

Rigged Hilbert Spaces and Time Asymmetry: The Case of the Upside-Down Simple Harmonic Oscillator

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The upside-down simple harmonic oscillator system is studied in the contexts of quantum mechanics and classical statistical mechanics. It is shown that in order to study in a simple manner the creation and decay of a physical system by way of Gamow vectors we must formulate the theory in a time-asymmetric fashion, namely using two different rigged Hilbert spaces to describe states evolving toward the past and the future. The spaces defined in the contexts of quantum and classical statistical mechanics are shown to be directly related by the Wigner function.

1. INTRODUCTION

In this work we will study the motion of a particle subject to an upside-down simple harmonic oscillator potential

$$V(q) = -\frac{1}{2} m\omega^2 q^2 \quad (1.1)$$

in the contexts of quantum mechanics and classical statistical mechanics. The aim of the paper is threefold:

1. We solve the problem using a nonconventional technique. In fact, we find that the evolution of the system can be entirely expressed in terms of idealized states that decay or grow exponentially (usually called Gamow vectors). In order to give mathematical meaning to these states we are forced

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to work in the framework of a rigged Hilbert space (RHS). In quantum mechanics the Gamow vectors are then defined as generalized eigenvectors of the Hamiltonian operator with complex eigenvalues, these being the poles of the scattering matrix when it is extended to the complex plane. The Gamow vectors can be used in ‘generalized spectral expansions’ similar to those found by the Gel’fand–Maurin theorem, but in order to use them we have to define two different test function spaces, which we shall call Φ_+ and Φ_- . A similar result is found in classical statistical mechanics.

2. We will prove that with this mathematical structure we have set the basis to introduce a time asymmetry in the theory. Let us explain this further. The vectors in Φ_+ can be expanded as linear combinations of the decaying Gamow vectors, while the vectors in Φ_- can be expanded as linear combinations of the growing Gamow vectors. Since every physical state (either quantum or statistical mechanical) must decay both toward the future and the past, it is mathematically sound to represent the state of a physical system when it evolves toward the future (i.e., from an initial condition) by a vector $\phi_+ \in \Phi_+$ and the state a system when evolving toward the past (i.e., going to a final condition) by a vector $\psi_- \in \Phi_-$. When considering the scattering of particles by the potential barrier, this division between initial states and final states is easily explained, but we think that it is useful for studying other phenomena, such as the decay toward the equilibrium position. Since both spaces Φ_+ and Φ_- are dense in the corresponding Hilbert space \mathcal{H} , at this stage there are no empirical results that could help us decide if the conventional representation of the state of a physical system by a vector in \mathcal{H} is better than the representation of the same system by a vector in Φ_+ or Φ_- . Both representations give the same empirical results, so both are, in a sense, correct. The difference is at the mathematical level (in the topologies used, etc.) and so we can use the representation we find more suitable to the description of the physical facts.

Now, by selecting two different mathematical structures to represent a physical system when evolving toward the future and toward the past we have introduced the basis for a time asymmetry in the mathematical description of time evolution. In fact, there are only two causes for asymmetry in nature: either the laws of nature are asymmetric or the solutions of the equations of the theory are asymmetric. For example, the laws governing the weak interaction are asymmetric, while the solutions of the theory are asymmetric in the case of spontaneous symmetry breaking.

Time asymmetry is not an exception. Thus, if we want to retain the time-symmetric laws of nature the only way to explain the time asymmetry of the universe and its subsystems is to postulate that the space of solutions is not time-symmetric, namely, to adopt the second cause for asymmetry. So the proper way to solve the problem is simply to define a realistic time-

asymmetric space of admissible physical solutions Φ_+ , namely to restrict the space of initial conditions. If \hat{K} is the time inversion operator, this space will be time-asymmetric whenever $\hat{K}: \Phi_+ \mapsto \Phi_-$, namely time inversion changes the physically admissible solutions in Φ_+ into a space of inadmissible solutions Φ_- different to the previous one. If \mathcal{H} is the usual space of solutions of the theory (Hilbert space in quantum mechanics or Liouville space in classical statistical mechanics) and we select Φ_+ properly, then mathematically speaking we have introduced a Gel'fand triplet $\Phi_+ \subset \mathcal{H} \subset \Phi_+^\times$.

A Reichenbach branched system is perhaps the most realistic model for an irreversible universe, i.e., a set of irreversible processes such that each one begins in an unstable state produced by another member of the system and it eventually ends in an equilibrium state (Reichenbach, 1956). This set of processes, all of them beginning in a nonequilibrium state, defines a global arrow of time in the universe. The problem is that the whole branch system must begin in a global unstable initial state, which has no explanation. This unstable initial state would be the initial cosmological state of the universe. It is qualitatively shown in Davies (1994) that the expansion of the universe can be the agency that produces this initial unstable state. Using the method of this paper, we have found the same explanation, but in a quantitative way (Aquilano and Castagnino, 1996), endowing the universe with a (global) space of admissible solutions Φ_+ . Therefore, we think that the time asymmetry is not given by the system itself, namely our upside-down oscillator; instead, it must be connected with the global arrow of time of the universe. In fact, our system is really a member of the Reichenbach branch system in such a way that the unstable initial condition of our oscillator is necessarily produced by another member of the branch system. Thus, as an initial condition is given, it is admissible only if it belongs to a (particular) space Φ_+ . Since the Rigged Hilbert space and the conventional Hilbert space formulations are equally correct, we can select the space better qualified to define time asymmetry.

3. As this procedure has been applied in the past to some unstable quantum mechanical systems [simple potential scattering problems (Bohm and Gadella, 1989) and Friedrichs' model (Antoniou and Prigogine, 1993)] and chaotic classical statistical systems [Renyi maps (Antoniou and Tasaki, 1992) and the baker's transformation (Antoniou and Tasaki, 1993)] in this paper we extend this technique to the simplest unstable system: the upside-down harmonic oscillator. Furthermore, we show that the two sets of spaces defined in quantum mechanics and classical statistical mechanics are connected in a simple manner. This is the first result of this kind that we know of.

