Predicting decoherence in discrete models

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The general aim of this paper is to supply a method to decide whether a discrete system decoheres or not, and under what conditions decoherence occurs, with no need of appealing to computer simulations to obtain the time evolution of the reduced state. In particular, a lemma is presented as the core of the method.

I. INTRODUCTION

At present, the study of quantum decoherence has acquired a central position in the theoretical research on quantum mechanics. Although the orthodox environment induced decoherence (EID) approach addresses decoherence in open systems ([1]-[6]), many authors have stressed that closed systems may also experience the phenomenon of decoherence ([7]-[17]; we have worked from this perspective in [18]-[29]).

In order to show that the two approaches must not be conceived as rival or alternative, but rather as complementary, we have developed a *general theoretical framework* for decoherence ([30], [31], [32]), which encompasses decoherence in open and closed systems. According to this general framework, decoherence is just a particular case of the general phenomenon of irreversibility in quantum mechanics ([33], [34]). In fact, since the quantum state $\rho(t)$ follows a unitary evolution, it cannot reach a final equilibrium state for $t\to\infty$. Therefore, if we want to explain the emergence of non-unitary irreversible evolutions, a further element has to be added: we must split the whole space $\mathcal{O}$ of all possible observables into a relevant subspace $\mathcal{O}_R\subset\mathcal{O}$ and an irrelevant subspace. Once the essential role played by the selection of the relevant observables is clearly understood, the phenomenon of decoherence can be explained in three general steps:

1. **First step:** The space $\mathcal{O}_R$ of relevant observables is defined .
2. **Second step:** The expectation value $\langle O_R\rangle_{\rho(t)}$, for any $O_R\in\mathcal{O}_R$, is obtained. This step can be formulated in two different but equivalent ways:
   - $\langle O_R\rangle_{\rho(t)}$ is computed as the expectation value of O_R in the unitarily evolving state $\rho(t)$.
   - A coarse-grained state $\rho_R(t)$ is defined by
   $$\langle O_R\rangle_{\rho(t)}=\langle O_R\rangle_{\rho_R(t)}\qquad \forall O_R\in\mathcal{O}_R \tag{1}$$
   and its non-unitary evolution (governed by a master equation) is solved.
3. **Third step:** It is proved that $\langle O_R\rangle_{\rho(t)}=\langle O_R\rangle_{\rho_R(t)}$ reaches a final equilibrium value:
$$\lim_{t\to\infty}\langle O_R\rangle_{\rho(t)}=\lim_{t\to\infty}\langle O_R\rangle_{\rho_R(t)}=\langle O_R\rangle_{\rho_*}=\langle O_R\rangle_{\rho_{R*}}\qquad \forall O_R\in\mathcal{O}_R \tag{2}$$

The final equilibrium state ρ_* is obviously diagonal in its own eigenbasis, which turns out to be the final equilibrium decoherence basis. But, from eq. (2) it cannot be concluded that $\lim_{t\to\infty}\rho(t)=\rho_*$; the mathematicians say that the unitarily evolving quantum state $\rho(t)$ of the whole system has only a *weak limit*, symbolized as:

$$W-\lim_{t\to\infty}\rho(t)=\rho_* \tag{3}$$

and equivalent to eq. (2). Physically this weak limit means that, although the off-diagonal terms of $\rho(t)$ never vanish through the unitary evolution, the system decoheres *from an observational point of view*, that is, from the viewpoint given by any relevant observable $O_R\in\mathcal{O}_R$. From this general perspective, the phenomenon of decoherence is relative because the off-diagonal terms of $\rho(t)$ vanish only from the viewpoint of the relevant observables $O_R\in\mathcal{O}_R$.

