Available online at www.sciencedirect.com
ScienceDirect
Physica A 381 (2007) 170–188
PHYSICA A
www.elsevier.com/locate/physa

A natural normalization for the eigenstates of a Hamiltonian with continuous spectrum

Gustavo Murgida*, Mario Castagnino

Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, 1428 Buenos Aires, Argentina

Received 11 June 2006; received in revised form 15 March 2007
Available online 24 March 2007

Abstract

A mathematical formalism that allows to deal with many problems on quantum systems with continuous evolution spectrum is presented. The usual Hilbert space is generalized to a prehilbert one $\mathcal{T}$ where singular states can be represented and an extended Dirac's notation can be introduced. The obtained formalism contains the Van Hove one but in a more natural way. It allows to explain decoherence and other phenomena.

Keywords: Van Hove's formalism; Normalization; Continuous spectrum

1. Introduction

In paper [1] we have introduced a formalism to deal with density operators in systems with continuous evolution spectrum taking into account their "diagonal singularity". Using this formalism we have studied statistical and thermodynamical phenomena [2], have searched the mathematical and physical properties of Gamow vectors [3], and have introduced a theory of decoherence, that can be used in the case of close (integrable [4] and nonintegrable quantum [6]) systems and cosmological models [5]. The mathematical structure is explained in paper [7], its relation with the usual theory in Ref. [8], and its decoherence time is estimated in Ref. [9].

But our formalism only deals with mixed states, generalized adding decoherent mixtures of energy eigenstates, and we could not normalize the energy eigenbasis of these states. As a consequence, in the case of our decoherence theory, we could only have a *nuclear representation* for the observables, while we could not define a similar one for the states. In this paper, we feel this gap and present a formalism to deal with quantum system with continuous spectrum that could be useful in other (may be many) physical problems.

After this introduction let us precise the problem: let us consider a Hamiltonian with continuous spectrum (the only one we will use in this paper):

$$H = \int_0^\infty E|E\rangle\langle E|\,\mathrm{d}E, \tag{1}$$

*Corresponding author. Tel.: +54 11 4576 3353; fax: +54 11 4576 3357.
E-mail address: gmurgida@dm.uba.ar (G. Murgida).

0378-4371/$ - see front matter
doi:10.1016/j.physa.2007.03.035

where $|E\rangle$ is a energy eigenstate. As usual we consider that the space of states is a Hilbert space $\mathscr{H}$, but as H is a noncompact operator, so $|E\rangle$ must be a generalized state, such that $|E\rangle \notin \mathscr{H}$ (see Refs. [10–12]) but it can be represented in a rigged Hilbert space (see Refs. [10,13]):

$$\Phi \subset \mathscr{H} \subset \Phi', \tag{2}$$

where $\mathscr{H}$ is the original space, Φ is a space of functions included in a continuous and dense way in $\mathscr{H}$, and Φ' is the topological dual of Φ. Then with an adequate rigging we can show that $|E\rangle \in \Phi'$ (see Ref. [12]). Obviously, the inner product of $\mathscr{H}$ is also defined in Φ and the Dirac bracket notation can be used for this inner product and for the functional contained in Φ':

$$\langle\alpha|\varphi\rangle \doteq \alpha[\varphi], \quad \alpha \in \Phi', \ \ \varphi \in \Phi.$$

Nevertheless, since $|E\rangle \notin \mathscr{H}$ expressions like

(i) $\langle E|E\rangle$ or $\langle E|f\rangle$ where $|f\rangle \in \mathscr{H}$,

(ii) $\langle E|H|E\rangle$

are not well defined. Then even if we restraint the space of states $\mathscr{H}$ to be a nuclear space, in which case we can use the Dirac notation as in Eq. (1) we cannot normalize the generalized states $|E\rangle$ and therefore they do not belong to the state space. Then we cannot use this notation to compute the mean value of an operator O in $|E\rangle$, i.e.,

$$\langle O\rangle_{|E\rangle} = \langle E|O|E\rangle \tag{3}$$

nor the density matrix

$$\rho(E, E') = \langle E|E_0\rangle\langle E_0|E'\rangle \tag{4}$$

and therefore we cannot have a representation of the microcanonical or canonical ensembles.

Traditionally, the density matrices of normalized states of $\mathscr{H}$ belong to a Hilbert–Schmidt space $\mathscr{H} \otimes \mathscr{H}'$ and the mean value $Tr(\rho O)$ is the inner product in this space [14]. Then to include generalized states it is necessary to extend this space via, e.g. an algebraic formulation of quantum mechanics. The first of these formulations was introduced by Segal [15]. In his formulation, and in the great majority of the following ones, the observables belong to a C^* algebra of compact operators, the states are positive linear functional on the space of observables, and the mean value is the one of the functional-state in the observable. Nevertheless to consider unbounded observables like the Hamiltonian (1) it is necessary to introduce other algebras containing this kind of observables.

To solve the problem and to represent, e.g. canonical and microcanonical observables with a Hamiltonian with continuous spectrum Antoniou et al. [14] considered an extension of the Hilbert–Schmidt space: an algebra with identity, i.e.,

$$\mathbb{C} \cdot I \oplus (\mathscr{H} \otimes \mathscr{H}').$$

This algebra allows us to define observables with continuous spectrum with diagonal singularity and to construct biorthonormal bases for the observables and the states. For a usual Hilbert space of infinite dimension the identity operator is not compact, and then it does not belong to a C^* algebra, therefore it is a more general structure, that allows us to incorporate the states and observables with diagonal singularity which, in fact, cannot be described by the conventional C^* formulations. Antoniou et al. named their formalism as the Van Hove's one [17] because he was a pioneer in the study of the diagonal singularities. We used this formalism to explain in an extremely simple way the decoherence process for Hamiltonians with continuous spectrum [4]. Van Hove formalism was also used in papers [1–3].

In the Van Hove formalism the space of states corresponds to the mixture states of the usual one plus the decoherent mixtures of states with definite energy. So it is not possible to represent coherent mixtures of states of defined energy and regular states. Moreover in this formalism the states do not have density matrices and then the mean value of an observable O in a state ρ cannot be computed in the usual way, i.e.,

$$\langle O\rangle_\rho = \int_0^\infty \int_0^\infty \rho(E,E')O(E,E')\,\mathrm{d}E\,\mathrm{d}E'. \tag{5}$$

As we will see we must add decoherent mixtures of energy eigenstates to the usual $\rho(E,E')$ or $O(E,E')$. But in the usual formalism there is not a way to normalize the energy eigenstates. Then we will find the way to do it by including the eigenstates of the Hamiltonian, with continuous spectrum, in the space of the theory, introducing a generalization of the usual product of the $\mathbb{L}^2$ space, that allows us to normalize these eigenstates, in such a way to define and use a *prehilbert space* $\mathscr{T}$. In this way we can also generalize the Dirac's notation, and to obtain a nuclear representations for the Van Hove observables and states, in such a way to unify the Van Hove formalism with the traditional one.

The paper is organized as follows:

In Section 2 we define the spaces of observables and regular states and the space of generalized states $\mathscr{T}$; Section 3 introduces a generalized Dirac's notation in $\mathscr{T}$; Section 4 defines the mean values and shows that the generalized Dirac's notation is compatible with this definition. In Section 5.1 we find the density matrices of the generalized states in $\mathscr{T}$, and in Section 5.2 we do so for the mixed states and we obtain an equation similar to (5), showing again the compatibility with the Dirac's notation. In Section 5.3 we discuss the relation between coherent and decoherent mixtures, both discrete or continuous.

Section 6 sketches the decoherence theory of papers [4] with the new formalism; and finally Section 7 draws the conclusions.

In the appendix we present the Van Hove formalism and, using the results of the previous sections, we unify this formalism with the usual one.

2. Spaces of observables and states

2.1. Regular states and space of observables

Let us consider a quantum system with Hamiltonian (1). We will call $\mathscr{S}$ to the space of *regular* states that in the energy representation reads

$$|\psi\rangle = \int_0^\infty \psi(E)|E\rangle\,\mathrm{d}E,$$

where $\psi(E)$ is a Schwarz function with $\psi(E)$ and all its derivatives in $\mathbb{L}^2$. $\mathscr{S}$ is dense in $\mathscr{H}=\mathbb{L}^2$, as the space Φ of Eq. (2).

