CENTRO DE INVESTIGACIÓN Y DE ESTUDIOS AVANZADOS
DEL INSTITUTO POLITÉCNICO NACIONAL

UNIDAD ZACATENCO
DEPARTAMENTO DE FÍSICA

“Estados de tiempo y operadores para sistemas cuánticos con espectro de energía discreto”

Tesis que presenta

José Armando Martínez Pérez

para obtener el Grado de

Doctor en Ciencias

en la Especialidad de

Física

Director de tesis: Dr. Gabino Torres Vega

Ciudad de México Julio, 2021

CENTER FOR RESEARCH AND ADVANCED STUDIES OF THE NATIONAL POLYTECHNIC INSTITUTE

PHYSICS DEPARTMENT

"Time states and operators for quantum systems with discrete energy spectrum”

by

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In order to obtain the

Doctor of Science

degree, speciality in

Physics

Advisor: Ph. D. Gabino Torres Vega

Mexico City July, 2021

Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional
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The present work was completed in the Physics Department at Cinvestav.

Acknowledgments

I thank my family for supporting me at all times. I would also like to thank Ana Laura and Anneth Marissa who supported me with love throughout my PhD.

On the other hand, I would like to thank my advisor Dr. Gabino Torres Vega for his help and patient throughout my PhD, and for introducing me to the quantum realm.

I would also like to thank Dr. David Bermúdez Rosales, Dr. Arturo Zuñiga Segundo, Dr. David José Fenández Cabrera and Dr. Jaime Santoyo Salazar for their careful reading of my thesis and for their remarks and suggestions, which significantly helped to improve the content and presentation of this thesis. I am also grateful to Dr. José Martínez Bernal for his advice that helped me at the end of my PhD.

Also, I am grateful to CONACyT for providing funds to me to be able to do my PhD through scholarship 457812 with No. CVU 634969.

QVED! *José Armando Martínez Pérez*

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Resumen

En esta tesis abordamos el problema de definir los espacios congruentes de las representaciones de tiempo y energía del espacio de estados para sistemas cuánticos con un espectro de energías discreto. Los casos de un espectro continuo o un espectro discreto equidistante ya han sido estudiados. Para el primer caso el espacio de tiempo asociado es el espacio de Lebesgue $L^2(\mathbb{R})$; el espacio de energía se obtiene con la transformación unitaria de Plancherel, usualmente llamada transformada de Fourier. Sin embargo, el caso de un espectro de energías discreto no necesariamente equidistante sigue estando en debate. En esta tesis definimos los espacios de tiempo y energía como subespacios de dos espacios no separables de Hilbert, el espacio de Besicovitch B^2 y el espacio de Lebesgue $l^2(\mathbb{R})$, respectivamente. Mostramos que estos espacios están relacionados por las transformaciones unitarias: el valor medio asociado a funciones de Besicovitch y la transformada de Fourier respecto a la medida del conteo.

Por otra parte, en esta tesis proponemos una versión discreta de un operador tiempo, el cual corresponde a un esquema de diferencias finitas exactas para la derivada respecto al espectro de energías discreto. Así logramos tener una versión discreta de una derivada continua. Además, este operador discreto cumple con una ecuación generalizada de eigenvalores, en el sentido que el eigenket asociado no es normalizable. Este eigenket ha sido estudiado antes como un eigenket de un operador tiempo, aunque sólo para el caso de un espectro de energías equidistantes. Finalmente, estudiamos el comportamiento del eigenket del tiempo, para ello usamos el modelo de una partícula en un pozo de potencial infinito. Los tiempos de Bohr, característicos del sistema y los cuales corresponden al inverso de las frecuencias de Bohr, surgen en la construcción de un operador discreto del tiempo. Estos tiempos de Bohr resultan ser los tiempos de llegada en los cuales una partícula clásica chocaría con las paredes del potencial. Los estados de tiempo formados con sólo dos estados propios de la energía se pueden reconocer como una onda que viaja a lo largo de las trayectorias clásicas más una onda estacionaria y otra onda con el mínimo de energía, las cuales hacen que se cumplan las condiciones de frontera.

Abstract

In this thesis we address the task of defining congruent time and energy representations of the state space related to a quantum system with only discrete energy spectrum. The cases of a continuous and an equidistant energy point spectra have already been studied. For the former, the time space is $L^2(\mathbb{R})$; the related energy space is obtained through the unitary Plancherel's transform, commonly called Fourier transform. Nevertheless, the point energy spectrum case, not necessarily equidistant, is still in debate. In this thesis we define the time and energy spaces as closed subspaces of two nonseparable Hilbert spaces: the Besicovitch space B^2 and the Lebesgue space $l^2(\mathbb{R})$. We show that these spaces are related by means of unitary maps: the mean value defined for Besicovitch functions and the Fourier transform with respect to the counting measure.

On the other hand, we propose a discrete version of a time operator, that corresponds to an exact finite difference scheme for the derivative with respect to a discrete energy spectrum. In this way, we get a discrete version of a continuous derivative. In addition, this operator satisfies a generalized eigenvalue equation, which means that the eigenket is not normalizable. This eigenket has been studied before as a time eigenket of a time operator, but mainly for the equidistant energy point spectrum case. Finally, we study the behavior of the time eigenket using of the model of a particle in the infinite well. The Bohr times, characteristic of the system and being the inverse of the Bohr frequencies, arise from the construction of the discrete time operator. These times turn out to be the arrival times at which a classical particle hit the walls. The time states that are formed with only two energy eigenstates, can be identified with a traveling wave following classical trajectories plus stationary and low energy traveling waves, to ensure that the boundary conditions are fulfilled.

Chapter 1

Introduction

A topic that needs further development in physical theories is how to extract the time information from the equations of motion. There are many approaches to this topic but none uses a discrete derivative as an operator in order to compute discrete derivatives with respect to the energy spectrum of a given Hamiltonian. The derivative with respect to the energy provides quantities perpendicular to the energy axis, a direction which can be used as a time coordinate. This is one of the aims of this thesis.

The discrete spectrum of quantum operators has been an outstanding achievement of the standard theory of quantum mechanics. This spectrum type can be described through the mathematical concept of the eigenvalue problem, which is stated in the theory of Hilbert spaces. In the abstract Hilbert space, this concept is written as follows

$$\hat{H}|E_n\rangle = E_n|E_n\rangle, \quad n = 1, 2, \ldots, \tag{1.1}$$

where E_n is the eigenvalue, $|E_n\rangle$ is the corresponding eigenket, and $\hat{H}$ is the Hamiltonian that describes a physical system and, once its spectrum is known, the Hamiltonian can be written as the spectral decomposition $\hat{H} = \sum_{n=1}^{\infty} E_n|E_n\rangle\langle E_n|$; which is an operator defined in a maximal domain of definition.

Although the Dirac notation can be misleading, see for example [16], it has many advantages, for example, we do not worry about whether the energies are equidistant or not, for instance. To illustrate this point, we can mention the orthonormalization relation

$$\langle E_n|E_m\rangle = \delta_{n,m} = \begin{cases} 1 & E_n = E_m \\ 0 & \text{otherwise} \end{cases}, \tag{1.2}$$

that avoids to deal with an explicit representation of the abstract Hilbert space. The case of an equidistant energy spectrum has been frequently considered. For example the cases of the harmonic oscillator or the angular momentum operator. For a non-equidistant spectrum, we can mention the infinite well and the hydrogen atoms. In fact, for the latter it is common to work with the abstract space rather than with the spherical harmonics.

From the abstract eigenkets we can get some representations of the space of states, for instance the coordinate and momentum representations. These representations are said to be a pair of conjugate spaces; the coordinate q and the momentum p are related through the Plancherel's transform (commonly called Fourier transform). Another purpose of this thesis is to establish the time and energy space representations of the abstract eigenkets, and therefore including the abstract Hilbert space, such that the time t and energy E variables are conjugated by means of some unitary transformation for the case of a discrete energy spectrum either equidistant or not.

Among the proposed time and energy representations (a few references are [2, 20, 36, 43], see also the references therein), we can mention the work of Torres-Vega [43] that settles that trajectory-like states can evolve in time with fixed operators, as is the case in the Wigner phase-space formulation of quantum mechanics. Another related work is due to Olkhovsky [36] who extensive revisited time and energy representations for both a continuous and bounded from below energy spectrum and an equidistant one. On the other hand, the time representation we introduce is in agreement with the one found in Ref. [20]. In his paper, Hall started by recognizing that the orthogonality relation of the energy eigenfunctions, in a time representation $\langle t|E_n\rangle = e^{itE_n/\hbar}$, $t \in \mathbb{R}$ (see also the generalized ket Eq. (1.11) below), can be accomplished by means of the Besicovitch measure; yielding the representation of the orthonormalization relation

$$\langle E_n|E_m\rangle = \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} e^{-itE_n/\hbar}\, e^{itE_m/\hbar}\, dt = \lim_{T\to\infty} \text{sinc}\left[\frac{(E_n - E_m)T}{\hbar}\right] = \delta_{n,m}. \tag{1.3}$$

We are interested in the Besicovitch framework because it has a Fourier analysis that includes the usual Fourier analysis for periodic functions [9]. This allows us to have a representation of the Hilbert space structure of the abstract space for a non-equidistant energy point spectrum. In Chapter 2, the starting point is the Fourier series of general type related to the Besicovitch functions. In that chapter, we want to place the Hilbert space structure with a Besicovitch inner product. Hall mainly relied on the Besicovitch measure concept [20]. However, our approach immediately leads to establish the conjugate space to the time representation.

The first goal of this thesis starts in Chapter 3, where we provide two ways to establish the time representation of wave functions for systems with discrete energy spectrum. First, we use a purely mathematical point of view. But then, since the Besicovitch setting enable us to use some elementary facts about the measure problem (see for Ref. [8] Chapter II, section c.3), we construct a second time representation of states.

In addition, at the end of Chapter 3, we show that the energy representation is a closed subset of the non-separable Lebesgue space $l^2(\mathbb{R})$, that is defined by means of the counting measure. By using an integral notation for this measure, we can handle a discrete energy spectrum on the same footing as the continuous case.

On the other hand, regarding the subject of the Chapter 4, we look at the eigenvalue problem related to the time operator. It is worth to pay attention to the time operator canonically conjugate to a Hamiltonian with equidistant point spectrum because it has been widely addressed. For example in References [6, 7, 18, 23, 34, 36, 41].

The commutator between the Hamiltonian $\hat{H}$ and an operator $\hat{T}$, not necessarily an observable can be computed

$$[\hat{T},\hat{H}] := \hat{T}\hat{H}-\hat{H}\hat{T} = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} T_{n,m}(E_n-E_m)|E_n\rangle\langle E_m|, \tag{1.4}$$

where $T_{n,m}=\langle E_n|\hat{T}|E_m\rangle$. If we restrict our attention to the diagonal entries of this commutator we find that they are always zero! Then, how can the Heisenberg uncertainty relationship be fulfilled for discrete spectra? In the matrix formalism this reads $[\hat{X},\hat{P}]=i\hbar\hat{I}$, when $\hat{X}$ and $\hat{P}$ are a pair of canonical conjugated operators and $\hat{P}$ has a point spectrum as $\hat{H}$ does. Specifically, how can we understand that all the diagonal entries of $\hat{I}$ are nonzero while they are zero for $[\hat{T},\hat{H}]$? This criticism can be solved with a proper use of the theory of operators. For example, in Ref. [6], Cannata noticed that instead of dealing with $[\hat{T},\hat{H}]=i\hbar\hat{I}$, it is better to look for the eigenvalue problem

$$[\hat{T},\hat{H}]|\vartheta\rangle = -i\hbar|\vartheta\rangle. \tag{1.5}$$

Cannata developed this approach mainly for the particular case of an equidistant spectrum. To illustrate this approach consider the equidistant energy spectrum

$$E_n=\hbar\frac{2\pi n}{2\tau},\quad n=0,\pm1,\pm2,\ldots, \tag{1.6}$$

where $\tau>0$ has units of time. Cannata found that the symmetric operator

$$\hat{T}=-i\hbar\sum_{n=-\infty}^{\infty}\sum_{\substack{m=-\infty\\ m\neq n}}^{\infty}\frac{e^{i(E_n-E_m)\tau/\hbar}}{E_n-E_m}|E_n\rangle\langle E_m| \tag{1.7}$$

along with the Hamiltonian comply with the canonical commutation relation, that is, the commutator $[\hat{T},\hat{H}]$ can be defined in the dense domain of states $|\vartheta\rangle=\sum_{n=1}^{\infty}\vartheta_n|E_n\rangle$ ($\sum_{n=1}^{\infty}|\vartheta_n|^2<\infty$) such that

$$\sum_{n=1}^{\infty}|E_n\vartheta_n|^2<\infty,\quad \text{and}\quad \sum_{n=1}^{\infty}e^{-iE_n\tau/\hbar}\vartheta_n=\sum_{n=1}^{\infty}(-1)^n\vartheta_n=0, \tag{1.8}$$

on this domain the commutator $[\hat{T},\hat{H}]$ is proportional to the identity operator $\hat{I}$; satisfying Eq.(1.5). Recall that Eq. (1.4) is just an infinite matrix written using Dirac notation, but, generally speaking, an operator is composed of a domain and a rule mapping.

Cannata named $\hat{T}$ as the conjugate momentum of the label operator $\hat{H}$, and in Ref. [7] he showed that $\hat{T}$ can represent a time operator for a one-dimensional harmonic oscillator with period 2τ and, that the matrix representation of the coordinate operator for the particle in the infinite well with walls at $\pm\tau$ is of type $\hat{T}$. Also, Weyl quantized the angle observable of the unit circle and found that the angle operator is of type $\hat{T}$ [45, p.36]. In this case $\hat{T}$ has the representation of a sawtooth function; this identification helps to find that the spectrum of $\hat{T}$ is the closed set $[-\tau,\tau]$, for details see Ref. [23]. Afterwards, Galapon [13] also studied the operator $e^{-i\tau\hat{H}/\hbar}\hat{T}e^{i\tau\hat{H}/\hbar}$, that is, the operator $\hat{T}$ but without phases. The starting point is to consider that the energy spectrum is bounded from below and satisfies the condition

$$\sum_{n=1}^{\infty}{}' \frac{1}{E_n^2} < \infty, \tag{1.9}$$

where the prime indicates $E_n \neq 0$. The significant improvement of this approach is that the spectrum is not constrained to be equidistant and $\hat{T}$ is still a time operator.

Regarding the spectrum of the canonical pair of operators $(\hat{H}, \hat{T})$, by definition the spectrum of $\hat{H}$ is just the set of quantum energy levels E_n, while for $\hat{T}$ if we restrict ourselves to the equidistant case Eq. (1.6), $\hat{T}$ has only a continuous spectrum. In order to give a rough proof of this assertion we proceed to establish the eigenvalue problem:

$$\hat{T}|t\rangle = \beta(t)|t\rangle, \tag{1.10}$$

where β is a sawtooth function (see Eq.(1.14) below).

Let us define the family of generalized kets [6, 7, 20, 34, 41]

$$|t\rangle = \sum_{n=-\infty}^{\infty} e^{itE_n/\hbar}|E_n\rangle, \quad t \in \mathbb{R}. \tag{1.11}$$

Calculating

$$\begin{aligned}\hat{T}|t\rangle &= -i\hbar \sum_{n=-\infty}^{\infty} \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)\tau/\hbar}e^{iE_m t/\hbar}}{E_n - E_m}|E_n\rangle \\ &= \sum_{n=-\infty}^{\infty} e^{itE_n/\hbar}\left[-i\hbar \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)(\tau-t)/\hbar}}{E_n - E_m}\right]|E_n\rangle \end{aligned} \tag{1.12a}$$

Realizing that the bracketed term does not depend on n using Eq.(1.6)

$$-i\hbar \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)(\tau-t)/\hbar}}{E_n - E_m} = -i\tau \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i\pi(n-m)(1-t/\tau)}}{\pi(n-m)} = i\tau \sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} \frac{e^{-i\pi k(1-t/\tau)}}{\pi k} \tag{1.12b}$$

we arrive at

$$\hat{T}|t\rangle = \left[-i\tau \sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} \frac{e^{i\pi k(1-t/\tau)}}{\pi k}\right]|t\rangle. \tag{1.12c}$$

Now, it is easy to identify the infinite sum above to be the usual Fourier series of a sawtooth function. To show that, we can calculate the usual Fourier coefficients, over a period 2τ, of the function t:

$$\frac{1}{2\tau}\int_{-\tau}^{\tau} te^{i\pi nt/\tau}dt = \begin{cases} -i\tau\dfrac{e^{i\pi n}}{\pi n} & n = \pm 1, \pm 2, \ldots \\ 0 & n = 0 \end{cases}, \tag{1.13}$$

then the respective Fourier series converges uniformly to the periodization of t, that is, to the sawtooth function

$$-i\tau \sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} \frac{e^{i\pi k}}{\pi k} e^{-i\pi kt/\tau} := \beta(t) = \begin{cases} t \pmod{2\tau} & t \in (-\tau, \tau) \\ 0 & t = \tau + 2\tau k, \quad k \in \mathbb{Z} \end{cases}. \tag{1.14}$$

Hence, the generalized eigenket $|t\rangle$ and its corresponding eigenvalue $\beta(t)$ are defined throughout the real line $t \in \mathbb{R}$ modulo a period 2τ. This suggests that the spectrum of $\hat{T}$ is $(-\tau, \tau)$. However, from the theory of self-adjoint operators a bounded self-adjoint operator always has a compact spectrum. Thus, the right argument is to consider the essential spectrum of $\beta(t)$, with respect to the Lebesgue measure, yielding that the spectrum of $\hat{T}$ is the closed real subset $[-\tau, \tau]$. The boundedness of $\hat{T}$ follows from the Hilbert inequality [19] which for $\hat{T}$ reads as follows

$$\sum_{n=-\infty}^{\infty} \left| -i\hbar \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)\tau/\hbar}}{E_n - E_m} \langle E_m|\psi\rangle \right|^2 \leq \tau^2 \sum_{n=-\infty}^{\infty} |\langle E_n|\psi\rangle|^2. \tag{1.15}$$

In fact, this estimate can be improved for the case of an energy spectrum of *uniformly discrete* type (also said *separated*), which means that for some $\epsilon > 0$ the separation of $\{E_n\}_{n=1}^{\infty}$ satisfies

$$\delta = \inf_{n\neq m} |E_n - E_m| > \epsilon. \tag{1.16}$$

This case includes Eq. (1.9). Then, for a uniformly discrete spectrum instead of considering the Hilbert inequality we need to use the generalization due to Montgomery [33], which for the operator $\hat{T}$ will read as follows

$$\sum_{n=-\infty}^{\infty} \left| -i\hbar \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)\tau/\hbar}}{E_n - E_m} \langle E_m|\psi\rangle \right|^2 \leq \frac{\hbar^2\pi^2}{\delta^2} \sum_{n=-\infty}^{\infty} |\langle E_n|\psi\rangle|^2. \tag{1.17}$$

In this case $\hat{T}$ should be considered as a τ-parameter operator. Note that the equidistant energy case Eq. (1.6) has the separation $\delta = \hbar\pi/\tau$. Thus, estimate Eq. (1.15) is a particular case of inequality Eq. (1.17).

Thus, a Hamiltonian with pure point spectrum may have a canonical conjugated operator. For the particular case of the equidistant energy spectrum Eq. (1.6) the Hamiltonian spectrum is unbounded, while the spectrum of $\hat{T}$ is continuous and bounded. Nevertheless, some properties of the operator $\hat{T}$ for the equidistant spectrum case are no longer valid for the general case. For instance, the series

$$-i\hbar \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)(\tau-t)/\hbar}}{E_n-E_m}, \quad n=1,2,\ldots \tag{1.18}$$

depends on E_n, unless the set of energy levels are an additive group as the equidistant case Eq. (1.6). Then, for a non-equidistant spectrum, we cannot repeat the steps (1.12) to get the eigenvalue equation (1.10).

On the other hand, let us point out further features of the operator $\hat{T}$: it is of infinite dimensional range and uses of all the coefficients of the states. For example, if we take the energy spectrum itself as the labeled set, we can identify

$$\langle E_n|\hat{T}|\psi\rangle = -i\hbar \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{e^{i(E_n-E_m)\tau/\hbar}\,\psi_m}{E_n-E_m}, \quad n=0,\pm1,\pm2,\ldots \tag{1.19}$$

with a discrete convolution (commutative only when the spectrum is an additive group) between the sequences $\{\psi_n=\langle E_n|\psi\rangle\}_{n=-\infty}^{\infty}$ and $\{-i\hbar e^{iE_n\tau/\hbar}/E_n\}_{n=-\infty}^{\prime\infty}$ (the prime indicates $E_n\neq 0$, and note that for the equidistant example this series reduces to the Fourier coefficients of the sawtooth function Eq. (1.14)), then, this convolution can be thought of as the discrete version of the Hilbert transform [42]

$$\frac{1}{\pi}\,\text{P.V.}\int_{-\infty}^{\infty} \frac{e^{i(E-E')\tau/\hbar} f(E')}{E-E'}dE', \quad f\in L^2(\mathbb{R}), \tag{1.20}$$

where P.V. denotes the principal value at $E'=E$. The standard definition of the Hilbert transform does not have the phase $e^{i(E-E')\tau/\hbar}$. It is in this sense that a meaning of local derivative with respect to the discrete spectrum cannot be attached to $\hat{T}$. In fact, the opposite situation occurs; $\hat{T}$ is a convolution type operator and it is also a discrete version of an integral operator, the Hilbert transform. This tells us that $\hat{T}$ does not resemble the operation which should be conjugated to the one of $\hat{H}$ (the action of the Hamiltonian is the multiplication by its discrete spectrum). The continuous operations counterparts are known to be differentiation and multiplication by the independent variable.

Aside from the previous remarks about $\hat{T}$, the generalized ket $|t\rangle$ itself yields a time-kind representation and they form a continuous basis in the sense of Dirac as is shown in Chapter 3 and in Ref. [28]. Therefore, we want to present an alternative approach to the time operator.

In Chapter 4, the (generalized) eigenvalue equation we address is

$$\hat{D}|t\rangle = t|t\rangle, \qquad t\in\mathbb{R}. \tag{1.21}$$

We will introduce an operator $\hat{D}$ such that the eigenvalue problem Eq. (1.21) is fulfilled, and such that the generalized ket $|t\rangle$ is always a generalized eigenvector of such an operator regardless if the energy spectrum is equidistant or not.

Our approach consists of introducing an operator $\hat{D}$ which is the realization of an exact finite difference scheme [25, 26, 27, 28]. This will allow us to get the eigenvalue equation Eq. (1.21), but with the time variable t itself as the eigenvalue related to the time eigenket $|t\rangle$. The variable t will take on any real value except for some singularities introduced by the discrete operator $\hat{D}$, depending on the energy spectrum under consideration. Since finite differences regard a finite number of terms, for instance to approximate a derivative, the operator $\hat{D}$ can be local, it can have only two terms at each point (column)

$$\hat{D} = \sum_{n=1}^{\infty} \left(D_{n,n+1} |E_n\rangle\langle E_{n+1}| + D_{n,n} |E_n\rangle\langle E_n| \right), \tag{1.22}$$

where $D_{n,m} = \langle E_n|\hat{D}|E_m\rangle$. Then, we also ask for what $D_{n,n+1}$ and $D_{n,n}$ correspond to the exact finite difference derivative for the complex exponential function so that we will have that

$$\left[-i\hbar \frac{\partial}{\partial E} e^{itE/\hbar} \right]_{E=E_n} = t e^{itE_n/\hbar} = e^{itE_{n+1}/\hbar} D_{n,n+1} + e^{itE_n/\hbar} D_{n,n}. \tag{1.23}$$

This equality relates a continuous derivative (the left side hand) to a finite difference scheme (the right hand side). Instead of having the steps Eqs. (1.12) we will have something like

$$\hat{D}|t\rangle = \sum_{n=1}^{\infty} \left[\sum_{m=1}^{\infty} e^{itE_m/\hbar} D_{n,m} \right] |E_n\rangle = -i\hbar \sum_{n=1}^{\infty} \frac{\partial}{\partial E} e^{itE/\hbar} \bigg|_{E=E_n} |E_n\rangle = t \sum_{n=1}^{\infty} e^{itE_n/\hbar} |E_n\rangle = t|t\rangle \tag{1.24}$$

We also show the properties of the time eigenket, choosing the infinite well as an example model. We found states that might resemble classical behavior. Since different operators satisfying the eigenvalue problem Eq. (1.21) might give distinct information about the system, we want to show some properties of the discrete time operator $\hat{D}$ for different sets of energy eigenfunctions. For example, we ask what states this operator satisfies a symmetric property of discrete type, such states will lead us to find quantum densities that resemble classical ones [28, 29]. This will be shown at the end of Chapter 4.