This general framework strictly applies when the limit of eq. (2) exists. This happen when the off-diagonal terms of the density matrix vanish by destructive interference according to the Riemann-Lebesgue theorem. In fact, when the relevant observables $O_R\in\mathcal{O}_R$ read

$$O_R=\int_0^\infty O(\omega)|\omega)\,d\omega+\int_0^\infty\int_0^\infty O(\omega,\omega')|\omega,\omega')\,d\omega d\omega' \tag{4}$$

where $\{|\omega\rangle\}$ is the eigenbasis of the Hamiltonian, $|\omega) = |\omega\rangle\langle\omega|$, $|\omega,\omega') = |\omega\rangle\langle\omega'|$, and $\{|\omega), |\omega,\omega')\}$ is a basis of $\mathcal{O}_R$, and the states are linear functionals belonging to $\mathcal{O}'_R$, the dual of $\mathcal{O}_R$,

$$\rho = \int_0^\infty \rho(\omega)\left(|\omega\rangle\langle\omega|\right)' \, d\omega + \int_0^\infty \int_0^\infty \rho(\omega,\omega')(\omega,\omega'|\, d\omega d\omega' \tag{5}$$

where $\{(\omega|, (\omega,\omega'|\}$ is the basis of $\mathcal{O}'_R$, then the expectation value of any observable $O_R \in \mathcal{O}_R$ in the state $\rho(t)$ can be computed as

$$\langle O_R\rangle_{\rho(t)} = \int_0^\infty \overline{\rho(\omega)} O(\omega)\, d\omega + \int_0^\infty \int_0^\infty \overline{\rho(\omega,\omega')} O(\omega,\omega')\, e^{i\frac{\omega-\omega'}{\hbar}t}\, d\omega d\omega' \tag{6}$$

When the function $\overline{\rho(\omega,\omega')}O(\omega,\omega')$ is regular (precisely, when it is $\mathbb{L}_1$ in variable $\nu = \omega - \omega'$), the Riemann-Lebesgue theorem can be applied to eq. (6). As a consequence, the second term vanishes and $\langle O_R\rangle_{\rho(t)}$ converges to a stable value

$$\langle O_R\rangle_{\rho(t)} \longrightarrow \int_0^\infty \overline{\rho(\omega)} O(\omega)\, d\omega = \langle O_R\rangle_{\rho_*} \tag{7}$$

where ρ_* is diagonal in the eigenbasis of the Hamiltonian.

It is clear that the Riemann-Lebesgue theorem strictly applies only in cases of continuous energy spectrum. However, we also know that we can use the results coming from the continuous realm in quasi-continuous cases, that is, in discrete models where (i) the energy spectrum is quasi-continuous, i.e., has a small discrete energy spacing, and (ii) the functions of energy used in the formalism are such that the sums in which they are involved can be approximated by Riemann integrals. These conditions are rather weak: in fact, the overwhelming majority of the physical models studied in the literature on dynamics, thermodynamics, quantum mechanics and quantum field theory are quasi-continuous.

The general aim of the present work is to supply a rigorous formulation of this intuitive idea. In particular, we will develop a discrete analogue of the Riemann-Lebesgue theorem, and this task will lead us to introduce a lemma in terms of which it is possible to predict whether a discrete system decoheres or not. For this purpose, the paper is organized as follows. In Section 2 we will consider the three cases that can be distinguished regarding the discrete analogue of the Riemann integral involved in the Riemann-Lebesgue theorem. Section 3 will be devoted to formulate the conditions for the validity of the discrete analogue of the Riemann integral. In Section 4, the lemma that constitutes the core of the proposed method is presented, and its relationship with the Discrete Fourier Transform is pointed out. Finally, in the Conclusions we will stress the fact that, whereas the usual strategy in this field is to rely on that computer simulations, our lemma makes possible to draw conclusions without that strategy; moreover, our results are particularly adequate to take advantage of the many mathematical methods of software engineering based on the Discrete Fourier Transform.