Now, following the line of papers [1,14–17] we will consider the space of observables $\mathcal{O}$ that in the energy representation are defined by the kernels

$$O(E,E') = O_R(E,E') + O_S(E)\delta(E-E') \tag{6}$$

i.e.,

$$O = \int_0^\infty \int_0^\infty O_R(E,E')|E\rangle\langle E'|\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty O_S(E)|E\rangle\langle E|\,\mathrm{d}E, \tag{7}$$

where $O_R(E,E')$ and $O_S(E)$ are regular functions of two and one variables, respectively, and such that $O_R(E,E')=O_R^*(E',E)$ and $O_S(E)$ is a real function. The choice of the spaces of functions $O_R(E,E')$ and $O_S(E)$ is not unique and depends on the system under consideration (see Refs. [1,4,14]), from now on we will assume that they are Schwarz functions, but the results we obtain below can also be reached by other spaces with adequate regularity conditions. The *regular* component $O_R(E,E')$ of the kernel (6) gives a compact operator while those that come from the *singular* component $O_S(E)$ correspond to operators that commute with the Hamiltonian. Nevertheless $H\notin\mathcal{O}$ since $O_S(E)=E$ is not bounded, and therefore it is not a Schwarz function. Thus we can measure the energy in any bounded set of the energy spectrum but not in the whole spectrum. But $H\in\mathcal{O}$ if $O_S(E)$ is chosen in a space of unbounded functions. It can be shown (see Ref. [14]) that the singular component of the observables are noncompact and therefore the space of observables is

$$\mathcal{O} = \mathcal{O}_R \oplus \mathcal{O}_S,$$

where $\mathcal{O}_R$ is the space of regular observables ($O_S(E) = 0$) and $\mathcal{O}_S$ is the space of pure singular observables ($O_R(E, E') = 0$).

The dynamic of the system is defined by

$$\psi_t(E) = \psi_0(E)\mathrm{e}^{-\mathrm{i}Et}$$

and the mean value of the observable O in the state $|\psi\rangle$ reads

$$\begin{aligned}\langle\psi|O|\psi\rangle &= \int_0^\infty \int_0^\infty O(E, E')\psi(E)\psi^*(E')\,\mathrm{d}E\,\mathrm{d}E' \\ &= \int_0^\infty \int_0^\infty O_R(E, E')\psi(E)\psi^*(E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty O_S(E)\psi(E)\psi^*(E)\,\mathrm{d}E.\end{aligned} \tag{8}$$

2.2. Space of generalized states $\mathcal{T}$

The generalized eigenstates $|E\rangle$ are "delta normalized"

$$\langle E|E'\rangle = \delta(E - E')$$

and therefore it is not possible to compute their norm or to obtain mean values or matrix densities like those of Eqs. (3) and (4). So, to solve this problem, in this section we propose an alternative normalization of states $|E\rangle$ based in an extension of the inner product of space $\mathbb{L}^2$, obtaining a generalization of the Dirac's notation.

As $\langle E|E'\rangle = \delta(E - E')$ the coordinates of vector $|E\rangle$, in the energy basis, are $\delta(E - E')$. Moreover Dirac's delta is a weak limit of a sequence of "approximations of the delta" (see Ref. [18]), i.e., a sequence $\{g_n\}$ of positive functions such that:

(D1) $\int_0^\infty g_n\,\mathrm{d}x = 1,$

(D2) For each $\delta > 0$ we have $\lim_{n\to\infty} \int_{|x|>\delta} g_n\,\mathrm{d}x = 0.$

Functions g_n are normalized to one in $\mathbb{L}^1$, but their norm diverges in $\mathbb{L}^2$

$$\lim_{n\to\infty} \int_0^\infty g_n^2\,\mathrm{d}x = \infty. \tag{9}$$

So it is reasonable to normalize these functions as

$$h_n(E - E') = g_n(E - E') \Bigg/ \sqrt{\int_0^\infty g_n^2\,\mathrm{d}x}. \tag{10}$$

We will name $|h_n^E\rangle$ the state with the energy representation $h_n(E - E')$, namely

$$\langle E'|h_n^E\rangle = h_n(E - E'). \tag{11}$$

In these states is clear that, given $\varepsilon > 0$, the probability of a measure of energy inside the interval $(E - \varepsilon, E + \varepsilon)$ converges to 1:

$$\lim_{n\to\infty} \int_{E-\varepsilon}^{E+\varepsilon} (h_n(E - E'))^2\,\mathrm{d}E = 1.$$

In this sense the sequence of states $\{|h_n^E\rangle\}$ is an approximation to a normalized state with defined energy E. So we define this "limit state" $|\widetilde{E}\rangle$ as the class of sequences $\{|h_n^E\rangle\}$.

I.e. in the same way that we consider that the sequence $\{g_n(E - E')\}$ is an approximation of the unnormalized state $|E\rangle$, $|\widetilde{E}\rangle$ has norm one but it is, of course, a generalized state.

Let us precise these ideas. We will say that the space $\mathscr{V}$ is the vector space generated by the set $\{|\widetilde{E}\rangle\}$ where $E \in \mathbb{R}>0$. We will call $\mathscr{T}$ to the sum of this space plus the space of regular Schwarz states $\mathscr{S}$

$$\mathscr{T} = \mathscr{V} \oplus \mathscr{S} \tag{12}$$

then the vectors of this space read

$$|\alpha\rangle = |\varphi\rangle + \sum_{i=1}^{n} a_i |\widetilde{E}_i\rangle, \tag{13}$$

where $|\varphi\rangle \in \mathscr{S}$ and $|\widetilde{E}_i\rangle \in \mathscr{V}$. We can consider $\mathscr{T}$ as an extension of the space $\mathscr{S}$ and its vectors as generalized states. We can also generalize the inner product of $\mathbb{L}^2$, which is well defined in $\mathscr{S}$, via the following inner products[1]:

$$\langle\varphi|\widetilde{E}\rangle = \lim_{n\to 0} \int_0^\infty \varphi^*(E') h_n(E-E')\,\mathrm{d}E' = 0, \tag{14}$$

$$\langle\widetilde{E}|\widetilde{E}'\rangle = \lim_{n\to 0} \int_0^\infty h_n(E-E'') h_n(E'-E'')\,\mathrm{d}E'' = \begin{cases} 0 & \text{if } E = E', \\ 1 & \text{if } E \neq E', \end{cases} \tag{15}$$

where $|\varphi\rangle \in \mathscr{S}$ and $|\widetilde{E}\rangle, |\widetilde{E}'\rangle \in \mathscr{V}$. Since the inner product in $\mathscr{T}$ must be bilinear we can deduce the general formula

$$\langle\alpha|\beta\rangle = \left(\langle\varphi| + \sum_{i=1}^{n} a_i^* \langle\widetilde{E}_i|\right)\left(|\psi\rangle + \sum_{j=1}^{n} b_j |\widetilde{E}_j\rangle\right) = \langle\varphi|\psi\rangle + \sum_{i=1}^{n} a_i^* b_i, \tag{16}$$

which is endowed with the usual properties of the inner product

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*, \quad \langle\alpha|\alpha\rangle \geqslant 0, \quad \langle\alpha|\alpha\rangle = 0 \Rightarrow |\alpha\rangle = 0$$

as follows from Eq. (16).

This inner product defines a norm in space $\mathscr{T}$ that becomes a prehilbert space. Moreover this inner product restricted to $\mathscr{S}$ coincides with the norm of $\mathbb{L}^2$, and as in the case of $\mathscr{S}$ we must identify the physical states with the projective space of $\mathscr{T}$. Thus in general we will only consider the norm one vectors of $\mathscr{T}$:

$$|\alpha\rangle = a_0|\varphi\rangle + \sum_{i=1}^{n} a_i |\widetilde{E}_i\rangle, \quad \langle\alpha|\alpha\rangle = |a_0|^2 + \sum_{i=1}^{n} |a_i|^2 = 1, \tag{17}$$

where $|\varphi\rangle$ is a regular norm one state.

The states of a system can be consider as functionals on the space of observables defined by the mean values. From Eq. (14) we can see that, the product between states of the spaces $\mathscr{V}$ and $\mathscr{S}$ is zero. As a consequence, we will see in Section 4 that the functionals associated to the states of the space $\mathscr{V}$ vanish on the set of observables without singular component (i.e., $O_S(E) = 0$). Then the states of the space $\mathscr{V}$ only can "see" the singular part of the observables. Precisely, the mean value of the observable given in Eq. (7) in the state $|\widetilde{E}_0\rangle$ is $\langle O\rangle_{|\widetilde{E}_0\rangle} = O_S(E_0)$. This equality shows that the set $\{|\widetilde{E}\rangle\}$ is the cobasis of the singular component of the observables (see Refs. [1,4,14]).

