \cdot 10^{-21} J$  at room temperature, with  $N = 10^{23}$ . Then

$$\tau \simeq 10^{13} s \simeq 3 \cdot 10^5 \text{ years} \quad (139)$$

This is a good confirm of the 2<sup>nd</sup> principle's validity on small timescales. In addition, it should be noticed that this kind of calculation is strongly relying on the hypothesis of ideality; suppose there is a small deviation from the predicted energy eigenvalue, due to the fact that the particles are actually interacting somehow, or that they're not points: then after a time  $\tau$  the little deviation is greatly emphasized - namely, by a factor  $10^{13}$  - and errors of one part over a billion contribute with a factor of  $10^4$  in the imaginary exponential, erasing the recurrence phenomenon by means of an essentially random phase

and causing the *real* recurrence time to take essentially unpredictable values. Still, it's reassuring that even for ideal systems the theory gives us a sufficiently large recurrence time.

Once the recurrence of the state is proven, it is easy to produce a similar proof of the recurrences of the mean values of the states. As a complement, here's a sketch of the proof:

**Proposition 3.4.1.** *Maintain the hypothesis of the recurrence theorem and let  $A$  be an observable for the system.*

*Then  $\forall \varepsilon > 0, \forall t_0 \geq 0 \exists T = T(\varepsilon, t_0) \in (t_0, +\infty)$  such that*

$$|\langle \psi(t_0) | A \psi(t_0) \rangle - \langle \psi(T) | A \psi(T) \rangle| < \varepsilon \quad (140)$$

*Sketch of the proof.* The expectation value of  $A$  at time  $t$  may be written as

$$\langle \psi(t) | A \psi(t) \rangle = \sum_{E, F \in \mathcal{E}} a_E a_F^* (\Pi[\phi_E(\mathbf{r})] | A \Pi[\phi_F(\mathbf{r})]) e^{(-i(E-F)t)} \quad (141)$$

Therefore we have to prove

$$\sum_{E, F \in \mathcal{E}} |a_E a_F^*| |(\Pi[\phi_E(\mathbf{r})] | A \Pi[\phi_F(\mathbf{r})])| |e^{(-i(E-F)t_0)} - e^{(-i(E-F)T)}| < \varepsilon \quad (142)$$

As before we can label the elements of the numerable set  $E$  with integers and conclude that  $\forall \varepsilon > 0 \exists M = M(\varepsilon) > 0$  such that

$$\sum_{n, m=M+1}^{+\infty} |a_n a_m^*| |(\Pi[\phi_n(\mathbf{r})] | A \Pi[\phi_m(\mathbf{r})])| |e^{(-i(E_n-E_m)t_0)} - e^{(-i(E_n-E_m)T)}| < \frac{\varepsilon}{2} \quad (143)$$

then set  $\mathcal{M} = \max_{m, n=1, \dots, M} \{(\Pi[\phi_n(\mathbf{r})] | A \Pi[\phi_m(\mathbf{r})])\}$ ,  $a = \max_{m, n=1, \dots, M} |a_n a_m^*|$  and observe

$$\begin{aligned} & |e^{(-i(E-F)t_0)} - e^{(-i(E_n-E_m)T)}| = \\ & = 2 \left| \sin \left[ \frac{(E-F)(T-t_0)}{2} \right] \right| \left| i \cos \left[ \frac{(E-F)(T+t_0)}{2} \right] - \sin \left[ \frac{(E-F)(T-t_0)}{2} \right] \right| \quad (144) \\ & \leq 2 \left| \sin \left[ \frac{(E-F)(T-t_0)}{2} \right] \right| \end{aligned}$$

therefore

$$\begin{aligned} & \sum_{n, m=1}^M |a_n a_m^*| |(\Pi[\phi_n(\mathbf{r})] | A \Pi[\phi_m(\mathbf{r})])| |e^{(-i(E_n-E_m)t_0)} - e^{(-i(E_n-E_m)T)}| \leq \\ & \leq 2a\mathcal{M} \sum_{n, m=1}^M \left| \sin \left[ \frac{(E_n-E_m)}{2} \tau \right] \right| \quad (145) \end{aligned}$$

where  $\tau \doteq T - t_0$ . The claim is

$$\exists \tau > 0 : \left| \sin \left[ \frac{(E_n-E_m)}{2} \tau \right] \right| < \varepsilon \quad \forall n, m = 1, \dots, M \quad (146)$$

and it can be proven essentially just like we did in the previous theorem, invoking Dirichlet's approximation theorem and the continuity and periodicity of the sine function. ■

## 4 Conclusion

It has been shown that both the stochastic and quantum picture of a physical system maintain the initial paradox generated by Poincaré's Recurrence Theorem: we may as well start wondering if the Second Law is wrong regardless of the physical model involved.

Poincaré proposed a solution during a talk he held in 1904, "The current state and the future of mathematical physics": he emphasized the difference between «the real objects, that Nature will always hide from us» and «the images we are forced to put in their place»; then when two contradictory theories are examined «it may happen that they both express *des rapport vrais*<sup>3</sup> and that there is no contradiction but in the images with which we have dressed up reality».

The Second Law has been built up by induction, as any other physical principle, and in this sense is true that the idea of having it valid on any timescale is merely an *image* we dressed up reality with: things turn out to be more complicate than this.

Actually, Ludwig Boltzmann already gave up on giving a global meaning to the concept of entropy, and he would rather think of it as something that makes sense just locally, and that incidentally defines the direction of time:

Just as in a certain place on the earth we can call "down" the direction toward the centre of the earth, so a living being that finds itself in such a world at a certain period of time can define the time direction as going from less probable to more probable states (the former will be the "past", the latter the "future") and by virtue of this definition he will find that this small region, isolated from the rest of the universe, is "initially" always in an improbable state.

This viewpoint opens up the discussion to deeper questions regarding the nature of time, which are beyond the means of this paper: nonetheless, it is fascinating to observe how from a contradiction which becomes evident only sinking physical principles into mathematical structures new thrilling hypotheses arise.

Moreover, it is understood that this new hypotheses will once again have to be translated into mathematical statements, and then again examined: this is indeed a most notable example of how new ideas in physics are generated under the influence of a formal mathematical system, and on the other hand of how new mathematical concepts are defined, pushed up by the practical necessity of describing a physical process.

This is not the whole story, of course, and one should be careful not to be trapped by mathematical models, which are always poorer than the reality they try to describe: still, the history of science seems to suggest that a dialectic evolution involving mathematics and physics is the most convenient path one should follow in order to investigate reality, as impervious and confusing as it may sometimes seem to be.

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<sup>3</sup>A *rapport* is for Poincaré a correlation between physical quantities.



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