The organization of the paper is as follows. In Section 2 we give the principal properties of the rigged Hilbert space formulation of quantum mechanics. We define the regular state space and the generalized state space

and we define generalized eigenfunctions. In Section 3 we work out the motion of a particle subject to the potential (1.1) in classical mechanics, introducing the canonical variables we shall use throughout the paper. In Section 4 we study the same problem in the context of quantum mechanics. We define the growing and decaying Gamow vectors and using these objects, we also define the two RHS that represent states evolving to the future and states evolving to the past. In Section 5 we undertake the same task in the context of classical statistical mechanics. We find the “statistical Gamow vectors,” namely generalized density functions in a state space that represent idealized growing and decaying states. Once again, using these objects, we define the two RHS that represent states evolving toward the past and toward the future. In Section 6 we show that the structures defined in Section 4 and 5 are connected by the Wigner function. Finally, we present our conclusions in Section 7.

2. THE RIGGED HILBERT SPACE FORMULATION OF QUANTUM MECHANICS

In the traditional (von Neumann) formulation of quantum mechanics, a physical state is represented by a vector in a Hilbert space \mathcal{H} and physical magnitudes (observables) by linear self-adjoint operators acting in it. We will deal in this paper with the unidimensional motion of a particle in a potential field, so the Hilbert space in which we should work is isomorphic to $L^2(\mathbb{R})$. More precisely, in the position ($|q\rangle$) representation the particle's state is represented by a normalized wavefunction $\psi(q) \in L^2(\mathbb{R})$ whose modulus squared gives the probability density of finding the particle in the position q . Observables are then represented (in this representation) by self-adjoint operators in $L^2(\mathbb{R})$.

This formulation contains certain idealizations, since once we interpret the wavefunction as a probability amplitude, the only physical requirement is that it must be square-integrable. But a Hilbert space is a complete topological space with respect to a particular topology, namely the one obtained from its scalar product. The assumption that every vector in this Hilbert space represents a physically realizable state cannot by any means be justified by empirical facts, since a topology (infinite limits, continuity) has no physical meaning. It is just a mathematical idealization with which a theoretical physicist works in order to formulate a theory. So we can take another mathematical idealization and formulate a theory in a different mathematical environment. For instance, we can take another topological space, which is itself a subspace of the Hilbert space, and associate with the vectors in such a space the states of the physical system.

This is what the rigged Hilbert space (RHS) formulation of quantum mechanics does (Bohm and Gadella, 1989). To define a RHS we take a topological vector space (endowed with a nuclear topology) Φ with a continuous scalar product defined in it. As we shall see, when the Hilbert space is the space of square-integrable functions, the test function space Φ is chosen as the set of functions of fast decrease or Schwarz functions $\mathcal{S} \equiv \mathcal{S}(\mathbb{R})$ or, in other models, some subspace of it, e.g., incoming or outgoing states subspaces. By completing the vector space with the topology given by the scalar product, we get a Hilbert space \mathcal{H} such that $\Phi \subset \mathcal{H}$. If we consider the set of all antilinear functionals continuous with respect to the nuclear topology, we get another vector space called the dual space of Φ and denoted Φ^\times . We will denote the value of the functional $F \in \Phi^\times$ on the vector $\phi \in \Phi$ by $\langle \phi | F \rangle$ and its complex conjugate by $\langle F | \phi \rangle$. Due to Riesz's lemma, the dual space of \mathcal{H} is \mathcal{H} itself, so we get (using the fact that the nuclear topology is stronger than the Hilbert space topology) the Gel'fand triplet

$$\Phi \subset \mathcal{H} \subset \Phi^\times \quad (2.1)$$

We associate the vectors in the space Φ with the physical states of the system under consideration; thus it is usually called the regular state space. The observables are associated with continuous (essentially) self-adjoint linear operators in Φ .

This formulation has some advantages over the conventional one. The first advantage is that in the traditional formulation of quantum mechanics a vector is a class of Lebesgue square-integrable functions differing in a set of measure zero, while in the RHS formulation a vector is usually just one continuous and infinitely differentiable function.

The second advantage is that every observable is well defined, since they are continuous in Φ . This means, in particular, that even when the operator is unbounded in \mathcal{H} , it is well behaved in Φ , which is contained in the domains of all operators of interest. In the case we will be studying, these include the position and momentum Hamiltonian operators.

The third advantage is that every essentially self-adjoint continuous linear operator in a RHS has a complete set of generalized eigenvectors in Φ^\times (the generalized state space) with their eigenvalues in the spectrum of the operator, a result proved by Gel'fand and Maurin (Bohm and Gadella, 1989; Gel'fand and Shilov, 1964).

By a generalized eigenvector of an operator \hat{A} in a RHS we mean a functional $|F_\lambda\rangle \in \Phi^\times$ such that

$$\langle A^\dagger \phi | F_\lambda \rangle = \lambda \langle \phi | F_\lambda \rangle \quad \forall \phi \in \Phi \quad (2.2)$$

Since this is a generalization of the definition of an eigenvector in finite-dimensional vector spaces, the number λ is called a generalized eigenvalue

corresponding to the eigenvector $|F_\lambda\rangle$. What the Gel'fand–Maurin theorem states is that given an operator, the set of generalized eigenvectors spans the regular vector space Φ . More precisely, if Λ is the spectrum of the aforementioned operator \hat{A} , then the scalar product between two vectors $\phi, \psi \in \Phi$ can be expressed as

$$(\phi, \psi) = \int_{\Lambda} d\mu(\lambda) \langle \phi | F_\lambda \rangle \langle F_\lambda | \psi \rangle \quad (2.3)$$

where μ is a certain integration measure. We see then that in the RHS formulation of quantum mechanics, Dirac's notation is fully justified. Even though the generalized eigenvectors do not belong to the Hilbert space, they are defined as antilinear functionals in Φ^\times . In the same way, the operator itself can be expressed as a linear combination of the same generalized eigenvectors, namely

$$\hat{A} = \int_{\Lambda} d\mu(\lambda) \lambda | \lambda \rangle \langle \lambda | \quad (2.4)$$

There is one more advantage that this formulation has over the traditional one: we can define generalized eigenvectors of an essentially self-adjoint operator with eigenvalues that do not belong to the (Hilbert space) spectrum of the operator. In the general case, such a spectrum is a closed subset of the real line, but, as we shall show below, we can find in some cases eigenvectors with complex eigenvalues. This will allow us to define Gamow vectors, namely generalized eigenvectors of the Hamiltonian operator with nonzero imaginary eigenvalues. As we shall see, this fact implies that the evolution of these vectors is exponential, either growing or decaying, depending on the sign of the imaginary part of the eigenvalue.