We have seen in Section 2.1 that the space of observables $\mathscr{O}$ is $\mathscr{O} = \mathscr{O}_R \oplus \mathscr{O}_S$. Then the space $\mathscr{S}_M$ of mixed states is a subspace of the dual of $\mathscr{O}$:

$$\mathscr{S}_M \subseteq \mathscr{O}' = \mathscr{O}'_R \oplus \mathscr{O}'_S. \tag{18}$$

The mixtures of regular states, whose kernels are regular functions of two variables, belong to the space $\mathscr{O}'_R$ whereas the decoherent mixtures of states $|\widetilde{E}\rangle$, defined in Section 5, belong to the space $\mathscr{O}'_S$.

Let us note that the inclusion of Eq. (18) becomes an equality if we consider the definitions of the spaces $\mathscr{O}_R$ and $\mathscr{O}_S$ chosen by Antoniou et. al. (see Ref. [14]). They define the space $\mathscr{O}_R$ as the set of compact operators $\mathscr{B}_H^\infty$ and the space $\mathscr{O}_S$ is given by the observables with kernels of the form $O(E,E') = O_S(E)\delta(E-E')$, where $O_S(E)$

[1] That can be proved using Eqs. (D1), (D2) and (10) (see also Section 3).

belongs to $\mathscr{L}^{\infty}$. This is a natural choice because in this way $\mathcal{O}'$ corresponds to the space of trace class operators $\mathscr{B}^1_H$ and $\mathcal{O}'_S$ is isomorphic to the space of measures on $\mathbb{R}>0$.

Finally, let us note that the prehilbert $\mathscr{T}$ can, of course, be completed becoming a Hilbert space, but Eq. (15) shows that this space is not separable. Then the closure of $\mathscr{T}$ does not have a countable basis and it is not isomorphic to the usual space L^2.

3. The Dirac's notation in space $\mathscr{T}$

Using the just defined inner product in $\mathscr{T}$ we will generalize the Dirac's notation, that we will use to compute the mean values. With this notation in a basis $\{|E\rangle\}$ the inner product of regular states reads:

$$\begin{aligned}\langle\varphi|\psi\rangle &= \left(\int_0^\infty \varphi^*(E)\langle E|\,\mathrm{d}E\right)\left(\int_0^\infty \psi(E')|E'\rangle\,\mathrm{d}E'\right) = \int_0^\infty\int_0^\infty \varphi^*(E)\psi(E')\langle E|E'\rangle\,\mathrm{d}E\,\mathrm{d}E' \\ &= \int_0^\infty\int_0^\infty \varphi^*(E)\psi(E')\delta(E-E')\,\mathrm{d}E\,\mathrm{d}E' = \int_0^\infty \varphi^*(E)\psi(E)\,\mathrm{d}E.\end{aligned} \tag{19}$$

But in space $\mathscr{T}$ we also have the basis $\{|\widetilde{E}\rangle\}$, thus in order to extend the Dirac's notation we must define the products:

$$\text{(i) } \langle E|E'\rangle, \quad \text{(ii) } \langle\widetilde{E}|\widetilde{E}'\rangle, \quad \text{(iii) } \langle E|\widetilde{E}'\rangle. \tag{20}$$

Of course, (i) is $\langle E|E'\rangle = \delta(E-E')$. Using a sequence of approximations (ii) was defined in Eq. (15). We will define (iii) using a notation similar to the one of the Dirac's delta as follows.

From definitions D1, D2 and (10) we can prove that, if $f(E)$ is a continuous function, we have

$$\text{(a) } \lim_{n\to\infty}\int_0^\infty h_n(E-E')f(E')\,\mathrm{d}E' = 0,$$

$$\text{(b) } \lim_{n\to\infty}\int_0^\infty [h_n(E-E')]^2 f(E')\,\mathrm{d}E' = f(E),$$

$$\text{(c) } \lim_{n\to\infty}\int_0^\infty h_n(E-E'')h_n(E'-E'')f(E'')\,\mathrm{d}E'' = 0 \quad \text{if } E\neq E'.$$

These properties and Eq. (11) suggest the following "Dirac-*like*" *notation*

$$\lim_{n\to\infty} h_n(E-E') = \langle E'|\widetilde{E}\rangle = \delta^{1/2}(E-E'). \tag{21}$$

Then we get

$$\text{(a}'\text{) } \int_0^\infty \delta^{1/2}(E-E')f(E')\,\mathrm{d}E' = 0,$$

$$\text{(b}'\text{) } \int_0^\infty [\delta^{1/2}(E-E')]^2 f(E')\,\mathrm{d}E' = f(E),$$

$$\text{(c}'\text{) } \int_0^\infty \delta^{1/2}(E-E'')\delta^{1/2}(E'-E'')f(E'')\,\mathrm{d}E'' = 0 \quad \text{if } E\neq E'.$$

So we have solved the problem presented in Eq. (20) as

$$\text{(i) } \langle E|E'\rangle = \delta(E-E'), \quad \text{(ii) } \langle\widetilde{E}|\widetilde{E}'\rangle = \begin{cases} 1 & \text{if } E=E', \\ 0 & \text{if } E\neq E', \end{cases} \quad \text{(iii) } \langle E|\widetilde{E}'\rangle = \delta^{1/2}(E-E').$$

Finally, using this Dirac-like formulae we can reobtain Eq. (16), in fact

$$\begin{aligned}\langle\alpha|\beta\rangle &= \left(\int_0^\infty \varphi^*(E)\langle E|\,\mathrm{d}E + \sum_{i=1}^n a_i^*\langle\widetilde{E}_i|\right)\left(\int_0^\infty \psi(E')|E'\rangle\,\mathrm{d}E' + \sum_{j=1}^n b_j|\widetilde{E}_j\rangle\right)\\ &= \int_0^\infty\int_0^\infty \varphi^*(E)\psi(E')\delta(E-E')\,\mathrm{d}E\,\mathrm{d}E' + \sum_{i,j=1}^n a_i^* b_j\delta_{ij}\\ &\quad + \sum_{j=1}^n b_j\int_0^\infty \varphi^*(E)\delta^{1/2}(E-E_j)\,\mathrm{d}E + \sum_{i=1}^n a_i^*\int_0^\infty \psi(E')\delta^{1/2}(E'-E_i)\,\mathrm{d}E' = \langle\varphi|\psi\rangle + \sum_{i=1}^n a_i^* b_i.\end{aligned}$$

We remark that the symbol $\delta^{1/2}(E-E')$ must be considered at the same level that the usual Dirac's delta $\delta(E-E')$, namely is a useful symbol, that can be considered as a rigorous notation if it is properly used inside an integral.[2]

4. Mean values in space $\mathscr{T}$

Let us consider the normalized state (17) and the observable (7). We define the corresponding mean value as

$$\langle O\rangle_{|\alpha\rangle} = \lim_{n\to\infty}\langle O\rangle_{|\alpha_n\rangle}, \tag{22}$$

where

$$|\alpha_n\rangle = a_0|\varphi\rangle + \sum_{i=1}^n a_i|h_n^{E_i}\rangle.$$

As the states $|h_n^{E_i}\rangle$ are regular Eq. (22) reads:

$$\begin{aligned}\langle O\rangle_{|\alpha\rangle} = \lim_{n\to\infty}\Bigg[&|a_0|^2\langle\varphi|O|\varphi\rangle + \sum_{i=1}^n |a_i|^2\langle h_n^{E_i}|O|h_n^{E_i}\rangle + \sum_{i\neq j=1}^n a_i^* a_j\langle h_n^{E_i}|O|h_n^{E_j}\rangle\\ &+ \sum_{i=1}^n a_0^* a_i\langle\varphi|O|h_n^{E_i}\rangle + \sum_{i=1}^n a_0 a_i^*\langle h_n^{E_i}|O|\varphi\rangle\Bigg]\end{aligned} \tag{23}$$

if we introduce definition (7), we develop this expression, we use properties (a), (b), and (c) of Section 3, and we take the limit we obtain

$$\langle O\rangle_{|\alpha\rangle} = |a_0|^2\langle O\rangle_{|\varphi\rangle} + \sum_{i=1}^n |a_i|^2\langle O\rangle_{|\widetilde{E}_i\rangle}, \tag{24}$$

where $\langle O\rangle_{|\widetilde{E}_i\rangle} = O_S(E_i)$. Let us remark that in the last equation there are neither $(|\varphi\rangle - |\widetilde{E}_i\rangle)$ nor $(|\widetilde{E}_i\rangle - |\widetilde{E}_j\rangle)$ cross terms due to the fact that the components $O_R(E,E')$ and $O_S(E)$ are regular functions and then the state $|\alpha\rangle$, which is a coherent mixture of states $|\varphi\rangle$ and $|\widetilde{E}_i\rangle$, cannot be distinguished from a decoherent mixture of the same states with probabilities $|a_0|^2$ and $|a_i|^2$, respectively.