II. THREE CASES IN THE DISCRETE ANALOGUE

The Riemann-Lebesgue theorem −the mathematical expression of destructive interference− establishes that

$$f(\nu) \in \mathbb{L}_1 \Longrightarrow \lim_{t\to\infty} \int_0^1 d\nu f(\nu) e^{i\nu t} = 0 \tag{8}$$

In order to obtain a version that can be used in the discrete case, let us analyze the discrete analogue of the Riemann integral $R(t)$:

$$R(t) = \int_0^1 d\nu f(\nu) e^{i\nu t} \longrightarrow R_D(t) = \sum_{j=0}^{N} \frac{1}{N} f\left(\frac{j}{N}\right) e^{i\frac{j}{N}t} \tag{9}$$

where $0 \leq j/N \leq 1$, and t is a dimensionless time. Since the function $R_D(t)$ is a finite sum of sine functions $f\left(\frac{j}{N}\right) e^{i\frac{j}{N}t}$, it has a recurrence or Poincaré time. Given an initial state $R_D(0)$, the Poincaré time t_P is defined by $R_D(0) = R_D(t_P)$. This means that

$$\sum_{j=0}^{N} \frac{1}{N} f\left(\frac{j}{N}\right) \left(e^{i\frac{j}{N}t_P} - 1\right) = 0 \quad \Longrightarrow \quad t_P = 2\pi \tag{10}$$

Since the system comes back to the initial state when $t = t_P$, there is no rigorous discrete analogue of the Riemann-Lebesgue theorem. Nevertheless, three possible situations can be distinguished:

1. If $N \to \infty$, then $\left|\frac{j+1}{N} - \frac{j}{N}\right|$ becomes infinitesimal and $t_P \to \infty$. Therefore, this situation can be considered a continuous-spectrum case where the Riemann-Lebesgue theorem can be applied.

2. If N is large, then $\left|\frac{j+1}{N} - \frac{j}{N}\right|$ is very small. Then, the sum turns out to be close to the Riemann integral, and the the situation can be approximated to the continuous-spectrum case where the Riemann-Lebesgue theorem can be applied. This condition is satisfied in a concrete example in [35]: in spite of the fact that, strictly speaking, a system with discrete spectrum never reaches equilibrium due to Poincaré recurrence, that paper shows that, for times $t \ll t_P$, the discrete spectrum can be approximated by a continuous spectrum where the considered functions satisfy the usual conditions of regularity and integrability.

3. If N is not large, then $\left|\frac{j+1}{N} - \frac{j}{N}\right|$ is far from being infinitesimal, and the sum cannot be approximated by a Riemann integral. Consequently, the Riemann-Lebesgue theorem is not applicable because there is no destructive interference.

Let us notice that the difference between cases 2 and 3 is not absolute, to the extent that the precise criterion to decide when N is large has not been defined. In the following subsections such a criterion will be established.

III. CONDITIONS FOR THE VALIDITY OF THE DISCRETE ANALOGUE

The problem is to find the conditions for the time t_F such that $R_D(t) \to 0$ when $t \to t_F$: therefore, in the time-scale $[0, t_F]$ it can be considered that N is large enough to make the continuous-spectrum approximation applicable. In order to face this problem, we begin by consider a fixed time t and by decomposing the exponential of eq. (9) as

$$R_D(t) = \sum_{i=0}^{N} \frac{1}{N} f(x_i)\, e^{ix_i t} = \sum_{i=0}^{N} \frac{1}{N} f(x_i) \cos(x_i t) + i \sum_{i=0}^{N} \frac{1}{N} f(x_i) \sin(x_i t) \tag{11}$$

where the points $x_i = i/N$ belong to a discrete set $\{x_i\}$ with $i = 0$ to N. Let us analyze the particular case where $f(x_i) = 1$, precisely,

$$R_D^{(1)}(t) = \sum_{i=0}^{N} \frac{1}{N} \cos(x_i t) + i \sum_{i=0}^{N} \frac{1}{N} \sin(x_i t) \tag{12}$$

In particular, we will consider the sums

$$\frac{1}{N} \sum_{i=0}^{N} \cos(x_i t) = R_D^{(1C)}(t) \qquad\qquad \frac{1}{N} \sum_{i=0}^{N} \sin(x_i t) = R_D^{(1S)}(t) \tag{13}$$

We begin by considering $R_D^{(1C)}(t)$, because the case of $R_D^{(1S)}(t)$ will be analogous.