These new generalized eigenvectors are useful to study the temporal evolution of the regular vectors representing physical states, if we define the RHS so that we can find new expansions like (2.3) containing them. We will find that in order to do so, we must define two different RHSs, which we shall call Φ_+ and Φ_- . The first one will correspond to the representation of physical systems when they evolve toward the future, since its vectors will be expressed in terms of the decaying Gamow vectors, and the second one will correspond to the representation of physical systems when they evolve toward the past, since they will be expressed in terms of the growing (or decaying toward the past) Gamow vectors.

To finish this section, we will mention the different rigged Hilbert spaces with which we will work in this paper (Gel'fand and Shilov, 1964). The first one is the one constructed from the space of Schwarz class functions \mathcal{S} , composed of all infinitely differentiable functions of a real variable such that

they, together with all their derivatives, vanish at infinity faster than the inverse of any polynomial. The RHS obtained is $\mathcal{S} \subset L^2(\mathbb{R}) \subset \mathcal{S}'$. In this case, the functionals in \mathcal{S}' are called tempered distributions. This is the RHS most theoretical physicists work in, since in it the position and momentum operators are continuous (Bohm and Gadella, 1989).

The other two RHSs we shall use are constructed from subspaces of \mathcal{S} , so that this last property is maintained. These subspaces are the space \mathcal{H} of infinitely differentiable functions of a real variable with compact support and the space \mathcal{L} of Fourier transforms of functions in \mathcal{H} , which is isomorphic to the space of entire functions of fast decrease. The RHS we obtain are then $\mathcal{H} \subset L^2(\mathbb{R}) \subset \mathcal{H}'$ and $\mathcal{L} \subset L^2(\mathbb{R}) \subset \mathcal{L}'$.

3. THE CLASSICAL UPSIDE-DOWN OSCILLATOR

The system we are going to study is one of the simplest unstable ones, namely the motion of a particle in the presence of a potential of the form (1.1). The Hamiltonian function of the system is $H = p^2/(2m) - \frac{1}{2} m\omega^2 q^2$.

As in the study of the harmonic oscillator, it is convenient at this point to make the dynamical variables dimensionless. In order to do that, we must take the natural scales of length, momentum, and time defined through the physical parameters available: m , \hbar and ω (we include \hbar since we will deal in the next section with the quantum case). These scales are, respectively, $\sqrt{\hbar/m\omega}$, $\sqrt{m\omega\hbar}$, and $1/\omega$, so we are making the transformations

$$q \mapsto \sqrt{\frac{m\omega}{\hbar}} q, \quad p \mapsto \frac{1}{\sqrt{m\omega\hbar}} p \tag{3.1}$$

and

$$H \mapsto \frac{1}{\hbar\omega} H, \quad t \mapsto \omega t \tag{3.2}$$

The relation between the Hamiltonian and the dimensionless q and p variables is

$$H = \frac{1}{2} (p^2 - q^2) \tag{3.3}$$

To solve the equations of motion, it will be helpful throughout the paper to work in another pair of canonical variables

$$v = \frac{1}{\sqrt{2}} (p + q), \quad u = \frac{1}{\sqrt{2}} (p - q) \tag{3.4}$$

obtained through the generating function $F(q, v) = -\frac{1}{2} v^2 + \sqrt{2}qv - \frac{1}{2} q^2$.

Expressed in these new variables, the Hamiltonian reads

$$H = vu \quad (3.5)$$

and thus the equations of motion are

$$\dot{v} = \frac{dv}{dt} = \frac{\partial H}{\partial u} = v, \quad \dot{u} = \frac{du}{dt} = -\frac{\partial H}{\partial v} = -u \quad (3.6)$$

These equations are uncoupled and they have as solutions for any initial condition v_0, u_0

$$v = v_0 e^t, \quad u = u_0 e^{-t} \quad (3.7)$$

In phase space, the trajectories of the particles are hyperbolic and the v and u axes are the corresponding asymptotes. The point $v = 0, u = 0$ (or $q = 0, p = 0$) is a point of unstable equilibrium. If $H_0 = v_0 u_0 \neq 0$, then the particle decays (gets away from the barrier region) both toward the past and the future. The directions parallel to the v axis will be called “dilating fibers,” while those parallel to the u axis will be called “contracting fibers.”

4. THE QUANTUM UPSIDE-DOWN OSCILLATOR

4.1. The $|v\rangle$ and $|u\rangle$ Representations

As we saw in the previous section, the evolution of the system is expressed in a simple way when we use the variables v and u . In quantum mechanics, a canonical transformation is associated with a change in representation. Instead of using the representations $|q\rangle$ and $|p\rangle$ of generalized eigenfunctions of \hat{Q} and \hat{P} , we will use the representations $|v\rangle$ and $|u\rangle$ of generalized eigenfunctions of the operators \hat{V} and \hat{U} , defined through

$$\hat{V} = \frac{1}{\sqrt{2}}(\hat{P} + \hat{Q}), \quad \hat{U} = \frac{1}{\sqrt{2}}(\hat{P} - \hat{Q}) \quad (4.1)$$

Since these operators are the quantum representations of canonically conjugate variables, they satisfy the commutation relation

$$[\hat{V}, \hat{U}] = i \quad (4.2)$$

The spectrum of these operators is the whole real line (Cohen-Tannoudji *et al.*, 1977) and the transformations from the $|q\rangle$ representation to the $|v\rangle$ or $|u\rangle$ representations are given by

$$\langle q|v\rangle = (2\pi^2)^{-1/4} e^{i(\sqrt{2}vq - q^2/2 - v^2/2)} \tag{4.3}$$

$$\langle q|u\rangle = (-2\pi^2)^{-1/4} e^{i(\sqrt{2}uq + q^2/2 + u^2/2)} \tag{4.4}$$