Let us now verify that we obtain the same result if we use the Dirac's notation

$$\langle O\rangle_{|\alpha\rangle} = \langle\alpha|O|\alpha\rangle = |a_0|^2\langle\varphi|O|\varphi\rangle + \sum_{i,j=1}^n a_i^* a_j\langle\widetilde{E}_i|O|\widetilde{E}_j\rangle + \sum_{i=1}^n a_0^* a_i\langle\varphi|O|\widetilde{E}_i\rangle + \sum_{i=1}^n a_0 a_i^*\langle\widetilde{E}_i|O|\varphi\rangle$$

if we introduce definition (7), we develop this expression, and we use properties (a′), (b′), and (c′) of Section 3, we obtain again Eq. (24).

[2] Of course, the δ can be rigorously defined as a functional in distribution theory. $\delta^{1/2}(E-E')$ is not a functional like $\delta(E-E')$, so it is just a symbol that allows to represent the identities (a), (b), and (c) with the expressions (a′), (b′), and (c′). Using these expressions and the inner product and density matrices definitions we can develop our generalized Dirac's notation.

Let us use Eq. (24) in the particular case

$$\langle H\rangle_{|\widetilde{E}\rangle} = \langle\widetilde{E}|H|\widetilde{E}\rangle = E \tag{25}$$

namely the correct and finite result, while $\langle H\rangle_{|E\rangle}$ was infinite and therefore ill defined (see Section 1, problem (ii)).

5. Density matrices

5.1. Density matrices of pure states

The density matrix of a regular pure states is

$$\rho(E,E') = \varphi(E)\varphi^*(E') = \langle E|\varphi\rangle\langle\varphi|E'\rangle. \tag{26}$$

Since our Hamiltonian has a continuous spectrum actually $\rho(E,E')$ is not a matrix but a regular function or a kernel of two variables. Knowing this $\rho(E,E')$ we can compute the mean value of any observable $O(E,E')$ using Eq. (5) and when the space of the observable is $\mathcal{O}$ (see Eqs. Eqs. (6) and (7)) we will obtain (7).

Let us now study the corresponding formulation in $\mathcal{T}$ space. We want to find a kernel $\rho(E,E')$ that would allow to compute the mean value $\langle O\rangle_{|\alpha\rangle}$ given by Eq. (24) if

$$|\alpha\rangle = a_0|\varphi\rangle + \sum_{i=1}^{n} a_i|\widetilde{E}_i\rangle. \tag{27}$$

Then we must satisfy the condition

$$\begin{aligned}&\int_0^\infty\int_0^\infty O_R(E,E')\rho(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty O_S(E)\rho(E,E)\,\mathrm{d}E\\ &\quad = |a_0|^2\left[\int_0^\infty\int_0^\infty O_R(E,E')\varphi(E)\varphi^*(E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty O_S(E)\varphi(E)\varphi^*(E)\,\mathrm{d}E\right] + \sum_{i=1}^{n}|a_i|^2 O_S(E_i)\end{aligned} \tag{28}$$

but it is easy to see that there is no regular function $\rho(E,E')$ that would satisfy this equation. However, we can define a generalized function or kernel

$$\begin{aligned}\rho(E,E') = \langle E|\alpha\rangle\langle\alpha|E'\rangle &= \left(a_0\langle E|\varphi\rangle + \sum_{i=1}^{n} a_i\langle E|\widetilde{E}_i\rangle\right)\left(a_0^*\langle\varphi|E'\rangle + \sum_{j=1}^{n} a_j^*\langle\widetilde{E}_j|E'\rangle\right)\\ &= |a_0|^2\varphi(E)\varphi^*(E') + \sum_{i,j=1}^{n} a_i a_j^*\delta^{1/2}(E-E_i)\delta^{1/2}(E'-E_j)\\ &\quad + a_0\varphi(E)\sum_{j=1}^{n} a_j^*\delta^{1/2}(E'-E_j) + a_0^*\varphi^*(E')\sum_{i=1}^{n} a_i\delta^{1/2}(E-E_i).\end{aligned} \tag{29}$$

If we substitute this kernel in the l.h.s. of Eq. (28) and use properties (a′), (b′) and (c′) we obtain Eq. (24) as we wanted.

A simpler alternative would be just to define

$$\rho(E,E') = |a_0|^2\varphi(E)\varphi^*(E') + \sum_{i,j=1}^{n} a_i a_j^*\delta^{1/2}(E-E_j)\delta^{1/2}(E'-E_i), \tag{30}$$

which only has the two first terms of the r.h.s. of Eq. (29). But the difference between the two proposed kernels cannot be observed in the space $\mathcal{O}$ since from condition (a′)

$$\int_0^\infty\int_0^\infty O(E,E')\varphi(E)\sum_{j=1}^{n} a_j^*\delta^{1/2}(E'-E_j)\,\mathrm{d}E\,\mathrm{d}E' = 0 \quad \forall O\in\mathcal{O}.$$

Thus the two kernels define the same functional corresponding to the state $|\alpha\rangle$ and we can use the simpler one. Moreover, kernel (30) can be further simplified since from condition (c′)

$$\int_0^\infty \int_0^\infty O(E,E')\delta^{1/2}(E-E_i)\delta^{1/2}(E'-E_j)\,\mathrm{d}E\,\mathrm{d}E' = 0 \quad \text{if } i \neq j$$

thus the off-diagonal terms can be eliminated in Eq. (30) and we obtain the simplest kernel

$$\rho(E,E') = |a_0|^2\varphi(E)\varphi^*(E') + \sum_{i=1}^n |a_i|^2\delta^{1/2}(E-E_i)\delta^{1/2}(E'-E_i). \tag{31}$$

Let us finally consider the normalization of ρ. The trace of a pure regular matrix as $\rho_\psi = |\psi\rangle\langle\psi|$ is

$$Tr\,\rho_\psi = \int_0^\infty \rho_\psi(E,E)\,\mathrm{d}E = 1 \tag{32}$$

so

$$Tr\,\rho_\psi = \langle I\rangle_{|\psi\rangle} = 1,$$

where I is the identity operator

$$I = \int_0^\infty |E\rangle\langle E|\,\mathrm{d}E.$$

Then we can naturally extend this trace definition to the density matrices of the pure states of space $\mathscr{T}$. So if $|\alpha\rangle$ is the pure state of Eq. (27) and ρ is the correspondent density we define

$$Tr\,\rho = \langle I\rangle_{|\alpha\rangle}$$

so from Eq. (24) we obtain

$$Tr\,\rho = \langle I\rangle_{|\alpha\rangle} = |a_0|^2\langle I\rangle_{|\varphi\rangle} + \sum_{i=1}^n |a_i|^2\langle I\rangle_{|\widetilde{E}_i\rangle} = |a_0|^2 + \sum_{i=1}^n |a_i|^2 = 1.$$

Finally, if we use Eq. (22) we also obtain

$$Tr\,\rho = \lim_{n\to\infty} Tr\,\rho_n \tag{33}$$

5.2. Density matrix for mixed states

The mean value of an observable O in a mixture of pure states $\{|\alpha_i\rangle\}$ with probabilities $\{c_i\}$, let say $\rho = \sum_{i=1}^n c_i|\alpha_i\rangle\langle\alpha_i|$, reads

$$\langle O\rangle_\rho = \sum_{i=1}^n c_i\langle O\rangle_{|\alpha_i\rangle}, \tag{34}$$

where $c_i \geqslant 0$ and $\sum_{i=1}^n c_i = 1$.