In Chapter 2 we give a presentation of the mathematical framework aimed at facilitating the study of Chapter 3. At the end of Chapters 3 and 4 there are some conclusions about the contributions of this thesis, while the last chapter is devoted to the conclusions and perspectives.

As a final remark, let us make some comments about parametric description of curves depicted in Figure 1.1. For this purpose let us pick the circle of radius ρ_0

$$\left\{ (x, y) : x^2 + y^2 = \rho_0^2 \right\}, \qquad \rho_0 > 0. \tag{1.25}$$

This first description makes use of two variables, namely x, y, see Figure 1.1a. There is one fixed parameter here: the radius of the circle ρ_0 =constant. A second type of description of the circle is a parametric one;

$$x = \rho_0 \cos\theta, \quad y = \rho_0 \sin\theta; \quad -\infty < \theta < \infty, \quad \rho_0 > 0, \tag{1.26}$$

a description in which we assign values to the additional parameter θ and then we get values for x and y. See Figure 1.1b. It is similar to the description of a classical trajectory in the phase space or the evolution of a quantum wave function, where the parameter θ is the time variable t and ρ_0 is related to the constant energy of a given particle.

However, the third type of description, depicted in Figure 1.1c, uses the parameters ρ and θ as the independent variables so that we only need of these variables to describe the circle, a non-parametric description. The last description, which is shown in Figure 1.1d, uses ρ and θ as axes. This is the simplest one: ρ =constant.

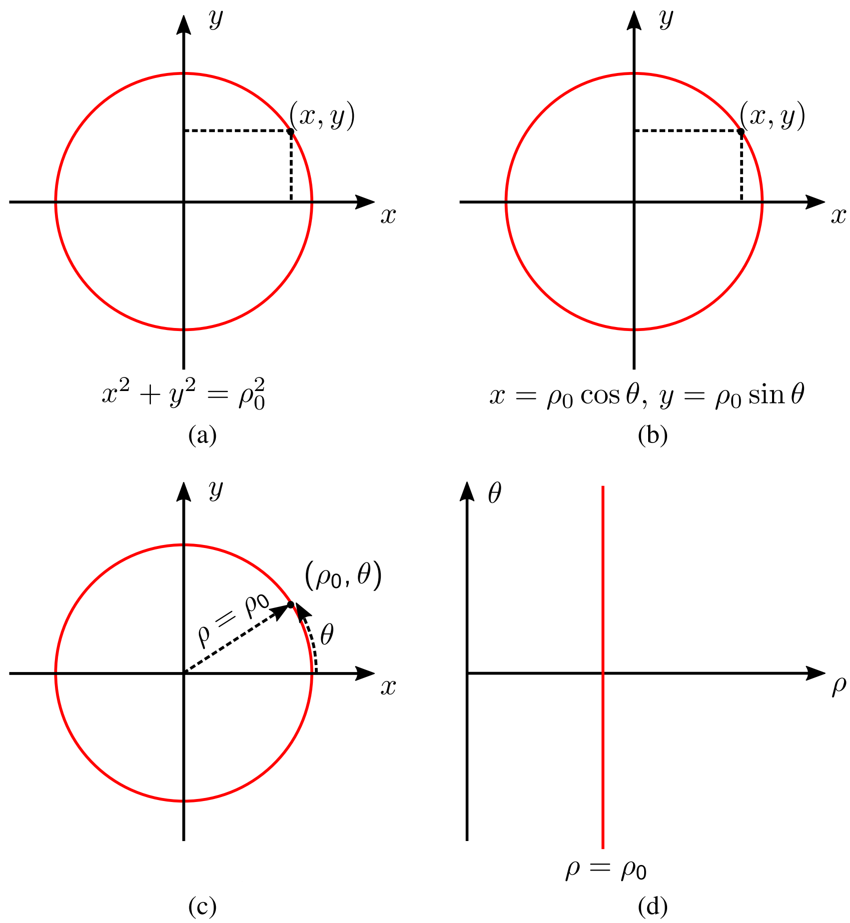


Figure 1.1: Different descriptions of the same object with: (a) two variables x and y and one fixed parameter ρ_0, (b) the same variables and the fixed parameter as in (a) but with a second parameter θ, (c) a non-parametric description with two variables θ and ρ, (d) a description with the perpendicular axes θ and ρ.

Throughout Chapters 3 and 4 we will use a non-parametric description of the dynamics of a given system to develop some time-related concepts in quantum systems with only discrete energy spectrum.

The usual description of motion of classical and quantum particles is similar to the parametric description of the circle with time playing the role of the parameter. Our purpose is to describe quantum motion in terms of non-parametric descriptions.

Chapter 2

Mathematical background

We consider an energy point spectrum $\sigma = \{E_n\}_{n=1}^{\infty}$ of a spin-less particle without degeneracy. This spectrum is not constrained to be equidistant of magnitude, and it is supposed to be arranged in increasing order of magnitude.

It should be noted that Hilbert spaces are (upon isomorphisms) "essentially identical" provided that their dimensions are the same. An *isomorphism* is a one-to-one, onto map that leaves the inner product invariant. In fact, the equivalence between Heisenberg's matrix theory and Schrödinger's wave mechanics is based on this concept. In view of this remark, we will denote the inner product and the norm throughout this thesis by $\langle \bullet | \bullet \rangle$ and $\| \bullet \| = [\langle \bullet | \bullet \rangle]^{1/2}$ without worrying about the space we will work with.

2.1 The abstract space

Our starting Hilbert space (in the next chapter) will be the so called "abstract" space defined by

$$\mathcal{H} = \left\{ |\psi\rangle = \sum_{n=1}^{\infty} \langle E_n|\psi\rangle \, |E_n\rangle : \langle E_n|\psi\rangle \in \mathbb{C}, \sum_{n=1}^{\infty} |\langle E_n|\psi\rangle|^2 < \infty \right\}, \tag{2.1}$$

where $|E_n\rangle$ are the energy eigenkets, that satisfy the eigenvalue equation

$$\hat{H}|E_n\rangle = E_n|E_n\rangle, \quad n = 1, 2, \ldots. \tag{2.2}$$

We consider the Hamiltonian as a self-adjoint, time-independent, and diagonalized by the energy eigenkets $\{|E_n\rangle\}_{n=1}^{\infty}$:

$$\hat{H} = \sum_{n=1}^{\infty} E_n |E_n\rangle\langle E_n|, \tag{2.3a}$$

with *maximal domain* of definition

$$\mathcal{D}(\hat{H}) = \left\{ |\varphi\rangle \in \mathcal{H} : \sum_{n=1}^{\infty} |E_n \langle E_n|\varphi\rangle|^2 < \infty \right\}. \tag{2.3b}$$

Recall that the $\mathcal{H}$ is endowed with the *inner product* $\langle \bullet | \bullet \rangle$, and the corresponding *norm* is given by

$$\langle \phi | \psi \rangle = \sum_{n=1}^{\infty} \langle \phi | E_n \rangle \langle E_n | \psi \rangle, \qquad \text{and} \qquad \| \psi \| = [\langle \psi | \psi \rangle]^{1/2}, \tag{2.4}$$

respectively.

The point to highlight in this construction is the assumptions of the completeness $\sum_{n=1}^{\infty} |E_n\rangle \langle E_n| = \hat{I}$, and the orthonormalization relation of the energy eigenkets $\langle E_m | E_n \rangle = \delta_{m,n}$ (the Kronecker delta). This relation is independent, e.g. the coordinate or momentum representations of the space of states, or even any other Hilbert space isomorphic to $\mathcal{H}$.

Although $\mathcal{H}$ is a separable Hilbert space, in what follows, we present two non-separable Hilbert spaces that will help us to develop our approach in the time and energy representations, in the next chapter. At the end of this chapter we provide a summary in order that the reader can get a quick overlook of the setting of such spaces.

In the rest of this thesis, we will use some standard concepts and usual results of real analysis and functional analysis. In particular, as standard references we utilize [1, 24, 40].

2.2 The Lebesgue space $l^2(\mathbb{R})$

The *non-separable Lebesgue space* $l^2(\mathbb{R})$ consists of all $\tilde{f}(E) : \mathbb{R} \to \mathbb{C}$ such that its *support*

$$\sigma_f := \overline{\{E \in \mathbb{R} : \tilde{f}(E) \neq 0\}}, \tag{2.5}$$

is countable (denumerable or finite) and has a finite l^2-norm

$$\|\tilde{f}\| = \left[\int_{\mathbb{R}} |\tilde{f}(E)|^2 dE \right]^{1/2} < \infty. \tag{2.6}$$

The *integral notation* stands for the *Lebesgue integral with respect to the counting measure* of $|\tilde{f}|^2$, defined as

$$\int_{\mathbb{R}} |\tilde{f}(E)|^2 dE = \sup_N \left\{ \sum_{n=1}^{N} |\tilde{f}(E'_n)|^2 : E'_n \in \mathbb{R}, N \in \mathbb{N} \right\}, \tag{2.7}$$

and such that agrees with the absolutely convergent series [40]

$$\int_{\mathbb{R}} |\tilde{f}(E)|^2 dE = \sum_{E \in \sigma_f} |\tilde{f}(E)|^2. \tag{2.8}$$

Throughout this thesis dE will stand for the *counting measure*; this measure assigns to each finite real set the number of its elements as its measure, if the real set does not have finite elements, the assigned measure is infinite.

Comparing the counting measure with the Lebesgue measure, denoted by $d\mu$, we see that the units associated with the integral $\int \bullet dE$ are the same as the integrand because this measure counts the elements of a given set, for example $\int_{\{0,1\}} dE = 2$. In contrast, the Lebesgue measure assigns to sets like $[0,l]$ ($l > 0$) its length $\int_{[0,l]} d\mu = l$. If we suppose that $[0,l]$ is an interval of length type , then, the units associated to $d\mu$ must be of length, and thus $\int \bullet d\mu$ will have units of the integrand times units of length.

By using the polarization formula the Parseval's identity holds on $l^2(\mathbb{R})$ [40], and then, the inner product on $l^2(\mathbb{R})$

$$\langle \tilde{g} | \tilde{f} \rangle = \int_{\mathbb{R}} \tilde{g}^*(E)\, \tilde{f}(E)\, dE = \sum_{E \in \sigma_{fg}} \tilde{g}^*(E) \tilde{f}(E), \tag{2.9}$$

follows, where $\sigma_{fg} = \sigma_f \cap \sigma_g$ is the support of the product $\tilde{g}^* \tilde{f}$. By letting $\tilde{g} = \tilde{f}$ we get the square norm $\langle \tilde{f} | \tilde{f} \rangle = \|\tilde{f}\|^2$.

Discrete Signal basics. The more elemental function in $l^2(\mathbb{R})$ can be *the unit sample function*

$$\delta[E - E'] = \begin{cases} 1 & E = E' \\ 0 & \text{otherwise} \end{cases} \tag{2.10}$$

a generalization of the Kronecker delta function. The standard, uncountable, orthonormal basis for $l^2(\mathbb{R})$ is thus the set

$$\{\delta[E - E'] : E' \in \mathbb{R}\}. \tag{2.11}$$

This basis expands each function in $l^2(\mathbb{R})$ in an unique way as

$$\tilde{f}(E) = \sum_{E' \in \sigma_f} \tilde{f}(E') \delta[E - E']. \tag{2.12}$$

Remark 2.1. *Given an absolutely convergent series* $\sum_{n=1}^{\infty} |\alpha_n|^2 < \infty$ *and a countable real subset* $\sigma' = \{E'_n\}_{n=1}^{\infty}$ *a function in* $l^2(\mathbb{R})$ *is uniquely defined as*

$$\tilde{g}(E) = \sum_{n=1}^{\infty} \alpha_n\, \delta[E - E'_n]. \tag{2.13}$$

The Lebesgue space $l^1(\mathbb{R})$ and the Fourier transform with respect to dE. A function $\tilde{h}$ is said to be *Lebesgue integrable with respect to the counting measure dE*, if

$$\int_{\mathbb{R}} |\tilde{h}(E)| dE = \sum_{E \in \sigma_h} |\tilde{h}(E)| < \infty. \tag{2.14}$$

See the definition of the integral with respect to the counting measure Eq. (2.7).

Henceforth, the Fourier transform of such $\tilde{h}$ with respect to the counting measure (dE) can be well-defined by

$$\hat{h}(t) := \int_{\mathbb{R}} e^{-itE/\hbar}\,\tilde{h}(E)dE = \sum_{E\in\sigma_h} e^{-itE/\hbar}\,\tilde{h}(E), \quad t \in \mathbb{R}. \tag{2.15}$$

Now, the next step is to attach to this Fourier transform some meaning when $\tilde{h}$ is an arbitrary function in $l^2(\mathbb{R})$. For this purpose we need to know some things about the Besicovitch framework. Recall that $l^1(\mathbb{R}) \subset l^2(\mathbb{R})$ [44].

Here, we are considering that t and E have units of time and energy, respectively, such that the product $E_n t/\hbar$ is dimensionless with $\hbar$ being the reduced Planck constant. The variables t and E will play the role of the time and energy variables, respectively.

2.3 The Besicovitch space

An important development is the theory of the Besicovitch spaces; the spaces in which the time states can be defined. The interested reader can learn more about these spaces in References [4, 5, 9].

The functions $f \in L^2_{\text{loc}}(\mathbb{R})$ with finite *Besicovitch-Marcinkiewicz norm* (B^2-norm)

$$\left[\mathcal{M}_t\left\{|f(t)|^2\right\}\right]^{1/2} := \left[\limsup_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} |f(t)|^2 dt\right]^{1/2} < \infty \tag{2.16}$$

are said to be Besicovitch functions (B^2-functions). $\mathcal{M}_t\{|f(t)|^2\}$ is named *the mean value of* $|f|^2$. This class of functions includes those belonging to the Hilbert space $L^2(\mathbb{R}/T'\mathbb{Z})$; the classes of periodic functions that are square Lebesgue integrable over a period (see Remark 2.3 below).

The collection of all the equivalence classes (B^2-classes) defined by the B^2-functions, through the equivalence relation

$$g \sim f \quad \text{if and only if} \quad \mathcal{M}_t\{|f(t) - g(t)|^2\} = 0, \tag{2.17}$$

is a Banach space called the *Besicovitch space* B^2. The symbol $\sim$ will stand for the equivalence relation (2.17).

The "$\limsup$" can be dropped to just the $\lim$ in Eq. (2.16) because for B^2-functions such limit exists [9, Theorem 3.1]. Even more, the mean value in Eq. (2.16) can be calculated over half of the real line [9, Remark. 3.16]

$$\mathcal{M}_t\{|f(t)|^2\} = \lim_{T\to\infty} \frac{1}{T}\int_{0}^{T} |f(t)|^2 dt. \tag{2.18}$$

Remark 2.2. *Aside from the fact that the B^2-functions are defined throughout the real line, expression Eq.* (2.18) *allows us to restrict the B^2-functions to $[0, \infty)$, or possibly, to keep considering that B^2-functions are defined throughout the real line but mean values can be calculated over the half of the real line. In the rest of this thesis, we will consider the first choice. A similar development as the following can be elaborated for the second setting if we want that "t" takes negative values.*

2.3.1 Harmonic analysis of Besicovitch functions

In order to introduce the Fourier series analysis of the Besicovitch functions to our purposes it is convenient to work with the complex exponential functions $e^{-itE/\hbar}$ instead of the usual convention found in the literature, namely, e^{itE} whit t and E as dimensionless variables. Recall that we are considering that the product $Et/\hbar$ is dimensionless.

Mean value. It is an outstanding property of any B^2-function that the mean value

$$\mathcal{M}_t\{e^{iEt/\hbar} f(t)\} = \lim_{T\to\infty} \frac{1}{T} \int_0^T e^{itE/\hbar} f(t) dt \tag{2.19}$$

exists and is zero for all but a countable number of E [9, Proposition 4.1]. The set of these numbers is called *the spectrum of* f:

$$\sigma_f = \{E \in \mathbb{R} \, : \, \mathcal{M}_t\{e^{itE/\hbar} f(t)\} \neq 0\}. \tag{2.20}$$

We will see soon the reason to use the same notation "σ_f" as for the supports (2.5) of the functions in $l^2(\mathbb{R})$.

Note that the mean value (2.19) is linear

$$\mathcal{M}_t\{e^{itE/\hbar}[\alpha f(t) + \beta g(t)]\} = \alpha \mathcal{M}_t\{e^{itE/\hbar} f(t)\} + \beta \mathcal{M}_t\{e^{itE/\hbar} g(t)\} \tag{2.21}$$

for all B^2-functions f, g and $\alpha, \beta \in \mathbb{C}$.

Fourier series. A *general type of Fourier series* is associated to each B^2-function such that

$$f(t) \sim \sum_{E\in\sigma_f} e^{-iEt/\hbar} \mathcal{M}_{t'}\{e^{it'E/\hbar} f(t')\}, \quad t \in \mathbb{R}. \tag{2.22}$$

We call these series merely Fourier series in the sequel. If f and g are B^2-functions and have the same Fourier series then they comply with Eq. (2.17) [9, Corollary 4.1].

Remark 2.3. *In particular, the series* (2.22) *include the usual Fourier series when the spectrum σ_f is equidistant, say $E_k = \hbar 2\pi k/T'$ (T' having units of time). Suppose that $f \in L^2(\mathbb{R}/T'\mathbb{Z})$, first,* *the coefficients can be computed over a period [9]*

$$
\begin{aligned}
\mathcal{M}_t\{e^{iE_k t/\hbar} f(t)\} &= \lim_{T\to\infty} \frac{1}{T} \int\limits_0^T e^{iE_k t/\hbar} f(t) dt \\
&= \lim_{T\to\infty} \frac{1}{T} \left(\int\limits_0^{T'} + \int\limits_{T'}^{2T'} + \cdots + \int\limits_{lT'}^{lT'+s} \right) e^{i2\pi k t/T'} f(t) dt \\
&= \lim_{l\to\infty} \left(\frac{l}{lT'+s} \int\limits_0^{T'} e^{i2\pi k t/T'} f(t) dt + \frac{1}{lT'+s} \int\limits_{lT'}^{lT'+s} e^{i2\pi k t/T'} f(t) dt \right), \qquad (2.23)
\end{aligned}
$$

where $T = lT' + s$, $l \in \mathbb{N}$, $0 \le s < T$. The second integral at the right hand side above tends to zero as $l \to \infty$ because $f \in L^2(\mathbb{R}/T'\mathbb{Z})$ and

$$
\begin{aligned}
\left| \frac{1}{lT'+s} \int\limits_{lT'}^{lT'+s} e^{i2\pi k t/T'} f(t) dt \right| &\le \frac{1}{lT'+s} \int\limits_{lT'}^{lT'+s} |f(t)| dt \\
&\le \frac{1}{lT'+s} \int\limits_0^{T'} |f(t)| dt \\
&\le \frac{\sqrt{T'}}{lT'+s} \sqrt{\int\limits_0^{T'} |f(t)|^2 dt}, \qquad (2.24)
\end{aligned}
$$

in the last inequality we have used the Schwarz inequality. Thus, from Eq. (2.23) we get the usual way to compute the Fourier coefficients

$$
\mathcal{M}_t\{e^{iE_k t/\hbar} f(t)\} = \frac{1}{T'} \int\limits_0^{T'} e^{i2\pi k t/T'} f(t) dt. \qquad (2.25)
$$

Following a similar procedure for the mean vale of $|f|^2$ we obtain

$$
\mathcal{M}_t\{|f(t)|^2\} = \frac{1}{T'} \int\limits_0^{T'} |f(t)|^2 dt. \qquad (2.26)
$$

Now, if $E \neq E_k$, $k \in \mathbb{Z}$, and since the nth partial Fourier series f_n of f converges in the corresponding L^2-norm of $L^2(\mathbb{R}/T'\mathbb{Z})$, we get $\mathcal{M}_t\{e^{iEt/\hbar} f(t)\} = \lim_{n\to\infty} \mathcal{M}_t\{e^{iEt/\hbar} f_n(t)\}$, but it is easy to verify that $\mathcal{M}_t\{e^{iEt/\hbar} f_n(t)\} = 0$ for all n, hence

$$
\mathcal{M}_t\{e^{iEt/\hbar} f(t)\} = 0, \qquad E \neq E_k \quad \forall k \in \mathbb{Z}. \qquad (2.27)
$$

Isomorphic Hilbert spaces. The Parseval's formula holds [4] in the form

$$\mathcal{M}_t\{|f(t)|^2\} = \sum_{E\in\sigma_f} |\mathcal{M}_t\{e^{itE/\hbar}f(t)\}|^2. \tag{2.28}$$

From Eqs. (2.20) and (2.28), see also Remark 2.1, it now follows that the mean-value map

$$f \mapsto \mathcal{M}_t\{e^{itE/\hbar}f(t)\} =: \tilde{f}(E) \in l^2(\mathbb{R}) \tag{2.29}$$

is an isomorphism from B^2 onto $l^2(\mathbb{R})$. The spectrum of f, Eq. (2.20), can now be identified with the support of its companion $\tilde{f}$, Eq. (2.5). Taking the square root of the mean value (2.28) it follows that the B^2-norm agrees with the l^2-norm

$$\|f\| = \left[\mathcal{M}_t\{|f(t)|^2\}\right]^{1/2} = \|\tilde{f}\|, \tag{2.30}$$

and then, we have that the inner product on $l^2(\mathbb{R})$ is also defined on B^2

$$\langle g|f\rangle = \mathcal{M}_t\{g^*(t)f(t)\} = \langle\tilde{g}|\tilde{f}\rangle. \tag{2.31}$$

The inner product being invariant guarantees that B^2 and l^2 have the same Hilbert space structure.

Riesz-Fischer Theorem. The next theorem for B^2-functions deals with the convergence of the Fourier series Eq. (2.22), and at the same time it shows the completeness of B^2. For more details, we refer the reader to Ref. [5, p. 54-58].

Theorem 2.4 (Riesz-Fischer Theorem)**.** *Let $\epsilon_1 > \epsilon_2 > \ldots > \epsilon_n \to 0$ be positive numbers and let $\{f_n\}_{n=1}^{\infty}$ be a Cauchy sequence of B^2-functions, that is $\mathcal{M}_t\{|f_m - f_n|^2\} \to 0$ as $n, m \to \infty$. Then, there exist positive numbers*

$$0 = T_0 < T_1 < T_2 < \cdots < T_n \to \infty \quad \textit{as} \quad n \to \infty, \tag{2.32}$$

each one depending on the previous $T_n = T_n(T_{n-1}, \ldots, T_1)$, such that the piece-wise function

$$\underset{\sim}{f}(t) = \begin{cases} f_1(t), & T_0 \le t < T_1 \\ & \vdots \\ f_n(t), & T_{n-1} \le t < T_n \\ & \vdots \end{cases} \tag{2.33}$$

satisfies

$$\mathcal{M}_t\left\{|\underset{\sim}{f}(t) - f_n(t)|^2\right\} = \lim_{T\to\infty}\frac{1}{T}\int_0^T \left|\underset{\sim}{f}(t) - f_n(t)\right|^2 dt \le \epsilon_n. \tag{2.34}$$

Letting $n \to \infty$ in Eq. (2.34) and because $\epsilon_n \to 0$, we have that f_n converges to $\underset{\sim}{f}$ in the B^2-norm, showing that the B^2-space is complete. In fact, $\underset{\sim}{f}$ is itself a B^2-function.

Remark 2.5. *The set of nth Fourier series*

$$f_n(t) = \sum_{i=1}^{n} e^{-iE_i t/\hbar} \mathcal{M}_{t'}\{e^{it'E_i/\hbar} f(t')\} = \sum_{i=1}^{n} e^{-iE_i t/\hbar} \tilde{f}(E_i) \tag{2.35}$$

of a B^2-function f forms a Cauchy sequence. We considered $E_i \in \sigma_f$ in Eq. (2.35). It can be shown that for $n > m$

$$\mathcal{M}_t\left\{|f_n(t) - f_m(t)|^2\right\} = \lim_{T_2 - T_1 \to \infty} \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} |f_n(t) - f_m(t)|^2 dt = \sum_{i=m+1}^{n} |\tilde{f}(E_i)|^2 \tag{2.36}$$

tends to zero as $m \to \infty$, because $\sum_{i=1}^{\infty} |\tilde{f}(E_i)|^2 < \infty$. Note that, here, also $n \to \infty$.

Remark 2.6. *From Eq. (2.36), it follows a property that we will use several times in the next proof, that is, for some $\epsilon > 0$ we can find $\Delta T' > 0$ sufficiently large such that*

$$\left| \frac{1}{T_2 - T_1} \int_{T_1}^{T_2} |f_n(t) - f_m(t)|^2 dt - \sum_{i=m+1}^{n} |\tilde{f}(E_i)|^2 \right| < \epsilon, \tag{2.37}$$

provided that the difference $T_2 - T_1$ is greater than or equal to $\Delta T'$. This property holds for any trigonometric polynomial.