Due to (4.2), we get the relation

$$\langle v|u\rangle = \frac{1}{\sqrt{2\pi}} e^{iuv} \tag{4.5}$$

4.2. Eigenfunctions of the Hamiltonian

4.2.1. Real Eigenvalues

The Hamiltonian of the system is

$$\hat{H} = \frac{1}{2} \hat{P}^2 - \frac{1}{2} \hat{Q}^2 = \frac{1}{2} (\hat{V}\hat{U} + \hat{U}\hat{V}) \tag{4.6}$$

namely, the symmetric version of (3.5). The eigenvalue equation for the eigenfunctions of this Hamiltonian with eigenvalue ϵ in the $|v\rangle$ and $|u\rangle$ representations reads

$$v \frac{d}{dv} \phi_\epsilon(v) = \left(i\epsilon - \frac{1}{2}\right) \phi_\epsilon(v), \quad u \frac{d}{du} \psi_\epsilon(u) = \left(-i\epsilon - \frac{1}{2}\right) \psi_\epsilon(u) \tag{4.7}$$

Formally, the solutions of these equations are

$$\phi_\epsilon(v) = \alpha v^{i\epsilon - 1/2}, \quad \psi_\epsilon(u) = \beta u^{-i\epsilon - 1/2} \tag{4.8}$$

but care must be taken, since these expressions are only defined for positive values of v and u , respectively (in fact, as we have seen in Section 2, they are not functions, but distributions).

Actually, there are two linearly independent solutions of equations (4.7) for each value of ϵ , due to the degeneracy of the Hamiltonian. These independent solutions can be chosen as (Bollini and Oxman, 1993)

$$\langle v|\epsilon + (v)\rangle = \frac{1}{\sqrt{2\pi}} \theta(v)v^{i\epsilon - 1/2}, \quad \langle v|\epsilon - (v)\rangle = \frac{1}{\sqrt{2\pi}} \theta(-v)|v|^{i\epsilon - 1/2} \tag{4.9}$$

or

$$\langle u|\epsilon + (u)\rangle = \frac{1}{\sqrt{2\pi}} \theta(u)u^{-i\epsilon - 1/2}, \quad \langle u|\epsilon - (u)\rangle = \frac{1}{\sqrt{2\pi}} \theta(-u)|u|^{-i\epsilon - 1/2} \tag{4.10}$$

The generalized functionals (4.9) represent the idealized scattering outgoing states, representing particles leaving to the left and the right, respec-

tively, while the generalized eigenfunctions (4.10) represent the scattering incoming states, representing particles entering the scattering region from the left and the right, respectively (Balazs and Voros, 1990; Barton, 1986). Both of these sets of solutions form complete and orthonormal sets in \mathcal{S} , in the sense discussed in Section 2.

By calculating the scalar product between the incoming states and the outgoing states, we obtain the scattering matrix, whose coefficients are in this case of the form (Bollini and Oxmar, 1993; Barton, 1986)

$$S_{\mu\nu}(\epsilon) = f_{\mu\nu}(\epsilon)\Gamma\left(\frac{1}{2} - i\epsilon\right), \quad \mu, \nu = +, - \quad (4.11)$$

where the $f_{\mu\nu}(\epsilon)$ are entire functions of ϵ .

4.2.2. Eigenfunctions with Complex Eigenvalues

As can be seen from the above formula, the scattering matrix when extended to the complex plane has an infinite number of imaginary poles located at $z_n = -i(n + 1/2)$, where n is a nonnegative integer. The Gamow vectors will have as generalized eigenvalues these numbers or their complex conjugates. Instead of taking the conventional way to obtain the expressions for these Gamow vectors [namely by analytical extension of the scalar product to the complex plane (Bohm, 1986)], we will take a shortcut and find them in a heuristic way.

We will consider the solutions of the eigenvalue equations (4.8) when taking $\epsilon = z_n$ in the first one and $\epsilon = \bar{z}_n$ in the second one. Then we get the functionals

$$\langle v|n\rangle = v^n, \quad \langle u|\bar{n}\rangle = \frac{(-i)^n}{\sqrt{2\pi n!}} u^n \quad (4.12)$$

where the multiplicative factors have been selected so that (4.14) below applies. Transforming with (4.5), we get

$$\langle u|n\rangle = \sqrt{2\pi} i^n \delta^{(n)}(u), \quad \langle v|\bar{n}\rangle = \frac{(-1)^n}{n!} \delta^{(n)}(v) \quad (4.13)$$

It is clear that these functionals are tempered distributions. By direct calculation, we can demonstrate the biorthonormality of the sets $\{|n\rangle\}$ and $\{|\bar{n}\rangle\}$, namely that

$$\langle n'|\bar{n}\rangle = \langle \bar{n}|n'\rangle = \delta_{n,n'} \quad (4.14)$$

We will show now that $|n\rangle$ is indeed a generalized eigenfunction of \hat{H} with complex eigenvalue z_n , namely that $\langle \hat{H}\phi|n\rangle = z_n\langle\phi|n\rangle$, $\forall|n\rangle \in \mathcal{S}$.

We have

$$\langle \hat{H}\phi | n \rangle = \int_{-\infty}^{+\infty} dv \left[i \left(v \frac{d\overline{\phi(v)}}{dv} + \frac{1}{2} \overline{\phi(v)} \right) \right] v^n$$

and integrating by parts in the right-hand side, we get

$$\langle \hat{H}\phi | n \rangle = -i \int_{-\infty}^{+\infty} dv \left\{ \overline{\phi(v)}(n + 1)v^n - \frac{1}{2} \overline{\phi(v)} \right\} = -i \left(n + \frac{1}{2} \right) \langle \phi | n \rangle$$

In a similar fashion, we can demonstrate that $|\bar{n}\rangle$ is a generalized eigenfunction of \hat{H} with eigenvalue $\bar{z}_n = i(n + 1/2)$. It is

$$\langle \hat{H}\phi | \bar{n} \rangle = \int_{-\infty}^{+\infty} dv \left[i \left(v \frac{d\overline{\phi(v)}}{dv} + \frac{1}{2} \overline{\phi(v)} \right) \right] \frac{(-1)^n}{n!} \delta^{(n)}(v)$$

and using

$$\frac{d^n}{dv^n} \left(v \frac{d}{dv} \right) = v \frac{d^{(n+1)}}{dv^{(n+1)}} + n \frac{d^n}{dv^n}$$

we get $\langle \hat{H}\phi | \bar{n} \rangle = \bar{z}_n \langle \phi | \bar{n} \rangle$.