The density matrix of the state ρ corresponds to a kernel that can be obtained as the linear convex combination of matrices $\rho_i(E,E')$

$$\rho = \sum_{i=1}^n c_i\rho_i(E,E')$$

and each $\rho_i(E,E')$ can be obtained from Eqs. (29), (30), or (31) of Section 5.1. So if

$$|\alpha_i\rangle = a_{i0}|\varphi_i\rangle + \sum_{j=1}^n a_{ij}|\widetilde{E}_{ij}\rangle$$

is substituted in Eq. (34) we obtain

$$\langle O\rangle_\rho = \sum_{i=1}^{n} c_i |a_{i0}|^2 \langle O\rangle_{|\varphi_i\rangle} + \sum_{i=1}^{n} c_i \sum_{j=1}^{n} |a_{ij}|^2 \langle O\rangle_{|\widetilde{E}_{ij}\rangle}. \tag{35}$$

This is a discrete decoherent mixture, if we would like to represent a continuous one of the pure states $|\alpha_x\rangle$ with $x \in \mathbb{R}$, Eq. (34) becomes

$$\langle O\rangle_\rho = \int_{-\infty}^{\infty} f(x) \langle O\rangle_{|\alpha_x\rangle}\, \mathrm{d}x, \tag{36}$$

where $f(x) \geqslant 0$, $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = 1$, and

$$|\alpha_x\rangle = a_{x0}|\varphi_x\rangle + \sum_{j=1}^{n} a_{xj}|\widetilde{E}_{xj}\rangle$$

so we obtain the analogue of Eq. (35), i.e.,

$$\langle O\rangle_\rho = \int_{-\infty}^{\infty} f(x)|a_{x0}|^2 \langle O\rangle_{|\varphi_x\rangle}\, \mathrm{d}x + \int_{-\infty}^{\infty} (x) \sum_{j=1}^{n} |a_{xj}|^2 \langle O\rangle_{|\widetilde{E}_{xj}\rangle}\, \mathrm{d}x. \tag{37}$$

In due time we will reobtain this equation using Dirac's notation. Now, let us just observe that the singular states $|\widetilde{E}_{xj}\rangle$ and the regular states $|\varphi_x\rangle$ allow us to represent the mean value as the sum of integrals of the last equation, where the first term of the r.h.s. corresponds to a decoherent distribution of regular states and the second one is a definite energy one, so

$$\langle O\rangle_\rho = \alpha\langle O\rangle_{\rho_R} + \beta\langle O\rangle_{\rho_S}, \tag{38}$$

where ρ_R is a mixture of regular states, ρ_S is a mixture of singular states and

$$\alpha = \int_{-\infty}^{\infty} f(x)|a_{x0}|^2\, \mathrm{d}x, \quad \beta = \int_{-\infty}^{\infty} f(x) \sum_{j=1}^{n} |a_{xj}|^2\, \mathrm{d}x$$

with the sum

$$\alpha + \beta = \int_{-\infty}^{\infty} f(x) \left(\sum_{j=1}^{n} |a_{xj}|^2 + |a_{x0}|^2 \right) \mathrm{d}x = 1.$$

Eq. (38) shows that matrix ρ can be decomposed as the convex sum

$$\rho(E,E') = \alpha\rho_R(E,E') + \beta\rho_S(E,E') \tag{39}$$

namely

$$\rho = \alpha\rho_R + \beta\rho_S, \quad \alpha,\beta \geqslant 0, \quad \alpha+\beta = 1 \tag{40}$$

therefore the problem to find the generic density matrix is simply to find its regular and singular components.

5.2.1. Mixtures of regular states

The density matrices of regular states are functions of two variables $\rho_R(E,E')$ that corresponds to Hilbert–Schmidt kernels with the following properties:

$$\text{(i) } \rho(E,E') = \rho^*(E',E), \quad \text{(ii) } \rho(E,E) \geqslant 0, \quad \text{(iii) } \int_0^{\infty} \rho(E,E)\, \mathrm{d}E = 1$$

and they can be decomposed as mixtures of regular pure states:

$$\rho_R(E,E') = \int_{-\infty}^{\infty} f(x)\varphi_x(E)\varphi_x^*(E')\,\mathrm{d}x.$$

But since $\rho_R(E,E')$ is also the kernel of a compact operator in $\mathbb{L}^2$ it has also a discrete spectrum, and therefore it also is the discrete mixture of regular states

$$\rho_R(E,E') = \sum_{i=1}^{n} c_i\varphi_i(E)\varphi_i^*(E'),$$

where $c_i \geqslant 0$ and $\sum_{i=1}^{n} c_i = 1$.

5.2.2. Mixtures of states with defined energy

Let ρ be a decoherent mixture of eigenstates of the energy $|\widetilde{E}\rangle$ combined with a probability density $f(E)$, namely

$$\rho = \int_0^{\infty} f(E)|\widetilde{E}\rangle\langle\widetilde{E}|\,\mathrm{d}E.$$

In this state the mean value of observable O reads

$$\langle O\rangle_\rho = \int_0^{\infty} f(E)\langle O\rangle_{|\widetilde{E}\rangle}\,\mathrm{d}E = \int_0^{\infty} f(E)O_S(E)\,\mathrm{d}E,$$

where $O_S(E)$ is the singular component of O. Then let us search for the kernel that produces this mean value i.e., a $\rho(E,E')$ such that:

$$\int_0^{\infty}\int_0^{\infty} \rho(E,E')O(E,E')\,\mathrm{d}E\,\mathrm{d}E' = \int_0^{\infty} f(E)O_S(E)\,\mathrm{d}E \tag{41}$$

and

$$\int_0^{\infty}\int_0^{\infty} \rho(E,E')O_R(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^{\infty} \rho(E,E)O_S(E)\,\mathrm{d}E = \int_0^{\infty} f(E)O_S(E)\,\mathrm{d}E. \tag{42}$$

As the double integral must vanish for any Schwarz function $O_R(E,E')$ then $\rho(E,E') = 0$, a.e., and $\rho(E,E) = f(E)$:

$$\rho(E,E') = \begin{cases} f(E) & \text{if } E = E', \\ 0 & \text{if } E \neq E'. \end{cases} \tag{43}$$

Then we are forced to define a "Kronecker delta" extended to the whole $\mathbb{R}^2$ as

$$\delta_{E,E'} = \begin{cases} 1 & \text{if } E = E', \\ 0 & \text{if } E \neq E'. \end{cases} \tag{44}$$

It is quite easy to show that $\delta(E-E')$ would not do this job. Then we can say that

$$\rho(E,E') = f(E)\delta_{E,E'} \tag{45}$$

if

$$\int_0^{\infty}\int_0^{\infty} f(E)\delta_{E,E'}O_R(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^{\infty} f(E)\delta_{E,E'}O_S(E)\,\mathrm{d}E = \int_0^{\infty} f(E)O_S(E)\,\mathrm{d}E,$$

which is plausible since $\delta_{E,E'} = 0$ but in a set of zero measure, but in order to verify Eq. (41) we must take some mathematical precautions because we must be sure that

$$\int_0^{\infty}\int_0^{\infty} f(E)\delta_{E,E'}O_R(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^{\infty}\int_0^{\infty} f(E)\delta_{E,E'}\delta(E-E')O_S(E)\,\mathrm{d}E\,\mathrm{d}E' = \int_0^{\infty} f(E)O_S(E)\,\mathrm{d}E.$$

The first integral is zero since $\delta_{E,E'} = 0$ but only in a set of zero measure, so it must be

$$\int_0^\infty \int_0^\infty f(E)\delta_{E,E'}\delta(E-E')O_S(E)\,\mathrm{d}E\,\mathrm{d}E' = \int_0^\infty f(E)O_S(E)\,\mathrm{d}E. \tag{46}$$

But the first term cannot be considered as an integral since there is a $\delta(E-E')$. May be we could try to think this $\delta(E-E')$ as a functional, but we cannot do it since $f(E)\delta_{E,E'}O_S(E)$ is not a regular function. So we must consider (46) as a notation that only allows us to obtain the mean value as the product of the matrix density and the kernel of the observable. Then we have that

$$\int_0^\infty \int_0^\infty g(E)\delta_{E,E'}\delta(E-E')\,\mathrm{d}E\,\mathrm{d}E' = \int_0^\infty g(E)\,\mathrm{d}E \tag{47}$$

for any regular function $g(E)$. Clearly using the usual way of operate with the Dirac's delta and the fact that $\delta_{E,E} = 1$ the last equation can be "deduced". But it is most wise and rigorous directly to think Eq. (47) as a definition.[3]

Let us now return to Section 2 where we defined the $|\widetilde{E}\rangle$ as a class of sequences of states. Let us call $|h_n^E\rangle$ the regular states with wave function $h_n(E-E')$ and we obtain the limit (22) namely the weak limit

$$|\widetilde{E}\rangle = w - \lim_{n\to\infty} |h_n^E\rangle$$

in a similar way, we can interpret the decoherent mixture of states with the defined energy with probabilities $f(E)$ as the weak limit of regular mixtures

$$\rho = w - \lim_{n\to\infty} \int_0^\infty f(E)\rho_n^E\,\mathrm{d}E, \tag{48}$$

where $\rho_n^E = |h_n^E\rangle\langle h_n^E|$.