The sum $R_D^{(1C)}(t)$ vanishes when its terms cancel by pairs, that is, when for any $x_i \in \{x_i\}$

$$\cos(x_i t) + \cos(x_i t + \pi) = 0 \tag{14}$$

where $x_k = x_i + \pi/t \in \{x_i\}$. Since $x_i = i/N$, this happens when

$$\frac{k}{N} = \frac{i}{N} + \frac{\pi}{t} \Rightarrow k - i = \frac{\pi}{t} N \tag{15}$$

where $k - i \in \mathbb{N}$ and $N \in \mathbb{N}$. However, since in general $\pi/t \notin \mathbb{N}$, the condition of eq. (15) is not always satisfied. Then, instead of requiring that the terms of $R_D^{(1C)}(t)$ cancel with each other exactly, we will only require that the corresponding difference be small in the following sense:

$$|\cos(x_i t) + \cos(x_i t + \pi + \delta_j)| < \varepsilon \ll 1 \tag{16}$$

where now $x_k = x_i + \pi/t + \delta_i/t \in \{x_i\}$ and

$$\delta_j = \min_i \{\delta_i\} \qquad \text{with} \quad \delta_i = x_k t - x_i t - \pi \quad (i = 0 \ldots N) \tag{17}$$

If $\delta_j < 1$, the Taylor development of $\cos(x_i t + \pi + \delta_j)$ leads to

$$|\cos(x_i t) + \cos(x_i t + \pi + \delta_j)| \simeq \left|\sin(x_i t)\,\delta_j + \cos(x_i t)\,\delta_j^2\right| < \varepsilon \tag{18}$$

But, on the other hand,

$$\begin{aligned}\left|\sin(x_i t)\,\delta_j + \cos(x_i t)\,\delta_j^2\right| &= |\delta_j|\,|\sin(x_i t) + \cos(x_i t)\,\delta_j| \\ &\le |\delta_j|\,(|\sin(x_i t)| + |\cos(x_i t)|\,|\delta_j|) \le |\delta_j|\,(1 + |\delta_j|) \le |\delta_j|\end{aligned} \tag{19}$$

Then, if $|\delta_j| < \varepsilon \ll 1$, from eqs. (18) and (19) we obtain the condition of eq. (16). Therefore, the condition of approximate cancelling is (see eq. (17))

$$|\delta_j| < \varepsilon \ll 1 \qquad \text{with} \quad \delta_j = x_k t - x_j t - \pi \tag{20}$$

Now we will express the condition of approximate cancelling of eq. (20) in terms of the time t. Let us begin by noticing that the condition is not satisfied for $t = 0$, since $t = 0 \Rightarrow \delta_j = -\pi \Rightarrow |\delta_j| > \varepsilon$. Then, the first condition is $t > 0$. Now, by recalling that $x_i = i/N$, from the expression of δ_j in eq. (20) we obtain

$$k - j = \frac{\pi N}{t} + \frac{\delta_j N}{t} \tag{21}$$

But since $j, k \in \mathbb{N}$, and $j, k \in [0, N]$, then for $j < k$

$$1 \le k - j \le N \quad \Longrightarrow \quad 1 \le \frac{\pi N}{t} + \frac{\delta_j N}{t} \le N \tag{22}$$