Since $|n\rangle$ and $|\bar{n}\rangle$ are generalized eigenvectors of \hat{H} , their temporal evolution is easily calculated. In fact, we get

$$e^{-i\hat{H}t}|n\rangle = e^{-(n+1/2)t}|n\rangle, \quad e^{-i\hat{H}t}|\bar{n}\rangle = e^{(n+1/2)t}|\bar{n}\rangle \tag{4.15}$$

showing that the Gamow vectors are indeed vectors that would represent idealized states that decay or grow in a perfectly exponential way. These functionals are more pathological (are “less physical”) than the eigenfunctions of the Hamiltonian with real eigenvalues (4.9) or (4.10); they are clearly distributions and not regular functions and thus cannot represent by themselves physical states. It will be shown, though, that they are useful in studying the temporal evolution of the regular states.

To complete the presentation of these functionals, let us study their expression in the $|q\rangle$ representation. In order to do that, we use (4.4) and get

$$\langle q | n \rangle = \alpha'_n e^{iq^2/2} \frac{\partial^n}{\partial u^n} (e^{i(\sqrt{2}uq + u^2/2)})|_{u=0}$$

where α'_n is just a numerical factor. Now, using the formula $H_n(z) = (\partial^n / \partial \lambda^n)(e^{-\lambda^2 + 2\lambda z})|_{\lambda=0}$, where $H_n(z)$ is the n th Hermite polynomial, we find that

$$\langle q | n \rangle = \alpha_n e^{iq^2/2} H_n(e^{-i\pi/4} q) \tag{4.16}$$

In an analogous way, using (4.3), we get

$$\langle q|\tilde{n}\rangle = \tilde{\alpha}_n e^{-iq^2/2} H_n(e^{i\pi/4}q) \tag{4.17}$$

Restoring the variables' dimensions, we get

$$\langle q|n\rangle = C_n e^{im\omega q^2/2\hbar} H_n\left(\sqrt{\frac{-im\omega}{\hbar}}q\right), \quad \langle q|\tilde{n}\rangle = \tilde{C}_n e^{im\omega q^2/2\hbar} H_n\left(\sqrt{\frac{im\omega}{\hbar}}q\right)$$

If we compare these generalized states with the eigenstates of the harmonic oscillator with equal frequency and mass (Merzbacher, 1970), we can see that the former can be obtained from the latter by means of the transformation $\omega \mapsto -i\omega$ in the case of $|n\rangle$ and the transformation $\omega \mapsto i\omega$ in the case of $|\tilde{n}\rangle$. But these transformations applied to the potential of the harmonic oscillator turn it into the potential (1.1) and the same happens with the eigenvalues: they are transformed from discrete real eigenvalues to discrete imaginary ones. Once again we see (now in the $|q\rangle$ representation) that these generalized eigenfunctions cannot represent physical states; when calculating the norm squared of these functions we obtain that they diverge in the limit $|q| \mapsto \infty$ as q^{2n} .

4.3. Generalized Expansions and the Regular Function Spaces Φ_+ and Φ_-

We study now the use of the generalized functions (4.12) in generalized expansions. Our first step toward this end is taking ϕ such that $\langle v|\phi\rangle = \phi(v) \in \mathcal{S}$. Since this wavefunction is infinitely differentiable, we can define its Taylor expansion around $v = 0$

$$\phi(v) = \sum_{n=0}^{\infty} \frac{\phi^{(n)}(0)}{n!} v^n = \sum_{n=0}^{\infty} \langle v|n\rangle \langle \tilde{n}|\phi\rangle \tag{4.18}$$

The equality in this formula is restricted to the values of v in an interval on the real line, namely inside the radius of convergence of the series, so the utility of this expansion is rather limited. Only when considered in a scalar product will it prove really useful.

Our second step is to define the test function spaces

$$\Phi_+ = \{\psi \in \mathcal{H}|\langle v|\psi\rangle \in \mathcal{L}\} = \{\psi \in \mathcal{H}|\langle u|\psi\rangle \in \mathcal{H}\} \tag{4.19}$$

$$\Phi_- = \{\psi \in \mathcal{H}|\langle v|\psi\rangle \in \mathcal{H}\} = \{\psi \in \mathcal{H}|\langle u|\psi\rangle \in \mathcal{L}\} \tag{4.20}$$

where \mathcal{H} and \mathcal{L} are the spaces introduced in Section 2. We can then construct two different RHS with these spaces, namely

$$\Phi_{\pm} \subset \mathcal{H} \subset \Phi_{\pm}^{\times} \tag{4.21}$$

Let us take $\phi \in \Phi_+$; in this case the expansion (4.18) is valid for all values of v . Considering that $|n\rangle$ is a generalized eigenfunction of \hat{H} with eigenvalue z_n and the definition (4.12₁), the time evolution of this vector is given by

$$\phi(v, t) = \langle v | e^{-i\hat{H}t} \phi \rangle = \sum_{n=0}^{\infty} e^{-(n+1/2)t} \langle v | n \rangle \langle \tilde{n} | \phi \rangle = e^{-i/2} \phi(v e^{-t}, 0) \quad (4.22)$$

Since Φ_+ is a dense subspace in \mathcal{H} , we get that (4.22) must be valid for any vector in \mathcal{H} ; this can be verified by direct substitution in Schrödinger's equation. If we consider the Taylor expansion of a vector ψ in Φ_- in the $|u\rangle$ representation, we get that in that representation the temporal evolution is given by $\psi(u, t) = e^{i/2} \psi(u e^t, 0)$.

These two results can be seen as the fact that the wavefunction does not change its form with time; it just suffers a change in scale. If the wavepacket is initially concentrated in some value v_0 (resp. u_0), then it will be concentrated at time t in $v_0 e^t$ (resp. $u_0 e^{-t}$), namely, the center of the wavepacket follows the classical trajectory found in Section 3. This is a consequence of Ehrenfest's theorem, since the potential is quadratic in position. Quantum effects come from the broadening of the wavefunction in the $|v\rangle$ representation and the narrowing of it in the $|u\rangle$ representation.