Guided principally by Ref. [3, p. 502-504] we proceed to establish a corollary of Theorem 2.4.

Corollary 2.7. *By taking the partial Fourier series as the Cauchy sequence in Theorem 2.4, it follows that the Fourier series of a B^2-function f converges (unconditionally) in the B^2-norm to the piece-wise function $\underset{\sim}{f}$ defined in Eq. (2.33).*

Proof. Let $m \geq 1$, and let $\epsilon_1 > \epsilon_2 > \cdots$ be as in Theorem 2.4. Also, denote by l_s the sum $\sum_{i=1}^{s} |\tilde{f}(E_i)|^2$, $s = 1, 2, \ldots$. The order in which the numbers of the spectrum of f appear is arbitrary, $E_1, E_2, \ldots$, because the important thing in what follows is that the series $\sum_{i=1}^{\infty} |\tilde{f}(E_i)|^2$ does converge absolutely. This will account for the unconditionally convergent sentence.

Let us proceed by induction on n. For $n = 1$ and ϵ_1 we can find T_1 such that

$$\left| \frac{1}{T} \int_{0}^{T} |f_1 - f_m|^2 dt - |l_1 - l_m| \right| < \epsilon_1, \qquad T \geq T_1. \tag{2.38}$$

This follows from the fact that $\mathcal{M}_t\{|f_1 - f_m|^2\} = |l_1 - l_m|$ (see Remark 2.6).

Next, assume that for $n > 1$ we have found $T_1 < \cdots < T_n$ such that the next estimates hold:

$$\left| \frac{1}{T_k - T_{k-1}} \int_{T_{k-1}}^{T_k} |f_k - f_m|^2 dt - |l_k - l_m| \right| < \epsilon_k, \qquad k = 1, 2, \ldots, n \tag{2.39}$$

and

$$\left|\frac{1}{T}\left[\int_0^{T_1}|f_1-f_m|^2dt+\int_{T_1}^{T_2}|f_2-f_m|^2dt+\cdots+\int_{T_{n-1}}^{T}|f_n-f_m|^2dt\right]-|l_n-l_m|\right|<\epsilon_n, \tag{2.40}$$

for $T\geq T_n$.

Our first goal is to find the next T_{n+1} such that Eqs. (2.39) and (2.40) remain valid for $n+1$.

First note that from Eq. (2.39) it follows

$$\int_{T_{k-1}}^{T_k}|f_k-f_m|^2dt<(|l_k-l_m|+\epsilon_k)(T_k-T_{k-1}),\qquad k=1,2,\ldots,n. \tag{2.41}$$

Also, since $\mathcal{M}_t\{|f_{n+1}-f_m|^2\}=|l_{n+1}-l_m|$, for T_n and ϵ_{n+1} we can find $T'>T_n$ such that

$$\left|\frac{1}{T-T_n}\int_{T_n}^{T}|f_{n+1}-f_m|^2dt-|l_{n+1}-l_m|\right|<\frac{\epsilon_{n+1}}{3}, \tag{2.42}$$

whenever $T\geq T'$.

Let $T>T_n$. Using inequalities in Eq. (2.41) and the triangle inequality we have that the term

$$\left|\frac{1}{T}\left[\int_0^{T_1}|f_1-f_m|^2dt+\cdots+\int_{T_{n-1}}^{T_n}|f_n-f_m|^2dt+\int_{T_n}^{T}|f_{n+1}-f_m|^2dt\right]-|l_{n+1}-l_m|\right| \tag{2.43}$$

is smaller than

$$\frac{(|l_1-l_m|+\epsilon_1)T_1+(|l_2-l_m|+\epsilon_2)(T_2-T_1)+\cdots(|l_n-l_m|+\epsilon_n)(T_n-T_{n-1})}{T}$$
$$+\left|\frac{1}{T}\int_{T_n}^{T}|f_{n+1}-f_m|^2dt-|l_{n+1}-l_m|\right|. \tag{2.44}$$

Let $\kappa_{n,m}$ denote the numerator of the first quotient in Eq. (2.44). Recall that, given that $|l_k-l_m|\leq\max\{|l_k-l_m|:k=1,2,\ldots,n\}=D_{n,m}$, and $\epsilon_k<\epsilon_1$ for $k=1,\ldots,n$; $\kappa_{n,m}$ is bounded by $(D_{n,m}+\epsilon_1)T_n$. On the other hand, if the second term of Eq. (2.44) is written in the form

$$\left|\frac{T-T_n}{T}\left[\frac{1}{T-T_n}\int_{T_n}^{T}|f_{n+1}-f_m|^2dt-|l_{n+1}-l_m|\right]+\left(\frac{T-T_n}{T}-1\right)|l_{n+1}-l_m|\right|, \tag{2.45}$$

we have that Eq. (2.44), as well as Eq. (2.43), are smaller than

$$\frac{\kappa_{n,m}}{T}+\left|\frac{1}{T-T_n}\int_{T_n}^{T}|f_{n+1}-f_m|^2dt-|l_{n+1}-l_m|\right|+\left(1-\frac{T-T_n}{T}\right)|l_{n+1}-l_m|. \tag{2.46}$$

Recall that $0<(T-T_n)/T<1$.

Thus, we can determine T_{n+1} by requiring that each of the three terms in Eq. (2.46) is smaller than $\epsilon_{n+1}/3$. Namely, $T_{n+1} > 3\kappa_{n,m}/\epsilon_{n+1}$, and $T_{n+1} > T'$ (from Eq. (2.42)), and $T_{n+1} > 3T_n|l_{n+1} - l_m|/\epsilon_{n+1}$; with this, we get that Eq. (2.43) is then smaller than ϵ_{n+1}, obtaining the induction step for Eq. (2.40). Besides, by letting $T = T_{n+1}$ in Eq. (2.42) we have that Eq. (2.39) holds for $n + 1$.

Now that we can find $T_0, T_1, \dots$, we can construct the function $\underset{\sim}{f}$. Thus, by taking the limit $n \to \infty$ at both sides of Eq. (2.40) we get

$$\mathcal{M}_t\{|\underset{\sim}{f} - f_m|^2\} = \lim_{T\to\infty} \frac{1}{T}\int_0^T |\underset{\sim}{f} - f_m|^2 dt = l - l_m = \sum_{i=m+1}^{\infty} |\tilde{f}(E_i)|^2, \tag{2.47}$$

which for sufficiently large m can be made arbitrarily small, yielding Eq. (2.34), or, equivalently

$$\lim_{m\to\infty} \mathcal{M}_t\{|\underset{\sim}{f} - f_m|^2\} = 0. \tag{2.48}$$

□

Remark 2.8. *From Corollary 2.7 it follows that the Fourier series of $\underset{\sim}{f}$ is the same as that of f, consequently $\underset{\sim}{f} \sim f$ [4].*

The Fourier transform with respect to the counting measure and the inverse isomorphism. If f and $\tilde{f}$ are related through (2.29), we can recognize that the Fourier series of f are nothing but the Fourier transform of $\tilde{f}$ (with respect to the counting measure, see Eq. (2.15)):

$$\sum_{E\in\sigma_f} e^{-iEt/\hbar}\mathcal{M}_{t'}\{e^{it'E/\hbar}f(t')\} = \sum_{E\in\sigma_f} e^{-itE/\hbar}\tilde{f}(E) = \int_{\mathbb{R}} e^{-itE/\hbar}\tilde{f}(E)dE = \hat{f}(t), \quad t\in\mathbb{R}. \tag{2.49}$$

Additionally, from the Riesz-Fischer theorem (see also Remark 2.5) it follows that the Fourier series $\hat{f}$ defines the inverse isomorphism of Eq. (2.29) from $l^2(\mathbb{R})$ onto B^2

$$\tilde{f} \mapsto \hat{f}(t) \sim f \sim \underset{\sim}{f}. \tag{2.50}$$

Recall that a B^2-class is uniquely defined by each Fourier series.

Remark 2.9. *Each Fourier series related to a B^2-function f is uniquely defined by an absolutely convergent series of square modulus of some sequence and a countable real subset. This can be seen, for example, from Eqs. (2.20) and (2.28). Recall that this statement is equivalent to the fact that by specifying such key ingredients the corresponding function $\tilde{f} = \mathcal{M}_t\{e^{itE/\hbar}f(t)\}$ is also determined in a unique way, see Remark 2.1.*

An orthonormal basis. It is now easy to see that Eq. (2.50) sends the orthonormal basis $\{\delta[E - E'] : E' \in \mathbb{R}\}$ of unit sample functions to the orthonormal basis of complex exponential functions $\{e^{-iE't/\hbar} : E' \in \mathbb{R}\}$. The orthonormal relation of this set reads

$$\begin{aligned}\mathcal{M}_t\{e^{iEt/\hbar}\, e^{-iE't/\hbar}\} &= \lim_{T\to\infty} \frac{1}{T}\int_0^T e^{i(E-E')t/\hbar} dt \\ &= \lim_{T\to\infty} e^{i(E-E')T/2\hbar}\, \text{sinc}\left[\frac{(E-E')T}{2\hbar}\right] \\ &= \delta[E - E'] \end{aligned} \tag{2.51}$$

The complex vector space spanned by $\{e^{-iE't/\hbar} : E' \in \mathbb{R}\}$ is called the *trigonometric polynomials* and is dense in B^2, that immediately follows from Eq. (2.34) by taking the Cauchy sequence as the nth-Fourier series of B^2-functions.

The space AP_1 and the Bohr's property. We can identify the set of all the Fourier transforms $\hat{h}(t)$ with $\tilde{h} \in l^1(\mathbb{R})$, Eq. (2.15), to be *the space of almost periodic functions with absolutely convergent Fourier series*, denoted by AP_1. This space is part of a more general class of functions, namely, *the space AP of almost periodic functions*, defined as follows.

A continuous function $f : \mathbb{R} \to \mathbb{C}$ is said to be *almost periodic* if for each $\epsilon > 0$ there is a $l = l(\epsilon) > 0$ such that we can find numbers (called *ϵ-translations* of f) $\tau \in [a, a + l]$, for any $a \in \mathbb{R}$, such that

$$|f(t + \tau) - f(t)| \leq \epsilon, \quad \forall t \in \mathbb{R}. \tag{2.52}$$

The space AP is complete with respect to the supremum norm [9], but not with the B^2-norm. Thus, there is no need to introduce equivalence classes in AP when working with the supremum norm. The *Bohr's property* (2.52) that defines the almost periodic functions can be extended to B^2-functions by replacing the module of complex numbers by the B^2-norm in Eq. (2.52) [9, Proposition 3.13].

For a continuous periodic function the period T' itself can be taken as the length l, working for each $\epsilon > 0$ in the Bohr property Eq. (2.52), and the entire multiples kT' ($k \in \mathbb{Z}$) of the period are thus the ϵ-translation numbers of the periodic function. In our opinion it is difficult to find such an ϵ-dependent length l for the general case.

2.4 Summary

In this section we summarize of some things about the spaces $l^2(\mathbb{R})$ and B^2.

We call to an arbitrary countable set of numbers

$$\sigma' = \{E'_1, E'_2, E'_3, \dots\}, \quad E'_n \in \mathbb{R},\, n = 1, 2, \dots \tag{2.53}$$

and an arbitrary absolutely convergent series of type

$$\sum_{n=1}^{\infty} |\psi'_n|^2 < \infty, \quad \psi'_n \in \mathbb{C},\, n = 1, 2, \ldots, \tag{2.54}$$

the *key ingredients*. There is no loss of generality in using the labeled set $n = 1, 2, \ldots$ because the important thing is that both are labeled by the same set. Starting with the key ingredients, we construct one element of each space $l^2(\mathbb{R})$ and B^2, identifying the roles of each ingredient:

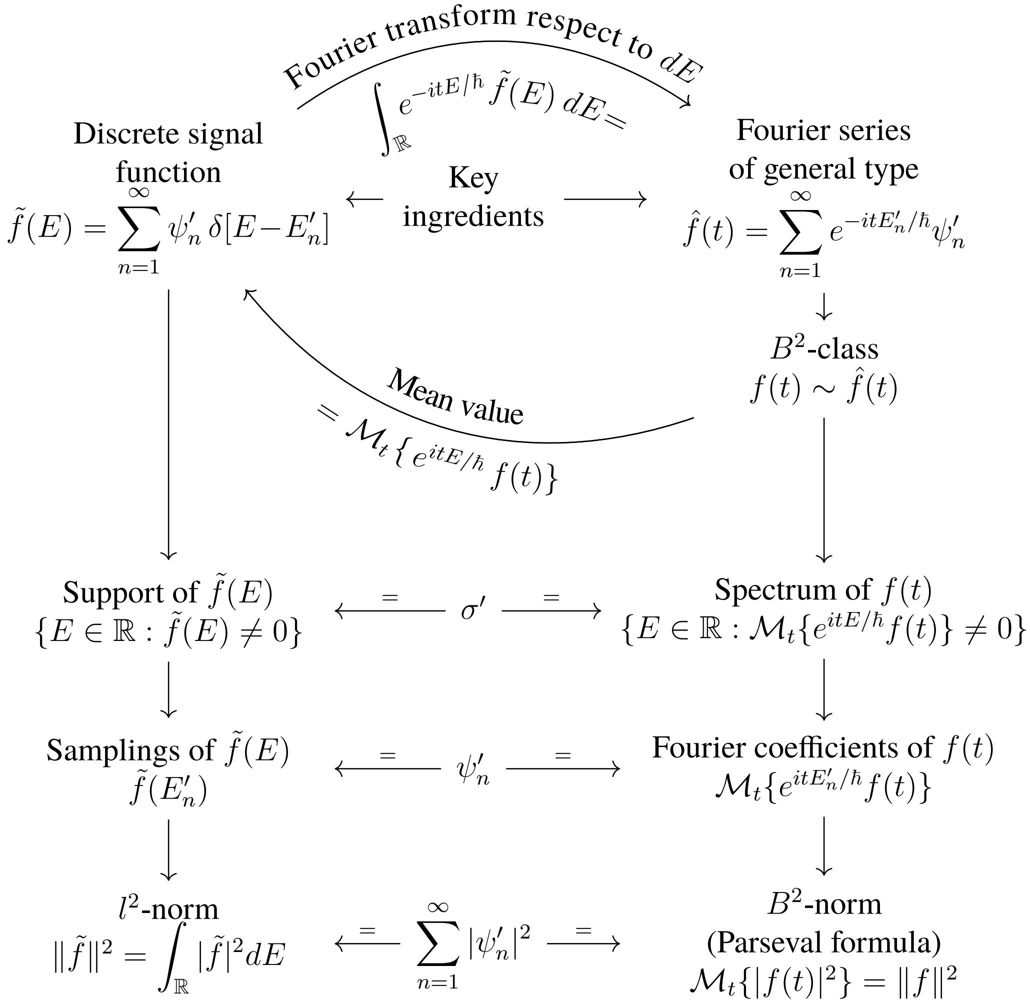
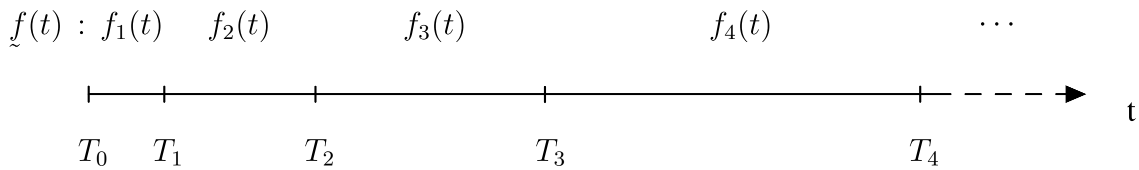


Table 2.1: Construction of objects using the key ingredients

In Table 2.1 $\mathcal{M}_t\{\bullet\}$ stands for the mean value defined as $\lim_{T\to\infty} T^{-1} \int_0^T \bullet dt$, and $f \sim \hat{f}$ denotes $\mathcal{M}_t\{|f(t) - \hat{f}(t)|^2\} = 0$. Recall that the elements of the Besicovitch space B^2 are the equivalence classes $f(t) \sim \hat{f}(t)$ and not the B^2-functions $f(t)$ ($\in L^2_{loc}(\mathbb{R})$). However, the custom is to treat as equal the B^2-functions of the same B^2-class.

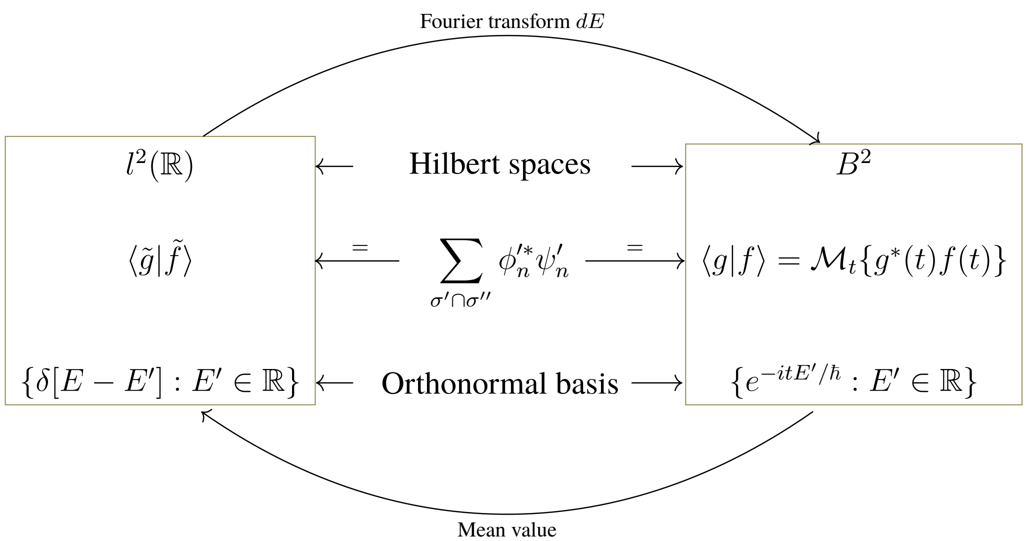
Besicovitch made the remarkable observation that for each Fourier series of general type there corresponds a B^2-function $\underset{\sim}{f}(t)$ constructed from the partial Fourier series f_n and some positive numbers $T_0 = 0 < T_1 < T_2 < \cdots \to \infty$:



As usual, the members of each equivalence class can be treated as if they were the same function. Thus, we can pick the Fourier series themselves if they converge absolutely or uniformly, for instance. Otherwise, we can chose the piece-wise function $\underset{\sim}{f}(t)$. The usual Fourier series of periodic functions $L^2(\mathbb{R}/T'\mathbb{Z})$, with period T', are a particular case of the Fourier series of B^2-functions.

Recall that the counting measure counts the elements of a set, thus the only sets that have finite counting measure are those having finite elements, for example $\int_{\mathbb{R}} \chi_{\{1,2\}}(E)dE = 2$. On the other hand, the Besicovitch measure assigns only to sets of infinite length a non zero measure, for example $\lim_{T\to\infty} T^{-1} \int_0^T \chi_{[0,\infty)}(t)dt = 1$. The function $\chi_\bullet$ is the characteristic function of the given set $\bullet$.

As shown in Table 2.1, the maps the mean value and the Fourier transform with respect to the counting measure yield the isomorphisms between $l^2(\mathbb{R})$ and B^2, thus both have the same the Hilbert space structure:



Above, we have used another set of key ingredients σ'' and $\sum_{n=1}^{\infty} |\phi_n'|^2 < \infty$ so as to define the discrete signal function $\tilde{g}$ and its companion $g(t)$. Note that, the more elemental functions in each space $l^2(\mathbb{R})$ and B^2 are the unit sample functions $\delta[E-E']$ and the complex exponential functions $e^{-itE/\hbar}$, respectively. The mean value sends the latter to the former

$$\mathcal{M}_t\{e^{itE'/\hbar}e^{-itE/\hbar}\} = \lim_{T\to\infty} \frac{1}{T} \int_0^T e^{it(E'-E)/\hbar}dt = \delta[E-E'] \qquad (2.55)$$

On the other hand, the reciprocity map is the Fourier transform with respect the counting measure, which for the unit sample functions $\delta_{E,E'} = \delta[E - E']$ it reads as follows

$$\widehat{\delta}_{E,E'}(t) = \int_{\mathbb{R}} e^{-itE/\hbar} \delta_{E,E'} dE = e^{-itE'/\hbar}. \tag{2.56}$$

Chapter 3

Time and energy representations

This chapter is devoted to the development of the mathematical framework in which the continuous set of generalized abstract kets

$$\left\{ |t\rangle = \sum_{n=1}^{\infty} e^{itE_n/\hbar} |E_n\rangle : t \in [0, \infty) \right\} \tag{3.1}$$

forms a basis in a Dirac sense. This set has already been considered by some authors [6, 20]. The presentation here of $|t\rangle$ as a time basis is an in-deep review of a part given by Martínez and Torres in Ref. [28]. In addition, we want to stress the convenience and usefulness of the Besicovitch framework as well as of the Lebesgue space $l^2(\mathbb{R})$ in order to introduce time and energy representations for quantum systems with discrete energy spectrum, in standard quantum mechanics.

3.1 Time representation

Let us define the *time representation* of the state $|\psi\rangle \in \mathcal{H}$ to be its projection on the continuous generalized kets $|t\rangle$

$$\langle t|\psi\rangle = \sum_{n=1}^{\infty} e^{-itE_n/\hbar} \langle E_n|\psi\rangle, \quad t \in [0, \infty). \tag{3.2}$$

Since we assume that the energy spectrum has no other restrictions than to be discrete, it might be questionable in what sense, if it existed, the series in Eq. (3.2) converges. If the energy spectrum were equidistant, it would be natural to make use of the L^2-convergence of the usual Fourier series. At this point, the Besicovitch framework becomes valuable because it can explain the aforementioned question and the nature of Eq. (3.2). Then, we only need to recognize Eq. (3.2) to be a Fourier series of general type, that defines a B^2-class $\langle t|\psi\rangle \sim \psi(t)$ in the B^2-space, with $\psi(t)$ being a B^2-function. This assertion follows from the Riesz-Fischer Theorem 2.4 (also see Remark 2.9) because $\langle t|\psi\rangle$ satisfies $\|\psi\|^2 = \sum_{n=1}^{\infty} |\langle E_n|\psi\rangle|^2 < \infty$ and the set of quantum energies $\{E_n\}_{n=1}^{\infty}$ in the exponential functions $e^{-itE_n/\hbar}$ is a countable set.

Note that $\langle t|\psi\rangle$ is a dimensionless quantity. Also, the mean value does not introduce additional units because units of time cancel each other in it:

$$\mathcal{M}\{\bullet\} = \lim_{T\to\infty}\frac{1}{T}\int_0^T \bullet\, dt. \tag{3.3}$$

This means that there is no need to add units to $\langle t|\psi\rangle$ either. Recall the Parseval formula $\mathcal{M}_t\{|\langle t|\psi\rangle|^2\} = \sum_{n=1}^{\infty}|\langle E_n|\psi\rangle|^2 = \|\psi\|^2$ is dimensionless.

Without restricting the generality of $|t\rangle$, the variable t has been restricted to $[0,\infty)$, see Remark 2.2.

Now, we proceed to expose another way of introducing a time representation of states, in addition of the Fourier series of general type $\langle t|\psi\rangle$.

3.1.1 An operational construction of the wave functions

In standard quantum mechanics, the way that the mean value $\langle\psi|\hat{H}|\psi\rangle$ can be approximated is through a large number of measurements of the observable $\hat{H}$ in the same (normalized state) $|\psi\rangle$. Thus, it is hoped that if N is the number of such repetitions and $\mathcal{N}(E_n;N)$ is the number of times that E_n was recorded, then $\mathcal{N}(E_n;N)/N \to |\langle E_n|\psi\rangle|^2$ as $N\to\infty$ [8]. This fact leads us to suppose that the functions

$$\alpha(E_n;N) := e^{i\theta_{N,n}}\sqrt{\frac{\mathcal{N}(E_n;N)}{N}}, \quad N = 1,2,\ldots \tag{3.4}$$

can be defined for some phases $e^{i\theta_{N,n}}$ such that

$$\alpha(E_n;N) \to \langle E_n|\psi\rangle \quad \text{as} \quad N\to\infty. \tag{3.5}$$

Recall that $\alpha(E_n;N)$ are dimensionless.

It results that we can construct a sequence of piece-wise B^2-functions as follows.

3.1.1.1 A piece-wise function

Since an extra measurement can only yield at most an energy distinct to all previous values, let us reorder the energies as they appear in a set of measurements, say $\{E_{n_j}\}_{j=1}^{\infty}$.