Then, if $|\delta_j| < \varepsilon \ll 1$, eq. (22) implies that

$$1 \le \frac{\pi N}{t} \le N \tag{23}$$

Therefore, the condition $|\delta_j| < \varepsilon \ll 1$ of approximate cancelling turns out to be

$$\pi \le t \le \pi N \tag{24}$$

Up to this point we have proved that, for $\pi \le t \le \pi N$, $\cos(x_j t)$ approximately cancels with $\cos(x_j t + \pi + \delta_j)$. Figure **??** shows an example of this situation, where point 1 is cancelled by point 9, point 2 by point 10, ... , point 8 by point 16. However, this is not the most general case, since the points cancel by pairs only when $t = 2\pi n$. In the general case there are points with no counterpart to be cancelled. An example of this situation is shown in Figure **??**, where points 13, 14, 15 and 16 are not cancelled.

In order to analyze this general situation, let us consider the "worst" case, when the points of a whole half-period are not cancelled, namely, when $t = (2n + 1)\pi$. Since in t there are $N + 1$ points, in such a half-period there are $(N + 1)/(2n + 1)$ points, whose contribution $r_\pi(t)$ to the sum $R_D^{(1C)}(t)$ is

$$r_\pi(t) = \frac{1}{N} \sum_{i=0}^{\frac{N+1}{2n+1}-1} \cos(x_i t) \tag{25}$$

The upper boundary of this contribution is

$$r_\pi(t) = \frac{1}{N} \sum_{i=0}^{\frac{N+1}{2n+1}-1} \cos(x_i t) < \frac{1}{N}\frac{N+1}{2n+1} \cong \frac{1}{2n+1} = \frac{\pi}{t} \tag{26}$$

Then, the contribution $r_\pi(t)$ of the non cancelled points is irrelevant when $r_\pi(t) = \pi/t < \varepsilon \ll 1$, and this adds the condition

$$t \gg \pi \tag{27}$$

Summing up, if we combine eqs. (24) and (27), we obtain the condition on the time-scale that guarantees the approximate cancelling of the terms of $R_D^{(1C)}(t)$:

$$\text{If } \pi \ll t \le \pi N \quad \Rightarrow \quad R_D^{(1C)}(t) < \varepsilon \ll 1 \tag{28}$$

By means of the same argument applied to $R_D^{(1S)}(t)$ we obtain an analogous result that, when combined with eq. (28), leads to

$$\text{If } \pi \ll t \le \pi N \quad \Rightarrow \quad R_D^{(1)}(t) < \varepsilon \ll 1 \tag{29}$$