Finally, it is interesting to remark that density (45) is also the point-limit of the density matrices $\int_0^\infty f(E'')\rho_n^{E''}(E,E')\,\mathrm{d}E''$ since

$$\lim_{n\to\infty} \int_0^\infty f(E'')\rho_n^{E''}(E,E')\,\mathrm{d}E'' = \lim_{n\to\infty} \int_0^\infty f(E'')h_n(E-E'')h_n(E'-E'')\,\mathrm{d}E''$$

but then

$$\lim_{n\to\infty} \int_0^\infty f(E'')\rho_n^{E''}(E,E')\,\mathrm{d}E'' = \begin{cases} f(E) & \text{if } E = E', \\ 0 & \text{if } E \neq E' \end{cases}$$

and so

$$\lim_{n\to\infty} \int_0^\infty f(E'')\rho_n^{E''}(E,E')\,\mathrm{d}E'' = f(E)\delta_{E,E'}.$$

5.2.3. Density matrices in general

Finally, we can present the most general matrix density of mixed states of space $\mathcal{T}$. From Section 5.2 this mixed state is a linear convex combination of a mixture of regular states plus a mixture of states of definite energy (Eqs. (39) and (40)) namely

$$\rho(E,E') = \alpha\rho_R(E,E') + \beta\rho_S(E)\delta_{E,E'}, \quad \alpha,\beta \geqslant 0, \quad \alpha+\beta = 1,$$

where $\rho_R(E,E')$ is the kernel of a self-adjoint positive operator of trace equal 1 and $\rho_S(E)$ is a distribution of probabilities in $\mathbb{R}^+$, i.e.,

$$\text{(i) } \rho_R(E,E') = \rho_R^*(E',E), \quad \text{(ii) } \rho_R(E,E) \geqslant 0, \quad \text{(iii) } \int_0^\infty \rho_R(E,E)\,\mathrm{d}E = 1$$

[3] $\delta_{E,E'}$ could be defined as a functional over a space of tempered distributions. The properties of such functional allow to prove Eqs. (41), (45), and (46) and also identities as $\int\int \delta_{E,E'}\delta(E-E')f(E)\,\mathrm{d}E\,\mathrm{d}E' = \int_f(E)\,\mathrm{d}E$ where $f(E)$ is a continuous function. We will develop this mathematical theory elsewhere.

and

$$\text{(iv) } \rho_S(E)\geqslant 0, \quad \text{(v) } \int_0^\infty \rho_s(E)\,\mathrm{d}E = 1.$$

Now, let us see how with this kernel ρ we can compute the mean value of an observable O:

$$\begin{aligned}\langle O\rangle_\rho &= \int_0^\infty\int_0^\infty \rho(E,E')O(E,E')\,\mathrm{d}E\,\mathrm{d}E' \\ &= \alpha\left(\int_0^\infty\int_0^\infty \rho_R(E,E')O_R(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty \rho_R(E,E)O_S(E)\,\mathrm{d}E\right) \\ &\quad + \beta\left(\int_0^\infty\int_0^\infty \rho s(E)\delta_{E,E'}(O_R(E,E') + O_S(E)\delta_{E,E'})\,\mathrm{d}E\,\mathrm{d}E'\right) \\ &= \alpha\left(\int_0^\infty\int_0^\infty \rho_R(E,E')O_R(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty \rho_R(E,E)O_S(E)\,\mathrm{d}E\right) + \beta\int_0^\infty \rho_S(E)O_S(E)\,\mathrm{d}E,\end{aligned}$$

where we have used identity (46). Thus

$$\langle O\rangle_\rho = \alpha\langle O\rangle_{\rho_R} + \beta\langle O\rangle_{\rho_S},$$

where α and β turns out to be the probabilities of the regular states or the singular one. From now on, for the sake of simplicity we take $\alpha = \beta = 1$. Then calling $\alpha\rho_R(E,E')$ and $\beta\rho_S(E)$ simply $\rho_R(E,E')$ and $\rho_S(E)$ the conditions (iii) and (v) above simply becomes

$$\text{(iii}'\text{) } \int_0^\infty (\rho_R(E,E) + \rho_s(E))\,\mathrm{d}E = 1.$$

We will say that a matrix density is regular if $\rho_S(E) = 0$, and we will say that it is purely singular if $\rho_R(E,E') = 0$. Regular matrices belong to the usual formalism while singular matrices are mixture of states of definite energy that allows to represent e.g.:

1. A canonical ensemble:

$$\rho(E,E') = C\,\mathrm{e}^{-\beta E}\delta_{E,E'}.$$

2. The matrix of a state with definite energy E_0

$$\rho(E,E') = \delta(E-E_0)\delta_{E,E'}. \tag{49}$$

3. The decoherent mixture of n states of well-defined energies $\{E_i\}$ with probabilities $\{c_i\}$

$$\rho(E,E') = \sum_{i=1}^n \delta(E-E_i)\delta_{E,E'}. \tag{50}$$

These kernels are different from those we found in Section 5.1 where the matrix of definite energy E_0 reads (see Eq. (31))

$$\rho(E,E') = \delta^{1/2}(E-E_0)\delta^{1/2}(E'-E_0). \tag{51}$$

Nevertheless both kernels allow us to find the same mean values then both representations are equivalent and

$$\delta(E-E_0)\delta_{E,E'} = \delta^{1/2}(E-E_0)\delta^{1/2}(E'-E_0). \tag{52}$$

Making $E = E'$ we can find the reason of the name $\delta^{1/2}(E-E_0)$ and we can verify that the introduced generalized Dirac's notation is consistent.

5.3. Discrete and continuous mixtures

A regular pure state $|\varphi\rangle$ can be considered as a continuous coherent superposition of energy eigenstates $|E\rangle$ as

$$|\varphi\rangle = \int_0^\infty \varphi(E)|E\rangle \, \mathrm{d}E, \tag{53}$$

where $\varphi(E)$ is a normalized function of $\mathbb{L}^2$.

Since $\langle E|E'\rangle = \delta(E-E')$, we associate the generalized state $|E\rangle$ with the sequences $\{g_n\}$ of "approximations of the delta" defined in Section 2.2. Let us note that $\varphi(E)$ is the punctual limit of the following sequence of developments:

$$\varphi(E) = \lim_{n\to\infty} \int_0^\infty \varphi(E) g_n(E-E') \, \mathrm{d}E'. \tag{54}$$

The functions g_n are not normalized in $\mathbb{L}^2$ and their norms diverge

$$\lim_{n\to\infty} \int_0^\infty g_n^2(x) \, \mathrm{d}x = \infty. \tag{55}$$

However, the limit of (54) is a regular function normalized in $\mathbb{L}^2$.

Considering sums in place of the integral in (53) we can represent discrete coherent mixtures of states with definite energy:

$$|\alpha\rangle = \sum_i a_i |E_i\rangle. \tag{56}$$

But this state is not normalized. In order to do it, it was necessary to define the states $|\widetilde{E}\rangle$ and an extension of $\mathbb{L}^2$ as in Section 2.2:

$$|\psi\rangle = \sum_i a_i |\widetilde{E}_i\rangle. \tag{57}$$

Then we can use the states $|E\rangle$ to represent continuous coherent mixtures as in (53), but to do it with discrete mixtures the normalized states $|\widetilde{E}\rangle$ are necessary. Moreover, it is impossible to engage states $|\widetilde{E}\rangle$ in continuous developments as

$$|\varphi\rangle = \int_0^\infty \varphi\langle E)|\widetilde{E}\rangle \, \mathrm{d}E$$

because the norm of this function is zero.

$$\langle\varphi|\varphi\rangle = \int_0^\infty \int_0^\infty \varphi(E)\varphi^*(E')\langle\widetilde{E}'|\widetilde{E}\rangle \, \mathrm{d}E = \int_0^\infty \int_0^\infty \varphi(E)\varphi^*(E')\delta_{E,E'} \, \mathrm{d}E \, \mathrm{d}E' = 0$$

and then $|\varphi\rangle \equiv 0$

Moreover, we know that $|\widetilde{E}\rangle$ is the class of sequences $\{|h_n^E\rangle\}$, so we can see that in a similar way as in Eq. (54) it results

$$\lim_{n\to\infty} \int_0^\infty \varphi(E) h_n^E(E') \, \mathrm{d}E' = \langle\varphi|\widetilde{E}\rangle = 0.$$

In Section 4 we have shown that discrete coherent mixtures of states of definite energy are indistinguishable of the decoherent mixtures. This fact is produced by the continuity of the spectrum of the Hamiltonian, and it would be not the case for discrete spectra. On the other hand, the continuous coherent mixtures of states of definite energy are pure regular states as (53) while the decoherent continuous mixtures are purely singular ($\rho_R(E,E') = 0$).