Let N be the number of measurements taken into account. If $N=1$, the first energy recorded is E_{n_1}, then, define $\psi_1(t) = e^{-itE_{n_1}/\hbar}$, $0\le t$. For $N>1$ we proceed recursively. Suppose that the jth measurement had an approximate time duration t_j and gave the outcome E_{n_j}; the energies of the system were different and recorded in the order

$$E_{n_1}, E_{n_2}, \ldots, E_{n_N}. \tag{3.6}$$

For the case without energy repetitions, that is, $|\alpha(E_{n_j}; N)|^2 = 1/N$. Then, define the piece-wise function as

$$
\psi_N(t) = \begin{cases}
\alpha(E_{n_1}; N)e^{-itE_{n_1}/\hbar} & 0 \le t < T_1 \\
\alpha(E_{n_1}; N)e^{-itE_{n_1}/\hbar} + \alpha(E_{n_2}; N)e^{-itE_{n_2}/\hbar} & T_1 \le t < T_2 \\
\quad\vdots & \quad\vdots \\
\sum_{i=1}^{j} \alpha(E_{n_i}; N)e^{-itE_{n_i}/\hbar} & T_{j-1} \le t < T_j \\
\quad\vdots & \quad\vdots \\
\sum_{i=1}^{N} \alpha(E_{n_i}; N)e^{-itE_{n_i}/\hbar} & T_{N-1} \le t
\end{cases}
\tag{3.7}
$$

where $T_j = \sum_{i=1}^{j} t_i$ ($T_0 = 0$). If the next measurement (the $(N+1)$th measurement) is supposed to record a previous energy; such that $|\alpha(E_{n_{i'}}; N+1)|^2 = 2/(N+1)$ holds only for one $E_{n_{i'}}$ ($1 \le i' \le N$), define

$$
\psi_{N+1}(t) = \begin{cases}
\alpha(E_{n_1}; N+1)e^{-itE_{n_1}/\hbar} & 0 \le t < T_1 \\
\quad\vdots & \quad\vdots \\
\sum_{i=1}^{j} \alpha(E_{n_i}; N+1)e^{-itE_{n_i}/\hbar} & T_{j-1} \le t < T_j \\
\quad\vdots & \quad\vdots \\
\sum_{i=1}^{N} \alpha(E_{n_i}; N+1)e^{-itE_{n_i}/\hbar} & T_{N-1} \le t < T_N \\
\sum_{i=1}^{N} \alpha(E_{n_i}; N+1)e^{-itE_{n_i}/\hbar} & T_N \le t.
\end{cases}
\tag{3.8}
$$

Otherwise, if the $(N+1)$th measurement would yield a different energy than the previous registered energies, such that $|\alpha(E_{n_i}; N+1)|^2 = 1/(N+1)$ for each E_{n_i}, then define $\psi_{N+1}(t)$ similar to (3.7), that is

$$\psi_{N+1}(t) = \begin{cases} \alpha(E_{n_1}; N+1)e^{-itE_{n_1}/\hbar} & 0 \le t < T_1 \\ \quad\vdots & \quad\vdots \\ \displaystyle\sum_{i=1}^{j} \alpha(E_{n_i}; N+1)e^{-itE_{n_i}/\hbar} & T_{j-1} \le t < T_j \\ \quad\vdots & \quad\vdots \\ \displaystyle\sum_{i=1}^{N} \alpha(E_{n_i}; N+1)e^{-itE_{n_i}/\hbar} & T_{N-1} \le t < T_N \\ \displaystyle\sum_{i=1}^{N+1} \alpha(E_{n_i}; N+1)e^{-itE_{n_i}/\hbar} & T_N \le t. \end{cases} \tag{3.9}$$

Repetitions of the measured values of the energy are handled in the way we constructed Eq. (3.8), so that we can now consider repetitions of the values measured. We keep building these functions in this way until the Mth-measurement, probably the last measurement $M \ge N$. The key point is that ψ_M is defined to be the trigonometric polynomial

$$\psi_M(t) = \sum_{i=1}^{M'(M)} \alpha(E_{n_i}; M)e^{-itE_{n_i}/\hbar}, \quad T_{M-1} \le t, \tag{3.10}$$

where $M' = M'(M)$ is the number of all the energies recorded in those M measurements ($M' \le M$). Recall that we might expect that $M'(M) \to \infty$ as $M \to \infty$ unless the state can be certainly expanded by a finite set of energy eigenstates. Also, this might be understood that for the sake of approximating each $|\langle E_n|\psi\rangle|^2$ by means of $\alpha(E_n; N)$ we should consider a large enough number of measurements $M \gg 1$ such that additional measurements will not significantly change the values of $\langle E_n|\psi\rangle$.

Since it would be more realistic to consider $M \gg 1$, assuming that $E_{n_1}, E_{n_2}, \ldots, E_{n_{M'}}$ are the related measurement results, the time representation of a system in the state $|\psi\rangle$ can then be approximated by the piece-wise function $\psi_M(t)$. During the time interval $[0, T_M)$ the function $\psi_M(t)$ accounts for the "history" of the measurements, and, after this period of time, $\psi_M(t)$ keeps evolving over time as a superposition of the waves $e^{-itE_{n_i}/\hbar}$, $i = 1, 2, \ldots, M'(M)$, but all at once. Some improvements can be made, if desired, to the piece-wise functions. For example, we can redefine them to be continuous at each T_j or even to be just the trigonometric polynomials Eq. (3.10) for all time. This latter would be the choice if the measurement history is either not necessary or not feasible. In any case, the choice of a trigonometric polynomial after a while or for all time, is the important fact for the Besicovitch setting, as shown next.

3.1.1.2 A Cauchy sequence

Since, at least theoretically, we can suppose that an infinity number of measurements of $\langle\psi|\hat{H}|\psi\rangle$ are achievable, and the corresponding time durations comply with $t_j \ge \tau$ for some $\tau > 0$ (the measurements might have a finite time duration). Then, roughly speaking, the sequence of the previous constructed piece-wise functions $\{\psi_n\}_{n=1}^{\infty}$ satisfies $\psi_n(t \geq T_{n-1}) \to \langle t|\psi\rangle$ as $n \to \infty$ ($t \to \infty$). In fact, they are B^2-functions because they are defined to be trigonometric polynomials after a time, and even more, as we show next, they form a Cauchy sequence. We start by showing the next claim.

Claim 3.1. *Each piece-wise function ψ_n, defined previously in Section 3.1.1.1, is a B^2-function.*

Proof. To show this, let us consider the probability density

$$|\psi_n(t)|^2 = \left|\sum_{i=1}^{n'(n)} \alpha(E_{n_i};n)e^{-itE_{n_i}/\hbar}\right|^2 = \sum_{i,j=1}^{n'(n)} \alpha(E_{n_i};n)\alpha^*(E_{n_j};n)e^{it(E_{n_j}-E_{n_i})/\hbar} \tag{3.11}$$

for $t > T_{n-1}$, see definition (3.10), and split the squared modulus of its norm as

$$\mathcal{M}_t\{|\psi(t)|^2\} = \lim_{T\to\infty}\frac{1}{T}\int_0^T |\psi_n|^2 dt = \lim_{T\to\infty}\frac{1}{T}\left(\int_0^{T_{n-1}} + \int_{T_{n-1}}^T\right)|\psi_n|^2 dt. \tag{3.12}$$

Noticing that ψ_n is bounded the first integral on the right hand side of Eq. (3.12) will vanish. For the last integral in Eq. (3.12), since ψ_n is a trigonometric polynomial for $t > T_{n-1}$ we get that

$$\begin{aligned}
\mathcal{M}_t\{|\psi(t)|^2\} &= \lim_{T\to\infty}\frac{T-T_{n-1}}{T} \times \lim_{T\to\infty}\frac{1}{T-T_{n-1}}\int_{T_{n-1}}^T |\psi_n|^2 dt \\
&= \sum_{i,j=1}^{n'(n)} \alpha(E_{n_i};n)\alpha^*(E_{n_j};n)\left[\lim_{T\to\infty}\frac{1}{T-T_{n-1}}\int_{T_{n-1}}^T e^{it(E_{n_j}-E_{n_i})/\hbar}dt\right] \\
&= \sum_{i,j=1}^{n'(n)} \alpha(E_{n_i};n)\alpha^*(E_{n_j};n)\delta[E_{n_i}-E_{n_j}] \\
&= \sum_{i=1}^{n'(n)} |\alpha(E_{n_i};n)|^2 < \infty,
\end{aligned} \tag{3.13}$$

where we have used the limit

$$\begin{aligned}
\lim_{T\to\infty}\frac{1}{T-T_{n-1}}\int_{T_{n-1}}^T e^{it(E_{n_j}-E_{n_i})/\hbar}dt &= \lim_{T\to\infty}\frac{e^{i(T+T_{n-1})(E_{n_j}-E_{n_i})/2\hbar}}{2T'}\int_{-T'}^{T'} e^{it(E_{n_j}-E_{n_i})/\hbar}dt \\
&= \lim_{T\to\infty} e^{i(T+T_{n-1})(E_{n_j}-E_{n_i})/2\hbar}\text{sinc}\left[\frac{T'(E_{n_j}-E_{n_i})}{\hbar}\right] \\
&= \delta[E_{n_i}-E_{n_j}],
\end{aligned} \tag{3.14}$$

where $T' = (T-T_{n-1})/2$. It is a Kronecker delta. □

Proposition 3.2. *The sequence of piece-wise functions $\{\psi_n\}$, defined in Section 3.1.1.1, is a Cauchy sequence with respect to the B^2-norm.*

Proof. Since Cauchy sequences are still Cauchy sequences under isomorphisms between Hilbert spaces, it suffices to show that the sequence $\{\tilde{\psi}_n(E) = \mathcal{M}_t\left\{e^{itE/\hbar}\psi_n(t)\right\}\}_{n=1}^{\infty}$ is a fundamental sequence in $l^2(\mathbb{R})$. For this purpose, we begin by calculating

$$\begin{aligned}\tilde{\psi}_n(E) &= \lim_{T\to\infty}\frac{1}{T}\left(\int_0^{T_{n-1}} + \int_{T_{n-1}}^{T}\right)\left[\sum_{i=1}^{n'(n)}\alpha(E_{n_i};n)e^{it(E-E_{n_i})/\hbar}\right]dt\\ &= \sum_{i=1}^{n'(n)}\alpha(E_{n_i};n)\left[\lim_{T\to\infty}\frac{1}{T-T_{n-1}}\int_{T_{n-1}}^{T} e^{it(E-E_{n_i})/\hbar}dt\right]\\ &= \sum_{i=1}^{n'(n)}\alpha(E_{n_i};n)\delta[E-E_{n_i}]. \end{aligned}\tag{3.15}$$

Then, let $m \geq n$, we have that

$$\|\tilde{\psi}_m - \tilde{\psi}_n\|^2 = \sum_{i=1}^{n'(n)}|\alpha(E_{n_i};m) - \alpha(E_{n_i};n)|^2 + \sum_{i=n'(n)+1}^{m'(m)}|\alpha(E_{n_i};m)|^2. \tag{3.16}$$

By virtue of Eq. (3.5) and $\sum_{n=1}^{\infty}|\langle E_n|\psi\rangle|^2 < \infty$, we can make Eq. (3.16) less than any $\epsilon > 0$ by taking n sufficiently large. This yields the desired conclusion. □

Claim 3.3. *The sequence $\tilde{\psi}_n$ converges to*

$$\tilde{\psi}(E) = \sum_{i=1}^{\infty}\langle E_{n_i}|\psi\rangle\delta[E-E_{n_i}] = \sum_{i=1}^{\infty}\langle E_i|\psi\rangle\delta[E-E_i]. \tag{3.17}$$

Proof. In order to show this assertion, as argued in the paragraph after Eq. (3.16), we get readily

$$\|\tilde{\psi} - \tilde{\psi}_n\|^2 = \sum_{i=1}^{n'(n)}|\langle E_{n_i}|\psi\rangle - \alpha(E_{n_i};n)|^2 + \sum_{i=n'(n)+1}^{\infty}|\langle E_{n_i}|\psi\rangle|^2 \to 0 \quad \text{as} \quad n\to\infty. \tag{3.18}$$

□

Now, an application of the inverse isomorphism (2.50) to $\tilde{\psi}$ immediately yields the next statement.

Proposition 3.4. *Let $\{\psi_n\}_{n=1}^{\infty}$ be the sequence built as in Section 3.1.1.1. Then*

$$\lim_{n\to\infty}\psi_n(t) \sim \langle t|\psi\rangle = \hat{\psi}(t) \tag{3.19}$$

where $\langle t|\psi\rangle$ is the Fourier series Eq.(3.2) related to each state $|\psi\rangle \in \mathcal{H}$, or equivalently, $\hat{\psi}(t)$ is the Fourier transform with respect to the counting measure of $\tilde{\psi}(E)$, defined in Eq.(3.17).

Remark 3.5. *From now on, we can follow the custom to consider as identical the B^2-functions belonging to the same B^2-class, analogous to how is done with the elements of $L^2(\mathbb{R}/\mathbb{Z})$ or $L^2(\mathbf{T})$ ($\mathbf{T}$ the torus). In those few instances where it might lead to confusion we will point out the difference, as in Eq. (3.19). Bearing this in mind, for an arbitrary state $|\psi\rangle \in \mathcal{H}$ we can think of its time representation as its related Fourier series $\langle t|\psi\rangle$, or equivalently, as the limit of the sequence of the piece-wise functions we just defined.*

3.1.2 Time basis

In order to show that the set $\{|t\rangle : t \in [0,\infty]\}$ constitutes a basis in the Dirac sense, we need to show its closure and orthonormalization relations. Immediately after, we discuss the space that this basis projects to.

3.1.2.1 The orthonormalization relation.

Let $\langle t|\psi\rangle$ be a trigonometric polynomial. Then we have the next chain of equalities

$$
\begin{aligned}
\langle t|\psi\rangle &= \sum_{n=1}^{N} e^{-itE_n/\hbar}\langle E_n|\psi\rangle = \sum_{n=1}^{N} e^{-itE_n/\hbar}\mathcal{M}_{t'}\{e^{it'E_n/\hbar}\langle t'|\psi\rangle\} \\
&= \sum_{n=1}^{N} e^{-itE_n/\hbar}\left[\lim_{T\to\infty}\frac{1}{T}\int_0^T e^{it'E_n/\hbar}\langle t'|\psi\rangle dt'\right] = \lim_{T\to\infty}\frac{1}{T}\int_0^T\left[\sum_{n=1}^{N} e^{i(t'-t)E_n/\hbar}\right]\langle t'|\psi\rangle dt' \\
&= \mathcal{M}_t\left\{\langle t|\hat{I}_N|t'\rangle\,\langle t'|\psi\rangle\right\},
\end{aligned}
\tag{3.20}
$$

where $\hat{I}_N$ is the projector $\sum_{n=1}^{N}|E_n\rangle\langle E_n|$, and where

$$
\langle t|\hat{I}_N|t'\rangle = \sum_{n=1}^{N} e^{i(t'-t)E_n/\hbar}. \tag{3.21}
$$

Now suppose that $\psi(t)$ is a B^2-function such that $\psi(t) \sim \langle t|\psi\rangle$ and let $\langle t|\psi_N\rangle$ denote its Nth-Fourier series. Since the trigonometric polynomials are dense in the B^2-space, for each $\epsilon > 0$ we can find a N such that $\mathcal{M}_t\{|\psi(t) - \langle t|\psi_n\rangle|^2\} < \epsilon$ provided $n \geq N$. This statement can be written in the form

$$
\lim_{T\to\infty}\frac{1}{T}\int_0^T\left|\psi(t) - \lim_{T'\to\infty}\frac{1}{T'}\int_0^{T'}\left[\sum_{n=1}^{N} e^{i(t'-t)E_n/\hbar}\right]\langle t'|\psi\rangle dt'\right|^2 dt < \epsilon. \tag{3.22}
$$

From Eq. (3.22) we can see that $\langle t|\hat{I}_N|t'\rangle$ converges to a Dirac-like distribution $\langle t|t'\rangle$ with respect to the B^2-norm as $N \to \infty$, analogous to how the test functions $\sum_{k=-N}^{N} e^{i2\pi k(t-t')}$ converge in the sense of a distribution to the periodization of the Dirac function with respect to the L^2-norm of $L^2(\mathbb{R}/\mathbb{Z})$. In fact, if the energy spectrum is equidistant, $\langle t|t'\rangle$ will coincide with such a periodization because the mean values in Eqs. (3.20) and (3.22) can be computed over a period.

3.1.2.2 The closure relation

By virtue of Plancherel's identity for the B^2-functions Eq. (2.31) the inner product between the states $|\phi\rangle$ and $|\psi\rangle$ has the representation

$$\langle\phi|\psi\rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T \langle\phi|t\rangle\,\langle t|\psi\rangle dt. \tag{3.23}$$

In particular, by choosing $|\phi\rangle = |\psi\rangle$ we will obtain the representation of the norm $\|\psi\|^2$.

If we use Dirac notation for Eq. (3.23), the closure relation of $|t\rangle$ reads

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |t\rangle\langle t|dt = \hat{I}. \tag{3.24}$$

This equality can also be deduced directly by substituting $|t\rangle$ by its definition (3.1) at the left-hand side

$$\begin{aligned}
\lim_{T\to\infty} \frac{1}{T}\int_0^T |t\rangle\,\langle t|dt &= \lim_{T\to\infty} \frac{1}{T}\int_0^T \left[\sum_{n,m=1}^{\infty} e^{i(E_n-E_m)t/\hbar}|E_n\rangle\,\langle E_m|\right] dt \\
&= \sum_{n,m=1}^{\infty} \left[\lim_{T\to\infty} \frac{1}{T}\int_0^T e^{i(E_n-E_m)t/\hbar}dt\right] |E_n\rangle\,\langle E_m| \\
&= \sum_{n,m=1}^{\infty} \lim_{T\to\infty} e^{i(E_n-E_m)T/2\hbar}\text{sinc}\left[\frac{(E_n-E_m)T}{2\hbar}\right] |E_n\rangle\,\langle E_m| \\
&= \sum_{n,m=1}^{\infty} \delta_{n,m}|E_n\rangle\,\langle E_m| \\
&= \hat{I}
\end{aligned} \tag{3.25}$$

where we have used the following limits.

For $E_n \neq E_m$

$$\lim_{T\to\infty} \left| e^{i(E_n-E_m)T/2\hbar}\text{sinc}\left[\frac{(E_n-E_m)T}{2\hbar}\right]\right| \leq \lim_{T\to\infty} \left|\frac{2\hbar}{|E_n-E_m|T}\right| \to 0 \tag{3.26}$$

and for $E_n = E_m$, since

$$e^{i(E_n-E_m)T/2\hbar}\text{sinc}\left[\frac{(E_n-E_m)T}{2\hbar}\right]\Bigg|_{E_n=E_m} = \text{sinc}(0) = 1 \tag{3.27}$$

we have that

$$\lim_{T\to\infty} e^{i(E_n-E_m)T/2\hbar}\text{sinc}\left[\frac{(E_n-E_m)T}{2\hbar}\right] = 1. \tag{3.28}$$

It is easy to see that the closure and the orthonormalization relations are in correspondence because $\lim_{N\to\infty}\langle t|\hat{I}_N|\psi\rangle = \langle t|\hat{I}|\psi\rangle$ agrees with Eq. (3.20).

3.2 Conjugate spaces: the energy representation

Using the mean value for the Besicovitch functions, the next quantity is well defined and can be taken as the *energy representation* of the state $|\psi\rangle$

$$\tilde{\psi}(E) = \mathcal{M}_t\{e^{iEt/\hbar}\psi(t)\} = \lim_{T\to\infty}\frac{1}{T}\int_0^T e^{iEt/\hbar}\langle t|\psi\rangle dt, \tag{3.29}$$

where $\psi(t) \sim \langle t|\psi\rangle$. As we will see later, this representation can be obtained in an analogous manner to the continuous energy spectrum case.

By the isomorphism Eq. (2.29), namely, $f \mapsto \mathcal{M}_t\{e^{iEt/\hbar}f(t)\} = \tilde{f}(E)$ from B^2 onto $l^2(\mathbb{R})$, the next assertions follow.

We define the *time representation of states* to be the closed subspace

$$B^2_\sigma = \{\psi \in B^2 : \sigma_\psi \subseteq \sigma\} \subset B^2. \tag{3.30}$$

Besides, the *energy representation* turns out to be

$$l^2(\sigma) = \{\tilde{\psi} \in l^2(\mathbb{R}) : \sigma_\psi \subseteq \sigma\} \subset l^2(\mathbb{R}). \tag{3.31}$$

Note that the *spectrum* of $\psi(t)$, or equivalently, the *support* of $\tilde{\psi}$, defined by the set

$$\sigma_\psi = \left\{E \in \mathbb{R} : \tilde{\psi}(E) = \mathcal{M}_t\{e^{iEt/\hbar}\,\psi(t)\} \neq 0\right\}, \tag{3.32}$$

is the set of energy levels that the state $|\psi\rangle$ has. The energy coefficients of $|\psi\rangle$ are given in these representations as

$$\langle E_n|\psi\rangle = \mathcal{M}_t\{e^{iE_nt/\hbar}\,\psi(t)\} = \tilde{\psi}(E_n). \tag{3.33}$$

Since σ is supposed to be labeled by the set of integers $n = 1, 2, \ldots$, the space Eq. (3.31) is just $l^2(\mathbb{N})$. If σ were labeled as $\{E_k : k \in \mathbb{Z}\}$, the space Eq. (3.31) would be $l^2(\mathbb{Z})$. As usual, we may also think the functions $\tilde{\psi}$ as being the sequences $\{\tilde{\psi}(E_n)\}_{n=1}^\infty$ such that $\sum|\tilde{\psi}(E_n)|^2 < \infty$, but, we think it is more appropriate, for our approach, to view the elements of $l^2(\sigma)$ as functions on a continuous variable having a countable support; discrete signals.

3.2.1 Canonical conjugate variables

It turns out that time and energy variables are a pair of conjugate variables through the mean value Eq. (3.29). The inverse transform of Eq. (3.29) to get the time representation of the state $|\psi\rangle$ from its energy representation is just the Fourier transform of $\tilde{\psi}(E)$ with respect to the counting measure

$$\langle t|\psi\rangle = \int_{\mathbb{R}} e^{-itE/\hbar}\tilde{\psi}(E)\,dE = \int_\sigma e^{-itE/\hbar}\tilde{\psi}(E)\,dE = \hat{\psi}(t), \tag{3.34}$$

where we have used the fact that $\tilde{\psi}$ has a support at most σ, which implies that

$$\int_{\mathbb{R}\setminus\sigma} e^{-itE/\hbar}\tilde{\psi}(E)\, dE = 0. \tag{3.35}$$

The transform (3.34) is nothing but (3.2) written using integral notation with dE standing for the counting measure.

Recall that, in contrast to the time representation, the energy representation of the wave function given by the mean value (3.29) is pointwise well-defined, because the zero distance norm $\|\tilde{\psi}-\tilde{\phi}\| = 0$ in $l^2(\mathbb{R})$ implies $\tilde{\psi}(E) = \tilde{\phi}(E)$ for all $E \in \mathbb{R}$.

3.2.2 The representations of the Hamiltonian

Before defining the energy and time representations of the Hamiltonian $\hat{H}$, let us recall the next definition that will help us to establish such operators.

Let $\hat{A}_1 : D_1 \to H_1$ and $\hat{A}_2 : D_2 \to H_2$ be two linear operators defined in two Hilbert spaces H_1 and H_2; $D_1 \subset H_1$ and $D_2 \subset H_2$. The operators $\hat{A}_1$ and $\hat{A}_2$ are said to be *unitarily equivalent* [1, p. 115] if there exists an isomorphism V between H_1 and H_2 such that $D_2 = V(D_1)$, and $\hat{A}_2\, g = V(\hat{A}_1\, h)$ whenever $g = V(h)$ for all $h \in D_1$. The self-adjointness, and the spectrum are unitary invariants for such operators [1, p. 292].

Noting that the map $|\psi\rangle \to \tilde{\psi}(E)$ is an isomorphism from $\mathcal{H}$ onto $l^2(\sigma)$, then the unitary equivalent operator to the Hamiltonian in the energy representation $l^2(\sigma)$ is the *multiplication operator*

$$\hat{E} : \tilde{D}(\hat{H}) \to l^2(\sigma)\,;\ \tilde{\varphi}(E) \mapsto E\,\tilde{\varphi}(E) \tag{3.36a}$$

defined with a maximal domain of definition

$$\tilde{D}(\hat{H}) = \left\{ \tilde{\varphi} \in l^2(\sigma) : \int_{\mathbb{R}} |E\,\tilde{\varphi}(E)|^2 dE < \infty \right\}. \tag{3.36b}$$

The action of this operator on $\tilde{\varphi} \in \tilde{D}(\hat{H})$ yields the function

$$E\tilde{\varphi}(E) = \sum_{n=1}^{\infty} E_n \tilde{\varphi}(E_n)\delta[E - E_n]. \tag{3.37}$$

Otherwise, the isomorphism $|\psi\rangle \to \psi(t) \sim \langle t|\psi\rangle$ gives another unitary equivalent operator to the Hamiltonian: its *time representation*

$$i\hbar\frac{\hat{d}}{dt} : D(\hat{H}) \to B^2_\sigma\,;\ \varphi(t) \mapsto i\hbar\frac{d\varphi}{dt} \tag{3.38a}$$

where

$$D(\hat{H}) = \left\{ \varphi \in B^2_\sigma : \varphi' = \frac{d\varphi}{dt} \in B^2_\sigma \right\}. \tag{3.38b}$$

The function obtained by the action of this operator is the weak derivative with respect to the Besicovitch measure. This derivative operator sends the function $\varphi \in D(\hat{H})$ to any Besicovitch function having the Fourier series

$$\langle t|\hat{H}|\varphi\rangle = \sum_{n=1}^{\infty} E_n \tilde{\varphi}(E_n) e^{-itE_n/\hbar}. \tag{3.39}$$

A similar situation happens for the momentum operator in its conjugate spaces, for which the derivative is defined almost everywhere with respect to the Lebesgue measure, see examples in Subsection 3.2.3.