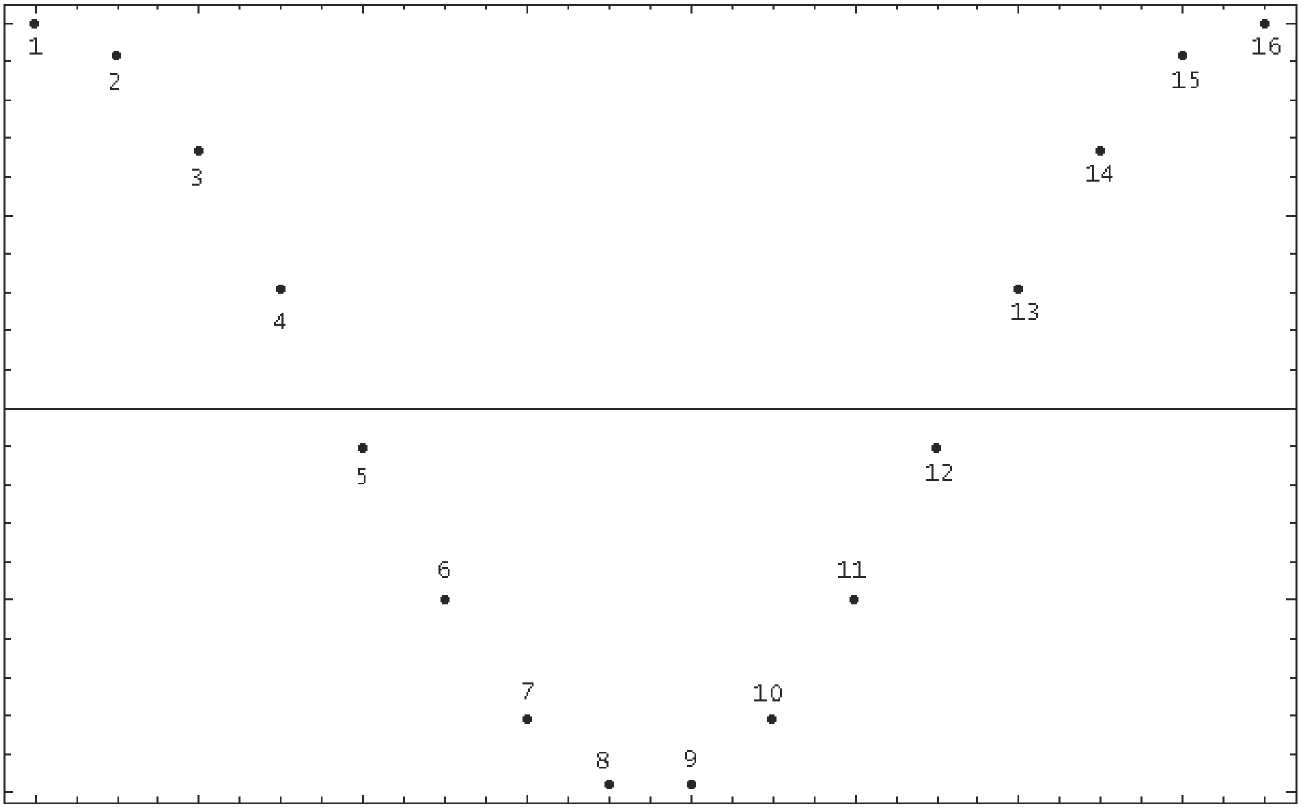

FIG. 1: Point 1 is cancelled by point 9, point 2 by point 10, ... , point 8 by point 16.

IV. A LEMMA FOR THE APPLICATION OF THE DISCRETE ANALOGUE

Up to this point we have studied the case $f(x_i) = 1$; now we will consider the case $f(x_i) \neq 1$. In order to compute $R_D(t)$ as defined by eq. (11), we have to ask a certain degree of regularity to function $f(x_i)$. The first step consists in splitting the set $\{x_i\}$ in G subsets of $(P+1)$ consecutive points:

$$\{x_i\} = \bigcup_{k=1}^{G} \left\{ x_{(k-1)(P+1)+1}, ..., x_{k(P+1)} \right\} = \bigcup_{k=1}^{G} X_k \tag{30}$$

Now we relabel the points $x_j \in X_k$: since $j = (k-1)(P+1)+1$ to $k(P+1)$, we can replace the index j by the index $r_k = j + (1-k)(P+1) - 1$, and we obtain

$$x_j \in X_k \longrightarrow x_{r_k} \in X_k \quad \text{with } r_k = 0, ..., P \tag{31}$$

Then, we define

Definition 1 . *Let $\{x_i\}$ be a set of points uniformly distributed (or equidistant), with $i \in [0, N]$ and $N \gg 1$. The set $\{x_i\}$ is said to be quasi-continuous of class 1 if $\exists G \in \mathbb{N}, \exists P \in \mathbb{N}$ such that $P \gg 1$ and $\{x_i\} = \bigcup_{k=1}^{G} \left\{ x_{(k-1)(P+1)+1}, ..., x_{k(P+1)} \right\} = \bigcup_{k=1}^{G} X_k$. The set X_k is called the k component of the quasi-continuous decomposition.*

If the function $f(x_{r_k})$ is almost constant in X_k, i.e.