So the ambiguity between coherent and decoherent mixtures only appears in the discrete ones. Then if we want to represent the density matrix of a discrete mixture of states $|\widetilde{E}_i\rangle$ we can either make a lineal combination of its density matrices or first, obtain a state of space $\mathscr{T}$ and then compute the density matrix of the state. Whereas if we want to represent the density matrix of a continuous mixture of definite energy in the case of a coherent one, we must first obtain the wave function integrating the states $|E\rangle$ but, in the case the one of a decoherent mixture, we must integrate the density matrices of the states $|\widetilde{E}\rangle$.

6. Decoherence

As an interesting example of the use of our method we will consider the decoherence phenomenon using the self-induced approach to decoherence (SID).

Historically the first attempt to explain decoherence was based in the destructive interference of the off-diagonal terms of the density matrix [19]. But this formalism does seems not quite satisfactory, so another one called Ein-selection decoherence (EID) was presented [20]. Nevertheless this formalism has many problems listed in papers [21–25]. These problems do not seem solved nowadays [26] thus many alternative formalisms were introduced [27]. In particular following the Van Hove formalism [17] a new approach, based again in the destructive interference of the off-diagonal terms of the density matrix was proposed: the self-induced decoherence presented in papers [4,28], based in previous research in quantum system with continuous spectrum [1,2], and with its conceptual foundations given in papers [29,30].

Let us explain SID using the formalism just introduced. From Section 5.2 any decoherent mixture in space $\mathscr{T}$ is a linear combination of a mixture of regular states with a mixture of states with defined energy, as shown in Eq. (40).

In Section 5.2 we show that matrix ρ_S can be considered as weak limits of sequences of regular mixtures (see Eq. (48)) and that this matrix is also the point limit of the density matrices of that sequence. Now we will see a new characterization of the purely singular states as weak limits of the time evolution of the mixed states.

The time evolution of the coordinates of a regular matrix $\rho_0(E,E')$ reads

$$\rho_t(E,E') = \rho_0(E,E')\mathrm{e}^{\mathrm{i}(E'-E)t}.$$

Clearly there is not a punctual limit of this oscillatory evolution, nevertheless there is a limit for the mean values for any observable O defined in Eq. (7). In fact, the mean value of O in state ρ_t according to Eq. (28) is

$$\langle O\rangle_{\rho_t} = \int_0^\infty \int_0^\infty O_R(E,E')\rho_0(E,E')\mathrm{e}^{\mathrm{i}(E'-E)t}\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty O_S(E)\rho_0(E,E)\,\mathrm{d}E. \tag{58}$$

As function $O_R(E,E')\rho_0(E,E')$ is regular we can consider that it is $\mathbb{L}^1$ in the variable $(E+E')$, then according to the Riemann–Lebesgue theorem the first integral vanishes in the limit and we have

$$\lim_{t\to\infty}\langle O\rangle_{\rho_t} = \int_0^\infty O_S(E)\rho_0(E,E)\,\mathrm{d}E. \tag{59}$$

Namely in the convex mixture (40) only the second term remains. So we have proved the weak limit

$$w - \lim_{t\to\infty}\rho_t(E,E') = \rho_0(E,E)\delta_{E,E'} \tag{60}$$

showing how when $t\to\infty$ the generic matrix $\rho_t(E,E')$ becomes the diagonal matrix $\rho_0(E,E)\delta_{E,E'}$ in such a way that the matrix have decohered in the energy eigen-basis. Of course, this is the simplest case. Much more general cases are studied in the quoted literature.

Precisely, from Eq. (58) we can see that singular matrices are invariant under time evolution while regular ones weakly converges to a singular one when $t\to\infty$ in such a way that the space of density matrices turns out to be a weakly close space under this evolution.

Moreover, the case $\rho_S(E,E') = \rho_0(E,E)\delta_{E,E'}$ corresponds to a continuous singular decoherent mixture of definite energy states which is invariant under time evolution.

In all the process decoherence was obtained without an environment as in EID being the coarse graining or trace typical of EID substituted by the systematic use of mean values that produce the weak limits (see Ref. [29] or [30] for details).

7. Conclusions

We have extended the usual space of wave functions to a prehilbert space $\mathscr{T}$ which includes the definite energy states for a system with continuous-spectrum Hamiltonian. The inner product of $\mathscr{T}$ is an extension of the ordinary product in $\mathbb{L}^2$, it allows to normalize the states and induce a generalization of the Dirac's notation.

With this notation we can compute inner products and mean values as in the usual case. We found density matrices representing decoherent mixtures of the generalized states of $\mathscr{T}$ in such a way that it can be used the following usual formula to compute the mean value

$$\langle O\rangle_\rho = \int_0^\infty \int_0^\infty \rho(E,E')O(E,E')\,\mathrm{d}E\,\mathrm{d}E'.$$

We found the way to represent discrete mixture of generalized states as well of continuous mixtures, in such a way that any state turns out to be a convex linear combination of regular states with a mixture of states of definite energy

$$\rho = \alpha\rho_R + \beta\rho_S, \quad \alpha,\beta \geqslant 0, \quad \alpha+\beta = 1.$$

The decoherent mixtures of states of definite energy allow us to represent the canonical ensemble and were characterized in three different ways (see Sections 5.2 and 6):

(a) As weak limits of density matrices ρ_n which are mixtures of regular states whose wave functions are "approximations of the delta" normalized in $\mathbb{L}^2$.
(b) As point limit of the density matrices ρ_n.
(c) As weak limit of the time evolution of regular states.

In the appendix, we will compare our formalism with the Van Hove one which historically has being most useful to represent generalized states, the approximation to thermic equilibrium, the classical limit and the study of resonances (see Refs. [1,2,14,17,28]), finding a correspondence between the density matrices of our formalism and the states of Van Hove space of states. In this way, these two formalisms and the usual one are unified.

We believe that with the new formalism developed in this paper it is possible to study all these subjects with the advantage of Van Hove formalism but with the natural flavor and intuition of the usual formalism.

Appendix A. Comparison with Van Hove formalism

Van Hove formalism is an algebraic formulation of quantum mechanics which includes, in its state space, the definite energy states and their decoherent mixtures. The formalism was introduced in papers [1,14], based in early papers of Van Hove [17]. Essentially, papers [1–5,26,27,30] use this formalism. Nevertheless in Van Hove formalism density matrices are not obtained as a straight forward generalization of the usual formalism, so we are always forced to invoke mean values, and the density matrices of the *regular states* do not have the same representation as in the usual formalism, i.e., the mean values are not the product of the kernels of the states and the observables. Moreover Van Hove state space corresponds to a generalized density matrices space, therefore does not allow us to consider coherent superpositions of pure states/either regular or not. In the formalism presented in this paper we do not deal with these problems since it is constructed as a generalization of the usual formalism by the introduction of the approximate sequences $\{|h_n^E\rangle\}$.

In this appendix, we will present the primitive Van Hove formalism and show how it can be obtained from the space of density matrices of our formalism and then it can be unified with the usual one, which turns out to be an extremely particular case of the formalism presented in this paper. In fact there is a one to one correspondence among the observables and states of both formalisms.

Van Hove observable space contains the self-adjoints operators endowed with the property:

$$O^{VH}(E,E') = O_R^{VH}(E,E') + O_S^{VH}(E)\delta(E-E'), \tag{A.1}$$

where $O_R^{VH}(E,E')$ and $O_S^{VH}(E)$ are regular functions. If we introduce the notation

$$|E,E') = |E\rangle\langle E'|, \quad |E) = |E\rangle\langle E|, \quad |O^{VH}) = O^{VH}$$

the observables read

$$|O^{VH}) = \int_0^\infty \int_0^\infty O_R^{VH}(E,E')|E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty O_S^{VH}(E)|E)\,\mathrm{d}E.$$

The states are considered as functional over this observable space. Then we can define the basis of the space of functionals $\{(E,E'|,(E|\}$ satisfying the biorthonormality conditions [1,2,14]

$$(E|E') = \delta(E-E'), \quad (E,E'|E'',E''') = \delta(E-E'')\delta(E'-E''), \quad (E|E',E'') = (E,E''|E'') = 0$$

and a generic state reads

$$(\rho^{VH}| = \int_0^\infty \int_0^\infty \rho_R^{VH}(E,E')(E,E'|\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty \rho_S^{VH}(E)(E|\,\mathrm{d}E,$$

where $\rho_R^{VH}(E,E')$ and $\rho_S^{VH}(E)$ are regular functions satisfying

$$\text{(i) } \rho_R^{VH}(E,E') = \rho_R^{VH*}(E',E), \quad \text{(ii) } \rho_S^{VH}(E), \rho_R^{VH}(E,E) \geqslant 0, \quad \text{(iii) } \int_0^\infty \rho_S^{VH}(E)\,\mathrm{d}E = 1$$

in such a way that we can define the trace

$$Tr(\rho^{VH}| = (\rho^{VH}|I),$$

where the unity operator reads $|I) = \int_0^\infty |E)\,\mathrm{d}E$ and therefore

$$Tr(\rho^{VH}| = \int_0^\infty \rho_S^{VH}(E)\,\mathrm{d}E = 1.$$

Then we can compute the mean value of the observable O^{VH} in the state ρ^{VH}, and using the conditions of biorthonormality we obtain

$$\langle O^{VH}\rangle_{\rho^{VH}} = \int_0^\infty \int_0^\infty \rho_R^{VH}(E,E')O_R^{VH}(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty \rho_S^{VH}(E)O_S^{VH}(E)\,\mathrm{d}E. \tag{A.2}$$

We can see that in Van Hove formalism the singular states cannot be represented by kernels like $\rho_S^{VH}(E,E')$ and we are forced to use (A.2) to compute mean values instead of the usual equation

$$\langle O\rangle_\rho = \int_0^\infty \int_0^\infty \rho(E,E')O(E,E')\,\mathrm{d}E\,\mathrm{d}E',$$

which is absent in the formalism.