Now, let us consider the scalar product between a vector $\phi_- \in \Phi_-$ and a vector $\psi_+ \in \Phi_+$, $(\phi_-, \psi_+) = \int_{-\infty}^{+\infty} dv \overline{\phi_-(v)} \psi_+(v)$. Since $\phi_-(v) \in \mathcal{H}$, it is an infinitely differentiable function of compact support; the integration limits can then be replaced by $-a, a$ for some a . On the other hand, since $\psi_+(v)$ is an entire function, the radius of convergence of its Taylor expansion around $v = 0$ is infinite, and so we have

$$(\phi_-, \psi_+) = \int_{-a}^a dv \overline{\phi_-(v)} \sum_{n=0}^{\infty} \langle \tilde{n} | \psi_+ \rangle v^n \quad (4.23)$$

The convergence of the series in the interval $[-a, a]$ is uniform and, since the function $\phi_-(v)$ is bounded in that interval, we can interchange the order of the summation and integration. Then we get

$$(\phi_-, \psi_+) = \sum_{n=0}^{\infty} \langle \phi_- | n \rangle \langle \tilde{n} | \psi_+ \rangle \quad (4.24)$$

We get a second expansion of this kind by taking the complex conjugate of this expression:

$$(\psi_+, \phi_-) = \sum_{n=0}^{\infty} \langle \psi_+ | \tilde{n} \rangle \langle n | \phi_- \rangle \quad (4.25)$$

This shows that a vector $\phi_+ \in \Phi_+$ can be expanded (when acting as a functional in Φ_-) as $|\phi_+\rangle = \sum |n\rangle \langle \bar{n} | \phi_+\rangle$ and a vector $\phi_- \in \Phi_-$ can be expanded as $|\phi_-\rangle = \sum |\bar{n}\rangle \langle n | \phi_-\rangle$.

Let us now turn to the physical meaning of these RHS. As we have seen, if $\phi_+ \in \Phi_+$, the expansion (4.18) is valid for all values of v . This means that we can represent a state as an infinite sum of decaying states. Then, if we want to study the decay of a physical system, we can represent its initial condition by a vector $\phi_+ \in \Phi_+$. If, on the other hand, we want to study the creation of a physical system, then by representing the final condition with a vector $\psi_- \in \Phi_-$ we can think of this process as the growth of a linear combination of the exponentially growing states $|\bar{n}\rangle$.

In an experiment, we control the initial condition, which evolves toward the future, and then compare it with a final condition by means of a measurement; thus, the quantities of interest are of the form $(\psi_-, \phi_+(t)) = \langle \psi_- | e^{-i\hat{H}t} | \phi_+\rangle$, which can be expanded as in (4.24)

$$\langle \psi_- | e^{-i\hat{H}t} | \phi_+\rangle = \sum_{n=0}^{\infty} e^{-(n+1/2)t} \langle \phi_- | n\rangle \langle \bar{n} | \psi_+\rangle \quad (4.26)$$

It is evident from this formula that we can think that the initial condition is fixed and the final condition evolves to the past. The series in the formula converges always (for all values of t) as we have seen, but it only has physical meaning for positive values of t . For long times, only the first term of the series makes a contribution and then we can take $(\psi_-, \phi_+(t)) = e^{-t/2} \langle \phi_- | 0\rangle \langle \bar{0} | \psi_+\rangle$, showing that in this regime the decay is effectively exponential, unless one of the coefficients $\langle \phi_- | 0\rangle$ or $\langle \bar{0} | \psi_+\rangle$ vanishes. We recover thus the lifetime already known from (Barton, 1986). We remind the reader that equations (4.24) and (4.26) are exact; there are no approximations in the series. In our system, unlike the one considered in Bohm and Gadella (1989), there is no background term; all the details of the evolution are found in the series expansions.

Finally, let us consider time reversal in our formulation. From the interpretation we have given to the spaces Φ_+ and Φ_- , it seems that the time reversal operator should transform one of the spaces into the other, since it changes initial conditions into final conditions. This we shall show now.

Wigner's time reversal operator is defined in the $|q\rangle$ representation as the conjugation operator, namely

$$\hat{K}: |\phi\rangle \mapsto |\phi'\rangle \quad \text{where} \quad \phi'(q) = \overline{\phi(q)} \quad (4.27)$$

Let us take $\phi \in \Phi_+$. Then we have

$$\langle v | \phi\rangle = \phi(v) = \frac{2^{1/4}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dq e^{i(-\sqrt{2}vq + q^2/2 + v^2/2)} \phi(q) \quad (4.28)$$

$$\varphi'(u) = \langle u | \phi' \rangle = \frac{2^{1/4}}{\sqrt{2\pi i}} \int_{-\infty}^{+\infty} dq e^{-i(\sqrt{2}vq - q^2/2 - v^2/2)} \overline{\phi(q)} \tag{4.29}$$

By comparing (4.28) and (4.29), we get

$$\varphi'(u) = e^{-i\pi/4} [\overline{\phi(v)}] |_{v=-u} \tag{4.30}$$

and considering (4.19) and (4.20), $\phi' \in \Phi_-$, or

$$\hat{K}: \Phi_+ \mapsto \Phi_- \tag{4.31}$$

The inverse relation can be proved in a similar way.

5. THE UPSIDE-DOWN OSCILLATOR IN CLASSICAL STATISTICAL MECHANICS

5.1. Generalized Eigenfunctions in Classical Statistical Mechanics

In classical statistical mechanics, a state of a physical system is represented by a density function $\rho(v, u)$ that gives the probability density to find it in a given region in phase space. This density function must satisfy certain requirements to have a physical meaning. First of all, it must be a positive function, since probabilities must be positive. Second, it must be integrable over the entire phase space. Finally, we ask the further condition that it be square-integrable, since we want to calculate mean values of functions that will be themselves square-integrable functions. In this case, we work in a Hilbert space. Just as we did in quantum mechanics, we will formulate the classical statistical theory in a rigged Hilbert space rather than in a Hilbert space, thereby introducing a time asymmetry in the representation of physical states. This method has been applied before to simple chaotic problems (Antoniou and Tasaki, 1992, 1993).