$$f(x_{r_k}) \cong C_k \tag{32}$$

Then, we can define

Definition 2 . *Let $f(x_i) : \mathbb{R} \to \mathbb{R}$ be a discrete function defined over the quasi-continuous set $\{x_i\}$ of class 1. If for every component X_k of a quasi-continuous decomposition $f(x_{r_k}) \cong C_k$, with $x_{r_k} \in X_k$, we say that $f(x_i) \in \mathcal{L}_1$.*

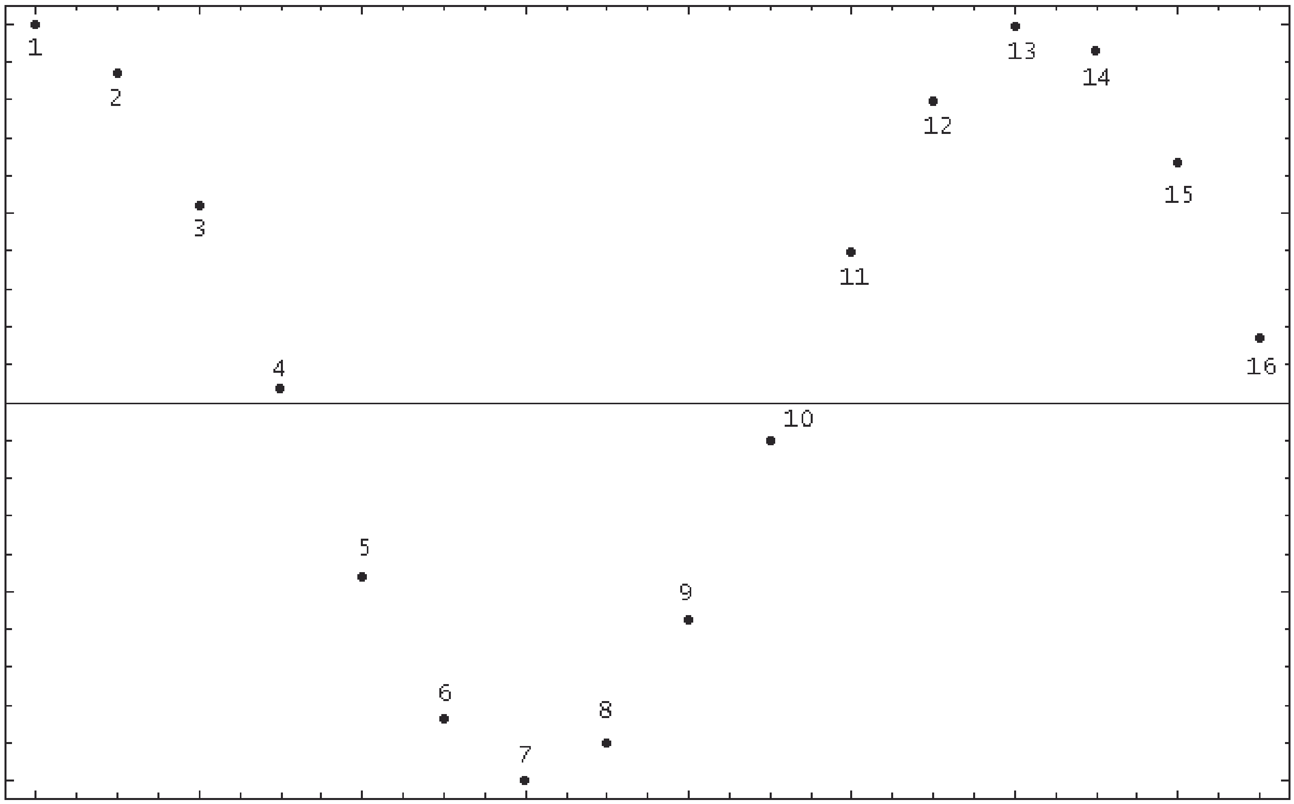

FIG. 2: Points 13, 14, 15 and 16 are not cancelled.