In our formalism (see Section 5.2.3) the matrices density are given by the functions

$$\rho(E,E') = \rho_R(E,E') + \rho_S(E)\delta_{E,E'},$$

where $\rho_R(E,E')$ and $\rho_S(E)$ satisfy the conditions

$$\text{(i) } \rho_R(E,E') = \rho_R^*(E',E), \quad \text{(ii) } \rho_S(E), \rho_R(E,E) \geqslant 0, \quad \text{(iii) } \int_0^\infty (\rho_S(E) + \rho_R(E,E))\,\mathrm{d}E = 1$$

and the mean value of the observable O in the state ρ is

$$\langle O\rangle_\rho = \int_0^\infty \int_0^\infty \rho(E,E')O(E,E')\,\mathrm{d}E\,\mathrm{d}E'$$

namely

$$\langle O\rangle_\rho = \int_0^\infty \rho_R(E,E')O_R(E,E')\,\mathrm{d}E\,\mathrm{d}E' + \int_0^\infty (\rho_S(E) + \rho_R(E,E))O_S(E)\,\mathrm{d}E. \tag{A.3}$$

Now let us compare Eq. (A.3) with Eq. (A.2) and we can obtain the formulae to go from one formalism to the other

$$O_R^{VH}(E,E') = O_R(E,E'), \quad O_S^{VH}(E) = O_S(E), \tag{A.4}$$

$$\rho_R^{VH}(E,E') = \rho_R(E,E'), \quad \rho_S^{VH}(E) - \rho_R^{VH}(E,E) = \rho_S(E). \tag{A.5}$$

Immediately, we can verify that if $\rho_S^{VH}(E) \geqslant \rho_R^{VH}(E,E)$ then conditions (i), (ii), and (iii) are equivalent to conditions (i), (ii), and (iii). So our density matrices formalism and the Van Hove one with the condition $\rho_S^{VH}(E) \geqslant \rho_R^{VH}(E,E)$ are equivalents. Moreover, the new formalism is more general since it allows to consider coherent mixtures that cannot be treated in Van Hove formalism.

In a similar way we can see that:

A state is singular if: $\rho_R(E,E') = 0 \Leftrightarrow \rho_R^{VH}(E,E') = 0$.
A state is regular if: $\rho_S(E) = 0 \Leftrightarrow \rho_S^{VH}(E) = \rho_R^{VH}(E,E)$ (in fact, See Ref. [1]).

This remark completes the comparison.

References

[1] R. Laura, M. Castagnino, Phys. Rev. A 57 (1998) 4140.
[2] R. Laura, M. Castagnino, Phys. Rev. E 57 (1998) 3948.
[3] M. Castagnino, R. Laura, R. Liotta, R. Id Betan, J. Phys. A 35 (2002) 6055.
[4] M. Castagnino, R. Laura, Phys. Rev. A 62 (2000) 22107;
M. Castagnino, Physica A 335 (2004) 511.
[5] M. Castagnino, R. Laura, Int. J. Theor. Phys. 39 (2000) 1767;
M. Castagnino, O. Lombardi, Int. J. Theor. Phys. 42 (2003) 1281.
[6] M. Castagnino, Braz. J. Phys. 35 (2005) 375;
M. Castagnino, O. Lombardi, Chaos, Solitons Fractals 28 (2006) 879.
[7] M. Castagnino, A. Ordoñez, Int. J. Theor. Phys. 43 (2004) 695.
[8] M. Castagnino, R. Laura, O. Lombardi, Decoherence in Open and Closed Systems, 2006, arXiv:quant-ph/0601132.
[9] M. Castagnino, O. Lombardi, Phys. Rev. A 72 (2005) 012102.
[10] M. Cotlar, Equipación con Espacios de Hilbert, Universidad de Buenos Aires, Buenos Aires, 1968.
[11] L. Balentine, Quantum Mechanics, Prentice-Hall, New Jersey, 1990.
[12] I.M. Gelfand, N. Vilekin, Generalized Functions, vol. 4, Academic Press, New York, 1964.
[13] M. Castagnino, R. Laura, Phys. Rev. A 56 (1997) 108.
[14] I. Antoniou, Z. Suchanecki, R. Laura, S. Tasaki, Physica A 241 (1997) 737.
[15] I.E. Segal, Postulates for quantum general quantum mechanics, Ann. Math. 48 (4) (1947) 930.
[16] I. Antoniou, Z. Suchanecki, in: Nonlinear, Deformed and Irreversible Quantum Systems, World Scientific, Singapore, 1995.
[17] L. Van Hove, Physica 21 (1955) 901;
L. Van Hove, Physica 22 (1956) 343;
L. Van Hove, Physica 25 (1959) 268.
[18] N. Fava, F. Zo, Medida e Integral de Lebesgue, Red Olimpica, Buenos Aires, 1996.
[19] N.G. van Kampen, Physica 20 (1954) 603;
A. Daneri, A. Loinger, G. Prosperi, Nucl. Phys. 33 (1962) 297;
I. Segal, Bull. Am. Math. Soc. 75 (1969) 1390.
[20] W.H. Zurek, Phys. Rev. D 24 (1981) 1516;
W.H. Zurek, Phys. Today 44 (1991) 36;
W.H. Zurek, Rev. Mod. Phys. 75 (2003) 715;
E. Joos, H.D. Zeh, C. Kiefer, D. Giulini, J. Kupsch, I.-O. Stamatescu, Decoherence and the Appearance of a Classical World in Quantum Theory, Springer, Heidelberg, 2003.
[21] J.J. Halliwell, J. Pérez-Mercader, W.H. Zurek (Eds.), Physical Origins of Time Asymmetry, Cambridge University Press, Cambridge, 1994.
[22] J.P. Paz, W.H. Zurek, Environment-induced Decoherence and Transition from Quantum to Classical, 2000, arXiv: quant-ph/0010011.
[23] W.H. Zurek, Decoherence, Einselection, and Existential Interpretation, 1998, arXiv: quant-ph/9805065.
[24] E. Knill, R. Laflamme, H. Barnum, D. Dalvit, J. Dziarmaga, J. Gubernatis, L. Gurvits, G. Ortiz, L. Viola, W.H. Zurek, Los Alamos Sci. 27 (2002) 2.
[25] G. Casati, B. Chirikov, Phys. Rev. Lett. 75 (1995) 349.

[26] M. Schlosshauer, Decoherence, the Measurement Problem, and Interpretations of Quantum Mechanics, 2004, arXiv: quant-phys/0312059.
[27] G. Casati, B. Chirikov, Physica D 86 (1995) 220;
R. Penrose, Shadows of the Mind, Oxford University Press, Oxford, 1995;
L. Diósi, Phys. Lett. A 120 (1987) 377;
L. Diósi, Phys. Rev. A 40 (1989) 1165;
G.J. Milburn, Phys. Rev. A 44 (1991) 5401;
S. Adler, Quantum Theory as an Emergent Phenomenon, Cambridge University Press, Cambridge, 2004.
[28] M. Castagnino, M. Gadella, R. Laura, R. Id Betan, Phys. Lett. A 282 (2001) 245;
M. Castagnino, M. Gadella, R. Laura, R. Id Betan, J. Phys. A 34 (2001) 10067;
M. Castagnino, M. Gadella, The role of self-induced decoherence in the problem of the classical limit of quantum mechanics, 2003, arXiv: quant-ph/0306014.
[29] M. Castagnino, O. Lombardi, Stud. Hist. Philos. Mod. Phys. 35 (2004) 73.
[30] M. Castagnino, O. Lombardi, Philos. Sci. 72 (2005) 764.