Let us consider the equation that gives the temporal evolution of the density functions, namely the Liouville equation

$$i \frac{\partial \rho}{\partial t} = \hat{L} \rho \tag{5.1}$$

where the Liouvillian operator is defined by

$$\hat{L} \rho = i \{H, \rho\}_{PB} = i \left(\frac{\partial H}{\partial v} \frac{\partial \rho}{\partial u} - \frac{\partial H}{\partial u} \frac{\partial \rho}{\partial v} \right) \tag{5.2}$$

Equation (5.1) is formally equivalent to the Schrödinger equation, so the solutions to this equation can be found in a similar way. The Liouvillian is an (essentially) self-adjoint operator in the Hilbert space of square-integrable

functions of two real variables $L^2(\mathbb{R}^2)$. We will find the generalized eigenfunctions of this operator that play a similar role as (4.13) did in Section 4.

The Liouvillian operator is, in our case, $\hat{L}\rho = i(u \partial\rho/\partial u - v \partial\rho/\partial v)$. Taking ν as the eigenvalue of \hat{L} and proposing as a solution the product of a function of v by a function of $u[\rho = V(\nu)U(u)]$, we get

$$uU^{-1}U' - \nu V^{-1}V' = -i\nu \tag{5.3}$$

It can be seen, then, that both terms on the left-hand side of this equation must be constants, which we shall call m and n , respectively:

$$uU^{-1}U' = m, \quad \nu V^{-1}V' = n \tag{5.4}$$

We see that the equations for U and V are the same, so they will similar solutions. A solution obtained by direct integration is $V = Av^n$, $U = Bu^m$, where A and B are arbitrary constants. We get then that $\rho = Cv^n u^m$ is a generalized eigenfunction of the Liouvillian operator with eigenvalue $\nu = i(m - n)$. As we did in Section 4, let see what happens when we take m and n to be nonnegative integers; in this case the eigenvalue is imaginary. We will denote these eigenfunctions as

$$|m, n\rangle = \frac{1}{n! m!} v^n u^m, \quad \nu = i(m - n) \tag{5.5}$$

They are merely polynomials in v and u . Once again, we find that these functions have no direct physical meaning; in fact, they do not satisfy any of the properties we asked for the physical density functions.

Using the relation

$$\nu \delta^{(n+1)}(\nu) = -(n + 1)\delta^{(n)}(\nu)$$

we can see that $V = \delta^{(n')}(\nu)$ is another solution to (5.4₂) if we take $n = -(n' + 1)$. We find then the following generalized eigenfunctions of the Liouvillian operator with their corresponding eigenvalues:

$$|\tilde{m}, \tilde{n}\rangle = (-1)^{m+n} \delta^{(m)}(u) \delta^{(n)}(\nu), \quad \nu = -i(m - n) \tag{5.6}$$

$$|m, \tilde{n}\rangle = \frac{(-1)^n}{m!} \delta^{(n)}(\nu) u^n, \quad \nu = i(m + n + 1) \tag{5.7}$$

$$|\hat{m}, n\rangle = \frac{(-1)^m}{n!} \delta^{(m)}(u) v^n, \quad \nu = -i(m + n + 1) \tag{5.8}$$

These generalized eigenfunctions are biorthonormal by pairs, namely

$$\langle m, n | \tilde{m}', \tilde{n}' \rangle = \langle m, \tilde{n} | \hat{m}', n' \rangle = \delta_{m,m'} \delta_{n,n'} \tag{5.9}$$

All these functionals are tempered distributions, acting on the space $\mathcal{P}^2 \equiv \mathcal{P}(\mathbb{R}^2)$.

5.2. Rigged Hilbert Spaces and Time Asymmetry in Classical Statistical Mechanics

With the generalized eigenfunctions just found we can construct four different function spaces. Nevertheless, to find time asymmetry we must work with (5.7) and (5.8). It has to be that way, since we must treat in a different way the contracting and dilating fibers, which in this case are the u and v variables.

On the other hand, let us consider the temporal evolution of these generalized eigenfunctions of the Liouvillian. We get

$$|m, \bar{n}(t)\rangle = e^{(m+n+1)t}|m, \bar{n}\rangle, \quad |\bar{m}, n(t)\rangle = e^{-(m+n+1)t}|\bar{m}, n\rangle \quad (5.10)$$

namely, the first ones correspond to idealized states that grow exponentially toward the future, while the second ones represent idealized states that decay exponentially toward the future. These are the “statistical Gamow vectors” that we wanted to find. In a completely analogous way to what we did in Section 4, using (5.10) we find that the solution to the Liouville equation is $\rho(v, u, t) = \rho(v e^{-t}, u e^t, 0)$.

We define, as in Section 4, the space of vectors that represent physical states when studying their evolution to the past and to the future, by

$$\Psi_+ = \{\rho(v, u) \in L^2/\rho \in \mathcal{L}(v) \otimes \mathcal{H}(u)\} \quad (5.11)$$

$$\Psi_- = \{\rho(v, u) \in L^2/\rho \in \mathcal{H}(v) \otimes \mathcal{L}(u)\} \quad (5.12)$$

Let us now consider the scalar product in $L^2(\mathbb{R}^2)$

$$(\rho, \rho') = \int_{-\infty}^{+\infty} dv \int_{-\infty}^{+\infty} du \overline{\rho(v, u)} \rho'(v, u)$$

where the conjugation has no effect, since the functions are real. Given $\rho_+ \in \Psi_+$, we get

$$\rho_+(v, u) = \sum_{n=0}^{\infty} \frac{v^n}{n!} \frac{\partial^n \rho_+}{\partial v^n}(0, u)$$

where the coefficients of the series are infinitely differentiable functions of u , which vanish outside a given interval $[-a, a]$ of the real line. Similarly, if $\rho_- \in \Psi_-$, then

$$\rho_-(v, u) = \sum_{m=0}^{\infty} \frac{u^m}{m!} \frac{\partial^m \rho_-}{\partial u^m}(v, 0)$$

where now the coefficients of the series are infinitely differentiable functions of v that vanish outside a different interval $[-b, b]$ of the real line.