Therefore, when $f(x_i) \in \mathcal{L}_1$, the discrete function $R_D(t)$ can be written as

$$R_D(t) = \sum_{i=0}^{N} \frac{1}{N} f\left(x_i\right) e^{ix_i t} = \sum_{k=1}^{G} \frac{P}{N} \left(\sum_{r_k=0}^{P} \frac{1}{P} f\left(x_{r_k}\right) e^{ix_{r_k} t} \right) = \sum_{k=1}^{G} \frac{P}{N} C_k \left(\sum_{r_k=0}^{P} \frac{1}{P} e^{ix_{r_k} t} \right) \tag{33}$$

If we define the function

$$R_D^{(k)}(t) = \sum_{r_k=0}^{P} \frac{1}{P} e^{ix_{r_k} t} \tag{34}$$

then the discrete function $R_D(t)$ results

$$R_D(t) = \sum_{k=1}^{G} \frac{P}{N} C_k R_D^{(k)}(t) \tag{35}$$

Under this form, the condition of eq. (29) obtained in the previous subsection can be applied to each $R_D^{(k)}(t)$:

$$\text{If } \pi \ll t \leq \pi P \quad \Rightarrow \quad R_D^{(k)}(t) < \varepsilon \ll 1 \tag{36}$$

When this condition is satisfied, the sum $R_D(t)$ results

$$R_D(t) = \sum_{k=1}^{G} \frac{P}{N} C_k R_D^{(k)}(t) < \sum_{k=1}^{G} \frac{P}{N} C_k \varepsilon_k \leq \sum_{k=1}^{G} \frac{P}{N} C\varepsilon = \frac{PG}{N} C\varepsilon = C\varepsilon \tag{37}$$

where $\varepsilon = \max_k \{\varepsilon_k\}$ and $C = \max_k \{C_k\}$. As a consequence, if we consider that $t_P = 2\pi$, we have proved that

Lemma 1. *Let $f(x_i)$ be defined over the quasi-continuous set $\{x_i\}$ of class 1, with $i = 1...N$. If $f(x_i) \in \mathcal{L}_1$, then*

$$\lim_{t \longrightarrow t_P/2} \sum_{i=0}^{N} \frac{1}{N} f(x_i) e^{ix_i t} \cong 0 \tag{38}$$

There are different kinds of functions for which the sum $R_D(t)$ vanishes and that could be characterized by further lemmas, but we will not consider those cases now. Nevertheless, a practically useful remark is in order. The condition of eq. (32) (that the function $f(x_i)$ be approximately constant in each element X_k of the partition) can be expressed under a matematically more elegant form. Given a function $f(x_i)$, its *Discrete Fourier Transform* (DFT), as used in signal analysis ([36]-[39]), is defined as

$$\tilde{f}(t) = \sum_{i=0}^{N} \frac{1}{N} f(x_i) e^{ix_i t} \tag{39}$$

This result may be very useful in practice, in particular in cases in which Lemma 1 is difficult to be applied. In fact, when we realize that the sum $R_D(t)$ corresponding to the function $f(x_i)$ is precisely the DFT of $f(x_i)$, we can use all the properties of DFT −as linearity, symmetry, time-shifting, frequency-shifting, the time-convolution theorem, and the frequency-convolution theorem− to study $R_D(t)$. Moreover, we can take advantage of the large amount of software designed to compute DFT and profusely used in physics and engineering. All these resources, which are standard tools in signal analysis, may prove to be extremely useful for studying decoherence in discrete models.

V. CONCLUSIONS

In this paper we have offered a discrete analogue of the Riemann-Lebesgue theorem and, on this basis, we have introduced a lemma relevant for discrete models, which provides a criterion for deciding whether or not the system decoheres with no need of numerical simulations. Moreover, we have shown how the large amount of mathematical methods of software engineering based on the Discrete Fourier Transform can be used to predict decoherence in discrete models.

VI. ACKNOWLEDGMENTS

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