Note that the conditions defining the domains Eqs. (3.36b) and (3.38b) are equivalent to $\|\hat{H}\varphi\|^2 = \sum_{n=1}^{\infty} |E_n \tilde{\varphi}(E_n)|^2 < \infty$.

3.2.2.1 Uniformly discreteness

Let us consider that the energy spectrum is uniformly discrete, which means that

$$\delta = \inf_{n \neq m} |E_n - E_m| > 0, \tag{3.40}$$

the number δ is called the *separation* of $\sigma = \{E_n\}_{n=1}^{\infty}$.

It follows readily from Eq. (3.40) that $|E_m - E_n| \geq |n - m|\delta$, and it can be shown that a non-negative separation (3.40) implies

$$\sum_{n=1}^{\infty}{}' \frac{1}{E_n^2} < \infty. \tag{3.41}$$

Here the prime indicates omission of the term $E_n = 0$ if it belongs to σ.

The uniformly discreteness Eq.(3.40) enables us to specify further the domain of the Hamiltonian in the time representation as

$$D(\hat{H}) = \left\{ \varphi \in B_\sigma^2 : \varphi \in AP_1, \frac{d\varphi}{dt} \in B_\sigma^2 \right\}. \tag{3.42}$$

To show this, it suffices to show that $\langle t|\varphi\rangle$ is absolutely convergent for each $|\varphi\rangle \in \mathcal{D}(\hat{H})$, see Section 2.3.1. This will justify that $D(\hat{H})$ is specified by the Fourier series themselves because $\langle t|\varphi\rangle = \varphi \in AP_1$. Note that by Eq. (3.41) and the CauchySchwarz inequality we have

$$|\langle t|\varphi\rangle| \leq \sum_{n=1}^{\infty} |\langle E_n|\varphi\rangle| = |\langle 0|\varphi\rangle| + \sum_{n=1}^{\infty}{}' \frac{|E_n \langle E_n|\varphi\rangle|}{|E_n|} \leq |\langle 0|\varphi\rangle| + \|\varphi\| \sqrt{\sum_{n=1}^{\infty}{}' \frac{1}{E_n^2}}. \tag{3.43}$$

The term $|\langle 0|\varphi\rangle|$ should be zero if $0 \notin \sigma$.

3.2.3 Two examples

To illustrate the time representation of the Hamiltonian, let us choose the following examples with equidistant spectra. Recall that an equidistant spectrum complies with the uniformly discrete property (3.40), and that the domain of definition in (3.42) indicates that we must choose the Fourier series as elements of $D(\hat{H})$ because they converge absolutely.

Let us consider that t is the coordinate variable q and E_n are the momentum eigenvalues $p_k = \hbar(\theta+2\pi k)/2a$ ($k \in \mathbb{Z}$ and $\theta \in [0, 2\pi)$) for a particle in the infinite square well potential of width $2a$. The momenta p_k and the related eigenfunctions $\chi_{[-a,a]}(q)(2a)^{-1/2}e^{ip_k q/\hbar}$ depend on the parameter θ and correspond to the momentum operator

$$-i\hbar\frac{\hat{d}}{dq} : D_\theta \to L^2([-a, a]) \quad ; \quad \varphi(q) \mapsto -i\hbar\frac{d\varphi(q)}{dq} \tag{3.44a}$$

where

$$D_\theta = \left\{ \varphi(q) \in L^2([-a, a]) : \varphi'(q) = \frac{d\varphi}{dq} \in L^2([-a, a]), \varphi(q) \in \text{AC}, \varphi(-a) = \varphi(a)e^{i\theta} \right\}. \tag{3.44b}$$

Here AC stands for the absolutely continuous functions on $[-a, a]$, defined as the complex functions $f : [-a, a] \to \mathbb{C}$ for which there exist $g \in L^1([-a, a])$ such that

$$f(q) - f(a) = \int_{-a}^{q} g(q)dq, \qquad \forall\ q \in [-a, a], \tag{3.45}$$

where the integral is the Lebesgue integral.

The operator (3.44) is a particular operator scheme of the time representation of the Hamiltonian operator (3.38). To show this, let us point out that the absolutely continuous functions in the domain D_θ agree with their Fourier series, see Theorems 8.5.4 and 2.3.4 in Ref. [12]. Then, instead of requiring $\varphi(q) \in \text{AC}$, it is possible to demand that

$$\varphi(q) = \chi_{[-a,a]}(q)\frac{1}{\sqrt{2a}}\sum_{k=-\infty}^{\infty} \varphi_k e^{ip_k q/\hbar}. \tag{3.46}$$

Except for the characteristic function $\chi_{[-a,a]}(q)$, this equivalent requirement is in agreement with the one in the domain (3.42), namely that the element belongs to AP_1.

Another example is the z-component of angular momentum. Similar arguments show that this operator agrees with the time representation of the Hamiltonian operator (3.38) because its eigenvalues are the entire numbers.

3.3 About the energy representation

The energy representation Eq. (3.33) of the energy coefficients leads us to suspect that we can define continuous kets

$$\{|E\rangle : E \in \mathbb{R}\}. \tag{3.47}$$

The energy values can also be continuous for some quantum systems. It is the aim of this section to show in what sense the continuous kets $|E\rangle$ form a basis. The method below is with the understanding that $|E\rangle = |E_n\rangle$ if $E = E_n$, for some n.

3.3.1 Energy basis

We will restrict ourselves to show the orthonormalization and closure relations of $|E\rangle$.

3.3.1.1 The orthonormalization relation

By expanding a function $\tilde{f} \in l^2(\mathbb{R})$ in the basis $\{\delta[E - E'] : E' \in \mathbb{R}\}$, and using the integral notation for the counting measure, we have

$$\tilde{f}(E) = \int_{\mathbb{R}} \delta[E - E']\tilde{f}(E')dE'. \tag{3.48}$$

This suggests that the way to view $|E\rangle$ is through the orthonormalization requirement, which amounts on the unit sample function, Eq. (2.10),

$$\langle E'|E\rangle = \langle E|E'\rangle = \delta[E - E']. \tag{3.49}$$

In fact, since the unit sample function belongs to the Hilbert space $l^2(\mathbb{R})$ we can write Eq. (3.48) as $\tilde{f}(E) = \langle \delta|\tilde{f}\rangle$, which means that the unit sample function is a kernel for $l^2(\mathbb{R})$.

Taking the ket notation to the setting of $l^2(\mathbb{R})$, Eq. (3.48) is left as

$$\langle E|f\rangle = \int_{\mathbb{R}} \langle E|E'\rangle\langle E'|f\rangle dE'. \tag{3.50}$$

The ket $|E\rangle$ might be thought of as the ket abstraction of the basis $\{\delta[E - E'] : E' \in \mathbb{R}\}$ such that $\langle E|\tilde{f}\rangle = \langle \delta|\tilde{f}\rangle = \tilde{f}(E)$ is now the projection of the abstract ket $|\tilde{f}\rangle$ on $|E\rangle$. The next definition follows.

The *non-separable abstract Hilbert space* generated by the continuous abstract kets $|E\rangle$ satisfying the orthonormalization relation Eq. (3.49) is defined to be

$$\left\{ |f\rangle = \sum_{\sigma'} \langle E'|f\rangle|E'\rangle : \sum_{E'\in\sigma'} |\langle E'|f\rangle|^2 < \infty, \sigma' \subset \mathbb{R} \text{ countable} \right\}. \tag{3.51}$$

We can say that this space is the ket abstraction of the non-separable Hilbert space $l^2(\mathbb{R})$.

3.3.1.2 The closure relation

By using the integral sign to write the inner product between $\tilde{g}, \tilde{f} \in l^2(\mathbb{R})$:

$$\langle \tilde{g}|\tilde{f}\rangle = \int_{\mathbb{R}} \langle g|E\rangle\langle E|f\rangle dE = \langle g|f\rangle \tag{3.52}$$

we get the closure relation of $|E\rangle$

$$\hat{I}' = \int_{\mathbb{R}} |E\rangle\langle E| dE. \tag{3.53}$$

In particular, this identity operator when restricted to the abstract Hilbert space $\mathcal{H}$, which turns out to be a closed subspace of Eq. (3.51), gives the well-known closure relation

$$\hat{I}'|_{\mathcal{H}} = \int_{\sigma} |E\rangle\langle E| dE = \sum_{n=1}^{\infty} |E_n\rangle\langle E_n| = \hat{I}. \tag{3.54}$$

The striking differences between the $|E\rangle$ and an usual continuous basis in the Dirac notation for a separable Hilbert space is, first, that the inner product representation associated to $|E\rangle$ is with respect to the counting measure instead of the Lebesgue measure (which is the right measure, e.g., for the coordinate representation). For this reason in place of having a Dirac delta function, we have the unit sample function Eq. (3.49). Second, the only physical kets among all $|E\rangle$ are $\{|E_n\rangle\}_{n=1}^{\infty}$, in the sense that any state $|\psi\rangle$ will be orthogonal to $|E\rangle$ for all but at most the energy eigenkets $\{|E_n\rangle\}_{n=1}^{\infty}$. This statement is described by the energy representation Eq. (3.29) of such a state, which can be now written as

$$\langle E|\psi\rangle = \tilde{\psi}(E). \tag{3.55}$$

Remark 3.6. *The introduction of the ket notation for the energy representation can be very useful to handle both the point and the continuous spectrum cases at once. This fact is justified on account that $l^2(\mathbb{R})$ and $L^2(\mathbb{R})$ are particular cases of the Lebesgue spaces $L^2(\sigma, d\mu, \mathfrak{M})$ where σ along with the σ-algebra $\mathfrak{M}$ (of some subsets of σ) is a measurable space. The triplet $(\sigma, d\mu, \mathfrak{M})$ is said to be a measure space. If σ is the real line, and $\mathfrak{M}$ is the power set of σ, and $d\mu$ is the counting measure dE, we get the non-separable Lebesgue space commonly denoted by $l^2(\mathbb{R})$. But, if $\mathfrak{M}$ is the σ-algebra of the Lebesgue measurable subsets of σ, along with $d\mu$ being the Lebesgue measure, the corresponding Lebesgue space is the separable one denoted, as usual, by $L^2(\mathbb{R})$. If σ is a closed subset as $[-A, A]$ $(A > 0)$ then we will have the Lebesgue space $L^2([-A, A])$.*

The continuous spectrum. For the sake of exposure, instead of being a point spectrum let σ be the real line; a continuous spectrum. We only need to replace the counting measure by the Lebesgue measure. We hope that no confusion arises from using here the same symbol dE of the counting measure for the Lebesgue measure. Thus, in this case the integral

$$\int_{\mathbb{R}} \bullet \, dE, \tag{3.56}$$

has units of energy and the energy presentation $\langle E|\psi\rangle$ needs to have units of one over square root of energy. The orthonormalization relation of the basis ket $|E\rangle$ turns to be the dirac function $\langle E|E'\rangle =$

$\delta(E' - E)$, and the energy representation is now the Lebesgue space $L^2(\mathbb{R})$ (a separable Hilbert space). The time representation $\langle t|\psi\rangle$ of the state $|\psi\rangle$ becomes the Plancherel's transform

$$\langle t|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} e^{-itE/\hbar} \langle E|\psi\rangle \, dE, \tag{3.57}$$

such that the time space is $L^2(\mathbb{R})$. The factor $1/\sqrt{2\pi\hbar}$ stands for the time representation to have units of one over square root of time. The energy and time representation are analogous to the coordinate and momentum representations of the space of states for the free particle. Compare Eq.(3.57) with Eq.(3.34). Instead of the mean value $\mathcal{M}$, we use the inverse Plancherel's transform to get the energy representation from the time representation

$$\langle E|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} e^{itE/\hbar} \langle t|\psi\rangle \, dt. \tag{3.58}$$

Contrast this with the mean value Eq. (3.29).

Guided by this analogy, thinking that the Lebesgue measure appears in the energy and time representations Eqs. (3.36) and (3.38) instead of the counting measure (these operators were defined for a Hamiltonian having pure point spectrum) we have the following. The energy representation (3.36) is similar to the coordinate representation of the position operator (for the free particle), and, on the other hand, the time representation (3.38) is then the unitary equivalent operator of the former. As regarding the time operator canonically conjugate to a Hamiltonian having as spectrum the real line, it will take the role played by the momentum operator of the free particle in the coordinate representation.

The relation of the energy representation with the discrete signal theory. The energy representation $l^2(\sigma)$ we introduced is not new, it is used implicitly in standard quantum mechanics textbooks, for example, in the way that the inner product and norm are computed for the abstract space, see Eqs. (2.4). However, the insight provided by the $l^2(\mathbb{R})$ space is the context of the discrete signal theory. To illustrate this briefly, let $|\psi\rangle$ be the initial state of a system, and consider that the entire spectrum of the Hamiltonian $\hat{H}$ is discrete $\sigma = \{E_n\}_{n=1}^{\infty}$, and let $|E_n\rangle$ be the related eigenkets. Then, in signal theory, the energy representation of the Hamiltonian is seen as a *discrete time system* [37], that takes the input $\langle E|\psi\rangle$ into the output (also called *response*) $\langle E|\hat{H}|\psi\rangle$; both being discrete signals. Recall that "time" in "discrete time system" does not stand for the time variable t we work with but, the energy variable E instead, and the term "discrete" stands for the countable support σ of the energy representation $\langle E|\psi\rangle$. The discrete time systems are considered as "black boxes", as illustrated in Figure 3.1, because their input and output are the only things that, for sure, are feasible. In quantum mechanics, it is supposed that a system can be prepared in a (normalized) quantum state $|\psi\rangle$, and, for example, after a hypothetical infinite number of measurements of the observable, related to $\hat{H}$, the mean value $\langle\psi|\hat{H}|\psi\rangle$ can also be obtained; thereby, we can hope that $\langle E_n|\psi\rangle$ and $\langle E_n|\hat{H}|\psi\rangle$ are known.

The *superposition principle* for states (in quantum mechanics) is realized by a particular class of discrete-systems (in the discrete signal theory) called *linear invariant*; if the input is a linear superposition of discrete signals, the output is the same weighted linear combination but of the responses

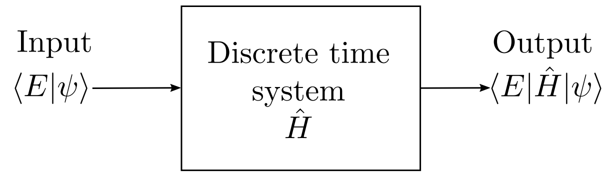


Figure 3.1: Representation of a generic discrete system.

of the signals forming the superposition input. Furthermore, the property that "$\langle E_{n+m}|\psi\rangle$ is sent to $\langle E_{n+m}|\hat{H}|\psi\rangle$ whenever $\langle E_n|\psi\rangle$ is sent to $\langle E_n|\hat{H}|\psi\rangle$" is called *time invariance* or *shift invariance*, and the discrete systems that satisfy such a condition are named *time or shift invariant* (again, recall that the "time" adjective in these terms is played by the energy variable in our approach). The linear and time invariant systems (LTI systems) are then the discrete signal description for operators of observables.

In addition, the quantum measurement process can be thought of as a filtering action. A filter is another view of discrete time systems, in particular, we focus on the so called *finite impulse response (FIR) filters* [11] because their outputs have only a finite number of responses. Thus, if the measurement E_m of the observable described by $\hat{H}$ is such that the state immediately after is $|E_m\rangle$, then, all this process becomes a FIR filter whose output is always a unit sample function, as depicted in Figure 3.2.

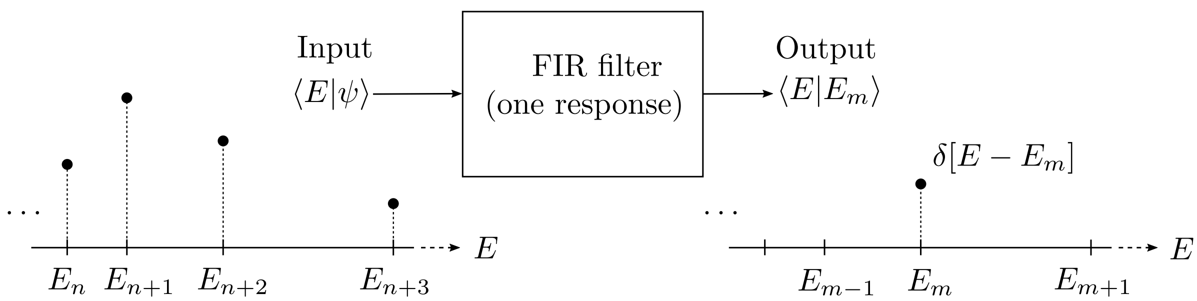


Figure 3.2: Discrete signal picture of a measurement process.

All this is suggestive on the energy representation meaning, which is left for future development.

3.4 Conclusions

The time and the energy representations we have introduced, as well as the corresponding representations of the Hamiltonian, can be used on any system that have an energy point spectrum without further constraints. The time representation of the Hamiltonian turned out to be a derivative, similar to that of the representation of the momentum operator in the momentum space for either the free particle or the particle in the infinite well potential.

Let us recall that the Hilbert space $L^2(\sigma, \mathcal{M}, d\mu)$ is the space to be considered when analyzing a quantum system. For example, it yields the coordinate and momentum representations for some usual quantum systems as are the harmonic oscillator, the free particle, the infinite square-well potential, and square potentials. All of the respective representations share the Hilbert space structure of a separable space, and it may happen that this fact tempts us to think that a time representation or the energy representation need the use of the Lebesgue measure when the energy spectra is discrete. However, as we have shown in this thesis, a closed subspace of the non-separable Besicovitch space has all the properties that a representation of the abstract Hilbert space needs. The particular case of an equidistant spectrum is not refuted by the Besicovitch framework, but on the contrary. Indeed, historically the main scope of the theory of Harald Bohr, and then of Besicovitch, was to give a generalization of the periodic functions such that the Fourier analysis was preserved [4]. All of this suggests that the Besicovitch framework allows to have Hilbert spaces, in addition to the usual Lebesgue spaces, the mathematical scheme that wave quantum mechanics theory is based on, to study the role played by the time variable in the standard quantum mechanics.

As we have shown, the introduction of the Besicovitch setting enables us to have a time representation of states with discrete energy spectra. This approach had already been studied by Hall [20, 21]. Also, He pointed out that an observable might be described by bounded operators in the Besicovitch time representation. Nevertheless, regardless if the Hamiltonian is bounded or not, we have shown that the closed Besicovitch space B^2_σ allows us to have a time representation of the Hamiltonian. In addition, we have shown that the mean value for Besicovitch functions defines a unitary map, which leads us to define an energy representation, conjugated to the time representation. This energy representation has to do with some discrete signal insights, a framework for further study.

With regard the time eigenket $|t\rangle$, let us recall that Cannata in References [6, 7] showed that for the equidistant spectrum the continuous eigenkets $|t\rangle$ forms a basis. We have extended this statement to the general energy point spectrum by showing that $|t\rangle$ is a basis in a Dirac sense. In the next chapter we provide momentum operators of discrete type, for which $|t\rangle$ is, indeed, their generalized eigenket.

We will apply the ideas developed in this thesis to other theories in physics to provide with a time axis for them.

Chapter 4

Discrete time operator

The finite-difference method has been devoted mainly to approximate the derivative of a function when the independent variable takes discrete values. The main requirement for this approximation is that the exact derivative can be recovered by taking some limits. The most common partition of the independent variable, in treatises of finite-difference calculus is the equidistant one [22, 38].

The finite difference scheme we use in this chapter was defined by Ronald E. Mickens [30]. This scheme is such that the difference equation and the associated differential equation have the same solution. Independently, we have defined such a scheme [25] only for the particular case of the first order differential equation

$$\frac{df(q)}{dq} = i\, f(q). \tag{4.1}$$

The main reason for this approach is to have a discrete derivative with respect to a non-equidistant mesh. A consequence of this approach is the finding of discrete operators that comply with the properties of the derivative of continuous functions, but defined on a non-equidistant set of points. These operators were introduced by hand in References [25, 27], but in this chapter we give a sound mathematical foundation for their existence. In particular, we use the exact finite difference scheme for the complex exponential function to define a discrete derivative with respect to an arbitrary energy point spectrum. The results in this chapter can be found in References [25, 26, 27, 28].

4.1 Mathematical background

Theorem 4.1. *Let $f : [a,b] \to \mathbb{C}$ be a derivable function at $q_0 \in [a,b]$, such that $0 < |f'(q_0)| < \infty$ ($f' = df/dq$), and let $g : [a,b] \to \mathbb{C}$ be another derivable function at q_0. Define the function*

$$\chi_f(q, q_0) = \frac{f(q) - f(q_0)}{f'(q_0)}, \quad q_0,\, q \in [a,b]. \tag{4.2}$$

Then

$$\lim_{q \to q_0} \frac{g(q) - g(q_0)}{\chi_f(q, q_0)} = g'(q_0). \tag{4.3}$$

This theorem shows that the difference $q - q_0$ in the denominator can be replaced by the more general function $\chi_f(q, q_0)$ to compute the derivative at q_0. This function is called a *denominator function* [31]. Below we will see the advantage of doing this. For the function f, we obtain the exact derivative f'.

Proof. The only difficulty with the limit in Eq. (4.3) is that the function χ_f might take the value zero at infinite points q as $q \to q_0$. Therefore, it is only necessary to show that we will not encounter this situation. For this purpose, define the function

$$\xi(q, q_0) = \begin{cases} \dfrac{1}{f'(q_0)} \left[\dfrac{f(q) - f(q_0)}{q - q_0} \right], & q \neq q_0 \\ \\ 1, & q = q_0. \end{cases} \tag{4.4}$$

Since f is derivable at q_0, it follows that ξ is continuous on $[a, b]$. In particular, since $\xi(q_0, q_0) \neq 0$ we can find a neighborhood U of q_0 where it happens that $\xi(q, q_0)$ is bounded and non zero, and henceforth $\xi(q, q_0)^{-1}$ is too. If q is a boundary point, the vicinity must be right or left open. So, in the punctured neighborhood $U \setminus \{q_0\}$, we have the well-defined quotient

$$\frac{g(q) - g(q_0)}{\chi_f(q, q_0)} = \frac{g(q) - g(q_0)}{q - q_0} \frac{1}{\xi_f(q, q_0)}. \tag{4.5}$$

Finally, since $g'(q_0)$ exists, along with the limit $\xi(q, q_0) \to 1$ as $q \to q_0$, this quotient takes the value $g'(q_0)$ when the limit $q \to q_0$ is taken, obtaining the desired result. $\square$

Corollary 4.2. *Let f, g be as in the preceding theorem. Let $\Delta_f, \Delta_b \geq 0$ such that*

$$q_0 + \Delta_f,\ q_0 - \Delta_b \in [a, b] \tag{4.6}$$

and define

$$\chi_f(\Delta_f, \Delta_b; q_0) = \frac{f(q_0 + \Delta_f) - f(q_0 - \Delta_b)}{f'(q_0)}. \tag{4.7}$$

Then

$$\lim_{\Delta_f, \Delta_b \to 0} \frac{g(q_0 + \Delta_f) - g(q_0 - \Delta_b)}{\chi_f(\Delta_f, \Delta_b; q_0)} = g'(q_0). \tag{4.8a}$$

When $g = f$, even for non zero Δ_b and Δ_f, we always have

$$\frac{f(q_0 + \Delta_f) - f(q_0 - \Delta_b)}{\chi_f(\Delta_f, \Delta_b; q_0)} = f'(q_0) \tag{4.8b}$$

Remarks. When $\Delta_b = 0$ ($\Delta_f = 0$) the quotients in Eqs.(4.8) are identified with the forward (backward) finite-difference derivative.