Working as we did in Section 4, we find

$$\begin{aligned}
 (\rho_-, \rho_+) &= \sum_{m,n=0}^{\infty} \frac{1}{n!m!} \left(\int_{-\infty}^{+\infty} du \frac{\partial^n \rho_+}{\partial v^n} (0, u) u^n \right) \left(\int_{-\infty}^{+\infty} dv \frac{\partial^m \rho_-}{\partial u^m} (v, 0) v^m \right) \\
 (\rho_-, \rho_+) &= \sum_{m,n=0}^{\infty} \langle \rho_- | \tilde{m}, n \rangle \langle m, \tilde{n} | \rho_+ \rangle
 \end{aligned}
 \tag{5.13}$$

In a restricted sense (when used in an expression between a function $\rho_+ \in \Psi_+$ and a function $\rho_- \in \Psi_-$) we get

$$= \sum_{m,n=0}^{\infty} | \tilde{m}, n \rangle \langle m, \tilde{n} |
 \tag{5.14}$$

Considering the complex conjugate of (5.13) we get

$$= \sum_{m,n=0}^{\infty} | m, \tilde{n} \rangle \langle \tilde{m}, n |
 \tag{5.15}$$

Just as in the quantum mechanical case, the justification for the distinction between the mathematical representations of a physical state of the particle when studying its future evolution and its past evolution comes from the fact that in the former case we want the expansion in terms of decaying states (5.10₂) to be valid and in the latter case we want the expansion in terms of the growing states (5.10₁) to be valid.

Let us now face the problem of time reversal in classical statistical mechanics. Once again we shall find that the time-reversed version of a function in Ψ_- belongs in Ψ_+ and vice versa. In this case it is easier to see, since time reversal in classical mechanics is just the transformation

$$q \mapsto q, \quad p \mapsto -p, \quad t \mapsto -t$$

and then the transformations for the variables v and u are

$$v \mapsto -u, \quad u \mapsto -v
 \tag{5.16}$$

and so, aside from sign changes, one of the variables is transformed into the other. Looking at the definitions of the spaces Ψ_{\pm} , we get that $\Psi_{\pm} \mapsto \Psi_{\mp}$.

6. CONNECTION BETWEEN THE CLASSICAL AND QUANTUM CASES

To complete our study on the introduction of a time asymmetry in an upside-down simple harmonic oscillator system, we will show how the structures defined in quantum mechanics (Section 4) and in classical statistical mechanics (Section 5) are connected. This connection is given by the Wigner

function. This function is defined from the density matrix $\hat{\rho}$ representing a quantum system by the formula

$$F_{\rho}(q, p) = (2\pi)^{-1} \int_{-\infty}^{+\infty} dy \langle q - y/2 | \hat{\rho} | q + y/2 \rangle e^{ipy} \tag{6.1}$$

It gives an idea of the probability density in classical phase space if the system is represented by $\hat{\rho}$ (Hillery *et al.*, 1984). In our case, we are considering pure states, so the density matrixes are $\hat{\rho} = |\psi\rangle\langle\psi|$ and then (6.1) reads

$$F_{\psi}(q, p) = (2\pi)^{-1} \int_{-\infty}^{+\infty} dy \psi(q - y/2) \overline{\psi(q + y/2)} e^{ipy} \tag{6.2}$$

Since we have been working mostly in the $|v\rangle$ and $|u\rangle$ representation, it will be useful to express the Wigner function in these variables. It can be shown (Balazs and Voros, 1990) that the Wigner function is invariant under linear canonical transformations; then we can take

$$F_{\psi}(v, u) = \pi^{-1} \int_{-\infty}^{+\infty} dy \psi(2v - y) \overline{\psi(y)} e^{iu(2y-2v)} \tag{6.3}$$

Let us consider that $|\psi\rangle \in \Phi_+$ and then $\psi(v) \in \mathcal{H}$. If the support of $\psi(v)$ is $[-a, a]$, then the integration will be performed in this interval. We can see that the Wigner function is infinitely derivable in its two variables, since we can make the derivation inside the integration sign.

Now, if we fix the u variable and look at the dependence on the v variable, then we can see that it vanishes if $|v| > a$. In fact, given that $|2v - y| \geq |2v| - |y| > a$, $\forall y \in [-a, a]$, there is no interval in the real line that contributes with a nonvanishing term to the integral.

On the other hand, let us fix the v variable. We see then that the Wigner function as a function of u is the Fourier transform of an infinitely differentiable function of bounded support, and thus is a function in \mathcal{L} . We find then the relation

$$|\psi\rangle \in \Phi_+ \mapsto F_{\psi}(v, u) \in \mathcal{H}(v) \otimes \mathcal{L}(u) = \Psi_+ \tag{6.4}$$

In a similar way, we can get the relation connecting the two spaces that describe the physical systems when they evolve to the past

$$|\psi\rangle \in \Phi_- \mapsto F_{\psi}(v, u) \in \mathcal{L}(v) \otimes \mathcal{H}(u) = \Psi_- \tag{6.5}$$

This result is not unexpected, since in our case the potential is quadratic in the position. Under these circumstances, the equation that rules the temporal evolution of the Wigner function coincides with the Liouville equation (Hillery *et al.*, 1984), so there must be a close relationship between the structures

found in the classical statistical case and the density function we get from the quantum case.

7. CONCLUSIONS

We found that in order to give meaning to Gamow vectors, two different rigged Hilbert spaces must be defined: one to represent states evolving toward the future from initial conditions and one to represent states evolving toward the past from final conditions. This distinction between initial conditions and final conditions must be thought of as an implementation of the global arrow of time of the universe and not as a manifestation of an intrinsic irreversibility pertaining to the system. Nevertheless, the instability is the key to the implementation of the time asymmetry by causing the existence of Gamow vectors.

By using this time-asymmetric formulation of the problem, we found that new “generalized expansions” can be used to make calculations in an easy way. For example, we found the solution of the Schrödinger and Liouville equations by means of the Gamow vectors. The fact that we restrict the space of vectors representing physical states has no empirical consequences since the test function spaces in which we work are dense in the corresponding Hilbert space in which the conventional theory is formulated.

Even though our model has some characteristics that make it unpleasant, such as a potential not bounded from below, we think that it is not so hard to avoid these characteristics. For instance, if we study the motion in the region around a maximum of a twice-differentiable potential function, then the approximation by a quadratic potential is valid. In particular, this happens when the decay from the unstable equilibrium position is studied.

As we stated in the introduction, this same method has been applied in the past to some models in quantum mechanics and classical statistical mechanics. In the future we will try to generalize our results to more general models in both contexts and study the conceptual implications of the time-asymmetric formulation of the theory.

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