Proof. The equality in equation (4.8b) follows directly from the definition (4.7). For the limit (4.8a) we make the observation that

$$\lim_{\Delta_f, \Delta_b \to 0} \frac{\chi_f(\Delta_f, \Delta_b; q_0)}{\Delta_f + \Delta_b} = 1 \tag{4.9}$$

and then, the proof is similar to that as in the previous theorem. □

It is easy to check that if the function f satisfies the condition $0 < |f'(q_0)| < \infty$ for each $q_0 \in [a, b]$ and g is derivable at each $q_0 \in [a, b]$, then, the way to compute the derivative of g on $[a, b]$ established in the previous theorem and its corollary holds true. Moreover, with suitable increments Δ_f and Δ_b, the quotient in Eq. (4.8a) gives us a kind of two or three points finite-differences for the derivative g' on $[a, b]$. Equation (4.8b) is called an *exact finite difference scheme* for the first derivative.

4.2 Discrete conjugate momenta of the Hamiltonian

We proceed to apply the obtained results to the complex exponential function. Two reasons for the interest in this function are that it is the eigenfunction of the derivative operator and it is related to the time evolution in classical and quantum mechanics. Afterwards, we define discrete versions of a conjugate momentum of the Hamiltonian.

4.2.1 The exact finite differences for the complex exponential function

Let us consider the quantum energies $\sigma = \{E_j\}_{j=1}^{\infty}$ and define the increments

$$\Delta_j = E_{j+1} - E_j, \qquad j = 1, 2, \ldots. \tag{4.10}$$

Recall that we are supposing that the energies are ordered in increasing value

$$E_1 < E_2 < E_3 < \ldots. \tag{4.11}$$

The complex exponential function we will work with is

$$f(E; t) = e^{iEt/\hbar}, \qquad E \in [E_1, \infty), \qquad t \in \mathbb{R}. \tag{4.12}$$

This function is derivable in both continuous variables t and E. Further on, the variable E will be restricted to take only the values of the energy spectrum.

By noting that $f(E; t)$ complies with $0 < |\partial f/\partial E| = |t|/\hbar < \infty$ for each fixed nonzero t and all E, and using the increments Δ_j, it follows that we can define the forward version of the function χ_f, Eq. (4.7), at each quantum energy E_j by

$$\chi_j(t) := \chi_f(\Delta_j, 0; E_j) = -i\hbar \frac{e^{it(E_j+\Delta_j)/\hbar} - e^{itE_j/\hbar}}{te^{itE_j/\hbar}} = \Delta_j e^{i\Delta_j t/2\hbar} \text{sinc}\left[\frac{t\Delta_j}{2\hbar}\right], \qquad j = 1, 2 \ldots \tag{4.13a}$$

The backward version is

$$\eta_j(t) \coloneqq \chi_f(0, \Delta_{j-1}; E_j) = -i\hbar \frac{e^{itE_j/\hbar} - e^{it(E_j - \Delta_{j-1})/\hbar}}{te^{itE_j/\hbar}}$$
$$= \Delta_{j-1} e^{-i\Delta_{j-1}t/2\hbar} \operatorname{sinc}\left[\frac{t\Delta_{j-1}}{2\hbar}\right], \qquad j = 2, 3 \dots \tag{4.13b}$$

where sinc(z) is the entire function $\sin(z)/z$ which takes the value sinc(0) $= 1$. This allows us to define $\chi_j(0) = \Delta_j$ and $\eta_j(0) = \Delta_{j-1}$ such that χ_j and η_j are well defined for all $t \in \mathbb{R}$. The forward denominator function is related to the backward one by

$$\chi_j(t) = \eta^*_{j+1}(t). \tag{4.14}$$

Thus, both have the same set of zeros

$$t_{k,j} = \frac{2\pi k\hbar}{\Delta_j}, \quad k = \pm 1, \pm 2, \dots \tag{4.15}$$

The zeroes Eq. (4.15) should be excluded in order to avoid any indeterminacy when the functions $1/\chi_j$ and $1/\eta_j$ appear. These zeroes will be explored in Section 4.3.

4.2.2 Discrete momentum operators

At this point, we can define the *discrete forward momentum operator*

$$\hat{D}_f(t) \coloneqq -i\hbar \sum_{j=1}^{\infty} \frac{|E_j\rangle\langle E_{j+1}| - |E_j\rangle\langle E_j|}{\chi_j(t)} \tag{4.16a}$$

and its companion, the *discrete backward momentum operator*

$$\hat{D}_b(t) \coloneqq -i\hbar \sum_{j=2}^{\infty} \frac{|E_j\rangle\langle E_j| - |E_j\rangle\langle E_{j-1}|}{\eta_j(t)}. \tag{4.16b}$$

At each energy E_j these operators yield the forward and backward finite difference scheme versions of Eq. (4.8a)

$$\langle E_j|\hat{D}_f|\psi\rangle = -i\hbar \frac{\psi_{j+1} - \psi_j}{\chi_j(t)}, \qquad \text{and} \qquad \langle E_j|\hat{D}_b|\psi\rangle = -i\hbar \frac{\psi_j - \psi_{j-1}}{\eta_j(t)}, \tag{4.17}$$

respectively, where $|\psi\rangle = \sum_{j=1}^{\infty} \psi_j |E_j\rangle$ ($\sum_{j=1}^{\infty} |\psi_j|^2 < \infty$). We can identify Eqs. (4.17) as the samplings of the corresponding energy representations $\langle E|\hat{D}_{f,b}|\psi\rangle$ (see Section 3.2). These schemes are equivalent on account of

$$|\langle E_j|\hat{D}_f|\psi\rangle| = |\langle E_{j+1}|\hat{D}_b|\psi\rangle|, \qquad j = 1, 2, \dots. \tag{4.18}$$

It is in this sense that $\hat{D}_f(t)$ and $\hat{D}_b(t)$ are equivalent.

The valuable property of the operator (4.16a) is the eigenvalue equation

$$\hat{D}_f|t\rangle = t|t\rangle, \qquad \forall\ t \in \mathbb{R}, \tag{4.19}$$

where the time basis appears

$$|t\rangle = \sum_{j=1}^{\infty} e^{iE_j t/\hbar}|E_j\rangle.$$

Equation (4.19) is verified by using the definition Eq. (4.13a) of the denominator function $\chi_j(t)$, yielding that each jth entry of Eq. (4.19) reads

$$\langle E_j|\hat{D}_f|t\rangle = -i\hbar\frac{e^{itE_{j+1}/\hbar} - e^{itE_j/\hbar}}{\chi_j(t)} = -i\hbar\frac{e^{it(E_j+\Delta_j)/\hbar} - e^{itE_j/\hbar}}{\chi_j(t)} = te^{itE_j/\hbar} = t\langle E_j|t\rangle. \tag{4.20}$$

In turn this shows that Eq. (4.19) is equivalent to the exact forward finite-difference schemes of Eq. (4.8b) in the particular case of the complex exponential function.

The backward operator satisfies a similar eigenvalue equation $\hat{D}_b|t\rangle = t|t\rangle$, except for the first entry because the backward finite difference scheme needs of the increments Δ_{j-1} but these increments are not defined at $j = 1$.

Note that the zeros of the denominator functions χ_j really do not introduce any indeterminacy in Eq. (4.19), since by means of a limiting procedure as t goes to some of these zeros the eigenvalue equation (4.19) remains true.

As to the domain of definitions of these discrete operators we have to avoid the zeroes of the denominator functions $\chi_j(t)$ and $\eta_j(t)$. Since the energy spectrum is not necessarily equidistant, another possibility which may happen is that the arguments $t\Delta_j/2\hbar$ of the sinc functions in the function denominators (4.13) get closer to $n\pi$ (the inverses $1/\chi_j$ and $1/\eta_j$ could tend to infinity) for some $n = \pm1, \pm2, \ldots$ as $j \to \infty$ because the set $\{t\Delta_j\}_{j=1}^{\infty}$ may be dense on the positive half of the real line. To avoid such an issue, we also define the operators $\hat{D}_{f,b}$ on the span of the energy eigenkets, that is, the linear space of finite linear complex combinations of the energy eigenkets $|E_j\rangle$. Recall that such a span is dense in the abstract Hilbert space we work with, so that $\hat{D}_{f,b}$ are said to be densely defined.

The discrete forward derivative operator $\hat{D}_f$ also satisfies a discrete type of a canonical commutation version [25], namely

$$\begin{aligned}[\hat{D}_f(t), \hat{H}] &= -i\hbar\sum_{j=1}^{\infty}\frac{E_{j+1}|E_j\rangle\langle E_{j+1}| - E_j|E_j\rangle\langle E_j|}{\chi_j(t)} + i\hbar\sum_{j=1}^{\infty}\frac{E_j|E_j\rangle\langle E_{j+1}| - E_j|E_j\rangle\langle E_j|}{\chi_j(t)} \\ &= -i\hbar\sum_{j=1}^{\infty}\frac{\Delta_j}{\chi_j(t)}\,|E_j\rangle\langle E_{j+1}|.\end{aligned} \tag{4.21}$$

The quotient $\Delta_j/\chi_j(t)$ tends to one either at $t = 0$ or as $\Delta_j \to 0$.

Recall that the time derivative of the time ket is just the (backward solution) Schrödinger equation

$$\hat{H}|t\rangle = -i\frac{d}{dt}|t\rangle, \tag{4.22}$$

for which Eq. (4.19) can be thought of as its discrete conjugate version.

The discrete forward derivative operator defined for a degenerate energy spectrum can be defined by

$$\hat{D}_f(t) := -i\hbar \sum_{j=1}^{\infty} \sum_{\alpha=1}^{\min\{g_{j+1},g_j\}} \frac{|E_j,\alpha\rangle\langle E_{j+1},\alpha| - |E_j,\alpha\rangle\langle E_j,\alpha|}{\chi_j(t)}, \tag{4.23}$$

where $\alpha = 1, 2, , \ldots, g_j$ is the degeneracy index.

4.2.3 The symmetric property

It is better to consider finite dimensional spaces, i.e. states of the form $\sum_{j=1}^{N} \psi_j |E_j\rangle$. Further on, we will consider that operators are redefined to be restricted to a finite set of N energies, for example

$$\hat{D}_f = \hat{I}_N \hat{D}_f \hat{I}_N = -i\hbar \sum_{j=1}^{N-1} \frac{|E_j\rangle\langle E_{j+1}| - |E_j\rangle\langle E_j|}{\chi_j(t)}, \tag{4.24}$$

where $\hat{I}_N = \sum_{j=1}^{N} |E_j\rangle\langle E_j|$. Similarly, $\hat{D}_b$.

4.2.3.1 The adjoint of the discrete momentum operator

The adjoint of $\hat{D}_f$ can be written as:

$$\begin{aligned}
\hat{D}_f^\dagger &= i\hbar \sum_{j=1}^{N-1} \frac{|E_{j+1}\rangle\langle E_j| - |E_j\rangle\langle E_j|}{\chi_j^*(t)} \\
&= i\hbar \sum_{j=1}^{N-1} \frac{|E_{j+1}\rangle\langle E_j| - |E_j\rangle\langle E_j|}{\eta_{j+1}(t)} \\
&= i\hbar \sum_{j=2}^{N} \frac{|E_j\rangle\langle E_{j-1}| - |E_{j-1}\rangle\langle E_{j-1}|}{\eta_j(t)} \\
&= -i\hbar \sum_{j=2}^{N} \frac{|E_j\rangle\langle E_j| - |E_j\rangle\langle E_{j-1}|}{\eta_j(t)} + i\hbar \sum_{j=2}^{N} \frac{|E_j\rangle\langle E_j| - |E_{j-1}\rangle\langle E_{j-1}|}{\eta_j(t)} \\
&= \hat{D}_b + \hat{\mathcal{I}},
\end{aligned} \tag{4.25}$$

where

$$\hat{\mathcal{I}} = i\hbar \sum_{j=2}^{N} \frac{|E_j\rangle\langle E_j| - |E_{j-1}\rangle\langle E_{j-1}|}{\eta_j(t)} = \left[i\hbar \sum_{j=1}^{N-1} \frac{|E_{j+1}\rangle\langle E_{j+1}| - |E_j\rangle\langle E_j|}{\chi_j(t)} \right]^\dagger . \tag{4.26}$$

Further, we can split this diagonal operator into

$$\begin{aligned}
\hat{\mathcal{I}} &= i\hbar \sum_{j=2}^{N} \frac{|E_j\rangle\langle E_j|}{\eta_j(t)} - i\hbar \sum_{j=2}^{N} \frac{|E_{j-1}\rangle\langle E_{j-1}|}{\eta_j(t)} \\
&= i\hbar \sum_{j=2}^{N} \frac{|E_j\rangle\langle E_j|}{\eta_j(t)} - i\hbar \sum_{j=1}^{N-1} \frac{|E_j\rangle\langle E_j|}{\eta_{j+1}(t)} \\
&= i\hbar \sum_{j=2}^{N-1} \frac{|E_j\rangle\langle E_j|}{\eta_j(t)} + i\hbar \frac{|E_N\rangle\langle E_N|}{\eta_N(t)} - i\hbar \sum_{j=2}^{N-1} \frac{|E_j\rangle\langle E_j|}{\eta_{j+1}(t)} - i\hbar \frac{|E_1\rangle\langle E_1|}{\eta_2(t)} \\
&= i\hbar \sum_{j=2}^{N-1} |E_j\rangle\langle E_j| \left[\frac{1}{\eta_j(t)} - \frac{1}{\eta_{j+1}(t)} \right] + i\hbar \frac{|E_N\rangle\langle E_N|}{\eta_N(t)} - i\hbar \frac{|E_1\rangle\langle E_1|}{\eta_2(t)}.
\end{aligned} \tag{4.27}$$

The first sum at right-hand side will be zero if the energy spectrum is equidistant because $\eta_2(t) = \eta_3(t) = \cdots$ when Δ_j =cte.

This form suggests to name $\hat{\mathcal{I}}$ as the boundary and interference term because, as we will show below, the sum at right-hand side can be seen as an interference term, while the last two terms will yield a boundary type conditions.

From the adjoint (4.25) it follows

$$\langle \hat{D}_f \psi | \psi \rangle = \langle \psi | \hat{D}_f^\dagger \psi \rangle = \langle \psi | \hat{D}_b \psi \rangle + \langle \psi | \hat{\mathcal{I}} \psi \rangle \tag{4.28}$$

where we have used the notation $\langle \hat{D}_f \psi | = \left[\hat{D}_f^\dagger | \psi \rangle \right]^\dagger$.

4.2.3.2 Discrete symmetry property

Definition 4.2.1. *We say that $\hat{D}_f$ satisfies the discrete symmetry property if there exists a domain of states $|\psi\rangle$ such that*

$$\langle \psi | \hat{\mathcal{I}} \psi \rangle = i\hbar \sum_{j=2}^{N} \frac{|\psi_j|^2 - |\psi_{j-1}|^2}{\eta_j(t)} = 0. \tag{4.29}$$

A way to obtain this value is by making use of the convenient separation Eq. (4.27), which helps us to write Eq.(4.29) as

$$\langle \psi | \hat{\mathcal{I}} \psi \rangle = i\hbar \sum_{j=2}^{N-1} |\psi_j|^2 \left[\frac{1}{\eta_j} - \frac{1}{\eta_{j+1}} \right] + i\hbar \left(\frac{|\psi_N|^2}{\eta_N} - \frac{|\psi_1|^2}{\eta_2} \right) = 0. \tag{4.30}$$

Thus, vanishing interference terms

$$\sum_{j=2}^{N-1} |\psi_j|^2 \left[\frac{1}{\eta_j(t)} - \frac{1}{\eta_{j+1}(t)} \right] = 0 \tag{4.31}$$

and vanishing boundary type conditions

$$|\psi_N|^2 - \frac{\eta_N}{\eta_2} |\psi_1|^2 = 0 \tag{4.32}$$

will do the job. Another possibility is that the two terms at left-hand side of Eqs. (4.31) and (4.32) cancel each other.

Observe that the summands in Eq.(4.29) are noting but the backward finite difference derivative applied to $|\psi_j|^2$. We proceed to give examples of states for which the symmetry requirement is fulfilled.

The partial time states. Let us consider a state $|\psi\rangle = \sum_{j=1}^{N} \psi_j |E_j\rangle$ such that $|\psi_j| = c$ (constant). From Eq.(4.29), it follows that $\langle\psi|\hat{\mathcal{I}}\psi\rangle = 0$. Hence, the discrete operator $\hat{D}_f$ satisfies the symmetry property when it acts on these states. Each ψ_j can include a phase factor, like a time evolution factor, and still comply with this constant property. Particular states of this class are the following which we will discuss later.

Definition 4.2.2. *A partial time eigenstate is defined to be a normalized equiprobable state of the form*

$$|t\rangle_N = \frac{1}{\sqrt{n_f - n_i + 1}} \sum_{j=n_i}^{n_f} e^{itE_j/\hbar} |E_j\rangle \tag{4.33}$$

where $n_f - n_i + 1 = N$, and where the finite set of energies $E_{n_i}, E_{n_i+1}, \ldots, E_{n_f}$ appears.

Equidistant spectrum. Another example for which the symmetry property holds is that of the equidistant energy spectrum, that is, when $E_{j+1} - E_j = \Delta$, $j \geq 1$. First note that the denominator functions $\eta_2 = \eta_3 = \ldots \eta_N$ are constant with respect to j, from which the vanishing interference terms Eq. (4.31) follows. In addition, it can be seen from Eq. (4.32) that as long as $\psi_N = e^{i\theta}\psi_1$ (θ a real parameter) holds true, the symmetry property of $\hat{D}_f$ will be fulfilled.

On the fulfillment of the symmetry property. For systems such that $\Delta_j \to \infty$ as $j \to \infty$ the symmetry property can be approximated because $|1/\eta_j| \leq 1/\Delta_j \ll 1$, $j > N$, for sufficiently large N. For states having a finite number of energy eigenkets all of them $E_n > E_N$ the term $\langle\psi|\hat{\mathcal{I}}\psi\rangle$ in Eq. (4.29) could be sufficiently small. Besides, roughly speaking, the differences $1/\eta_{j+1} - 1/\eta_j$ will also be small, because they are the difference between adjacent terms, so that interference terms in Eq. (4.31) will be small. But, since the time ket comply with the symmetry property, we just have to consider states written in terms of the time states.

In the forthcoming section we want to show, by using the particle in a box quantum model, that we can get some insights about the dynamics of the quantum system only through the time partial eigenstates.

4.3 The particle in a box

The energy eigenvalues for a particle of mass m in the infinite well potential

$$V(q) = \begin{cases} 0 & |q| \leq a \\ \infty & \text{otherwise} \end{cases} \tag{4.34}$$

are

$$E'_k = E'_1 \, k^2 = \frac{\hbar^2 \pi^2 k^2}{2m(2a)^2}, \quad k = 1, 2, \ldots \tag{4.35}$$

where E'_1 is the energy of the ground state, and $2a$ is the width of the well. We will pick $a = 1$ (units of mass). The related wave-function space is known to be the Lebesgue space $L^2([-a, a])$ [15].

The corresponding odd eigenenergies and odd eigenfunctions are

$$E^-_n = E'_{2n} = \frac{\hbar^2 \pi^2 n^2}{2ma^2}, \quad n = 1, 2, \ldots \tag{4.36}$$

and

$$v^-_n(q) = \frac{\chi_{[-a,a]}(q)}{\sqrt{a}} \sin(\pi n q / a), \tag{4.37}$$

respectively, where $\chi_{[-a,a]}(q)$ is the characteristic function of the interval $[-a, a]$:

$$\chi_{[-a,a]}(q) = \begin{cases} 1 & \text{if } q \in [-a, a] \\ 0 & \text{otherwise} \end{cases}. \tag{4.38}$$

On the other hand, the even eigenenergies and even eigenfunctions are given by

$$E^+_n = E'_{2n-1} = \frac{\hbar^2 \pi^2 (n - 1/2)^2}{2ma^2}, \quad n = 1, 2, \ldots \tag{4.39}$$

and

$$v^+_n(q) = \frac{\chi_{[-a,a]}(q)}{\sqrt{a}} \cos(\pi [n - 1/2] q / a). \tag{4.40}$$

We also consider the normalized truncated plane waves

$$u^\pm_n(q) = \frac{1}{\sqrt{2a}} e^{i p_{\pm n} q / \hbar} \chi_{[-a,a]}(q), \quad n = 1, 2, \ldots, \tag{4.41}$$

where $p_{\pm n} = \pm\hbar\pi n/a$. These functions allow us to split the odd eigenfunctions as the linear superposition $v_n^-(q) = [u_n^+(q) - u_n^-(q)]/i\sqrt{2}$, and then, associate two momentum eigenvalues $p_{\pm n} = \pm p_n$ to each energy through the classical type of relationship

$$E_n := E_n^- = \frac{p_{\pm n}^2}{2m}, \quad n = 1, 2, \dots \tag{4.42}$$

Each energy level E_n is therefore two-fold degenerate; $u_n^\pm$ are a set of eigenfunctions common to the momentum operator and the kinetic energy operators [17].

The corresponding energy increments are not equally spaced but

$$\Delta_n = \frac{\hbar^2\pi^2}{2ma^2}\left[(n+1)^2 - n^2\right] = \frac{\hbar^2\pi^2}{ma^2}(n + 1/2) \tag{4.43}$$

and the zeroes Eq. (4.15) of the denominator function χ_j (or, equivalently, the zeroes of η_j) are

$$t_{k,n} = \frac{2\pi\hbar k}{\Delta_n} = \frac{2ma^2 k}{\pi\hbar(n+1/2)}, \quad k = \pm 1, \pm 2, \dots \tag{4.44}$$

We can identify the times $t_{1,n}$ as the *Bohr times;* the inverse of the Bohr frequencies $|E_{n+1} - E_n|/2\pi\hbar$.

The procedure we are adopting here, that is, the use of the complex exponential functions $u_n^\pm(q)$, enables us to make use of the next nonstandard eigenfunctions. Another choice of complex exponential functions is $e^{ip'_{\pm n}q/\hbar}\chi_{[-a,a]}(q)/\sqrt{2a}$ with $p'_{\pm n} = \pm\hbar\pi(n - 1/2)/a$ in order to separate two momenta in the even eigenfunctions. This approach can be treated similarly, reaching similar conclusions.

4.3.1 Non standard energy eigenfunctions

From now on, instead of considering the odd eigenfunctions $u_n^-(q)$ we will consider the functions

$$w_n(q) = \frac{\chi_{[-a,a]}(q)}{\sqrt{a}}\cos(p_n q/\hbar), \qquad n = 1, 2, \dots, \tag{4.45}$$

which belong to the domain of a self-adjoint extension of the Hamiltonian of the infinite well potential [17] related to periodic boundary conditions, namely, the (self-adjoint) operator defined as

$$\hat{H}' : D_{\hat{H}'} \to L^2([-a,a]) \quad ; \quad \psi(q) \mapsto -\frac{\hbar^2}{2m}\frac{d^2\psi(q)}{d^2q}, \tag{4.46}$$

where

$$D_{\hat{H}'} = \left\{\psi \in L^2([-a,a]) : \psi, \psi' \in \mathrm{AC}, \psi', \psi'' \in L^2([-a,a]),\right.$$
$$\left.\psi(a) = \psi(-a), \psi'(a) = \psi'(-a)\right\}. \tag{4.47}$$

Here AC stands for the class of absolutely continuous functions (see Eq. (3.45)).

As can be verified, the functions $w_n(q)$ belong to the domain of $\hat{H}'$, and satisfy the differential equation

$$-\frac{\hbar^2}{2m}\frac{d^2 w_n(q)}{d^2 q} = E_n w_n(q). \tag{4.48}$$

This means that the functions $w_n(q)$ are eigenfunctions of $\hat{H}'$ and that each $w_n(q)$ does not satisfy the usual vanishing conditions ($w_n(\pm a) = (-1)^n/\sqrt{a} \neq 0$).

4.3.2 Time eigenstates

In order to study the time eigestates $|t\rangle$, since they are not normalized, we analyze the behavior of the partial time states, for the particle in the infinite well, defined by:

$$|t\rangle_N = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{itE_n/\hbar}\left[\frac{|E_n^+\rangle + |E_n^-\rangle}{\sqrt{2}}\right], \tag{4.49}$$

where $|E_n^{\pm}\rangle$ stands for the two-fold degeneracy of each energy level E_n

$$\langle q|E_n\rangle = \frac{\langle q|E_n^+\rangle + \langle q|E_n^-\rangle}{\sqrt{2}} = \frac{u_n^+(q) + u_n^-(q)}{\sqrt{2}} = w_n(q). \tag{4.50}$$

It is worth noting that the partial time eigenstates are the most important states for our approach because they provide to the discrete momenta $-i\hbar\hat{D}_{f,g}$ the discrete symmetry property, and, as we will see below, they also give account of classical trajectories.

The coordinate representation of Eq. (4.49) is

$$\begin{aligned}
\langle q|t\rangle_N =& \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{itE_n/\hbar} w_n(q) \\
=& \frac{\chi_{[-a,a]}(q)}{\sqrt{Na}}\sum_{n=1}^{N} e^{itE_n/\hbar}\cos(n\pi q/a) \\
=& \frac{\chi_{[-a,a]}(q)}{2\sqrt{Na}}\sum_{n=1}^{N} e^{itE_n/\hbar}\left[e^{ip_n q/\hbar} + e^{-ip_n q/\hbar}\right] \\
=& \frac{\chi_{[-a,a]}(q)}{2\sqrt{Na}}\sum_{n=1}^{N}\left[\exp\left\{i\pi n\left(\frac{q}{a} + t\,\frac{\hbar\pi n}{2ma^2}\right)\right\} + \exp\left\{-i\pi n\left(\frac{q}{a} - t\,\frac{\hbar\pi n}{2ma^2}\right)\right\}\right]
\end{aligned} \tag{4.51}$$

and its corresponding probability density is

$$
\begin{aligned}
|\langle q|t\rangle_N|^2 &= \frac{\chi_{[-a,a]}(q)}{Na} \sum_{k,n=1}^{N} e^{it(E_n-E_k)/\hbar} \cos(n\pi q/a)\ \cos(k\pi q/a) \\
&= \frac{\chi_{[-a,a]}(q)}{Na} \sum_{k,n=1}^{N} \cos(t(E_n-E_k)/\hbar) \cos(n\pi q/a)\ \cos(k\pi q/a) \\
&= \frac{2\chi_{[-a,a]}(q)}{Na} \sum_{n=1}^{N} \sum_{k>n}^{N} \cos(t(E_n-E_k)/\hbar) \cos(n\pi q/a)\ \cos(k\pi q/a) \\
&\quad + \frac{\chi_{[-a,a]}(q)}{Na} \sum_{n=1}^{N} \cos^2(n\pi q) \\
&= \frac{\chi_{[-a,a]}(q)}{Na} \sum_{n=1}^{N} \sum_{k>n}^{N} \cos(t(E_n-E_k)/\hbar) \cos((n-k)\pi q/a) \\
&\quad + \frac{\chi_{[-a,a]}(q)}{Na} \sum_{n=1}^{N} \sum_{k>n}^{N} \cos(t(E_n-E_k)/\hbar) \cos((n+k)\pi q/a) \\
&\quad + \frac{\chi_{[-a,a]}}{2a} + \frac{\chi_{[-a,a]}}{2Na} \sum_{n=1}^{N} \cos(2n\pi q).
\end{aligned}
\tag{4.52}
$$

In the first step we considered that the probability density is non-negative, while in the last step we have used the identities $\cos\theta\ \cos\phi = (\cos(\theta-\phi)+\cos(\theta+\phi))/2$ and $\cos^2\theta = (1+\cos(2\theta))/2$.

So as to identify each sum in the probability density $|\langle q|t\rangle_N|^2$, let us consider the partial time eigenstates formed by the complex exponential function (free particle) corresponding to either positive or negative momenta ($\pm p_n = \pm\hbar\pi n/a$) defined by

$$
\langle q|t\rangle_N^{\pm} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{itE_n/\hbar} \langle q|E_n^{\pm}\rangle = \frac{\chi_{[-a,a]}(q)}{\sqrt{2Na}} \sum_{n=1}^{N} e^{itE_n/\hbar} e^{\pm ip_n q/\hbar}. \tag{4.53}
$$

Their corresponding probability densities are

$$
\begin{aligned}
|\langle q|t\rangle_N^{\pm}|^2 &= \left| \frac{\chi_{[-a,a]}(q)}{\sqrt{2Na}} \sum_{n=1}^{N} e^{itE_n/\hbar} e^{\pm ip_n q/\hbar} \right|^2 \\
&= \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{n,k=1}^{N} \exp\left\{ i\frac{t(E_n - E_k)}{\hbar} \pm i\frac{(p_n - p_k)q}{\hbar} \right\} \\
&= \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{n,k=1}^{N} \cos\left[\frac{t(E_n - E_k)}{\hbar} \pm \frac{(p_n - p_k)q}{\hbar} \right] \\
&= \frac{\chi_{[-a,a]}(q)}{Na} \sum_{n=1}^{N} \sum_{k>n}^{N} \cos\left[\frac{t(E_n - E_k)}{\hbar} \pm \frac{(p_n - p_k)q}{\hbar} \right] + \frac{\chi_{[-a,a]}(q)}{2a},
\end{aligned}
\tag{4.54}
$$

and using the trigonometric identity $\cos(\theta + \phi) = \cos\theta\cos\phi - \sin\theta\sin\phi$, they can be written as:

$$
\begin{aligned}
|\langle q|t\rangle_N^{\pm}|^2 = \frac{\chi_{[-a,a]}(q)}{Na} &\sum_{n=1}^{N} \sum_{k>n}^{N} \cos\left(t(E_n - E_k)/\hbar\right) \cos\left(\pi(n-k)q/a\right) \\
&\mp \frac{\chi_{[-a,a]}(q)}{Na} \sum_{n=1}^{N} \sum_{k>n}^{N} \sin\left(t(E_n - E_k)/\hbar\right) \sin\left(\pi(n-k)q/a\right) + \frac{\chi_{[-a,a]}(q)}{2a}.
\end{aligned}
\tag{4.55}
$$

On the other hand, the interference between $\langle q|t\rangle_N^{+}$ and $\langle q|t\rangle_N^{-}$ is

$$
\begin{aligned}
\Re\left\{ {}_N^{-}\langle t|q\rangle\langle q|t\rangle_N^{+} \right\} &= \frac{\chi_{[-a,a]}(q)}{2Na} \Re\left\{ \sum_{k=1}^{N} e^{-i(tE_k - p_k q)/\hbar} \sum_{n=1}^{N} e^{i(tE_n + p_n q)/\hbar} \right\} \\
&= \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{n,k=1}^{N} \cos\left[\frac{t(E_n - E_k)}{\hbar} + \frac{(p_n + p_k)q}{\hbar} \right] \\
&= \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{n\neq k}^{N} \cos\left[\frac{t(E_n - E_k)}{\hbar} + \frac{(p_n + p_k)q}{\hbar} \right] + \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{n=1}^{N} \cos\left[\frac{2p_n q}{\hbar} \right] \\
&= \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{k>n}^{N} \left\{ \cos\left[\frac{t(E_n - E_k)}{\hbar} + \frac{(p_n + p_k)q}{\hbar} \right] \right. \\
&\qquad \left. + \cos\left[\frac{t(E_k - E_n)}{\hbar} + \frac{(p_k + p_n)q}{\hbar} \right] \right\} \\
&\qquad \frac{\chi_{[-a,a]}(q)}{2Na} \sum_{n=1}^{N} \cos\left[\frac{2p_n q}{\hbar} \right],
\end{aligned}
\tag{4.56}
$$

the sum of cos functions above can be reduced by using the trigonometric identity

$$
\begin{aligned}
\cos(\theta + \phi) + \cos(-\theta + \phi) &= \cos\theta\cos\phi - \sin\theta\sin\phi + \cos\theta\cos\phi + \sin\theta\sin\phi \\
&= 2\cos\theta\cos\phi
\end{aligned}
\tag{4.57}
$$

and by replacing in it $\theta = t(E_n - E_m)/\hbar$ and $\phi = (p_n + p_m)q/\hbar$. Thus, the interference term is left as

$$\Re\left\{{}_N^-\langle t|q\rangle\langle q|t\rangle_N^+\right\} = \frac{\chi_{[-a,a]}(q)}{Na}\sum_{n=1}^{N}\sum_{k>n}^{N}\cos\left[t(E_n - E_k)/\hbar\right]\cos\left[\pi(n+k)q/a\right] + \frac{\chi_{[-a,a]}(q)}{2Na}\sum_{n=1}^{N}\cos(2\pi nq/a) \tag{4.58}$$

Recall that we can split the partial time state into

$$|t\rangle_N = \frac{|t\rangle_N^+ + |t\rangle_N^-}{\sqrt{2}} = \frac{1}{\sqrt{2N}}\sum_{n=1}^{N} e^{itE_n/\hbar}|E_n^+\rangle + \frac{1}{\sqrt{2N}}\sum_{n=1}^{N} e^{itE_n/\hbar}|E_n^-\rangle \tag{4.59}$$

such that

$$|\langle q|t\rangle_N|^2 = \left|\frac{\langle q|t\rangle_N^+}{\sqrt{2}} + \frac{\langle q|t\rangle_N^-}{\sqrt{2}}\right|^2 = \frac{|\langle q|t\rangle_N^+|^2}{2} + \frac{|\langle q|t\rangle_N^-|^2}{2} + \Re\left\{{}_N^-\langle t|q\rangle\langle q|t\rangle_N^+\right\}. \tag{4.60}$$

In this expression the sin functions in $|\langle q|t\rangle_N^{\pm}|^2$, see Eq. (4.55), cancel each other.

If we had chosen the odd eigenfunctions $v_n^-(q)$ instead of the non standard eigenfunctions $w_n(q)$, we would have gotten $|t\rangle_N = |t\rangle_N^+/i\sqrt{2} - |t\rangle_N^-/i\sqrt{2}$ with $\langle q|t\rangle_N = (N)^{-1/2}\sum_{n=1}^{N} e^{itE_n/\hbar}v_n^-(q)$ and the density Eq. (4.60) would be

$$|\langle q|t\rangle_N|^2 = \left|\frac{\langle q|t\rangle_N^+}{i\sqrt{2}} - \frac{\langle q|t\rangle_N^-}{i\sqrt{2}}\right|^2 = \frac{|\langle q|t\rangle_N^+|^2}{2} + \frac{|\langle q|t\rangle_N^-|^2}{2} - \Re\left\{{}_N^-\langle t|q\rangle\langle q|t\rangle_N^+\right\}. \tag{4.61}$$

We have plotted in Figure 4.1 an example of each wave: the probability densities Eqs. (4.52), (4.55), and the interference term (4.58), when the time goes from 0 to a period of the system $\tau = 4ma^2/\pi\hbar$ (see Eq. (4.63) below).

We clearly see in Figure 4.2 that the peaks of $|\langle q|t\rangle_N^-|^2$ defines classical paths of classical particles with negative momenta. Note that $|\langle q|t\rangle_N^+|^2 = |\langle -q|t\rangle_N^-|^2$, thus $|\langle q|t\rangle_N^+|^2$ defines the corresponding positive classical paths. Roughly, these classical paths are also seen in the Figures 4.1a and 4.1b. In Figure 4.3 we see a zoom of the density shown in Figure 4.1d.

On the other hand, in Figure 4.4 there is a plot of $|\langle q|t\rangle_N|^2$, but in this case we take 50 energy eigenstates from the 950th to the 1000th energy eigenstates, see Definition 4.2.2. The use of 50 states is enough to get a well-defined density around the classical path, better defined when the energy is large. In addition to the large peaks pointed out in Figure 4.1, in this figure there are pronounced peaks sketching paths that connect the peaks at $(q = 0, t = 0)$, $(q = \pm 1, t = \tau/2)$, and $(q = 0, t = \tau)$. These further peaks are due to the interference between positive and negative momentum parts of the density. This interference was not present when only low energy eigenstates were used, and it appears because the part of the density that arrives to the wall interferes with the part that leaves the wall.

We proceed to show some properties that can be seen roughly in the plots of the Figure 4.1.

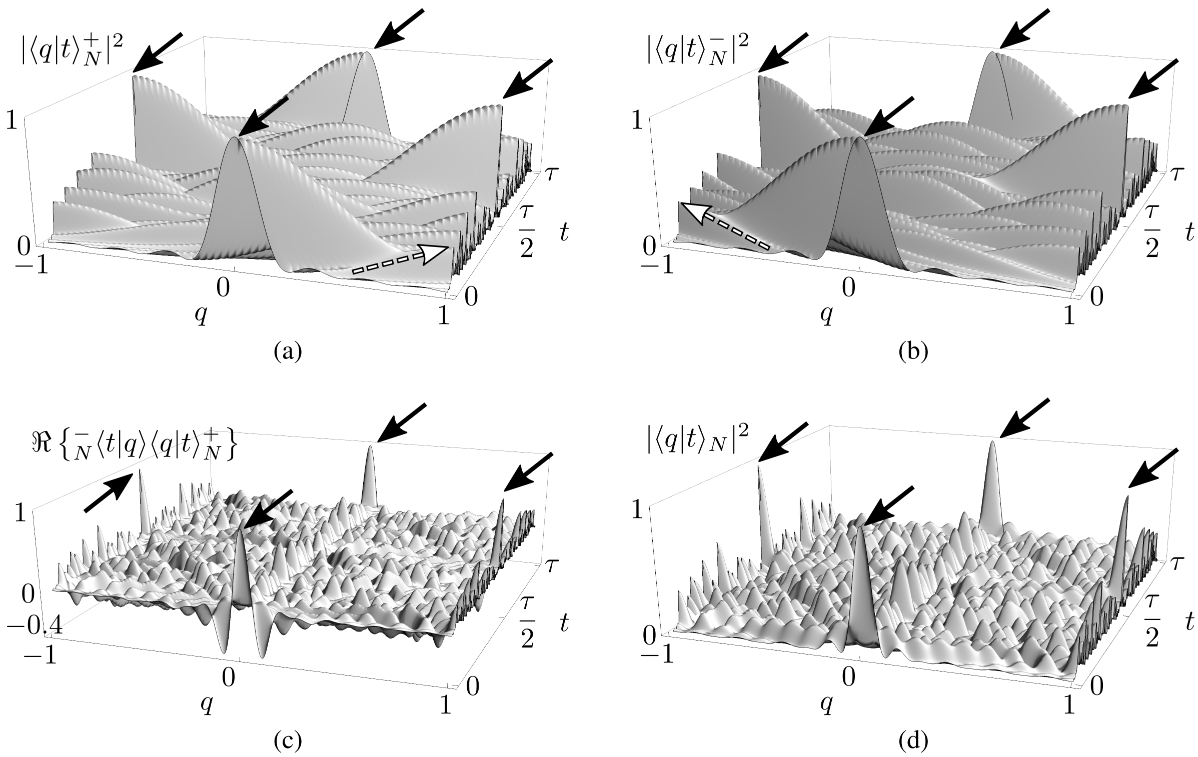


Figure 4.1: (a) A plot of $|\langle q|t\rangle_N^+|^2$, (b) a plot of $|\langle q|t\rangle_N^-|^2$, (c) a plot of $\Re\left\{{}_N^-\langle t|q\rangle\langle q|t\rangle_N^+\right\}$, and (d) a plot of $|\langle q|t\rangle_N|^2$. The energy eigenstates used in these plots are from E_1 to E_8, for the infinite well. The black arrows in each subplot indicates four pronounced peaks centered at $(q = 0, t = 0)$, $(q = \pm 1, t = \tau/2)$, and $(q = 0, t = \tau)$. Roughly, in (a) and (b) it can be seen that the densities tend to be concentrated around classical trajectories with only the positive and negative momentum parts, respectively, starting from the origin of coordinates as indicated by the dashed white arrows. (d) shows that the interference term $\Re\left\{{}_N^-\langle t|q\rangle\langle q|t\rangle_N^+\right\}$, plotted in (c), prevails over the positive and negative momentum counterparts $|\langle q|t\rangle_N^{\pm}|^2$.

Even function. The time state is an even function of the coordinate, $\langle q|t\rangle_N = \langle -q|t\rangle_N$ because of $w_n(-q) = w_n(q)$.

Periodicity. On account of

$$\exp\left\{i\left(t + \frac{4ma^2}{\pi\hbar}\right)\frac{E_n}{\hbar}\right\} = e^{itE_n/\hbar}\exp\left\{i\frac{4ma^2}{\pi\hbar^2}\frac{\hbar^2\pi^2 n^2}{2ma^2}\right\} = e^{itE_n/\hbar}e^{i2\pi n^2} = e^{itE_n/\hbar} \tag{4.62}$$

the partial time eigenstates are periodic $\langle q|t+\tau\rangle_N = \langle q|t\rangle_N$ with period

$$\tau = \frac{4ma^2}{\pi\hbar} = \frac{2\pi\hbar}{E_1}. \tag{4.63}$$

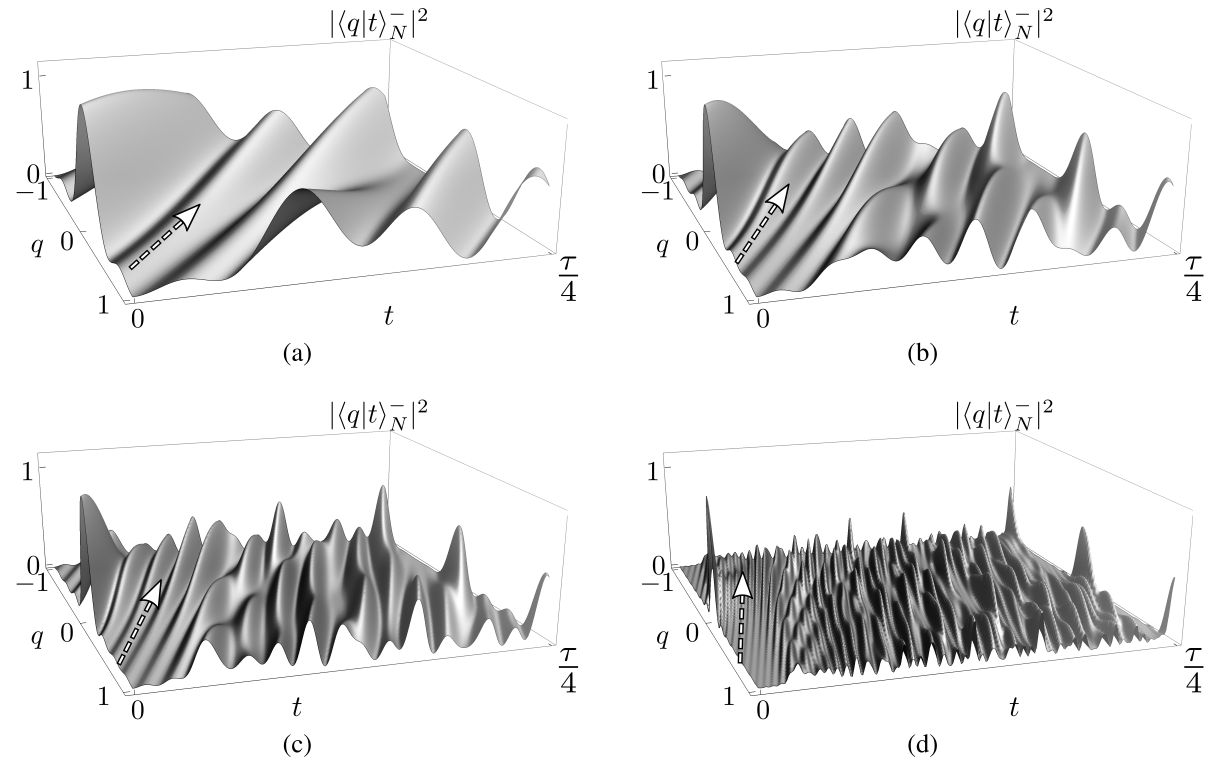


Figure 4.2: Plots of $|\langle q|t\rangle_N^-|^2$ for different sets of energies: (a) from E_1 to E_4, (b) from E_1 to E_6, (c) from E_1 to E_8, (d) from E_1 to E_{15}. The time interval considered is quarter period. In particular, the plot (c) is a zoom of Figure 4.1b. These plots help to visualize the forms that arise from the densities $|\langle q|t\rangle_N^-|^2$ with negative momenta. Note that the density $|\langle q|t\rangle_N^+|^2$ is the reflection with respect to the coordinate of $|\langle q|t\rangle_N^-|^2$. In these plots it is easier to see that the densities are concentrated around classical trajectories with only negative momentum parts, the dashed white arrows indicates the paths that a classical particle will follow.

where E_1 is the ground state energy. This is the time needed to resolve the energy of the ground state.

The half of a period. Using the identities

$$\exp\left\{i\frac{\tau}{2}\frac{E_n}{\hbar}\right\} = e^{in^2\pi} = e^{\pm in\pi a/a} = (-1)^{\pm n}, \tag{4.64}$$

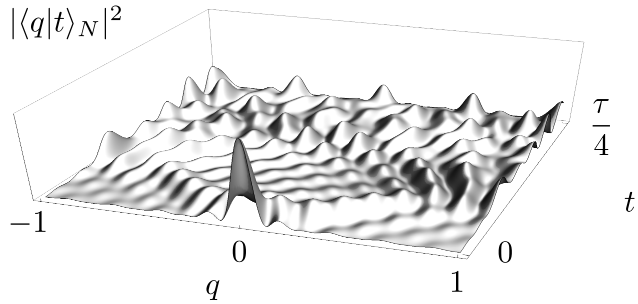


Figure 4.3: A plot of $|\langle q|t\rangle_N|^2$ formed with the first eight energy eigenstates for the infinite well, in the coordinate representation. This probability density is the same as the one plotted in Figure 4.1d, but, the time interval considered here is a quarter period. The density has a pronounced peak which starts at the origin of coordinates, and then, it is separated into two less pronounced peaks, the positive and negative momentum parts, each one returning after hitting the walls, and, at this moment, we can notice some oscillations going on that start to dominate the density.

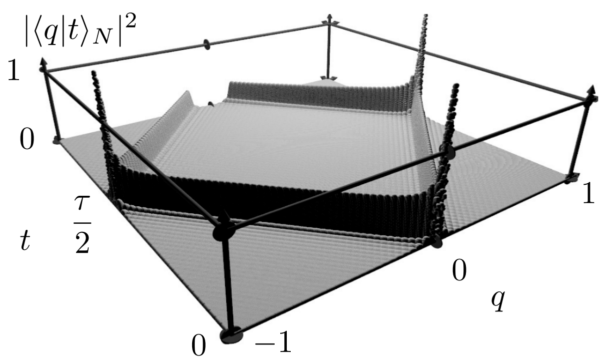


Figure 4.4: A plot of the density $|\langle q|t\rangle_N|^2$ for the infinite well, with only 50 energy eigenstates, from the state 950 to the state 1000. This figure was taken from Ref. [28]. The density resembles better the classical behavior at large energies than at low energies, in which oscillations dominate the evolution of the density as is shown in Figure 4.1.

first we have

$$\begin{aligned}\langle q|t+\tau/2\rangle_N &= \frac{1}{\sqrt{N}}\sum_{n=1}^{N} e^{i(t+\tau/2)E_n/\hbar} w_n(q) \\ &= \frac{\chi_{[-a,a]}(q)}{2\sqrt{Na}}\sum_{n=1}^{N} e^{itE_n/\hbar}\left[(-1)^n e^{in\pi q/a} + (-1)^{-n} e^{-in\pi q/a}\right]. \end{aligned} \tag{4.65}$$

However, if we write this expression as follows

$$\langle q|t+\tau/2\rangle_N = \frac{\chi_{[-a,a]}(q)}{2\sqrt{Na}}\sum_{j=1}^{N} e^{itE_n/\hbar}\left[\exp\left\{in\pi\left(\frac{q-a}{a}\right)\right\} + \exp\left\{-in\pi\left(\frac{q+a}{a}\right)\right\}\right] \tag{4.66}$$

we can now realize that a half of the state is moving to the left and that the other half of the state moves to the right. At half of the period, the part that was moving towards the right is replaced by a function that moves towards the left and vice versa. This is a set of waves moving along a set of classical trajectories with momenta $p = \pm n\pi\hbar/a$.

Dirac function. At $t = 0$, and in each period, the coordinate representation of the time state becomes a scaled dirac function

$$\begin{aligned}\lim_{N\to\infty}\sqrt{\frac{N}{a}}\langle q|t\rangle_N\Big|_{t=0} &= \lim_{N\to\infty}\frac{\chi_{[-a,a]}(q)}{2a}\left[\sum_{n=0}^{N}e^{in\pi q/a}+\sum_{n=1}^{N}e^{-in\pi q/a}\right]-\frac{\chi_{[-a,a]}(q)}{2a}\\ &= \chi_{[-a,a]}(q)\lim_{N\to\infty}\left[\frac{1}{2a}\sum_{k=-N}^{N}e^{ik\pi q/a}\right]-\frac{\chi_{[-a,a]}(q)}{2a}\\ &= \chi_{[-a,a]}(q)\sum_{k=-\infty}^{\infty}\delta(q-2ka)-\frac{\chi_{[-a,a]}(q)}{2a}\\ &= \delta(q)-\frac{\chi_{[-a,a]}(q)}{2a}\end{aligned} \tag{4.67}$$

The term $\chi_{[-a,a]}(q)/2a$ compensates the constant term $e^{i\pi nq/a}|_{n=0}$ in the Dirac function that corresponds to zero momentum or zero energy level, thus the zero energy level is still missing.

We can observe that the limit (4.67) accounts for the pronounced peaks at $t = 0, \tau, 2\tau, \ldots$ that the probability density $\langle q|t\rangle_N$ exhibits in the plots of Figures 4.1, 4.3, and 4.4.

Recall that the Fourier series of the Dirac function with respect to the basis $\{e^{ik\pi q/a}/\sqrt{2a}\}_{k\in\mathbb{Z}}$ yields the periodization of the Dirac function

$$\sum_{k=-\infty}^{\infty}\delta(q-2ka)=\frac{1}{2a}\sum_{k=-\infty}^{\infty}e^{ik\pi q/a}=\sum_{k=-\infty}^{\infty}\frac{1}{\sqrt{2a}}\frac{e^{ik\pi q/a}}{\sqrt{2a}}, \tag{4.68}$$

where the Fourier coefficients are calculated in the usual way

$$\int_{-a}^{a}\frac{e^{-ik\pi q/a}}{\sqrt{2a}}\delta(q)dq=\frac{1}{\sqrt{2a}}. \tag{4.69}$$

Dirac functions at the boundaries. If we calculate the Fourier series of a Dirac function at some boundary, say $q = -a$, we get its corresponding periodization

$$\sum_{k=-\infty}^{\infty}\delta(q+a-2ka)=\frac{1}{2a}\sum_{k=-\infty}^{\infty}(-1)^k e^{ik\pi q/a}=\sum_{k=-\infty}^{\infty}\frac{(-1)^k}{\sqrt{2a}}\frac{e^{ik\pi q/a}}{\sqrt{2a}} \tag{4.70}$$

in this case the Fourier coefficients are

$$\int_{-a}^{a}\frac{e^{-ik\pi q/a}}{\sqrt{2a}}\delta(q+a)dq=\frac{(-1)^{-k}}{\sqrt{2a}}=\frac{(-1)^k}{\sqrt{2a}}. \tag{4.71}$$

Therefore, the partial time eigenstates at half of the period behave as scaled partial Fourier series of such a periodization. This follows from expression Eq. (4.65) and Eq. (4.70):

$$
\begin{aligned}
\lim_{N\to\infty}\sqrt{\frac{N}{a}}\langle q|t\rangle_N\Big|_{t=\tau/2} &= \lim_{N\to\infty}\frac{\chi_{[-a,a]}(q)}{2a}\left[\sum_{n=0}^{N}(-1)^n e^{in\pi q/a}+\sum_{n=1}^{N}(-1)^{-n}e^{-in\pi q/a}\right]-\frac{\chi_{[-a,a]}(q)}{2a}\\
&=\chi_{[-a,a]}(q)\lim_{N\to\infty}\left[\frac{1}{2a}\sum_{k=-N}^{N}(-1)^k e^{ik\pi q/a}\right]-\frac{\chi_{[-a,a]}(q)}{2a}\\
&=\chi_{[-a,a]}(q)\sum_{k=-\infty}^{\infty}\delta(q+a-2ka)-\frac{\chi_{[-a,a]}(q)}{2a}\\
&=\delta(q+a)+\delta(q-a)-\frac{\chi_{[-a,a]}(q)}{2a}.
\end{aligned}
\tag{4.72}
$$

This means that the partial time eigenstates at half the period behave as the partial Fourier series of two Dirac functions centered at the boundaries. This behavior can be observed in the plots of Figure 4.1 and 4.4 at time $\tau/2$. Indeed, as suspected, this half of a period and its subsequent times $\tau/2+n\tau$ ($n=1,2,\dots$) are the arrival times at the boundaries of a classical particle [39] with velocity

$$
\frac{a}{\tau/2}=\frac{\pi\hbar}{2ma}. \tag{4.73}
$$

Such a particle starts at the origin when $t=0$ and it hits a boundary, for the first time, when $t=\tau/2$.

The coordinate mean value. Since $\langle q|t\rangle_N$ is an even function (with respect to the coordinate), thus $q|\langle q|t\rangle_N|^2$ is an odd function and then

$$
{}_N\langle t|\hat{q}|t\rangle_N=\int_{-a}^{a}q|\langle q|t\rangle_N|^2dq=0. \tag{4.74}
$$

The root-mean-square deviation. Using the integration formula

$$
\frac{1}{2a}\int_{-a}^{a}q^2e^{ipq/\hbar}dq\Big|_{p=\hbar\pi n/a}=\begin{cases}2a^2\,(-1)^n/n^2\pi^2, & n\neq 0\\ \dfrac{a^2}{3}, & n=0\end{cases}, \tag{4.75}
$$

we can calculate the mean of the square of $\hat{q}$ in the states $|t\rangle_N$

$$
\begin{aligned}
{}_N\langle t|\hat{q}^2|t\rangle_N &= \int_{-a}^{a} q^2 |\langle q|t\rangle_N|^2 dq \\
&= \frac{1}{Na}\sum_{k,n=1}^{N} e^{it(E_n-E_k)/\hbar}\int_{-a}^{a} q^2\cos(p_nq/\hbar)\cos(p_kq/\hbar)dq \\
&= \frac{1}{2N}\sum_{n,k=1}^{N} e^{it(E_n-E_k)/\hbar}\frac{1}{2a}\int_{-a}^{a} q^2\left[e^{i(p_n-p_k)q/\hbar}+e^{-i(p_n-p_k)q/\hbar}\right]dq \\
&\qquad + \frac{1}{2N}\sum_{n,k=1}^{N} e^{it(E_n-E_k)/\hbar}\frac{1}{2a}\int_{-a}^{a} q^2\left[e^{i(p_n+p_k)q/\hbar}+e^{-i(p_n+p_k)q/\hbar}\right]dq \\
&= \frac{1}{2N}\sum_{n=1}^{N}\frac{2a^2}{3} + \frac{1}{2N}\sum_{n\neq k}^{N} e^{it(E_n-E_k)/\hbar}\frac{4a^2(-1)^{n-k}}{(n-k)^2\pi^2} \\
&\qquad + \frac{1}{2N}\sum_{n=1}^{N}\frac{a^2}{n^2\pi^2} + \frac{1}{2N}\sum_{n\neq k}^{N} e^{it(E_n-E_k)/\hbar}\frac{4a^2(-1)^{n+k}}{(n+k)^2\pi^2} \\
&= \frac{a^2}{3} + \frac{a^2}{2N\pi^2}\sum_{n=1}^{N}\frac{1}{n^2} + \frac{4a^2}{N\pi^2}\sum_{n\neq k}^{N} e^{it(E_n-E_k)/\hbar}(-1)^{n+k}\frac{(n^2+k^2)}{(n^2-k^2)^2} \\
&= \frac{a^2}{N\pi^2}\left[\frac{N\pi^2}{3} + \frac{1}{2}\sum_{n=1}^{N}\frac{1}{n^2} + 4\sum_{n\neq k}^{N}\cos\left[t\frac{(E_n-E_k)}{\hbar}\right](-1)^{n+k}\frac{(n^2+k^2)}{(n^2-k^2)^2}\right]. \quad (4.76)
\end{aligned}
$$

In the last step we have used the fact that ${}_N\langle t|\hat{q}^2|t\rangle_N$ is a real number such that its imaginary part must be equal to zero.

Thus, we get the root-mean-square deviation

$$\Delta\hat{q} = \sqrt{{}_N\langle t|\hat{q}^2|t\rangle_N - {}_N\langle t|\hat{q}|t\rangle_N^2} = \sqrt{{}_N\langle t|\hat{q}^2|t\rangle_N}. \quad (4.77)$$

We have plotted this function in Figure 4.5 for the same energy eigenstates as in Figure 4.1. The scaled Dirac function behavior at $t = 0$, and at the next periods, can be observed through the minimums of the root-mean-square deviation. On the other hand, the maximum deviation is found at $\tau/2$ when the partial time eigenstates behave as scaled partial Fourier series of two Dirac functions centered at the walls at $q = \pm a$. Recall that, $\Delta\hat{q}$ is the width in q of the wave function, and then, if we base our dynamic analysis on $\Delta\hat{q}$ and $\langle\hat{q}\rangle$, as can be seen from Figure 4.5, we will have a rough description, for instance, we will not be able to notice waves moving accordingly to classical trajectories.

Classical analogues. Expressing the difference between E_n and E_m in terms of momentum

$$E_n - E_k = \frac{\hbar^2\pi^2(n^2-k^2)}{2ma^2} = \frac{1}{2m}(p_n+p_k)(p_n-p_k), \quad (4.78)$$

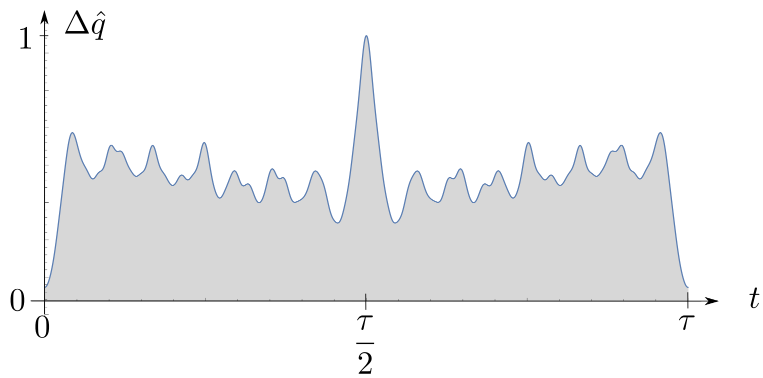


Figure 4.5: A plot of $\Delta\hat{q}$. The energy eigenstates used in these plots are from E_1 to E_8, again, for the infinite well. Observe that there are two minima at $t = 0, \tau$, while there is a pronounced peak centered at $t = \tau/2$. We can see roughly a total of seven peaks before the maximum peak at $t = \tau/2$, they can be associated with eight classical hits at the boundaries. Even if more and more energy eigenstates are added to the partial time eigenstates, the maximum at $t = \tau/2$ and the minimums at $t = 0, \tau$ always remains.

and considering only two states corresponding to adjacent energies, and with either positive or negative momentum only, from Eqs. (4.54) we get

$$\begin{aligned} |\langle q|t\rangle_2^{\pm}|^2 &= \frac{\chi_{[-a,a]}(q)}{2a}\cos\left[q\left(\frac{p_{n+1}-p_n}{\hbar}\right) \pm t\left(\frac{E_{n+1}-E_n}{\hbar}\right)\right] + \frac{\chi_{[-a,a]}(q)}{2a} \\ &= \frac{\chi_{[-a,a]}(q)}{2a}\cos\left[\left(q \pm t\left[\frac{p_{n+1}+p_n}{2m}\right]\right)\frac{p_{n+1}-p_n}{\hbar}\right] + \frac{\chi_{[-a,a]}(q)}{2a}. \end{aligned} \tag{4.79}$$

Classically, the distance that this wave travels in a Bohr time, Eq. (4.44), is

$$t_{1,n}\left[\frac{p_{n+1}+p_n}{2m}\right] = \frac{2ma^2}{\hbar\pi(n+1/2)}\left[\frac{p_{n+1}+p_n}{2m}\right] = \frac{2ma^2}{\hbar\pi(n+1/2)}\,\frac{\hbar\pi(2n+1)}{2ma} = 2a, \tag{4.80}$$

which is exactly the width of the well. Since the constant term $\chi_{[-a,a]}(q)/2a$ does not evolve in time we can leave it out of the discussion. Taking N to be an even positive integer, we can always split $|t\rangle_N$, and $|t\rangle_N^{\pm}$, and $|\langle q|t\rangle_N^{\pm}|^2$, and $|\langle q|t\rangle_N|^2$ into pairs of eigenstates corresponding to adjacent energies. Each of these pairs spends the respective Bohr time from one wall to the other. These states formed with two adjacent energy eigenkets can be considered then as quantum analogues of classical trajectories.

4.4 The harmonic oscillator

As an additional example, let us consider the one-dimensional harmonic oscillator. In this case, the eigenenergies are $E_n = \hbar\omega(n+1/2)$, where ω is the angular frequency, and there are no degenerate levels. In the coordinate representation, the partial time eigenket is written as

$$\langle q|t\rangle = \sum_{n=1}^{N} e^{i\omega(n+1/2)t} \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega q^2/2\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right), \tag{4.81}$$

where s$H_n(q) = (-1)^n e^{q^2} d^n(e^{-q^2})/dq^n$ is the Hermite polynomial of degree $n = 0, 1, 2, \ldots$. The corresponding coordinate density has been traced in Figures 4.6. In each of these plots we can notice that the pronounced peaks depict the classical paths of a particle having an oscillatory behavior. Recall that for an equidistant energy spectrum the symmetry property is fulfilled by the discrete momentum operators (upon to a boundary condition).

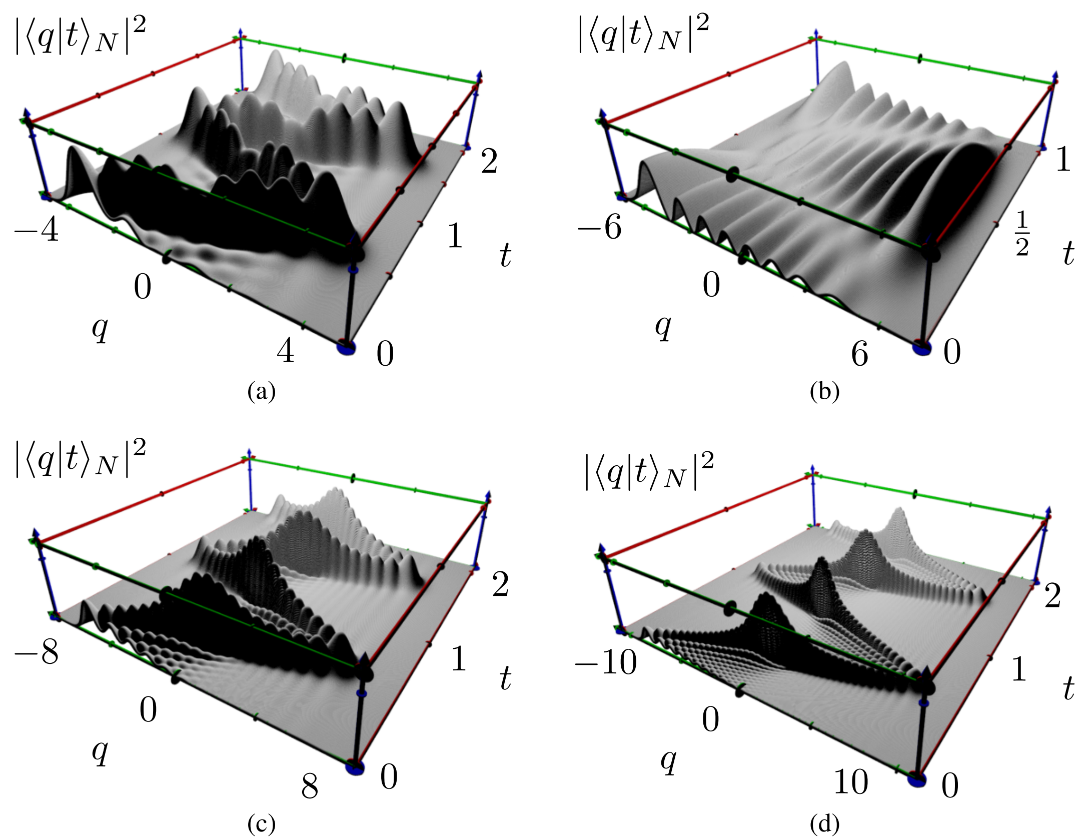


Figure 4.6: Three-dimensional plots of the coordinate density $|\langle q|t\rangle|^2$ for the one dimensional harmonic oscillator. We are using states formed with (a) states 0 to 8 during two periods, with (b) 7 to 8 during one period, with (c) 0 to 19 during two periods, and (d) 0 to 40 during two periods. In these plots we have used dimensionless units, $\hbar = 1$, $\omega = 1$, $m = 1$, and then, having a unit period $\hbar\omega = 1$. In (b), we can see one of the quantum analogues of a classical trajectory. In (c) and (d), we can see peaks around the origin due to the presence of the ground state in the time state.

4.5 General characterization.

Returning to the general case, each time evolved element of the span of $\{|E_n\rangle\}_{n=1}^{\infty}$

$$|\psi_t\rangle = \sum_{j=1}^{N} e^{-itE_j/\hbar}\psi_j|E_j\rangle, \tag{4.82}$$

is a trigonometric polynomial, in t, with coefficients being elements of the abstract Hilbert space (a Banach space). In fact these trigonometric polynomials are of type of almost periodic functions in Banach spaces. It means that the Bohr property in Section 2.3.1 for $|\psi_t\rangle$ in the span of the energy eigenkets and the following holds.

For each ϵ there exists $l = l(\epsilon) > 0$ such that for each interval $(a, a+l)$ ($a \in \mathbb{R}$) we can find a ϵ-translation $\tau \in (a, a+l)$ satisfying

$$\||\psi_{t+\tau}\rangle - |\psi_t\rangle\| = \sqrt{2 - 2\Re\{\langle\psi_{t+\tau}|\psi_t\rangle\}} < \epsilon, \tag{4.83}$$

where we have assumed $|\psi_t\rangle$ to be normalized, and where $\Re$ stands for the real part of the correlation function $\langle\psi_{t+\tau}|\psi_t\rangle$. Consequently, the states $|\psi_t\rangle$ including the time partial eigenstates comply with this Bohr property.

In addition, if we consider the coordinate representation of $|\psi_t\rangle$ in the span of $\{|E_n\rangle\}_{n=1}^{\infty}$:

$$\langle q|\psi_t\rangle = \sum_{j=1}^{N} e^{-itE_{n_j}/\hbar}\psi_j\langle q|E_{n_j}\rangle. \tag{4.84}$$

It turns out that $\langle q|\psi_t\rangle$ is again a trigonometric polynomial in t but depending on the parameter q. Noticing that the product of trigonometric polynomials is a trigonometric polynomial it follows that for each fixed q the wave function $\langle q|\psi_t\rangle$ and $|\langle q|\psi_t\rangle|^2$ are trigonometric polynomials, and, accordingly they are almost periodic functions, depending on the parameter q, and having the Bohr property, Section 2.3.1, again. Similar arguments apply to the momentum amplitude $\langle p|\psi_t\rangle$.

4.6 Conclusions

We have defined discrete momentum operators conjugated to the Hamiltonian, that satisfy discrete versions of properties of a usual momentum operator. They are local operators in the sense of discrete finite difference schemes, becoming exact for the complex exponential function. The time ket $|t\rangle$ is a generalized eigenket of the discrete momentum operators, and the partial time eigenkets, which are genuine elements of the corresponding Hilbert space, furnish to the discrete momentum operators a symmetry property. It is in this sense that the discrete momentum operators are good candidates to be time operators, and we can call them discrete time operators.

An interesting result is that we have found that the partial time states, for the particle in an infinite well as well as the harmonic oscillator, are sets of waves moving classically. Then, if we use only two consecutive energy states to form a time state, we have the wave analogue of a classical trajectory, providing an interpretation to the time states. We have used non standard energy eigenfunctions for the particle in the infinite well that give account, for example, of the hits with the walls. Thus, the time states can be used to define a time coordinate for the quantum system. Happily, the partial time states belong to the domain of the discrete time operator and are normalizable. However there are more kets than that which also belong to the domain of the discrete time operators and to the corresponding Hilbert space as $|t\rangle$ itself.

In addition, the discrete momentum operators yield another approach to the characteristic times of the quantum system, that are the Bohr's times $(E_{n+1} - E_n)/2\pi\hbar$ in the case of the infinite well potential. The discrete symmetry property of the momentum operators, as might have been expected, cannot be satisfied on regions around the zeroes $t_{k,n}$ of the denominator functions, since they are in fact the singularities for the discrete operators; except for the partial time eigenstates. However, as we examined for the particle in the infinite well, we can interpret these singularities as that the particle undergoes an abrupt change of its behavior due to the hits with the walls. For other systems, having discrete energy spectrum, these times should be analyzed, finding the times at which the systems experience some characteristic behavior.

Chapter 5

Conclusions and Perspectives

5.1 Conclusions

The principal object of this thesis was the generalized ket $|t\rangle$ and its truncated version. The fact that $|t\rangle$ has been studied, earlier by other authors, mainly for the equidistant energy spectrum, motivated us to study further this generalized ket for an arbitrary energy spectrum. The original contributions of this thesis are: the mathematical foundation in which $|t\rangle$ is a basis and leads to the definition of a quantum time axis for quantum systems with discrete energy spectrum, and to show that it is possible to have momentum operators of discrete type with similar properties to the continuous counterparts.

In Chapter 2 we have given a brief review of the Besicovitch space B^2 and the Lebesgue space $l^2(\mathbb{R})$, with the property that the latter is the discrete version of the former, and that both have the same Hilbert space structure. In that chapter, we departed from the standard presentation in the use of the Lebesgue space $l^2(\mathbb{R})$ as the conjugate space of the Besicovitch space B^2 through the mean value, and the use of the Lebesgue integral with respect to the counting measure to define the Fourier series of general type. Also, important to our approach of an energy representation, we provided an extension $\{|E\rangle : E \in \mathbb{R}\}$ of the energy eigenkets $\{|E_n\rangle\}_{n=1}^{\infty}$ in such a way that the space of linear combinations of $|E\rangle$ is the ket abstraction of the $l^2(\mathbb{R})$ space.

In Chapter 3, we investigated the protection of states $|\psi\rangle$ on the ket $|t\rangle$. Among our results, we found that these projections $\langle t|\psi\rangle$ define Fourier series of general type, that define a closed subspace of the Besicovitch space B^2. We identified this space with a time representation because the Besicovitch framework extends in a natural way, and henceforth it includes, the usual Fourier analysis. Recall that time representations for quantum systems with an equidistant spectrum is based on the usual Fourier analysis because the states are periodic in time. Additionally, founded on the B^2-norm we were able to give time presentation of wave functions by means of some quantities acquired through repetitions of a large number of identical experiments.

On the other hand, with the knowledge that $l^2(\mathbb{R})$ is an isomorphic Hilbert space to B^2, an energy representation of states was established. Some ideas of the discrete signal theory were taken to this representation, the closed subspace conjugate to the time representation studied in this thesis.

In Chapter 4 we defined the discrete momentum operators $\hat{D}_f$ and $\hat{D}_b$. Let us stress that $\hat{D}_f$, called a discrete time operator, was constructed driven by the quest for a time-type operator satisfying an eigenvalue equation, with $|t\rangle$ as the time eigenket. This was accomplished by exact finite difference schemes for the complex exponential function. What it has shown to us is that, for an arbitrary energy point spectrum, it is always possible to have a discrete time-like operator with $|t\rangle$ as its eigenket, and also that at each quantum energy $\hat{D}_f$ acts like a finite difference scheme. This last point enabled us to have a discrete version of the derivative operation $-i\hbar d/dE$ conjugated to the multiplication by the independent continuous variable E. It is in this sense that $\hat{D}_f$ is discrete version of a time operator.

The time eigenket $|t\rangle$ is not normalizable, but a partial time eigenstate is normalizable and, then, it belongs to the usual Hilbert space. A classical behavior was found through these states for the particle in the infinite well potential. The conjecture is that the partial time state formed with two energy eigenstates is the quantum analogue of a classical trajectory for other potentials as well.

5.2 Perspectives

As mentioned in the introduction of this thesis, the time ket $|t\rangle$ is an eigenket of the Galapon operator provided the energy spectrum is equidistant. However, as far as we know, the Montgomery inequality has not been used to deduce directly that the Galapon operator is a bounded operator for a uniformly discrete energy spectrum. This leads us to ask about the spectrum of such a bounded operator. An article including these topics has already been submitted for publication. It would be interesting to study the Galapon operator from the Besicovitch framework.

On the other hand, the discrete momentum operators defined in this thesis are dependent of exact finite difference schemes. We used forward and backward difference models. However, a discrete momentum operator has been defined by Martínez and Torres in Ref. [27] using central difference schemes. The improvement of others finite difference schemes can lead us to complicated things, but also we can gain more insights about the role played by the time in quantum mechanics. It is hoped that the use of an appropriate exact finite difference scheme will allow us to find new time related properties for discrete quantum systems. In forthcoming papers, we will discuss more of this approach, and we will consider more discrete quantum systems.

With regard to the partial time eigenstates defined in this work, it was possible to obtain classical densities with peaks around classical paths for the particle in the infinite well potential. This is different from the quantum trajectories found with the help of equations such as the master equations of motion that describes an ensemble of particles, and also different from quantum jumps theory [10, 14, 32].

In the future, we would like to study further properties of the partial time eigenstates. For instance, the time derivatives of $|\langle q|t\rangle_N|^2$ and $|\langle p|t\rangle_N|^2$ as quantum analogues of Hamilton's equations $\dot{q} = \partial_p H(q,p)$ and $\dot{p} = -\partial_q H(q,p)$.

It would also be interesting to study what happens to classical chaos because it is not directly observable in quantum systems. We would also like to apply the ideas developed in this thesis in special relativity, in general relativity, in strings theory and other theories.

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